

# Supporting information for “Defining Structural and Evolutionary Modules in Proteins: A Community Detection Approach to explore sub-domain architecture”

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## Supporting Information Content

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## Supporting Tables

Table S1: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 1U33, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |

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| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 30             | 192           | PHE                  | C      |
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |

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| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 76             | 239           | ASP                  | C      |
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |

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| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 122            | 316           | GLU                  | B      |
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASN                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |

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| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 168            | 370           | SER                  | B      |
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASP                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |

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Table S1 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 214            | 436           | PHE                  | A      |
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |

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Table S1 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 260            | 507           | SER                  | A      |
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 574           | ARG                  | A      |
| 295            | 575           | PRO                  | A      |
| 296            | 576           | TYR                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S2: Residues membership for the *N. polysaccharea*  $\alpha$ -amylase (PDB code 1MVY, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 98            | GLN                  | A      |
| 1              | 99            | VAL                  | A      |
| 2              | 100           | GLY                  | B      |
| 3              | 101           | GLY                  | B      |
| 4              | 102           | VAL                  | B      |
| 5              | 103           | CYS                  | C      |
| 6              | 104           | TYR                  | C      |
| 7              | 105           | VAL                  | C      |
| 8              | 110           | GLY                  | C      |
| 9              | 111           | ASP                  | C      |
| 10             | 112           | LEU                  | C      |
| 11             | 113           | LYS                  | C      |
| 12             | 114           | GLY                  | C      |
| 13             | 115           | LEU                  | C      |
| 14             | 116           | LYS                  | C      |
| 15             | 117           | ASP                  | C      |
| 16             | 118           | LYS                  | C      |
| 17             | 119           | ILE                  | C      |
| 18             | 120           | PRO                  | C      |
| 19             | 121           | TYR                  | C      |
| 20             | 122           | PHE                  | C      |
| 21             | 123           | GLN                  | C      |
| 22             | 124           | GLU                  | C      |
| 23             | 125           | LEU                  | C      |
| 24             | 126           | GLY                  | C      |
| 25             | 127           | LEU                  | C      |
| 26             | 128           | THR                  | C      |
| 27             | 129           | TYR                  | C      |
| 28             | 130           | LEU                  | C      |
| 29             | 131           | TYR                  | C      |
| 30             | 132           | LEU                  | C      |
| 31             | 133           | MET                  | C      |
| 32             | 134           | PRO                  | C      |
| 33             | 135           | LEU                  | C      |
| 34             | 136           | PHE                  | C      |
| 35             | 137           | LYS                  | C      |
| 36             | 138           | CYS                  | C      |
| 37             | 139           | PRO                  | C      |
| 38             | 141           | GLY                  | C      |
| 39             | 144           | ASP                  | C      |
| 40             | 145           | GLY                  | C      |
| 41             | 146           | GLY                  | C      |
| 42             | 147           | TYR                  | C      |
| 43             | 148           | ALA                  | C      |

*Continued on next page*

Table S2 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 149           | VAL                  | C      |
| 45             | 150           | SER                  | C      |
| 46             | 151           | SER                  | C      |
| 47             | 153           | ARG                  | C      |
| 48             | 154           | ASP                  | C      |
| 49             | 155           | VAL                  | C      |
| 50             | 156           | ASN                  | C      |
| 51             | 157           | PRO                  | C      |
| 52             | 158           | ALA                  | C      |
| 53             | 159           | LEU                  | C      |
| 54             | 160           | GLY                  | C      |
| 55             | 161           | THR                  | C      |
| 56             | 162           | ILE                  | C      |
| 57             | 163           | GLY                  | C      |
| 58             | 164           | ASP                  | C      |
| 59             | 165           | LEU                  | C      |
| 60             | 166           | ARG                  | C      |
| 61             | 167           | GLU                  | C      |
| 62             | 168           | VAL                  | C      |
| 63             | 169           | ILE                  | C      |
| 64             | 170           | ALA                  | C      |
| 65             | 171           | ALA                  | C      |
| 66             | 172           | LEU                  | C      |
| 67             | 173           | HIS                  | C      |
| 68             | 174           | GLU                  | C      |
| 69             | 175           | ALA                  | C      |
| 70             | 176           | GLY                  | C      |
| 71             | 177           | ILE                  | C      |
| 72             | 178           | SER                  | C      |
| 73             | 179           | ALA                  | C      |
| 74             | 180           | VAL                  | C      |
| 75             | 181           | VAL                  | C      |
| 76             | 182           | ASP                  | C      |
| 77             | 183           | PHE                  | C      |
| 78             | 184           | ILE                  | C      |
| 79             | 185           | PHE                  | C      |
| 80             | 186           | ASN                  | C      |
| 81             | 187           | HIS                  | C      |
| 82             | 188           | THR                  | C      |
| 83             | 189           | SER                  | C      |
| 84             | 190           | ASN                  | C      |
| 85             | 191           | GLU                  | C      |
| 86             | 192           | HIS                  | C      |
| 87             | 193           | GLU                  | C      |
| 88             | 194           | TRP                  | C      |
| 89             | 195           | ALA                  | C      |

*Continued on next page*

Table S2 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 206           | ASP                  | C      |
| 91             | 207           | ASN                  | C      |
| 92             | 208           | PHE                  | C      |
| 93             | 209           | TYR                  | C      |
| 94             | 210           | TYR                  | B      |
| 95             | 247           | TRP                  | B      |
| 96             | 248           | THR                  | B      |
| 97             | 249           | THR                  | B      |
| 98             | 250           | PHE                  | B      |
| 99             | 254           | GLN                  | B      |
| 100            | 255           | TRP                  | B      |
| 101            | 256           | ASP                  | B      |
| 102            | 257           | LEU                  | B      |
| 103            | 258           | ASN                  | B      |
| 104            | 259           | TYR                  | B      |
| 105            | 260           | SER                  | B      |
| 106            | 261           | ASN                  | B      |
| 107            | 262           | PRO                  | B      |
| 108            | 263           | TRP                  | B      |
| 109            | 264           | VAL                  | B      |
| 110            | 265           | PHE                  | B      |
| 111            | 266           | ARG                  | B      |
| 112            | 267           | ALA                  | B      |
| 113            | 268           | MET                  | B      |
| 114            | 269           | ALA                  | B      |
| 115            | 270           | GLY                  | B      |
| 116            | 271           | GLU                  | B      |
| 117            | 272           | MET                  | B      |
| 118            | 273           | LEU                  | B      |
| 119            | 274           | PHE                  | B      |
| 120            | 275           | LEU                  | B      |
| 121            | 276           | ALA                  | B      |
| 122            | 277           | ASN                  | B      |
| 123            | 278           | LEU                  | C      |
| 124            | 279           | GLY                  | C      |
| 125            | 280           | VAL                  | C      |
| 126            | 281           | ASP                  | C      |
| 127            | 282           | ILE                  | C      |
| 128            | 283           | LEU                  | B      |
| 129            | 284           | ARG                  | D      |
| 130            | 285           | MET                  | B      |
| 131            | 286           | ASP                  | B      |
| 132            | 287           | ALA                  | B      |
| 133            | 288           | VAL                  | B      |
| 134            | 289           | ALA                  | B      |
| 135            | 290           | PHE                  | B      |

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Table S2 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 291           | ILE                  | B      |
| 137            | 292           | TRP                  | B      |
| 138            | 306           | HIS                  | B      |
| 139            | 307           | ALA                  | B      |
| 140            | 308           | LEU                  | B      |
| 141            | 309           | ILE                  | B      |
| 142            | 310           | ARG                  | B      |
| 143            | 311           | ALA                  | B      |
| 144            | 312           | PHE                  | B      |
| 145            | 313           | ASN                  | B      |
| 146            | 314           | ALA                  | B      |
| 147            | 315           | VAL                  | B      |
| 148            | 316           | MET                  | B      |
| 149            | 317           | ARG                  | B      |
| 150            | 323           | VAL                  | B      |
| 151            | 324           | PHE                  | B      |
| 152            | 325           | PHE                  | B      |
| 153            | 326           | LYS                  | C      |
| 154            | 327           | SER                  | B      |
| 155            | 328           | GLN                  | B      |
| 156            | 329           | ALA                  | B      |
| 157            | 330           | ILE                  | B      |
| 158            | 331           | VAL                  | B      |
| 159            | 332           | HIS                  | B      |
| 160            | 336           | VAL                  | B      |
| 161            | 337           | VAL                  | B      |
| 162            | 338           | GLN                  | B      |
| 163            | 339           | TYR                  | B      |
| 164            | 340           | ILE                  | B      |
| 165            | 341           | GLY                  | B      |
| 166            | 345           | CYS                  | B      |
| 167            | 346           | GLN                  | B      |
| 168            | 347           | ILE                  | B      |
| 169            | 348           | GLY                  | B      |
| 170            | 349           | TYR                  | D      |
| 171            | 350           | ASN                  | D      |
| 172            | 351           | PRO                  | D      |
| 173            | 352           | LEU                  | D      |
| 174            | 354           | MET                  | D      |
| 175            | 355           | ALA                  | D      |
| 176            | 356           | LEU                  | D      |
| 177            | 357           | LEU                  | D      |
| 178            | 358           | TRP                  | D      |
| 179            | 359           | ASN                  | D      |
| 180            | 360           | THR                  | D      |
| 181            | 361           | LEU                  | D      |

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Table S2 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 364           | ARG                  | D      |
| 183            | 365           | GLU                  | A      |
| 184            | 366           | VAL                  | A      |
| 185            | 367           | ASN                  | A      |
| 186            | 372           | ALA                  | A      |
| 187            | 373           | LEU                  | D      |
| 188            | 374           | THR                  | D      |
| 189            | 375           | TYR                  | D      |
| 190            | 376           | ARG                  | D      |
| 191            | 377           | HIS                  | B      |
| 192            | 378           | ASN                  | B      |
| 193            | 381           | GLU                  | B      |
| 194            | 382           | HIS                  | B      |
| 195            | 383           | THR                  | B      |
| 196            | 384           | ALA                  | B      |
| 197            | 385           | TRP                  | B      |
| 198            | 386           | VAL                  | D      |
| 199            | 387           | ASN                  | D      |
| 200            | 388           | TYR                  | D      |
| 201            | 389           | VAL                  | A      |
| 202            | 390           | ARG                  | D      |
| 203            | 391           | SER                  | D      |
| 204            | 392           | HIS                  | D      |
| 205            | 393           | ASP                  | D      |
| 206            | 394           | ASP                  | D      |
| 207            | 448           | SER                  | D      |
| 208            | 450           | THR                  | D      |
| 209            | 451           | ALA                  | D      |
| 210            | 452           | ALA                  | D      |
| 211            | 453           | ALA                  | D      |
| 212            | 464           | ALA                  | A      |
| 213            | 467           | ARG                  | A      |
| 214            | 468           | ILE                  | A      |
| 215            | 469           | LYS                  | A      |
| 216            | 470           | LEU                  | A      |
| 217            | 471           | LEU                  | A      |
| 218            | 472           | TYR                  | A      |
| 219            | 473           | SER                  | A      |
| 220            | 474           | ILE                  | A      |
| 221            | 475           | ALA                  | A      |
| 222            | 476           | LEU                  | A      |
| 223            | 477           | SER                  | A      |
| 224            | 478           | THR                  | A      |
| 225            | 479           | GLY                  | D      |
| 226            | 480           | GLY                  | D      |
| 227            | 481           | LEU                  | D      |

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Table S2 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 482           | PRO                  | A      |
| 229            | 483           | LEU                  | D      |
| 230            | 484           | ILE                  | A      |
| 231            | 485           | TYR                  | D      |
| 232            | 486           | LEU                  | C      |
| 233            | 487           | GLY                  | D      |
| 234            | 488           | ASP                  | A      |
| 235            | 514           | PRO                  | C      |
| 236            | 515           | ARG                  | C      |
| 237            | 516           | TYR                  | D      |
| 238            | 517           | ASN                  | D      |
| 239            | 521           | TYR                  | D      |
| 240            | 534           | ILE                  | A      |
| 241            | 535           | TYR                  | A      |
| 242            | 536           | GLN                  | A      |
| 243            | 537           | GLY                  | A      |
| 244            | 538           | LEU                  | A      |
| 245            | 539           | ARG                  | A      |
| 246            | 540           | HIS                  | A      |
| 247            | 541           | MET                  | A      |
| 248            | 542           | ILE                  | A      |
| 249            | 543           | ALA                  | A      |
| 250            | 544           | VAL                  | A      |
| 251            | 545           | ARG                  | A      |
| 252            | 546           | GLN                  | A      |
| 253            | 547           | SER                  | A      |
| 254            | 548           | ASN                  | A      |
| 255            | 549           | PRO                  | A      |
| 256            | 553           | GLY                  | A      |
| 257            | 554           | GLY                  | A      |
| 258            | 555           | ARG                  | A      |
| 259            | 556           | LEU                  | A      |
| 260            | 558           | THR                  | A      |
| 261            | 559           | PHE                  | A      |
| 262            | 560           | ASN                  | A      |
| 263            | 561           | THR                  | A      |
| 264            | 563           | ASN                  | A      |
| 265            | 564           | LYS                  | A      |
| 266            | 565           | HIS                  | A      |
| 267            | 566           | ILE                  | A      |
| 268            | 567           | ILE                  | A      |
| 269            | 568           | GLY                  | A      |
| 270            | 569           | TYR                  | A      |
| 271            | 570           | ILE                  | A      |
| 272            | 571           | ARG                  | A      |
| 273            | 573           | ASN                  | A      |

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Table S2 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 574           | ALA                  | A      |
| 275            | 575           | LEU                  | A      |
| 276            | 576           | LEU                  | A      |
| 277            | 577           | ALA                  | A      |
| 278            | 578           | PHE                  | A      |
| 279            | 579           | GLY                  | A      |
| 280            | 580           | ASN                  | A      |
| 281            | 584           | TYR                  | A      |
| 282            | 585           | PRO                  | A      |
| 283            | 586           | GLN                  | A      |
| 284            | 587           | THR                  | A      |
| 285            | 588           | VAL                  | A      |
| 286            | 589           | THR                  | A      |
| 287            | 590           | ALA                  | A      |
| 288            | 599           | LYS                  | A      |
| 289            | 600           | ALA                  | A      |
| 290            | 601           | HIS                  | A      |
| 291            | 602           | ASP                  | A      |
| 292            | 603           | LEU                  | A      |
| 293            | 604           | ILE                  | A      |
| 294            | 617           | LEU                  | A      |
| 295            | 618           | GLN                  | A      |
| 296            | 619           | PRO                  | A      |
| 297            | 621           | GLN                  | A      |
| 298            | 622           | VAL                  | A      |
| 299            | 623           | MET                  | A      |
| 300            | 624           | TRP                  | A      |
| 301            | 625           | LEU                  | A      |
| 302            | 626           | GLU                  | A      |

Table S3: Residues membership for the *T. vulgaris* R47  $\alpha$ -amylase (PDB code 1VFM, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |

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Table S3 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |
| 30             | 192           | PHE                  | C      |
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |

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Table S3 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |
| 76             | 239           | ASP                  | C      |
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |

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Table S3 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |
| 122            | 316           | GLU                  | B      |
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASN                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |

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Table S3 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |
| 168            | 370           | SER                  | B      |
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |

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Table S3 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASN                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |
| 214            | 436           | PHE                  | A      |
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |

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Table S3 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |
| 260            | 507           | SER                  | A      |
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |

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Table S3 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 574           | ARG                  | A      |
| 295            | 575           | PRO                  | A      |
| 296            | 576           | TYR                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S4: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 1OSE, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |

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Table S4 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | ILE                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |

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Table S4 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |

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Table S4 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |

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Table S4 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |

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Table S4 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | VAL                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLU                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |

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Table S4 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLU                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |

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Table S4 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S5: Residues membership for the *B. licheniformis*  $\alpha$ -amylase (PDB code 1OB0, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 5             | GLY                  | A      |
| 1              | 6             | THR                  | A      |
| 2              | 7             | LEU                  | B      |
| 3              | 8             | MET                  | B      |
| 4              | 9             | GLN                  | B      |
| 5              | 10            | TYR                  | C      |
| 6              | 11            | PHE                  | C      |
| 7              | 15            | MET                  | C      |
| 8              | 20            | GLN                  | C      |
| 9              | 21            | HIS                  | C      |
| 10             | 22            | TRP                  | C      |
| 11             | 23            | LYS                  | C      |
| 12             | 24            | ARG                  | C      |
| 13             | 25            | LEU                  | C      |
| 14             | 26            | GLN                  | C      |
| 15             | 27            | ASN                  | C      |
| 16             | 28            | ASP                  | C      |
| 17             | 29            | SER                  | C      |
| 18             | 30            | ALA                  | C      |
| 19             | 31            | TYR                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | GLU                  | C      |
| 23             | 35            | HIS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | ILE                  | C      |
| 26             | 38            | THR                  | C      |
| 27             | 39            | ALA                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | TRP                  | C      |
| 30             | 42            | ILE                  | C      |

*Continued on next page*

Table S5 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | PRO                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | ALA                  | C      |
| 34             | 46            | TYR                  | C      |
| 35             | 47            | LYS                  | C      |
| 36             | 48            | GLY                  | C      |
| 37             | 49            | THR                  | C      |
| 38             | 52            | ALA                  | C      |
| 39             | 53            | ASP                  | C      |
| 40             | 54            | VAL                  | C      |
| 41             | 55            | GLY                  | C      |
| 42             | 56            | TYR                  | C      |
| 43             | 57            | GLY                  | C      |
| 44             | 58            | ALA                  | C      |
| 45             | 59            | TYR                  | C      |
| 46             | 60            | ASP                  | C      |
| 47             | 62            | TYR                  | C      |
| 48             | 63            | ASP                  | C      |
| 49             | 64            | LEU                  | C      |
| 50             | 65            | GLY                  | C      |
| 51             | 75            | THR                  | C      |
| 52             | 76            | LYS                  | C      |
| 53             | 77            | TYR                  | C      |
| 54             | 78            | GLY                  | C      |
| 55             | 79            | THR                  | C      |
| 56             | 80            | LYS                  | C      |
| 57             | 81            | GLY                  | C      |
| 58             | 82            | GLU                  | C      |
| 59             | 83            | LEU                  | C      |
| 60             | 84            | GLN                  | C      |
| 61             | 85            | SER                  | C      |
| 62             | 86            | ALA                  | C      |
| 63             | 87            | ILE                  | C      |
| 64             | 88            | LYS                  | C      |
| 65             | 89            | SER                  | C      |
| 66             | 90            | LEU                  | C      |
| 67             | 91            | HIS                  | C      |
| 68             | 92            | SER                  | C      |
| 69             | 93            | ARG                  | C      |
| 70             | 94            | ASP                  | C      |
| 71             | 95            | ILE                  | C      |
| 72             | 96            | ASN                  | C      |
| 73             | 97            | VAL                  | C      |
| 74             | 98            | TYR                  | C      |
| 75             | 99            | GLY                  | C      |
| 76             | 100           | ASP                  | C      |

*Continued on next page*

Table S5 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 101           | VAL                  | C      |
| 78             | 102           | VAL                  | C      |
| 79             | 103           | ILE                  | C      |
| 80             | 104           | ASN                  | C      |
| 81             | 105           | HIS                  | C      |
| 82             | 106           | LYS                  | C      |
| 83             | 107           | GLY                  | C      |
| 84             | 108           | GLY                  | C      |
| 85             | 109           | ALA                  | C      |
| 86             | 141           | PHE                  | C      |
| 87             | 154           | LYS                  | C      |
| 88             | 155           | TRP                  | C      |
| 89             | 156           | HIS                  | C      |
| 90             | 157           | TRP                  | C      |
| 91             | 158           | TYR                  | C      |
| 92             | 159           | HIS                  | C      |
| 93             | 160           | PHE                  | C      |
| 94             | 161           | ASP                  | B      |
| 95             | 194           | ASP                  | B      |
| 96             | 195           | TYR                  | B      |
| 97             | 196           | LEU                  | B      |
| 98             | 197           | MET                  | B      |
| 99             | 198           | TYR                  | B      |
| 100            | 199           | ALA                  | B      |
| 101            | 200           | ASP                  | B      |
| 102            | 201           | ILE                  | B      |
| 103            | 202           | ASP                  | B      |
| 104            | 203           | TYR                  | B      |
| 105            | 204           | ASP                  | B      |
| 106            | 205           | HIS                  | B      |
| 107            | 206           | PRO                  | B      |
| 108            | 207           | ASP                  | B      |
| 109            | 208           | VAL                  | B      |
| 110            | 209           | VAL                  | B      |
| 111            | 210           | ALA                  | B      |
| 112            | 211           | GLU                  | B      |
| 113            | 212           | ILE                  | B      |
| 114            | 213           | LYS                  | B      |
| 115            | 214           | ARG                  | B      |
| 116            | 215           | TRP                  | B      |
| 117            | 216           | GLY                  | B      |
| 118            | 217           | THR                  | B      |
| 119            | 218           | TRP                  | B      |
| 120            | 219           | TYR                  | B      |
| 121            | 220           | ALA                  | B      |
| 122            | 221           | ASN                  | B      |

*Continued on next page*

Table S5 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 223           | LEU                  | C      |
| 124            | 224           | GLN                  | C      |
| 125            | 225           | LEU                  | C      |
| 126            | 226           | ASP                  | C      |
| 127            | 227           | GLY                  | C      |
| 128            | 228           | PHE                  | B      |
| 129            | 229           | ARG                  | D      |
| 130            | 230           | LEU                  | B      |
| 131            | 231           | ASP                  | B      |
| 132            | 232           | ALA                  | B      |
| 133            | 233           | VAL                  | B      |
| 134            | 234           | LYS                  | B      |
| 135            | 235           | HIS                  | B      |
| 136            | 236           | ILE                  | B      |
| 137            | 237           | LYS                  | B      |
| 138            | 238           | PHE                  | B      |
| 139            | 239           | SER                  | B      |
| 140            | 240           | PHE                  | B      |
| 141            | 241           | LEU                  | B      |
| 142            | 242           | ARG                  | B      |
| 143            | 243           | ASP                  | B      |
| 144            | 244           | TRP                  | B      |
| 145            | 245           | VAL                  | B      |
| 146            | 246           | ASN                  | B      |
| 147            | 247           | HIS                  | B      |
| 148            | 248           | VAL                  | B      |
| 149            | 249           | ARG                  | B      |
| 150            | 256           | MET                  | B      |
| 151            | 257           | PHE                  | B      |
| 152            | 258           | THR                  | B      |
| 153            | 259           | VAL                  | C      |
| 154            | 260           | ALA                  | B      |
| 155            | 261           | GLU                  | B      |
| 156            | 262           | TYR                  | B      |
| 157            | 263           | TRP                  | B      |
| 158            | 264           | SER                  | B      |
| 159            | 265           | TYR                  | B      |
| 160            | 270           | LEU                  | B      |
| 161            | 271           | GLU                  | B      |
| 162            | 272           | ASN                  | B      |
| 163            | 273           | TYR                  | B      |
| 164            | 274           | LEU                  | B      |
| 165            | 275           | ASN                  | B      |
| 166            | 280           | ASN                  | B      |
| 167            | 281           | HIS                  | B      |
| 168            | 282           | SER                  | B      |

*Continued on next page*

Table S5 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 283           | VAL                  | B      |
| 170            | 284           | PHE                  | D      |
| 171            | 285           | ASP                  | D      |
| 172            | 286           | VAL                  | D      |
| 173            | 287           | PRO                  | D      |
| 174            | 289           | HIS                  | D      |
| 175            | 290           | TYR                  | D      |
| 176            | 291           | GLN                  | D      |
| 177            | 292           | PHE                  | D      |
| 178            | 293           | HIS                  | D      |
| 179            | 294           | ALA                  | D      |
| 180            | 295           | ALA                  | D      |
| 181            | 296           | SER                  | D      |
| 182            | 302           | TYR                  | D      |
| 183            | 303           | ASP                  | A      |
| 184            | 304           | MET                  | A      |
| 185            | 305           | ARG                  | A      |
| 186            | 307           | LEU                  | A      |
| 187            | 308           | LEU                  | D      |
| 188            | 309           | ASN                  | D      |
| 189            | 310           | GLY                  | D      |
| 190            | 313           | VAL                  | D      |
| 191            | 314           | SER                  | B      |
| 192            | 315           | LYS                  | B      |
| 193            | 316           | HIS                  | B      |
| 194            | 317           | PRO                  | B      |
| 195            | 318           | LEU                  | B      |
| 196            | 319           | LYS                  | B      |
| 197            | 320           | SER                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | VAL                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | THR                  | D      |
| 207            | 330           | GLN                  | D      |
| 208            | 338           | THR                  | D      |
| 209            | 339           | VAL                  | D      |
| 210            | 340           | GLN                  | D      |
| 211            | 341           | THR                  | D      |
| 212            | 342           | TRP                  | A      |
| 213            | 343           | PHE                  | A      |
| 214            | 344           | LYS                  | A      |

*Continued on next page*

Table S5 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 345           | PRO                  | A      |
| 216            | 346           | LEU                  | A      |
| 217            | 347           | ALA                  | A      |
| 218            | 348           | TYR                  | A      |
| 219            | 349           | ALA                  | A      |
| 220            | 350           | PHE                  | A      |
| 221            | 351           | ILE                  | A      |
| 222            | 352           | LEU                  | A      |
| 223            | 353           | THR                  | A      |
| 224            | 354           | ARG                  | A      |
| 225            | 356           | SER                  | D      |
| 226            | 357           | GLY                  | D      |
| 227            | 358           | TYR                  | D      |
| 228            | 359           | PRO                  | A      |
| 229            | 360           | GLN                  | D      |
| 230            | 361           | VAL                  | A      |
| 231            | 362           | PHE                  | D      |
| 232            | 363           | TYR                  | C      |
| 233            | 364           | GLY                  | D      |
| 234            | 365           | ASP                  | A      |
| 235            | 366           | MET                  | C      |
| 236            | 367           | TYR                  | C      |
| 237            | 368           | GLY                  | D      |
| 238            | 369           | THR                  | D      |
| 239            | 379           | ALA                  | D      |
| 240            | 380           | LEU                  | A      |
| 241            | 381           | LYS                  | A      |
| 242            | 382           | HIS                  | A      |
| 243            | 383           | LYS                  | A      |
| 244            | 384           | ILE                  | A      |
| 245            | 385           | GLU                  | A      |
| 246            | 386           | PRO                  | A      |
| 247            | 387           | ILE                  | A      |
| 248            | 388           | LEU                  | A      |
| 249            | 389           | LYS                  | A      |
| 250            | 390           | ALA                  | A      |
| 251            | 391           | ARG                  | A      |
| 252            | 392           | LYS                  | A      |
| 253            | 393           | GLN                  | A      |
| 254            | 394           | TYR                  | A      |
| 255            | 395           | ALA                  | A      |
| 256            | 397           | GLY                  | A      |
| 257            | 398           | ALA                  | A      |
| 258            | 399           | GLN                  | A      |
| 259            | 400           | HIS                  | A      |
| 260            | 401           | ASP                  | A      |

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Table S5 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 402           | TYR                  | A      |
| 262            | 403           | PHE                  | A      |
| 263            | 404           | ASP                  | A      |
| 264            | 405           | HIS                  | A      |
| 265            | 406           | HIS                  | A      |
| 266            | 407           | ASP                  | A      |
| 267            | 408           | ILE                  | A      |
| 268            | 409           | VAL                  | A      |
| 269            | 410           | GLY                  | A      |
| 270            | 411           | TRP                  | A      |
| 271            | 412           | THR                  | A      |
| 272            | 413           | ARG                  | A      |
| 273            | 414           | GLU                  | A      |
| 274            | 415           | GLY                  | A      |
| 275            | 424           | LEU                  | A      |
| 276            | 425           | ALA                  | A      |
| 277            | 426           | ALA                  | A      |
| 278            | 427           | LEU                  | A      |
| 279            | 428           | ILE                  | A      |
| 280            | 429           | THR                  | A      |
| 281            | 431           | GLY                  | A      |
| 282            | 432           | PRO                  | A      |
| 283            | 433           | GLY                  | A      |
| 284            | 434           | GLY                  | A      |
| 285            | 435           | ALA                  | A      |
| 286            | 436           | LYS                  | A      |
| 287            | 437           | ARG                  | A      |
| 288            | 446           | GLY                  | A      |
| 289            | 447           | GLU                  | A      |
| 290            | 449           | TRP                  | A      |
| 291            | 450           | HIS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | ILE                  | A      |
| 294            | 472           | VAL                  | A      |
| 295            | 473           | ASN                  | A      |
| 296            | 474           | GLY                  | A      |
| 297            | 476           | SER                  | A      |
| 298            | 477           | VAL                  | A      |
| 299            | 478           | SER                  | A      |
| 300            | 479           | ILE                  | A      |
| 301            | 480           | TYR                  | A      |
| 302            | 481           | VAL                  | A      |

Table S6: Residues membership for the *B. subtilis*  $\alpha$ -amylase (PDB code 1UA7, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | GLY                  | A      |
| 1              | 10            | THR                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | LEU                  | B      |
| 4              | 13            | HIS                  | B      |
| 5              | 14            | ALA                  | C      |
| 6              | 15            | TRP                  | C      |
| 7              | 16            | ASN                  | C      |
| 8              | 17            | TRP                  | C      |
| 9              | 18            | SER                  | C      |
| 10             | 19            | PHE                  | C      |
| 11             | 20            | ASN                  | C      |
| 12             | 21            | THR                  | C      |
| 13             | 22            | LEU                  | C      |
| 14             | 23            | LYS                  | C      |
| 15             | 24            | HIS                  | C      |
| 16             | 25            | ASN                  | C      |
| 17             | 26            | MET                  | C      |
| 18             | 27            | LYS                  | C      |
| 19             | 28            | ASP                  | C      |
| 20             | 29            | ILE                  | C      |
| 21             | 30            | HIS                  | C      |
| 22             | 31            | ASP                  | C      |
| 23             | 32            | ALA                  | C      |
| 24             | 33            | GLY                  | C      |
| 25             | 34            | TYR                  | C      |
| 26             | 35            | THR                  | C      |
| 27             | 36            | ALA                  | C      |
| 28             | 37            | ILE                  | C      |
| 29             | 38            | GLN                  | C      |
| 30             | 39            | THR                  | C      |
| 31             | 40            | SER                  | C      |
| 32             | 41            | PRO                  | C      |
| 33             | 42            | ILE                  | C      |
| 34             | 43            | ASN                  | C      |
| 35             | 44            | GLN                  | C      |
| 36             | 45            | VAL                  | C      |
| 37             | 46            | LYS                  | C      |
| 38             | 48            | GLY                  | C      |
| 39             | 59            | TYR                  | C      |
| 40             | 60            | TRP                  | C      |
| 41             | 61            | LEU                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |

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Table S6 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 64            | PRO                  | C      |
| 45             | 65            | THR                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | GLN                  | C      |
| 49             | 69            | ILE                  | C      |
| 50             | 70            | GLY                  | C      |
| 51             | 72            | ARG                  | C      |
| 52             | 73            | TYR                  | C      |
| 53             | 74            | LEU                  | C      |
| 54             | 75            | GLY                  | C      |
| 55             | 76            | THR                  | C      |
| 56             | 77            | GLU                  | C      |
| 57             | 78            | GLN                  | C      |
| 58             | 79            | GLU                  | C      |
| 59             | 80            | PHE                  | C      |
| 60             | 81            | LYS                  | C      |
| 61             | 82            | GLU                  | C      |
| 62             | 83            | MET                  | C      |
| 63             | 84            | CYS                  | C      |
| 64             | 85            | ALA                  | C      |
| 65             | 86            | ALA                  | C      |
| 66             | 87            | ALA                  | C      |
| 67             | 88            | GLU                  | C      |
| 68             | 89            | GLU                  | C      |
| 69             | 90            | TYR                  | C      |
| 70             | 91            | GLY                  | C      |
| 71             | 92            | ILE                  | C      |
| 72             | 93            | LYS                  | C      |
| 73             | 94            | VAL                  | C      |
| 74             | 95            | ILE                  | C      |
| 75             | 96            | VAL                  | C      |
| 76             | 97            | ASP                  | C      |
| 77             | 98            | ALA                  | C      |
| 78             | 99            | VAL                  | C      |
| 79             | 100           | ILE                  | C      |
| 80             | 101           | ASN                  | C      |
| 81             | 102           | HIS                  | C      |
| 82             | 103           | THR                  | C      |
| 83             | 104           | THR                  | C      |
| 84             | 105           | PHE                  | C      |
| 85             | 106           | ASP                  | C      |
| 86             | 111           | SER                  | C      |
| 87             | 113           | GLU                  | C      |
| 88             | 114           | VAL                  | C      |
| 89             | 115           | LYS                  | C      |

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Table S6 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 118           | PRO                  | C      |
| 91             | 119           | ASN                  | C      |
| 92             | 120           | TRP                  | C      |
| 93             | 121           | THR                  | C      |
| 94             | 122           | HIS                  | B      |
| 95             | 139           | ASN                  | B      |
| 96             | 140           | SER                  | B      |
| 97             | 141           | LEU                  | B      |
| 98             | 142           | LEU                  | B      |
| 99             | 144           | LEU                  | B      |
| 100            | 145           | TYR                  | B      |
| 101            | 146           | ASP                  | B      |
| 102            | 147           | TRP                  | B      |
| 103            | 148           | ASN                  | B      |
| 104            | 149           | THR                  | B      |
| 105            | 150           | GLN                  | B      |
| 106            | 151           | ASN                  | B      |
| 107            | 152           | THR                  | B      |
| 108            | 153           | GLN                  | B      |
| 109            | 154           | VAL                  | B      |
| 110            | 155           | GLN                  | B      |
| 111            | 156           | SER                  | B      |
| 112            | 157           | TYR                  | B      |
| 113            | 158           | LEU                  | B      |
| 114            | 159           | LYS                  | B      |
| 115            | 160           | ARG                  | B      |
| 116            | 161           | PHE                  | B      |
| 117            | 162           | LEU                  | B      |
| 118            | 163           | GLU                  | B      |
| 119            | 164           | ARG                  | B      |
| 120            | 165           | ALA                  | B      |
| 121            | 166           | LEU                  | B      |
| 122            | 167           | ASN                  | B      |
| 123            | 168           | ASP                  | C      |
| 124            | 169           | GLY                  | C      |
| 125            | 170           | ALA                  | C      |
| 126            | 171           | ASP                  | C      |
| 127            | 172           | GLY                  | C      |
| 128            | 173           | PHE                  | B      |
| 129            | 174           | ARG                  | D      |
| 130            | 175           | PHE                  | B      |
| 131            | 176           | ASP                  | B      |
| 132            | 177           | ALA                  | B      |
| 133            | 178           | ALA                  | B      |
| 134            | 179           | LYS                  | B      |
| 135            | 180           | HIS                  | B      |

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Table S6 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 181           | ILE                  | B      |
| 137            | 182           | GLU                  | B      |
| 138            | 191           | SER                  | B      |
| 139            | 192           | GLN                  | B      |
| 140            | 193           | PHE                  | B      |
| 141            | 194           | TRP                  | B      |
| 142            | 195           | PRO                  | B      |
| 143            | 196           | ASN                  | B      |
| 144            | 197           | ILE                  | B      |
| 145            | 198           | THR                  | B      |
| 146            | 199           | ASN                  | B      |
| 147            | 200           | THR                  | B      |
| 148            | 201           | SER                  | B      |
| 149            | 202           | ALA                  | B      |
| 150            | 203           | GLU                  | B      |
| 151            | 204           | PHE                  | B      |
| 152            | 205           | GLN                  | B      |
| 153            | 206           | TYR                  | C      |
| 154            | 207           | GLY                  | B      |
| 155            | 208           | GLU                  | B      |
| 156            | 209           | ILE                  | B      |
| 157            | 210           | LEU                  | B      |
| 158            | 211           | GLN                  | B      |
| 159            | 212           | ASP                  | B      |
| 160            | 217           | ASP                  | B      |
| 161            | 218           | ALA                  | B      |
| 162            | 219           | ALA                  | B      |
| 163            | 220           | TYR                  | B      |
| 164            | 221           | ALA                  | B      |
| 165            | 222           | ASN                  | B      |
| 166            | 223           | TYR                  | B      |
| 167            | 224           | MET                  | B      |
| 168            | 225           | ASP                  | B      |
| 169            | 226           | VAL                  | B      |
| 170            | 227           | THR                  | D      |
| 171            | 228           | ALA                  | D      |
| 172            | 229           | SER                  | D      |
| 173            | 230           | ASN                  | D      |
| 174            | 232           | GLY                  | D      |
| 175            | 233           | HIS                  | D      |
| 176            | 234           | SER                  | D      |
| 177            | 235           | ILE                  | D      |
| 178            | 236           | ARG                  | D      |
| 179            | 237           | SER                  | D      |
| 180            | 238           | ALA                  | D      |
| 181            | 239           | LEU                  | D      |

*Continued on next page*

Table S6 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 243           | ASN                  | D      |
| 183            | 244           | LEU                  | A      |
| 184            | 245           | GLY                  | A      |
| 185            | 246           | VAL                  | A      |
| 186            | 249           | ILE                  | A      |
| 187            | 250           | SER                  | D      |
| 188            | 251           | HIS                  | D      |
| 189            | 252           | TYR                  | D      |
| 190            | 253           | ALA                  | D      |
| 191            | 254           | SER                  | B      |
| 192            | 255           | ASP                  | B      |
| 193            | 257           | SER                  | B      |
| 194            | 258           | ALA                  | B      |
| 195            | 259           | ASP                  | B      |
| 196            | 260           | LYS                  | B      |
| 197            | 261           | LEU                  | B      |
| 198            | 262           | VAL                  | D      |
| 199            | 263           | THR                  | D      |
| 200            | 264           | TRP                  | D      |
| 201            | 265           | VAL                  | A      |
| 202            | 266           | GLU                  | D      |
| 203            | 267           | SER                  | D      |
| 204            | 268           | HIS                  | D      |
| 205            | 269           | ASP                  | D      |
| 206            | 270           | THR                  | D      |
| 207            | 271           | TYR                  | D      |
| 208            | 279           | THR                  | D      |
| 209            | 280           | TRP                  | D      |
| 210            | 281           | MET                  | D      |
| 211            | 282           | SER                  | D      |
| 212            | 284           | ASP                  | A      |
| 213            | 285           | ASP                  | A      |
| 214            | 286           | ILE                  | A      |
| 215            | 287           | ARG                  | A      |
| 216            | 288           | LEU                  | A      |
| 217            | 289           | GLY                  | A      |
| 218            | 290           | TRP                  | A      |
| 219            | 291           | ALA                  | A      |
| 220            | 292           | VAL                  | A      |
| 221            | 293           | ILE                  | A      |
| 222            | 294           | ALA                  | A      |
| 223            | 295           | SER                  | A      |
| 224            | 296           | ARG                  | A      |
| 225            | 297           | SER                  | D      |
| 226            | 299           | SER                  | D      |
| 227            | 300           | THR                  | D      |

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Table S6 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 301           | PRO                  | A      |
| 229            | 302           | LEU                  | D      |
| 230            | 303           | PHE                  | A      |
| 231            | 304           | PHE                  | D      |
| 232            | 305           | SER                  | C      |
| 233            | 306           | ARG                  | D      |
| 234            | 307           | PRO                  | A      |
| 235            | 316           | PHE                  | C      |
| 236            | 325           | ARG                  | C      |
| 237            | 326           | GLY                  | D      |
| 238            | 327           | SER                  | D      |
| 239            | 328           | ALA                  | D      |
| 240            | 331           | GLU                  | A      |
| 241            | 332           | ASP                  | A      |
| 242            | 333           | GLN                  | A      |
| 243            | 334           | ALA                  | A      |
| 244            | 335           | ILE                  | A      |
| 245            | 336           | THR                  | A      |
| 246            | 337           | ALA                  | A      |
| 247            | 338           | VAL                  | A      |
| 248            | 339           | ASN                  | A      |
| 249            | 340           | ARG                  | A      |
| 250            | 341           | PHE                  | A      |
| 251            | 342           | HIS                  | A      |
| 252            | 343           | ASN                  | A      |
| 253            | 344           | VAL                  | A      |
| 254            | 345           | MET                  | A      |
| 255            | 346           | ALA                  | A      |
| 256            | 347           | GLY                  | A      |
| 257            | 348           | GLN                  | A      |
| 258            | 349           | PRO                  | A      |
| 259            | 350           | GLU                  | A      |
| 260            | 351           | GLU                  | A      |
| 261            | 352           | LEU                  | A      |
| 262            | 353           | SER                  | A      |
| 263            | 354           | ASN                  | A      |
| 264            | 357           | GLY                  | A      |
| 265            | 358           | ASN                  | A      |
| 266            | 359           | ASN                  | A      |
| 267            | 360           | GLN                  | A      |
| 268            | 362           | PHE                  | A      |
| 269            | 363           | MET                  | A      |
| 270            | 364           | ASN                  | A      |
| 271            | 365           | GLN                  | A      |
| 272            | 366           | ARG                  | A      |
| 273            | 367           | GLY                  | A      |

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Table S6 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 368           | SER                  | A      |
| 275            | 370           | GLY                  | A      |
| 276            | 371           | VAL                  | A      |
| 277            | 372           | VAL                  | A      |
| 278            | 373           | LEU                  | A      |
| 279            | 374           | ALA                  | A      |
| 280            | 375           | ASN                  | A      |
| 281            | 378           | SER                  | A      |
| 282            | 379           | SER                  | A      |
| 283            | 380           | SER                  | A      |
| 284            | 381           | VAL                  | A      |
| 285            | 383           | ILE                  | A      |
| 286            | 384           | ASN                  | A      |
| 287            | 385           | THR                  | A      |
| 288            | 391           | ASP                  | A      |
| 289            | 392           | GLY                  | A      |
| 290            | 394           | TYR                  | A      |
| 291            | 395           | ASP                  | A      |
| 292            | 396           | ASN                  | A      |
| 293            | 397           | LYS                  | A      |
| 294            | 414           | ILE                  | A      |
| 295            | 415           | ASN                  | A      |
| 296            | 416           | ALA                  | A      |
| 297            | 418           | SER                  | A      |
| 298            | 419           | VAL                  | A      |
| 299            | 420           | ALA                  | A      |
| 300            | 421           | VAL                  | A      |
| 301            | 422           | LEU                  | A      |
| 302            | 423           | TYR                  | A      |

Table S7: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 1PIF, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |

*Continued on next page*

Table S7 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |

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Table S7 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |

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Table S7 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |

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Table S7 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |

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Table S7 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | VAL                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |

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Table S7 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLU                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |

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Table S7 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASN                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S8: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 1PPI, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |

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Table S8 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |

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Table S8 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |

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Table S8 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |

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Table S8 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |

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Table S8 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | VAL                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLU                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |

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Table S8 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLU                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |

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Table S8 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S9: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1PJ9, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | ASN                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |

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Table S9 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |

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Table S9 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | ARG                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |

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Table S9 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |

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Table S9 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |

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Table S9 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |

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Table S9 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S10: Residues membership for the . *stearothermophilus* maltose  
 $\alpha$ -amylase (PDB code 1QHP, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | ASP                  | A      |
| 1              | 10            | VAL                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | TYR                  | B      |
| 4              | 13            | GLN                  | B      |
| 5              | 14            | ILE                  | C      |
| 6              | 15            | ILE                  | C      |
| 7              | 16            | ILE                  | C      |
| 8              | 49            | GLY                  | C      |
| 9              | 50            | ASP                  | C      |
| 10             | 51            | LEU                  | C      |
| 11             | 52            | GLU                  | C      |
| 12             | 53            | GLY                  | C      |
| 13             | 54            | VAL                  | C      |
| 14             | 55            | ARG                  | C      |
| 15             | 56            | GLN                  | C      |
| 16             | 57            | LYS                  | C      |
| 17             | 58            | LEU                  | C      |
| 18             | 59            | PRO                  | C      |
| 19             | 60            | TYR                  | C      |
| 20             | 61            | LEU                  | C      |
| 21             | 62            | LYS                  | C      |
| 22             | 63            | GLN                  | C      |
| 23             | 64            | LEU                  | C      |
| 24             | 65            | GLY                  | C      |
| 25             | 66            | VAL                  | C      |
| 26             | 67            | THR                  | C      |
| 27             | 68            | THR                  | C      |
| 28             | 69            | ILE                  | C      |
| 29             | 70            | TRP                  | C      |
| 30             | 71            | LEU                  | C      |
| 31             | 72            | SER                  | C      |
| 32             | 73            | PRO                  | C      |
| 33             | 74            | VAL                  | C      |
| 34             | 75            | LEU                  | C      |
| 35             | 76            | ASP                  | C      |
| 36             | 77            | ASN                  | C      |
| 37             | 78            | LEU                  | C      |
| 38             | 87            | THR                  | C      |
| 39             | 89            | TYR                  | C      |
| 40             | 90            | HIS                  | C      |
| 41             | 91            | GLY                  | C      |
| 42             | 92            | TYR                  | C      |
| 43             | 93            | TRP                  | C      |

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Table S10 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 94            | THR                  | C      |
| 45             | 95            | ARG                  | C      |
| 46             | 96            | ASP                  | C      |
| 47             | 98            | LYS                  | C      |
| 48             | 99            | GLN                  | C      |
| 49             | 100           | ILE                  | C      |
| 50             | 101           | GLU                  | C      |
| 51             | 102           | GLU                  | C      |
| 52             | 103           | HIS                  | C      |
| 53             | 104           | PHE                  | C      |
| 54             | 105           | GLY                  | C      |
| 55             | 106           | ASN                  | C      |
| 56             | 107           | TRP                  | C      |
| 57             | 108           | THR                  | C      |
| 58             | 109           | THR                  | C      |
| 59             | 110           | PHE                  | C      |
| 60             | 111           | ASP                  | C      |
| 61             | 112           | THR                  | C      |
| 62             | 113           | LEU                  | C      |
| 63             | 114           | VAL                  | C      |
| 64             | 115           | ASN                  | C      |
| 65             | 116           | ASP                  | C      |
| 66             | 117           | ALA                  | C      |
| 67             | 118           | HIS                  | C      |
| 68             | 119           | GLN                  | C      |
| 69             | 120           | ASN                  | C      |
| 70             | 121           | GLY                  | C      |
| 71             | 122           | ILE                  | C      |
| 72             | 123           | LYS                  | C      |
| 73             | 124           | VAL                  | C      |
| 74             | 125           | ILE                  | C      |
| 75             | 126           | VAL                  | C      |
| 76             | 127           | ASP                  | C      |
| 77             | 128           | PHE                  | C      |
| 78             | 129           | VAL                  | C      |
| 79             | 130           | PRO                  | C      |
| 80             | 131           | ASN                  | C      |
| 81             | 132           | HIS                  | C      |
| 82             | 133           | SER                  | C      |
| 83             | 134           | THR                  | C      |
| 84             | 135           | PRO                  | C      |
| 85             | 136           | PHE                  | C      |
| 86             | 148           | ALA                  | C      |
| 87             | 155           | TYR                  | C      |
| 88             | 156           | MET                  | C      |
| 89             | 157           | GLY                  | C      |

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Table S10 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 165           | LYS                  | C      |
| 91             | 166           | GLY                  | C      |
| 92             | 167           | TYR                  | C      |
| 93             | 168           | PHE                  | C      |
| 94             | 169           | HIS                  | B      |
| 95             | 186           | LYS                  | B      |
| 96             | 187           | ASN                  | B      |
| 97             | 188           | PHE                  | B      |
| 98             | 189           | THR                  | B      |
| 99             | 196           | LEU                  | B      |
| 100            | 197           | ALA                  | B      |
| 101            | 198           | ASP                  | B      |
| 102            | 199           | LEU                  | B      |
| 103            | 200           | SER                  | B      |
| 104            | 201           | GLN                  | B      |
| 105            | 202           | GLU                  | B      |
| 106            | 203           | ASN                  | B      |
| 107            | 204           | GLY                  | B      |
| 108            | 205           | THR                  | B      |
| 109            | 206           | ILE                  | B      |
| 110            | 207           | ALA                  | B      |
| 111            | 208           | GLN                  | B      |
| 112            | 209           | TYR                  | B      |
| 113            | 210           | LEU                  | B      |
| 114            | 211           | THR                  | B      |
| 115            | 212           | ASP                  | B      |
| 116            | 213           | ALA                  | B      |
| 117            | 214           | ALA                  | B      |
| 118            | 215           | VAL                  | B      |
| 119            | 216           | GLN                  | B      |
| 120            | 217           | LEU                  | B      |
| 121            | 218           | VAL                  | B      |
| 122            | 219           | ALA                  | B      |
| 123            | 220           | HIS                  | C      |
| 124            | 221           | GLY                  | C      |
| 125            | 222           | ALA                  | C      |
| 126            | 223           | ASP                  | C      |
| 127            | 224           | GLY                  | C      |
| 128            | 225           | LEU                  | B      |
| 129            | 226           | ARG                  | D      |
| 130            | 227           | ILE                  | B      |
| 131            | 228           | ASP                  | B      |
| 132            | 229           | ALA                  | B      |
| 133            | 230           | VAL                  | B      |
| 134            | 231           | LYS                  | B      |
| 135            | 232           | HIS                  | B      |

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Table S10 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 233           | PHE                  | B      |
| 137            | 234           | ASN                  | B      |
| 138            | 235           | SER                  | B      |
| 139            | 236           | GLY                  | B      |
| 140            | 237           | PHE                  | B      |
| 141            | 238           | SER                  | B      |
| 142            | 239           | LYS                  | B      |
| 143            | 240           | SER                  | B      |
| 144            | 241           | LEU                  | B      |
| 145            | 242           | ALA                  | B      |
| 146            | 243           | ASP                  | B      |
| 147            | 244           | LYS                  | B      |
| 148            | 245           | LEU                  | B      |
| 149            | 246           | TYR                  | B      |
| 150            | 251           | ILE                  | B      |
| 151            | 252           | PHE                  | B      |
| 152            | 253           | LEU                  | B      |
| 153            | 254           | VAL                  | C      |
| 154            | 255           | GLY                  | B      |
| 155            | 256           | GLU                  | B      |
| 156            | 257           | TRP                  | B      |
| 157            | 258           | TYR                  | B      |
| 158            | 259           | GLY                  | B      |
| 159            | 260           | ASP                  | B      |
| 160            | 270           | LYS                  | B      |
| 161            | 271           | VAL                  | B      |
| 162            | 272           | ARG                  | B      |
| 163            | 273           | TYR                  | B      |
| 164            | 275           | ASN                  | B      |
| 165            | 276           | ASN                  | B      |
| 166            | 278           | GLY                  | B      |
| 167            | 279           | VAL                  | B      |
| 168            | 280           | ASN                  | B      |
| 169            | 281           | VAL                  | B      |
| 170            | 282           | LEU                  | D      |
| 171            | 283           | ASP                  | D      |
| 172            | 284           | PHE                  | D      |
| 173            | 285           | ASP                  | D      |
| 174            | 287           | ASN                  | D      |
| 175            | 288           | THR                  | D      |
| 176            | 289           | VAL                  | D      |
| 177            | 290           | ILE                  | D      |
| 178            | 291           | ARG                  | D      |
| 179            | 292           | ASN                  | D      |
| 180            | 293           | VAL                  | D      |
| 181            | 294           | PHE                  | D      |

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Table S10 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 299           | GLN                  | D      |
| 183            | 300           | THR                  | A      |
| 184            | 301           | MET                  | A      |
| 185            | 302           | TYR                  | A      |
| 186            | 307           | MET                  | A      |
| 187            | 308           | VAL                  | D      |
| 188            | 309           | ASN                  | D      |
| 189            | 310           | GLN                  | D      |
| 190            | 311           | THR                  | D      |
| 191            | 312           | GLY                  | B      |
| 192            | 313           | ASN                  | B      |
| 193            | 317           | TYR                  | B      |
| 194            | 318           | LYS                  | B      |
| 195            | 319           | GLU                  | B      |
| 196            | 320           | ASN                  | B      |
| 197            | 321           | LEU                  | B      |
| 198            | 322           | ILE                  | D      |
| 199            | 323           | THR                  | D      |
| 200            | 324           | PHE                  | D      |
| 201            | 325           | ILE                  | A      |
| 202            | 326           | ASP                  | D      |
| 203            | 327           | ASN                  | D      |
| 204            | 328           | HIS                  | D      |
| 205            | 329           | ASP                  | D      |
| 206            | 330           | MET                  | D      |
| 207            | 331           | SER                  | D      |
| 208            | 332           | ARG                  | D      |
| 209            | 333           | PHE                  | D      |
| 210            | 334           | LEU                  | D      |
| 211            | 335           | SER                  | D      |
| 212            | 340           | LYS                  | A      |
| 213            | 342           | ASN                  | A      |
| 214            | 343           | LEU                  | A      |
| 215            | 344           | HIS                  | A      |
| 216            | 345           | GLN                  | A      |
| 217            | 346           | ALA                  | A      |
| 218            | 347           | LEU                  | A      |
| 219            | 348           | ALA                  | A      |
| 220            | 349           | PHE                  | A      |
| 221            | 350           | ILE                  | A      |
| 222            | 351           | LEU                  | A      |
| 223            | 352           | THR                  | A      |
| 224            | 353           | SER                  | A      |
| 225            | 354           | ARG                  | D      |
| 226            | 355           | GLY                  | D      |
| 227            | 356           | THR                  | D      |

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Table S10 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 357           | PRO                  | A      |
| 229            | 358           | SER                  | D      |
| 230            | 359           | ILE                  | A      |
| 231            | 360           | TYR                  | D      |
| 232            | 361           | TYR                  | C      |
| 233            | 362           | GLY                  | D      |
| 234            | 363           | THR                  | A      |
| 235            | 377           | GLY                  | C      |
| 236            | 378           | MET                  | C      |
| 237            | 379           | MET                  | D      |
| 238            | 380           | PRO                  | D      |
| 239            | 382           | PHE                  | D      |
| 240            | 388           | ALA                  | A      |
| 241            | 389           | PHE                  | A      |
| 242            | 390           | LYS                  | A      |
| 243            | 391           | GLU                  | A      |
| 244            | 392           | VAL                  | A      |
| 245            | 393           | SER                  | A      |
| 246            | 394           | THR                  | A      |
| 247            | 395           | LEU                  | A      |
| 248            | 396           | ALA                  | A      |
| 249            | 397           | GLY                  | A      |
| 250            | 398           | LEU                  | A      |
| 251            | 399           | ARG                  | A      |
| 252            | 400           | ARG                  | A      |
| 253            | 401           | ASN                  | A      |
| 254            | 402           | ASN                  | A      |
| 255            | 403           | ALA                  | A      |
| 256            | 407           | TYR                  | A      |
| 257            | 408           | GLY                  | A      |
| 258            | 409           | THR                  | A      |
| 259            | 410           | THR                  | A      |
| 260            | 412           | GLN                  | A      |
| 261            | 413           | ARG                  | A      |
| 262            | 414           | TRP                  | A      |
| 263            | 415           | ILE                  | A      |
| 264            | 416           | ASN                  | A      |
| 265            | 417           | ASN                  | A      |
| 266            | 418           | ASP                  | A      |
| 267            | 419           | VAL                  | A      |
| 268            | 420           | TYR                  | A      |
| 269            | 421           | ILE                  | A      |
| 270            | 422           | TYR                  | A      |
| 271            | 423           | GLU                  | A      |
| 272            | 424           | ARG                  | A      |
| 273            | 429           | ASP                  | A      |

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Table S10 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 430           | VAL                  | A      |
| 275            | 431           | VAL                  | A      |
| 276            | 432           | LEU                  | A      |
| 277            | 433           | VAL                  | A      |
| 278            | 434           | ALA                  | A      |
| 279            | 435           | ILE                  | A      |
| 280            | 436           | ASN                  | A      |
| 281            | 440           | GLN                  | A      |
| 282            | 441           | SER                  | A      |
| 283            | 442           | SER                  | A      |
| 284            | 443           | TYR                  | A      |
| 285            | 444           | SER                  | A      |
| 286            | 445           | ILE                  | A      |
| 287            | 446           | SER                  | A      |
| 288            | 455           | GLY                  | A      |
| 289            | 456           | SER                  | A      |
| 290            | 458           | ALA                  | A      |
| 291            | 459           | ASP                  | A      |
| 292            | 460           | TYR                  | A      |
| 293            | 461           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | PRO                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | ALA                  | A      |
| 298            | 487           | VAL                  | A      |
| 299            | 488           | SER                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S11: Residues membership for the *B. stearothermophilus* maltose  $\alpha$ -amylase (PDB code 1QHO, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | ASP                  | A      |
| 1              | 10            | VAL                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | TYR                  | B      |
| 4              | 13            | GLN                  | B      |
| 5              | 14            | ILE                  | C      |
| 6              | 15            | ILE                  | C      |
| 7              | 16            | ILE                  | C      |
| 8              | 49            | GLY                  | C      |

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Table S11 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 50            | ASP                  | C      |
| 10             | 51            | LEU                  | C      |
| 11             | 52            | GLU                  | C      |
| 12             | 53            | GLY                  | C      |
| 13             | 54            | VAL                  | C      |
| 14             | 55            | ARG                  | C      |
| 15             | 56            | GLN                  | C      |
| 16             | 57            | LYS                  | C      |
| 17             | 58            | LEU                  | C      |
| 18             | 59            | PRO                  | C      |
| 19             | 60            | TYR                  | C      |
| 20             | 61            | LEU                  | C      |
| 21             | 62            | LYS                  | C      |
| 22             | 63            | GLN                  | C      |
| 23             | 64            | LEU                  | C      |
| 24             | 65            | GLY                  | C      |
| 25             | 66            | VAL                  | C      |
| 26             | 67            | THR                  | C      |
| 27             | 68            | THR                  | C      |
| 28             | 69            | ILE                  | C      |
| 29             | 70            | TRP                  | C      |
| 30             | 71            | LEU                  | C      |
| 31             | 72            | SER                  | C      |
| 32             | 73            | PRO                  | C      |
| 33             | 74            | VAL                  | C      |
| 34             | 75            | LEU                  | C      |
| 35             | 76            | ASP                  | C      |
| 36             | 77            | ASN                  | C      |
| 37             | 78            | LEU                  | C      |
| 38             | 87            | THR                  | C      |
| 39             | 89            | TYR                  | C      |
| 40             | 90            | HIS                  | C      |
| 41             | 91            | GLY                  | C      |
| 42             | 92            | TYR                  | C      |
| 43             | 93            | TRP                  | C      |
| 44             | 94            | THR                  | C      |
| 45             | 95            | ARG                  | C      |
| 46             | 96            | ASP                  | C      |
| 47             | 98            | LYS                  | C      |
| 48             | 99            | GLN                  | C      |
| 49             | 100           | ILE                  | C      |
| 50             | 101           | GLU                  | C      |
| 51             | 102           | GLU                  | C      |
| 52             | 103           | HIS                  | C      |
| 53             | 104           | PHE                  | C      |
| 54             | 105           | GLY                  | C      |

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Table S11 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 106           | ASN                  | C      |
| 56             | 107           | TRP                  | C      |
| 57             | 108           | THR                  | C      |
| 58             | 109           | THR                  | C      |
| 59             | 110           | PHE                  | C      |
| 60             | 111           | ASP                  | C      |
| 61             | 112           | THR                  | C      |
| 62             | 113           | LEU                  | C      |
| 63             | 114           | VAL                  | C      |
| 64             | 115           | ASN                  | C      |
| 65             | 116           | ASP                  | C      |
| 66             | 117           | ALA                  | C      |
| 67             | 118           | HIS                  | C      |
| 68             | 119           | GLN                  | C      |
| 69             | 120           | ASN                  | C      |
| 70             | 121           | GLY                  | C      |
| 71             | 122           | ILE                  | C      |
| 72             | 123           | LYS                  | C      |
| 73             | 124           | VAL                  | C      |
| 74             | 125           | ILE                  | C      |
| 75             | 126           | VAL                  | C      |
| 76             | 127           | ASP                  | C      |
| 77             | 128           | PHE                  | C      |
| 78             | 129           | VAL                  | C      |
| 79             | 130           | PRO                  | C      |
| 80             | 131           | ASN                  | C      |
| 81             | 132           | HIS                  | C      |
| 82             | 133           | SER                  | C      |
| 83             | 134           | THR                  | C      |
| 84             | 135           | PRO                  | C      |
| 85             | 136           | PHE                  | C      |
| 86             | 148           | ALA                  | C      |
| 87             | 155           | TYR                  | C      |
| 88             | 156           | MET                  | C      |
| 89             | 157           | GLY                  | C      |
| 90             | 165           | LYS                  | C      |
| 91             | 166           | GLY                  | C      |
| 92             | 167           | TYR                  | C      |
| 93             | 168           | PHE                  | C      |
| 94             | 169           | HIS                  | B      |
| 95             | 186           | LYS                  | B      |
| 96             | 187           | ASN                  | B      |
| 97             | 188           | PHE                  | B      |
| 98             | 189           | THR                  | B      |
| 99             | 196           | LEU                  | B      |
| 100            | 197           | ALA                  | B      |

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Table S11 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 198           | ASP                  | B      |
| 102            | 199           | LEU                  | B      |
| 103            | 200           | SER                  | B      |
| 104            | 201           | GLN                  | B      |
| 105            | 202           | GLU                  | B      |
| 106            | 203           | ASN                  | B      |
| 107            | 204           | GLY                  | B      |
| 108            | 205           | THR                  | B      |
| 109            | 206           | ILE                  | B      |
| 110            | 207           | ALA                  | B      |
| 111            | 208           | GLN                  | B      |
| 112            | 209           | TYR                  | B      |
| 113            | 210           | LEU                  | B      |
| 114            | 211           | THR                  | B      |
| 115            | 212           | ASP                  | B      |
| 116            | 213           | ALA                  | B      |
| 117            | 214           | ALA                  | B      |
| 118            | 215           | VAL                  | B      |
| 119            | 216           | GLN                  | B      |
| 120            | 217           | LEU                  | B      |
| 121            | 218           | VAL                  | B      |
| 122            | 219           | ALA                  | B      |
| 123            | 220           | HIS                  | C      |
| 124            | 221           | GLY                  | C      |
| 125            | 222           | ALA                  | C      |
| 126            | 223           | ASP                  | C      |
| 127            | 224           | GLY                  | C      |
| 128            | 225           | LEU                  | B      |
| 129            | 226           | ARG                  | D      |
| 130            | 227           | ILE                  | B      |
| 131            | 228           | ASP                  | B      |
| 132            | 229           | ALA                  | B      |
| 133            | 230           | VAL                  | B      |
| 134            | 231           | LYS                  | B      |
| 135            | 232           | HIS                  | B      |
| 136            | 233           | PHE                  | B      |
| 137            | 234           | ASN                  | B      |
| 138            | 235           | SER                  | B      |
| 139            | 236           | GLY                  | B      |
| 140            | 237           | PHE                  | B      |
| 141            | 238           | SER                  | B      |
| 142            | 239           | LYS                  | B      |
| 143            | 240           | SER                  | B      |
| 144            | 241           | LEU                  | B      |
| 145            | 242           | ALA                  | B      |
| 146            | 243           | ASP                  | B      |

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Table S11 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 244           | LYS                  | B      |
| 148            | 245           | LEU                  | B      |
| 149            | 246           | TYR                  | B      |
| 150            | 251           | ILE                  | B      |
| 151            | 252           | PHE                  | B      |
| 152            | 253           | LEU                  | B      |
| 153            | 254           | VAL                  | C      |
| 154            | 255           | GLY                  | B      |
| 155            | 256           | GLU                  | B      |
| 156            | 257           | TRP                  | B      |
| 157            | 258           | TYR                  | B      |
| 158            | 259           | GLY                  | B      |
| 159            | 260           | ASP                  | B      |
| 160            | 270           | LYS                  | B      |
| 161            | 271           | VAL                  | B      |
| 162            | 272           | ARG                  | B      |
| 163            | 273           | TYR                  | B      |
| 164            | 275           | ASN                  | B      |
| 165            | 276           | ASN                  | B      |
| 166            | 278           | GLY                  | B      |
| 167            | 279           | VAL                  | B      |
| 168            | 280           | ASN                  | B      |
| 169            | 281           | VAL                  | B      |
| 170            | 282           | LEU                  | D      |
| 171            | 283           | ASP                  | D      |
| 172            | 284           | PHE                  | D      |
| 173            | 285           | ASP                  | D      |
| 174            | 287           | ASN                  | D      |
| 175            | 288           | THR                  | D      |
| 176            | 289           | VAL                  | D      |
| 177            | 290           | ILE                  | D      |
| 178            | 291           | ARG                  | D      |
| 179            | 292           | ASN                  | D      |
| 180            | 293           | VAL                  | D      |
| 181            | 294           | PHE                  | D      |
| 182            | 299           | GLN                  | D      |
| 183            | 300           | THR                  | A      |
| 184            | 301           | MET                  | A      |
| 185            | 302           | TYR                  | A      |
| 186            | 307           | MET                  | A      |
| 187            | 308           | VAL                  | D      |
| 188            | 309           | ASN                  | D      |
| 189            | 310           | GLN                  | D      |
| 190            | 311           | THR                  | D      |
| 191            | 312           | GLY                  | B      |
| 192            | 313           | ASN                  | B      |

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Table S11 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 317           | TYR                  | B      |
| 194            | 318           | LYS                  | B      |
| 195            | 319           | GLU                  | B      |
| 196            | 320           | ASN                  | B      |
| 197            | 321           | LEU                  | B      |
| 198            | 322           | ILE                  | D      |
| 199            | 323           | THR                  | D      |
| 200            | 324           | PHE                  | D      |
| 201            | 325           | ILE                  | A      |
| 202            | 326           | ASP                  | D      |
| 203            | 327           | ASN                  | D      |
| 204            | 328           | HIS                  | D      |
| 205            | 329           | ASP                  | D      |
| 206            | 330           | MET                  | D      |
| 207            | 331           | SER                  | D      |
| 208            | 332           | ARG                  | D      |
| 209            | 333           | PHE                  | D      |
| 210            | 334           | LEU                  | D      |
| 211            | 335           | SER                  | D      |
| 212            | 340           | LYS                  | A      |
| 213            | 342           | ASN                  | A      |
| 214            | 343           | LEU                  | A      |
| 215            | 344           | HIS                  | A      |
| 216            | 345           | GLN                  | A      |
| 217            | 346           | ALA                  | A      |
| 218            | 347           | LEU                  | A      |
| 219            | 348           | ALA                  | A      |
| 220            | 349           | PHE                  | A      |
| 221            | 350           | ILE                  | A      |
| 222            | 351           | LEU                  | A      |
| 223            | 352           | THR                  | A      |
| 224            | 353           | SER                  | A      |
| 225            | 354           | ARG                  | D      |
| 226            | 355           | GLY                  | D      |
| 227            | 356           | THR                  | D      |
| 228            | 357           | PRO                  | A      |
| 229            | 358           | SER                  | D      |
| 230            | 359           | ILE                  | A      |
| 231            | 360           | TYR                  | D      |
| 232            | 361           | TYR                  | C      |
| 233            | 362           | GLY                  | D      |
| 234            | 363           | THR                  | A      |
| 235            | 377           | GLY                  | C      |
| 236            | 378           | MET                  | C      |
| 237            | 379           | MET                  | D      |
| 238            | 380           | PRO                  | D      |

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Table S11 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 382           | PHE                  | D      |
| 240            | 388           | ALA                  | A      |
| 241            | 389           | PHE                  | A      |
| 242            | 390           | LYS                  | A      |
| 243            | 391           | GLU                  | A      |
| 244            | 392           | VAL                  | A      |
| 245            | 393           | SER                  | A      |
| 246            | 394           | THR                  | A      |
| 247            | 395           | LEU                  | A      |
| 248            | 396           | ALA                  | A      |
| 249            | 397           | GLY                  | A      |
| 250            | 398           | LEU                  | A      |
| 251            | 399           | ARG                  | A      |
| 252            | 400           | ARG                  | A      |
| 253            | 401           | ASN                  | A      |
| 254            | 402           | ASN                  | A      |
| 255            | 403           | ALA                  | A      |
| 256            | 407           | TYR                  | A      |
| 257            | 408           | GLY                  | A      |
| 258            | 409           | THR                  | A      |
| 259            | 410           | THR                  | A      |
| 260            | 412           | GLN                  | A      |
| 261            | 413           | ARG                  | A      |
| 262            | 414           | TRP                  | A      |
| 263            | 415           | ILE                  | A      |
| 264            | 416           | ASN                  | A      |
| 265            | 417           | ASN                  | A      |
| 266            | 418           | ASP                  | A      |
| 267            | 419           | VAL                  | A      |
| 268            | 420           | TYR                  | A      |
| 269            | 421           | ILE                  | A      |
| 270            | 422           | TYR                  | A      |
| 271            | 423           | GLU                  | A      |
| 272            | 424           | ARG                  | A      |
| 273            | 429           | ASP                  | A      |
| 274            | 430           | VAL                  | A      |
| 275            | 431           | VAL                  | A      |
| 276            | 432           | LEU                  | A      |
| 277            | 433           | VAL                  | A      |
| 278            | 434           | ALA                  | A      |
| 279            | 435           | ILE                  | A      |
| 280            | 436           | ASN                  | A      |
| 281            | 440           | GLN                  | A      |
| 282            | 441           | SER                  | A      |
| 283            | 442           | SER                  | A      |
| 284            | 443           | TYR                  | A      |

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Table S11 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 444           | SER                  | A      |
| 286            | 445           | ILE                  | A      |
| 287            | 446           | SER                  | A      |
| 288            | 455           | GLY                  | A      |
| 289            | 456           | SER                  | A      |
| 290            | 458           | ALA                  | A      |
| 291            | 459           | ASP                  | A      |
| 292            | 460           | TYR                  | A      |
| 293            | 461           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | PRO                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | ALA                  | A      |
| 298            | 487           | VAL                  | A      |
| 299            | 488           | SER                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S12: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 1UA3, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |

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Table S12 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | ILE                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |

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Table S12 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |

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Table S12 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |

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Table S12 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |

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Table S12 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | ILE                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLU                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |

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Table S12 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |

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Table S12 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S13: Residues membership for the *P. haloplanctis*  $\alpha$ -amylase (PDB code 1G94, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 3             | THR                  | A      |
| 1              | 4             | THR                  | A      |
| 2              | 5             | PHE                  | B      |
| 3              | 6             | VAL                  | B      |
| 4              | 7             | HIS                  | B      |
| 5              | 8             | LEU                  | C      |
| 6              | 9             | PHE                  | C      |
| 7              | 10            | GLU                  | C      |
| 8              | 11            | TRP                  | C      |
| 9              | 12            | ASN                  | C      |
| 10             | 13            | TRP                  | C      |
| 11             | 14            | GLN                  | C      |
| 12             | 15            | ASP                  | C      |
| 13             | 16            | VAL                  | C      |
| 14             | 17            | ALA                  | C      |
| 15             | 18            | GLN                  | C      |
| 16             | 19            | GLU                  | C      |
| 17             | 20            | CYS                  | C      |
| 18             | 21            | GLU                  | C      |
| 19             | 22            | GLN                  | C      |
| 20             | 24            | LEU                  | C      |
| 21             | 25            | GLY                  | C      |
| 22             | 26            | PRO                  | C      |
| 23             | 27            | LYS                  | C      |
| 24             | 28            | GLY                  | C      |
| 25             | 29            | TYR                  | C      |
| 26             | 30            | ALA                  | C      |
| 27             | 31            | ALA                  | C      |
| 28             | 32            | VAL                  | C      |
| 29             | 33            | GLN                  | C      |
| 30             | 34            | VAL                  | C      |

*Continued on next page*

Table S13 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 35            | SER                  | C      |
| 32             | 36            | PRO                  | C      |
| 33             | 37            | PRO                  | C      |
| 34             | 38            | ASN                  | C      |
| 35             | 39            | GLU                  | C      |
| 36             | 40            | HIS                  | C      |
| 37             | 41            | ILE                  | C      |
| 38             | 43            | GLY                  | C      |
| 39             | 47            | TRP                  | C      |
| 40             | 48            | THR                  | C      |
| 41             | 49            | ARG                  | C      |
| 42             | 50            | TYR                  | C      |
| 43             | 51            | GLN                  | C      |
| 44             | 52            | PRO                  | C      |
| 45             | 53            | VAL                  | C      |
| 46             | 54            | SER                  | C      |
| 47             | 55            | TYR                  | C      |
| 48             | 56            | GLU                  | C      |
| 49             | 57            | LEU                  | C      |
| 50             | 58            | GLN                  | C      |
| 51             | 59            | SER                  | C      |
| 52             | 60            | ARG                  | C      |
| 53             | 61            | GLY                  | C      |
| 54             | 62            | GLY                  | C      |
| 55             | 63            | ASN                  | C      |
| 56             | 64            | ARG                  | C      |
| 57             | 65            | ALA                  | C      |
| 58             | 66            | GLN                  | C      |
| 59             | 67            | PHE                  | C      |
| 60             | 68            | ILE                  | C      |
| 61             | 69            | ASP                  | C      |
| 62             | 70            | MET                  | C      |
| 63             | 71            | VAL                  | C      |
| 64             | 72            | ASN                  | C      |
| 65             | 73            | ARG                  | C      |
| 66             | 74            | CYS                  | C      |
| 67             | 75            | SER                  | C      |
| 68             | 76            | ALA                  | C      |
| 69             | 77            | ALA                  | C      |
| 70             | 78            | GLY                  | C      |
| 71             | 79            | VAL                  | C      |
| 72             | 80            | ASP                  | C      |
| 73             | 81            | ILE                  | C      |
| 74             | 82            | TYR                  | C      |
| 75             | 83            | VAL                  | C      |
| 76             | 84            | ASP                  | C      |

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Table S13 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 85            | THR                  | C      |
| 78             | 86            | LEU                  | C      |
| 79             | 87            | ILE                  | C      |
| 80             | 88            | ASN                  | C      |
| 81             | 89            | HIS                  | C      |
| 82             | 90            | MET                  | C      |
| 83             | 91            | ALA                  | C      |
| 84             | 92            | ALA                  | C      |
| 85             | 93            | GLY                  | C      |
| 86             | 108           | PHE                  | C      |
| 87             | 110           | ILE                  | C      |
| 88             | 111           | TYR                  | C      |
| 89             | 112           | SER                  | C      |
| 90             | 113           | PRO                  | C      |
| 91             | 114           | GLN                  | C      |
| 92             | 115           | ASP                  | C      |
| 93             | 116           | PHE                  | C      |
| 94             | 117           | HIS                  | B      |
| 95             | 137           | CYS                  | B      |
| 96             | 138           | GLU                  | B      |
| 97             | 139           | LEU                  | B      |
| 98             | 140           | VAL                  | B      |
| 99             | 142           | LEU                  | B      |
| 100            | 143           | ALA                  | B      |
| 101            | 144           | ASP                  | B      |
| 102            | 145           | LEU                  | B      |
| 103            | 146           | ASP                  | B      |
| 104            | 147           | THR                  | B      |
| 105            | 148           | ALA                  | B      |
| 106            | 149           | SER                  | B      |
| 107            | 150           | ASN                  | B      |
| 108            | 151           | TYR                  | B      |
| 109            | 152           | VAL                  | B      |
| 110            | 153           | GLN                  | B      |
| 111            | 154           | ASN                  | B      |
| 112            | 155           | THR                  | B      |
| 113            | 156           | ILE                  | B      |
| 114            | 157           | ALA                  | B      |
| 115            | 158           | ALA                  | B      |
| 116            | 159           | TYR                  | B      |
| 117            | 160           | ILE                  | B      |
| 118            | 161           | ASN                  | B      |
| 119            | 162           | ASP                  | B      |
| 120            | 163           | LEU                  | B      |
| 121            | 164           | GLN                  | B      |
| 122            | 165           | ALA                  | B      |

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Table S13 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 166           | ILE                  | C      |
| 124            | 167           | GLY                  | C      |
| 125            | 168           | VAL                  | C      |
| 126            | 169           | LYS                  | C      |
| 127            | 170           | GLY                  | C      |
| 128            | 171           | PHE                  | B      |
| 129            | 172           | ARG                  | D      |
| 130            | 173           | PHE                  | B      |
| 131            | 174           | ASP                  | B      |
| 132            | 175           | ALA                  | B      |
| 133            | 176           | SER                  | B      |
| 134            | 177           | LYS                  | B      |
| 135            | 178           | HIS                  | B      |
| 136            | 179           | VAL                  | B      |
| 137            | 180           | ALA                  | B      |
| 138            | 181           | ALA                  | B      |
| 139            | 182           | SER                  | B      |
| 140            | 183           | ASP                  | B      |
| 141            | 184           | ILE                  | B      |
| 142            | 185           | GLN                  | B      |
| 143            | 186           | SER                  | B      |
| 144            | 187           | LEU                  | B      |
| 145            | 188           | MET                  | B      |
| 146            | 189           | ALA                  | B      |
| 147            | 190           | LYS                  | B      |
| 148            | 191           | VAL                  | B      |
| 149            | 192           | ASN                  | B      |
| 150            | 195           | PRO                  | B      |
| 151            | 196           | VAL                  | B      |
| 152            | 197           | VAL                  | B      |
| 153            | 198           | PHE                  | C      |
| 154            | 199           | GLN                  | B      |
| 155            | 200           | GLU                  | B      |
| 156            | 201           | VAL                  | B      |
| 157            | 202           | ILE                  | B      |
| 158            | 203           | ASP                  | B      |
| 159            | 204           | GLN                  | B      |
| 160            | 211           | ALA                  | B      |
| 161            | 212           | SER                  | B      |
| 162            | 213           | GLU                  | B      |
| 163            | 214           | TYR                  | B      |
| 164            | 215           | LEU                  | B      |
| 165            | 216           | SER                  | B      |
| 166            | 217           | THR                  | B      |
| 167            | 218           | GLY                  | B      |
| 168            | 219           | LEU                  | B      |

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Table S13 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 220           | VAL                  | B      |
| 170            | 221           | THR                  | D      |
| 171            | 222           | GLU                  | D      |
| 172            | 223           | PHE                  | D      |
| 173            | 224           | LYS                  | D      |
| 174            | 226           | SER                  | D      |
| 175            | 227           | THR                  | D      |
| 176            | 228           | GLU                  | D      |
| 177            | 229           | LEU                  | D      |
| 178            | 230           | GLY                  | D      |
| 179            | 231           | ASN                  | D      |
| 180            | 232           | THR                  | D      |
| 181            | 233           | PHE                  | D      |
| 182            | 236           | GLY                  | D      |
| 183            | 237           | SER                  | A      |
| 184            | 238           | LEU                  | A      |
| 185            | 239           | ALA                  | A      |
| 186            | 244           | PHE                  | A      |
| 187            | 245           | GLY                  | D      |
| 188            | 246           | GLU                  | D      |
| 189            | 247           | GLY                  | D      |
| 190            | 249           | GLY                  | D      |
| 191            | 250           | PHE                  | B      |
| 192            | 251           | MET                  | B      |
| 193            | 252           | PRO                  | B      |
| 194            | 253           | SER                  | B      |
| 195            | 254           | SER                  | B      |
| 196            | 255           | SER                  | B      |
| 197            | 256           | ALA                  | B      |
| 198            | 257           | VAL                  | D      |
| 199            | 258           | VAL                  | D      |
| 200            | 259           | PHE                  | D      |
| 201            | 260           | VAL                  | A      |
| 202            | 261           | ASP                  | D      |
| 203            | 262           | ASN                  | D      |
| 204            | 263           | HIS                  | D      |
| 205            | 264           | ASP                  | D      |
| 206            | 265           | ASN                  | D      |
| 207            | 266           | GLN                  | D      |
| 208            | 277           | THR                  | D      |
| 209            | 278           | PHE                  | D      |
| 210            | 279           | GLU                  | D      |
| 211            | 280           | ASP                  | D      |
| 212            | 282           | ARG                  | A      |
| 213            | 283           | LEU                  | A      |
| 214            | 284           | TYR                  | A      |

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Table S13 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 285           | ASP                  | A      |
| 216            | 286           | LEU                  | A      |
| 217            | 287           | ALA                  | A      |
| 218            | 288           | ASN                  | A      |
| 219            | 289           | VAL                  | A      |
| 220            | 290           | PHE                  | A      |
| 221            | 291           | MET                  | A      |
| 222            | 292           | LEU                  | A      |
| 223            | 293           | ALA                  | A      |
| 224            | 294           | TYR                  | A      |
| 225            | 296           | TYR                  | D      |
| 226            | 297           | GLY                  | D      |
| 227            | 298           | TYR                  | D      |
| 228            | 299           | PRO                  | A      |
| 229            | 300           | LYS                  | D      |
| 230            | 301           | VAL                  | A      |
| 231            | 302           | MET                  | D      |
| 232            | 303           | SER                  | C      |
| 233            | 304           | SER                  | D      |
| 234            | 305           | TYR                  | A      |
| 235            | 306           | ASP                  | C      |
| 236            | 332           | ASN                  | C      |
| 237            | 333           | TRP                  | D      |
| 238            | 334           | LYS                  | D      |
| 239            | 335           | CYS                  | D      |
| 240            | 338           | ARG                  | A      |
| 241            | 339           | TRP                  | A      |
| 242            | 340           | SER                  | A      |
| 243            | 341           | TYR                  | A      |
| 244            | 342           | ILE                  | A      |
| 245            | 343           | ALA                  | A      |
| 246            | 344           | GLY                  | A      |
| 247            | 345           | GLY                  | A      |
| 248            | 346           | VAL                  | A      |
| 249            | 347           | ASP                  | A      |
| 250            | 348           | PHE                  | A      |
| 251            | 349           | ARG                  | A      |
| 252            | 350           | ASN                  | A      |
| 253            | 351           | ASN                  | A      |
| 254            | 352           | THR                  | A      |
| 255            | 353           | ALA                  | A      |
| 256            | 355           | ASN                  | A      |
| 257            | 356           | TRP                  | A      |
| 258            | 357           | ALA                  | A      |
| 259            | 358           | VAL                  | A      |
| 260            | 360           | ASN                  | A      |

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Table S13 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 361           | TRP                  | A      |
| 262            | 362           | TRP                  | A      |
| 263            | 363           | ASP                  | A      |
| 264            | 365           | THR                  | A      |
| 265            | 366           | ASN                  | A      |
| 266            | 367           | ASN                  | A      |
| 267            | 368           | GLN                  | A      |
| 268            | 369           | ILE                  | A      |
| 269            | 370           | SER                  | A      |
| 270            | 371           | PHE                  | A      |
| 271            | 372           | GLY                  | A      |
| 272            | 373           | ARG                  | A      |
| 273            | 374           | GLY                  | A      |
| 274            | 375           | SER                  | A      |
| 275            | 377           | GLY                  | A      |
| 276            | 378           | HIS                  | A      |
| 277            | 379           | MET                  | A      |
| 278            | 380           | ALA                  | A      |
| 279            | 381           | ILE                  | A      |
| 280            | 382           | ASN                  | A      |
| 281            | 385           | ASP                  | A      |
| 282            | 386           | SER                  | A      |
| 283            | 387           | THR                  | A      |
| 284            | 388           | LEU                  | A      |
| 285            | 389           | THR                  | A      |
| 286            | 390           | ALA                  | A      |
| 287            | 391           | THR                  | A      |
| 288            | 397           | ALA                  | A      |
| 289            | 398           | SER                  | A      |
| 290            | 401           | TYR                  | A      |
| 291            | 402           | CYS                  | A      |
| 292            | 403           | ASN                  | A      |
| 293            | 404           | VAL                  | A      |
| 294            | 433           | ILE                  | A      |
| 295            | 434           | GLY                  | A      |
| 296            | 435           | ALA                  | A      |
| 297            | 437           | ASP                  | A      |
| 298            | 438           | ALA                  | A      |
| 299            | 439           | MET                  | A      |
| 300            | 440           | ALA                  | A      |
| 301            | 441           | ILE                  | A      |
| 302            | 442           | HIS                  | A      |

Table S14: Residues membership for the *N. polysaccharea*  $\alpha$ -amylase (PDB code 1JG9, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 98            | GLN                  | A      |
| 1              | 99            | VAL                  | A      |
| 2              | 100           | GLY                  | B      |
| 3              | 101           | GLY                  | B      |
| 4              | 102           | VAL                  | B      |
| 5              | 103           | CYS                  | C      |
| 6              | 104           | TYR                  | C      |
| 7              | 105           | VAL                  | C      |
| 8              | 110           | GLY                  | C      |
| 9              | 111           | ASP                  | C      |
| 10             | 112           | LEU                  | C      |
| 11             | 113           | LYS                  | C      |
| 12             | 114           | GLY                  | C      |
| 13             | 115           | LEU                  | C      |
| 14             | 116           | LYS                  | C      |
| 15             | 117           | ASP                  | C      |
| 16             | 118           | LYS                  | C      |
| 17             | 119           | ILE                  | C      |
| 18             | 120           | PRO                  | C      |
| 19             | 121           | TYR                  | C      |
| 20             | 122           | PHE                  | C      |
| 21             | 123           | GLN                  | C      |
| 22             | 124           | GLU                  | C      |
| 23             | 125           | LEU                  | C      |
| 24             | 126           | GLY                  | C      |
| 25             | 127           | LEU                  | C      |
| 26             | 128           | THR                  | C      |
| 27             | 129           | TYR                  | C      |
| 28             | 130           | LEU                  | C      |
| 29             | 131           | HIS                  | C      |
| 30             | 132           | LEU                  | C      |
| 31             | 133           | MET                  | C      |
| 32             | 134           | PRO                  | C      |
| 33             | 135           | LEU                  | C      |
| 34             | 136           | PHE                  | C      |
| 35             | 137           | LYS                  | C      |
| 36             | 138           | CYS                  | C      |
| 37             | 139           | PRO                  | C      |
| 38             | 141           | GLY                  | C      |
| 39             | 144           | ASP                  | C      |
| 40             | 145           | GLY                  | C      |
| 41             | 146           | GLY                  | C      |
| 42             | 147           | TYR                  | C      |
| 43             | 148           | ALA                  | C      |

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Table S14 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 149           | VAL                  | C      |
| 45             | 150           | SER                  | C      |
| 46             | 151           | SER                  | C      |
| 47             | 153           | ARG                  | C      |
| 48             | 154           | ASP                  | C      |
| 49             | 155           | VAL                  | C      |
| 50             | 156           | ASN                  | C      |
| 51             | 157           | PRO                  | C      |
| 52             | 158           | ALA                  | C      |
| 53             | 159           | LEU                  | C      |
| 54             | 160           | GLY                  | C      |
| 55             | 161           | THR                  | C      |
| 56             | 162           | ILE                  | C      |
| 57             | 163           | GLY                  | C      |
| 58             | 164           | ASP                  | C      |
| 59             | 165           | LEU                  | C      |
| 60             | 166           | ARG                  | C      |
| 61             | 167           | GLU                  | C      |
| 62             | 168           | VAL                  | C      |
| 63             | 169           | ILE                  | C      |
| 64             | 170           | ALA                  | C      |
| 65             | 171           | ALA                  | C      |
| 66             | 172           | LEU                  | C      |
| 67             | 173           | HIS                  | C      |
| 68             | 174           | GLU                  | C      |
| 69             | 175           | ALA                  | C      |
| 70             | 176           | GLY                  | C      |
| 71             | 177           | ILE                  | C      |
| 72             | 178           | SER                  | C      |
| 73             | 179           | ALA                  | C      |
| 74             | 180           | VAL                  | C      |
| 75             | 181           | VAL                  | C      |
| 76             | 182           | ASP                  | C      |
| 77             | 183           | PHE                  | C      |
| 78             | 184           | ILE                  | C      |
| 79             | 185           | PHE                  | C      |
| 80             | 186           | ASN                  | C      |
| 81             | 187           | HIS                  | C      |
| 82             | 188           | THR                  | C      |
| 83             | 189           | SER                  | C      |
| 84             | 190           | ASN                  | C      |
| 85             | 191           | GLU                  | C      |
| 86             | 192           | HIS                  | C      |
| 87             | 193           | GLU                  | C      |
| 88             | 194           | TRP                  | C      |
| 89             | 195           | ALA                  | C      |

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Table S14 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 206           | ASP                  | C      |
| 91             | 207           | ASN                  | C      |
| 92             | 208           | PHE                  | C      |
| 93             | 209           | TYR                  | C      |
| 94             | 210           | TYR                  | B      |
| 95             | 247           | TRP                  | B      |
| 96             | 248           | THR                  | B      |
| 97             | 249           | THR                  | B      |
| 98             | 250           | PHE                  | B      |
| 99             | 254           | GLN                  | B      |
| 100            | 255           | TRP                  | B      |
| 101            | 256           | ASP                  | B      |
| 102            | 257           | LEU                  | B      |
| 103            | 258           | ASN                  | B      |
| 104            | 259           | TYR                  | B      |
| 105            | 260           | SER                  | B      |
| 106            | 261           | ASN                  | B      |
| 107            | 262           | PRO                  | B      |
| 108            | 263           | TRP                  | B      |
| 109            | 264           | VAL                  | B      |
| 110            | 265           | PHE                  | B      |
| 111            | 266           | ARG                  | B      |
| 112            | 267           | ALA                  | B      |
| 113            | 268           | MET                  | B      |
| 114            | 269           | ALA                  | B      |
| 115            | 270           | GLY                  | B      |
| 116            | 271           | GLU                  | B      |
| 117            | 272           | MET                  | B      |
| 118            | 273           | LEU                  | B      |
| 119            | 274           | PHE                  | B      |
| 120            | 275           | LEU                  | B      |
| 121            | 276           | ALA                  | B      |
| 122            | 277           | ASN                  | B      |
| 123            | 278           | LEU                  | C      |
| 124            | 279           | GLY                  | C      |
| 125            | 280           | VAL                  | C      |
| 126            | 281           | ASP                  | C      |
| 127            | 282           | ILE                  | C      |
| 128            | 283           | LEU                  | B      |
| 129            | 284           | ARG                  | D      |
| 130            | 285           | MET                  | B      |
| 131            | 286           | ASP                  | B      |
| 132            | 287           | ALA                  | B      |
| 133            | 288           | VAL                  | B      |
| 134            | 289           | ALA                  | B      |
| 135            | 290           | PHE                  | B      |

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Table S14 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 291           | ILE                  | B      |
| 137            | 292           | TRP                  | B      |
| 138            | 306           | HIS                  | B      |
| 139            | 307           | ALA                  | B      |
| 140            | 308           | LEU                  | B      |
| 141            | 309           | ILE                  | B      |
| 142            | 310           | ARG                  | B      |
| 143            | 311           | ALA                  | B      |
| 144            | 312           | PHE                  | B      |
| 145            | 313           | ASN                  | B      |
| 146            | 314           | ALA                  | B      |
| 147            | 315           | VAL                  | B      |
| 148            | 316           | MET                  | B      |
| 149            | 317           | ARG                  | B      |
| 150            | 323           | VAL                  | B      |
| 151            | 324           | PHE                  | B      |
| 152            | 325           | PHE                  | B      |
| 153            | 326           | LYS                  | C      |
| 154            | 327           | SER                  | B      |
| 155            | 328           | GLU                  | B      |
| 156            | 329           | ALA                  | B      |
| 157            | 330           | ILE                  | B      |
| 158            | 331           | VAL                  | B      |
| 159            | 332           | HIS                  | B      |
| 160            | 336           | VAL                  | B      |
| 161            | 337           | VAL                  | B      |
| 162            | 338           | GLN                  | B      |
| 163            | 339           | TYR                  | B      |
| 164            | 340           | ILE                  | B      |
| 165            | 341           | GLY                  | B      |
| 166            | 345           | CYS                  | B      |
| 167            | 346           | GLN                  | B      |
| 168            | 347           | ILE                  | B      |
| 169            | 348           | GLY                  | B      |
| 170            | 349           | TYR                  | D      |
| 171            | 350           | ASN                  | D      |
| 172            | 351           | PRO                  | D      |
| 173            | 352           | LEU                  | D      |
| 174            | 354           | MET                  | D      |
| 175            | 355           | ALA                  | D      |
| 176            | 356           | LEU                  | D      |
| 177            | 357           | LEU                  | D      |
| 178            | 358           | TRP                  | D      |
| 179            | 359           | ASN                  | D      |
| 180            | 360           | THR                  | D      |
| 181            | 361           | LEU                  | D      |

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Table S14 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 364           | ARG                  | D      |
| 183            | 365           | GLU                  | A      |
| 184            | 366           | VAL                  | A      |
| 185            | 367           | ASN                  | A      |
| 186            | 372           | ALA                  | A      |
| 187            | 373           | LEU                  | D      |
| 188            | 374           | THR                  | D      |
| 189            | 375           | TYR                  | D      |
| 190            | 376           | ARG                  | D      |
| 191            | 377           | HIS                  | B      |
| 192            | 378           | ASN                  | B      |
| 193            | 381           | GLU                  | B      |
| 194            | 382           | HIS                  | B      |
| 195            | 383           | THR                  | B      |
| 196            | 384           | ALA                  | B      |
| 197            | 385           | TRP                  | B      |
| 198            | 386           | VAL                  | D      |
| 199            | 387           | ASN                  | D      |
| 200            | 388           | TYR                  | D      |
| 201            | 389           | VAL                  | A      |
| 202            | 390           | ARG                  | D      |
| 203            | 391           | SER                  | D      |
| 204            | 392           | HIS                  | D      |
| 205            | 393           | ASP                  | D      |
| 206            | 394           | ASP                  | D      |
| 207            | 448           | SER                  | D      |
| 208            | 450           | THR                  | D      |
| 209            | 451           | ALA                  | D      |
| 210            | 452           | ALA                  | D      |
| 211            | 453           | ALA                  | D      |
| 212            | 464           | ALA                  | A      |
| 213            | 467           | ARG                  | A      |
| 214            | 468           | ILE                  | A      |
| 215            | 469           | LYS                  | A      |
| 216            | 470           | LEU                  | A      |
| 217            | 471           | LEU                  | A      |
| 218            | 472           | TYR                  | A      |
| 219            | 473           | SER                  | A      |
| 220            | 474           | ILE                  | A      |
| 221            | 475           | ALA                  | A      |
| 222            | 476           | LEU                  | A      |
| 223            | 477           | SER                  | A      |
| 224            | 478           | THR                  | A      |
| 225            | 479           | GLY                  | D      |
| 226            | 480           | GLY                  | D      |
| 227            | 481           | LEU                  | D      |

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Table S14 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 482           | PRO                  | A      |
| 229            | 483           | LEU                  | D      |
| 230            | 484           | ILE                  | A      |
| 231            | 485           | TYR                  | D      |
| 232            | 486           | LEU                  | C      |
| 233            | 487           | GLY                  | D      |
| 234            | 488           | ASP                  | A      |
| 235            | 514           | PRO                  | C      |
| 236            | 515           | ARG                  | C      |
| 237            | 516           | TYR                  | D      |
| 238            | 517           | ASN                  | D      |
| 239            | 521           | TYR                  | D      |
| 240            | 534           | ILE                  | A      |
| 241            | 535           | TYR                  | A      |
| 242            | 536           | GLN                  | A      |
| 243            | 537           | ASP                  | A      |
| 244            | 538           | LEU                  | A      |
| 245            | 539           | ARG                  | A      |
| 246            | 540           | HIS                  | A      |
| 247            | 541           | MET                  | A      |
| 248            | 542           | ILE                  | A      |
| 249            | 543           | ALA                  | A      |
| 250            | 544           | VAL                  | A      |
| 251            | 545           | ARG                  | A      |
| 252            | 546           | GLN                  | A      |
| 253            | 547           | SER                  | A      |
| 254            | 548           | ASN                  | A      |
| 255            | 549           | PRO                  | A      |
| 256            | 553           | GLY                  | A      |
| 257            | 554           | GLY                  | A      |
| 258            | 555           | ARG                  | A      |
| 259            | 556           | LEU                  | A      |
| 260            | 558           | THR                  | A      |
| 261            | 559           | PHE                  | A      |
| 262            | 560           | ASN                  | A      |
| 263            | 561           | THR                  | A      |
| 264            | 563           | ASN                  | A      |
| 265            | 564           | LYS                  | A      |
| 266            | 565           | HIS                  | A      |
| 267            | 566           | ILE                  | A      |
| 268            | 567           | ILE                  | A      |
| 269            | 568           | GLY                  | A      |
| 270            | 569           | TYR                  | A      |
| 271            | 570           | ILE                  | A      |
| 272            | 571           | ARG                  | A      |
| 273            | 573           | ASN                  | A      |

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Table S14 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 574           | ALA                  | A      |
| 275            | 575           | LEU                  | A      |
| 276            | 576           | LEU                  | A      |
| 277            | 577           | ALA                  | A      |
| 278            | 578           | PHE                  | A      |
| 279            | 579           | GLY                  | A      |
| 280            | 580           | ASN                  | A      |
| 281            | 584           | TYR                  | A      |
| 282            | 585           | PRO                  | A      |
| 283            | 586           | GLN                  | A      |
| 284            | 587           | THR                  | A      |
| 285            | 588           | VAL                  | A      |
| 286            | 589           | THR                  | A      |
| 287            | 590           | ALA                  | A      |
| 288            | 599           | LYS                  | A      |
| 289            | 600           | ALA                  | A      |
| 290            | 601           | HIS                  | A      |
| 291            | 602           | ASP                  | A      |
| 292            | 603           | LEU                  | A      |
| 293            | 604           | ILE                  | A      |
| 294            | 617           | LEU                  | A      |
| 295            | 618           | GLN                  | A      |
| 296            | 619           | PRO                  | A      |
| 297            | 621           | GLN                  | A      |
| 298            | 622           | VAL                  | A      |
| 299            | 623           | MET                  | A      |
| 300            | 624           | TRP                  | A      |
| 301            | 625           | LEU                  | A      |
| 302            | 626           | GLU                  | A      |

Table S15: Residues membership for the *T. maritima*  $\alpha$ -amylase (PDB code 1GJU, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 84            | SER                  | A      |
| 1              | 85            | VAL                  | A      |
| 2              | 86            | VAL                  | B      |
| 3              | 87            | TYR                  | B      |
| 4              | 88            | GLY                  | B      |
| 5              | 89            | SER                  | C      |
| 6              | 90            | LEU                  | C      |
| 7              | 91            | PRO                  | C      |
| 8              | 117           | GLY                  | C      |

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Table S15 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 118           | THR                  | C      |
| 10             | 119           | PHE                  | C      |
| 11             | 120           | PHE                  | C      |
| 12             | 121           | LYS                  | C      |
| 13             | 122           | MET                  | C      |
| 14             | 123           | MET                  | C      |
| 15             | 124           | LEU                  | C      |
| 16             | 125           | LEU                  | C      |
| 17             | 126           | LEU                  | C      |
| 18             | 127           | PRO                  | C      |
| 19             | 128           | PHE                  | C      |
| 20             | 129           | VAL                  | C      |
| 21             | 130           | LYS                  | C      |
| 22             | 131           | SER                  | C      |
| 23             | 132           | LEU                  | C      |
| 24             | 133           | GLY                  | C      |
| 25             | 134           | ALA                  | C      |
| 26             | 135           | ASP                  | C      |
| 27             | 136           | ALA                  | C      |
| 28             | 137           | ILE                  | C      |
| 29             | 138           | TYR                  | C      |
| 30             | 139           | LEU                  | C      |
| 31             | 140           | LEU                  | C      |
| 32             | 141           | PRO                  | C      |
| 33             | 142           | VAL                  | C      |
| 34             | 143           | SER                  | C      |
| 35             | 144           | ARG                  | C      |
| 36             | 145           | MET                  | C      |
| 37             | 146           | SER                  | C      |
| 38             | 154           | ALA                  | C      |
| 39             | 155           | PRO                  | C      |
| 40             | 156           | SER                  | C      |
| 41             | 157           | PRO                  | C      |
| 42             | 158           | TYR                  | C      |
| 43             | 159           | SER                  | C      |
| 44             | 160           | VAL                  | C      |
| 45             | 161           | LYS                  | C      |
| 46             | 162           | ASN                  | C      |
| 47             | 164           | MET                  | C      |
| 48             | 165           | GLU                  | C      |
| 49             | 166           | LEU                  | C      |
| 50             | 167           | ASP                  | C      |
| 51             | 168           | GLU                  | C      |
| 52             | 169           | ARG                  | C      |
| 53             | 170           | TYR                  | C      |
| 54             | 171           | HIS                  | C      |

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Table S15 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 172           | ASP                  | C      |
| 56             | 181           | ASP                  | C      |
| 57             | 182           | GLU                  | C      |
| 58             | 183           | GLU                  | C      |
| 59             | 184           | PHE                  | C      |
| 60             | 185           | LYS                  | C      |
| 61             | 186           | ALA                  | C      |
| 62             | 187           | PHE                  | C      |
| 63             | 188           | VAL                  | C      |
| 64             | 189           | GLU                  | C      |
| 65             | 190           | ALA                  | C      |
| 66             | 191           | CYS                  | C      |
| 67             | 192           | HIS                  | C      |
| 68             | 193           | ILE                  | C      |
| 69             | 194           | LEU                  | C      |
| 70             | 195           | GLY                  | C      |
| 71             | 196           | ILE                  | C      |
| 72             | 197           | ARG                  | C      |
| 73             | 198           | VAL                  | C      |
| 74             | 199           | ILE                  | C      |
| 75             | 200           | LEU                  | C      |
| 76             | 201           | ASP                  | C      |
| 77             | 202           | PHE                  | C      |
| 78             | 203           | ILE                  | C      |
| 79             | 204           | PRO                  | C      |
| 80             | 205           | ARG                  | C      |
| 81             | 206           | THR                  | C      |
| 82             | 207           | ALA                  | C      |
| 83             | 208           | ALA                  | C      |
| 84             | 209           | ARG                  | C      |
| 85             | 210           | ASP                  | C      |
| 86             | 211           | SER                  | C      |
| 87             | 212           | ASP                  | C      |
| 88             | 213           | LEU                  | C      |
| 89             | 214           | ILE                  | C      |
| 90             | 218           | PRO                  | C      |
| 91             | 219           | ASP                  | C      |
| 92             | 220           | TRP                  | C      |
| 93             | 221           | PHE                  | C      |
| 94             | 222           | TYR                  | B      |
| 95             | 302           | PRO                  | B      |
| 96             | 303           | GLY                  | B      |
| 97             | 304           | PHE                  | B      |
| 98             | 305           | SER                  | B      |
| 99             | 318           | VAL                  | B      |
| 100            | 319           | THR                  | B      |

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Table S15 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 320           | PHE                  | B      |
| 102            | 321           | LEU                  | B      |
| 103            | 322           | ARG                  | B      |
| 104            | 323           | LEU                  | B      |
| 105            | 324           | TYR                  | B      |
| 106            | 359           | ASN                  | B      |
| 107            | 360           | ARG                  | B      |
| 108            | 361           | GLU                  | B      |
| 109            | 362           | LEU                  | B      |
| 110            | 363           | TRP                  | B      |
| 111            | 364           | GLU                  | B      |
| 112            | 365           | TYR                  | B      |
| 113            | 366           | LEU                  | B      |
| 114            | 367           | ALA                  | B      |
| 115            | 368           | GLY                  | B      |
| 116            | 369           | VAL                  | B      |
| 117            | 370           | ILE                  | B      |
| 118            | 371           | PRO                  | B      |
| 119            | 372           | HIS                  | B      |
| 120            | 373           | TYR                  | B      |
| 121            | 374           | GLN                  | B      |
| 122            | 375           | LYS                  | B      |
| 123            | 377           | TYR                  | C      |
| 124            | 378           | GLY                  | C      |
| 125            | 379           | ILE                  | C      |
| 126            | 380           | ASP                  | C      |
| 127            | 381           | GLY                  | C      |
| 128            | 382           | ALA                  | B      |
| 129            | 383           | ARG                  | D      |
| 130            | 384           | LEU                  | B      |
| 131            | 385           | ASP                  | B      |
| 132            | 386           | MET                  | B      |
| 133            | 387           | GLY                  | B      |
| 134            | 388           | HIS                  | B      |
| 135            | 389           | ALA                  | B      |
| 136            | 390           | LEU                  | B      |
| 137            | 391           | PRO                  | B      |
| 138            | 392           | LYS                  | B      |
| 139            | 393           | GLU                  | B      |
| 140            | 394           | LEU                  | B      |
| 141            | 395           | LEU                  | B      |
| 142            | 396           | ASP                  | B      |
| 143            | 397           | LEU                  | B      |
| 144            | 398           | ILE                  | B      |
| 145            | 399           | ILE                  | B      |
| 146            | 400           | LYS                  | B      |

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Table S15 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 401           | ASN                  | B      |
| 148            | 402           | VAL                  | B      |
| 149            | 403           | LYS                  | B      |
| 150            | 409           | PHE                  | B      |
| 151            | 410           | VAL                  | B      |
| 152            | 411           | MET                  | B      |
| 153            | 412           | ILE                  | C      |
| 154            | 413           | ALA                  | B      |
| 155            | 414           | GLU                  | B      |
| 156            | 415           | GLU                  | B      |
| 157            | 416           | LEU                  | B      |
| 158            | 417           | ASP                  | B      |
| 159            | 418           | MET                  | B      |
| 160            | 421           | ASP                  | B      |
| 161            | 422           | LYS                  | B      |
| 162            | 423           | ALA                  | B      |
| 163            | 424           | SER                  | B      |
| 164            | 425           | LYS                  | B      |
| 165            | 426           | GLU                  | B      |
| 166            | 429           | TYR                  | B      |
| 167            | 430           | ASP                  | B      |
| 168            | 431           | VAL                  | B      |
| 169            | 432           | ILE                  | B      |
| 170            | 433           | LEU                  | D      |
| 171            | 434           | GLY                  | D      |
| 172            | 435           | SER                  | D      |
| 173            | 436           | SER                  | D      |
| 174            | 437           | TRP                  | D      |
| 175            | 438           | TYR                  | D      |
| 176            | 439           | PHE                  | D      |
| 177            | 440           | ALA                  | D      |
| 178            | 441           | GLY                  | D      |
| 179            | 442           | ARG                  | D      |
| 180            | 443           | VAL                  | D      |
| 181            | 444           | GLU                  | D      |
| 182            | 445           | GLU                  | D      |
| 183            | 446           | ILE                  | A      |
| 184            | 447           | GLY                  | A      |
| 185            | 448           | LYS                  | A      |
| 186            | 449           | LEU                  | A      |
| 187            | 450           | PRO                  | D      |
| 188            | 451           | ASP                  | D      |
| 189            | 452           | ILE                  | D      |
| 190            | 453           | ALA                  | D      |
| 191            | 454           | GLU                  | B      |
| 192            | 455           | GLU                  | B      |

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Table S15 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 456           | LEU                  | B      |
| 194            | 457           | VAL                  | B      |
| 195            | 458           | LEU                  | B      |
| 196            | 459           | PRO                  | B      |
| 197            | 460           | PHE                  | B      |
| 198            | 461           | LEU                  | D      |
| 199            | 462           | ALA                  | D      |
| 200            | 463           | SER                  | D      |
| 201            | 464           | VAL                  | A      |
| 202            | 465           | GLU                  | D      |
| 203            | 466           | THR                  | D      |
| 204            | 467           | PRO                  | D      |
| 205            | 468           | ASP                  | D      |
| 206            | 469           | THR                  | D      |
| 207            | 470           | PRO                  | D      |
| 208            | 471           | ARG                  | D      |
| 209            | 472           | ILE                  | D      |
| 210            | 473           | ALA                  | D      |
| 211            | 474           | THR                  | D      |
| 212            | 479           | SER                  | A      |
| 213            | 481           | MET                  | A      |
| 214            | 482           | LYS                  | A      |
| 215            | 483           | LYS                  | A      |
| 216            | 484           | LEU                  | A      |
| 217            | 485           | ALA                  | A      |
| 218            | 486           | PRO                  | A      |
| 219            | 487           | PHE                  | A      |
| 220            | 488           | VAL                  | A      |
| 221            | 489           | THR                  | A      |
| 222            | 490           | TYR                  | A      |
| 223            | 491           | PHE                  | A      |
| 224            | 492           | LEU                  | A      |
| 225            | 493           | PRO                  | D      |
| 226            | 495           | SER                  | D      |
| 227            | 496           | ILE                  | D      |
| 228            | 497           | PRO                  | A      |
| 229            | 498           | TYR                  | D      |
| 230            | 499           | VAL                  | A      |
| 231            | 500           | ASN                  | D      |
| 232            | 501           | THR                  | C      |
| 233            | 502           | GLY                  | D      |
| 234            | 503           | GLN                  | A      |
| 235            | 541           | TYR                  | C      |
| 236            | 542           | VAL                  | C      |
| 237            | 543           | LEU                  | D      |
| 238            | 544           | HIS                  | D      |

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Table S15 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 545           | TRP                  | D      |
| 240            | 552           | VAL                  | A      |
| 241            | 553           | LEU                  | A      |
| 242            | 554           | ASN                  | A      |
| 243            | 555           | PHE                  | A      |
| 244            | 556           | ILE                  | A      |
| 245            | 557           | LYS                  | A      |
| 246            | 558           | LYS                  | A      |
| 247            | 559           | LEU                  | A      |
| 248            | 560           | ILE                  | A      |
| 249            | 561           | LYS                  | A      |
| 250            | 562           | VAL                  | A      |
| 251            | 563           | ARG                  | A      |
| 252            | 564           | HIS                  | A      |
| 253            | 565           | GLU                  | A      |
| 254            | 566           | PHE                  | A      |
| 255            | 567           | LEU                  | A      |
| 256            | 572           | ASN                  | A      |
| 257            | 573           | GLY                  | A      |
| 258            | 574           | LYS                  | A      |
| 259            | 575           | PHE                  | A      |
| 260            | 576           | GLU                  | A      |
| 261            | 577           | ASN                  | A      |
| 262            | 578           | LEU                  | A      |
| 263            | 579           | THR                  | A      |
| 264            | 580           | THR                  | A      |
| 265            | 581           | LYS                  | A      |
| 266            | 582           | ASP                  | A      |
| 267            | 583           | LEU                  | A      |
| 268            | 584           | VAL                  | A      |
| 269            | 585           | MET                  | A      |
| 270            | 586           | TYR                  | A      |
| 271            | 587           | SER                  | A      |
| 272            | 588           | TYR                  | A      |
| 273            | 593           | GLN                  | A      |
| 274            | 594           | LYS                  | A      |
| 275            | 595           | ILE                  | A      |
| 276            | 596           | VAL                  | A      |
| 277            | 597           | ILE                  | A      |
| 278            | 598           | ALA                  | A      |
| 279            | 599           | ALA                  | A      |
| 280            | 600           | ASN                  | A      |
| 281            | 603           | LYS                  | A      |
| 282            | 604           | GLU                  | A      |
| 283            | 605           | PRO                  | A      |
| 284            | 606           | LYS                  | A      |

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Table S15 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 607           | GLU                  | A      |
| 286            | 608           | ILE                  | A      |
| 287            | 609           | THR                  | A      |
| 288            | 610           | GLY                  | A      |
| 289            | 611           | GLY                  | A      |
| 290            | 612           | ARG                  | A      |
| 291            | 613           | VAL                  | A      |
| 292            | 614           | TRP                  | A      |
| 293            | 615           | ASN                  | A      |
| 294            | 626           | LEU                  | A      |
| 295            | 627           | LYS                  | A      |
| 296            | 628           | PRO                  | A      |
| 297            | 630           | GLU                  | A      |
| 298            | 631           | PHE                  | A      |
| 299            | 632           | ALA                  | A      |
| 300            | 633           | LEU                  | A      |
| 301            | 634           | VAL                  | A      |
| 302            | 635           | VAL                  | A      |

Table S16: Residues membership for the *P. stutzeri*  $\alpha$ -amylase (PDB code 1GCY, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 17            | GLU                  | A      |
| 1              | 18            | ILE                  | A      |
| 2              | 19            | ILE                  | B      |
| 3              | 20            | LEU                  | B      |
| 4              | 21            | GLN                  | B      |
| 5              | 22            | GLY                  | C      |
| 6              | 23            | PHE                  | C      |
| 7              | 27            | VAL                  | C      |
| 8              | 34            | ASP                  | C      |
| 9              | 35            | TRP                  | C      |
| 10             | 36            | TYR                  | C      |
| 11             | 37            | ASN                  | C      |
| 12             | 38            | ILE                  | C      |
| 13             | 39            | LEU                  | C      |
| 14             | 40            | ARG                  | C      |
| 15             | 41            | GLN                  | C      |
| 16             | 42            | GLN                  | C      |
| 17             | 43            | ALA                  | C      |
| 18             | 44            | ALA                  | C      |
| 19             | 45            | THR                  | C      |

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Table S16 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 46            | ILE                  | C      |
| 21             | 47            | ALA                  | C      |
| 22             | 48            | ALA                  | C      |
| 23             | 49            | ASP                  | C      |
| 24             | 50            | GLY                  | C      |
| 25             | 51            | PHE                  | C      |
| 26             | 52            | SER                  | C      |
| 27             | 53            | ALA                  | C      |
| 28             | 54            | ILE                  | C      |
| 29             | 55            | TRP                  | C      |
| 30             | 56            | MET                  | C      |
| 31             | 57            | PRO                  | C      |
| 32             | 58            | VAL                  | C      |
| 33             | 59            | PRO                  | C      |
| 34             | 60            | TRP                  | C      |
| 35             | 61            | ARG                  | C      |
| 36             | 62            | ASP                  | C      |
| 37             | 63            | PHE                  | C      |
| 38             | 65            | SER                  | C      |
| 39             | 75            | GLY                  | C      |
| 40             | 76            | GLU                  | C      |
| 41             | 77            | GLY                  | C      |
| 42             | 78            | TYR                  | C      |
| 43             | 79            | PHE                  | C      |
| 44             | 80            | TRP                  | C      |
| 45             | 81            | HIS                  | C      |
| 46             | 82            | ASP                  | C      |
| 47             | 83            | PHE                  | C      |
| 48             | 84            | ASN                  | C      |
| 49             | 85            | LYS                  | C      |
| 50             | 86            | ASN                  | C      |
| 51             | 87            | GLY                  | C      |
| 52             | 88            | ARG                  | C      |
| 53             | 89            | TYR                  | C      |
| 54             | 90            | GLY                  | C      |
| 55             | 91            | SER                  | C      |
| 56             | 92            | ASP                  | C      |
| 57             | 93            | ALA                  | C      |
| 58             | 94            | GLN                  | C      |
| 59             | 95            | LEU                  | C      |
| 60             | 96            | ARG                  | C      |
| 61             | 97            | GLN                  | C      |
| 62             | 98            | ALA                  | C      |
| 63             | 99            | ALA                  | C      |
| 64             | 100           | SER                  | C      |
| 65             | 101           | ALA                  | C      |

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Table S16 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 102           | LEU                  | C      |
| 67             | 103           | GLY                  | C      |
| 68             | 104           | GLY                  | C      |
| 69             | 105           | ALA                  | C      |
| 70             | 106           | GLY                  | C      |
| 71             | 107           | VAL                  | C      |
| 72             | 108           | LYS                  | C      |
| 73             | 109           | VAL                  | C      |
| 74             | 110           | LEU                  | C      |
| 75             | 111           | TYR                  | C      |
| 76             | 112           | ASP                  | C      |
| 77             | 113           | VAL                  | C      |
| 78             | 114           | VAL                  | C      |
| 79             | 115           | PRO                  | C      |
| 80             | 116           | ASN                  | C      |
| 81             | 117           | HIS                  | C      |
| 82             | 118           | MET                  | C      |
| 83             | 119           | ASN                  | C      |
| 84             | 120           | ARG                  | C      |
| 85             | 121           | GLY                  | C      |
| 86             | 125           | LYS                  | C      |
| 87             | 127           | ILE                  | C      |
| 88             | 128           | ASN                  | C      |
| 89             | 129           | LEU                  | C      |
| 90             | 131           | ALA                  | C      |
| 91             | 132           | GLY                  | C      |
| 92             | 133           | GLN                  | C      |
| 93             | 134           | GLY                  | C      |
| 94             | 135           | PHE                  | B      |
| 95             | 154           | ASP                  | B      |
| 96             | 155           | ARG                  | B      |
| 97             | 156           | PHE                  | B      |
| 98             | 157           | ILE                  | B      |
| 99             | 160           | ASP                  | B      |
| 100            | 161           | ALA                  | B      |
| 101            | 162           | ASP                  | B      |
| 102            | 163           | LEU                  | B      |
| 103            | 164           | ASN                  | B      |
| 104            | 165           | THR                  | B      |
| 105            | 166           | GLY                  | B      |
| 106            | 167           | HIS                  | B      |
| 107            | 168           | PRO                  | B      |
| 108            | 169           | GLN                  | B      |
| 109            | 170           | VAL                  | B      |
| 110            | 171           | TYR                  | B      |
| 111            | 172           | GLY                  | B      |

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Table S16 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 173           | MET                  | B      |
| 113            | 174           | PHE                  | B      |
| 114            | 175           | ARG                  | B      |
| 115            | 176           | ASP                  | B      |
| 116            | 177           | GLU                  | B      |
| 117            | 178           | PHE                  | B      |
| 118            | 179           | THR                  | B      |
| 119            | 180           | ASN                  | B      |
| 120            | 181           | LEU                  | B      |
| 121            | 182           | ARG                  | B      |
| 122            | 183           | SER                  | B      |
| 123            | 185           | TYR                  | C      |
| 124            | 186           | GLY                  | C      |
| 125            | 187           | ALA                  | C      |
| 126            | 188           | GLY                  | C      |
| 127            | 189           | GLY                  | C      |
| 128            | 190           | PHE                  | B      |
| 129            | 191           | ARG                  | D      |
| 130            | 192           | PHE                  | B      |
| 131            | 193           | ASP                  | B      |
| 132            | 194           | PHE                  | B      |
| 133            | 195           | VAL                  | B      |
| 134            | 196           | ARG                  | B      |
| 135            | 197           | GLY                  | B      |
| 136            | 198           | TYR                  | B      |
| 137            | 199           | ALA                  | B      |
| 138            | 200           | PRO                  | B      |
| 139            | 201           | GLU                  | B      |
| 140            | 202           | ARG                  | B      |
| 141            | 203           | VAL                  | B      |
| 142            | 204           | ASN                  | B      |
| 143            | 205           | SER                  | B      |
| 144            | 206           | TRP                  | B      |
| 145            | 207           | MET                  | B      |
| 146            | 208           | THR                  | B      |
| 147            | 209           | ASP                  | B      |
| 148            | 210           | SER                  | B      |
| 149            | 211           | ALA                  | B      |
| 150            | 214           | SER                  | B      |
| 151            | 215           | PHE                  | B      |
| 152            | 216           | CYS                  | B      |
| 153            | 217           | VAL                  | C      |
| 154            | 218           | GLY                  | B      |
| 155            | 219           | GLU                  | B      |
| 156            | 220           | LEU                  | B      |
| 157            | 221           | TRP                  | B      |

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Table S16 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 222           | LYS                  | B      |
| 159            | 223           | GLY                  | B      |
| 160            | 242           | ILE                  | B      |
| 161            | 243           | LYS                  | B      |
| 162            | 244           | ASP                  | B      |
| 163            | 245           | TRP                  | B      |
| 164            | 247           | ASP                  | B      |
| 165            | 248           | ARG                  | B      |
| 166            | 250           | LYS                  | B      |
| 167            | 251           | CYS                  | B      |
| 168            | 252           | PRO                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | PHE                  | D      |
| 171            | 255           | ASP                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | ALA                  | D      |
| 174            | 259           | LYS                  | D      |
| 175            | 260           | GLU                  | D      |
| 176            | 261           | ARG                  | D      |
| 177            | 262           | MET                  | D      |
| 178            | 263           | GLN                  | D      |
| 179            | 264           | ASN                  | D      |
| 180            | 265           | GLY                  | D      |
| 181            | 266           | SER                  | D      |
| 182            | 267           | ILE                  | D      |
| 183            | 268           | ALA                  | A      |
| 184            | 269           | ASP                  | A      |
| 185            | 270           | TRP                  | A      |
| 186            | 271           | LYS                  | A      |
| 187            | 272           | HIS                  | D      |
| 188            | 273           | GLY                  | D      |
| 189            | 274           | LEU                  | D      |
| 190            | 276           | GLY                  | D      |
| 191            | 277           | ASN                  | B      |
| 192            | 278           | PRO                  | B      |
| 193            | 282           | TRP                  | B      |
| 194            | 283           | ARG                  | B      |
| 195            | 284           | GLU                  | B      |
| 196            | 285           | VAL                  | B      |
| 197            | 286           | ALA                  | B      |
| 198            | 287           | VAL                  | D      |
| 199            | 288           | THR                  | D      |
| 200            | 289           | PHE                  | D      |
| 201            | 290           | VAL                  | A      |
| 202            | 291           | ASP                  | D      |
| 203            | 292           | ASN                  | D      |

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Table S16 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 293           | HIS                  | D      |
| 205            | 294           | ASP                  | D      |
| 206            | 295           | THR                  | D      |
| 207            | 296           | GLY                  | D      |
| 208            | 309           | ALA                  | D      |
| 209            | 310           | LEU                  | D      |
| 210            | 311           | GLN                  | D      |
| 211            | 312           | ASP                  | D      |
| 212            | 313           | GLY                  | A      |
| 213            | 314           | LEU                  | A      |
| 214            | 315           | ILE                  | A      |
| 215            | 316           | ARG                  | A      |
| 216            | 317           | GLN                  | A      |
| 217            | 318           | ALA                  | A      |
| 218            | 319           | TYR                  | A      |
| 219            | 320           | ALA                  | A      |
| 220            | 321           | TYR                  | A      |
| 221            | 322           | ILE                  | A      |
| 222            | 323           | LEU                  | A      |
| 223            | 324           | THR                  | A      |
| 224            | 325           | SER                  | A      |
| 225            | 326           | PRO                  | D      |
| 226            | 327           | GLY                  | D      |
| 227            | 328           | THR                  | D      |
| 228            | 329           | PRO                  | A      |
| 229            | 330           | VAL                  | D      |
| 230            | 331           | VAL                  | A      |
| 231            | 332           | TYR                  | D      |
| 232            | 333           | TRP                  | C      |
| 233            | 334           | ASP                  | D      |
| 234            | 335           | HIS                  | A      |
| 235            | 336           | MET                  | C      |
| 236            | 337           | TYR                  | C      |
| 237            | 338           | ASP                  | D      |
| 238            | 339           | TRP                  | D      |
| 239            | 340           | GLY                  | D      |
| 240            | 341           | TYR                  | A      |
| 241            | 342           | GLY                  | A      |
| 242            | 343           | ASP                  | A      |
| 243            | 344           | PHE                  | A      |
| 244            | 345           | ILE                  | A      |
| 245            | 346           | ARG                  | A      |
| 246            | 347           | GLN                  | A      |
| 247            | 348           | LEU                  | A      |
| 248            | 349           | ILE                  | A      |
| 249            | 350           | GLN                  | A      |

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Table S16 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 351           | VAL                  | A      |
| 251            | 352           | ARG                  | A      |
| 252            | 353           | ARG                  | A      |
| 253            | 354           | ALA                  | A      |
| 254            | 355           | ALA                  | A      |
| 255            | 356           | GLY                  | A      |
| 256            | 360           | ASP                  | A      |
| 257            | 361           | SER                  | A      |
| 258            | 362           | ALA                  | A      |
| 259            | 363           | ILE                  | A      |
| 260            | 364           | SER                  | A      |
| 261            | 365           | PHE                  | A      |
| 262            | 366           | HIS                  | A      |
| 263            | 367           | SER                  | A      |
| 264            | 368           | GLY                  | A      |
| 265            | 369           | TYR                  | A      |
| 266            | 370           | SER                  | A      |
| 267            | 371           | GLY                  | A      |
| 268            | 372           | LEU                  | A      |
| 269            | 373           | VAL                  | A      |
| 270            | 374           | ALA                  | A      |
| 271            | 375           | THR                  | A      |
| 272            | 376           | VAL                  | A      |
| 273            | 381           | GLN                  | A      |
| 274            | 382           | THR                  | A      |
| 275            | 383           | LEU                  | A      |
| 276            | 384           | VAL                  | A      |
| 277            | 385           | VAL                  | A      |
| 278            | 386           | ALA                  | A      |
| 279            | 387           | LEU                  | A      |
| 280            | 388           | ASN                  | A      |
| 281            | 389           | SER                  | A      |
| 282            | 390           | ASP                  | A      |
| 283            | 391           | LEU                  | A      |
| 284            | 392           | GLY                  | A      |
| 285            | 393           | ASN                  | A      |
| 286            | 394           | PRO                  | A      |
| 287            | 395           | GLY                  | A      |
| 288            | 401           | SER                  | A      |
| 289            | 402           | PHE                  | A      |
| 290            | 403           | SER                  | A      |
| 291            | 404           | GLU                  | A      |
| 292            | 405           | ALA                  | A      |
| 293            | 406           | VAL                  | A      |
| 294            | 409           | SER                  | A      |
| 295            | 410           | ASN                  | A      |

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Table S16 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 411           | GLY                  | A      |
| 297            | 412           | GLN                  | A      |
| 298            | 413           | VAL                  | A      |
| 299            | 414           | ARG                  | A      |
| 300            | 415           | VAL                  | A      |
| 301            | 416           | TRP                  | A      |
| 302            | 417           | ARG                  | A      |

Table S17: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 1HNY, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |

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Table S17 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |

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Table S17 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |

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Table S17 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |

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Table S17 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |

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Table S17 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |

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Table S17 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S18: Residues membership for the *T. maritima*  $\alpha$ -amylase (PDB code 1GJW, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 84            | SER                  | A      |
| 1              | 85            | VAL                  | A      |
| 2              | 86            | VAL                  | B      |
| 3              | 87            | TYR                  | B      |
| 4              | 88            | GLY                  | B      |
| 5              | 89            | SER                  | C      |
| 6              | 90            | LEU                  | C      |
| 7              | 91            | PRO                  | C      |
| 8              | 117           | GLY                  | C      |
| 9              | 118           | THR                  | C      |
| 10             | 119           | PHE                  | C      |
| 11             | 120           | PHE                  | C      |
| 12             | 121           | LYS                  | C      |
| 13             | 122           | MET                  | C      |
| 14             | 123           | MET                  | C      |
| 15             | 124           | LEU                  | C      |
| 16             | 125           | LEU                  | C      |
| 17             | 126           | LEU                  | C      |
| 18             | 127           | PRO                  | C      |
| 19             | 128           | PHE                  | C      |
| 20             | 129           | VAL                  | C      |
| 21             | 130           | LYS                  | C      |
| 22             | 131           | SER                  | C      |
| 23             | 132           | LEU                  | C      |
| 24             | 133           | GLY                  | C      |
| 25             | 134           | ALA                  | C      |
| 26             | 135           | ASP                  | C      |
| 27             | 136           | ALA                  | C      |
| 28             | 137           | ILE                  | C      |
| 29             | 138           | TYR                  | C      |
| 30             | 139           | LEU                  | C      |
| 31             | 140           | LEU                  | C      |
| 32             | 141           | PRO                  | C      |
| 33             | 142           | VAL                  | C      |
| 34             | 143           | SER                  | C      |
| 35             | 144           | ARG                  | C      |
| 36             | 145           | MET                  | C      |
| 37             | 146           | SER                  | C      |
| 38             | 154           | ALA                  | C      |
| 39             | 155           | PRO                  | C      |
| 40             | 156           | SER                  | C      |
| 41             | 157           | PRO                  | C      |
| 42             | 158           | TYR                  | C      |
| 43             | 159           | SER                  | C      |

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Table S18 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 160           | VAL                  | C      |
| 45             | 161           | LYS                  | C      |
| 46             | 162           | ASN                  | C      |
| 47             | 164           | MET                  | C      |
| 48             | 165           | GLU                  | C      |
| 49             | 166           | LEU                  | C      |
| 50             | 167           | ASP                  | C      |
| 51             | 168           | GLU                  | C      |
| 52             | 169           | ARG                  | C      |
| 53             | 170           | TYR                  | C      |
| 54             | 171           | HIS                  | C      |
| 55             | 172           | ASP                  | C      |
| 56             | 181           | ASP                  | C      |
| 57             | 182           | GLU                  | C      |
| 58             | 183           | GLU                  | C      |
| 59             | 184           | PHE                  | C      |
| 60             | 185           | LYS                  | C      |
| 61             | 186           | ALA                  | C      |
| 62             | 187           | PHE                  | C      |
| 63             | 188           | VAL                  | C      |
| 64             | 189           | GLU                  | C      |
| 65             | 190           | ALA                  | C      |
| 66             | 191           | CYS                  | C      |
| 67             | 192           | HIS                  | C      |
| 68             | 193           | ILE                  | C      |
| 69             | 194           | LEU                  | C      |
| 70             | 195           | GLY                  | C      |
| 71             | 196           | ILE                  | C      |
| 72             | 197           | ARG                  | C      |
| 73             | 198           | VAL                  | C      |
| 74             | 199           | ILE                  | C      |
| 75             | 200           | LEU                  | C      |
| 76             | 201           | ASP                  | C      |
| 77             | 202           | PHE                  | C      |
| 78             | 203           | ILE                  | C      |
| 79             | 204           | PRO                  | C      |
| 80             | 205           | ARG                  | C      |
| 81             | 206           | THR                  | C      |
| 82             | 207           | ALA                  | C      |
| 83             | 208           | ALA                  | C      |
| 84             | 209           | ARG                  | C      |
| 85             | 210           | ASP                  | C      |
| 86             | 211           | SER                  | C      |
| 87             | 212           | ASP                  | C      |
| 88             | 213           | LEU                  | C      |
| 89             | 214           | ILE                  | C      |

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Table S18 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 218           | PRO                  | C      |
| 91             | 219           | ASP                  | C      |
| 92             | 220           | TRP                  | C      |
| 93             | 221           | PHE                  | C      |
| 94             | 222           | TYR                  | B      |
| 95             | 302           | PRO                  | B      |
| 96             | 303           | GLY                  | B      |
| 97             | 304           | PHE                  | B      |
| 98             | 305           | SER                  | B      |
| 99             | 318           | VAL                  | B      |
| 100            | 319           | THR                  | B      |
| 101            | 320           | PHE                  | B      |
| 102            | 321           | LEU                  | B      |
| 103            | 322           | ARG                  | B      |
| 104            | 323           | LEU                  | B      |
| 105            | 324           | TYR                  | B      |
| 106            | 359           | ASN                  | B      |
| 107            | 360           | ARG                  | B      |
| 108            | 361           | GLU                  | B      |
| 109            | 362           | LEU                  | B      |
| 110            | 363           | TRP                  | B      |
| 111            | 364           | GLU                  | B      |
| 112            | 365           | TYR                  | B      |
| 113            | 366           | LEU                  | B      |
| 114            | 367           | ALA                  | B      |
| 115            | 368           | GLY                  | B      |
| 116            | 369           | VAL                  | B      |
| 117            | 370           | ILE                  | B      |
| 118            | 371           | PRO                  | B      |
| 119            | 372           | HIS                  | B      |
| 120            | 373           | TYR                  | B      |
| 121            | 374           | GLN                  | B      |
| 122            | 375           | LYS                  | B      |
| 123            | 377           | TYR                  | C      |
| 124            | 378           | GLY                  | C      |
| 125            | 379           | ILE                  | C      |
| 126            | 380           | ASP                  | C      |
| 127            | 381           | GLY                  | C      |
| 128            | 382           | ALA                  | B      |
| 129            | 383           | ARG                  | D      |
| 130            | 384           | LEU                  | B      |
| 131            | 385           | ASP                  | B      |
| 132            | 386           | MET                  | B      |
| 133            | 387           | GLY                  | B      |
| 134            | 388           | HIS                  | B      |
| 135            | 389           | ALA                  | B      |

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Table S18 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 390           | LEU                  | B      |
| 137            | 391           | PRO                  | B      |
| 138            | 392           | LYS                  | B      |
| 139            | 393           | GLU                  | B      |
| 140            | 394           | LEU                  | B      |
| 141            | 395           | LEU                  | B      |
| 142            | 396           | ASP                  | B      |
| 143            | 397           | LEU                  | B      |
| 144            | 398           | ILE                  | B      |
| 145            | 399           | ILE                  | B      |
| 146            | 400           | LYS                  | B      |
| 147            | 401           | ASN                  | B      |
| 148            | 402           | VAL                  | B      |
| 149            | 403           | LYS                  | B      |
| 150            | 409           | PHE                  | B      |
| 151            | 410           | VAL                  | B      |
| 152            | 411           | MET                  | B      |
| 153            | 412           | ILE                  | C      |
| 154            | 413           | ALA                  | B      |
| 155            | 414           | GLU                  | B      |
| 156            | 415           | GLU                  | B      |
| 157            | 416           | LEU                  | B      |
| 158            | 417           | ASP                  | B      |
| 159            | 418           | MET                  | B      |
| 160            | 421           | ASP                  | B      |
| 161            | 422           | LYS                  | B      |
| 162            | 423           | ALA                  | B      |
| 163            | 424           | SER                  | B      |
| 164            | 425           | LYS                  | B      |
| 165            | 426           | GLU                  | B      |
| 166            | 429           | TYR                  | B      |
| 167            | 430           | ASP                  | B      |
| 168            | 431           | VAL                  | B      |
| 169            | 432           | ILE                  | B      |
| 170            | 433           | LEU                  | D      |
| 171            | 434           | GLY                  | D      |
| 172            | 435           | SER                  | D      |
| 173            | 436           | SER                  | D      |
| 174            | 437           | TRP                  | D      |
| 175            | 438           | TYR                  | D      |
| 176            | 439           | PHE                  | D      |
| 177            | 440           | ALA                  | D      |
| 178            | 441           | GLY                  | D      |
| 179            | 442           | ARG                  | D      |
| 180            | 443           | VAL                  | D      |
| 181            | 444           | GLU                  | D      |

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Table S18 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 445           | GLU                  | D      |
| 183            | 446           | ILE                  | A      |
| 184            | 447           | GLY                  | A      |
| 185            | 448           | LYS                  | A      |
| 186            | 449           | LEU                  | A      |
| 187            | 450           | PRO                  | D      |
| 188            | 451           | ASP                  | D      |
| 189            | 452           | ILE                  | D      |
| 190            | 453           | ALA                  | D      |
| 191            | 454           | GLU                  | B      |
| 192            | 455           | GLU                  | B      |
| 193            | 456           | LEU                  | B      |
| 194            | 457           | VAL                  | B      |
| 195            | 458           | LEU                  | B      |
| 196            | 459           | PRO                  | B      |
| 197            | 460           | PHE                  | B      |
| 198            | 461           | LEU                  | D      |
| 199            | 462           | ALA                  | D      |
| 200            | 463           | SER                  | D      |
| 201            | 464           | VAL                  | A      |
| 202            | 465           | GLU                  | D      |
| 203            | 466           | THR                  | D      |
| 204            | 467           | PRO                  | D      |
| 205            | 468           | ASP                  | D      |
| 206            | 469           | THR                  | D      |
| 207            | 470           | PRO                  | D      |
| 208            | 471           | ARG                  | D      |
| 209            | 472           | ILE                  | D      |
| 210            | 473           | ALA                  | D      |
| 211            | 474           | THR                  | D      |
| 212            | 479           | SER                  | A      |
| 213            | 481           | MET                  | A      |
| 214            | 482           | LYS                  | A      |
| 215            | 483           | LYS                  | A      |
| 216            | 484           | LEU                  | A      |
| 217            | 485           | ALA                  | A      |
| 218            | 486           | PRO                  | A      |
| 219            | 487           | PHE                  | A      |
| 220            | 488           | VAL                  | A      |
| 221            | 489           | THR                  | A      |
| 222            | 490           | TYR                  | A      |
| 223            | 491           | PHE                  | A      |
| 224            | 492           | LEU                  | A      |
| 225            | 493           | PRO                  | D      |
| 226            | 495           | SER                  | D      |
| 227            | 496           | ILE                  | D      |

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Table S18 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 497           | PRO                  | A      |
| 229            | 498           | TYR                  | D      |
| 230            | 499           | VAL                  | A      |
| 231            | 500           | ASN                  | D      |
| 232            | 501           | THR                  | C      |
| 233            | 502           | GLY                  | D      |
| 234            | 503           | GLN                  | A      |
| 235            | 541           | TYR                  | C      |
| 236            | 542           | VAL                  | C      |
| 237            | 543           | LEU                  | D      |
| 238            | 544           | HIS                  | D      |
| 239            | 545           | TRP                  | D      |
| 240            | 552           | VAL                  | A      |
| 241            | 553           | LEU                  | A      |
| 242            | 554           | ASN                  | A      |
| 243            | 555           | PHE                  | A      |
| 244            | 556           | ILE                  | A      |
| 245            | 557           | LYS                  | A      |
| 246            | 558           | LYS                  | A      |
| 247            | 559           | LEU                  | A      |
| 248            | 560           | ILE                  | A      |
| 249            | 561           | LYS                  | A      |
| 250            | 562           | VAL                  | A      |
| 251            | 563           | ARG                  | A      |
| 252            | 564           | HIS                  | A      |
| 253            | 565           | GLU                  | A      |
| 254            | 566           | PHE                  | A      |
| 255            | 567           | LEU                  | A      |
| 256            | 572           | ASN                  | A      |
| 257            | 573           | GLY                  | A      |
| 258            | 574           | LYS                  | A      |
| 259            | 575           | PHE                  | A      |
| 260            | 576           | GLU                  | A      |
| 261            | 577           | ASN                  | A      |
| 262            | 578           | LEU                  | A      |
| 263            | 579           | THR                  | A      |
| 264            | 580           | THR                  | A      |
| 265            | 581           | LYS                  | A      |
| 266            | 582           | ASP                  | A      |
| 267            | 583           | LEU                  | A      |
| 268            | 584           | VAL                  | A      |
| 269            | 585           | MET                  | A      |
| 270            | 586           | TYR                  | A      |
| 271            | 587           | SER                  | A      |
| 272            | 588           | TYR                  | A      |
| 273            | 593           | GLN                  | A      |

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Table S18 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 594           | LYS                  | A      |
| 275            | 595           | ILE                  | A      |
| 276            | 596           | VAL                  | A      |
| 277            | 597           | ILE                  | A      |
| 278            | 598           | ALA                  | A      |
| 279            | 599           | ALA                  | A      |
| 280            | 600           | ASN                  | A      |
| 281            | 603           | LYS                  | A      |
| 282            | 604           | GLU                  | A      |
| 283            | 605           | PRO                  | A      |
| 284            | 606           | LYS                  | A      |
| 285            | 607           | GLU                  | A      |
| 286            | 608           | ILE                  | A      |
| 287            | 609           | THR                  | A      |
| 288            | 610           | GLY                  | A      |
| 289            | 611           | GLY                  | A      |
| 290            | 612           | ARG                  | A      |
| 291            | 613           | VAL                  | A      |
| 292            | 614           | TRP                  | A      |
| 293            | 615           | ASN                  | A      |
| 294            | 626           | LEU                  | A      |
| 295            | 627           | LYS                  | A      |
| 296            | 628           | PRO                  | A      |
| 297            | 630           | GLU                  | A      |
| 298            | 631           | PHE                  | A      |
| 299            | 632           | ALA                  | A      |
| 300            | 633           | LEU                  | A      |
| 301            | 634           | VAL                  | A      |
| 302            | 635           | VAL                  | A      |

Table S19: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 1HX0, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |

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Table S19 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | ILE                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |

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Table S19 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |

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Table S19 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |

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Table S19 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |

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Table S19 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | ILE                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |

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Table S19 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLU                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |

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Table S19 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S20: Residues membership for the *B. stearothermophilus*  $\alpha$ -amylase (PDB code 1HVX, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 6             | GLY                  | A      |
| 1              | 7             | THR                  | A      |
| 2              | 8             | MET                  | B      |
| 3              | 9             | MET                  | B      |
| 4              | 10            | GLN                  | B      |
| 5              | 11            | TYR                  | C      |
| 6              | 12            | PHE                  | C      |
| 7              | 16            | LEU                  | C      |
| 8              | 21            | THR                  | C      |
| 9              | 22            | LEU                  | C      |
| 10             | 23            | TRP                  | C      |
| 11             | 24            | THR                  | C      |
| 12             | 25            | LYS                  | C      |
| 13             | 26            | VAL                  | C      |
| 14             | 27            | ALA                  | C      |
| 15             | 28            | ASN                  | C      |
| 16             | 29            | GLU                  | C      |
| 17             | 30            | ALA                  | C      |
| 18             | 31            | ASN                  | C      |
| 19             | 32            | ASN                  | C      |

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Table S20 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 33            | LEU                  | C      |
| 21             | 34            | SER                  | C      |
| 22             | 35            | SER                  | C      |
| 23             | 36            | LEU                  | C      |
| 24             | 37            | GLY                  | C      |
| 25             | 38            | ILE                  | C      |
| 26             | 39            | THR                  | C      |
| 27             | 40            | ALA                  | C      |
| 28             | 41            | LEU                  | C      |
| 29             | 42            | TRP                  | C      |
| 30             | 43            | LEU                  | C      |
| 31             | 44            | PRO                  | C      |
| 32             | 45            | PRO                  | C      |
| 33             | 46            | ALA                  | C      |
| 34             | 47            | TYR                  | C      |
| 35             | 48            | LYS                  | C      |
| 36             | 49            | GLY                  | C      |
| 37             | 50            | THR                  | C      |
| 38             | 53            | SER                  | C      |
| 39             | 54            | ASP                  | C      |
| 40             | 55            | VAL                  | C      |
| 41             | 56            | GLY                  | C      |
| 42             | 57            | TYR                  | C      |
| 43             | 58            | GLY                  | C      |
| 44             | 59            | VAL                  | C      |
| 45             | 60            | TYR                  | C      |
| 46             | 61            | ASP                  | C      |
| 47             | 63            | TYR                  | C      |
| 48             | 64            | ASP                  | C      |
| 49             | 65            | LEU                  | C      |
| 50             | 66            | GLY                  | C      |
| 51             | 76            | THR                  | C      |
| 52             | 77            | LYS                  | C      |
| 53             | 78            | TYR                  | C      |
| 54             | 79            | GLY                  | C      |
| 55             | 80            | THR                  | C      |
| 56             | 81            | LYS                  | C      |
| 57             | 82            | ALA                  | C      |
| 58             | 83            | GLN                  | C      |
| 59             | 84            | TYR                  | C      |
| 60             | 85            | LEU                  | C      |
| 61             | 86            | GLN                  | C      |
| 62             | 87            | ALA                  | C      |
| 63             | 88            | ILE                  | C      |
| 64             | 89            | GLN                  | C      |
| 65             | 90            | ALA                  | C      |

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Table S20 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 91            | ALA                  | C      |
| 67             | 92            | HIS                  | C      |
| 68             | 93            | ALA                  | C      |
| 69             | 94            | ALA                  | C      |
| 70             | 95            | GLY                  | C      |
| 71             | 96            | MET                  | C      |
| 72             | 97            | GLN                  | C      |
| 73             | 98            | VAL                  | C      |
| 74             | 99            | TYR                  | C      |
| 75             | 100           | ALA                  | C      |
| 76             | 101           | ASP                  | C      |
| 77             | 102           | VAL                  | C      |
| 78             | 103           | VAL                  | C      |
| 79             | 104           | PHE                  | C      |
| 80             | 105           | ASP                  | C      |
| 81             | 106           | HIS                  | C      |
| 82             | 107           | LYS                  | C      |
| 83             | 108           | GLY                  | C      |
| 84             | 109           | GLY                  | C      |
| 85             | 110           | ALA                  | C      |
| 86             | 142           | PHE                  | C      |
| 87             | 155           | LYS                  | C      |
| 88             | 156           | TRP                  | C      |
| 89             | 157           | ARG                  | C      |
| 90             | 158           | TRP                  | C      |
| 91             | 159           | TYR                  | C      |
| 92             | 160           | HIS                  | C      |
| 93             | 161           | PHE                  | C      |
| 94             | 162           | ASP                  | B      |
| 95             | 197           | ASP                  | B      |
| 96             | 198           | TYR                  | B      |
| 97             | 199           | LEU                  | B      |
| 98             | 200           | MET                  | B      |
| 99             | 201           | TYR                  | B      |
| 100            | 202           | ALA                  | B      |
| 101            | 203           | ASP                  | B      |
| 102            | 204           | LEU                  | B      |
| 103            | 205           | ASP                  | B      |
| 104            | 206           | MET                  | B      |
| 105            | 207           | ASP                  | B      |
| 106            | 208           | HIS                  | B      |
| 107            | 209           | PRO                  | B      |
| 108            | 210           | GLU                  | B      |
| 109            | 211           | VAL                  | B      |
| 110            | 212           | VAL                  | B      |
| 111            | 213           | THR                  | B      |

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Table S20 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 214           | GLU                  | B      |
| 113            | 215           | LEU                  | B      |
| 114            | 216           | LYS                  | B      |
| 115            | 217           | SER                  | B      |
| 116            | 218           | TRP                  | B      |
| 117            | 219           | GLY                  | B      |
| 118            | 220           | LYS                  | B      |
| 119            | 221           | TRP                  | B      |
| 120            | 222           | TYR                  | B      |
| 121            | 223           | VAL                  | B      |
| 122            | 224           | ASN                  | B      |
| 123            | 226           | THR                  | C      |
| 124            | 227           | ASN                  | C      |
| 125            | 228           | ILE                  | C      |
| 126            | 229           | ASP                  | C      |
| 127            | 230           | GLY                  | C      |
| 128            | 231           | PHE                  | B      |
| 129            | 232           | ARG                  | D      |
| 130            | 233           | LEU                  | B      |
| 131            | 234           | ASP                  | B      |
| 132            | 235           | ALA                  | B      |
| 133            | 236           | VAL                  | B      |
| 134            | 237           | LYS                  | B      |
| 135            | 238           | HIS                  | B      |
| 136            | 239           | ILE                  | B      |
| 137            | 240           | LYS                  | B      |
| 138            | 241           | PHE                  | B      |
| 139            | 242           | SER                  | B      |
| 140            | 243           | PHE                  | B      |
| 141            | 244           | PHE                  | B      |
| 142            | 245           | PRO                  | B      |
| 143            | 246           | ASP                  | B      |
| 144            | 247           | TRP                  | B      |
| 145            | 248           | LEU                  | B      |
| 146            | 249           | SER                  | B      |
| 147            | 250           | TYR                  | B      |
| 148            | 251           | VAL                  | B      |
| 149            | 252           | ARG                  | B      |
| 150            | 259           | LEU                  | B      |
| 151            | 260           | PHE                  | B      |
| 152            | 261           | THR                  | B      |
| 153            | 262           | VAL                  | C      |
| 154            | 263           | GLY                  | B      |
| 155            | 264           | GLU                  | B      |
| 156            | 265           | TYR                  | B      |
| 157            | 266           | TRP                  | B      |

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Table S20 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 267           | SER                  | B      |
| 159            | 268           | TYR                  | B      |
| 160            | 273           | LEU                  | B      |
| 161            | 274           | HIS                  | B      |
| 162            | 275           | ASN                  | B      |
| 163            | 276           | TYR                  | B      |
| 164            | 277           | ILE                  | B      |
| 165            | 278           | MET                  | B      |
| 166            | 283           | THR                  | B      |
| 167            | 284           | MET                  | B      |
| 168            | 285           | SER                  | B      |
| 169            | 286           | LEU                  | B      |
| 170            | 287           | PHE                  | D      |
| 171            | 288           | ASP                  | D      |
| 172            | 289           | ALA                  | D      |
| 173            | 290           | PRO                  | D      |
| 174            | 292           | HIS                  | D      |
| 175            | 293           | ASN                  | D      |
| 176            | 294           | LYS                  | D      |
| 177            | 295           | PHE                  | D      |
| 178            | 296           | TYR                  | D      |
| 179            | 297           | THR                  | D      |
| 180            | 298           | ALA                  | D      |
| 181            | 299           | SER                  | D      |
| 182            | 305           | PHE                  | D      |
| 183            | 306           | ASP                  | A      |
| 184            | 307           | MET                  | A      |
| 185            | 308           | ARG                  | A      |
| 186            | 310           | LEU                  | A      |
| 187            | 311           | MET                  | D      |
| 188            | 312           | THR                  | D      |
| 189            | 313           | ASN                  | D      |
| 190            | 316           | MET                  | D      |
| 191            | 317           | LYS                  | B      |
| 192            | 318           | ASP                  | B      |
| 193            | 319           | GLN                  | B      |
| 194            | 320           | PRO                  | B      |
| 195            | 321           | THR                  | B      |
| 196            | 322           | LEU                  | B      |
| 197            | 323           | ALA                  | B      |
| 198            | 324           | VAL                  | D      |
| 199            | 325           | THR                  | D      |
| 200            | 326           | PHE                  | D      |
| 201            | 327           | VAL                  | A      |
| 202            | 328           | ASP                  | D      |
| 203            | 329           | ASN                  | D      |

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Table S20 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 330           | HIS                  | D      |
| 205            | 331           | ASP                  | D      |
| 206            | 332           | THR                  | D      |
| 207            | 333           | GLU                  | D      |
| 208            | 341           | TRP                  | D      |
| 209            | 342           | VAL                  | D      |
| 210            | 343           | ASP                  | D      |
| 211            | 344           | PRO                  | D      |
| 212            | 345           | TRP                  | A      |
| 213            | 346           | PHE                  | A      |
| 214            | 347           | LYS                  | A      |
| 215            | 348           | PRO                  | A      |
| 216            | 349           | LEU                  | A      |
| 217            | 350           | ALA                  | A      |
| 218            | 351           | TYR                  | A      |
| 219            | 352           | ALA                  | A      |
| 220            | 353           | PHE                  | A      |
| 221            | 354           | ILE                  | A      |
| 222            | 355           | LEU                  | A      |
| 223            | 356           | THR                  | A      |
| 224            | 357           | ARG                  | A      |
| 225            | 359           | GLU                  | D      |
| 226            | 360           | GLY                  | D      |
| 227            | 361           | TYR                  | D      |
| 228            | 362           | PRO                  | A      |
| 229            | 363           | CYS                  | D      |
| 230            | 364           | VAL                  | A      |
| 231            | 365           | PHE                  | D      |
| 232            | 366           | TYR                  | C      |
| 233            | 367           | GLY                  | D      |
| 234            | 368           | ASP                  | A      |
| 235            | 369           | TYR                  | C      |
| 236            | 370           | TYR                  | C      |
| 237            | 371           | GLY                  | D      |
| 238            | 372           | ILE                  | D      |
| 239            | 379           | SER                  | D      |
| 240            | 380           | LEU                  | A      |
| 241            | 381           | LYS                  | A      |
| 242            | 382           | SER                  | A      |
| 243            | 383           | LYS                  | A      |
| 244            | 384           | ILE                  | A      |
| 245            | 385           | ASP                  | A      |
| 246            | 386           | PRO                  | A      |
| 247            | 387           | LEU                  | A      |
| 248            | 388           | LEU                  | A      |
| 249            | 389           | ILE                  | A      |

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Table S20 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 390           | ALA                  | A      |
| 251            | 391           | ARG                  | A      |
| 252            | 392           | ARG                  | A      |
| 253            | 393           | ASP                  | A      |
| 254            | 394           | TYR                  | A      |
| 255            | 395           | ALA                  | A      |
| 256            | 397           | GLY                  | A      |
| 257            | 398           | THR                  | A      |
| 258            | 399           | GLN                  | A      |
| 259            | 400           | HIS                  | A      |
| 260            | 401           | ASP                  | A      |
| 261            | 402           | TYR                  | A      |
| 262            | 403           | LEU                  | A      |
| 263            | 404           | ASP                  | A      |
| 264            | 405           | HIS                  | A      |
| 265            | 406           | SER                  | A      |
| 266            | 407           | ASP                  | A      |
| 267            | 408           | ILE                  | A      |
| 268            | 409           | ILE                  | A      |
| 269            | 410           | GLY                  | A      |
| 270            | 411           | TRP                  | A      |
| 271            | 412           | THR                  | A      |
| 272            | 413           | ARG                  | A      |
| 273            | 414           | GLU                  | A      |
| 274            | 415           | GLY                  | A      |
| 275            | 424           | LEU                  | A      |
| 276            | 425           | ALA                  | A      |
| 277            | 426           | ALA                  | A      |
| 278            | 427           | LEU                  | A      |
| 279            | 428           | ILE                  | A      |
| 280            | 429           | THR                  | A      |
| 281            | 431           | GLY                  | A      |
| 282            | 432           | PRO                  | A      |
| 283            | 433           | GLY                  | A      |
| 284            | 434           | GLY                  | A      |
| 285            | 435           | SER                  | A      |
| 286            | 436           | LYS                  | A      |
| 287            | 437           | TRP                  | A      |
| 288            | 446           | GLY                  | A      |
| 289            | 447           | LYS                  | A      |
| 290            | 449           | PHE                  | A      |
| 291            | 450           | TYR                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | LEU                  | A      |
| 294            | 472           | VAL                  | A      |
| 295            | 473           | ASN                  | A      |

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Table S20 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 474           | GLY                  | A      |
| 297            | 476           | SER                  | A      |
| 298            | 477           | VAL                  | A      |
| 299            | 478           | SER                  | A      |
| 300            | 479           | VAL                  | A      |
| 301            | 480           | TRP                  | A      |
| 302            | 481           | VAL                  | A      |

Table S21: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 1JFH, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |

*Continued on next page*

Table S21 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |

*Continued on next page*

Table S21 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |

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Table S21 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |

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Table S21 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |

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Table S21 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 322           | LYS                  | A      |
| 216            | 323           | ILE                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLU                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLU                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |

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Table S21 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S22: Residues membership for the *T. molitor*  $\alpha$ -amylase (PDB code 1JAE, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | ASN                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | LYS                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | ASN                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | ASP                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLN                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | GLN                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | ILE                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | TYR                  | C      |
| 37             | 49            | LEU                  | C      |
| 38             | 51            | ALA                  | C      |
| 39             | 57            | TRP                  | C      |
| 40             | 58            | GLU                  | C      |
| 41             | 59            | ARG                  | C      |
| 42             | 60            | TYR                  | C      |
| 43             | 61            | GLN                  | C      |

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Table S22 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 62            | PRO                  | C      |
| 45             | 63            | VAL                  | C      |
| 46             | 64            | SER                  | C      |
| 47             | 65            | TYR                  | C      |
| 48             | 66            | ILE                  | C      |
| 49             | 67            | ILE                  | C      |
| 50             | 68            | ASN                  | C      |
| 51             | 69            | THR                  | C      |
| 52             | 70            | ARG                  | C      |
| 53             | 71            | SER                  | C      |
| 54             | 72            | GLY                  | C      |
| 55             | 73            | ASP                  | C      |
| 56             | 74            | GLU                  | C      |
| 57             | 75            | SER                  | C      |
| 58             | 76            | ALA                  | C      |
| 59             | 77            | PHE                  | C      |
| 60             | 78            | THR                  | C      |
| 61             | 79            | ASP                  | C      |
| 62             | 80            | MET                  | C      |
| 63             | 81            | THR                  | C      |
| 64             | 82            | ARG                  | C      |
| 65             | 83            | ARG                  | C      |
| 66             | 84            | CYS                  | C      |
| 67             | 85            | ASN                  | C      |
| 68             | 86            | ASP                  | C      |
| 69             | 87            | ALA                  | C      |
| 70             | 88            | GLY                  | C      |
| 71             | 89            | VAL                  | C      |
| 72             | 90            | ARG                  | C      |
| 73             | 91            | ILE                  | C      |
| 74             | 92            | TYR                  | C      |
| 75             | 93            | VAL                  | C      |
| 76             | 94            | ASP                  | C      |
| 77             | 95            | ALA                  | C      |
| 78             | 96            | VAL                  | C      |
| 79             | 97            | ILE                  | C      |
| 80             | 98            | ASN                  | C      |
| 81             | 99            | HIS                  | C      |
| 82             | 100           | MET                  | C      |
| 83             | 101           | THR                  | C      |
| 84             | 102           | GLY                  | C      |
| 85             | 103           | MET                  | C      |
| 86             | 120           | TYR                  | C      |
| 87             | 124           | PRO                  | C      |
| 88             | 125           | TYR                  | C      |
| 89             | 126           | GLY                  | C      |

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Table S22 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 127           | SER                  | C      |
| 91             | 128           | GLY                  | C      |
| 92             | 129           | ASP                  | C      |
| 93             | 130           | PHE                  | C      |
| 94             | 131           | HIS                  | B      |
| 95             | 148           | CYS                  | B      |
| 96             | 149           | GLU                  | B      |
| 97             | 150           | LEU                  | B      |
| 98             | 151           | VAL                  | B      |
| 99             | 153           | LEU                  | B      |
| 100            | 154           | ARG                  | B      |
| 101            | 155           | ASP                  | B      |
| 102            | 156           | LEU                  | B      |
| 103            | 157           | ASN                  | B      |
| 104            | 158           | GLN                  | B      |
| 105            | 159           | GLY                  | B      |
| 106            | 160           | SER                  | B      |
| 107            | 161           | ASP                  | B      |
| 108            | 162           | TYR                  | B      |
| 109            | 163           | VAL                  | B      |
| 110            | 164           | ARG                  | B      |
| 111            | 165           | GLY                  | B      |
| 112            | 166           | VAL                  | B      |
| 113            | 167           | LEU                  | B      |
| 114            | 168           | ILE                  | B      |
| 115            | 169           | ASP                  | B      |
| 116            | 170           | TYR                  | B      |
| 117            | 171           | MET                  | B      |
| 118            | 172           | ASN                  | B      |
| 119            | 173           | HIS                  | B      |
| 120            | 174           | MET                  | B      |
| 121            | 175           | ILE                  | B      |
| 122            | 176           | ASP                  | B      |
| 123            | 177           | LEU                  | C      |
| 124            | 178           | GLY                  | C      |
| 125            | 179           | VAL                  | C      |
| 126            | 180           | ALA                  | C      |
| 127            | 181           | GLY                  | C      |
| 128            | 182           | PHE                  | B      |
| 129            | 183           | ARG                  | D      |
| 130            | 184           | VAL                  | B      |
| 131            | 185           | ASP                  | B      |
| 132            | 186           | ALA                  | B      |
| 133            | 187           | ALA                  | B      |
| 134            | 188           | LYS                  | B      |
| 135            | 189           | HIS                  | B      |

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Table S22 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 190           | MET                  | B      |
| 137            | 191           | SER                  | B      |
| 138            | 192           | PRO                  | B      |
| 139            | 193           | GLY                  | B      |
| 140            | 194           | ASP                  | B      |
| 141            | 195           | LEU                  | B      |
| 142            | 196           | SER                  | B      |
| 143            | 197           | VAL                  | B      |
| 144            | 198           | ILE                  | B      |
| 145            | 199           | PHE                  | B      |
| 146            | 200           | SER                  | B      |
| 147            | 201           | GLY                  | B      |
| 148            | 202           | LEU                  | B      |
| 149            | 203           | LYS                  | B      |
| 150            | 217           | PRO                  | B      |
| 151            | 218           | PHE                  | B      |
| 152            | 219           | ILE                  | B      |
| 153            | 220           | TYR                  | C      |
| 154            | 221           | GLN                  | B      |
| 155            | 222           | GLU                  | B      |
| 156            | 223           | VAL                  | B      |
| 157            | 224           | ILE                  | B      |
| 158            | 225           | ASP                  | B      |
| 159            | 226           | LEU                  | B      |
| 160            | 233           | LYS                  | B      |
| 161            | 234           | ASN                  | B      |
| 162            | 235           | GLU                  | B      |
| 163            | 236           | TYR                  | B      |
| 164            | 237           | THR                  | B      |
| 165            | 238           | GLY                  | B      |
| 166            | 239           | PHE                  | B      |
| 167            | 240           | GLY                  | B      |
| 168            | 241           | CYS                  | B      |
| 169            | 242           | VAL                  | B      |
| 170            | 243           | LEU                  | D      |
| 171            | 244           | GLU                  | D      |
| 172            | 245           | PHE                  | D      |
| 173            | 246           | GLN                  | D      |
| 174            | 248           | GLY                  | D      |
| 175            | 249           | VAL                  | D      |
| 176            | 250           | SER                  | D      |
| 177            | 251           | LEU                  | D      |
| 178            | 252           | GLY                  | D      |
| 179            | 253           | ASN                  | D      |
| 180            | 254           | ALA                  | D      |
| 181            | 255           | PHE                  | D      |

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Table S22 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 259           | ASN                  | D      |
| 183            | 260           | GLN                  | A      |
| 184            | 261           | LEU                  | A      |
| 185            | 262           | LYS                  | A      |
| 186            | 267           | TRP                  | A      |
| 187            | 268           | GLY                  | D      |
| 188            | 269           | PRO                  | D      |
| 189            | 270           | GLU                  | D      |
| 190            | 272           | GLY                  | D      |
| 191            | 273           | LEU                  | B      |
| 192            | 274           | LEU                  | B      |
| 193            | 275           | GLU                  | B      |
| 194            | 276           | GLY                  | B      |
| 195            | 277           | LEU                  | B      |
| 196            | 278           | ASP                  | B      |
| 197            | 279           | ALA                  | B      |
| 198            | 280           | VAL                  | D      |
| 199            | 281           | VAL                  | D      |
| 200            | 282           | PHE                  | D      |
| 201            | 283           | VAL                  | A      |
| 202            | 284           | ASP                  | D      |
| 203            | 285           | ASN                  | D      |
| 204            | 286           | HIS                  | D      |
| 205            | 287           | ASP                  | D      |
| 206            | 288           | ASN                  | D      |
| 207            | 289           | GLN                  | D      |
| 208            | 298           | THR                  | D      |
| 209            | 299           | TYR                  | D      |
| 210            | 300           | LYS                  | D      |
| 211            | 301           | ASN                  | D      |
| 212            | 303           | LYS                  | A      |
| 213            | 304           | PRO                  | A      |
| 214            | 305           | TYR                  | A      |
| 215            | 306           | LYS                  | A      |
| 216            | 307           | MET                  | A      |
| 217            | 308           | ALA                  | A      |
| 218            | 309           | ILE                  | A      |
| 219            | 310           | ALA                  | A      |
| 220            | 311           | PHE                  | A      |
| 221            | 312           | MET                  | A      |
| 222            | 313           | LEU                  | A      |
| 223            | 314           | ALA                  | A      |
| 224            | 315           | HIS                  | A      |
| 225            | 317           | TYR                  | D      |
| 226            | 318           | GLY                  | D      |
| 227            | 319           | THR                  | D      |

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Table S22 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 320           | THR                  | A      |
| 229            | 321           | ARG                  | D      |
| 230            | 322           | ILE                  | A      |
| 231            | 323           | MET                  | D      |
| 232            | 324           | SER                  | C      |
| 233            | 325           | SER                  | D      |
| 234            | 326           | PHE                  | A      |
| 235            | 327           | ASP                  | C      |
| 236            | 357           | GLY                  | C      |
| 237            | 358           | TYR                  | D      |
| 238            | 359           | VAL                  | D      |
| 239            | 360           | CYS                  | D      |
| 240            | 363           | ARG                  | A      |
| 241            | 364           | TRP                  | A      |
| 242            | 365           | ARG                  | A      |
| 243            | 366           | GLN                  | A      |
| 244            | 367           | VAL                  | A      |
| 245            | 368           | TYR                  | A      |
| 246            | 369           | GLY                  | A      |
| 247            | 370           | MET                  | A      |
| 248            | 371           | VAL                  | A      |
| 249            | 372           | GLY                  | A      |
| 250            | 373           | PHE                  | A      |
| 251            | 374           | ARG                  | A      |
| 252            | 375           | ASN                  | A      |
| 253            | 376           | ALA                  | A      |
| 254            | 377           | VAL                  | A      |
| 255            | 378           | GLU                  | A      |
| 256            | 379           | GLY                  | A      |
| 257            | 380           | THR                  | A      |
| 258            | 381           | GLN                  | A      |
| 259            | 382           | VAL                  | A      |
| 260            | 384           | ASN                  | A      |
| 261            | 385           | TRP                  | A      |
| 262            | 386           | TRP                  | A      |
| 263            | 387           | SER                  | A      |
| 264            | 389           | ASP                  | A      |
| 265            | 390           | ASP                  | A      |
| 266            | 391           | ASN                  | A      |
| 267            | 392           | GLN                  | A      |
| 268            | 393           | ILE                  | A      |
| 269            | 394           | ALA                  | A      |
| 270            | 395           | PHE                  | A      |
| 271            | 396           | SER                  | A      |
| 272            | 397           | ARG                  | A      |
| 273            | 398           | GLY                  | A      |

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Table S22 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 399           | SER                  | A      |
| 275            | 401           | GLY                  | A      |
| 276            | 402           | PHE                  | A      |
| 277            | 403           | VAL                  | A      |
| 278            | 404           | ALA                  | A      |
| 279            | 405           | PHE                  | A      |
| 280            | 406           | THR                  | A      |
| 281            | 408           | GLY                  | A      |
| 282            | 409           | GLY                  | A      |
| 283            | 410           | ASP                  | A      |
| 284            | 411           | LEU                  | A      |
| 285            | 412           | ASN                  | A      |
| 286            | 413           | GLN                  | A      |
| 287            | 414           | ASN                  | A      |
| 288            | 420           | PRO                  | A      |
| 289            | 421           | ALA                  | A      |
| 290            | 424           | TYR                  | A      |
| 291            | 425           | CYS                  | A      |
| 292            | 426           | ASP                  | A      |
| 293            | 427           | VAL                  | A      |
| 294            | 454           | LEU                  | A      |
| 295            | 455           | GLY                  | A      |
| 296            | 456           | SER                  | A      |
| 297            | 461           | GLY                  | A      |
| 298            | 462           | VAL                  | A      |
| 299            | 463           | LEU                  | A      |
| 300            | 464           | ALA                  | A      |
| 301            | 465           | ILE                  | A      |
| 302            | 466           | HIS                  | A      |

Table S23: Residues membership for the *N. polysaccharea*  $\alpha$ -amylase (PDB code 1S46, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 98            | GLN                  | A      |
| 1              | 99            | VAL                  | A      |
| 2              | 100           | GLY                  | B      |
| 3              | 101           | GLY                  | B      |
| 4              | 102           | VAL                  | B      |
| 5              | 103           | CYS                  | C      |
| 6              | 104           | TYR                  | C      |
| 7              | 105           | VAL                  | C      |
| 8              | 110           | GLY                  | C      |

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Table S23 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 111           | ASP                  | C      |
| 10             | 112           | LEU                  | C      |
| 11             | 113           | LYS                  | C      |
| 12             | 114           | GLY                  | C      |
| 13             | 115           | LEU                  | C      |
| 14             | 116           | LYS                  | C      |
| 15             | 117           | ASP                  | C      |
| 16             | 118           | LYS                  | C      |
| 17             | 119           | ILE                  | C      |
| 18             | 120           | PRO                  | C      |
| 19             | 121           | TYR                  | C      |
| 20             | 122           | PHE                  | C      |
| 21             | 123           | GLN                  | C      |
| 22             | 124           | GLU                  | C      |
| 23             | 125           | LEU                  | C      |
| 24             | 126           | GLY                  | C      |
| 25             | 127           | LEU                  | C      |
| 26             | 128           | THR                  | C      |
| 27             | 129           | TYR                  | C      |
| 28             | 130           | LEU                  | C      |
| 29             | 131           | TYR                  | C      |
| 30             | 132           | LEU                  | C      |
| 31             | 133           | MET                  | C      |
| 32             | 134           | PRO                  | C      |
| 33             | 135           | LEU                  | C      |
| 34             | 136           | PHE                  | C      |
| 35             | 137           | LYS                  | C      |
| 36             | 138           | CYS                  | C      |
| 37             | 139           | PRO                  | C      |
| 38             | 141           | GLY                  | C      |
| 39             | 144           | ASP                  | C      |
| 40             | 145           | GLY                  | C      |
| 41             | 146           | GLY                  | C      |
| 42             | 147           | TYR                  | C      |
| 43             | 148           | ALA                  | C      |
| 44             | 149           | VAL                  | C      |
| 45             | 150           | SER                  | C      |
| 46             | 151           | SER                  | C      |
| 47             | 153           | ARG                  | C      |
| 48             | 154           | ASP                  | C      |
| 49             | 155           | VAL                  | C      |
| 50             | 156           | ASN                  | C      |
| 51             | 157           | PRO                  | C      |
| 52             | 158           | ALA                  | C      |
| 53             | 159           | LEU                  | C      |
| 54             | 160           | GLY                  | C      |

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Table S23 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 161           | THR                  | C      |
| 56             | 162           | ILE                  | C      |
| 57             | 163           | GLY                  | C      |
| 58             | 164           | ASP                  | C      |
| 59             | 165           | LEU                  | C      |
| 60             | 166           | ARG                  | C      |
| 61             | 167           | GLU                  | C      |
| 62             | 168           | VAL                  | C      |
| 63             | 169           | ILE                  | C      |
| 64             | 170           | ALA                  | C      |
| 65             | 171           | ALA                  | C      |
| 66             | 172           | LEU                  | C      |
| 67             | 173           | HIS                  | C      |
| 68             | 174           | GLU                  | C      |
| 69             | 175           | ALA                  | C      |
| 70             | 176           | GLY                  | C      |
| 71             | 177           | ILE                  | C      |
| 72             | 178           | SER                  | C      |
| 73             | 179           | ALA                  | C      |
| 74             | 180           | VAL                  | C      |
| 75             | 181           | VAL                  | C      |
| 76             | 182           | ASP                  | C      |
| 77             | 183           | PHE                  | C      |
| 78             | 184           | ILE                  | C      |
| 79             | 185           | PHE                  | C      |
| 80             | 186           | ASN                  | C      |
| 81             | 187           | HIS                  | C      |
| 82             | 188           | THR                  | C      |
| 83             | 189           | SER                  | C      |
| 84             | 190           | ASN                  | C      |
| 85             | 191           | GLU                  | C      |
| 86             | 192           | HIS                  | C      |
| 87             | 193           | GLU                  | C      |
| 88             | 194           | TRP                  | C      |
| 89             | 195           | ALA                  | C      |
| 90             | 206           | ASP                  | C      |
| 91             | 207           | ASN                  | C      |
| 92             | 208           | PHE                  | C      |
| 93             | 209           | TYR                  | C      |
| 94             | 210           | TYR                  | B      |
| 95             | 247           | TRP                  | B      |
| 96             | 248           | THR                  | B      |
| 97             | 249           | THR                  | B      |
| 98             | 250           | PHE                  | B      |
| 99             | 254           | GLN                  | B      |
| 100            | 255           | TRP                  | B      |

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Table S23 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 256           | ASP                  | B      |
| 102            | 257           | LEU                  | B      |
| 103            | 258           | ASN                  | B      |
| 104            | 259           | TYR                  | B      |
| 105            | 260           | SER                  | B      |
| 106            | 261           | ASN                  | B      |
| 107            | 262           | PRO                  | B      |
| 108            | 263           | TRP                  | B      |
| 109            | 264           | VAL                  | B      |
| 110            | 265           | PHE                  | B      |
| 111            | 266           | ARG                  | B      |
| 112            | 267           | ALA                  | B      |
| 113            | 268           | MET                  | B      |
| 114            | 269           | ALA                  | B      |
| 115            | 270           | GLY                  | B      |
| 116            | 271           | GLU                  | B      |
| 117            | 272           | MET                  | B      |
| 118            | 273           | LEU                  | B      |
| 119            | 274           | PHE                  | B      |
| 120            | 275           | LEU                  | B      |
| 121            | 276           | ALA                  | B      |
| 122            | 277           | ASN                  | B      |
| 123            | 278           | LEU                  | C      |
| 124            | 279           | GLY                  | C      |
| 125            | 280           | VAL                  | C      |
| 126            | 281           | ASP                  | C      |
| 127            | 282           | ILE                  | C      |
| 128            | 283           | LEU                  | B      |
| 129            | 284           | ARG                  | D      |
| 130            | 285           | MET                  | B      |
| 131            | 286           | ASP                  | B      |
| 132            | 287           | ALA                  | B      |
| 133            | 288           | VAL                  | B      |
| 134            | 289           | ALA                  | B      |
| 135            | 290           | PHE                  | B      |
| 136            | 291           | ILE                  | B      |
| 137            | 292           | TRP                  | B      |
| 138            | 306           | HIS                  | B      |
| 139            | 307           | ALA                  | B      |
| 140            | 308           | LEU                  | B      |
| 141            | 309           | ILE                  | B      |
| 142            | 310           | ARG                  | B      |
| 143            | 311           | ALA                  | B      |
| 144            | 312           | PHE                  | B      |
| 145            | 313           | ASN                  | B      |
| 146            | 314           | ALA                  | B      |

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Table S23 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 315           | VAL                  | B      |
| 148            | 316           | MET                  | B      |
| 149            | 317           | ARG                  | B      |
| 150            | 323           | VAL                  | B      |
| 151            | 324           | PHE                  | B      |
| 152            | 325           | PHE                  | B      |
| 153            | 326           | LYS                  | C      |
| 154            | 327           | SER                  | B      |
| 155            | 328           | GLN                  | B      |
| 156            | 329           | ALA                  | B      |
| 157            | 330           | ILE                  | B      |
| 158            | 331           | VAL                  | B      |
| 159            | 332           | HIS                  | B      |
| 160            | 336           | VAL                  | B      |
| 161            | 337           | VAL                  | B      |
| 162            | 338           | GLN                  | B      |
| 163            | 339           | TYR                  | B      |
| 164            | 340           | ILE                  | B      |
| 165            | 341           | GLY                  | B      |
| 166            | 345           | CYS                  | B      |
| 167            | 346           | GLN                  | B      |
| 168            | 347           | ILE                  | B      |
| 169            | 348           | GLY                  | B      |
| 170            | 349           | TYR                  | D      |
| 171            | 350           | ASN                  | D      |
| 172            | 351           | PRO                  | D      |
| 173            | 352           | LEU                  | D      |
| 174            | 354           | MET                  | D      |
| 175            | 355           | ALA                  | D      |
| 176            | 356           | LEU                  | D      |
| 177            | 357           | LEU                  | D      |
| 178            | 358           | TRP                  | D      |
| 179            | 359           | ASN                  | D      |
| 180            | 360           | THR                  | D      |
| 181            | 361           | LEU                  | D      |
| 182            | 364           | ARG                  | D      |
| 183            | 365           | GLU                  | A      |
| 184            | 366           | VAL                  | A      |
| 185            | 367           | ASN                  | A      |
| 186            | 372           | ALA                  | A      |
| 187            | 373           | LEU                  | D      |
| 188            | 374           | THR                  | D      |
| 189            | 375           | TYR                  | D      |
| 190            | 376           | ARG                  | D      |
| 191            | 377           | HIS                  | B      |
| 192            | 378           | ASN                  | B      |

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Table S23 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 381           | GLU                  | B      |
| 194            | 382           | HIS                  | B      |
| 195            | 383           | THR                  | B      |
| 196            | 384           | ALA                  | B      |
| 197            | 385           | TRP                  | B      |
| 198            | 386           | VAL                  | D      |
| 199            | 387           | ASN                  | D      |
| 200            | 388           | TYR                  | D      |
| 201            | 389           | VAL                  | A      |
| 202            | 390           | ARG                  | D      |
| 203            | 391           | SER                  | D      |
| 204            | 392           | HIS                  | D      |
| 205            | 393           | ASP                  | D      |
| 206            | 394           | ASP                  | D      |
| 207            | 448           | SER                  | D      |
| 208            | 450           | THR                  | D      |
| 209            | 451           | ALA                  | D      |
| 210            | 452           | ALA                  | D      |
| 211            | 453           | ALA                  | D      |
| 212            | 464           | ALA                  | A      |
| 213            | 467           | ARG                  | A      |
| 214            | 468           | ILE                  | A      |
| 215            | 469           | LYS                  | A      |
| 216            | 470           | LEU                  | A      |
| 217            | 471           | LEU                  | A      |
| 218            | 472           | TYR                  | A      |
| 219            | 473           | SER                  | A      |
| 220            | 474           | ILE                  | A      |
| 221            | 475           | ALA                  | A      |
| 222            | 476           | LEU                  | A      |
| 223            | 477           | SER                  | A      |
| 224            | 478           | THR                  | A      |
| 225            | 479           | GLY                  | D      |
| 226            | 480           | GLY                  | D      |
| 227            | 481           | LEU                  | D      |
| 228            | 482           | PRO                  | A      |
| 229            | 483           | LEU                  | D      |
| 230            | 484           | ILE                  | A      |
| 231            | 485           | TYR                  | D      |
| 232            | 486           | LEU                  | C      |
| 233            | 487           | GLY                  | D      |
| 234            | 488           | ASP                  | A      |
| 235            | 514           | PRO                  | C      |
| 236            | 515           | ARG                  | C      |
| 237            | 516           | TYR                  | D      |
| 238            | 517           | ASN                  | D      |

*Continued on next page*

Table S23 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 521           | TYR                  | D      |
| 240            | 534           | ILE                  | A      |
| 241            | 535           | TYR                  | A      |
| 242            | 536           | GLN                  | A      |
| 243            | 537           | GLY                  | A      |
| 244            | 538           | LEU                  | A      |
| 245            | 539           | ARG                  | A      |
| 246            | 540           | HIS                  | A      |
| 247            | 541           | MET                  | A      |
| 248            | 542           | ILE                  | A      |
| 249            | 543           | ALA                  | A      |
| 250            | 544           | VAL                  | A      |
| 251            | 545           | ARG                  | A      |
| 252            | 546           | GLN                  | A      |
| 253            | 547           | SER                  | A      |
| 254            | 548           | ASN                  | A      |
| 255            | 549           | PRO                  | A      |
| 256            | 553           | GLY                  | A      |
| 257            | 554           | GLY                  | A      |
| 258            | 555           | ARG                  | A      |
| 259            | 556           | LEU                  | A      |
| 260            | 558           | THR                  | A      |
| 261            | 559           | PHE                  | A      |
| 262            | 560           | ASN                  | A      |
| 263            | 561           | THR                  | A      |
| 264            | 563           | ASN                  | A      |
| 265            | 564           | LYS                  | A      |
| 266            | 565           | HIS                  | A      |
| 267            | 566           | ILE                  | A      |
| 268            | 567           | ILE                  | A      |
| 269            | 568           | GLY                  | A      |
| 270            | 569           | TYR                  | A      |
| 271            | 570           | ILE                  | A      |
| 272            | 571           | ARG                  | A      |
| 273            | 573           | ASN                  | A      |
| 274            | 574           | ALA                  | A      |
| 275            | 575           | LEU                  | A      |
| 276            | 576           | LEU                  | A      |
| 277            | 577           | ALA                  | A      |
| 278            | 578           | PHE                  | A      |
| 279            | 579           | GLY                  | A      |
| 280            | 580           | ASN                  | A      |
| 281            | 584           | TYR                  | A      |
| 282            | 585           | PRO                  | A      |
| 283            | 586           | GLN                  | A      |
| 284            | 587           | THR                  | A      |

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Table S23 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 588           | VAL                  | A      |
| 286            | 589           | THR                  | A      |
| 287            | 590           | ALA                  | A      |
| 288            | 599           | LYS                  | A      |
| 289            | 600           | ALA                  | A      |
| 290            | 601           | HIS                  | A      |
| 291            | 602           | ASP                  | A      |
| 292            | 603           | LEU                  | A      |
| 293            | 604           | ILE                  | A      |
| 294            | 617           | LEU                  | A      |
| 295            | 618           | GLN                  | A      |
| 296            | 619           | PRO                  | A      |
| 297            | 621           | GLN                  | A      |
| 298            | 622           | VAL                  | A      |
| 299            | 623           | MET                  | A      |
| 300            | 624           | TRP                  | A      |
| 301            | 625           | LEU                  | A      |
| 302            | 626           | GLU                  | A      |

Table S24: Residues membership for the *T. molitor*  $\alpha$ -amylase (PDB code 1TMQ, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | ASN                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | LYS                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | ASN                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | ASP                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |

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Table S24 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLN                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | GLN                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | ILE                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | TYR                  | C      |
| 37             | 49            | LEU                  | C      |
| 38             | 51            | ALA                  | C      |
| 39             | 57            | TRP                  | C      |
| 40             | 58            | GLU                  | C      |
| 41             | 59            | ARG                  | C      |
| 42             | 60            | TYR                  | C      |
| 43             | 61            | GLN                  | C      |
| 44             | 62            | PRO                  | C      |
| 45             | 63            | VAL                  | C      |
| 46             | 64            | SER                  | C      |
| 47             | 65            | TYR                  | C      |
| 48             | 66            | ILE                  | C      |
| 49             | 67            | ILE                  | C      |
| 50             | 68            | ASN                  | C      |
| 51             | 69            | THR                  | C      |
| 52             | 70            | ARG                  | C      |
| 53             | 71            | SER                  | C      |
| 54             | 72            | GLY                  | C      |
| 55             | 73            | ASP                  | C      |
| 56             | 74            | GLU                  | C      |
| 57             | 75            | SER                  | C      |
| 58             | 76            | ALA                  | C      |
| 59             | 77            | PHE                  | C      |
| 60             | 78            | THR                  | C      |
| 61             | 79            | ASP                  | C      |
| 62             | 80            | MET                  | C      |
| 63             | 81            | THR                  | C      |
| 64             | 82            | ARG                  | C      |
| 65             | 83            | ARG                  | C      |

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Table S24 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 84            | CYS                  | C      |
| 67             | 85            | ASN                  | C      |
| 68             | 86            | ASP                  | C      |
| 69             | 87            | ALA                  | C      |
| 70             | 88            | GLY                  | C      |
| 71             | 89            | VAL                  | C      |
| 72             | 90            | ARG                  | C      |
| 73             | 91            | ILE                  | C      |
| 74             | 92            | TYR                  | C      |
| 75             | 93            | VAL                  | C      |
| 76             | 94            | ASP                  | C      |
| 77             | 95            | ALA                  | C      |
| 78             | 96            | VAL                  | C      |
| 79             | 97            | ILE                  | C      |
| 80             | 98            | ASN                  | C      |
| 81             | 99            | HIS                  | C      |
| 82             | 100           | MET                  | C      |
| 83             | 101           | THR                  | C      |
| 84             | 102           | GLY                  | C      |
| 85             | 103           | MET                  | C      |
| 86             | 120           | TYR                  | C      |
| 87             | 124           | PRO                  | C      |
| 88             | 125           | TYR                  | C      |
| 89             | 126           | GLY                  | C      |
| 90             | 127           | SER                  | C      |
| 91             | 128           | GLY                  | C      |
| 92             | 129           | ASP                  | C      |
| 93             | 130           | PHE                  | C      |
| 94             | 131           | HIS                  | B      |
| 95             | 148           | CYS                  | B      |
| 96             | 149           | GLU                  | B      |
| 97             | 150           | LEU                  | B      |
| 98             | 151           | VAL                  | B      |
| 99             | 153           | LEU                  | B      |
| 100            | 154           | ARG                  | B      |
| 101            | 155           | ASP                  | B      |
| 102            | 156           | LEU                  | B      |
| 103            | 157           | ASN                  | B      |
| 104            | 158           | GLN                  | B      |
| 105            | 159           | GLY                  | B      |
| 106            | 160           | SER                  | B      |
| 107            | 161           | ASP                  | B      |
| 108            | 162           | TYR                  | B      |
| 109            | 163           | VAL                  | B      |
| 110            | 164           | ARG                  | B      |
| 111            | 165           | GLY                  | B      |

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Table S24 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 166           | VAL                  | B      |
| 113            | 167           | LEU                  | B      |
| 114            | 168           | ILE                  | B      |
| 115            | 169           | ASP                  | B      |
| 116            | 170           | TYR                  | B      |
| 117            | 171           | MET                  | B      |
| 118            | 172           | ASN                  | B      |
| 119            | 173           | HIS                  | B      |
| 120            | 174           | MET                  | B      |
| 121            | 175           | ILE                  | B      |
| 122            | 176           | ASP                  | B      |
| 123            | 177           | LEU                  | C      |
| 124            | 178           | GLY                  | C      |
| 125            | 179           | VAL                  | C      |
| 126            | 180           | ALA                  | C      |
| 127            | 181           | GLY                  | C      |
| 128            | 182           | PHE                  | B      |
| 129            | 183           | ARG                  | D      |
| 130            | 184           | VAL                  | B      |
| 131            | 185           | ASP                  | B      |
| 132            | 186           | ALA                  | B      |
| 133            | 187           | ALA                  | B      |
| 134            | 188           | LYS                  | B      |
| 135            | 189           | HIS                  | B      |
| 136            | 190           | MET                  | B      |
| 137            | 191           | SER                  | B      |
| 138            | 192           | PRO                  | B      |
| 139            | 193           | GLY                  | B      |
| 140            | 194           | ASP                  | B      |
| 141            | 195           | LEU                  | B      |
| 142            | 196           | SER                  | B      |
| 143            | 197           | VAL                  | B      |
| 144            | 198           | ILE                  | B      |
| 145            | 199           | PHE                  | B      |
| 146            | 200           | SER                  | B      |
| 147            | 201           | GLY                  | B      |
| 148            | 202           | LEU                  | B      |
| 149            | 203           | LYS                  | B      |
| 150            | 217           | PRO                  | B      |
| 151            | 218           | PHE                  | B      |
| 152            | 219           | ILE                  | B      |
| 153            | 220           | TYR                  | C      |
| 154            | 221           | GLN                  | B      |
| 155            | 222           | GLU                  | B      |
| 156            | 223           | VAL                  | B      |
| 157            | 224           | ILE                  | B      |

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Table S24 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 225           | ASP                  | B      |
| 159            | 226           | LEU                  | B      |
| 160            | 233           | LYS                  | B      |
| 161            | 234           | ASN                  | B      |
| 162            | 235           | GLU                  | B      |
| 163            | 236           | TYR                  | B      |
| 164            | 237           | THR                  | B      |
| 165            | 238           | GLY                  | B      |
| 166            | 239           | PHE                  | B      |
| 167            | 240           | GLY                  | B      |
| 168            | 241           | CYS                  | B      |
| 169            | 242           | VAL                  | B      |
| 170            | 243           | LEU                  | D      |
| 171            | 244           | GLU                  | D      |
| 172            | 245           | PHE                  | D      |
| 173            | 246           | GLN                  | D      |
| 174            | 248           | GLY                  | D      |
| 175            | 249           | VAL                  | D      |
| 176            | 250           | SER                  | D      |
| 177            | 251           | LEU                  | D      |
| 178            | 252           | GLY                  | D      |
| 179            | 253           | ASN                  | D      |
| 180            | 254           | ALA                  | D      |
| 181            | 255           | PHE                  | D      |
| 182            | 259           | ASN                  | D      |
| 183            | 260           | GLN                  | A      |
| 184            | 261           | LEU                  | A      |
| 185            | 262           | LYS                  | A      |
| 186            | 267           | TRP                  | A      |
| 187            | 268           | GLY                  | D      |
| 188            | 269           | PRO                  | D      |
| 189            | 270           | GLU                  | D      |
| 190            | 272           | GLY                  | D      |
| 191            | 273           | LEU                  | B      |
| 192            | 274           | LEU                  | B      |
| 193            | 275           | GLU                  | B      |
| 194            | 276           | GLY                  | B      |
| 195            | 277           | LEU                  | B      |
| 196            | 278           | ASP                  | B      |
| 197            | 279           | ALA                  | B      |
| 198            | 280           | VAL                  | D      |
| 199            | 281           | VAL                  | D      |
| 200            | 282           | PHE                  | D      |
| 201            | 283           | VAL                  | A      |
| 202            | 284           | ASP                  | D      |
| 203            | 285           | ASN                  | D      |

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Table S24 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 286           | HIS                  | D      |
| 205            | 287           | ASP                  | D      |
| 206            | 288           | ASN                  | D      |
| 207            | 289           | GLN                  | D      |
| 208            | 298           | THR                  | D      |
| 209            | 299           | TYR                  | D      |
| 210            | 300           | LYS                  | D      |
| 211            | 301           | ASN                  | D      |
| 212            | 303           | LYS                  | A      |
| 213            | 304           | PRO                  | A      |
| 214            | 305           | TYR                  | A      |
| 215            | 306           | LYS                  | A      |
| 216            | 307           | MET                  | A      |
| 217            | 308           | ALA                  | A      |
| 218            | 309           | ILE                  | A      |
| 219            | 310           | ALA                  | A      |
| 220            | 311           | PHE                  | A      |
| 221            | 312           | MET                  | A      |
| 222            | 313           | LEU                  | A      |
| 223            | 314           | ALA                  | A      |
| 224            | 315           | HIS                  | A      |
| 225            | 317           | TYR                  | D      |
| 226            | 318           | GLY                  | D      |
| 227            | 319           | THR                  | D      |
| 228            | 320           | THR                  | A      |
| 229            | 321           | ARG                  | D      |
| 230            | 322           | ILE                  | A      |
| 231            | 323           | MET                  | D      |
| 232            | 324           | SER                  | C      |
| 233            | 325           | SER                  | D      |
| 234            | 326           | PHE                  | A      |
| 235            | 327           | ASP                  | C      |
| 236            | 357           | GLY                  | C      |
| 237            | 358           | TYR                  | D      |
| 238            | 359           | VAL                  | D      |
| 239            | 360           | CYS                  | D      |
| 240            | 363           | ARG                  | A      |
| 241            | 364           | TRP                  | A      |
| 242            | 365           | ARG                  | A      |
| 243            | 366           | GLN                  | A      |
| 244            | 367           | VAL                  | A      |
| 245            | 368           | TYR                  | A      |
| 246            | 369           | GLY                  | A      |
| 247            | 370           | MET                  | A      |
| 248            | 371           | VAL                  | A      |
| 249            | 372           | GLY                  | A      |

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Table S24 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 373           | PHE                  | A      |
| 251            | 374           | ARG                  | A      |
| 252            | 375           | ASN                  | A      |
| 253            | 376           | ALA                  | A      |
| 254            | 377           | VAL                  | A      |
| 255            | 378           | GLU                  | A      |
| 256            | 379           | GLY                  | A      |
| 257            | 380           | THR                  | A      |
| 258            | 381           | GLN                  | A      |
| 259            | 382           | VAL                  | A      |
| 260            | 384           | ASN                  | A      |
| 261            | 385           | TRP                  | A      |
| 262            | 386           | TRP                  | A      |
| 263            | 387           | SER                  | A      |
| 264            | 389           | ASP                  | A      |
| 265            | 390           | ASP                  | A      |
| 266            | 391           | ASN                  | A      |
| 267            | 392           | GLN                  | A      |
| 268            | 393           | ILE                  | A      |
| 269            | 394           | ALA                  | A      |
| 270            | 395           | PHE                  | A      |
| 271            | 396           | SER                  | A      |
| 272            | 397           | ARG                  | A      |
| 273            | 398           | GLY                  | A      |
| 274            | 399           | SER                  | A      |
| 275            | 401           | GLY                  | A      |
| 276            | 402           | PHE                  | A      |
| 277            | 403           | VAL                  | A      |
| 278            | 404           | ALA                  | A      |
| 279            | 405           | PHE                  | A      |
| 280            | 406           | THR                  | A      |
| 281            | 408           | GLY                  | A      |
| 282            | 409           | GLY                  | A      |
| 283            | 410           | ASP                  | A      |
| 284            | 411           | LEU                  | A      |
| 285            | 412           | ASN                  | A      |
| 286            | 413           | GLN                  | A      |
| 287            | 414           | ASN                  | A      |
| 288            | 420           | PRO                  | A      |
| 289            | 421           | ALA                  | A      |
| 290            | 424           | TYR                  | A      |
| 291            | 425           | CYS                  | A      |
| 292            | 426           | ASP                  | A      |
| 293            | 427           | VAL                  | A      |
| 294            | 454           | LEU                  | A      |
| 295            | 455           | GLY                  | A      |

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Table S24 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 456           | SER                  | A      |
| 297            | 461           | GLY                  | A      |
| 298            | 462           | VAL                  | A      |
| 299            | 463           | LEU                  | A      |
| 300            | 464           | ALA                  | A      |
| 301            | 465           | ILE                  | A      |
| 302            | 466           | HIS                  | A      |

Table S25: Residues membership for the *T. vulgaris* R47  $\alpha$ -amylase (PDB code 1VB9, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |
| 30             | 192           | PHE                  | C      |

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Table S25 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |
| 76             | 239           | ASP                  | C      |

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Table S25 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |
| 122            | 316           | GLU                  | B      |

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Table S25 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASN                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |
| 168            | 370           | SER                  | B      |

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Table S25 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASP                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |
| 214            | 436           | PHE                  | A      |

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Table S25 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |
| 260            | 507           | SER                  | A      |

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Table S25 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 573           | LEU                  | A      |
| 295            | 574           | ARG                  | A      |
| 296            | 575           | PRO                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S26: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 1U33, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |

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Table S26 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |

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Table S26 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |

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Table S26 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |

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Table S26 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |

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Table S26 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |

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Table S26 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S27: Residues membership for the *T. thermosulfurigenes* EM1  $\alpha$ -amylase (PDB code 1A47, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | VAL                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |

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Table S27 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 96            | THR                  | C      |
| 39             | 98            | TYR                  | C      |
| 40             | 99            | HIS                  | C      |
| 41             | 100           | GLY                  | C      |
| 42             | 101           | TYR                  | C      |
| 43             | 102           | TRP                  | C      |
| 44             | 103           | ALA                  | C      |
| 45             | 104           | ARG                  | C      |
| 46             | 105           | ASP                  | C      |
| 47             | 107           | LYS                  | C      |
| 48             | 108           | ARG                  | C      |
| 49             | 109           | THR                  | C      |
| 50             | 110           | ASN                  | C      |
| 51             | 111           | PRO                  | C      |
| 52             | 112           | TYR                  | C      |
| 53             | 113           | PHE                  | C      |
| 54             | 114           | GLY                  | C      |

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Table S27 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 115           | SER                  | C      |
| 56             | 116           | PHE                  | C      |
| 57             | 117           | THR                  | C      |
| 58             | 118           | ASP                  | C      |
| 59             | 119           | PHE                  | C      |
| 60             | 120           | GLN                  | C      |
| 61             | 121           | ASN                  | C      |
| 62             | 122           | LEU                  | C      |
| 63             | 123           | ILE                  | C      |
| 64             | 124           | ASN                  | C      |
| 65             | 125           | THR                  | C      |
| 66             | 126           | ALA                  | C      |
| 67             | 127           | HIS                  | C      |
| 68             | 128           | ALA                  | C      |
| 69             | 129           | HIS                  | C      |
| 70             | 130           | ASN                  | C      |
| 71             | 131           | ILE                  | C      |
| 72             | 132           | LYS                  | C      |
| 73             | 133           | VAL                  | C      |
| 74             | 134           | ILE                  | C      |
| 75             | 135           | ILE                  | C      |
| 76             | 136           | ASP                  | C      |
| 77             | 137           | PHE                  | C      |
| 78             | 138           | ALA                  | C      |
| 79             | 139           | PRO                  | C      |
| 80             | 140           | ASN                  | C      |
| 81             | 141           | HIS                  | C      |
| 82             | 142           | THR                  | C      |
| 83             | 143           | SER                  | C      |
| 84             | 144           | PRO                  | C      |
| 85             | 145           | ALA                  | C      |
| 86             | 157           | ARG                  | C      |
| 87             | 164           | LEU                  | C      |
| 88             | 165           | LEU                  | C      |
| 89             | 166           | GLY                  | C      |
| 90             | 173           | ASN                  | C      |
| 91             | 174           | GLY                  | C      |
| 92             | 175           | TYR                  | C      |
| 93             | 176           | PHE                  | C      |
| 94             | 177           | HIS                  | B      |
| 95             | 193           | ARG                  | B      |
| 96             | 194           | ASN                  | B      |
| 97             | 195           | LEU                  | B      |
| 98             | 196           | PHE                  | B      |
| 99             | 198           | LEU                  | B      |
| 100            | 199           | ALA                  | B      |

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Table S27 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 200           | ASP                  | B      |
| 102            | 201           | LEU                  | B      |
| 103            | 202           | ASN                  | B      |
| 104            | 203           | GLN                  | B      |
| 105            | 204           | GLN                  | B      |
| 106            | 205           | ASN                  | B      |
| 107            | 206           | SER                  | B      |
| 108            | 207           | THR                  | B      |
| 109            | 208           | ILE                  | B      |
| 110            | 209           | ASP                  | B      |
| 111            | 210           | SER                  | B      |
| 112            | 211           | TYR                  | B      |
| 113            | 212           | LEU                  | B      |
| 114            | 213           | LYS                  | B      |
| 115            | 214           | SER                  | B      |
| 116            | 215           | ALA                  | B      |
| 117            | 216           | ILE                  | B      |
| 118            | 217           | LYS                  | B      |
| 119            | 218           | VAL                  | B      |
| 120            | 219           | TRP                  | B      |
| 121            | 220           | LEU                  | B      |
| 122            | 221           | ASP                  | B      |
| 123            | 222           | MET                  | C      |
| 124            | 223           | GLY                  | C      |
| 125            | 224           | ILE                  | C      |
| 126            | 225           | ASP                  | C      |
| 127            | 226           | GLY                  | C      |
| 128            | 227           | ILE                  | B      |
| 129            | 228           | ARG                  | D      |
| 130            | 229           | LEU                  | B      |
| 131            | 230           | ASP                  | B      |
| 132            | 231           | ALA                  | B      |
| 133            | 232           | VAL                  | B      |
| 134            | 233           | LYS                  | B      |
| 135            | 234           | HIS                  | B      |
| 136            | 235           | MET                  | B      |
| 137            | 236           | PRO                  | B      |
| 138            | 237           | PHE                  | B      |
| 139            | 238           | GLY                  | B      |
| 140            | 239           | TRP                  | B      |
| 141            | 240           | GLN                  | B      |
| 142            | 241           | LYS                  | B      |
| 143            | 242           | ASN                  | B      |
| 144            | 243           | PHE                  | B      |
| 145            | 244           | MET                  | B      |
| 146            | 245           | ASP                  | B      |

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Table S27 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 246           | SER                  | B      |
| 148            | 247           | ILE                  | B      |
| 149            | 248           | LEU                  | B      |
| 150            | 253           | VAL                  | B      |
| 151            | 254           | PHE                  | B      |
| 152            | 255           | THR                  | B      |
| 153            | 256           | PHE                  | C      |
| 154            | 257           | GLY                  | B      |
| 155            | 258           | GLU                  | B      |
| 156            | 259           | TRP                  | B      |
| 157            | 260           | PHE                  | B      |
| 158            | 261           | LEU                  | B      |
| 159            | 262           | GLY                  | B      |
| 160            | 270           | ASN                  | B      |
| 161            | 271           | THR                  | B      |
| 162            | 272           | TYR                  | B      |
| 163            | 273           | PHE                  | B      |
| 164            | 275           | ASN                  | B      |
| 165            | 276           | GLU                  | B      |
| 166            | 278           | GLY                  | B      |
| 167            | 279           | MET                  | B      |
| 168            | 280           | SER                  | B      |
| 169            | 281           | LEU                  | B      |
| 170            | 282           | LEU                  | D      |
| 171            | 283           | ASP                  | D      |
| 172            | 284           | PHE                  | D      |
| 173            | 285           | ARG                  | D      |
| 174            | 287           | SER                  | D      |
| 175            | 288           | GLN                  | D      |
| 176            | 289           | LYS                  | D      |
| 177            | 290           | VAL                  | D      |
| 178            | 291           | ARG                  | D      |
| 179            | 292           | GLN                  | D      |
| 180            | 293           | VAL                  | D      |
| 181            | 294           | PHE                  | D      |
| 182            | 299           | ASP                  | D      |
| 183            | 300           | THR                  | A      |
| 184            | 301           | MET                  | A      |
| 185            | 302           | TYR                  | A      |
| 186            | 307           | MET                  | A      |
| 187            | 308           | ILE                  | D      |
| 188            | 309           | GLN                  | D      |
| 189            | 310           | SER                  | D      |
| 190            | 311           | THR                  | D      |
| 191            | 312           | ALA                  | B      |
| 192            | 313           | SER                  | B      |

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Table S27 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 317           | PHE                  | B      |
| 194            | 318           | ILE                  | B      |
| 195            | 319           | ASN                  | B      |
| 196            | 320           | ASP                  | B      |
| 197            | 321           | MET                  | B      |
| 198            | 322           | VAL                  | D      |
| 199            | 323           | THR                  | D      |
| 200            | 324           | PHE                  | D      |
| 201            | 325           | ILE                  | A      |
| 202            | 326           | ASP                  | D      |
| 203            | 327           | ASN                  | D      |
| 204            | 328           | HIS                  | D      |
| 205            | 329           | ASP                  | D      |
| 206            | 330           | MET                  | D      |
| 207            | 331           | ASP                  | D      |
| 208            | 332           | ARG                  | D      |
| 209            | 333           | PHE                  | D      |
| 210            | 334           | TYR                  | D      |
| 211            | 335           | ASN                  | D      |
| 212            | 339           | THR                  | A      |
| 213            | 341           | PRO                  | A      |
| 214            | 342           | VAL                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | MET                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | THR                  | D      |

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Table S27 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | LYS                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | THR                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | LEU                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | ILE                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | TYR                  | A      |

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Table S27 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 443           | ASN                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | THR                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | SER                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLU                  | A      |
| 298            | 487           | VAL                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S28: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1KCL, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |

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Table S28 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |

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Table S28 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |

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Table S28 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |

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Table S28 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |

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Table S28 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |

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Table S28 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | CYS                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |

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Table S28 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S29: Residues membership for the *P. haloplanctis*  $\alpha$ -amylase (PDB code 1AQH, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 3             | THR                  | A      |
| 1              | 4             | THR                  | A      |
| 2              | 5             | PHE                  | B      |
| 3              | 6             | VAL                  | B      |
| 4              | 7             | HIS                  | B      |
| 5              | 8             | LEU                  | C      |
| 6              | 9             | PHE                  | C      |
| 7              | 10            | GLU                  | C      |
| 8              | 11            | TRP                  | C      |
| 9              | 12            | ASN                  | C      |
| 10             | 13            | TRP                  | C      |
| 11             | 14            | GLN                  | C      |
| 12             | 15            | ASP                  | C      |
| 13             | 16            | VAL                  | C      |
| 14             | 17            | ALA                  | C      |
| 15             | 18            | GLN                  | C      |
| 16             | 19            | GLU                  | C      |
| 17             | 20            | CYS                  | C      |
| 18             | 21            | GLU                  | C      |
| 19             | 22            | GLN                  | C      |
| 20             | 24            | LEU                  | C      |
| 21             | 25            | GLY                  | C      |
| 22             | 26            | PRO                  | C      |
| 23             | 27            | LYS                  | C      |
| 24             | 28            | GLY                  | C      |
| 25             | 29            | TYR                  | C      |
| 26             | 30            | ALA                  | C      |
| 27             | 31            | ALA                  | C      |
| 28             | 32            | VAL                  | C      |
| 29             | 33            | GLN                  | C      |
| 30             | 34            | VAL                  | C      |

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Table S29 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 35            | SER                  | C      |
| 32             | 36            | PRO                  | C      |
| 33             | 37            | PRO                  | C      |
| 34             | 38            | ASN                  | C      |
| 35             | 39            | GLU                  | C      |
| 36             | 40            | HIS                  | C      |
| 37             | 41            | ILE                  | C      |
| 38             | 43            | GLY                  | C      |
| 39             | 47            | TRP                  | C      |
| 40             | 48            | THR                  | C      |
| 41             | 49            | ARG                  | C      |
| 42             | 50            | TYR                  | C      |
| 43             | 51            | GLN                  | C      |
| 44             | 52            | PRO                  | C      |
| 45             | 53            | VAL                  | C      |
| 46             | 54            | SER                  | C      |
| 47             | 55            | TYR                  | C      |
| 48             | 56            | GLU                  | C      |
| 49             | 57            | LEU                  | C      |
| 50             | 58            | GLN                  | C      |
| 51             | 59            | SER                  | C      |
| 52             | 60            | ARG                  | C      |
| 53             | 61            | GLY                  | C      |
| 54             | 62            | GLY                  | C      |
| 55             | 63            | ASN                  | C      |
| 56             | 64            | ARG                  | C      |
| 57             | 65            | ALA                  | C      |
| 58             | 66            | GLN                  | C      |
| 59             | 67            | PHE                  | C      |
| 60             | 68            | ILE                  | C      |
| 61             | 69            | ASP                  | C      |
| 62             | 70            | MET                  | C      |
| 63             | 71            | VAL                  | C      |
| 64             | 72            | ASN                  | C      |
| 65             | 73            | ARG                  | C      |
| 66             | 74            | CYS                  | C      |
| 67             | 75            | SER                  | C      |
| 68             | 76            | ALA                  | C      |
| 69             | 77            | ALA                  | C      |
| 70             | 78            | GLY                  | C      |
| 71             | 79            | VAL                  | C      |
| 72             | 80            | ASP                  | C      |
| 73             | 81            | ILE                  | C      |
| 74             | 82            | TYR                  | C      |
| 75             | 83            | VAL                  | C      |
| 76             | 84            | ASP                  | C      |

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Table S29 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 85            | THR                  | C      |
| 78             | 86            | LEU                  | C      |
| 79             | 87            | ILE                  | C      |
| 80             | 88            | ASN                  | C      |
| 81             | 89            | HIS                  | C      |
| 82             | 90            | MET                  | C      |
| 83             | 91            | ALA                  | C      |
| 84             | 92            | ALA                  | C      |
| 85             | 93            | GLY                  | C      |
| 86             | 108           | PHE                  | C      |
| 87             | 110           | ILE                  | C      |
| 88             | 111           | TYR                  | C      |
| 89             | 112           | SER                  | C      |
| 90             | 113           | PRO                  | C      |
| 91             | 114           | GLN                  | C      |
| 92             | 115           | ASP                  | C      |
| 93             | 116           | PHE                  | C      |
| 94             | 117           | HIS                  | B      |
| 95             | 137           | CYS                  | B      |
| 96             | 138           | GLU                  | B      |
| 97             | 139           | LEU                  | B      |
| 98             | 140           | VAL                  | B      |
| 99             | 142           | LEU                  | B      |
| 100            | 143           | ALA                  | B      |
| 101            | 144           | ASP                  | B      |
| 102            | 145           | LEU                  | B      |
| 103            | 146           | ASP                  | B      |
| 104            | 147           | THR                  | B      |
| 105            | 148           | ALA                  | B      |
| 106            | 149           | SER                  | B      |
| 107            | 150           | ASN                  | B      |
| 108            | 151           | TYR                  | B      |
| 109            | 152           | VAL                  | B      |
| 110            | 153           | GLN                  | B      |
| 111            | 154           | ASN                  | B      |
| 112            | 155           | THR                  | B      |
| 113            | 156           | ILE                  | B      |
| 114            | 157           | ALA                  | B      |
| 115            | 158           | ALA                  | B      |
| 116            | 159           | TYR                  | B      |
| 117            | 160           | ILE                  | B      |
| 118            | 161           | ASN                  | B      |
| 119            | 162           | ASP                  | B      |
| 120            | 163           | LEU                  | B      |
| 121            | 164           | GLN                  | B      |
| 122            | 165           | ALA                  | B      |

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Table S29 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 166           | ILE                  | C      |
| 124            | 167           | GLY                  | C      |
| 125            | 168           | VAL                  | C      |
| 126            | 169           | LYS                  | C      |
| 127            | 170           | GLY                  | C      |
| 128            | 171           | PHE                  | B      |
| 129            | 172           | ARG                  | D      |
| 130            | 173           | PHE                  | B      |
| 131            | 174           | ASP                  | B      |
| 132            | 175           | ALA                  | B      |
| 133            | 176           | SER                  | B      |
| 134            | 177           | LYS                  | B      |
| 135            | 178           | HIS                  | B      |
| 136            | 179           | VAL                  | B      |
| 137            | 180           | ALA                  | B      |
| 138            | 181           | ALA                  | B      |
| 139            | 182           | SER                  | B      |
| 140            | 183           | ASP                  | B      |
| 141            | 184           | ILE                  | B      |
| 142            | 185           | GLN                  | B      |
| 143            | 186           | SER                  | B      |
| 144            | 187           | LEU                  | B      |
| 145            | 188           | MET                  | B      |
| 146            | 189           | ALA                  | B      |
| 147            | 190           | LYS                  | B      |
| 148            | 191           | VAL                  | B      |
| 149            | 192           | ASN                  | B      |
| 150            | 195           | PRO                  | B      |
| 151            | 196           | VAL                  | B      |
| 152            | 197           | VAL                  | B      |
| 153            | 198           | PHE                  | C      |
| 154            | 199           | GLN                  | B      |
| 155            | 200           | GLU                  | B      |
| 156            | 201           | VAL                  | B      |
| 157            | 202           | ILE                  | B      |
| 158            | 203           | ASP                  | B      |
| 159            | 204           | GLN                  | B      |
| 160            | 211           | ALA                  | B      |
| 161            | 212           | SER                  | B      |
| 162            | 213           | GLU                  | B      |
| 163            | 214           | TYR                  | B      |
| 164            | 215           | LEU                  | B      |
| 165            | 216           | SER                  | B      |
| 166            | 217           | THR                  | B      |
| 167            | 218           | GLY                  | B      |
| 168            | 219           | LEU                  | B      |

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Table S29 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 220           | VAL                  | B      |
| 170            | 221           | THR                  | D      |
| 171            | 222           | GLU                  | D      |
| 172            | 223           | PHE                  | D      |
| 173            | 224           | LYS                  | D      |
| 174            | 226           | SER                  | D      |
| 175            | 227           | THR                  | D      |
| 176            | 228           | GLU                  | D      |
| 177            | 229           | LEU                  | D      |
| 178            | 230           | GLY                  | D      |
| 179            | 231           | ASN                  | D      |
| 180            | 232           | THR                  | D      |
| 181            | 233           | PHE                  | D      |
| 182            | 236           | GLY                  | D      |
| 183            | 237           | SER                  | A      |
| 184            | 238           | LEU                  | A      |
| 185            | 239           | ALA                  | A      |
| 186            | 244           | PHE                  | A      |
| 187            | 245           | GLY                  | D      |
| 188            | 246           | GLU                  | D      |
| 189            | 247           | GLY                  | D      |
| 190            | 249           | GLY                  | D      |
| 191            | 250           | PHE                  | B      |
| 192            | 251           | MET                  | B      |
| 193            | 252           | PRO                  | B      |
| 194            | 253           | SER                  | B      |
| 195            | 254           | SER                  | B      |
| 196            | 255           | SER                  | B      |
| 197            | 256           | ALA                  | B      |
| 198            | 257           | VAL                  | D      |
| 199            | 258           | VAL                  | D      |
| 200            | 259           | PHE                  | D      |
| 201            | 260           | VAL                  | A      |
| 202            | 261           | ASP                  | D      |
| 203            | 262           | ASN                  | D      |
| 204            | 263           | HIS                  | D      |
| 205            | 264           | ASP                  | D      |
| 206            | 265           | ASN                  | D      |
| 207            | 266           | GLN                  | D      |
| 208            | 277           | THR                  | D      |
| 209            | 278           | PHE                  | D      |
| 210            | 279           | GLU                  | D      |
| 211            | 280           | ASP                  | D      |
| 212            | 282           | ARG                  | A      |
| 213            | 283           | LEU                  | A      |
| 214            | 284           | TYR                  | A      |

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Table S29 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 285           | ASP                  | A      |
| 216            | 286           | LEU                  | A      |
| 217            | 287           | ALA                  | A      |
| 218            | 288           | ASN                  | A      |
| 219            | 289           | VAL                  | A      |
| 220            | 290           | PHE                  | A      |
| 221            | 291           | MET                  | A      |
| 222            | 292           | LEU                  | A      |
| 223            | 293           | ALA                  | A      |
| 224            | 294           | TYR                  | A      |
| 225            | 296           | TYR                  | D      |
| 226            | 297           | GLY                  | D      |
| 227            | 298           | TYR                  | D      |
| 228            | 299           | PRO                  | A      |
| 229            | 300           | LYS                  | D      |
| 230            | 301           | VAL                  | A      |
| 231            | 302           | MET                  | D      |
| 232            | 303           | SER                  | C      |
| 233            | 304           | SER                  | D      |
| 234            | 305           | TYR                  | A      |
| 235            | 306           | ASP                  | C      |
| 236            | 332           | ASN                  | C      |
| 237            | 333           | TRP                  | D      |
| 238            | 334           | LYS                  | D      |
| 239            | 335           | CYS                  | D      |
| 240            | 338           | ARG                  | A      |
| 241            | 339           | TRP                  | A      |
| 242            | 340           | SER                  | A      |
| 243            | 341           | TYR                  | A      |
| 244            | 342           | ILE                  | A      |
| 245            | 343           | ALA                  | A      |
| 246            | 344           | GLY                  | A      |
| 247            | 345           | GLY                  | A      |
| 248            | 346           | VAL                  | A      |
| 249            | 347           | ASP                  | A      |
| 250            | 348           | PHE                  | A      |
| 251            | 349           | ARG                  | A      |
| 252            | 350           | ASN                  | A      |
| 253            | 351           | ASN                  | A      |
| 254            | 352           | THR                  | A      |
| 255            | 353           | ALA                  | A      |
| 256            | 355           | ASN                  | A      |
| 257            | 356           | TRP                  | A      |
| 258            | 357           | ALA                  | A      |
| 259            | 358           | VAL                  | A      |
| 260            | 360           | ASN                  | A      |

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Table S29 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 361           | TRP                  | A      |
| 262            | 362           | TRP                  | A      |
| 263            | 363           | ASP                  | A      |
| 264            | 365           | THR                  | A      |
| 265            | 366           | ASN                  | A      |
| 266            | 367           | ASN                  | A      |
| 267            | 368           | GLN                  | A      |
| 268            | 369           | ILE                  | A      |
| 269            | 370           | SER                  | A      |
| 270            | 371           | PHE                  | A      |
| 271            | 372           | GLY                  | A      |
| 272            | 373           | ARG                  | A      |
| 273            | 374           | GLY                  | A      |
| 274            | 375           | SER                  | A      |
| 275            | 377           | GLY                  | A      |
| 276            | 378           | HIS                  | A      |
| 277            | 379           | MET                  | A      |
| 278            | 380           | ALA                  | A      |
| 279            | 381           | ILE                  | A      |
| 280            | 382           | ASN                  | A      |
| 281            | 385           | ASP                  | A      |
| 282            | 386           | SER                  | A      |
| 283            | 387           | THR                  | A      |
| 284            | 388           | LEU                  | A      |
| 285            | 389           | THR                  | A      |
| 286            | 390           | ALA                  | A      |
| 287            | 391           | THR                  | A      |
| 288            | 397           | ALA                  | A      |
| 289            | 398           | SER                  | A      |
| 290            | 401           | TYR                  | A      |
| 291            | 402           | CYS                  | A      |
| 292            | 403           | ASN                  | A      |
| 293            | 404           | VAL                  | A      |
| 294            | 433           | ILE                  | A      |
| 295            | 434           | GLY                  | A      |
| 296            | 435           | ALA                  | A      |
| 297            | 437           | ASP                  | A      |
| 298            | 438           | ALA                  | A      |
| 299            | 439           | MET                  | A      |
| 300            | 440           | ALA                  | A      |
| 301            | 441           | ILE                  | A      |
| 302            | 442           | HIS                  | A      |

Table S30: Residues membership for the *H. vulgare*  $\alpha$ -amylase (PDB code 1AMY, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 1             | GLN                  | A      |
| 1              | 2             | VAL                  | A      |
| 2              | 3             | LEU                  | B      |
| 3              | 4             | PHE                  | B      |
| 4              | 5             | GLN                  | B      |
| 5              | 6             | GLY                  | C      |
| 6              | 7             | PHE                  | C      |
| 7              | 11            | SER                  | C      |
| 8              | 17            | GLY                  | C      |
| 9              | 18            | TRP                  | C      |
| 10             | 19            | TYR                  | C      |
| 11             | 20            | ASN                  | C      |
| 12             | 21            | PHE                  | C      |
| 13             | 22            | LEU                  | C      |
| 14             | 23            | MET                  | C      |
| 15             | 24            | GLY                  | C      |
| 16             | 25            | LYS                  | C      |
| 17             | 26            | VAL                  | C      |
| 18             | 27            | ASP                  | C      |
| 19             | 28            | ASP                  | C      |
| 20             | 29            | ILE                  | C      |
| 21             | 30            | ALA                  | C      |
| 22             | 31            | ALA                  | C      |
| 23             | 32            | ALA                  | C      |
| 24             | 33            | GLY                  | C      |
| 25             | 34            | ILE                  | C      |
| 26             | 35            | THR                  | C      |
| 27             | 36            | HIS                  | C      |
| 28             | 37            | VAL                  | C      |
| 29             | 38            | TRP                  | C      |
| 30             | 39            | LEU                  | C      |
| 31             | 40            | PRO                  | C      |
| 32             | 41            | PRO                  | C      |
| 33             | 42            | ALA                  | C      |
| 34             | 43            | SER                  | C      |
| 35             | 44            | GLN                  | C      |
| 36             | 45            | SER                  | C      |
| 37             | 46            | VAL                  | C      |
| 38             | 47            | ALA                  | C      |
| 39             | 48            | GLU                  | C      |
| 40             | 49            | GLN                  | C      |
| 41             | 50            | GLY                  | C      |
| 42             | 51            | TYR                  | C      |
| 43             | 52            | MET                  | C      |

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Table S30 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 53            | PRO                  | C      |
| 45             | 54            | GLY                  | C      |
| 46             | 55            | ARG                  | C      |
| 47             | 57            | TYR                  | C      |
| 48             | 58            | ASP                  | C      |
| 49             | 59            | LEU                  | C      |
| 50             | 60            | ASP                  | C      |
| 51             | 62            | SER                  | C      |
| 52             | 63            | LYS                  | C      |
| 53             | 64            | TYR                  | C      |
| 54             | 65            | GLY                  | C      |
| 55             | 66            | ASN                  | C      |
| 56             | 67            | LYS                  | C      |
| 57             | 68            | ALA                  | C      |
| 58             | 69            | GLN                  | C      |
| 59             | 70            | LEU                  | C      |
| 60             | 71            | LYS                  | C      |
| 61             | 72            | SER                  | C      |
| 62             | 73            | LEU                  | C      |
| 63             | 74            | ILE                  | C      |
| 64             | 75            | GLY                  | C      |
| 65             | 76            | ALA                  | C      |
| 66             | 77            | LEU                  | C      |
| 67             | 78            | HIS                  | C      |
| 68             | 79            | GLY                  | C      |
| 69             | 80            | LYS                  | C      |
| 70             | 81            | GLY                  | C      |
| 71             | 82            | VAL                  | C      |
| 72             | 83            | LYS                  | C      |
| 73             | 84            | ALA                  | C      |
| 74             | 85            | ILE                  | C      |
| 75             | 86            | ALA                  | C      |
| 76             | 87            | ASP                  | C      |
| 77             | 88            | ILE                  | C      |
| 78             | 89            | VAL                  | C      |
| 79             | 90            | ILE                  | C      |
| 80             | 91            | ASN                  | C      |
| 81             | 92            | HIS                  | C      |
| 82             | 93            | ARG                  | C      |
| 83             | 94            | THR                  | C      |
| 84             | 95            | ALA                  | C      |
| 85             | 96            | GLU                  | C      |
| 86             | 107           | PHE                  | C      |
| 87             | 117           | ASP                  | C      |
| 88             | 118           | TRP                  | C      |
| 89             | 119           | GLY                  | C      |

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Table S30 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 120           | PRO                  | C      |
| 91             | 121           | HIS                  | C      |
| 92             | 122           | MET                  | C      |
| 93             | 123           | ILE                  | C      |
| 94             | 124           | CYS                  | B      |
| 95             | 141           | ALA                  | B      |
| 96             | 142           | ASP                  | B      |
| 97             | 143           | PHE                  | B      |
| 98             | 144           | GLY                  | B      |
| 99             | 146           | ALA                  | B      |
| 100            | 147           | PRO                  | B      |
| 101            | 148           | ASP                  | B      |
| 102            | 149           | ILE                  | B      |
| 103            | 150           | ASP                  | B      |
| 104            | 151           | HIS                  | B      |
| 105            | 152           | LEU                  | B      |
| 106            | 153           | ASN                  | B      |
| 107            | 154           | LEU                  | B      |
| 108            | 155           | ARG                  | B      |
| 109            | 156           | VAL                  | B      |
| 110            | 157           | GLN                  | B      |
| 111            | 158           | LYS                  | B      |
| 112            | 159           | GLU                  | B      |
| 113            | 160           | LEU                  | B      |
| 114            | 161           | VAL                  | B      |
| 115            | 162           | GLU                  | B      |
| 116            | 163           | TRP                  | B      |
| 117            | 164           | LEU                  | B      |
| 118            | 165           | ASN                  | B      |
| 119            | 166           | TRP                  | B      |
| 120            | 167           | LEU                  | B      |
| 121            | 168           | LYS                  | B      |
| 122            | 169           | ALA                  | B      |
| 123            | 171           | ILE                  | C      |
| 124            | 172           | GLY                  | C      |
| 125            | 173           | PHE                  | C      |
| 126            | 174           | ASP                  | C      |
| 127            | 175           | GLY                  | C      |
| 128            | 176           | TRP                  | B      |
| 129            | 177           | ARG                  | D      |
| 130            | 178           | PHE                  | B      |
| 131            | 179           | ASP                  | B      |
| 132            | 180           | PHE                  | B      |
| 133            | 181           | ALA                  | B      |
| 134            | 182           | LYS                  | B      |
| 135            | 183           | GLY                  | B      |

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Table S30 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 184           | TYR                  | B      |
| 137            | 185           | SER                  | B      |
| 138            | 186           | ALA                  | B      |
| 139            | 187           | ASP                  | B      |
| 140            | 188           | VAL                  | B      |
| 141            | 189           | ALA                  | B      |
| 142            | 190           | LYS                  | B      |
| 143            | 191           | ILE                  | B      |
| 144            | 192           | TYR                  | B      |
| 145            | 193           | ILE                  | B      |
| 146            | 194           | ASP                  | B      |
| 147            | 195           | ARG                  | B      |
| 148            | 196           | SER                  | B      |
| 149            | 197           | GLU                  | B      |
| 150            | 199           | SER                  | B      |
| 151            | 200           | PHE                  | B      |
| 152            | 201           | ALA                  | B      |
| 153            | 202           | VAL                  | C      |
| 154            | 203           | ALA                  | B      |
| 155            | 204           | GLU                  | B      |
| 156            | 205           | ILE                  | B      |
| 157            | 206           | TRP                  | B      |
| 158            | 207           | THR                  | B      |
| 159            | 208           | SER                  | B      |
| 160            | 228           | LEU                  | B      |
| 161            | 229           | VAL                  | B      |
| 162            | 230           | ASN                  | B      |
| 163            | 231           | TRP                  | B      |
| 164            | 232           | VAL                  | B      |
| 165            | 233           | ASP                  | B      |
| 166            | 240           | PRO                  | B      |
| 167            | 241           | ALA                  | B      |
| 168            | 242           | THR                  | B      |
| 169            | 243           | THR                  | B      |
| 170            | 244           | PHE                  | D      |
| 171            | 245           | ASP                  | D      |
| 172            | 246           | PHE                  | D      |
| 173            | 247           | THR                  | D      |
| 174            | 249           | LYS                  | D      |
| 175            | 250           | GLY                  | D      |
| 176            | 251           | ILE                  | D      |
| 177            | 252           | LEU                  | D      |
| 178            | 253           | ASN                  | D      |
| 179            | 254           | VAL                  | D      |
| 180            | 255           | ALA                  | D      |
| 181            | 256           | VAL                  | D      |

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Table S30 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 259           | GLU                  | D      |
| 183            | 260           | LEU                  | A      |
| 184            | 261           | TRP                  | A      |
| 185            | 262           | ARG                  | A      |
| 186            | 269           | LYS                  | A      |
| 187            | 270           | ALA                  | D      |
| 188            | 271           | PRO                  | D      |
| 189            | 272           | GLY                  | D      |
| 190            | 274           | ILE                  | D      |
| 191            | 275           | GLY                  | B      |
| 192            | 276           | TRP                  | B      |
| 193            | 277           | TRP                  | B      |
| 194            | 278           | PRO                  | B      |
| 195            | 279           | ALA                  | B      |
| 196            | 280           | LYS                  | B      |
| 197            | 281           | ALA                  | B      |
| 198            | 282           | VAL                  | D      |
| 199            | 283           | THR                  | D      |
| 200            | 284           | PHE                  | D      |
| 201            | 285           | VAL                  | A      |
| 202            | 286           | ASP                  | D      |
| 203            | 287           | ASN                  | D      |
| 204            | 288           | HIS                  | D      |
| 205            | 289           | ASP                  | D      |
| 206            | 290           | THR                  | D      |
| 207            | 291           | GLY                  | D      |
| 208            | 298           | PRO                  | D      |
| 209            | 299           | PHE                  | D      |
| 210            | 300           | PRO                  | D      |
| 211            | 301           | SER                  | D      |
| 212            | 302           | ASP                  | A      |
| 213            | 303           | ARG                  | A      |
| 214            | 304           | VAL                  | A      |
| 215            | 305           | MET                  | A      |
| 216            | 306           | GLN                  | A      |
| 217            | 307           | GLY                  | A      |
| 218            | 308           | TYR                  | A      |
| 219            | 309           | ALA                  | A      |
| 220            | 310           | TYR                  | A      |
| 221            | 311           | ILE                  | A      |
| 222            | 312           | LEU                  | A      |
| 223            | 313           | THR                  | A      |
| 224            | 314           | HIS                  | A      |
| 225            | 315           | PRO                  | D      |
| 226            | 316           | GLY                  | D      |
| 227            | 317           | THR                  | D      |

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Table S30 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 318           | PRO                  | A      |
| 229            | 319           | CYS                  | D      |
| 230            | 320           | ILE                  | A      |
| 231            | 321           | PHE                  | D      |
| 232            | 322           | TYR                  | C      |
| 233            | 323           | ASP                  | D      |
| 234            | 324           | HIS                  | A      |
| 235            | 325           | PHE                  | C      |
| 236            | 326           | PHE                  | C      |
| 237            | 327           | ASP                  | D      |
| 238            | 328           | TRP                  | D      |
| 239            | 329           | GLY                  | D      |
| 240            | 330           | LEU                  | A      |
| 241            | 331           | LYS                  | A      |
| 242            | 332           | GLU                  | A      |
| 243            | 333           | GLU                  | A      |
| 244            | 334           | ILE                  | A      |
| 245            | 335           | ASP                  | A      |
| 246            | 336           | ARG                  | A      |
| 247            | 337           | LEU                  | A      |
| 248            | 338           | VAL                  | A      |
| 249            | 339           | SER                  | A      |
| 250            | 340           | VAL                  | A      |
| 251            | 341           | ARG                  | A      |
| 252            | 342           | THR                  | A      |
| 253            | 343           | ARG                  | A      |
| 254            | 344           | HIS                  | A      |
| 255            | 345           | GLY                  | A      |
| 256            | 349           | GLU                  | A      |
| 257            | 350           | SER                  | A      |
| 258            | 351           | LYS                  | A      |
| 259            | 352           | LEU                  | A      |
| 260            | 354           | ILE                  | A      |
| 261            | 355           | ILE                  | A      |
| 262            | 356           | GLU                  | A      |
| 263            | 357           | ALA                  | A      |
| 264            | 358           | ASP                  | A      |
| 265            | 359           | ALA                  | A      |
| 266            | 360           | ASP                  | A      |
| 267            | 361           | LEU                  | A      |
| 268            | 362           | TYR                  | A      |
| 269            | 363           | LEU                  | A      |
| 270            | 364           | ALA                  | A      |
| 271            | 365           | GLU                  | A      |
| 272            | 366           | ILE                  | A      |
| 273            | 368           | GLY                  | A      |

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Table S30 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 369           | LYS                  | A      |
| 275            | 370           | VAL                  | A      |
| 276            | 371           | ILE                  | A      |
| 277            | 372           | VAL                  | A      |
| 278            | 373           | LYS                  | A      |
| 279            | 374           | LEU                  | A      |
| 280            | 375           | GLY                  | A      |
| 281            | 376           | PRO                  | A      |
| 282            | 377           | ARG                  | A      |
| 283            | 378           | TYR                  | A      |
| 284            | 379           | ASP                  | A      |
| 285            | 380           | VAL                  | A      |
| 286            | 381           | GLY                  | A      |
| 287            | 382           | ASN                  | A      |
| 288            | 387           | GLY                  | A      |
| 289            | 388           | PHE                  | A      |
| 290            | 389           | LYS                  | A      |
| 291            | 390           | VAL                  | A      |
| 292            | 391           | ALA                  | A      |
| 293            | 392           | ALA                  | A      |
| 294            | 393           | HIS                  | A      |
| 295            | 394           | GLY                  | A      |
| 296            | 395           | ASN                  | A      |
| 297            | 396           | ASP                  | A      |
| 298            | 397           | TYR                  | A      |
| 299            | 398           | ALA                  | A      |
| 300            | 399           | VAL                  | A      |
| 301            | 400           | TRP                  | A      |
| 302            | 401           | GLU                  | A      |

Table S31: Residues membership for the *H. vulgare*  $\alpha$ -amylase (PDB code 1AVA, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 1             | GLN                  | A      |
| 1              | 2             | VAL                  | A      |
| 2              | 3             | LEU                  | B      |
| 3              | 4             | PHE                  | B      |
| 4              | 5             | GLN                  | B      |
| 5              | 6             | GLY                  | C      |
| 6              | 7             | PHE                  | C      |
| 7              | 11            | SER                  | C      |
| 8              | 17            | GLY                  | C      |

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Table S31 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 18            | TRP                  | C      |
| 10             | 19            | TYR                  | C      |
| 11             | 20            | ASN                  | C      |
| 12             | 21            | PHE                  | C      |
| 13             | 22            | LEU                  | C      |
| 14             | 23            | MET                  | C      |
| 15             | 24            | GLY                  | C      |
| 16             | 25            | LYS                  | C      |
| 17             | 26            | VAL                  | C      |
| 18             | 27            | ASP                  | C      |
| 19             | 28            | ASP                  | C      |
| 20             | 29            | ILE                  | C      |
| 21             | 30            | ALA                  | C      |
| 22             | 31            | ALA                  | C      |
| 23             | 32            | ALA                  | C      |
| 24             | 33            | GLY                  | C      |
| 25             | 34            | ILE                  | C      |
| 26             | 35            | THR                  | C      |
| 27             | 36            | HIS                  | C      |
| 28             | 37            | VAL                  | C      |
| 29             | 38            | TRP                  | C      |
| 30             | 39            | LEU                  | C      |
| 31             | 40            | PRO                  | C      |
| 32             | 41            | PRO                  | C      |
| 33             | 42            | ALA                  | C      |
| 34             | 43            | SER                  | C      |
| 35             | 44            | GLN                  | C      |
| 36             | 45            | SER                  | C      |
| 37             | 46            | VAL                  | C      |
| 38             | 47            | ALA                  | C      |
| 39             | 48            | GLU                  | C      |
| 40             | 49            | GLN                  | C      |
| 41             | 50            | GLY                  | C      |
| 42             | 51            | TYR                  | C      |
| 43             | 52            | MET                  | C      |
| 44             | 53            | PRO                  | C      |
| 45             | 54            | GLY                  | C      |
| 46             | 55            | ARG                  | C      |
| 47             | 57            | TYR                  | C      |
| 48             | 58            | ASP                  | C      |
| 49             | 59            | LEU                  | C      |
| 50             | 60            | ASP                  | C      |
| 51             | 62            | SER                  | C      |
| 52             | 63            | LYS                  | C      |
| 53             | 64            | TYR                  | C      |
| 54             | 65            | GLY                  | C      |

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Table S31 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 66            | ASN                  | C      |
| 56             | 67            | LYS                  | C      |
| 57             | 68            | ALA                  | C      |
| 58             | 69            | GLN                  | C      |
| 59             | 70            | LEU                  | C      |
| 60             | 71            | LYS                  | C      |
| 61             | 72            | SER                  | C      |
| 62             | 73            | LEU                  | C      |
| 63             | 74            | ILE                  | C      |
| 64             | 75            | GLY                  | C      |
| 65             | 76            | ALA                  | C      |
| 66             | 77            | LEU                  | C      |
| 67             | 78            | HIS                  | C      |
| 68             | 79            | GLY                  | C      |
| 69             | 80            | LYS                  | C      |
| 70             | 81            | GLY                  | C      |
| 71             | 82            | VAL                  | C      |
| 72             | 83            | LYS                  | C      |
| 73             | 84            | ALA                  | C      |
| 74             | 85            | ILE                  | C      |
| 75             | 86            | ALA                  | C      |
| 76             | 87            | ASP                  | C      |
| 77             | 88            | ILE                  | C      |
| 78             | 89            | VAL                  | C      |
| 79             | 90            | ILE                  | C      |
| 80             | 91            | ASN                  | C      |
| 81             | 92            | HIS                  | C      |
| 82             | 93            | ARG                  | C      |
| 83             | 94            | THR                  | C      |
| 84             | 95            | ALA                  | C      |
| 85             | 96            | GLU                  | C      |
| 86             | 107           | PHE                  | C      |
| 87             | 117           | ASP                  | C      |
| 88             | 118           | TRP                  | C      |
| 89             | 119           | GLY                  | C      |
| 90             | 120           | PRO                  | C      |
| 91             | 121           | HIS                  | C      |
| 92             | 122           | MET                  | C      |
| 93             | 123           | ILE                  | C      |
| 94             | 124           | CYS                  | B      |
| 95             | 141           | ALA                  | B      |
| 96             | 142           | ASP                  | B      |
| 97             | 143           | PHE                  | B      |
| 98             | 144           | GLY                  | B      |
| 99             | 146           | ALA                  | B      |
| 100            | 147           | PRO                  | B      |

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Table S31 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 148           | ASP                  | B      |
| 102            | 149           | ILE                  | B      |
| 103            | 150           | ASP                  | B      |
| 104            | 151           | HIS                  | B      |
| 105            | 152           | LEU                  | B      |
| 106            | 153           | ASN                  | B      |
| 107            | 154           | LEU                  | B      |
| 108            | 155           | ARG                  | B      |
| 109            | 156           | VAL                  | B      |
| 110            | 157           | GLN                  | B      |
| 111            | 158           | LYS                  | B      |
| 112            | 159           | GLU                  | B      |
| 113            | 160           | LEU                  | B      |
| 114            | 161           | VAL                  | B      |
| 115            | 162           | GLU                  | B      |
| 116            | 163           | TRP                  | B      |
| 117            | 164           | LEU                  | B      |
| 118            | 165           | ASN                  | B      |
| 119            | 166           | TRP                  | B      |
| 120            | 167           | LEU                  | B      |
| 121            | 168           | LYS                  | B      |
| 122            | 169           | ALA                  | B      |
| 123            | 171           | ILE                  | C      |
| 124            | 172           | GLY                  | C      |
| 125            | 173           | PHE                  | C      |
| 126            | 174           | ASP                  | C      |
| 127            | 175           | GLY                  | C      |
| 128            | 176           | TRP                  | B      |
| 129            | 177           | ARG                  | D      |
| 130            | 178           | PHE                  | B      |
| 131            | 179           | ASP                  | B      |
| 132            | 180           | PHE                  | B      |
| 133            | 181           | ALA                  | B      |
| 134            | 182           | LYS                  | B      |
| 135            | 183           | GLY                  | B      |
| 136            | 184           | TYR                  | B      |
| 137            | 185           | SER                  | B      |
| 138            | 186           | ALA                  | B      |
| 139            | 187           | ASP                  | B      |
| 140            | 188           | VAL                  | B      |
| 141            | 189           | ALA                  | B      |
| 142            | 190           | LYS                  | B      |
| 143            | 191           | ILE                  | B      |
| 144            | 192           | TYR                  | B      |
| 145            | 193           | ILE                  | B      |
| 146            | 194           | ASP                  | B      |

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Table S31 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 195           | ARG                  | B      |
| 148            | 196           | SER                  | B      |
| 149            | 197           | GLU                  | B      |
| 150            | 199           | SER                  | B      |
| 151            | 200           | PHE                  | B      |
| 152            | 201           | ALA                  | B      |
| 153            | 202           | VAL                  | C      |
| 154            | 203           | ALA                  | B      |
| 155            | 204           | GLU                  | B      |
| 156            | 205           | ILE                  | B      |
| 157            | 206           | TRP                  | B      |
| 158            | 207           | THR                  | B      |
| 159            | 208           | SER                  | B      |
| 160            | 228           | LEU                  | B      |
| 161            | 229           | VAL                  | B      |
| 162            | 230           | ASN                  | B      |
| 163            | 231           | TRP                  | B      |
| 164            | 232           | VAL                  | B      |
| 165            | 233           | ASP                  | B      |
| 166            | 240           | PRO                  | B      |
| 167            | 241           | ALA                  | B      |
| 168            | 242           | THR                  | B      |
| 169            | 243           | THR                  | B      |
| 170            | 244           | PHE                  | D      |
| 171            | 245           | ASP                  | D      |
| 172            | 246           | PHE                  | D      |
| 173            | 247           | THR                  | D      |
| 174            | 249           | LYS                  | D      |
| 175            | 250           | GLY                  | D      |
| 176            | 251           | ILE                  | D      |
| 177            | 252           | LEU                  | D      |
| 178            | 253           | ASN                  | D      |
| 179            | 254           | VAL                  | D      |
| 180            | 255           | ALA                  | D      |
| 181            | 256           | VAL                  | D      |
| 182            | 259           | GLU                  | D      |
| 183            | 260           | LEU                  | A      |
| 184            | 261           | TRP                  | A      |
| 185            | 262           | ARG                  | A      |
| 186            | 269           | LYS                  | A      |
| 187            | 270           | ALA                  | D      |
| 188            | 271           | PRO                  | D      |
| 189            | 272           | GLY                  | D      |
| 190            | 274           | ILE                  | D      |
| 191            | 275           | GLY                  | B      |
| 192            | 276           | TRP                  | B      |

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Table S31 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 277           | TRP                  | B      |
| 194            | 278           | PRO                  | B      |
| 195            | 279           | ALA                  | B      |
| 196            | 280           | LYS                  | B      |
| 197            | 281           | ALA                  | B      |
| 198            | 282           | VAL                  | D      |
| 199            | 283           | THR                  | D      |
| 200            | 284           | PHE                  | D      |
| 201            | 285           | VAL                  | A      |
| 202            | 286           | ASP                  | D      |
| 203            | 287           | ASN                  | D      |
| 204            | 288           | HIS                  | D      |
| 205            | 289           | ASP                  | D      |
| 206            | 290           | THR                  | D      |
| 207            | 291           | GLY                  | D      |
| 208            | 298           | PRO                  | D      |
| 209            | 299           | PHE                  | D      |
| 210            | 300           | PRO                  | D      |
| 211            | 301           | SER                  | D      |
| 212            | 302           | ASP                  | A      |
| 213            | 303           | ARG                  | A      |
| 214            | 304           | VAL                  | A      |
| 215            | 305           | MET                  | A      |
| 216            | 306           | GLN                  | A      |
| 217            | 307           | GLY                  | A      |
| 218            | 308           | TYR                  | A      |
| 219            | 309           | ALA                  | A      |
| 220            | 310           | TYR                  | A      |
| 221            | 311           | ILE                  | A      |
| 222            | 312           | LEU                  | A      |
| 223            | 313           | THR                  | A      |
| 224            | 314           | HIS                  | A      |
| 225            | 315           | PRO                  | D      |
| 226            | 316           | GLY                  | D      |
| 227            | 317           | THR                  | D      |
| 228            | 318           | PRO                  | A      |
| 229            | 319           | CYS                  | D      |
| 230            | 320           | ILE                  | A      |
| 231            | 321           | PHE                  | D      |
| 232            | 322           | TYR                  | C      |
| 233            | 323           | ASP                  | D      |
| 234            | 324           | HIS                  | A      |
| 235            | 325           | PHE                  | C      |
| 236            | 326           | PHE                  | C      |
| 237            | 327           | ASP                  | D      |
| 238            | 328           | TRP                  | D      |

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Table S31 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 329           | GLY                  | D      |
| 240            | 330           | LEU                  | A      |
| 241            | 331           | LYS                  | A      |
| 242            | 332           | GLU                  | A      |
| 243            | 333           | GLU                  | A      |
| 244            | 334           | ILE                  | A      |
| 245            | 335           | ASP                  | A      |
| 246            | 336           | ARG                  | A      |
| 247            | 337           | LEU                  | A      |
| 248            | 338           | VAL                  | A      |
| 249            | 339           | SER                  | A      |
| 250            | 340           | VAL                  | A      |
| 251            | 341           | ARG                  | A      |
| 252            | 342           | THR                  | A      |
| 253            | 343           | ARG                  | A      |
| 254            | 344           | HIS                  | A      |
| 255            | 345           | GLY                  | A      |
| 256            | 349           | GLU                  | A      |
| 257            | 350           | SER                  | A      |
| 258            | 351           | LYS                  | A      |
| 259            | 352           | LEU                  | A      |
| 260            | 354           | ILE                  | A      |
| 261            | 355           | ILE                  | A      |
| 262            | 356           | GLU                  | A      |
| 263            | 357           | ALA                  | A      |
| 264            | 358           | ASP                  | A      |
| 265            | 359           | ALA                  | A      |
| 266            | 360           | ASP                  | A      |
| 267            | 361           | LEU                  | A      |
| 268            | 362           | TYR                  | A      |
| 269            | 363           | LEU                  | A      |
| 270            | 364           | ALA                  | A      |
| 271            | 365           | GLU                  | A      |
| 272            | 366           | ILE                  | A      |
| 273            | 368           | GLY                  | A      |
| 274            | 369           | LYS                  | A      |
| 275            | 370           | VAL                  | A      |
| 276            | 371           | ILE                  | A      |
| 277            | 372           | VAL                  | A      |
| 278            | 373           | LYS                  | A      |
| 279            | 374           | LEU                  | A      |
| 280            | 375           | GLY                  | A      |
| 281            | 376           | PRO                  | A      |
| 282            | 377           | ARG                  | A      |
| 283            | 378           | TYR                  | A      |
| 284            | 379           | ASP                  | A      |

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Table S31 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 380           | VAL                  | A      |
| 286            | 381           | GLY                  | A      |
| 287            | 382           | ASN                  | A      |
| 288            | 387           | GLY                  | A      |
| 289            | 388           | PHE                  | A      |
| 290            | 389           | LYS                  | A      |
| 291            | 390           | VAL                  | A      |
| 292            | 391           | ALA                  | A      |
| 293            | 392           | ALA                  | A      |
| 294            | 393           | HIS                  | A      |
| 295            | 394           | GLY                  | A      |
| 296            | 395           | ASN                  | A      |
| 297            | 396           | ASP                  | A      |
| 298            | 397           | TYR                  | A      |
| 299            | 398           | ALA                  | A      |
| 300            | 399           | VAL                  | A      |
| 301            | 400           | TRP                  | A      |
| 302            | 401           | GLU                  | A      |

Table S32: Residues membership for the *P. haloplanctis*  $\alpha$ -amylase (PDB code 1AQM, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 3             | THR                  | A      |
| 1              | 4             | THR                  | A      |
| 2              | 5             | PHE                  | B      |
| 3              | 6             | VAL                  | B      |
| 4              | 7             | HIS                  | B      |
| 5              | 8             | LEU                  | C      |
| 6              | 9             | PHE                  | C      |
| 7              | 10            | GLU                  | C      |
| 8              | 11            | TRP                  | C      |
| 9              | 12            | ASN                  | C      |
| 10             | 13            | TRP                  | C      |
| 11             | 14            | GLN                  | C      |
| 12             | 15            | ASP                  | C      |
| 13             | 16            | VAL                  | C      |
| 14             | 17            | ALA                  | C      |
| 15             | 18            | GLN                  | C      |
| 16             | 19            | GLU                  | C      |
| 17             | 20            | CYS                  | C      |
| 18             | 21            | GLU                  | C      |
| 19             | 22            | GLN                  | C      |

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Table S32 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 24            | LEU                  | C      |
| 21             | 25            | GLY                  | C      |
| 22             | 26            | PRO                  | C      |
| 23             | 27            | LYS                  | C      |
| 24             | 28            | GLY                  | C      |
| 25             | 29            | TYR                  | C      |
| 26             | 30            | ALA                  | C      |
| 27             | 31            | ALA                  | C      |
| 28             | 32            | VAL                  | C      |
| 29             | 33            | GLN                  | C      |
| 30             | 34            | VAL                  | C      |
| 31             | 35            | SER                  | C      |
| 32             | 36            | PRO                  | C      |
| 33             | 37            | PRO                  | C      |
| 34             | 38            | ASN                  | C      |
| 35             | 39            | GLU                  | C      |
| 36             | 40            | HIS                  | C      |
| 37             | 41            | ILE                  | C      |
| 38             | 43            | GLY                  | C      |
| 39             | 47            | TRP                  | C      |
| 40             | 48            | THR                  | C      |
| 41             | 49            | ARG                  | C      |
| 42             | 50            | TYR                  | C      |
| 43             | 51            | GLN                  | C      |
| 44             | 52            | PRO                  | C      |
| 45             | 53            | VAL                  | C      |
| 46             | 54            | SER                  | C      |
| 47             | 55            | TYR                  | C      |
| 48             | 56            | GLU                  | C      |
| 49             | 57            | LEU                  | C      |
| 50             | 58            | GLN                  | C      |
| 51             | 59            | SER                  | C      |
| 52             | 60            | ARG                  | C      |
| 53             | 61            | GLY                  | C      |
| 54             | 62            | GLY                  | C      |
| 55             | 63            | ASN                  | C      |
| 56             | 64            | ARG                  | C      |
| 57             | 65            | ALA                  | C      |
| 58             | 66            | GLN                  | C      |
| 59             | 67            | PHE                  | C      |
| 60             | 68            | ILE                  | C      |
| 61             | 69            | ASP                  | C      |
| 62             | 70            | MET                  | C      |
| 63             | 71            | VAL                  | C      |
| 64             | 72            | ASN                  | C      |
| 65             | 73            | ARG                  | C      |

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Table S32 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 74            | CYS                  | C      |
| 67             | 75            | SER                  | C      |
| 68             | 76            | ALA                  | C      |
| 69             | 77            | ALA                  | C      |
| 70             | 78            | GLY                  | C      |
| 71             | 79            | VAL                  | C      |
| 72             | 80            | ASP                  | C      |
| 73             | 81            | ILE                  | C      |
| 74             | 82            | TYR                  | C      |
| 75             | 83            | VAL                  | C      |
| 76             | 84            | ASP                  | C      |
| 77             | 85            | THR                  | C      |
| 78             | 86            | LEU                  | C      |
| 79             | 87            | ILE                  | C      |
| 80             | 88            | ASN                  | C      |
| 81             | 89            | HIS                  | C      |
| 82             | 90            | MET                  | C      |
| 83             | 91            | ALA                  | C      |
| 84             | 92            | ALA                  | C      |
| 85             | 93            | GLY                  | C      |
| 86             | 108           | PHE                  | C      |
| 87             | 110           | ILE                  | C      |
| 88             | 111           | TYR                  | C      |
| 89             | 112           | SER                  | C      |
| 90             | 113           | PRO                  | C      |
| 91             | 114           | GLN                  | C      |
| 92             | 115           | ASP                  | C      |
| 93             | 116           | PHE                  | C      |
| 94             | 117           | HIS                  | B      |
| 95             | 137           | CYS                  | B      |
| 96             | 138           | GLU                  | B      |
| 97             | 139           | LEU                  | B      |
| 98             | 140           | VAL                  | B      |
| 99             | 142           | LEU                  | B      |
| 100            | 143           | ALA                  | B      |
| 101            | 144           | ASP                  | B      |
| 102            | 145           | LEU                  | B      |
| 103            | 146           | ASP                  | B      |
| 104            | 147           | THR                  | B      |
| 105            | 148           | ALA                  | B      |
| 106            | 149           | SER                  | B      |
| 107            | 150           | ASN                  | B      |
| 108            | 151           | TYR                  | B      |
| 109            | 152           | VAL                  | B      |
| 110            | 153           | GLN                  | B      |
| 111            | 154           | ASN                  | B      |

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Table S32 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 155           | THR                  | B      |
| 113            | 156           | ILE                  | B      |
| 114            | 157           | ALA                  | B      |
| 115            | 158           | ALA                  | B      |
| 116            | 159           | TYR                  | B      |
| 117            | 160           | ILE                  | B      |
| 118            | 161           | ASN                  | B      |
| 119            | 162           | ASP                  | B      |
| 120            | 163           | LEU                  | B      |
| 121            | 164           | GLN                  | B      |
| 122            | 165           | ALA                  | B      |
| 123            | 166           | ILE                  | C      |
| 124            | 167           | GLY                  | C      |
| 125            | 168           | VAL                  | C      |
| 126            | 169           | LYS                  | C      |
| 127            | 170           | GLY                  | C      |
| 128            | 171           | PHE                  | B      |
| 129            | 172           | ARG                  | D      |
| 130            | 173           | PHE                  | B      |
| 131            | 174           | ASP                  | B      |
| 132            | 175           | ALA                  | B      |
| 133            | 176           | SER                  | B      |
| 134            | 177           | LYS                  | B      |
| 135            | 178           | HIS                  | B      |
| 136            | 179           | VAL                  | B      |
| 137            | 180           | ALA                  | B      |
| 138            | 181           | ALA                  | B      |
| 139            | 182           | SER                  | B      |
| 140            | 183           | ASP                  | B      |
| 141            | 184           | ILE                  | B      |
| 142            | 185           | GLN                  | B      |
| 143            | 186           | SER                  | B      |
| 144            | 187           | LEU                  | B      |
| 145            | 188           | MET                  | B      |
| 146            | 189           | ALA                  | B      |
| 147            | 190           | LYS                  | B      |
| 148            | 191           | VAL                  | B      |
| 149            | 192           | ASN                  | B      |
| 150            | 195           | PRO                  | B      |
| 151            | 196           | VAL                  | B      |
| 152            | 197           | VAL                  | B      |
| 153            | 198           | PHE                  | C      |
| 154            | 199           | GLN                  | B      |
| 155            | 200           | GLU                  | B      |
| 156            | 201           | VAL                  | B      |
| 157            | 202           | ILE                  | B      |

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Table S32 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 203           | ASP                  | B      |
| 159            | 204           | GLN                  | B      |
| 160            | 211           | ALA                  | B      |
| 161            | 212           | SER                  | B      |
| 162            | 213           | GLU                  | B      |
| 163            | 214           | TYR                  | B      |
| 164            | 215           | LEU                  | B      |
| 165            | 216           | SER                  | B      |
| 166            | 217           | THR                  | B      |
| 167            | 218           | GLY                  | B      |
| 168            | 219           | LEU                  | B      |
| 169            | 220           | VAL                  | B      |
| 170            | 221           | THR                  | D      |
| 171            | 222           | GLU                  | D      |
| 172            | 223           | PHE                  | D      |
| 173            | 224           | LYS                  | D      |
| 174            | 226           | SER                  | D      |
| 175            | 227           | THR                  | D      |
| 176            | 228           | GLU                  | D      |
| 177            | 229           | LEU                  | D      |
| 178            | 230           | GLY                  | D      |
| 179            | 231           | ASN                  | D      |
| 180            | 232           | THR                  | D      |
| 181            | 233           | PHE                  | D      |
| 182            | 236           | GLY                  | D      |
| 183            | 237           | SER                  | A      |
| 184            | 238           | LEU                  | A      |
| 185            | 239           | ALA                  | A      |
| 186            | 244           | PHE                  | A      |
| 187            | 245           | GLY                  | D      |
| 188            | 246           | GLU                  | D      |
| 189            | 247           | GLY                  | D      |
| 190            | 249           | GLY                  | D      |
| 191            | 250           | PHE                  | B      |
| 192            | 251           | MET                  | B      |
| 193            | 252           | PRO                  | B      |
| 194            | 253           | SER                  | B      |
| 195            | 254           | SER                  | B      |
| 196            | 255           | SER                  | B      |
| 197            | 256           | ALA                  | B      |
| 198            | 257           | VAL                  | D      |
| 199            | 258           | VAL                  | D      |
| 200            | 259           | PHE                  | D      |
| 201            | 260           | VAL                  | A      |
| 202            | 261           | ASP                  | D      |
| 203            | 262           | ASN                  | D      |

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Table S32 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 263           | HIS                  | D      |
| 205            | 264           | ASP                  | D      |
| 206            | 265           | ASN                  | D      |
| 207            | 266           | GLN                  | D      |
| 208            | 277           | THR                  | D      |
| 209            | 278           | PHE                  | D      |
| 210            | 279           | GLU                  | D      |
| 211            | 280           | ASP                  | D      |
| 212            | 282           | ARG                  | A      |
| 213            | 283           | LEU                  | A      |
| 214            | 284           | TYR                  | A      |
| 215            | 285           | ASP                  | A      |
| 216            | 286           | LEU                  | A      |
| 217            | 287           | ALA                  | A      |
| 218            | 288           | ASN                  | A      |
| 219            | 289           | VAL                  | A      |
| 220            | 290           | PHE                  | A      |
| 221            | 291           | MET                  | A      |
| 222            | 292           | LEU                  | A      |
| 223            | 293           | ALA                  | A      |
| 224            | 294           | TYR                  | A      |
| 225            | 296           | TYR                  | D      |
| 226            | 297           | GLY                  | D      |
| 227            | 298           | TYR                  | D      |
| 228            | 299           | PRO                  | A      |
| 229            | 300           | LYS                  | D      |
| 230            | 301           | VAL                  | A      |
| 231            | 302           | MET                  | D      |
| 232            | 303           | SER                  | C      |
| 233            | 304           | SER                  | D      |
| 234            | 305           | TYR                  | A      |
| 235            | 306           | ASP                  | C      |
| 236            | 332           | ASN                  | C      |
| 237            | 333           | TRP                  | D      |
| 238            | 334           | LYS                  | D      |
| 239            | 335           | CYS                  | D      |
| 240            | 338           | ARG                  | A      |
| 241            | 339           | TRP                  | A      |
| 242            | 340           | SER                  | A      |
| 243            | 341           | TYR                  | A      |
| 244            | 342           | ILE                  | A      |
| 245            | 343           | ALA                  | A      |
| 246            | 344           | GLY                  | A      |
| 247            | 345           | GLY                  | A      |
| 248            | 346           | VAL                  | A      |
| 249            | 347           | ASP                  | A      |

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Table S32 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 348           | PHE                  | A      |
| 251            | 349           | ARG                  | A      |
| 252            | 350           | ASN                  | A      |
| 253            | 351           | ASN                  | A      |
| 254            | 352           | THR                  | A      |
| 255            | 353           | ALA                  | A      |
| 256            | 355           | ASN                  | A      |
| 257            | 356           | TRP                  | A      |
| 258            | 357           | ALA                  | A      |
| 259            | 358           | VAL                  | A      |
| 260            | 360           | ASN                  | A      |
| 261            | 361           | TRP                  | A      |
| 262            | 362           | TRP                  | A      |
| 263            | 363           | ASP                  | A      |
| 264            | 365           | THR                  | A      |
| 265            | 366           | ASN                  | A      |
| 266            | 367           | ASN                  | A      |
| 267            | 368           | GLN                  | A      |
| 268            | 369           | ILE                  | A      |
| 269            | 370           | SER                  | A      |
| 270            | 371           | PHE                  | A      |
| 271            | 372           | GLY                  | A      |
| 272            | 373           | ARG                  | A      |
| 273            | 374           | GLY                  | A      |
| 274            | 375           | SER                  | A      |
| 275            | 377           | GLY                  | A      |
| 276            | 378           | HIS                  | A      |
| 277            | 379           | MET                  | A      |
| 278            | 380           | ALA                  | A      |
| 279            | 381           | ILE                  | A      |
| 280            | 382           | ASN                  | A      |
| 281            | 385           | ASP                  | A      |
| 282            | 386           | SER                  | A      |
| 283            | 387           | THR                  | A      |
| 284            | 388           | LEU                  | A      |
| 285            | 389           | THR                  | A      |
| 286            | 390           | ALA                  | A      |
| 287            | 391           | THR                  | A      |
| 288            | 397           | ALA                  | A      |
| 289            | 398           | SER                  | A      |
| 290            | 401           | TYR                  | A      |
| 291            | 402           | CYS                  | A      |
| 292            | 403           | ASN                  | A      |
| 293            | 404           | VAL                  | A      |
| 294            | 433           | ILE                  | A      |
| 295            | 434           | GLY                  | A      |

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Table S32 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 435           | ALA                  | A      |
| 297            | 437           | ASP                  | A      |
| 298            | 438           | ALA                  | A      |
| 299            | 439           | MET                  | A      |
| 300            | 440           | ALA                  | A      |
| 301            | 441           | ILE                  | A      |
| 302            | 442           | HIS                  | A      |

Table S33: Residues membership for the *B. subtilis*  $\alpha$ -amylase (PDB code 1BAG, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | GLY                  | A      |
| 1              | 10            | THR                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | LEU                  | B      |
| 4              | 13            | HIS                  | B      |
| 5              | 14            | ALA                  | C      |
| 6              | 15            | TRP                  | C      |
| 7              | 16            | ASN                  | C      |
| 8              | 17            | TRP                  | C      |
| 9              | 18            | SER                  | C      |
| 10             | 19            | PHE                  | C      |
| 11             | 20            | ASN                  | C      |
| 12             | 21            | THR                  | C      |
| 13             | 22            | LEU                  | C      |
| 14             | 23            | LYS                  | C      |
| 15             | 24            | HIS                  | C      |
| 16             | 25            | ASN                  | C      |
| 17             | 26            | MET                  | C      |
| 18             | 27            | LYS                  | C      |
| 19             | 28            | ASP                  | C      |
| 20             | 29            | ILE                  | C      |
| 21             | 30            | HIS                  | C      |
| 22             | 31            | ASP                  | C      |
| 23             | 32            | ALA                  | C      |
| 24             | 33            | GLY                  | C      |
| 25             | 34            | TYR                  | C      |
| 26             | 35            | THR                  | C      |
| 27             | 36            | ALA                  | C      |
| 28             | 37            | ILE                  | C      |
| 29             | 38            | GLN                  | C      |
| 30             | 39            | THR                  | C      |

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Table S33 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 40            | SER                  | C      |
| 32             | 41            | PRO                  | C      |
| 33             | 42            | ILE                  | C      |
| 34             | 43            | ASN                  | C      |
| 35             | 44            | GLN                  | C      |
| 36             | 45            | VAL                  | C      |
| 37             | 46            | LYS                  | C      |
| 38             | 48            | GLY                  | C      |
| 39             | 59            | TYR                  | C      |
| 40             | 60            | TRP                  | C      |
| 41             | 61            | LEU                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | THR                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | GLN                  | C      |
| 49             | 69            | ILE                  | C      |
| 50             | 70            | GLY                  | C      |
| 51             | 72            | ARG                  | C      |
| 52             | 73            | TYR                  | C      |
| 53             | 74            | LEU                  | C      |
| 54             | 75            | GLY                  | C      |
| 55             | 76            | THR                  | C      |
| 56             | 77            | GLU                  | C      |
| 57             | 78            | GLN                  | C      |
| 58             | 79            | GLU                  | C      |
| 59             | 80            | PHE                  | C      |
| 60             | 81            | LYS                  | C      |
| 61             | 82            | GLU                  | C      |
| 62             | 83            | MET                  | C      |
| 63             | 84            | CYS                  | C      |
| 64             | 85            | ALA                  | C      |
| 65             | 86            | ALA                  | C      |
| 66             | 87            | ALA                  | C      |
| 67             | 88            | GLU                  | C      |
| 68             | 89            | GLU                  | C      |
| 69             | 90            | TYR                  | C      |
| 70             | 91            | GLY                  | C      |
| 71             | 92            | ILE                  | C      |
| 72             | 93            | LYS                  | C      |
| 73             | 94            | VAL                  | C      |
| 74             | 95            | ILE                  | C      |
| 75             | 96            | VAL                  | C      |
| 76             | 97            | ASP                  | C      |

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Table S33 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 98            | ALA                  | C      |
| 78             | 99            | VAL                  | C      |
| 79             | 100           | ILE                  | C      |
| 80             | 101           | ASN                  | C      |
| 81             | 102           | HIS                  | C      |
| 82             | 103           | THR                  | C      |
| 83             | 104           | THR                  | C      |
| 84             | 105           | PHE                  | C      |
| 85             | 106           | ASP                  | C      |
| 86             | 111           | SER                  | C      |
| 87             | 113           | GLU                  | C      |
| 88             | 114           | VAL                  | C      |
| 89             | 115           | LYS                  | C      |
| 90             | 118           | PRO                  | C      |
| 91             | 119           | ASN                  | C      |
| 92             | 120           | TRP                  | C      |
| 93             | 121           | THR                  | C      |
| 94             | 122           | HIS                  | B      |
| 95             | 139           | ASN                  | B      |
| 96             | 140           | SER                  | B      |
| 97             | 141           | LEU                  | B      |
| 98             | 142           | LEU                  | B      |
| 99             | 144           | LEU                  | B      |
| 100            | 145           | TYR                  | B      |
| 101            | 146           | ASP                  | B      |
| 102            | 147           | TRP                  | B      |
| 103            | 148           | ASN                  | B      |
| 104            | 149           | THR                  | B      |
| 105            | 150           | GLN                  | B      |
| 106            | 151           | ASN                  | B      |
| 107            | 152           | THR                  | B      |
| 108            | 153           | GLN                  | B      |
| 109            | 154           | VAL                  | B      |
| 110            | 155           | GLN                  | B      |
| 111            | 156           | SER                  | B      |
| 112            | 157           | TYR                  | B      |
| 113            | 158           | LEU                  | B      |
| 114            | 159           | LYS                  | B      |
| 115            | 160           | ARG                  | B      |
| 116            | 161           | PHE                  | B      |
| 117            | 162           | LEU                  | B      |
| 118            | 163           | GLU                  | B      |
| 119            | 164           | ARG                  | B      |
| 120            | 165           | ALA                  | B      |
| 121            | 166           | LEU                  | B      |
| 122            | 167           | ASN                  | B      |

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Table S33 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 168           | ASP                  | C      |
| 124            | 169           | GLY                  | C      |
| 125            | 170           | ALA                  | C      |
| 126            | 171           | ASP                  | C      |
| 127            | 172           | GLY                  | C      |
| 128            | 173           | PHE                  | B      |
| 129            | 174           | ARG                  | D      |
| 130            | 175           | PHE                  | B      |
| 131            | 176           | ASP                  | B      |
| 132            | 177           | ALA                  | B      |
| 133            | 178           | ALA                  | B      |
| 134            | 179           | LYS                  | B      |
| 135            | 180           | HIS                  | B      |
| 136            | 181           | ILE                  | B      |
| 137            | 182           | GLU                  | B      |
| 138            | 191           | SER                  | B      |
| 139            | 192           | GLN                  | B      |
| 140            | 193           | PHE                  | B      |
| 141            | 194           | TRP                  | B      |
| 142            | 195           | PRO                  | B      |
| 143            | 196           | ASN                  | B      |
| 144            | 197           | ILE                  | B      |
| 145            | 198           | THR                  | B      |
| 146            | 199           | ASN                  | B      |
| 147            | 200           | THR                  | B      |
| 148            | 201           | SER                  | B      |
| 149            | 202           | ALA                  | B      |
| 150            | 203           | GLU                  | B      |
| 151            | 204           | PHE                  | B      |
| 152            | 205           | GLN                  | B      |
| 153            | 206           | TYR                  | C      |
| 154            | 207           | GLY                  | B      |
| 155            | 208           | GLN                  | B      |
| 156            | 209           | ILE                  | B      |
| 157            | 210           | LEU                  | B      |
| 158            | 211           | GLN                  | B      |
| 159            | 212           | ASP                  | B      |
| 160            | 217           | ASP                  | B      |
| 161            | 218           | ALA                  | B      |
| 162            | 219           | ALA                  | B      |
| 163            | 220           | TYR                  | B      |
| 164            | 221           | ALA                  | B      |
| 165            | 222           | ASN                  | B      |
| 166            | 223           | TYR                  | B      |
| 167            | 224           | MET                  | B      |
| 168            | 225           | ASP                  | B      |

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Table S33 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 226           | VAL                  | B      |
| 170            | 227           | THR                  | D      |
| 171            | 228           | ALA                  | D      |
| 172            | 229           | SER                  | D      |
| 173            | 230           | ASN                  | D      |
| 174            | 232           | GLY                  | D      |
| 175            | 233           | HIS                  | D      |
| 176            | 234           | SER                  | D      |
| 177            | 235           | ILE                  | D      |
| 178            | 236           | ARG                  | D      |
| 179            | 237           | SER                  | D      |
| 180            | 238           | ALA                  | D      |
| 181            | 239           | LEU                  | D      |
| 182            | 243           | ASN                  | D      |
| 183            | 244           | LEU                  | A      |
| 184            | 245           | GLY                  | A      |
| 185            | 246           | VAL                  | A      |
| 186            | 249           | ILE                  | A      |
| 187            | 250           | SER                  | D      |
| 188            | 251           | HIS                  | D      |
| 189            | 252           | TYR                  | D      |
| 190            | 253           | ALA                  | D      |
| 191            | 254           | SER                  | B      |
| 192            | 255           | ASP                  | B      |
| 193            | 257           | SER                  | B      |
| 194            | 258           | ALA                  | B      |
| 195            | 259           | ASP                  | B      |
| 196            | 260           | LYS                  | B      |
| 197            | 261           | LEU                  | B      |
| 198            | 262           | VAL                  | D      |
| 199            | 263           | THR                  | D      |
| 200            | 264           | TRP                  | D      |
| 201            | 265           | VAL                  | A      |
| 202            | 266           | GLU                  | D      |
| 203            | 267           | SER                  | D      |
| 204            | 268           | HIS                  | D      |
| 205            | 269           | ASP                  | D      |
| 206            | 270           | THR                  | D      |
| 207            | 271           | TYR                  | D      |
| 208            | 279           | THR                  | D      |
| 209            | 280           | TRP                  | D      |
| 210            | 281           | MET                  | D      |
| 211            | 282           | SER                  | D      |
| 212            | 284           | ASP                  | A      |
| 213            | 285           | ASP                  | A      |
| 214            | 286           | ILE                  | A      |

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Table S33 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 287           | ARG                  | A      |
| 216            | 288           | LEU                  | A      |
| 217            | 289           | GLY                  | A      |
| 218            | 290           | TRP                  | A      |
| 219            | 291           | ALA                  | A      |
| 220            | 292           | VAL                  | A      |
| 221            | 293           | ILE                  | A      |
| 222            | 294           | ALA                  | A      |
| 223            | 295           | SER                  | A      |
| 224            | 296           | ARG                  | A      |
| 225            | 297           | SER                  | D      |
| 226            | 299           | SER                  | D      |
| 227            | 300           | THR                  | D      |
| 228            | 301           | PRO                  | A      |
| 229            | 302           | LEU                  | D      |
| 230            | 303           | PHE                  | A      |
| 231            | 304           | PHE                  | D      |
| 232            | 305           | SER                  | C      |
| 233            | 306           | ARG                  | D      |
| 234            | 307           | PRO                  | A      |
| 235            | 316           | PHE                  | C      |
| 236            | 325           | ARG                  | C      |
| 237            | 326           | GLY                  | D      |
| 238            | 327           | SER                  | D      |
| 239            | 328           | ALA                  | D      |
| 240            | 331           | GLU                  | A      |
| 241            | 332           | ASP                  | A      |
| 242            | 333           | GLN                  | A      |
| 243            | 334           | ALA                  | A      |
| 244            | 335           | ILE                  | A      |
| 245            | 336           | THR                  | A      |
| 246            | 337           | ALA                  | A      |
| 247            | 338           | VAL                  | A      |
| 248            | 339           | ASN                  | A      |
| 249            | 340           | ARG                  | A      |
| 250            | 341           | PHE                  | A      |
| 251            | 342           | HIS                  | A      |
| 252            | 343           | ASN                  | A      |
| 253            | 344           | VAL                  | A      |
| 254            | 345           | MET                  | A      |
| 255            | 346           | ALA                  | A      |
| 256            | 347           | GLY                  | A      |
| 257            | 348           | GLN                  | A      |
| 258            | 349           | PRO                  | A      |
| 259            | 350           | GLU                  | A      |
| 260            | 351           | GLU                  | A      |

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Table S33 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 352           | LEU                  | A      |
| 262            | 353           | SER                  | A      |
| 263            | 354           | ASN                  | A      |
| 264            | 357           | GLY                  | A      |
| 265            | 358           | ASN                  | A      |
| 266            | 359           | ASN                  | A      |
| 267            | 360           | GLN                  | A      |
| 268            | 362           | PHE                  | A      |
| 269            | 363           | MET                  | A      |
| 270            | 364           | ASN                  | A      |
| 271            | 365           | GLN                  | A      |
| 272            | 366           | ARG                  | A      |
| 273            | 367           | GLY                  | A      |
| 274            | 368           | SER                  | A      |
| 275            | 370           | GLY                  | A      |
| 276            | 371           | VAL                  | A      |
| 277            | 372           | VAL                  | A      |
| 278            | 373           | LEU                  | A      |
| 279            | 374           | ALA                  | A      |
| 280            | 375           | ASN                  | A      |
| 281            | 378           | SER                  | A      |
| 282            | 379           | SER                  | A      |
| 283            | 380           | SER                  | A      |
| 284            | 381           | VAL                  | A      |
| 285            | 383           | ILE                  | A      |
| 286            | 384           | ASN                  | A      |
| 287            | 385           | THR                  | A      |
| 288            | 391           | ASP                  | A      |
| 289            | 392           | GLY                  | A      |
| 290            | 394           | TYR                  | A      |
| 291            | 395           | ASP                  | A      |
| 292            | 396           | ASN                  | A      |
| 293            | 397           | LYS                  | A      |
| 294            | 414           | ILE                  | A      |
| 295            | 415           | ASN                  | A      |
| 296            | 416           | ALA                  | A      |
| 297            | 418           | SER                  | A      |
| 298            | 419           | VAL                  | A      |
| 299            | 420           | ALA                  | A      |
| 300            | 421           | VAL                  | A      |
| 301            | 422           | LEU                  | A      |
| 302            | 423           | TYR                  | A      |

Table S34: Residues membership for the *P. haloplanctis*  $\alpha$ -amylase (PDB code 1B0I, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 3             | THR                  | A      |
| 1              | 4             | THR                  | A      |
| 2              | 5             | PHE                  | B      |
| 3              | 6             | VAL                  | B      |
| 4              | 7             | HIS                  | B      |
| 5              | 8             | LEU                  | C      |
| 6              | 9             | PHE                  | C      |
| 7              | 10            | GLU                  | C      |
| 8              | 11            | TRP                  | C      |
| 9              | 12            | ASN                  | C      |
| 10             | 13            | TRP                  | C      |
| 11             | 14            | GLN                  | C      |
| 12             | 15            | ASP                  | C      |
| 13             | 16            | VAL                  | C      |
| 14             | 17            | ALA                  | C      |
| 15             | 18            | GLN                  | C      |
| 16             | 19            | GLU                  | C      |
| 17             | 20            | CYS                  | C      |
| 18             | 21            | GLU                  | C      |
| 19             | 22            | GLN                  | C      |
| 20             | 24            | LEU                  | C      |
| 21             | 25            | GLY                  | C      |
| 22             | 26            | PRO                  | C      |
| 23             | 27            | LYS                  | C      |
| 24             | 28            | GLY                  | C      |
| 25             | 29            | TYR                  | C      |
| 26             | 30            | ALA                  | C      |
| 27             | 31            | ALA                  | C      |
| 28             | 32            | VAL                  | C      |
| 29             | 33            | GLN                  | C      |
| 30             | 34            | VAL                  | C      |
| 31             | 35            | SER                  | C      |
| 32             | 36            | PRO                  | C      |
| 33             | 37            | PRO                  | C      |
| 34             | 38            | ASN                  | C      |
| 35             | 39            | GLU                  | C      |
| 36             | 40            | HIS                  | C      |
| 37             | 41            | ILE                  | C      |
| 38             | 43            | GLY                  | C      |
| 39             | 47            | TRP                  | C      |
| 40             | 48            | THR                  | C      |
| 41             | 49            | ARG                  | C      |
| 42             | 50            | TYR                  | C      |
| 43             | 51            | GLN                  | C      |

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Table S34 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 52            | PRO                  | C      |
| 45             | 53            | VAL                  | C      |
| 46             | 54            | SER                  | C      |
| 47             | 55            | TYR                  | C      |
| 48             | 56            | GLU                  | C      |
| 49             | 57            | LEU                  | C      |
| 50             | 58            | GLN                  | C      |
| 51             | 59            | SER                  | C      |
| 52             | 60            | ARG                  | C      |
| 53             | 61            | GLY                  | C      |
| 54             | 62            | GLY                  | C      |
| 55             | 63            | ASN                  | C      |
| 56             | 64            | ARG                  | C      |
| 57             | 65            | ALA                  | C      |
| 58             | 66            | GLN                  | C      |
| 59             | 67            | PHE                  | C      |
| 60             | 68            | ILE                  | C      |
| 61             | 69            | ASP                  | C      |
| 62             | 70            | MET                  | C      |
| 63             | 71            | VAL                  | C      |
| 64             | 72            | ASN                  | C      |
| 65             | 73            | ARG                  | C      |
| 66             | 74            | CYS                  | C      |
| 67             | 75            | SER                  | C      |
| 68             | 76            | ALA                  | C      |
| 69             | 77            | ALA                  | C      |
| 70             | 78            | GLY                  | C      |
| 71             | 79            | VAL                  | C      |
| 72             | 80            | ASP                  | C      |
| 73             | 81            | ILE                  | C      |
| 74             | 82            | TYR                  | C      |
| 75             | 83            | VAL                  | C      |
| 76             | 84            | ASP                  | C      |
| 77             | 85            | THR                  | C      |
| 78             | 86            | LEU                  | C      |
| 79             | 87            | ILE                  | C      |
| 80             | 88            | ASN                  | C      |
| 81             | 89            | HIS                  | C      |
| 82             | 90            | MET                  | C      |
| 83             | 91            | ALA                  | C      |
| 84             | 92            | ALA                  | C      |
| 85             | 93            | GLY                  | C      |
| 86             | 108           | PHE                  | C      |
| 87             | 110           | ILE                  | C      |
| 88             | 111           | TYR                  | C      |
| 89             | 112           | SER                  | C      |

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Table S34 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 113           | PRO                  | C      |
| 91             | 114           | GLN                  | C      |
| 92             | 115           | ASP                  | C      |
| 93             | 116           | PHE                  | C      |
| 94             | 117           | HIS                  | B      |
| 95             | 137           | CYS                  | B      |
| 96             | 138           | GLU                  | B      |
| 97             | 139           | LEU                  | B      |
| 98             | 140           | VAL                  | B      |
| 99             | 142           | LEU                  | B      |
| 100            | 143           | ALA                  | B      |
| 101            | 144           | ASP                  | B      |
| 102            | 145           | LEU                  | B      |
| 103            | 146           | ASP                  | B      |
| 104            | 147           | THR                  | B      |
| 105            | 148           | ALA                  | B      |
| 106            | 149           | SER                  | B      |
| 107            | 150           | ASN                  | B      |
| 108            | 151           | TYR                  | B      |
| 109            | 152           | VAL                  | B      |
| 110            | 153           | GLN                  | B      |
| 111            | 154           | ASN                  | B      |
| 112            | 155           | THR                  | B      |
| 113            | 156           | ILE                  | B      |
| 114            | 157           | ALA                  | B      |
| 115            | 158           | ALA                  | B      |
| 116            | 159           | TYR                  | B      |
| 117            | 160           | ILE                  | B      |
| 118            | 161           | ASN                  | B      |
| 119            | 162           | ASP                  | B      |
| 120            | 163           | LEU                  | B      |
| 121            | 164           | GLN                  | B      |
| 122            | 165           | ALA                  | B      |
| 123            | 166           | ILE                  | C      |
| 124            | 167           | GLY                  | C      |
| 125            | 168           | VAL                  | C      |
| 126            | 169           | LYS                  | C      |
| 127            | 170           | GLY                  | C      |
| 128            | 171           | PHE                  | B      |
| 129            | 172           | ARG                  | D      |
| 130            | 173           | PHE                  | B      |
| 131            | 174           | ASP                  | B      |
| 132            | 175           | ALA                  | B      |
| 133            | 176           | SER                  | B      |
| 134            | 177           | LYS                  | B      |
| 135            | 178           | HIS                  | B      |

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Table S34 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 179           | VAL                  | B      |
| 137            | 180           | ALA                  | B      |
| 138            | 181           | ALA                  | B      |
| 139            | 182           | SER                  | B      |
| 140            | 183           | ASP                  | B      |
| 141            | 184           | ILE                  | B      |
| 142            | 185           | GLN                  | B      |
| 143            | 186           | SER                  | B      |
| 144            | 187           | LEU                  | B      |
| 145            | 188           | MET                  | B      |
| 146            | 189           | ALA                  | B      |
| 147            | 190           | LYS                  | B      |
| 148            | 191           | VAL                  | B      |
| 149            | 192           | ASN                  | B      |
| 150            | 195           | PRO                  | B      |
| 151            | 196           | VAL                  | B      |
| 152            | 197           | VAL                  | B      |
| 153            | 198           | PHE                  | C      |
| 154            | 199           | GLN                  | B      |
| 155            | 200           | GLU                  | B      |
| 156            | 201           | VAL                  | B      |
| 157            | 202           | ILE                  | B      |
| 158            | 203           | ASP                  | B      |
| 159            | 204           | GLN                  | B      |
| 160            | 211           | ALA                  | B      |
| 161            | 212           | SER                  | B      |
| 162            | 213           | GLU                  | B      |
| 163            | 214           | TYR                  | B      |
| 164            | 215           | LEU                  | B      |
| 165            | 216           | SER                  | B      |
| 166            | 217           | THR                  | B      |
| 167            | 218           | GLY                  | B      |
| 168            | 219           | LEU                  | B      |
| 169            | 220           | VAL                  | B      |
| 170            | 221           | THR                  | D      |
| 171            | 222           | GLU                  | D      |
| 172            | 223           | PHE                  | D      |
| 173            | 224           | LYS                  | D      |
| 174            | 226           | SER                  | D      |
| 175            | 227           | THR                  | D      |
| 176            | 228           | GLU                  | D      |
| 177            | 229           | LEU                  | D      |
| 178            | 230           | GLY                  | D      |
| 179            | 231           | ASN                  | D      |
| 180            | 232           | THR                  | D      |
| 181            | 233           | PHE                  | D      |

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Table S34 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 236           | GLY                  | D      |
| 183            | 237           | SER                  | A      |
| 184            | 238           | LEU                  | A      |
| 185            | 239           | ALA                  | A      |
| 186            | 244           | PHE                  | A      |
| 187            | 245           | GLY                  | D      |
| 188            | 246           | GLU                  | D      |
| 189            | 247           | GLY                  | D      |
| 190            | 249           | GLY                  | D      |
| 191            | 250           | PHE                  | B      |
| 192            | 251           | MET                  | B      |
| 193            | 252           | PRO                  | B      |
| 194            | 253           | SER                  | B      |
| 195            | 254           | SER                  | B      |
| 196            | 255           | SER                  | B      |
| 197            | 256           | ALA                  | B      |
| 198            | 257           | VAL                  | D      |
| 199            | 258           | VAL                  | D      |
| 200            | 259           | PHE                  | D      |
| 201            | 260           | VAL                  | A      |
| 202            | 261           | ASP                  | D      |
| 203            | 262           | ASN                  | D      |
| 204            | 263           | HIS                  | D      |
| 205            | 264           | ASP                  | D      |
| 206            | 265           | ASN                  | D      |
| 207            | 266           | GLN                  | D      |
| 208            | 277           | THR                  | D      |
| 209            | 278           | PHE                  | D      |
| 210            | 279           | GLU                  | D      |
| 211            | 280           | ASP                  | D      |
| 212            | 282           | ARG                  | A      |
| 213            | 283           | LEU                  | A      |
| 214            | 284           | TYR                  | A      |
| 215            | 285           | ASP                  | A      |
| 216            | 286           | LEU                  | A      |
| 217            | 287           | ALA                  | A      |
| 218            | 288           | ASN                  | A      |
| 219            | 289           | VAL                  | A      |
| 220            | 290           | PHE                  | A      |
| 221            | 291           | MET                  | A      |
| 222            | 292           | LEU                  | A      |
| 223            | 293           | ALA                  | A      |
| 224            | 294           | TYR                  | A      |
| 225            | 296           | TYR                  | D      |
| 226            | 297           | GLY                  | D      |
| 227            | 298           | TYR                  | D      |

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Table S34 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 299           | PRO                  | A      |
| 229            | 300           | LYS                  | D      |
| 230            | 301           | VAL                  | A      |
| 231            | 302           | MET                  | D      |
| 232            | 303           | SER                  | C      |
| 233            | 304           | SER                  | D      |
| 234            | 305           | TYR                  | A      |
| 235            | 306           | ASP                  | C      |
| 236            | 332           | ASN                  | C      |
| 237            | 333           | TRP                  | D      |
| 238            | 334           | LYS                  | D      |
| 239            | 335           | CYS                  | D      |
| 240            | 338           | ARG                  | A      |
| 241            | 339           | TRP                  | A      |
| 242            | 340           | SER                  | A      |
| 243            | 341           | TYR                  | A      |
| 244            | 342           | ILE                  | A      |
| 245            | 343           | ALA                  | A      |
| 246            | 344           | GLY                  | A      |
| 247            | 345           | GLY                  | A      |
| 248            | 346           | VAL                  | A      |
| 249            | 347           | ASP                  | A      |
| 250            | 348           | PHE                  | A      |
| 251            | 349           | ARG                  | A      |
| 252            | 350           | ASN                  | A      |
| 253            | 351           | ASN                  | A      |
| 254            | 352           | THR                  | A      |
| 255            | 353           | ALA                  | A      |
| 256            | 355           | ASN                  | A      |
| 257            | 356           | TRP                  | A      |
| 258            | 357           | ALA                  | A      |
| 259            | 358           | VAL                  | A      |
| 260            | 360           | ASN                  | A      |
| 261            | 361           | TRP                  | A      |
| 262            | 362           | TRP                  | A      |
| 263            | 363           | ASP                  | A      |
| 264            | 365           | THR                  | A      |
| 265            | 366           | ASN                  | A      |
| 266            | 367           | ASN                  | A      |
| 267            | 368           | GLN                  | A      |
| 268            | 369           | ILE                  | A      |
| 269            | 370           | SER                  | A      |
| 270            | 371           | PHE                  | A      |
| 271            | 372           | GLY                  | A      |
| 272            | 373           | ARG                  | A      |
| 273            | 374           | GLY                  | A      |

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Table S34 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 375           | SER                  | A      |
| 275            | 377           | GLY                  | A      |
| 276            | 378           | HIS                  | A      |
| 277            | 379           | MET                  | A      |
| 278            | 380           | ALA                  | A      |
| 279            | 381           | ILE                  | A      |
| 280            | 382           | ASN                  | A      |
| 281            | 385           | ASP                  | A      |
| 282            | 386           | SER                  | A      |
| 283            | 387           | THR                  | A      |
| 284            | 388           | LEU                  | A      |
| 285            | 389           | THR                  | A      |
| 286            | 390           | ALA                  | A      |
| 287            | 391           | THR                  | A      |
| 288            | 397           | ALA                  | A      |
| 289            | 398           | SER                  | A      |
| 290            | 401           | TYR                  | A      |
| 291            | 402           | CYS                  | A      |
| 292            | 403           | ASN                  | A      |
| 293            | 404           | VAL                  | A      |
| 294            | 433           | ILE                  | A      |
| 295            | 434           | GLY                  | A      |
| 296            | 435           | ALA                  | A      |
| 297            | 437           | ASP                  | A      |
| 298            | 438           | ALA                  | A      |
| 299            | 439           | MET                  | A      |
| 300            | 440           | ALA                  | A      |
| 301            | 441           | ILE                  | A      |
| 302            | 442           | HIS                  | A      |

Table S35: Residues membership for the *B. licheniformis*  $\alpha$ -amylase (PDB code 1BLI, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 5             | GLY                  | A      |
| 1              | 6             | THR                  | A      |
| 2              | 7             | LEU                  | B      |
| 3              | 8             | MET                  | B      |
| 4              | 9             | GLN                  | B      |
| 5              | 10            | TYR                  | C      |
| 6              | 11            | PHE                  | C      |
| 7              | 15            | MET                  | C      |
| 8              | 20            | GLN                  | C      |

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Table S35 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 21            | HIS                  | C      |
| 10             | 22            | TRP                  | C      |
| 11             | 23            | LYS                  | C      |
| 12             | 24            | ARG                  | C      |
| 13             | 25            | LEU                  | C      |
| 14             | 26            | GLN                  | C      |
| 15             | 27            | ASN                  | C      |
| 16             | 28            | ASP                  | C      |
| 17             | 29            | SER                  | C      |
| 18             | 30            | ALA                  | C      |
| 19             | 31            | TYR                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | GLU                  | C      |
| 23             | 35            | HIS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | ILE                  | C      |
| 26             | 38            | THR                  | C      |
| 27             | 39            | ALA                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | TRP                  | C      |
| 30             | 42            | ILE                  | C      |
| 31             | 43            | PRO                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | ALA                  | C      |
| 34             | 46            | TYR                  | C      |
| 35             | 47            | LYS                  | C      |
| 36             | 48            | GLY                  | C      |
| 37             | 49            | THR                  | C      |
| 38             | 52            | ALA                  | C      |
| 39             | 53            | ASP                  | C      |
| 40             | 54            | VAL                  | C      |
| 41             | 55            | GLY                  | C      |
| 42             | 56            | TYR                  | C      |
| 43             | 57            | GLY                  | C      |
| 44             | 58            | ALA                  | C      |
| 45             | 59            | TYR                  | C      |
| 46             | 60            | ASP                  | C      |
| 47             | 62            | TYR                  | C      |
| 48             | 63            | ASP                  | C      |
| 49             | 64            | LEU                  | C      |
| 50             | 65            | GLY                  | C      |
| 51             | 75            | THR                  | C      |
| 52             | 76            | LYS                  | C      |
| 53             | 77            | TYR                  | C      |
| 54             | 78            | GLY                  | C      |

*Continued on next page*

Table S35 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 79            | THR                  | C      |
| 56             | 80            | LYS                  | C      |
| 57             | 81            | GLY                  | C      |
| 58             | 82            | GLU                  | C      |
| 59             | 83            | LEU                  | C      |
| 60             | 84            | GLN                  | C      |
| 61             | 85            | SER                  | C      |
| 62             | 86            | ALA                  | C      |
| 63             | 87            | ILE                  | C      |
| 64             | 88            | LYS                  | C      |
| 65             | 89            | SER                  | C      |
| 66             | 90            | LEU                  | C      |
| 67             | 91            | HIS                  | C      |
| 68             | 92            | SER                  | C      |
| 69             | 93            | ARG                  | C      |
| 70             | 94            | ASP                  | C      |
| 71             | 95            | ILE                  | C      |
| 72             | 96            | ASN                  | C      |
| 73             | 97            | VAL                  | C      |
| 74             | 98            | TYR                  | C      |
| 75             | 99            | GLY                  | C      |
| 76             | 100           | ASP                  | C      |
| 77             | 101           | VAL                  | C      |
| 78             | 102           | VAL                  | C      |
| 79             | 103           | ILE                  | C      |
| 80             | 104           | ASN                  | C      |
| 81             | 105           | HIS                  | C      |
| 82             | 106           | LYS                  | C      |
| 83             | 107           | GLY                  | C      |
| 84             | 108           | GLY                  | C      |
| 85             | 109           | ALA                  | C      |
| 86             | 141           | PHE                  | C      |
| 87             | 154           | LYS                  | C      |
| 88             | 155           | TRP                  | C      |
| 89             | 156           | HIS                  | C      |
| 90             | 157           | TRP                  | C      |
| 91             | 158           | TYR                  | C      |
| 92             | 159           | HIS                  | C      |
| 93             | 160           | PHE                  | C      |
| 94             | 161           | ASP                  | B      |
| 95             | 194           | ASP                  | B      |
| 96             | 195           | TYR                  | B      |
| 97             | 196           | LEU                  | B      |
| 98             | 197           | MET                  | B      |
| 99             | 198           | TYR                  | B      |
| 100            | 199           | ALA                  | B      |

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Table S35 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 200           | ASP                  | B      |
| 102            | 201           | ILE                  | B      |
| 103            | 202           | ASP                  | B      |
| 104            | 203           | TYR                  | B      |
| 105            | 204           | ASP                  | B      |
| 106            | 205           | HIS                  | B      |
| 107            | 206           | PRO                  | B      |
| 108            | 207           | ASP                  | B      |
| 109            | 208           | VAL                  | B      |
| 110            | 209           | ALA                  | B      |
| 111            | 210           | ALA                  | B      |
| 112            | 211           | GLU                  | B      |
| 113            | 212           | ILE                  | B      |
| 114            | 213           | LYS                  | B      |
| 115            | 214           | ARG                  | B      |
| 116            | 215           | TRP                  | B      |
| 117            | 216           | GLY                  | B      |
| 118            | 217           | THR                  | B      |
| 119            | 218           | TRP                  | B      |
| 120            | 219           | TYR                  | B      |
| 121            | 220           | ALA                  | B      |
| 122            | 221           | ASN                  | B      |
| 123            | 223           | LEU                  | C      |
| 124            | 224           | GLN                  | C      |
| 125            | 225           | LEU                  | C      |
| 126            | 226           | ASP                  | C      |
| 127            | 227           | GLY                  | C      |
| 128            | 228           | PHE                  | B      |
| 129            | 229           | ARG                  | D      |
| 130            | 230           | LEU                  | B      |
| 131            | 231           | ASP                  | B      |
| 132            | 232           | ALA                  | B      |
| 133            | 233           | VAL                  | B      |
| 134            | 234           | LYS                  | B      |
| 135            | 235           | HIS                  | B      |
| 136            | 236           | ILE                  | B      |
| 137            | 237           | LYS                  | B      |
| 138            | 238           | PHE                  | B      |
| 139            | 239           | SER                  | B      |
| 140            | 240           | PHE                  | B      |
| 141            | 241           | LEU                  | B      |
| 142            | 242           | ARG                  | B      |
| 143            | 243           | ASP                  | B      |
| 144            | 244           | TRP                  | B      |
| 145            | 245           | VAL                  | B      |
| 146            | 246           | ASN                  | B      |

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Table S35 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 247           | HIS                  | B      |
| 148            | 248           | VAL                  | B      |
| 149            | 249           | ARG                  | B      |
| 150            | 256           | MET                  | B      |
| 151            | 257           | PHE                  | B      |
| 152            | 258           | THR                  | B      |
| 153            | 259           | VAL                  | C      |
| 154            | 260           | ALA                  | B      |
| 155            | 261           | GLU                  | B      |
| 156            | 262           | TYR                  | B      |
| 157            | 263           | TRP                  | B      |
| 158            | 264           | SER                  | B      |
| 159            | 265           | TYR                  | B      |
| 160            | 270           | LEU                  | B      |
| 161            | 271           | GLU                  | B      |
| 162            | 272           | ASN                  | B      |
| 163            | 273           | TYR                  | B      |
| 164            | 274           | LEU                  | B      |
| 165            | 275           | ASN                  | B      |
| 166            | 280           | ASN                  | B      |
| 167            | 281           | HIS                  | B      |
| 168            | 282           | SER                  | B      |
| 169            | 283           | VAL                  | B      |
| 170            | 284           | PHE                  | D      |
| 171            | 285           | ASP                  | D      |
| 172            | 286           | VAL                  | D      |
| 173            | 287           | PRO                  | D      |
| 174            | 289           | HIS                  | D      |
| 175            | 290           | TYR                  | D      |
| 176            | 291           | GLN                  | D      |
| 177            | 292           | PHE                  | D      |
| 178            | 293           | HIS                  | D      |
| 179            | 294           | ALA                  | D      |
| 180            | 295           | ALA                  | D      |
| 181            | 296           | SER                  | D      |
| 182            | 302           | TYR                  | D      |
| 183            | 303           | ASP                  | A      |
| 184            | 304           | MET                  | A      |
| 185            | 305           | ARG                  | A      |
| 186            | 307           | LEU                  | A      |
| 187            | 308           | LEU                  | D      |
| 188            | 309           | ASN                  | D      |
| 189            | 310           | GLY                  | D      |
| 190            | 313           | VAL                  | D      |
| 191            | 314           | SER                  | B      |
| 192            | 315           | LYS                  | B      |

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Table S35 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 316           | HIS                  | B      |
| 194            | 317           | PRO                  | B      |
| 195            | 318           | LEU                  | B      |
| 196            | 319           | LYS                  | B      |
| 197            | 320           | SER                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | VAL                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | THR                  | D      |
| 207            | 330           | GLN                  | D      |
| 208            | 338           | THR                  | D      |
| 209            | 339           | VAL                  | D      |
| 210            | 340           | GLN                  | D      |
| 211            | 341           | THR                  | D      |
| 212            | 342           | TRP                  | A      |
| 213            | 343           | PHE                  | A      |
| 214            | 344           | LYS                  | A      |
| 215            | 345           | PRO                  | A      |
| 216            | 346           | LEU                  | A      |
| 217            | 347           | ALA                  | A      |
| 218            | 348           | TYR                  | A      |
| 219            | 349           | ALA                  | A      |
| 220            | 350           | PHE                  | A      |
| 221            | 351           | ILE                  | A      |
| 222            | 352           | LEU                  | A      |
| 223            | 353           | THR                  | A      |
| 224            | 354           | ARG                  | A      |
| 225            | 356           | SER                  | D      |
| 226            | 357           | GLY                  | D      |
| 227            | 358           | TYR                  | D      |
| 228            | 359           | PRO                  | A      |
| 229            | 360           | GLN                  | D      |
| 230            | 361           | VAL                  | A      |
| 231            | 362           | PHE                  | D      |
| 232            | 363           | TYR                  | C      |
| 233            | 364           | GLY                  | D      |
| 234            | 365           | ASP                  | A      |
| 235            | 366           | MET                  | C      |
| 236            | 367           | TYR                  | C      |
| 237            | 368           | GLY                  | D      |
| 238            | 369           | THR                  | D      |

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Table S35 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 379           | ALA                  | D      |
| 240            | 380           | LEU                  | A      |
| 241            | 381           | LYS                  | A      |
| 242            | 382           | HIS                  | A      |
| 243            | 383           | LYS                  | A      |
| 244            | 384           | ILE                  | A      |
| 245            | 385           | GLU                  | A      |
| 246            | 386           | PRO                  | A      |
| 247            | 387           | ILE                  | A      |
| 248            | 388           | LEU                  | A      |
| 249            | 389           | LYS                  | A      |
| 250            | 390           | ALA                  | A      |
| 251            | 391           | ARG                  | A      |
| 252            | 392           | LYS                  | A      |
| 253            | 393           | GLN                  | A      |
| 254            | 394           | TYR                  | A      |
| 255            | 395           | ALA                  | A      |
| 256            | 397           | GLY                  | A      |
| 257            | 398           | ALA                  | A      |
| 258            | 399           | GLN                  | A      |
| 259            | 400           | HIS                  | A      |
| 260            | 401           | ASP                  | A      |
| 261            | 402           | TYR                  | A      |
| 262            | 403           | PHE                  | A      |
| 263            | 404           | ASP                  | A      |
| 264            | 405           | HIS                  | A      |
| 265            | 406           | HIS                  | A      |
| 266            | 407           | ASP                  | A      |
| 267            | 408           | ILE                  | A      |
| 268            | 409           | VAL                  | A      |
| 269            | 410           | GLY                  | A      |
| 270            | 411           | TRP                  | A      |
| 271            | 412           | THR                  | A      |
| 272            | 413           | ARG                  | A      |
| 273            | 414           | GLU                  | A      |
| 274            | 415           | GLY                  | A      |
| 275            | 424           | LEU                  | A      |
| 276            | 425           | ALA                  | A      |
| 277            | 426           | ALA                  | A      |
| 278            | 427           | LEU                  | A      |
| 279            | 428           | ILE                  | A      |
| 280            | 429           | THR                  | A      |
| 281            | 431           | GLY                  | A      |
| 282            | 432           | PRO                  | A      |
| 283            | 433           | GLY                  | A      |
| 284            | 434           | GLY                  | A      |

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Table S35 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 435           | ALA                  | A      |
| 286            | 436           | LYS                  | A      |
| 287            | 437           | ARG                  | A      |
| 288            | 446           | GLY                  | A      |
| 289            | 447           | GLU                  | A      |
| 290            | 449           | TRP                  | A      |
| 291            | 450           | HIS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | ILE                  | A      |
| 294            | 472           | VAL                  | A      |
| 295            | 473           | ASN                  | A      |
| 296            | 474           | GLY                  | A      |
| 297            | 476           | SER                  | A      |
| 298            | 477           | VAL                  | A      |
| 299            | 478           | SER                  | A      |
| 300            | 479           | ILE                  | A      |
| 301            | 480           | TYR                  | A      |
| 302            | 481           | VAL                  | A      |

Table S36: Residues membership for the *P. amyloclavata*  $\alpha$ -amylase (PDB code 1BF2, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 179           | ASP                  | A      |
| 1              | 180           | VAL                  | A      |
| 2              | 181           | ILE                  | B      |
| 3              | 182           | TYR                  | B      |
| 4              | 183           | GLU                  | B      |
| 5              | 184           | VAL                  | C      |
| 6              | 185           | HIS                  | C      |
| 7              | 186           | VAL                  | C      |
| 8              | 202           | GLY                  | C      |
| 9              | 203           | THR                  | C      |
| 10             | 204           | TYR                  | C      |
| 11             | 205           | TYR                  | C      |
| 12             | 206           | GLY                  | C      |
| 13             | 207           | ALA                  | C      |
| 14             | 208           | GLY                  | C      |
| 15             | 209           | LEU                  | C      |
| 16             | 210           | LYS                  | C      |
| 17             | 211           | ALA                  | C      |
| 18             | 212           | SER                  | C      |
| 19             | 213           | TYR                  | C      |

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Table S36 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 214           | LEU                  | C      |
| 21             | 215           | ALA                  | C      |
| 22             | 216           | SER                  | C      |
| 23             | 217           | LEU                  | C      |
| 24             | 218           | GLY                  | C      |
| 25             | 219           | VAL                  | C      |
| 26             | 220           | THR                  | C      |
| 27             | 221           | ALA                  | C      |
| 28             | 222           | VAL                  | C      |
| 29             | 223           | GLU                  | C      |
| 30             | 224           | PHE                  | C      |
| 31             | 225           | LEU                  | C      |
| 32             | 226           | PRO                  | C      |
| 33             | 227           | VAL                  | C      |
| 34             | 228           | GLN                  | C      |
| 35             | 229           | GLU                  | C      |
| 36             | 230           | THR                  | C      |
| 37             | 231           | GLN                  | C      |
| 38             | 246           | ASN                  | C      |
| 39             | 247           | TYR                  | C      |
| 40             | 248           | TRP                  | C      |
| 41             | 249           | GLY                  | C      |
| 42             | 250           | TYR                  | C      |
| 43             | 251           | MET                  | C      |
| 44             | 252           | THR                  | C      |
| 45             | 253           | GLU                  | C      |
| 46             | 254           | ASN                  | C      |
| 47             | 256           | PHE                  | C      |
| 48             | 257           | SER                  | C      |
| 49             | 258           | PRO                  | C      |
| 50             | 259           | ASP                  | C      |
| 51             | 260           | ARG                  | C      |
| 52             | 261           | ARG                  | C      |
| 53             | 262           | TYR                  | C      |
| 54             | 263           | ALA                  | C      |
| 55             | 264           | TYR                  | C      |
| 56             | 272           | THR                  | C      |
| 57             | 273           | ALA                  | C      |
| 58             | 274           | GLU                  | C      |
| 59             | 275           | PHE                  | C      |
| 60             | 276           | GLN                  | C      |
| 61             | 277           | ALA                  | C      |
| 62             | 278           | MET                  | C      |
| 63             | 279           | VAL                  | C      |
| 64             | 280           | GLN                  | C      |
| 65             | 281           | ALA                  | C      |

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Table S36 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 282           | PHE                  | C      |
| 67             | 283           | HIS                  | C      |
| 68             | 284           | ASN                  | C      |
| 69             | 285           | ALA                  | C      |
| 70             | 286           | GLY                  | C      |
| 71             | 287           | ILE                  | C      |
| 72             | 288           | LYS                  | C      |
| 73             | 289           | VAL                  | C      |
| 74             | 290           | TYR                  | C      |
| 75             | 291           | MET                  | C      |
| 76             | 292           | ASP                  | C      |
| 77             | 293           | VAL                  | C      |
| 78             | 294           | VAL                  | C      |
| 79             | 295           | TYR                  | C      |
| 80             | 296           | ASN                  | C      |
| 81             | 297           | HIS                  | C      |
| 82             | 298           | THR                  | C      |
| 83             | 299           | ALA                  | C      |
| 84             | 300           | GLU                  | C      |
| 85             | 301           | GLY                  | C      |
| 86             | 315           | TYR                  | C      |
| 87             | 316           | SER                  | C      |
| 88             | 317           | TRP                  | C      |
| 89             | 318           | ARG                  | C      |
| 90             | 323           | ALA                  | C      |
| 91             | 324           | THR                  | C      |
| 92             | 325           | TYR                  | C      |
| 93             | 326           | TYR                  | C      |
| 94             | 327           | GLU                  | B      |
| 95             | 337           | ASP                  | B      |
| 96             | 338           | ASN                  | B      |
| 97             | 339           | THR                  | B      |
| 98             | 340           | GLY                  | B      |
| 99             | 341           | ILE                  | B      |
| 100            | 343           | ALA                  | B      |
| 101            | 344           | ASN                  | B      |
| 102            | 345           | PHE                  | B      |
| 103            | 346           | ASN                  | B      |
| 104            | 347           | THR                  | B      |
| 105            | 348           | TYR                  | B      |
| 106            | 349           | ASN                  | B      |
| 107            | 350           | THR                  | B      |
| 108            | 351           | VAL                  | B      |
| 109            | 352           | ALA                  | B      |
| 110            | 353           | GLN                  | B      |
| 111            | 354           | ASN                  | B      |

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Table S36 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 355           | LEU                  | B      |
| 113            | 356           | ILE                  | B      |
| 114            | 357           | VAL                  | B      |
| 115            | 358           | ASP                  | B      |
| 116            | 359           | SER                  | B      |
| 117            | 360           | LEU                  | B      |
| 118            | 361           | ALA                  | B      |
| 119            | 362           | TYR                  | B      |
| 120            | 363           | TRP                  | B      |
| 121            | 364           | ALA                  | B      |
| 122            | 365           | ASN                  | B      |
| 123            | 367           | MET                  | C      |
| 124            | 368           | GLY                  | C      |
| 125            | 369           | VAL                  | C      |
| 126            | 370           | ASP                  | C      |
| 127            | 371           | GLY                  | C      |
| 128            | 372           | PHE                  | B      |
| 129            | 373           | ARG                  | D      |
| 130            | 374           | PHE                  | B      |
| 131            | 375           | ASP                  | B      |
| 132            | 376           | LEU                  | B      |
| 133            | 377           | ALA                  | B      |
| 134            | 378           | SER                  | B      |
| 135            | 379           | VAL                  | B      |
| 136            | 380           | LEU                  | B      |
| 137            | 381           | GLY                  | B      |
| 138            | 409           | ASN                  | B      |
| 139            | 410           | VAL                  | B      |
| 140            | 411           | ALA                  | B      |
| 141            | 412           | ILE                  | B      |
| 142            | 413           | ASN                  | B      |
| 143            | 414           | ARG                  | B      |
| 144            | 415           | ILE                  | B      |
| 145            | 416           | LEU                  | B      |
| 146            | 417           | ARG                  | B      |
| 147            | 418           | GLU                  | B      |
| 148            | 419           | PHE                  | B      |
| 149            | 420           | THR                  | B      |
| 150            | 430           | LEU                  | B      |
| 151            | 431           | ASP                  | B      |
| 152            | 432           | LEU                  | B      |
| 153            | 433           | PHE                  | C      |
| 154            | 434           | ALA                  | B      |
| 155            | 435           | GLU                  | B      |
| 156            | 436           | PRO                  | B      |
| 157            | 443           | SER                  | B      |

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Table S36 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 444           | TYR                  | B      |
| 159            | 445           | GLN                  | B      |
| 160            | 446           | LEU                  | B      |
| 161            | 447           | GLY                  | B      |
| 162            | 448           | GLY                  | B      |
| 163            | 449           | PHE                  | B      |
| 164            | 450           | PRO                  | B      |
| 165            | 451           | GLN                  | B      |
| 166            | 452           | GLY                  | B      |
| 167            | 453           | TRP                  | B      |
| 168            | 454           | SER                  | B      |
| 169            | 455           | GLU                  | B      |
| 170            | 456           | TRP                  | D      |
| 171            | 457           | ASN                  | D      |
| 172            | 458           | GLY                  | D      |
| 173            | 459           | LEU                  | D      |
| 174            | 461           | ARG                  | D      |
| 175            | 462           | ASP                  | D      |
| 176            | 463           | SER                  | D      |
| 177            | 464           | LEU                  | D      |
| 178            | 465           | ARG                  | D      |
| 179            | 466           | GLN                  | D      |
| 180            | 467           | ALA                  | D      |
| 181            | 468           | GLN                  | D      |
| 182            | 475           | THR                  | D      |
| 183            | 476           | ILE                  | A      |
| 184            | 477           | TYR                  | A      |
| 185            | 478           | VAL                  | A      |
| 186            | 480           | GLN                  | A      |
| 187            | 481           | ASP                  | D      |
| 188            | 482           | ALA                  | D      |
| 189            | 483           | ASN                  | D      |
| 190            | 488           | SER                  | D      |
| 191            | 489           | SER                  | B      |
| 192            | 490           | ASN                  | B      |
| 193            | 498           | SER                  | B      |
| 194            | 499           | PRO                  | B      |
| 195            | 500           | TRP                  | B      |
| 196            | 501           | ASN                  | B      |
| 197            | 502           | SER                  | B      |
| 198            | 503           | ILE                  | D      |
| 199            | 504           | ASN                  | D      |
| 200            | 505           | PHE                  | D      |
| 201            | 506           | ILE                  | A      |
| 202            | 507           | ASP                  | D      |
| 203            | 508           | VAL                  | D      |

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Table S36 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 509           | HIS                  | D      |
| 205            | 510           | ASP                  | D      |
| 206            | 511           | GLY                  | D      |
| 207            | 512           | MET                  | D      |
| 208            | 513           | THR                  | D      |
| 209            | 514           | LEU                  | D      |
| 210            | 515           | LYS                  | D      |
| 211            | 516           | ASP                  | D      |
| 212            | 559           | ARG                  | A      |
| 213            | 561           | ALA                  | A      |
| 214            | 562           | ALA                  | A      |
| 215            | 563           | ARG                  | A      |
| 216            | 564           | THR                  | A      |
| 217            | 565           | GLY                  | A      |
| 218            | 566           | MET                  | A      |
| 219            | 567           | ALA                  | A      |
| 220            | 568           | PHE                  | A      |
| 221            | 569           | GLU                  | A      |
| 222            | 570           | MET                  | A      |
| 223            | 571           | LEU                  | A      |
| 224            | 572           | SER                  | A      |
| 225            | 573           | ALA                  | D      |
| 226            | 574           | GLY                  | D      |
| 227            | 575           | THR                  | D      |
| 228            | 576           | PRO                  | A      |
| 229            | 577           | LEU                  | D      |
| 230            | 578           | MET                  | A      |
| 231            | 579           | GLN                  | D      |
| 232            | 580           | GLY                  | C      |
| 233            | 581           | GLY                  | D      |
| 234            | 582           | ASP                  | A      |
| 235            | 602           | ASN                  | C      |
| 236            | 603           | TRP                  | C      |
| 237            | 604           | LEU                  | D      |
| 238            | 605           | THR                  | D      |
| 239            | 606           | TYR                  | D      |
| 240            | 615           | PHE                  | A      |
| 241            | 616           | TYR                  | A      |
| 242            | 617           | THR                  | A      |
| 243            | 618           | PHE                  | A      |
| 244            | 619           | ALA                  | A      |
| 245            | 620           | GLN                  | A      |
| 246            | 621           | ARG                  | A      |
| 247            | 622           | LEU                  | A      |
| 248            | 623           | ILE                  | A      |
| 249            | 624           | ALA                  | A      |

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Table S36 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 625           | PHE                  | A      |
| 251            | 626           | ARG                  | A      |
| 252            | 627           | LYS                  | A      |
| 253            | 628           | ALA                  | A      |
| 254            | 629           | HIS                  | A      |
| 255            | 630           | PRO                  | A      |
| 256            | 635           | SER                  | A      |
| 257            | 636           | SER                  | A      |
| 258            | 637           | TRP                  | A      |
| 259            | 638           | TYR                  | A      |
| 260            | 645           | TRP                  | A      |
| 261            | 646           | TYR                  | A      |
| 262            | 647           | GLN                  | A      |
| 263            | 648           | PRO                  | A      |
| 264            | 662           | SER                  | A      |
| 265            | 663           | ASN                  | A      |
| 266            | 664           | TYR                  | A      |
| 267            | 665           | ALA                  | A      |
| 268            | 666           | ILE                  | A      |
| 269            | 667           | ALA                  | A      |
| 270            | 668           | TYR                  | A      |
| 271            | 669           | ALA                  | A      |
| 272            | 670           | ILE                  | A      |
| 273            | 671           | ASN                  | A      |
| 274            | 672           | GLY                  | A      |
| 275            | 681           | ILE                  | A      |
| 276            | 682           | TYR                  | A      |
| 277            | 683           | VAL                  | A      |
| 278            | 684           | ALA                  | A      |
| 279            | 685           | TYR                  | A      |
| 280            | 686           | ASN                  | A      |
| 281            | 690           | SER                  | A      |
| 282            | 691           | SER                  | A      |
| 283            | 692           | VAL                  | A      |
| 284            | 693           | THR                  | A      |
| 285            | 694           | PHE                  | A      |
| 286            | 695           | THR                  | A      |
| 287            | 696           | LEU                  | A      |
| 288            | 703           | THR                  | A      |
| 289            | 704           | GLN                  | A      |
| 290            | 706           | TYR                  | A      |
| 291            | 707           | ARG                  | A      |
| 292            | 708           | VAL                  | A      |
| 293            | 709           | THR                  | A      |
| 294            | 739           | GLN                  | A      |
| 295            | 740           | CYS                  | A      |

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Table S36 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 741           | GLY                  | A      |
| 297            | 743           | SER                  | A      |
| 298            | 744           | LEU                  | A      |
| 299            | 745           | LEU                  | A      |
| 300            | 746           | LEU                  | A      |
| 301            | 747           | LEU                  | A      |
| 302            | 748           | ILE                  | A      |

Table S37: Residues membership for the *T. vulgaris* R47  $\alpha$ -amylase (PDB code 1BVZ, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |
| 30             | 192           | PHE                  | C      |

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Table S37 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |
| 76             | 239           | ASP                  | C      |

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Table S37 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |
| 122            | 316           | GLU                  | B      |

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Table S37 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASP                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |
| 168            | 370           | SER                  | B      |

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Table S37 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASP                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |
| 214            | 436           | PHE                  | A      |

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Table S37 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |
| 260            | 507           | SER                  | A      |

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Table S37 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 574           | ARG                  | A      |
| 295            | 575           | PRO                  | A      |
| 296            | 576           | TYR                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S38: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 1BSI, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |

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Table S38 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |

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Table S38 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |

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Table S38 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |

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Table S38 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |

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Table S38 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |

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Table S38 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S39: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase (PDB code 1CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |

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Table S39 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |

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Table S39 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |

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Table S39 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |

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Table S39 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |

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Table S39 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |

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Table S39 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |

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Table S39 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S40: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1CDG, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |

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Table S40 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |

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Table S40 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |

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Table S40 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |

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Table S40 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |

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Table S40 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |

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Table S40 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | CYS                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |

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Table S40 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S41: Residues membership for the *T. thermosulfurigenes* EM1  $\alpha$ -amylase (PDB code 1CIU, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | VAL                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |

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Table S41 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 96            | THR                  | C      |
| 39             | 98            | TYR                  | C      |
| 40             | 99            | HIS                  | C      |
| 41             | 100           | GLY                  | C      |
| 42             | 101           | TYR                  | C      |
| 43             | 102           | TRP                  | C      |
| 44             | 103           | ALA                  | C      |
| 45             | 104           | ARG                  | C      |
| 46             | 105           | ASP                  | C      |
| 47             | 107           | LYS                  | C      |
| 48             | 108           | ARG                  | C      |
| 49             | 109           | THR                  | C      |
| 50             | 110           | ASN                  | C      |
| 51             | 111           | PRO                  | C      |
| 52             | 112           | TYR                  | C      |
| 53             | 113           | PHE                  | C      |
| 54             | 114           | GLY                  | C      |
| 55             | 115           | SER                  | C      |
| 56             | 116           | PHE                  | C      |
| 57             | 117           | THR                  | C      |
| 58             | 118           | ASP                  | C      |
| 59             | 119           | PHE                  | C      |
| 60             | 120           | GLN                  | C      |
| 61             | 121           | ASN                  | C      |
| 62             | 122           | LEU                  | C      |
| 63             | 123           | ILE                  | C      |
| 64             | 124           | ASN                  | C      |
| 65             | 125           | THR                  | C      |
| 66             | 126           | ALA                  | C      |
| 67             | 127           | HIS                  | C      |
| 68             | 128           | ALA                  | C      |
| 69             | 129           | HIS                  | C      |
| 70             | 130           | ASN                  | C      |
| 71             | 131           | ILE                  | C      |
| 72             | 132           | LYS                  | C      |
| 73             | 133           | VAL                  | C      |
| 74             | 134           | ILE                  | C      |
| 75             | 135           | ILE                  | C      |
| 76             | 136           | ASP                  | C      |

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Table S41 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 137           | PHE                  | C      |
| 78             | 138           | ALA                  | C      |
| 79             | 139           | PRO                  | C      |
| 80             | 140           | ASN                  | C      |
| 81             | 141           | HIS                  | C      |
| 82             | 142           | THR                  | C      |
| 83             | 143           | SER                  | C      |
| 84             | 144           | PRO                  | C      |
| 85             | 145           | ALA                  | C      |
| 86             | 157           | ARG                  | C      |
| 87             | 164           | LEU                  | C      |
| 88             | 165           | LEU                  | C      |
| 89             | 166           | GLY                  | C      |
| 90             | 173           | ASN                  | C      |
| 91             | 174           | GLY                  | C      |
| 92             | 175           | TYR                  | C      |
| 93             | 176           | PHE                  | C      |
| 94             | 177           | HIS                  | B      |
| 95             | 193           | ARG                  | B      |
| 96             | 194           | ASN                  | B      |
| 97             | 195           | LEU                  | B      |
| 98             | 196           | PHE                  | B      |
| 99             | 198           | LEU                  | B      |
| 100            | 199           | ALA                  | B      |
| 101            | 200           | ASP                  | B      |
| 102            | 201           | LEU                  | B      |
| 103            | 202           | ASN                  | B      |
| 104            | 203           | GLN                  | B      |
| 105            | 204           | GLN                  | B      |
| 106            | 205           | ASN                  | B      |
| 107            | 206           | SER                  | B      |
| 108            | 207           | THR                  | B      |
| 109            | 208           | ILE                  | B      |
| 110            | 209           | ASP                  | B      |
| 111            | 210           | SER                  | B      |
| 112            | 211           | TYR                  | B      |
| 113            | 212           | LEU                  | B      |
| 114            | 213           | LYS                  | B      |
| 115            | 214           | SER                  | B      |
| 116            | 215           | ALA                  | B      |
| 117            | 216           | ILE                  | B      |
| 118            | 217           | LYS                  | B      |
| 119            | 218           | VAL                  | B      |
| 120            | 219           | TRP                  | B      |
| 121            | 220           | LEU                  | B      |
| 122            | 221           | ASP                  | B      |

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Table S41 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 222           | MET                  | C      |
| 124            | 223           | GLY                  | C      |
| 125            | 224           | ILE                  | C      |
| 126            | 225           | ASP                  | C      |
| 127            | 226           | GLY                  | C      |
| 128            | 227           | ILE                  | B      |
| 129            | 228           | ARG                  | D      |
| 130            | 229           | LEU                  | B      |
| 131            | 230           | ASP                  | B      |
| 132            | 231           | ALA                  | B      |
| 133            | 232           | VAL                  | B      |
| 134            | 233           | LYS                  | B      |
| 135            | 234           | HIS                  | B      |
| 136            | 235           | MET                  | B      |
| 137            | 236           | PRO                  | B      |
| 138            | 237           | PHE                  | B      |
| 139            | 238           | GLY                  | B      |
| 140            | 239           | TRP                  | B      |
| 141            | 240           | GLN                  | B      |
| 142            | 241           | LYS                  | B      |
| 143            | 242           | ASN                  | B      |
| 144            | 243           | PHE                  | B      |
| 145            | 244           | MET                  | B      |
| 146            | 245           | ASP                  | B      |
| 147            | 246           | SER                  | B      |
| 148            | 247           | ILE                  | B      |
| 149            | 248           | LEU                  | B      |
| 150            | 253           | VAL                  | B      |
| 151            | 254           | PHE                  | B      |
| 152            | 255           | THR                  | B      |
| 153            | 256           | PHE                  | C      |
| 154            | 257           | GLY                  | B      |
| 155            | 258           | GLU                  | B      |
| 156            | 259           | TRP                  | B      |
| 157            | 260           | PHE                  | B      |
| 158            | 261           | LEU                  | B      |
| 159            | 262           | GLY                  | B      |
| 160            | 270           | ASN                  | B      |
| 161            | 271           | THR                  | B      |
| 162            | 272           | TYR                  | B      |
| 163            | 273           | PHE                  | B      |
| 164            | 275           | ASN                  | B      |
| 165            | 276           | GLU                  | B      |
| 166            | 278           | GLY                  | B      |
| 167            | 279           | MET                  | B      |
| 168            | 280           | SER                  | B      |

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Table S41 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 281           | LEU                  | B      |
| 170            | 282           | LEU                  | D      |
| 171            | 283           | ASP                  | D      |
| 172            | 284           | PHE                  | D      |
| 173            | 285           | ARG                  | D      |
| 174            | 287           | SER                  | D      |
| 175            | 288           | GLN                  | D      |
| 176            | 289           | LYS                  | D      |
| 177            | 290           | VAL                  | D      |
| 178            | 291           | ARG                  | D      |
| 179            | 292           | GLN                  | D      |
| 180            | 293           | VAL                  | D      |
| 181            | 294           | PHE                  | D      |
| 182            | 299           | ASP                  | D      |
| 183            | 300           | THR                  | A      |
| 184            | 301           | MET                  | A      |
| 185            | 302           | TYR                  | A      |
| 186            | 307           | MET                  | A      |
| 187            | 308           | ILE                  | D      |
| 188            | 309           | GLN                  | D      |
| 189            | 310           | SER                  | D      |
| 190            | 311           | THR                  | D      |
| 191            | 312           | ALA                  | B      |
| 192            | 313           | SER                  | B      |
| 193            | 317           | PHE                  | B      |
| 194            | 318           | ILE                  | B      |
| 195            | 319           | ASN                  | B      |
| 196            | 320           | ASP                  | B      |
| 197            | 321           | MET                  | B      |
| 198            | 322           | VAL                  | D      |
| 199            | 323           | THR                  | D      |
| 200            | 324           | PHE                  | D      |
| 201            | 325           | ILE                  | A      |
| 202            | 326           | ASP                  | D      |
| 203            | 327           | ASN                  | D      |
| 204            | 328           | HIS                  | D      |
| 205            | 329           | ASP                  | D      |
| 206            | 330           | MET                  | D      |
| 207            | 331           | ASP                  | D      |
| 208            | 332           | ARG                  | D      |
| 209            | 333           | PHE                  | D      |
| 210            | 334           | TYR                  | D      |
| 211            | 335           | ASN                  | D      |
| 212            | 339           | THR                  | A      |
| 213            | 341           | PRO                  | A      |
| 214            | 342           | VAL                  | A      |

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Table S41 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | MET                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | THR                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | LYS                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | THR                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |

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Table S41 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | LEU                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | ILE                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | TYR                  | A      |
| 285            | 443           | ASN                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | THR                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | SER                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLU                  | A      |
| 298            | 487           | VAL                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S42: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase  
(PDB code 1CGU, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S42 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S42 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ALA                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S42 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S42 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S42 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |

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Table S42 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S43: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1CXE, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |

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Table S43 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |

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Table S43 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |

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Table S43 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |

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Table S43 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |

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Table S43 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |

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Table S43 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | CYS                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |

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Table S43 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S44: Residues membership for the *T. molitor*  $\alpha$ -amylase (PDB code 1CLV, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | ASN                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | LYS                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | ASN                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | ASP                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |

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Table S44 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLN                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | GLN                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | ILE                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | TYR                  | C      |
| 37             | 49            | LEU                  | C      |
| 38             | 51            | ALA                  | C      |
| 39             | 57            | TRP                  | C      |
| 40             | 58            | GLU                  | C      |
| 41             | 59            | ARG                  | C      |
| 42             | 60            | TYR                  | C      |
| 43             | 61            | GLN                  | C      |
| 44             | 62            | PRO                  | C      |
| 45             | 63            | VAL                  | C      |
| 46             | 64            | SER                  | C      |
| 47             | 65            | TYR                  | C      |
| 48             | 66            | ILE                  | C      |
| 49             | 67            | ILE                  | C      |
| 50             | 68            | ASN                  | C      |
| 51             | 69            | THR                  | C      |
| 52             | 70            | ARG                  | C      |
| 53             | 71            | SER                  | C      |
| 54             | 72            | GLY                  | C      |
| 55             | 73            | ASP                  | C      |
| 56             | 74            | GLU                  | C      |
| 57             | 75            | SER                  | C      |
| 58             | 76            | ALA                  | C      |
| 59             | 77            | PHE                  | C      |
| 60             | 78            | THR                  | C      |
| 61             | 79            | ASP                  | C      |
| 62             | 80            | MET                  | C      |
| 63             | 81            | THR                  | C      |
| 64             | 82            | ARG                  | C      |
| 65             | 83            | ARG                  | C      |

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Table S44 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 84            | CYS                  | C      |
| 67             | 85            | ASN                  | C      |
| 68             | 86            | ASP                  | C      |
| 69             | 87            | ALA                  | C      |
| 70             | 88            | GLY                  | C      |
| 71             | 89            | VAL                  | C      |
| 72             | 90            | ARG                  | C      |
| 73             | 91            | ILE                  | C      |
| 74             | 92            | TYR                  | C      |
| 75             | 93            | VAL                  | C      |
| 76             | 94            | ASP                  | C      |
| 77             | 95            | ALA                  | C      |
| 78             | 96            | VAL                  | C      |
| 79             | 97            | ILE                  | C      |
| 80             | 98            | ASN                  | C      |
| 81             | 99            | HIS                  | C      |
| 82             | 100           | MET                  | C      |
| 83             | 101           | THR                  | C      |
| 84             | 102           | GLY                  | C      |
| 85             | 103           | MET                  | C      |
| 86             | 120           | TYR                  | C      |
| 87             | 124           | PRO                  | C      |
| 88             | 125           | TYR                  | C      |
| 89             | 126           | GLY                  | C      |
| 90             | 127           | SER                  | C      |
| 91             | 128           | GLY                  | C      |
| 92             | 129           | ASP                  | C      |
| 93             | 130           | PHE                  | C      |
| 94             | 131           | HIS                  | B      |
| 95             | 148           | CYS                  | B      |
| 96             | 149           | GLU                  | B      |
| 97             | 150           | LEU                  | B      |
| 98             | 151           | VAL                  | B      |
| 99             | 153           | LEU                  | B      |
| 100            | 154           | ARG                  | B      |
| 101            | 155           | ASP                  | B      |
| 102            | 156           | LEU                  | B      |
| 103            | 157           | ASN                  | B      |
| 104            | 158           | GLN                  | B      |
| 105            | 159           | GLY                  | B      |
| 106            | 160           | SER                  | B      |
| 107            | 161           | ASP                  | B      |
| 108            | 162           | TYR                  | B      |
| 109            | 163           | VAL                  | B      |
| 110            | 164           | ARG                  | B      |
| 111            | 165           | GLY                  | B      |

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Table S44 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 166           | VAL                  | B      |
| 113            | 167           | LEU                  | B      |
| 114            | 168           | ILE                  | B      |
| 115            | 169           | ASP                  | B      |
| 116            | 170           | TYR                  | B      |
| 117            | 171           | MET                  | B      |
| 118            | 172           | ASN                  | B      |
| 119            | 173           | HIS                  | B      |
| 120            | 174           | MET                  | B      |
| 121            | 175           | ILE                  | B      |
| 122            | 176           | ASP                  | B      |
| 123            | 177           | LEU                  | C      |
| 124            | 178           | GLY                  | C      |
| 125            | 179           | VAL                  | C      |
| 126            | 180           | ALA                  | C      |
| 127            | 181           | GLY                  | C      |
| 128            | 182           | PHE                  | B      |
| 129            | 183           | ARG                  | D      |
| 130            | 184           | VAL                  | B      |
| 131            | 185           | ASP                  | B      |
| 132            | 186           | ALA                  | B      |
| 133            | 187           | ALA                  | B      |
| 134            | 188           | LYS                  | B      |
| 135            | 189           | HIS                  | B      |
| 136            | 190           | MET                  | B      |
| 137            | 191           | SER                  | B      |
| 138            | 192           | PRO                  | B      |
| 139            | 193           | GLY                  | B      |
| 140            | 194           | ASP                  | B      |
| 141            | 195           | LEU                  | B      |
| 142            | 196           | SER                  | B      |
| 143            | 197           | VAL                  | B      |
| 144            | 198           | ILE                  | B      |
| 145            | 199           | PHE                  | B      |
| 146            | 200           | SER                  | B      |
| 147            | 201           | GLY                  | B      |
| 148            | 202           | LEU                  | B      |
| 149            | 203           | LYS                  | B      |
| 150            | 217           | PRO                  | B      |
| 151            | 218           | PHE                  | B      |
| 152            | 219           | ILE                  | B      |
| 153            | 220           | TYR                  | C      |
| 154            | 221           | GLN                  | B      |
| 155            | 222           | GLU                  | B      |
| 156            | 223           | VAL                  | B      |
| 157            | 224           | ILE                  | B      |

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Table S44 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 225           | ASP                  | B      |
| 159            | 226           | LEU                  | B      |
| 160            | 233           | LYS                  | B      |
| 161            | 234           | ASN                  | B      |
| 162            | 235           | GLU                  | B      |
| 163            | 236           | TYR                  | B      |
| 164            | 237           | THR                  | B      |
| 165            | 238           | GLY                  | B      |
| 166            | 239           | PHE                  | B      |
| 167            | 240           | GLY                  | B      |
| 168            | 241           | CYS                  | B      |
| 169            | 242           | VAL                  | B      |
| 170            | 243           | LEU                  | D      |
| 171            | 244           | GLU                  | D      |
| 172            | 245           | PHE                  | D      |
| 173            | 246           | GLN                  | D      |
| 174            | 248           | GLY                  | D      |
| 175            | 249           | VAL                  | D      |
| 176            | 250           | SER                  | D      |
| 177            | 251           | LEU                  | D      |
| 178            | 252           | GLY                  | D      |
| 179            | 253           | ASN                  | D      |
| 180            | 254           | ALA                  | D      |
| 181            | 255           | PHE                  | D      |
| 182            | 259           | ASN                  | D      |
| 183            | 260           | GLN                  | A      |
| 184            | 261           | LEU                  | A      |
| 185            | 262           | LYS                  | A      |
| 186            | 267           | TRP                  | A      |
| 187            | 268           | GLY                  | D      |
| 188            | 269           | PRO                  | D      |
| 189            | 270           | GLU                  | D      |
| 190            | 272           | GLY                  | D      |
| 191            | 273           | LEU                  | B      |
| 192            | 274           | LEU                  | B      |
| 193            | 275           | GLU                  | B      |
| 194            | 276           | GLY                  | B      |
| 195            | 277           | LEU                  | B      |
| 196            | 278           | ASP                  | B      |
| 197            | 279           | ALA                  | B      |
| 198            | 280           | VAL                  | D      |
| 199            | 281           | VAL                  | D      |
| 200            | 282           | PHE                  | D      |
| 201            | 283           | VAL                  | A      |
| 202            | 284           | ASP                  | D      |
| 203            | 285           | ASN                  | D      |

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Table S44 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 286           | HIS                  | D      |
| 205            | 287           | ASP                  | D      |
| 206            | 288           | ASN                  | D      |
| 207            | 289           | GLN                  | D      |
| 208            | 298           | THR                  | D      |
| 209            | 299           | TYR                  | D      |
| 210            | 300           | LYS                  | D      |
| 211            | 301           | ASN                  | D      |
| 212            | 303           | LYS                  | A      |
| 213            | 304           | PRO                  | A      |
| 214            | 305           | TYR                  | A      |
| 215            | 306           | LYS                  | A      |
| 216            | 307           | MET                  | A      |
| 217            | 308           | ALA                  | A      |
| 218            | 309           | ILE                  | A      |
| 219            | 310           | ALA                  | A      |
| 220            | 311           | PHE                  | A      |
| 221            | 312           | MET                  | A      |
| 222            | 313           | LEU                  | A      |
| 223            | 314           | ALA                  | A      |
| 224            | 315           | HIS                  | A      |
| 225            | 317           | TYR                  | D      |
| 226            | 318           | GLY                  | D      |
| 227            | 319           | THR                  | D      |
| 228            | 320           | THR                  | A      |
| 229            | 321           | ARG                  | D      |
| 230            | 322           | ILE                  | A      |
| 231            | 323           | MET                  | D      |
| 232            | 324           | SER                  | C      |
| 233            | 325           | SER                  | D      |
| 234            | 326           | PHE                  | A      |
| 235            | 327           | ASP                  | C      |
| 236            | 357           | GLY                  | C      |
| 237            | 358           | TYR                  | D      |
| 238            | 359           | VAL                  | D      |
| 239            | 360           | CYS                  | D      |
| 240            | 363           | ARG                  | A      |
| 241            | 364           | TRP                  | A      |
| 242            | 365           | ARG                  | A      |
| 243            | 366           | GLN                  | A      |
| 244            | 367           | VAL                  | A      |
| 245            | 368           | TYR                  | A      |
| 246            | 369           | GLY                  | A      |
| 247            | 370           | MET                  | A      |
| 248            | 371           | VAL                  | A      |
| 249            | 372           | GLY                  | A      |

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Table S44 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 373           | PHE                  | A      |
| 251            | 374           | ARG                  | A      |
| 252            | 375           | ASN                  | A      |
| 253            | 376           | ALA                  | A      |
| 254            | 377           | VAL                  | A      |
| 255            | 378           | GLU                  | A      |
| 256            | 379           | GLY                  | A      |
| 257            | 380           | THR                  | A      |
| 258            | 381           | GLN                  | A      |
| 259            | 382           | VAL                  | A      |
| 260            | 384           | ASN                  | A      |
| 261            | 385           | TRP                  | A      |
| 262            | 386           | TRP                  | A      |
| 263            | 387           | SER                  | A      |
| 264            | 389           | ASP                  | A      |
| 265            | 390           | ASP                  | A      |
| 266            | 391           | ASN                  | A      |
| 267            | 392           | GLN                  | A      |
| 268            | 393           | ILE                  | A      |
| 269            | 394           | ALA                  | A      |
| 270            | 395           | PHE                  | A      |
| 271            | 396           | SER                  | A      |
| 272            | 397           | ARG                  | A      |
| 273            | 398           | GLY                  | A      |
| 274            | 399           | SER                  | A      |
| 275            | 401           | GLY                  | A      |
| 276            | 402           | PHE                  | A      |
| 277            | 403           | VAL                  | A      |
| 278            | 404           | ALA                  | A      |
| 279            | 405           | PHE                  | A      |
| 280            | 406           | THR                  | A      |
| 281            | 408           | GLY                  | A      |
| 282            | 409           | GLY                  | A      |
| 283            | 410           | ASP                  | A      |
| 284            | 411           | LEU                  | A      |
| 285            | 412           | ASN                  | A      |
| 286            | 413           | GLN                  | A      |
| 287            | 414           | ASN                  | A      |
| 288            | 420           | PRO                  | A      |
| 289            | 421           | ALA                  | A      |
| 290            | 424           | TYR                  | A      |
| 291            | 425           | CYS                  | A      |
| 292            | 426           | ASP                  | A      |
| 293            | 427           | VAL                  | A      |
| 294            | 454           | LEU                  | A      |
| 295            | 455           | GLY                  | A      |

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Table S44 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 456           | SER                  | A      |
| 297            | 461           | GLY                  | A      |
| 298            | 462           | VAL                  | A      |
| 299            | 463           | LEU                  | A      |
| 300            | 464           | ALA                  | A      |
| 301            | 465           | ILE                  | A      |
| 302            | 466           | HIS                  | A      |

Table S45: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1CXK, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |

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Table S45 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |

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Table S45 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |

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Table S45 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASN                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLN                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |

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Table S45 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |

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Table S45 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | CYS                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |

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Table S45 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S46: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1CXF, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S46 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S46 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASN                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S46 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLN                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S46 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S46 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | CYS                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |

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Table S46 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S47: Residues membership for the *B. stearothermophilus*  $\alpha$ -amylase (PDB code 1CYG, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 12            | ASP                  | A      |
| 1              | 13            | VAL                  | A      |
| 2              | 14            | VAL                  | B      |
| 3              | 15            | TYR                  | B      |
| 4              | 16            | GLN                  | B      |
| 5              | 17            | ILE                  | C      |
| 6              | 18            | VAL                  | C      |
| 7              | 19            | VAL                  | C      |
| 8              | 49            | GLY                  | C      |

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Table S47 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 50            | ASP                  | C      |
| 10             | 51            | TRP                  | C      |
| 11             | 52            | GLN                  | C      |
| 12             | 53            | GLY                  | C      |
| 13             | 54            | ILE                  | C      |
| 14             | 55            | ILE                  | C      |
| 15             | 56            | ASN                  | C      |
| 16             | 57            | LYS                  | C      |
| 17             | 58            | ILE                  | C      |
| 18             | 59            | ASN                  | C      |
| 19             | 60            | ASP                  | C      |
| 20             | 63            | LEU                  | C      |
| 21             | 64            | THR                  | C      |
| 22             | 65            | ASP                  | C      |
| 23             | 66            | MET                  | C      |
| 24             | 67            | GLY                  | C      |
| 25             | 68            | VAL                  | C      |
| 26             | 69            | THR                  | C      |
| 27             | 70            | ALA                  | C      |
| 28             | 71            | ILE                  | C      |
| 29             | 72            | TRP                  | C      |
| 30             | 73            | ILE                  | C      |
| 31             | 74            | SER                  | C      |
| 32             | 75            | GLN                  | C      |
| 33             | 76            | PRO                  | C      |
| 34             | 77            | VAL                  | C      |
| 35             | 78            | GLU                  | C      |
| 36             | 79            | ASN                  | C      |
| 37             | 80            | VAL                  | C      |
| 38             | 91            | ALA                  | C      |
| 39             | 93            | TYR                  | C      |
| 40             | 94            | HIS                  | C      |
| 41             | 95            | GLY                  | C      |
| 42             | 96            | TYR                  | C      |
| 43             | 97            | TRP                  | C      |
| 44             | 98            | ALA                  | C      |
| 45             | 99            | ARG                  | C      |
| 46             | 100           | ASP                  | C      |
| 47             | 102           | LYS                  | C      |
| 48             | 103           | LYS                  | C      |
| 49             | 104           | PRO                  | C      |
| 50             | 105           | ASN                  | C      |
| 51             | 106           | PRO                  | C      |
| 52             | 107           | PHE                  | C      |
| 53             | 108           | PHE                  | C      |
| 54             | 109           | GLY                  | C      |

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Table S47 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 110           | THR                  | C      |
| 56             | 111           | LEU                  | C      |
| 57             | 112           | SER                  | C      |
| 58             | 113           | ASP                  | C      |
| 59             | 114           | PHE                  | C      |
| 60             | 115           | GLN                  | C      |
| 61             | 116           | ARG                  | C      |
| 62             | 117           | LEU                  | C      |
| 63             | 118           | VAL                  | C      |
| 64             | 119           | ASP                  | C      |
| 65             | 120           | ALA                  | C      |
| 66             | 121           | ALA                  | C      |
| 67             | 122           | HIS                  | C      |
| 68             | 123           | ALA                  | C      |
| 69             | 124           | LYS                  | C      |
| 70             | 125           | GLY                  | C      |
| 71             | 126           | ILE                  | C      |
| 72             | 127           | LYS                  | C      |
| 73             | 128           | VAL                  | C      |
| 74             | 129           | ILE                  | C      |
| 75             | 130           | ILE                  | C      |
| 76             | 131           | ASP                  | C      |
| 77             | 132           | PHE                  | C      |
| 78             | 133           | ALA                  | C      |
| 79             | 134           | PRO                  | C      |
| 80             | 135           | ASN                  | C      |
| 81             | 136           | HIS                  | C      |
| 82             | 137           | THR                  | C      |
| 83             | 138           | SER                  | C      |
| 84             | 139           | PRO                  | C      |
| 85             | 140           | ALA                  | C      |
| 86             | 152           | ARG                  | C      |
| 87             | 159           | LEU                  | C      |
| 88             | 160           | LEU                  | C      |
| 89             | 161           | GLY                  | C      |
| 90             | 168           | ASN                  | C      |
| 91             | 169           | MET                  | C      |
| 92             | 170           | TYR                  | C      |
| 93             | 171           | PHE                  | C      |
| 94             | 172           | HIS                  | B      |
| 95             | 188           | ARG                  | B      |
| 96             | 189           | ASN                  | B      |
| 97             | 190           | LEU                  | B      |
| 98             | 191           | PHE                  | B      |
| 99             | 193           | LEU                  | B      |
| 100            | 194           | ALA                  | B      |

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Table S47 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 195           | ASP                  | B      |
| 102            | 196           | LEU                  | B      |
| 103            | 197           | ASN                  | B      |
| 104            | 198           | HIS                  | B      |
| 105            | 199           | GLN                  | B      |
| 106            | 200           | ASN                  | B      |
| 107            | 201           | PRO                  | B      |
| 108            | 202           | VAL                  | B      |
| 109            | 203           | ILE                  | B      |
| 110            | 204           | ASP                  | B      |
| 111            | 205           | ARG                  | B      |
| 112            | 206           | TYR                  | B      |
| 113            | 207           | LEU                  | B      |
| 114            | 208           | LYS                  | B      |
| 115            | 209           | ASP                  | B      |
| 116            | 210           | ALA                  | B      |
| 117            | 211           | VAL                  | B      |
| 118            | 212           | LYS                  | B      |
| 119            | 213           | MET                  | B      |
| 120            | 214           | TRP                  | B      |
| 121            | 215           | ILE                  | B      |
| 122            | 216           | ASP                  | B      |
| 123            | 217           | MET                  | C      |
| 124            | 218           | GLY                  | C      |
| 125            | 219           | ILE                  | C      |
| 126            | 220           | ASP                  | C      |
| 127            | 221           | GLY                  | C      |
| 128            | 222           | ILE                  | B      |
| 129            | 223           | ARG                  | D      |
| 130            | 224           | MET                  | B      |
| 131            | 225           | ASP                  | B      |
| 132            | 226           | ALA                  | B      |
| 133            | 227           | VAL                  | B      |
| 134            | 228           | LYS                  | B      |
| 135            | 229           | HIS                  | B      |
| 136            | 230           | MET                  | B      |
| 137            | 231           | PRO                  | B      |
| 138            | 232           | PHE                  | B      |
| 139            | 233           | GLY                  | B      |
| 140            | 234           | TRP                  | B      |
| 141            | 235           | GLN                  | B      |
| 142            | 236           | LYS                  | B      |
| 143            | 237           | SER                  | B      |
| 144            | 238           | LEU                  | B      |
| 145            | 239           | MET                  | B      |
| 146            | 240           | ASP                  | B      |

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Table S47 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 241           | GLU                  | B      |
| 148            | 242           | ILE                  | B      |
| 149            | 243           | ASP                  | B      |
| 150            | 248           | VAL                  | B      |
| 151            | 249           | PHE                  | B      |
| 152            | 250           | THR                  | B      |
| 153            | 251           | PHE                  | C      |
| 154            | 252           | GLY                  | B      |
| 155            | 253           | GLU                  | B      |
| 156            | 254           | TRP                  | B      |
| 157            | 255           | PHE                  | B      |
| 158            | 256           | LEU                  | B      |
| 159            | 257           | SER                  | B      |
| 160            | 265           | ASN                  | B      |
| 161            | 266           | HIS                  | B      |
| 162            | 267           | TYR                  | B      |
| 163            | 268           | PHE                  | B      |
| 164            | 270           | ASN                  | B      |
| 165            | 271           | GLU                  | B      |
| 166            | 273           | GLY                  | B      |
| 167            | 274           | MET                  | B      |
| 168            | 275           | SER                  | B      |
| 169            | 276           | LEU                  | B      |
| 170            | 277           | LEU                  | D      |
| 171            | 278           | ASP                  | D      |
| 172            | 279           | PHE                  | D      |
| 173            | 280           | ARG                  | D      |
| 174            | 282           | GLY                  | D      |
| 175            | 283           | GLN                  | D      |
| 176            | 284           | LYS                  | D      |
| 177            | 285           | LEU                  | D      |
| 178            | 286           | ARG                  | D      |
| 179            | 287           | GLN                  | D      |
| 180            | 288           | VAL                  | D      |
| 181            | 289           | LEU                  | D      |
| 182            | 294           | ASP                  | D      |
| 183            | 295           | ASN                  | A      |
| 184            | 296           | TRP                  | A      |
| 185            | 297           | TYR                  | A      |
| 186            | 302           | MET                  | A      |
| 187            | 303           | ILE                  | D      |
| 188            | 304           | GLN                  | D      |
| 189            | 305           | ASP                  | D      |
| 190            | 306           | THR                  | D      |
| 191            | 307           | ALA                  | B      |
| 192            | 308           | SER                  | B      |

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Table S47 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 312           | GLU                  | B      |
| 194            | 313           | VAL                  | B      |
| 195            | 314           | LEU                  | B      |
| 196            | 315           | ASP                  | B      |
| 197            | 316           | GLN                  | B      |
| 198            | 317           | VAL                  | D      |
| 199            | 318           | THR                  | D      |
| 200            | 319           | PHE                  | D      |
| 201            | 320           | ILE                  | A      |
| 202            | 321           | ASP                  | D      |
| 203            | 322           | ASN                  | D      |
| 204            | 323           | HIS                  | D      |
| 205            | 324           | ASP                  | D      |
| 206            | 325           | MET                  | D      |
| 207            | 326           | ASP                  | D      |
| 208            | 327           | ARG                  | D      |
| 209            | 328           | PHE                  | D      |
| 210            | 329           | MET                  | D      |
| 211            | 330           | ILE                  | D      |
| 212            | 335           | PRO                  | A      |
| 213            | 337           | LYS                  | A      |
| 214            | 338           | VAL                  | A      |
| 215            | 339           | ASP                  | A      |
| 216            | 340           | MET                  | A      |
| 217            | 341           | ALA                  | A      |
| 218            | 342           | LEU                  | A      |
| 219            | 343           | ALA                  | A      |
| 220            | 344           | VAL                  | A      |
| 221            | 345           | LEU                  | A      |
| 222            | 346           | LEU                  | A      |
| 223            | 347           | THR                  | A      |
| 224            | 348           | SER                  | A      |
| 225            | 349           | ARG                  | D      |
| 226            | 350           | GLY                  | D      |
| 227            | 351           | VAL                  | D      |
| 228            | 352           | PRO                  | A      |
| 229            | 353           | ASN                  | D      |
| 230            | 354           | ILE                  | A      |
| 231            | 355           | TYR                  | D      |
| 232            | 356           | TYR                  | C      |
| 233            | 357           | GLY                  | D      |
| 234            | 358           | THR                  | A      |
| 235            | 372           | LYS                  | C      |
| 236            | 373           | MET                  | C      |
| 237            | 374           | MET                  | D      |
| 238            | 375           | SER                  | D      |

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Table S47 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 377           | PHE                  | D      |
| 240            | 383           | ALA                  | A      |
| 241            | 384           | TYR                  | A      |
| 242            | 385           | GLN                  | A      |
| 243            | 386           | VAL                  | A      |
| 244            | 387           | ILE                  | A      |
| 245            | 388           | GLN                  | A      |
| 246            | 389           | LYS                  | A      |
| 247            | 390           | LEU                  | A      |
| 248            | 391           | SER                  | A      |
| 249            | 392           | SER                  | A      |
| 250            | 393           | LEU                  | A      |
| 251            | 394           | ARG                  | A      |
| 252            | 395           | ARG                  | A      |
| 253            | 396           | ASN                  | A      |
| 254            | 397           | ASN                  | A      |
| 255            | 398           | PRO                  | A      |
| 256            | 402           | TYR                  | A      |
| 257            | 403           | GLY                  | A      |
| 258            | 404           | ASP                  | A      |
| 259            | 405           | THR                  | A      |
| 260            | 407           | GLN                  | A      |
| 261            | 408           | ARG                  | A      |
| 262            | 409           | TRP                  | A      |
| 263            | 410           | ILE                  | A      |
| 264            | 411           | ASN                  | A      |
| 265            | 412           | GLY                  | A      |
| 266            | 413           | ASP                  | A      |
| 267            | 414           | VAL                  | A      |
| 268            | 415           | TYR                  | A      |
| 269            | 416           | VAL                  | A      |
| 270            | 417           | TYR                  | A      |
| 271            | 418           | GLU                  | A      |
| 272            | 419           | ARG                  | A      |
| 273            | 424           | ASP                  | A      |
| 274            | 425           | VAL                  | A      |
| 275            | 426           | VAL                  | A      |
| 276            | 427           | LEU                  | A      |
| 277            | 428           | VAL                  | A      |
| 278            | 429           | ALA                  | A      |
| 279            | 430           | VAL                  | A      |
| 280            | 431           | ASN                  | A      |
| 281            | 435           | SER                  | A      |
| 282            | 436           | SER                  | A      |
| 283            | 437           | ASN                  | A      |
| 284            | 438           | TYR                  | A      |

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Table S47 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 439           | SER                  | A      |
| 286            | 440           | ILE                  | A      |
| 287            | 441           | THR                  | A      |
| 288            | 450           | GLY                  | A      |
| 289            | 451           | THR                  | A      |
| 290            | 453           | THR                  | A      |
| 291            | 454           | ASP                  | A      |
| 292            | 455           | GLN                  | A      |
| 293            | 456           | LEU                  | A      |
| 294            | 478           | LEU                  | A      |
| 295            | 479           | GLY                  | A      |
| 296            | 480           | PRO                  | A      |
| 297            | 482           | GLU                  | A      |
| 298            | 483           | VAL                  | A      |
| 299            | 484           | GLY                  | A      |
| 300            | 485           | VAL                  | A      |
| 301            | 486           | TRP                  | A      |
| 302            | 487           | ALA                  | A      |

Table S48: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1CXL, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |

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Table S48 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |

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Table S48 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |

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Table S48 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLN                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |

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Table S48 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |

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Table S48 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |

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Table S48 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |

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Table S48 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S49: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 1DHK, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |

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Table S49 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |

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Table S49 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |

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Table S49 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |

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Table S49 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |

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Table S49 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 322           | LYS                  | A      |
| 216            | 323           | VAL                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLU                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |

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Table S49 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S50: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1D3C, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S50 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S50 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASN                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S50 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLN                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S50 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S50 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | CYS                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |

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Table S50 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S51: Residues membership for the *S. solfataricus* KM1  $\alpha$ -amylase (PDB code 1EHA, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 102           | LEU                  | A      |
| 1              | 103           | ILE                  | A      |
| 2              | 104           | ILE                  | B      |
| 3              | 105           | TYR                  | B      |
| 4              | 106           | GLU                  | B      |
| 5              | 107           | ILE                  | C      |
| 6              | 108           | HIS                  | C      |
| 7              | 109           | VAL                  | C      |
| 8              | 116           | GLY                  | C      |

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Table S51 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 117           | THR                  | C      |
| 10             | 118           | PHE                  | C      |
| 11             | 119           | GLU                  | C      |
| 12             | 120           | GLY                  | C      |
| 13             | 121           | VAL                  | C      |
| 14             | 122           | ILE                  | C      |
| 15             | 123           | ARG                  | C      |
| 16             | 124           | LYS                  | C      |
| 17             | 125           | LEU                  | C      |
| 18             | 126           | ASP                  | C      |
| 19             | 127           | TYR                  | C      |
| 20             | 128           | LEU                  | C      |
| 21             | 129           | LYS                  | C      |
| 22             | 130           | ASP                  | C      |
| 23             | 131           | LEU                  | C      |
| 24             | 132           | GLY                  | C      |
| 25             | 133           | ILE                  | C      |
| 26             | 134           | THR                  | C      |
| 27             | 135           | ALA                  | C      |
| 28             | 136           | ILE                  | C      |
| 29             | 137           | GLU                  | C      |
| 30             | 138           | ILE                  | C      |
| 31             | 139           | MET                  | C      |
| 32             | 140           | PRO                  | C      |
| 33             | 141           | ILE                  | C      |
| 34             | 142           | ALA                  | C      |
| 35             | 143           | GLN                  | C      |
| 36             | 144           | PHE                  | C      |
| 37             | 145           | PRO                  | C      |
| 38             | 146           | GLY                  | C      |
| 39             | 149           | ASP                  | C      |
| 40             | 150           | TRP                  | C      |
| 41             | 151           | GLY                  | C      |
| 42             | 152           | TYR                  | C      |
| 43             | 153           | ASP                  | C      |
| 44             | 154           | GLY                  | C      |
| 45             | 155           | VAL                  | C      |
| 46             | 156           | TYR                  | C      |
| 47             | 158           | TYR                  | C      |
| 48             | 159           | ALA                  | C      |
| 49             | 160           | VAL                  | C      |
| 50             | 161           | GLN                  | C      |
| 51             | 162           | ASN                  | C      |
| 52             | 163           | SER                  | C      |
| 53             | 164           | TYR                  | C      |
| 54             | 165           | GLY                  | C      |

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Table S51 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 166           | GLY                  | C      |
| 56             | 167           | PRO                  | C      |
| 57             | 168           | GLU                  | C      |
| 58             | 169           | GLY                  | C      |
| 59             | 170           | PHE                  | C      |
| 60             | 171           | ARG                  | C      |
| 61             | 172           | LYS                  | C      |
| 62             | 173           | LEU                  | C      |
| 63             | 174           | VAL                  | C      |
| 64             | 175           | ASP                  | C      |
| 65             | 176           | GLU                  | C      |
| 66             | 177           | ALA                  | C      |
| 67             | 178           | HIS                  | C      |
| 68             | 179           | LYS                  | C      |
| 69             | 180           | LYS                  | C      |
| 70             | 181           | GLY                  | C      |
| 71             | 182           | LEU                  | C      |
| 72             | 183           | GLY                  | C      |
| 73             | 184           | VAL                  | C      |
| 74             | 185           | ILE                  | C      |
| 75             | 186           | LEU                  | C      |
| 76             | 187           | ASP                  | C      |
| 77             | 188           | VAL                  | C      |
| 78             | 189           | VAL                  | C      |
| 79             | 190           | TYR                  | C      |
| 80             | 191           | ASN                  | C      |
| 81             | 192           | HIS                  | C      |
| 82             | 193           | VAL                  | C      |
| 83             | 194           | GLY                  | C      |
| 84             | 195           | PRO                  | C      |
| 85             | 196           | GLU                  | C      |
| 86             | 198           | ASN                  | C      |
| 87             | 199           | TYR                  | C      |
| 88             | 200           | MET                  | C      |
| 89             | 201           | VAL                  | C      |
| 90             | 204           | GLY                  | C      |
| 91             | 205           | PRO                  | C      |
| 92             | 206           | TYR                  | C      |
| 93             | 207           | PHE                  | C      |
| 94             | 208           | SER                  | B      |
| 95             | 212           | LYS                  | B      |
| 96             | 213           | THR                  | B      |
| 97             | 214           | PRO                  | B      |
| 98             | 215           | TRP                  | B      |
| 99             | 216           | GLY                  | B      |
| 100            | 217           | LEU                  | B      |

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Table S51 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 218           | THR                  | B      |
| 102            | 219           | PHE                  | B      |
| 103            | 220           | ASN                  | B      |
| 104            | 221           | PHE                  | B      |
| 105            | 222           | ASP                  | B      |
| 106            | 226           | SER                  | B      |
| 107            | 227           | ASP                  | B      |
| 108            | 228           | GLU                  | B      |
| 109            | 229           | VAL                  | B      |
| 110            | 230           | ARG                  | B      |
| 111            | 231           | LYS                  | B      |
| 112            | 232           | PHE                  | B      |
| 113            | 233           | ILE                  | B      |
| 114            | 234           | LEU                  | B      |
| 115            | 235           | GLU                  | B      |
| 116            | 236           | ASN                  | B      |
| 117            | 237           | VAL                  | B      |
| 118            | 238           | GLU                  | B      |
| 119            | 239           | TYR                  | B      |
| 120            | 240           | TRP                  | B      |
| 121            | 241           | ILE                  | B      |
| 122            | 242           | LYS                  | B      |
| 123            | 244           | TYR                  | C      |
| 124            | 245           | ASN                  | C      |
| 125            | 246           | VAL                  | C      |
| 126            | 247           | ASP                  | C      |
| 127            | 248           | GLY                  | C      |
| 128            | 249           | PHE                  | B      |
| 129            | 250           | ARG                  | D      |
| 130            | 251           | LEU                  | B      |
| 131            | 252           | ASP                  | B      |
| 132            | 253           | ALA                  | B      |
| 133            | 254           | VAL                  | B      |
| 134            | 255           | HIS                  | B      |
| 135            | 256           | ALA                  | B      |
| 136            | 257           | ILE                  | B      |
| 137            | 258           | ILE                  | B      |
| 138            | 263           | LYS                  | B      |
| 139            | 264           | HIS                  | B      |
| 140            | 265           | ILE                  | B      |
| 141            | 266           | LEU                  | B      |
| 142            | 267           | GLU                  | B      |
| 143            | 268           | GLU                  | B      |
| 144            | 269           | ILE                  | B      |
| 145            | 270           | ALA                  | B      |
| 146            | 271           | ASP                  | B      |

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Table S51 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 272           | VAL                  | B      |
| 148            | 273           | VAL                  | B      |
| 149            | 274           | HIS                  | B      |
| 150            | 278           | ARG                  | B      |
| 151            | 279           | ILE                  | B      |
| 152            | 280           | VAL                  | B      |
| 153            | 281           | ILE                  | C      |
| 154            | 282           | ALA                  | B      |
| 155            | 283           | GLU                  | B      |
| 156            | 284           | SER                  | B      |
| 157            | 285           | ASP                  | B      |
| 158            | 286           | LEU                  | B      |
| 159            | 287           | ASN                  | B      |
| 160            | 288           | ASP                  | B      |
| 161            | 289           | PRO                  | B      |
| 162            | 290           | ARG                  | B      |
| 163            | 291           | VAL                  | B      |
| 164            | 292           | VAL                  | B      |
| 165            | 293           | ASN                  | B      |
| 166            | 302           | ILE                  | B      |
| 167            | 303           | ASP                  | B      |
| 168            | 304           | ALA                  | B      |
| 169            | 305           | GLN                  | B      |
| 170            | 306           | TRP                  | D      |
| 171            | 307           | VAL                  | D      |
| 172            | 308           | ASP                  | D      |
| 173            | 309           | ASP                  | D      |
| 174            | 311           | HIS                  | D      |
| 175            | 312           | HIS                  | D      |
| 176            | 313           | SER                  | D      |
| 177            | 314           | ILE                  | D      |
| 178            | 315           | HIS                  | D      |
| 179            | 316           | ALA                  | D      |
| 180            | 317           | TYR                  | D      |
| 181            | 318           | LEU                  | D      |
| 182            | 330           | GLY                  | D      |
| 183            | 331           | ASN                  | A      |
| 184            | 332           | LEU                  | A      |
| 185            | 333           | ASP                  | A      |
| 186            | 338           | SER                  | A      |
| 187            | 339           | TYR                  | D      |
| 188            | 340           | LYS                  | D      |
| 189            | 341           | ASP                  | D      |
| 190            | 342           | VAL                  | D      |
| 191            | 343           | PHE                  | B      |
| 192            | 344           | VAL                  | B      |

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Table S51 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 365           | ASP                  | B      |
| 194            | 366           | GLY                  | B      |
| 195            | 367           | CYS                  | B      |
| 196            | 368           | ASN                  | B      |
| 197            | 369           | PHE                  | B      |
| 198            | 370           | VAL                  | D      |
| 199            | 371           | VAL                  | D      |
| 200            | 372           | TYR                  | D      |
| 201            | 373           | ILE                  | A      |
| 202            | 374           | GLN                  | D      |
| 203            | 375           | ASN                  | D      |
| 204            | 376           | HIS                  | D      |
| 205            | 377           | ASP                  | D      |
| 206            | 378           | GLN                  | D      |
| 207            | 379           | VAL                  | D      |
| 208            | 387           | ARG                  | D      |
| 209            | 388           | ILE                  | D      |
| 210            | 389           | ILE                  | D      |
| 211            | 390           | LYS                  | D      |
| 212            | 394           | ARG                  | A      |
| 213            | 396           | SER                  | A      |
| 214            | 397           | TYR                  | A      |
| 215            | 398           | LYS                  | A      |
| 216            | 399           | ILE                  | A      |
| 217            | 400           | ALA                  | A      |
| 218            | 401           | ALA                  | A      |
| 219            | 402           | ALA                  | A      |
| 220            | 403           | LEU                  | A      |
| 221            | 404           | TYR                  | A      |
| 222            | 405           | LEU                  | A      |
| 223            | 406           | LEU                  | A      |
| 224            | 407           | SER                  | A      |
| 225            | 408           | PRO                  | D      |
| 226            | 409           | TYR                  | D      |
| 227            | 410           | ILE                  | D      |
| 228            | 411           | PRO                  | A      |
| 229            | 412           | MET                  | D      |
| 230            | 413           | ILE                  | A      |
| 231            | 414           | PHE                  | D      |
| 232            | 415           | MET                  | C      |
| 233            | 416           | GLY                  | D      |
| 234            | 417           | GLU                  | A      |
| 235            | 463           | SER                  | C      |
| 236            | 464           | LYS                  | C      |
| 237            | 465           | LEU                  | D      |
| 238            | 466           | SER                  | D      |

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Table S51 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 467           | TRP                  | D      |
| 240            | 473           | ILE                  | A      |
| 241            | 474           | PHE                  | A      |
| 242            | 475           | SER                  | A      |
| 243            | 476           | PHE                  | A      |
| 244            | 477           | TYR                  | A      |
| 245            | 478           | LYS                  | A      |
| 246            | 479           | ILE                  | A      |
| 247            | 480           | LEU                  | A      |
| 248            | 481           | ILE                  | A      |
| 249            | 482           | LYS                  | A      |
| 250            | 483           | MET                  | A      |
| 251            | 484           | ARG                  | A      |
| 252            | 485           | LYS                  | A      |
| 253            | 486           | GLU                  | A      |
| 254            | 487           | LEU                  | A      |
| 255            | 488           | SER                  | A      |
| 256            | 492           | ASP                  | A      |
| 257            | 493           | ARG                  | A      |
| 258            | 494           | ARG                  | A      |
| 259            | 495           | VAL                  | A      |
| 260            | 496           | ASN                  | A      |
| 261            | 497           | VAL                  | A      |
| 262            | 498           | VAL                  | A      |
| 263            | 499           | ASN                  | A      |
| 264            | 500           | GLY                  | A      |
| 265            | 501           | GLU                  | A      |
| 266            | 502           | ASN                  | A      |
| 267            | 503           | TRP                  | A      |
| 268            | 504           | LEU                  | A      |
| 269            | 505           | ILE                  | A      |
| 270            | 506           | ILE                  | A      |
| 271            | 507           | LYS                  | A      |
| 272            | 508           | GLY                  | A      |
| 273            | 509           | ARG                  | A      |
| 274            | 510           | GLU                  | A      |
| 275            | 511           | TYR                  | A      |
| 276            | 512           | PHE                  | A      |
| 277            | 513           | SER                  | A      |
| 278            | 514           | LEU                  | A      |
| 279            | 515           | TYR                  | A      |
| 280            | 516           | VAL                  | A      |
| 281            | 518           | SER                  | A      |
| 282            | 519           | LYS                  | A      |
| 283            | 520           | SER                  | A      |
| 284            | 521           | SER                  | A      |

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Table S51 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 522           | ILE                  | A      |
| 286            | 523           | GLU                  | A      |
| 287            | 524           | VAL                  | A      |
| 288            | 527           | SER                  | A      |
| 289            | 528           | GLY                  | A      |
| 290            | 529           | THR                  | A      |
| 291            | 530           | LEU                  | A      |
| 292            | 531           | LEU                  | A      |
| 293            | 532           | LEU                  | A      |
| 294            | 549           | PHE                  | A      |
| 295            | 550           | ASP                  | A      |
| 296            | 551           | LYS                  | A      |
| 297            | 552           | GLY                  | A      |
| 298            | 553           | PHE                  | A      |
| 299            | 554           | ALA                  | A      |
| 300            | 555           | LEU                  | A      |
| 301            | 556           | TYR                  | A      |
| 302            | 557           | LYS                  | A      |

Table S52: Residues membership for the *S. solfataricus* KM1  $\alpha$ -amylase (PDB code 1EH9, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 102           | LEU                  | A      |
| 1              | 103           | ILE                  | A      |
| 2              | 104           | ILE                  | B      |
| 3              | 105           | TYR                  | B      |
| 4              | 106           | GLU                  | B      |
| 5              | 107           | ILE                  | C      |
| 6              | 108           | HIS                  | C      |
| 7              | 109           | VAL                  | C      |
| 8              | 116           | GLY                  | C      |
| 9              | 117           | THR                  | C      |
| 10             | 118           | PHE                  | C      |
| 11             | 119           | GLU                  | C      |
| 12             | 120           | GLY                  | C      |
| 13             | 121           | VAL                  | C      |
| 14             | 122           | ILE                  | C      |
| 15             | 123           | ARG                  | C      |
| 16             | 124           | LYS                  | C      |
| 17             | 125           | LEU                  | C      |
| 18             | 126           | ASP                  | C      |
| 19             | 127           | TYR                  | C      |

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Table S52 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 128           | LEU                  | C      |
| 21             | 129           | LYS                  | C      |
| 22             | 130           | ASP                  | C      |
| 23             | 131           | LEU                  | C      |
| 24             | 132           | GLY                  | C      |
| 25             | 133           | ILE                  | C      |
| 26             | 134           | THR                  | C      |
| 27             | 135           | ALA                  | C      |
| 28             | 136           | ILE                  | C      |
| 29             | 137           | GLU                  | C      |
| 30             | 138           | ILE                  | C      |
| 31             | 139           | MET                  | C      |
| 32             | 140           | PRO                  | C      |
| 33             | 141           | ILE                  | C      |
| 34             | 142           | ALA                  | C      |
| 35             | 143           | GLN                  | C      |
| 36             | 144           | PHE                  | C      |
| 37             | 145           | PRO                  | C      |
| 38             | 146           | GLY                  | C      |
| 39             | 149           | ASP                  | C      |
| 40             | 150           | TRP                  | C      |
| 41             | 151           | GLY                  | C      |
| 42             | 152           | TYR                  | C      |
| 43             | 153           | ASP                  | C      |
| 44             | 154           | GLY                  | C      |
| 45             | 155           | VAL                  | C      |
| 46             | 156           | TYR                  | C      |
| 47             | 158           | TYR                  | C      |
| 48             | 159           | ALA                  | C      |
| 49             | 160           | VAL                  | C      |
| 50             | 161           | GLN                  | C      |
| 51             | 162           | ASN                  | C      |
| 52             | 163           | SER                  | C      |
| 53             | 164           | TYR                  | C      |
| 54             | 165           | GLY                  | C      |
| 55             | 166           | GLY                  | C      |
| 56             | 167           | PRO                  | C      |
| 57             | 168           | GLU                  | C      |
| 58             | 169           | GLY                  | C      |
| 59             | 170           | PHE                  | C      |
| 60             | 171           | ARG                  | C      |
| 61             | 172           | LYS                  | C      |
| 62             | 173           | LEU                  | C      |
| 63             | 174           | VAL                  | C      |
| 64             | 175           | ASP                  | C      |
| 65             | 176           | GLU                  | C      |

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Table S52 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 177           | ALA                  | C      |
| 67             | 178           | HIS                  | C      |
| 68             | 179           | LYS                  | C      |
| 69             | 180           | LYS                  | C      |
| 70             | 181           | GLY                  | C      |
| 71             | 182           | LEU                  | C      |
| 72             | 183           | GLY                  | C      |
| 73             | 184           | VAL                  | C      |
| 74             | 185           | ILE                  | C      |
| 75             | 186           | LEU                  | C      |
| 76             | 187           | ASP                  | C      |
| 77             | 188           | VAL                  | C      |
| 78             | 189           | VAL                  | C      |
| 79             | 190           | TYR                  | C      |
| 80             | 191           | ASN                  | C      |
| 81             | 192           | HIS                  | C      |
| 82             | 193           | VAL                  | C      |
| 83             | 194           | GLY                  | C      |
| 84             | 195           | PRO                  | C      |
| 85             | 196           | GLU                  | C      |
| 86             | 198           | ASN                  | C      |
| 87             | 199           | TYR                  | C      |
| 88             | 200           | MET                  | C      |
| 89             | 201           | VAL                  | C      |
| 90             | 204           | GLY                  | C      |
| 91             | 205           | PRO                  | C      |
| 92             | 206           | TYR                  | C      |
| 93             | 207           | PHE                  | C      |
| 94             | 208           | SER                  | B      |
| 95             | 212           | LYS                  | B      |
| 96             | 213           | THR                  | B      |
| 97             | 214           | PRO                  | B      |
| 98             | 215           | TRP                  | B      |
| 99             | 216           | GLY                  | B      |
| 100            | 217           | LEU                  | B      |
| 101            | 218           | THR                  | B      |
| 102            | 219           | PHE                  | B      |
| 103            | 220           | ASN                  | B      |
| 104            | 221           | PHE                  | B      |
| 105            | 222           | ASP                  | B      |
| 106            | 226           | SER                  | B      |
| 107            | 227           | ASP                  | B      |
| 108            | 228           | GLU                  | B      |
| 109            | 229           | VAL                  | B      |
| 110            | 230           | ARG                  | B      |
| 111            | 231           | LYS                  | B      |

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Table S52 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 232           | PHE                  | B      |
| 113            | 233           | ILE                  | B      |
| 114            | 234           | LEU                  | B      |
| 115            | 235           | GLU                  | B      |
| 116            | 236           | ASN                  | B      |
| 117            | 237           | VAL                  | B      |
| 118            | 238           | GLU                  | B      |
| 119            | 239           | TYR                  | B      |
| 120            | 240           | TRP                  | B      |
| 121            | 241           | ILE                  | B      |
| 122            | 242           | LYS                  | B      |
| 123            | 244           | TYR                  | C      |
| 124            | 245           | ASN                  | C      |
| 125            | 246           | VAL                  | C      |
| 126            | 247           | ASP                  | C      |
| 127            | 248           | GLY                  | C      |
| 128            | 249           | PHE                  | B      |
| 129            | 250           | ARG                  | D      |
| 130            | 251           | LEU                  | B      |
| 131            | 252           | ASP                  | B      |
| 132            | 253           | ALA                  | B      |
| 133            | 254           | VAL                  | B      |
| 134            | 255           | HIS                  | B      |
| 135            | 256           | ALA                  | B      |
| 136            | 257           | ILE                  | B      |
| 137            | 258           | ILE                  | B      |
| 138            | 263           | LYS                  | B      |
| 139            | 264           | HIS                  | B      |
| 140            | 265           | ILE                  | B      |
| 141            | 266           | LEU                  | B      |
| 142            | 267           | GLU                  | B      |
| 143            | 268           | GLU                  | B      |
| 144            | 269           | ILE                  | B      |
| 145            | 270           | ALA                  | B      |
| 146            | 271           | ASP                  | B      |
| 147            | 272           | VAL                  | B      |
| 148            | 273           | VAL                  | B      |
| 149            | 274           | HIS                  | B      |
| 150            | 278           | ARG                  | B      |
| 151            | 279           | ILE                  | B      |
| 152            | 280           | VAL                  | B      |
| 153            | 281           | ILE                  | C      |
| 154            | 282           | ALA                  | B      |
| 155            | 283           | GLU                  | B      |
| 156            | 284           | SER                  | B      |
| 157            | 285           | ASP                  | B      |

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Table S52 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 286           | LEU                  | B      |
| 159            | 287           | ASN                  | B      |
| 160            | 288           | ASP                  | B      |
| 161            | 289           | PRO                  | B      |
| 162            | 290           | ARG                  | B      |
| 163            | 291           | VAL                  | B      |
| 164            | 292           | VAL                  | B      |
| 165            | 293           | ASN                  | B      |
| 166            | 302           | ILE                  | B      |
| 167            | 303           | ASP                  | B      |
| 168            | 304           | ALA                  | B      |
| 169            | 305           | GLN                  | B      |
| 170            | 306           | TRP                  | D      |
| 171            | 307           | VAL                  | D      |
| 172            | 308           | ASP                  | D      |
| 173            | 309           | ASP                  | D      |
| 174            | 311           | HIS                  | D      |
| 175            | 312           | HIS                  | D      |
| 176            | 313           | SER                  | D      |
| 177            | 314           | ILE                  | D      |
| 178            | 315           | HIS                  | D      |
| 179            | 316           | ALA                  | D      |
| 180            | 317           | TYR                  | D      |
| 181            | 318           | LEU                  | D      |
| 182            | 330           | GLY                  | D      |
| 183            | 331           | ASN                  | A      |
| 184            | 332           | LEU                  | A      |
| 185            | 333           | ASP                  | A      |
| 186            | 338           | SER                  | A      |
| 187            | 339           | TYR                  | D      |
| 188            | 340           | LYS                  | D      |
| 189            | 341           | ASP                  | D      |
| 190            | 342           | VAL                  | D      |
| 191            | 343           | PHE                  | B      |
| 192            | 344           | VAL                  | B      |
| 193            | 365           | ASP                  | B      |
| 194            | 366           | GLY                  | B      |
| 195            | 367           | CYS                  | B      |
| 196            | 368           | ASN                  | B      |
| 197            | 369           | PHE                  | B      |
| 198            | 370           | VAL                  | D      |
| 199            | 371           | VAL                  | D      |
| 200            | 372           | TYR                  | D      |
| 201            | 373           | ILE                  | A      |
| 202            | 374           | GLN                  | D      |
| 203            | 375           | ASN                  | D      |

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Table S52 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 376           | HIS                  | D      |
| 205            | 377           | ASP                  | D      |
| 206            | 378           | GLN                  | D      |
| 207            | 379           | VAL                  | D      |
| 208            | 387           | ARG                  | D      |
| 209            | 388           | ILE                  | D      |
| 210            | 389           | ILE                  | D      |
| 211            | 390           | LYS                  | D      |
| 212            | 394           | ARG                  | A      |
| 213            | 396           | SER                  | A      |
| 214            | 397           | TYR                  | A      |
| 215            | 398           | LYS                  | A      |
| 216            | 399           | ILE                  | A      |
| 217            | 400           | ALA                  | A      |
| 218            | 401           | ALA                  | A      |
| 219            | 402           | ALA                  | A      |
| 220            | 403           | LEU                  | A      |
| 221            | 404           | TYR                  | A      |
| 222            | 405           | LEU                  | A      |
| 223            | 406           | LEU                  | A      |
| 224            | 407           | SER                  | A      |
| 225            | 408           | PRO                  | D      |
| 226            | 409           | TYR                  | D      |
| 227            | 410           | ILE                  | D      |
| 228            | 411           | PRO                  | A      |
| 229            | 412           | MET                  | D      |
| 230            | 413           | ILE                  | A      |
| 231            | 414           | PHE                  | D      |
| 232            | 415           | MET                  | C      |
| 233            | 416           | GLY                  | D      |
| 234            | 417           | GLU                  | A      |
| 235            | 463           | SER                  | C      |
| 236            | 464           | LYS                  | C      |
| 237            | 465           | LEU                  | D      |
| 238            | 466           | SER                  | D      |
| 239            | 467           | TRP                  | D      |
| 240            | 473           | ILE                  | A      |
| 241            | 474           | PHE                  | A      |
| 242            | 475           | SER                  | A      |
| 243            | 476           | PHE                  | A      |
| 244            | 477           | TYR                  | A      |
| 245            | 478           | LYS                  | A      |
| 246            | 479           | ILE                  | A      |
| 247            | 480           | LEU                  | A      |
| 248            | 481           | ILE                  | A      |
| 249            | 482           | LYS                  | A      |

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Table S52 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 483           | MET                  | A      |
| 251            | 484           | ARG                  | A      |
| 252            | 485           | LYS                  | A      |
| 253            | 486           | GLU                  | A      |
| 254            | 487           | LEU                  | A      |
| 255            | 488           | SER                  | A      |
| 256            | 492           | ASP                  | A      |
| 257            | 493           | ARG                  | A      |
| 258            | 494           | ARG                  | A      |
| 259            | 495           | VAL                  | A      |
| 260            | 496           | ASN                  | A      |
| 261            | 497           | VAL                  | A      |
| 262            | 498           | VAL                  | A      |
| 263            | 499           | ASN                  | A      |
| 264            | 500           | GLY                  | A      |
| 265            | 501           | GLU                  | A      |
| 266            | 502           | ASN                  | A      |
| 267            | 503           | TRP                  | A      |
| 268            | 504           | LEU                  | A      |
| 269            | 505           | ILE                  | A      |
| 270            | 506           | ILE                  | A      |
| 271            | 507           | LYS                  | A      |
| 272            | 508           | GLY                  | A      |
| 273            | 509           | ARG                  | A      |
| 274            | 510           | GLU                  | A      |
| 275            | 511           | TYR                  | A      |
| 276            | 512           | PHE                  | A      |
| 277            | 513           | SER                  | A      |
| 278            | 514           | LEU                  | A      |
| 279            | 515           | TYR                  | A      |
| 280            | 516           | VAL                  | A      |
| 281            | 518           | SER                  | A      |
| 282            | 519           | LYS                  | A      |
| 283            | 520           | SER                  | A      |
| 284            | 521           | SER                  | A      |
| 285            | 522           | ILE                  | A      |
| 286            | 523           | GLU                  | A      |
| 287            | 524           | VAL                  | A      |
| 288            | 527           | SER                  | A      |
| 289            | 528           | GLY                  | A      |
| 290            | 529           | THR                  | A      |
| 291            | 530           | LEU                  | A      |
| 292            | 531           | LEU                  | A      |
| 293            | 532           | LEU                  | A      |
| 294            | 549           | PHE                  | A      |
| 295            | 550           | ASP                  | A      |

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Table S52 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 551           | LYS                  | A      |
| 297            | 552           | GLY                  | A      |
| 298            | 553           | PHE                  | A      |
| 299            | 554           | ALA                  | A      |
| 300            | 555           | LEU                  | A      |
| 301            | 556           | TYR                  | A      |
| 302            | 557           | LYS                  | A      |

Table S53: Residues membership for the *T. vulgaris* R47  $\alpha$ -amylase (PDB code 1VFO, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |
| 30             | 192           | PHE                  | C      |

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Table S53 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |
| 76             | 239           | ASP                  | C      |

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Table S53 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |
| 122            | 316           | GLU                  | B      |

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Table S53 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASN                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |
| 168            | 370           | SER                  | B      |

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Table S53 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASN                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |
| 214            | 436           | PHE                  | A      |

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Table S53 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |
| 260            | 507           | SER                  | A      |

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Table S53 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 574           | ARG                  | A      |
| 295            | 575           | PRO                  | A      |
| 296            | 576           | TYR                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S54: Residues membership for the *N. polysaccharea*  $\alpha$ -amylase (PDB code 1G5A, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 98            | GLN                  | A      |
| 1              | 99            | VAL                  | A      |
| 2              | 100           | GLY                  | B      |
| 3              | 101           | GLY                  | B      |
| 4              | 102           | VAL                  | B      |
| 5              | 103           | CYS                  | C      |
| 6              | 104           | TYR                  | C      |
| 7              | 105           | VAL                  | C      |
| 8              | 110           | GLY                  | C      |
| 9              | 111           | ASP                  | C      |
| 10             | 112           | LEU                  | C      |
| 11             | 113           | LYS                  | C      |
| 12             | 114           | GLY                  | C      |
| 13             | 115           | LEU                  | C      |
| 14             | 116           | LYS                  | C      |
| 15             | 117           | ASP                  | C      |
| 16             | 118           | LYS                  | C      |
| 17             | 119           | ILE                  | C      |
| 18             | 120           | PRO                  | C      |
| 19             | 121           | TYR                  | C      |
| 20             | 122           | PHE                  | C      |
| 21             | 123           | GLN                  | C      |
| 22             | 124           | GLU                  | C      |
| 23             | 125           | LEU                  | C      |
| 24             | 126           | GLY                  | C      |
| 25             | 127           | LEU                  | C      |
| 26             | 128           | THR                  | C      |
| 27             | 129           | TYR                  | C      |
| 28             | 130           | LEU                  | C      |
| 29             | 131           | HIS                  | C      |
| 30             | 132           | LEU                  | C      |
| 31             | 133           | MET                  | C      |
| 32             | 134           | PRO                  | C      |
| 33             | 135           | LEU                  | C      |
| 34             | 136           | PHE                  | C      |
| 35             | 137           | LYS                  | C      |
| 36             | 138           | CYS                  | C      |
| 37             | 139           | PRO                  | C      |
| 38             | 141           | GLY                  | C      |
| 39             | 144           | ASP                  | C      |
| 40             | 145           | GLY                  | C      |
| 41             | 146           | GLY                  | C      |
| 42             | 147           | TYR                  | C      |
| 43             | 148           | ALA                  | C      |

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Table S54 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 149           | VAL                  | C      |
| 45             | 150           | SER                  | C      |
| 46             | 151           | SER                  | C      |
| 47             | 153           | ARG                  | C      |
| 48             | 154           | ASP                  | C      |
| 49             | 155           | VAL                  | C      |
| 50             | 156           | ASN                  | C      |
| 51             | 157           | PRO                  | C      |
| 52             | 158           | ALA                  | C      |
| 53             | 159           | LEU                  | C      |
| 54             | 160           | GLY                  | C      |
| 55             | 161           | THR                  | C      |
| 56             | 162           | ILE                  | C      |
| 57             | 163           | GLY                  | C      |
| 58             | 164           | ASP                  | C      |
| 59             | 165           | LEU                  | C      |
| 60             | 166           | ARG                  | C      |
| 61             | 167           | GLU                  | C      |
| 62             | 168           | VAL                  | C      |
| 63             | 169           | ILE                  | C      |
| 64             | 170           | ALA                  | C      |
| 65             | 171           | ALA                  | C      |
| 66             | 172           | LEU                  | C      |
| 67             | 173           | HIS                  | C      |
| 68             | 174           | GLU                  | C      |
| 69             | 175           | ALA                  | C      |
| 70             | 176           | GLY                  | C      |
| 71             | 177           | ILE                  | C      |
| 72             | 178           | SER                  | C      |
| 73             | 179           | ALA                  | C      |
| 74             | 180           | VAL                  | C      |
| 75             | 181           | VAL                  | C      |
| 76             | 182           | ASP                  | C      |
| 77             | 183           | PHE                  | C      |
| 78             | 184           | ILE                  | C      |
| 79             | 185           | PHE                  | C      |
| 80             | 186           | ASN                  | C      |
| 81             | 187           | HIS                  | C      |
| 82             | 188           | THR                  | C      |
| 83             | 189           | SER                  | C      |
| 84             | 190           | ASN                  | C      |
| 85             | 191           | GLU                  | C      |
| 86             | 192           | HIS                  | C      |
| 87             | 193           | GLU                  | C      |
| 88             | 194           | TRP                  | C      |
| 89             | 195           | ALA                  | C      |

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Table S54 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 206           | ASP                  | C      |
| 91             | 207           | ASN                  | C      |
| 92             | 208           | PHE                  | C      |
| 93             | 209           | TYR                  | C      |
| 94             | 210           | TYR                  | B      |
| 95             | 247           | TRP                  | B      |
| 96             | 248           | THR                  | B      |
| 97             | 249           | THR                  | B      |
| 98             | 250           | PHE                  | B      |
| 99             | 254           | GLN                  | B      |
| 100            | 255           | TRP                  | B      |
| 101            | 256           | ASP                  | B      |
| 102            | 257           | LEU                  | B      |
| 103            | 258           | ASN                  | B      |
| 104            | 259           | TYR                  | B      |
| 105            | 260           | SER                  | B      |
| 106            | 261           | ASN                  | B      |
| 107            | 262           | PRO                  | B      |
| 108            | 263           | TRP                  | B      |
| 109            | 264           | VAL                  | B      |
| 110            | 265           | PHE                  | B      |
| 111            | 266           | ARG                  | B      |
| 112            | 267           | ALA                  | B      |
| 113            | 268           | MET                  | B      |
| 114            | 269           | ALA                  | B      |
| 115            | 270           | GLY                  | B      |
| 116            | 271           | GLU                  | B      |
| 117            | 272           | MET                  | B      |
| 118            | 273           | LEU                  | B      |
| 119            | 274           | PHE                  | B      |
| 120            | 275           | LEU                  | B      |
| 121            | 276           | ALA                  | B      |
| 122            | 277           | ASN                  | B      |
| 123            | 278           | LEU                  | C      |
| 124            | 279           | GLY                  | C      |
| 125            | 280           | VAL                  | C      |
| 126            | 281           | ASP                  | C      |
| 127            | 282           | ILE                  | C      |
| 128            | 283           | LEU                  | B      |
| 129            | 284           | ARG                  | D      |
| 130            | 285           | MET                  | B      |
| 131            | 286           | ASP                  | B      |
| 132            | 287           | ALA                  | B      |
| 133            | 288           | VAL                  | B      |
| 134            | 289           | ALA                  | B      |
| 135            | 290           | PHE                  | B      |

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Table S54 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 291           | ILE                  | B      |
| 137            | 292           | TRP                  | B      |
| 138            | 306           | HIS                  | B      |
| 139            | 307           | ALA                  | B      |
| 140            | 308           | LEU                  | B      |
| 141            | 309           | ILE                  | B      |
| 142            | 310           | ARG                  | B      |
| 143            | 311           | ALA                  | B      |
| 144            | 312           | PHE                  | B      |
| 145            | 313           | ASN                  | B      |
| 146            | 314           | ALA                  | B      |
| 147            | 315           | VAL                  | B      |
| 148            | 316           | MET                  | B      |
| 149            | 317           | ARG                  | B      |
| 150            | 323           | VAL                  | B      |
| 151            | 324           | PHE                  | B      |
| 152            | 325           | PHE                  | B      |
| 153            | 326           | LYS                  | C      |
| 154            | 327           | SER                  | B      |
| 155            | 328           | GLU                  | B      |
| 156            | 329           | ALA                  | B      |
| 157            | 330           | ILE                  | B      |
| 158            | 331           | VAL                  | B      |
| 159            | 332           | HIS                  | B      |
| 160            | 336           | VAL                  | B      |
| 161            | 337           | VAL                  | B      |
| 162            | 338           | GLN                  | B      |
| 163            | 339           | TYR                  | B      |
| 164            | 340           | ILE                  | B      |
| 165            | 341           | GLY                  | B      |
| 166            | 345           | CYS                  | B      |
| 167            | 346           | GLN                  | B      |
| 168            | 347           | ILE                  | B      |
| 169            | 348           | GLY                  | B      |
| 170            | 349           | TYR                  | D      |
| 171            | 350           | ASN                  | D      |
| 172            | 351           | PRO                  | D      |
| 173            | 352           | LEU                  | D      |
| 174            | 354           | MET                  | D      |
| 175            | 355           | ALA                  | D      |
| 176            | 356           | LEU                  | D      |
| 177            | 357           | LEU                  | D      |
| 178            | 358           | TRP                  | D      |
| 179            | 359           | ASN                  | D      |
| 180            | 360           | THR                  | D      |
| 181            | 361           | LEU                  | D      |

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Table S54 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 364           | ARG                  | D      |
| 183            | 365           | GLU                  | A      |
| 184            | 366           | VAL                  | A      |
| 185            | 367           | ASN                  | A      |
| 186            | 372           | ALA                  | A      |
| 187            | 373           | LEU                  | D      |
| 188            | 374           | THR                  | D      |
| 189            | 375           | TYR                  | D      |
| 190            | 376           | ARG                  | D      |
| 191            | 377           | HIS                  | B      |
| 192            | 378           | ASN                  | B      |
| 193            | 381           | GLU                  | B      |
| 194            | 382           | HIS                  | B      |
| 195            | 383           | THR                  | B      |
| 196            | 384           | ALA                  | B      |
| 197            | 385           | TRP                  | B      |
| 198            | 386           | VAL                  | D      |
| 199            | 387           | ASN                  | D      |
| 200            | 388           | TYR                  | D      |
| 201            | 389           | VAL                  | A      |
| 202            | 390           | ARG                  | D      |
| 203            | 391           | SER                  | D      |
| 204            | 392           | HIS                  | D      |
| 205            | 393           | ASP                  | D      |
| 206            | 394           | ASP                  | D      |
| 207            | 448           | SER                  | D      |
| 208            | 450           | THR                  | D      |
| 209            | 451           | ALA                  | D      |
| 210            | 452           | ALA                  | D      |
| 211            | 453           | ALA                  | D      |
| 212            | 464           | ALA                  | A      |
| 213            | 467           | ARG                  | A      |
| 214            | 468           | ILE                  | A      |
| 215            | 469           | LYS                  | A      |
| 216            | 470           | LEU                  | A      |
| 217            | 471           | LEU                  | A      |
| 218            | 472           | TYR                  | A      |
| 219            | 473           | SER                  | A      |
| 220            | 474           | ILE                  | A      |
| 221            | 475           | ALA                  | A      |
| 222            | 476           | LEU                  | A      |
| 223            | 477           | SER                  | A      |
| 224            | 478           | THR                  | A      |
| 225            | 479           | GLY                  | D      |
| 226            | 480           | GLY                  | D      |
| 227            | 481           | LEU                  | D      |

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Table S54 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 482           | PRO                  | A      |
| 229            | 483           | LEU                  | D      |
| 230            | 484           | ILE                  | A      |
| 231            | 485           | TYR                  | D      |
| 232            | 486           | LEU                  | C      |
| 233            | 487           | GLY                  | D      |
| 234            | 488           | ASP                  | A      |
| 235            | 514           | PRO                  | C      |
| 236            | 515           | ARG                  | C      |
| 237            | 516           | TYR                  | D      |
| 238            | 517           | ASN                  | D      |
| 239            | 521           | TYR                  | D      |
| 240            | 534           | ILE                  | A      |
| 241            | 535           | TYR                  | A      |
| 242            | 536           | GLN                  | A      |
| 243            | 537           | ASP                  | A      |
| 244            | 538           | LEU                  | A      |
| 245            | 539           | ARG                  | A      |
| 246            | 540           | HIS                  | A      |
| 247            | 541           | MET                  | A      |
| 248            | 542           | ILE                  | A      |
| 249            | 543           | ALA                  | A      |
| 250            | 544           | VAL                  | A      |
| 251            | 545           | ARG                  | A      |
| 252            | 546           | GLN                  | A      |
| 253            | 547           | SER                  | A      |
| 254            | 548           | ASN                  | A      |
| 255            | 549           | PRO                  | A      |
| 256            | 553           | GLY                  | A      |
| 257            | 554           | GLY                  | A      |
| 258            | 555           | ARG                  | A      |
| 259            | 556           | LEU                  | A      |
| 260            | 558           | THR                  | A      |
| 261            | 559           | PHE                  | A      |
| 262            | 560           | ASN                  | A      |
| 263            | 561           | THR                  | A      |
| 264            | 563           | ASN                  | A      |
| 265            | 564           | LYS                  | A      |
| 266            | 565           | HIS                  | A      |
| 267            | 566           | ILE                  | A      |
| 268            | 567           | ILE                  | A      |
| 269            | 568           | GLY                  | A      |
| 270            | 569           | TYR                  | A      |
| 271            | 570           | ILE                  | A      |
| 272            | 571           | ARG                  | A      |
| 273            | 573           | ASN                  | A      |

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Table S54 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 574           | ALA                  | A      |
| 275            | 575           | LEU                  | A      |
| 276            | 576           | LEU                  | A      |
| 277            | 577           | ALA                  | A      |
| 278            | 578           | PHE                  | A      |
| 279            | 579           | GLY                  | A      |
| 280            | 580           | ASN                  | A      |
| 281            | 584           | TYR                  | A      |
| 282            | 585           | PRO                  | A      |
| 283            | 586           | GLN                  | A      |
| 284            | 587           | THR                  | A      |
| 285            | 588           | VAL                  | A      |
| 286            | 589           | THR                  | A      |
| 287            | 590           | ALA                  | A      |
| 288            | 599           | LYS                  | A      |
| 289            | 600           | ALA                  | A      |
| 290            | 601           | HIS                  | A      |
| 291            | 602           | ASP                  | A      |
| 292            | 603           | LEU                  | A      |
| 293            | 604           | ILE                  | A      |
| 294            | 617           | LEU                  | A      |
| 295            | 618           | GLN                  | A      |
| 296            | 619           | PRO                  | A      |
| 297            | 621           | GLN                  | A      |
| 298            | 622           | VAL                  | A      |
| 299            | 623           | MET                  | A      |
| 300            | 624           | TRP                  | A      |
| 301            | 625           | LEU                  | A      |
| 302            | 626           | GLU                  | A      |

Table S55: Residues membership for the *T. molitor*  $\alpha$ -amylase (PDB code 1VIW, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | ASN                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |

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Table S55 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 20            | LYS                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | ASN                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | ASP                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLN                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | GLN                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | ILE                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | TYR                  | C      |
| 37             | 49            | LEU                  | C      |
| 38             | 51            | ALA                  | C      |
| 39             | 57            | TRP                  | C      |
| 40             | 58            | GLU                  | C      |
| 41             | 59            | ARG                  | C      |
| 42             | 60            | TYR                  | C      |
| 43             | 61            | GLN                  | C      |
| 44             | 62            | PRO                  | C      |
| 45             | 63            | VAL                  | C      |
| 46             | 64            | SER                  | C      |
| 47             | 65            | TYR                  | C      |
| 48             | 66            | ILE                  | C      |
| 49             | 67            | ILE                  | C      |
| 50             | 68            | ASN                  | C      |
| 51             | 69            | THR                  | C      |
| 52             | 70            | ARG                  | C      |
| 53             | 71            | SER                  | C      |
| 54             | 72            | GLY                  | C      |

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Table S55 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 73            | ASN                  | C      |
| 56             | 74            | GLU                  | C      |
| 57             | 75            | SER                  | C      |
| 58             | 76            | ALA                  | C      |
| 59             | 77            | PHE                  | C      |
| 60             | 78            | THR                  | C      |
| 61             | 79            | ASP                  | C      |
| 62             | 80            | MET                  | C      |
| 63             | 81            | THR                  | C      |
| 64             | 82            | ARG                  | C      |
| 65             | 83            | ARG                  | C      |
| 66             | 84            | CYS                  | C      |
| 67             | 85            | ASN                  | C      |
| 68             | 86            | ASP                  | C      |
| 69             | 87            | ALA                  | C      |
| 70             | 88            | GLY                  | C      |
| 71             | 89            | VAL                  | C      |
| 72             | 90            | ARG                  | C      |
| 73             | 91            | ILE                  | C      |
| 74             | 92            | TYR                  | C      |
| 75             | 93            | VAL                  | C      |
| 76             | 94            | ASP                  | C      |
| 77             | 95            | ALA                  | C      |
| 78             | 96            | VAL                  | C      |
| 79             | 97            | ILE                  | C      |
| 80             | 98            | ASN                  | C      |
| 81             | 99            | HIS                  | C      |
| 82             | 100           | MET                  | C      |
| 83             | 101           | THR                  | C      |
| 84             | 102           | GLY                  | C      |
| 85             | 103           | MET                  | C      |
| 86             | 120           | TYR                  | C      |
| 87             | 124           | PRO                  | C      |
| 88             | 125           | TYR                  | C      |
| 89             | 126           | GLY                  | C      |
| 90             | 127           | SER                  | C      |
| 91             | 128           | GLY                  | C      |
| 92             | 129           | ASP                  | C      |
| 93             | 130           | PHE                  | C      |
| 94             | 131           | HIS                  | B      |
| 95             | 148           | CYS                  | B      |
| 96             | 149           | GLU                  | B      |
| 97             | 150           | LEU                  | B      |
| 98             | 151           | VAL                  | B      |
| 99             | 153           | LEU                  | B      |
| 100            | 154           | ARG                  | B      |

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Table S55 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 155           | ASP                  | B      |
| 102            | 156           | LEU                  | B      |
| 103            | 157           | ASN                  | B      |
| 104            | 158           | ALA                  | B      |
| 105            | 159           | GLY                  | B      |
| 106            | 160           | SER                  | B      |
| 107            | 161           | ASP                  | B      |
| 108            | 162           | TYR                  | B      |
| 109            | 163           | VAL                  | B      |
| 110            | 164           | ARG                  | B      |
| 111            | 165           | GLY                  | B      |
| 112            | 166           | VAL                  | B      |
| 113            | 167           | LEU                  | B      |
| 114            | 168           | ILE                  | B      |
| 115            | 169           | ASP                  | B      |
| 116            | 170           | TYR                  | B      |
| 117            | 171           | MET                  | B      |
| 118            | 172           | ASN                  | B      |
| 119            | 173           | HIS                  | B      |
| 120            | 174           | MET                  | B      |
| 121            | 175           | ILE                  | B      |
| 122            | 176           | ASP                  | B      |
| 123            | 177           | LEU                  | C      |
| 124            | 178           | GLY                  | C      |
| 125            | 179           | VAL                  | C      |
| 126            | 180           | ALA                  | C      |
| 127            | 181           | GLY                  | C      |
| 128            | 182           | PHE                  | B      |
| 129            | 183           | ARG                  | D      |
| 130            | 184           | VAL                  | B      |
| 131            | 185           | ASP                  | B      |
| 132            | 186           | ALA                  | B      |
| 133            | 187           | ALA                  | B      |
| 134            | 188           | LYS                  | B      |
| 135            | 189           | HIS                  | B      |
| 136            | 190           | MET                  | B      |
| 137            | 191           | SER                  | B      |
| 138            | 192           | PRO                  | B      |
| 139            | 193           | GLY                  | B      |
| 140            | 194           | ASP                  | B      |
| 141            | 195           | LEU                  | B      |
| 142            | 196           | SER                  | B      |
| 143            | 197           | VAL                  | B      |
| 144            | 198           | ILE                  | B      |
| 145            | 199           | PHE                  | B      |
| 146            | 200           | ASP                  | B      |

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Table S55 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 201           | GLY                  | B      |
| 148            | 202           | LEU                  | B      |
| 149            | 203           | LYS                  | B      |
| 150            | 217           | PRO                  | B      |
| 151            | 218           | PHE                  | B      |
| 152            | 219           | ILE                  | B      |
| 153            | 220           | TYR                  | C      |
| 154            | 221           | GLN                  | B      |
| 155            | 222           | GLU                  | B      |
| 156            | 223           | VAL                  | B      |
| 157            | 224           | ILE                  | B      |
| 158            | 225           | ASP                  | B      |
| 159            | 226           | LEU                  | B      |
| 160            | 233           | LYS                  | B      |
| 161            | 234           | ASN                  | B      |
| 162            | 235           | GLU                  | B      |
| 163            | 236           | TYR                  | B      |
| 164            | 237           | THR                  | B      |
| 165            | 238           | GLY                  | B      |
| 166            | 239           | PHE                  | B      |
| 167            | 240           | GLY                  | B      |
| 168            | 241           | CYS                  | B      |
| 169            | 242           | VAL                  | B      |
| 170            | 243           | LEU                  | D      |
| 171            | 244           | GLU                  | D      |
| 172            | 245           | PHE                  | D      |
| 173            | 246           | GLN                  | D      |
| 174            | 248           | GLY                  | D      |
| 175            | 249           | VAL                  | D      |
| 176            | 250           | SER                  | D      |
| 177            | 251           | LEU                  | D      |
| 178            | 252           | GLY                  | D      |
| 179            | 253           | ASN                  | D      |
| 180            | 254           | ALA                  | D      |
| 181            | 255           | PHE                  | D      |
| 182            | 259           | ASN                  | D      |
| 183            | 260           | GLN                  | A      |
| 184            | 261           | LEU                  | A      |
| 185            | 262           | LYS                  | A      |
| 186            | 267           | TRP                  | A      |
| 187            | 268           | GLY                  | D      |
| 188            | 269           | PRO                  | D      |
| 189            | 270           | GLU                  | D      |
| 190            | 272           | GLY                  | D      |
| 191            | 273           | LEU                  | B      |
| 192            | 274           | LEU                  | B      |

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Table S55 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 275           | GLU                  | B      |
| 194            | 276           | GLY                  | B      |
| 195            | 277           | LEU                  | B      |
| 196            | 278           | ASP                  | B      |
| 197            | 279           | ALA                  | B      |
| 198            | 280           | VAL                  | D      |
| 199            | 281           | VAL                  | D      |
| 200            | 282           | PHE                  | D      |
| 201            | 283           | VAL                  | A      |
| 202            | 284           | ASP                  | D      |
| 203            | 285           | ASN                  | D      |
| 204            | 286           | HIS                  | D      |
| 205            | 287           | ASP                  | D      |
| 206            | 288           | ASN                  | D      |
| 207            | 289           | GLN                  | D      |
| 208            | 298           | THR                  | D      |
| 209            | 299           | TYR                  | D      |
| 210            | 300           | LYS                  | D      |
| 211            | 301           | ASN                  | D      |
| 212            | 303           | LYS                  | A      |
| 213            | 304           | PRO                  | A      |
| 214            | 305           | TYR                  | A      |
| 215            | 306           | LYS                  | A      |
| 216            | 307           | MET                  | A      |
| 217            | 308           | ALA                  | A      |
| 218            | 309           | ILE                  | A      |
| 219            | 310           | ALA                  | A      |
| 220            | 311           | PHE                  | A      |
| 221            | 312           | MET                  | A      |
| 222            | 313           | LEU                  | A      |
| 223            | 314           | ALA                  | A      |
| 224            | 315           | HIS                  | A      |
| 225            | 317           | TYR                  | D      |
| 226            | 318           | GLY                  | D      |
| 227            | 319           | THR                  | D      |
| 228            | 320           | THR                  | A      |
| 229            | 321           | ARG                  | D      |
| 230            | 322           | ILE                  | A      |
| 231            | 323           | MET                  | D      |
| 232            | 324           | SER                  | C      |
| 233            | 325           | SER                  | D      |
| 234            | 326           | PHE                  | A      |
| 235            | 327           | ASP                  | C      |
| 236            | 357           | GLY                  | C      |
| 237            | 358           | TYR                  | D      |
| 238            | 359           | VAL                  | D      |

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Table S55 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 360           | CYS                  | D      |
| 240            | 363           | ARG                  | A      |
| 241            | 364           | TRP                  | A      |
| 242            | 365           | ARG                  | A      |
| 243            | 366           | GLN                  | A      |
| 244            | 367           | VAL                  | A      |
| 245            | 368           | TYR                  | A      |
| 246            | 369           | GLY                  | A      |
| 247            | 370           | MET                  | A      |
| 248            | 371           | VAL                  | A      |
| 249            | 372           | GLY                  | A      |
| 250            | 373           | PHE                  | A      |
| 251            | 374           | ARG                  | A      |
| 252            | 375           | ASN                  | A      |
| 253            | 376           | ALA                  | A      |
| 254            | 377           | VAL                  | A      |
| 255            | 378           | GLU                  | A      |
| 256            | 379           | GLY                  | A      |
| 257            | 380           | THR                  | A      |
| 258            | 381           | GLN                  | A      |
| 259            | 382           | VAL                  | A      |
| 260            | 384           | ASN                  | A      |
| 261            | 385           | TRP                  | A      |
| 262            | 386           | TRP                  | A      |
| 263            | 387           | SER                  | A      |
| 264            | 389           | ASP                  | A      |
| 265            | 390           | ASP                  | A      |
| 266            | 391           | ASN                  | A      |
| 267            | 392           | GLN                  | A      |
| 268            | 393           | ILE                  | A      |
| 269            | 394           | ALA                  | A      |
| 270            | 395           | PHE                  | A      |
| 271            | 396           | SER                  | A      |
| 272            | 397           | ARG                  | A      |
| 273            | 398           | GLY                  | A      |
| 274            | 399           | SER                  | A      |
| 275            | 401           | GLY                  | A      |
| 276            | 402           | PHE                  | A      |
| 277            | 403           | VAL                  | A      |
| 278            | 404           | ALA                  | A      |
| 279            | 405           | PHE                  | A      |
| 280            | 406           | THR                  | A      |
| 281            | 408           | GLY                  | A      |
| 282            | 409           | GLY                  | A      |
| 283            | 410           | ASP                  | A      |
| 284            | 411           | LEU                  | A      |

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Table S55 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 412           | ASN                  | A      |
| 286            | 413           | GLN                  | A      |
| 287            | 414           | ASN                  | A      |
| 288            | 420           | PRO                  | A      |
| 289            | 421           | ALA                  | A      |
| 290            | 424           | TYR                  | A      |
| 291            | 425           | CYS                  | A      |
| 292            | 426           | ASP                  | A      |
| 293            | 427           | VAL                  | A      |
| 294            | 454           | LEU                  | A      |
| 295            | 455           | GLY                  | A      |
| 296            | 456           | SER                  | A      |
| 297            | 461           | GLY                  | A      |
| 298            | 462           | VAL                  | A      |
| 299            | 463           | LEU                  | A      |
| 300            | 464           | ALA                  | A      |
| 301            | 465           | ILE                  | A      |
| 302            | 466           | HIS                  | A      |

Table S56: Residues membership for the *B. cereus*  $\alpha$ -amylase (PDB code 1UOK, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | SER                  | A      |
| 1              | 10            | VAL                  | A      |
| 2              | 11            | VAL                  | B      |
| 3              | 12            | TYR                  | B      |
| 4              | 13            | GLN                  | B      |
| 5              | 14            | ILE                  | C      |
| 6              | 15            | TYR                  | C      |
| 7              | 16            | PRO                  | C      |
| 8              | 28            | GLY                  | C      |
| 9              | 29            | ASP                  | C      |
| 10             | 30            | LEU                  | C      |
| 11             | 31            | ARG                  | C      |
| 12             | 32            | GLY                  | C      |
| 13             | 33            | ILE                  | C      |
| 14             | 34            | ILE                  | C      |
| 15             | 35            | SER                  | C      |
| 16             | 36            | LYS                  | C      |
| 17             | 37            | LEU                  | C      |
| 18             | 38            | ASP                  | C      |
| 19             | 39            | TYR                  | C      |

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Table S56 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 40            | LEU                  | C      |
| 21             | 41            | LYS                  | C      |
| 22             | 42            | GLU                  | C      |
| 23             | 43            | LEU                  | C      |
| 24             | 44            | GLY                  | C      |
| 25             | 45            | ILE                  | C      |
| 26             | 46            | ASP                  | C      |
| 27             | 47            | VAL                  | C      |
| 28             | 48            | ILE                  | C      |
| 29             | 49            | TRP                  | C      |
| 30             | 50            | LEU                  | C      |
| 31             | 51            | SER                  | C      |
| 32             | 52            | PRO                  | C      |
| 33             | 53            | VAL                  | C      |
| 34             | 54            | TYR                  | C      |
| 35             | 55            | GLU                  | C      |
| 36             | 56            | SER                  | C      |
| 37             | 57            | PRO                  | C      |
| 38             | 58            | ASN                  | C      |
| 39             | 60            | ASP                  | C      |
| 40             | 61            | ASN                  | C      |
| 41             | 62            | GLY                  | C      |
| 42             | 63            | TYR                  | C      |
| 43             | 64            | ASP                  | C      |
| 44             | 65            | ILE                  | C      |
| 45             | 66            | SER                  | C      |
| 46             | 67            | ASP                  | C      |
| 47             | 69            | CYS                  | C      |
| 48             | 70            | LYS                  | C      |
| 49             | 71            | ILE                  | C      |
| 50             | 72            | MET                  | C      |
| 51             | 73            | ASN                  | C      |
| 52             | 74            | GLU                  | C      |
| 53             | 75            | PHE                  | C      |
| 54             | 76            | GLY                  | C      |
| 55             | 77            | THR                  | C      |
| 56             | 78            | MET                  | C      |
| 57             | 79            | GLU                  | C      |
| 58             | 80            | ASP                  | C      |
| 59             | 81            | TRP                  | C      |
| 60             | 82            | ASP                  | C      |
| 61             | 83            | GLU                  | C      |
| 62             | 84            | LEU                  | C      |
| 63             | 85            | LEU                  | C      |
| 64             | 86            | HIS                  | C      |
| 65             | 87            | GLU                  | C      |

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Table S56 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 88            | MET                  | C      |
| 67             | 89            | HIS                  | C      |
| 68             | 90            | GLU                  | C      |
| 69             | 91            | ARG                  | C      |
| 70             | 92            | ASN                  | C      |
| 71             | 93            | MET                  | C      |
| 72             | 94            | LYS                  | C      |
| 73             | 95            | LEU                  | C      |
| 74             | 96            | MET                  | C      |
| 75             | 97            | MET                  | C      |
| 76             | 98            | ASP                  | C      |
| 77             | 99            | LEU                  | C      |
| 78             | 100           | VAL                  | C      |
| 79             | 101           | VAL                  | C      |
| 80             | 102           | ASN                  | C      |
| 81             | 103           | HIS                  | C      |
| 82             | 104           | THR                  | C      |
| 83             | 105           | SER                  | C      |
| 84             | 106           | ASP                  | C      |
| 85             | 107           | GLU                  | C      |
| 86             | 108           | HIS                  | C      |
| 87             | 109           | ASN                  | C      |
| 88             | 110           | TRP                  | C      |
| 89             | 111           | PHE                  | C      |
| 90             | 123           | ARG                  | C      |
| 91             | 124           | ASP                  | C      |
| 92             | 125           | TYR                  | C      |
| 93             | 126           | TYR                  | C      |
| 94             | 127           | ILE                  | B      |
| 95             | 160           | LEU                  | B      |
| 96             | 161           | HIS                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | PHE                  | B      |
| 99             | 167           | GLN                  | B      |
| 100            | 168           | PRO                  | B      |
| 101            | 169           | ASP                  | B      |
| 102            | 170           | LEU                  | B      |
| 103            | 171           | ASN                  | B      |
| 104            | 172           | TRP                  | B      |
| 105            | 173           | ASP                  | B      |
| 106            | 174           | ASN                  | B      |
| 107            | 175           | GLU                  | B      |
| 108            | 176           | LYS                  | B      |
| 109            | 177           | VAL                  | B      |
| 110            | 178           | ARG                  | B      |
| 111            | 179           | GLN                  | B      |

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Table S56 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 180           | ASP                  | B      |
| 113            | 181           | VAL                  | B      |
| 114            | 182           | TYR                  | B      |
| 115            | 183           | GLU                  | B      |
| 116            | 184           | MET                  | B      |
| 117            | 185           | MET                  | B      |
| 118            | 186           | LYS                  | B      |
| 119            | 187           | PHE                  | B      |
| 120            | 188           | TRP                  | B      |
| 121            | 189           | LEU                  | B      |
| 122            | 190           | GLU                  | B      |
| 123            | 191           | LYS                  | C      |
| 124            | 192           | GLY                  | C      |
| 125            | 193           | ILE                  | C      |
| 126            | 194           | ASP                  | C      |
| 127            | 195           | GLY                  | C      |
| 128            | 196           | PHE                  | B      |
| 129            | 197           | ARG                  | D      |
| 130            | 198           | MET                  | B      |
| 131            | 199           | ASP                  | B      |
| 132            | 200           | VAL                  | B      |
| 133            | 201           | ILE                  | B      |
| 134            | 202           | ASN                  | B      |
| 135            | 203           | PHE                  | B      |
| 136            | 204           | ILE                  | B      |
| 137            | 205           | SER                  | B      |
| 138            | 234           | HIS                  | B      |
| 139            | 235           | LYS                  | B      |
| 140            | 236           | TYR                  | B      |
| 141            | 237           | LEU                  | B      |
| 142            | 238           | HIS                  | B      |
| 143            | 239           | GLU                  | B      |
| 144            | 240           | MET                  | B      |
| 145            | 241           | ASN                  | B      |
| 146            | 242           | GLU                  | B      |
| 147            | 243           | GLU                  | B      |
| 148            | 244           | VAL                  | B      |
| 149            | 245           | LEU                  | B      |
| 150            | 250           | ILE                  | B      |
| 151            | 251           | MET                  | B      |
| 152            | 252           | THR                  | B      |
| 153            | 253           | VAL                  | C      |
| 154            | 254           | GLY                  | B      |
| 155            | 255           | GLU                  | B      |
| 156            | 256           | MET                  | B      |
| 157            | 257           | PRO                  | B      |

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Table S56 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 258           | GLY                  | B      |
| 159            | 259           | VAL                  | B      |
| 160            | 264           | ALA                  | B      |
| 161            | 265           | LYS                  | B      |
| 162            | 266           | LEU                  | B      |
| 163            | 267           | TYR                  | B      |
| 164            | 268           | THR                  | B      |
| 165            | 269           | GLY                  | B      |
| 166            | 275           | LEU                  | B      |
| 167            | 276           | GLN                  | B      |
| 168            | 277           | MET                  | B      |
| 169            | 278           | VAL                  | B      |
| 170            | 279           | PHE                  | D      |
| 171            | 280           | GLN                  | D      |
| 172            | 281           | PHE                  | D      |
| 173            | 282           | GLU                  | D      |
| 174            | 284           | MET                  | D      |
| 175            | 285           | ASP                  | D      |
| 176            | 286           | LEU                  | D      |
| 177            | 287           | ASP                  | D      |
| 178            | 288           | SER                  | D      |
| 179            | 289           | GLY                  | D      |
| 180            | 290           | GLU                  | D      |
| 181            | 291           | GLY                  | D      |
| 182            | 300           | SER                  | D      |
| 183            | 301           | LEU                  | A      |
| 184            | 302           | LEU                  | A      |
| 185            | 303           | THR                  | A      |
| 186            | 308           | LEU                  | A      |
| 187            | 309           | THR                  | D      |
| 188            | 310           | LYS                  | D      |
| 189            | 311           | TRP                  | D      |
| 190            | 312           | GLN                  | D      |
| 191            | 313           | LYS                  | B      |
| 192            | 314           | ALA                  | B      |
| 193            | 317           | HIS                  | B      |
| 194            | 318           | THR                  | B      |
| 195            | 319           | GLY                  | B      |
| 196            | 320           | TRP                  | B      |
| 197            | 321           | ASN                  | B      |
| 198            | 322           | SER                  | D      |
| 199            | 323           | LEU                  | D      |
| 200            | 324           | TYR                  | D      |
| 201            | 325           | TRP                  | A      |
| 202            | 326           | ASN                  | D      |
| 203            | 327           | ASN                  | D      |

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Table S56 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 328           | HIS                  | D      |
| 205            | 329           | ASP                  | D      |
| 206            | 330           | GLN                  | D      |
| 207            | 331           | PRO                  | D      |
| 208            | 332           | ARG                  | D      |
| 209            | 333           | VAL                  | D      |
| 210            | 334           | VAL                  | D      |
| 211            | 335           | SER                  | D      |
| 212            | 344           | ARG                  | A      |
| 213            | 347           | SER                  | A      |
| 214            | 348           | ALA                  | A      |
| 215            | 349           | LYS                  | A      |
| 216            | 350           | MET                  | A      |
| 217            | 351           | LEU                  | A      |
| 218            | 352           | ALA                  | A      |
| 219            | 353           | THR                  | A      |
| 220            | 354           | VAL                  | A      |
| 221            | 355           | LEU                  | A      |
| 222            | 356           | HIS                  | A      |
| 223            | 357           | MET                  | A      |
| 224            | 358           | MET                  | A      |
| 225            | 359           | LYS                  | D      |
| 226            | 360           | GLY                  | D      |
| 227            | 361           | THR                  | D      |
| 228            | 362           | PRO                  | A      |
| 229            | 363           | TYR                  | D      |
| 230            | 364           | ILE                  | A      |
| 231            | 365           | TYR                  | D      |
| 232            | 366           | GLN                  | C      |
| 233            | 367           | GLY                  | D      |
| 234            | 368           | GLU                  | A      |
| 235            | 420           | THR                  | C      |
| 236            | 421           | PRO                  | C      |
| 237            | 422           | MET                  | D      |
| 238            | 423           | GLN                  | D      |
| 239            | 424           | TRP                  | D      |
| 240            | 460           | ILE                  | A      |
| 241            | 461           | PHE                  | A      |
| 242            | 462           | TYR                  | A      |
| 243            | 463           | TYR                  | A      |
| 244            | 464           | TYR                  | A      |
| 245            | 465           | LYS                  | A      |
| 246            | 466           | LYS                  | A      |
| 247            | 467           | LEU                  | A      |
| 248            | 468           | ILE                  | A      |
| 249            | 469           | GLU                  | A      |

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Table S56 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 470           | LEU                  | A      |
| 251            | 471           | ARG                  | A      |
| 252            | 472           | LYS                  | A      |
| 253            | 473           | ASN                  | A      |
| 254            | 474           | ASN                  | A      |
| 255            | 475           | GLU                  | A      |
| 256            | 479           | TYR                  | A      |
| 257            | 480           | GLY                  | A      |
| 258            | 481           | SER                  | A      |
| 259            | 482           | TYR                  | A      |
| 260            | 484           | LEU                  | A      |
| 261            | 485           | ILE                  | A      |
| 262            | 486           | LEU                  | A      |
| 263            | 487           | GLU                  | A      |
| 264            | 489           | ASN                  | A      |
| 265            | 490           | PRO                  | A      |
| 266            | 491           | SER                  | A      |
| 267            | 492           | ILE                  | A      |
| 268            | 493           | PHE                  | A      |
| 269            | 494           | ALA                  | A      |
| 270            | 495           | TYR                  | A      |
| 271            | 496           | VAL                  | A      |
| 272            | 497           | ARG                  | A      |
| 273            | 502           | GLU                  | A      |
| 274            | 503           | LYS                  | A      |
| 275            | 504           | LEU                  | A      |
| 276            | 505           | LEU                  | A      |
| 277            | 506           | VAL                  | A      |
| 278            | 507           | ILE                  | A      |
| 279            | 508           | ALA                  | A      |
| 280            | 509           | ASN                  | A      |
| 281            | 513           | GLU                  | A      |
| 282            | 514           | GLU                  | A      |
| 283            | 515           | CYS                  | A      |
| 284            | 516           | ILE                  | A      |
| 285            | 517           | PHE                  | A      |
| 286            | 518           | GLU                  | A      |
| 287            | 519           | LEU                  | A      |
| 288            | 527           | GLU                  | A      |
| 289            | 528           | VAL                  | A      |
| 290            | 530           | LEU                  | A      |
| 291            | 531           | LEU                  | A      |
| 292            | 532           | ILE                  | A      |
| 293            | 533           | HIS                  | A      |
| 294            | 547           | LEU                  | A      |
| 295            | 548           | ARG                  | A      |

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Table S56 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 549           | PRO                  | A      |
| 297            | 551           | GLU                  | A      |
| 298            | 552           | ALA                  | A      |
| 299            | 553           | MET                  | A      |
| 300            | 554           | VAL                  | A      |
| 301            | 555           | PHE                  | A      |
| 302            | 556           | LYS                  | A      |

Table S57: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 1SMD, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |

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Table S57 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |

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Table S57 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | SER                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLY                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |

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Table S57 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |

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Table S57 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |

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Table S57 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ASN                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |

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Table S57 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | THR                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S58: Residues membership for the *B. circulans*  $\alpha$ -amylase (PDB code 1OT1, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S58 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | ALA                  | C      |
| 53             | 112           | TYR                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | ILE                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | ALA                  | C      |
| 65             | 124           | ALA                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | ASN                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | VAL                  | C      |
| 74             | 133           | ILE                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ALA                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | LEU                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S58 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | GLN                  | C      |
| 91             | 173           | ASN                  | C      |
| 92             | 174           | LEU                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | LEU                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | SER                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | VAL                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | VAL                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | LEU                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | MET                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | LEU                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | ILE                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | MET                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S58 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | PHE                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | PHE                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | ALA                  | B      |
| 147            | 245           | ALA                  | B      |
| 148            | 246           | VAL                  | B      |
| 149            | 247           | ASN                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | HIS                  | B      |
| 162            | 271           | LYS                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | GLU                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ALA                  | D      |
| 175            | 287           | GLN                  | D      |
| 176            | 288           | LYS                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | GLN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S58 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | ASP                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | LEU                  | D      |
| 188            | 308           | GLU                  | D      |
| 189            | 309           | GLY                  | D      |
| 190            | 310           | SER                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | ALA                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASP                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | GLU                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | HIS                  | D      |
| 211            | 334           | ALA                  | D      |
| 212            | 339           | ARG                  | A      |
| 213            | 341           | LYS                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S58 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | ARG                  | C      |
| 237            | 378           | ILE                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | GLN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | GLN                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLU                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | LEU                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |

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Table S58 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | ASN                  | A      |
| 282            | 440           | ALA                  | A      |
| 283            | 441           | PRO                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | SER                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | ASN                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | ALA                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLY                  | A      |
| 298            | 487           | THR                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S59: Residues membership for the *T. vulgaris* R47  $\alpha$ -amylase (PDB code 1WZL, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |

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Table S59 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |
| 30             | 192           | PHE                  | C      |
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |

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Table S59 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |
| 76             | 239           | ASP                  | C      |
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |

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Table S59 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |
| 122            | 316           | GLU                  | B      |
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASP                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |

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Table S59 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |
| 168            | 370           | SER                  | B      |
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |

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Table S59 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASP                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |
| 214            | 436           | PHE                  | A      |
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |

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Table S59 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |
| 260            | 507           | SER                  | A      |
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |

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Table S59 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 574           | ARG                  | A      |
| 295            | 575           | PRO                  | A      |
| 296            | 576           | TYR                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S60: Residues membership for the *N. polysaccharea*  $\alpha$ -amylase (PDB code 1ZS2, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 98            | GLN                  | A      |
| 1              | 99            | VAL                  | A      |
| 2              | 100           | GLY                  | B      |
| 3              | 101           | GLY                  | B      |
| 4              | 102           | VAL                  | B      |
| 5              | 103           | CYS                  | C      |
| 6              | 104           | TYR                  | C      |
| 7              | 105           | VAL                  | C      |
| 8              | 110           | GLY                  | C      |
| 9              | 111           | ASP                  | C      |
| 10             | 112           | LEU                  | C      |
| 11             | 113           | LYS                  | C      |
| 12             | 114           | GLY                  | C      |
| 13             | 115           | LEU                  | C      |
| 14             | 116           | LYS                  | C      |
| 15             | 117           | ASP                  | C      |
| 16             | 118           | LYS                  | C      |
| 17             | 119           | ILE                  | C      |
| 18             | 120           | PRO                  | C      |
| 19             | 121           | TYR                  | C      |

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Table S60 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 122           | PHE                  | C      |
| 21             | 123           | GLN                  | C      |
| 22             | 124           | GLU                  | C      |
| 23             | 125           | LEU                  | C      |
| 24             | 126           | GLY                  | C      |
| 25             | 127           | LEU                  | C      |
| 26             | 128           | THR                  | C      |
| 27             | 129           | TYR                  | C      |
| 28             | 130           | LEU                  | C      |
| 29             | 131           | TYR                  | C      |
| 30             | 132           | LEU                  | C      |
| 31             | 133           | MET                  | C      |
| 32             | 134           | PRO                  | C      |
| 33             | 135           | LEU                  | C      |
| 34             | 136           | PHE                  | C      |
| 35             | 137           | LYS                  | C      |
| 36             | 138           | CYS                  | C      |
| 37             | 139           | PRO                  | C      |
| 38             | 141           | GLY                  | C      |
| 39             | 144           | ASP                  | C      |
| 40             | 145           | GLY                  | C      |
| 41             | 146           | GLY                  | C      |
| 42             | 147           | TYR                  | C      |
| 43             | 148           | ALA                  | C      |
| 44             | 149           | VAL                  | C      |
| 45             | 150           | SER                  | C      |
| 46             | 151           | SER                  | C      |
| 47             | 153           | ARG                  | C      |
| 48             | 154           | ASP                  | C      |
| 49             | 155           | VAL                  | C      |
| 50             | 156           | ASN                  | C      |
| 51             | 157           | PRO                  | C      |
| 52             | 158           | ALA                  | C      |
| 53             | 159           | LEU                  | C      |
| 54             | 160           | GLY                  | C      |
| 55             | 161           | THR                  | C      |
| 56             | 162           | ILE                  | C      |
| 57             | 163           | GLY                  | C      |
| 58             | 164           | ASP                  | C      |
| 59             | 165           | LEU                  | C      |
| 60             | 166           | ARG                  | C      |
| 61             | 167           | GLU                  | C      |
| 62             | 168           | VAL                  | C      |
| 63             | 169           | ILE                  | C      |
| 64             | 170           | ALA                  | C      |
| 65             | 171           | ALA                  | C      |

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Table S60 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 172           | LEU                  | C      |
| 67             | 173           | HIS                  | C      |
| 68             | 174           | GLU                  | C      |
| 69             | 175           | ALA                  | C      |
| 70             | 176           | GLY                  | C      |
| 71             | 177           | ILE                  | C      |
| 72             | 178           | SER                  | C      |
| 73             | 179           | ALA                  | C      |
| 74             | 180           | VAL                  | C      |
| 75             | 181           | VAL                  | C      |
| 76             | 182           | ASP                  | C      |
| 77             | 183           | PHE                  | C      |
| 78             | 184           | ILE                  | C      |
| 79             | 185           | PHE                  | C      |
| 80             | 186           | ASN                  | C      |
| 81             | 187           | HIS                  | C      |
| 82             | 188           | THR                  | C      |
| 83             | 189           | SER                  | C      |
| 84             | 190           | ASN                  | C      |
| 85             | 191           | GLU                  | C      |
| 86             | 192           | HIS                  | C      |
| 87             | 193           | GLU                  | C      |
| 88             | 194           | TRP                  | C      |
| 89             | 195           | ALA                  | C      |
| 90             | 206           | ASP                  | C      |
| 91             | 207           | ASN                  | C      |
| 92             | 208           | PHE                  | C      |
| 93             | 209           | TYR                  | C      |
| 94             | 210           | TYR                  | B      |
| 95             | 247           | TRP                  | B      |
| 96             | 248           | THR                  | B      |
| 97             | 249           | THR                  | B      |
| 98             | 250           | PHE                  | B      |
| 99             | 254           | GLN                  | B      |
| 100            | 255           | TRP                  | B      |
| 101            | 256           | ASP                  | B      |
| 102            | 257           | LEU                  | B      |
| 103            | 258           | ASN                  | B      |
| 104            | 259           | TYR                  | B      |
| 105            | 260           | SER                  | B      |
| 106            | 261           | ASN                  | B      |
| 107            | 262           | PRO                  | B      |
| 108            | 263           | TRP                  | B      |
| 109            | 264           | VAL                  | B      |
| 110            | 265           | PHE                  | B      |
| 111            | 266           | ARG                  | B      |

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Table S60 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 267           | ALA                  | B      |
| 113            | 268           | MET                  | B      |
| 114            | 269           | ALA                  | B      |
| 115            | 270           | GLY                  | B      |
| 116            | 271           | GLU                  | B      |
| 117            | 272           | MET                  | B      |
| 118            | 273           | LEU                  | B      |
| 119            | 274           | PHE                  | B      |
| 120            | 275           | LEU                  | B      |
| 121            | 276           | ALA                  | B      |
| 122            | 277           | ASN                  | B      |
| 123            | 278           | LEU                  | C      |
| 124            | 279           | GLY                  | C      |
| 125            | 280           | VAL                  | C      |
| 126            | 281           | ASP                  | C      |
| 127            | 282           | ILE                  | C      |
| 128            | 283           | LEU                  | B      |
| 129            | 284           | ARG                  | D      |
| 130            | 285           | MET                  | B      |
| 131            | 286           | ASP                  | B      |
| 132            | 287           | ALA                  | B      |
| 133            | 288           | VAL                  | B      |
| 134            | 289           | ALA                  | B      |
| 135            | 290           | PHE                  | B      |
| 136            | 291           | ILE                  | B      |
| 137            | 292           | TRP                  | B      |
| 138            | 306           | HIS                  | B      |
| 139            | 307           | ALA                  | B      |
| 140            | 308           | LEU                  | B      |
| 141            | 309           | ILE                  | B      |
| 142            | 310           | ARG                  | B      |
| 143            | 311           | ALA                  | B      |
| 144            | 312           | PHE                  | B      |
| 145            | 313           | ASN                  | B      |
| 146            | 314           | ALA                  | B      |
| 147            | 315           | VAL                  | B      |
| 148            | 316           | MET                  | B      |
| 149            | 317           | ARG                  | B      |
| 150            | 323           | VAL                  | B      |
| 151            | 324           | PHE                  | B      |
| 152            | 325           | PHE                  | B      |
| 153            | 326           | LYS                  | C      |
| 154            | 327           | SER                  | B      |
| 155            | 328           | GLN                  | B      |
| 156            | 329           | ALA                  | B      |
| 157            | 330           | ILE                  | B      |

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Table S60 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 331           | VAL                  | B      |
| 159            | 332           | HIS                  | B      |
| 160            | 336           | VAL                  | B      |
| 161            | 337           | VAL                  | B      |
| 162            | 338           | GLN                  | B      |
| 163            | 339           | TYR                  | B      |
| 164            | 340           | ILE                  | B      |
| 165            | 341           | GLY                  | B      |
| 166            | 345           | CYS                  | B      |
| 167            | 346           | GLN                  | B      |
| 168            | 347           | ILE                  | B      |
| 169            | 348           | GLY                  | B      |
| 170            | 349           | TYR                  | D      |
| 171            | 350           | ASN                  | D      |
| 172            | 351           | PRO                  | D      |
| 173            | 352           | LEU                  | D      |
| 174            | 354           | MET                  | D      |
| 175            | 355           | ALA                  | D      |
| 176            | 356           | LEU                  | D      |
| 177            | 357           | LEU                  | D      |
| 178            | 358           | TRP                  | D      |
| 179            | 359           | ASN                  | D      |
| 180            | 360           | THR                  | D      |
| 181            | 361           | LEU                  | D      |
| 182            | 364           | ARG                  | D      |
| 183            | 365           | GLU                  | A      |
| 184            | 366           | VAL                  | A      |
| 185            | 367           | ASN                  | A      |
| 186            | 372           | ALA                  | A      |
| 187            | 373           | LEU                  | D      |
| 188            | 374           | THR                  | D      |
| 189            | 375           | TYR                  | D      |
| 190            | 376           | ARG                  | D      |
| 191            | 377           | HIS                  | B      |
| 192            | 378           | ASN                  | B      |
| 193            | 381           | GLU                  | B      |
| 194            | 382           | HIS                  | B      |
| 195            | 383           | THR                  | B      |
| 196            | 384           | ALA                  | B      |
| 197            | 385           | TRP                  | B      |
| 198            | 386           | VAL                  | D      |
| 199            | 387           | ASN                  | D      |
| 200            | 388           | TYR                  | D      |
| 201            | 389           | VAL                  | A      |
| 202            | 390           | ARG                  | D      |
| 203            | 391           | SER                  | D      |

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Table S60 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 392           | HIS                  | D      |
| 205            | 393           | ASP                  | D      |
| 206            | 394           | ASP                  | D      |
| 207            | 448           | SER                  | D      |
| 208            | 450           | THR                  | D      |
| 209            | 451           | ALA                  | D      |
| 210            | 452           | ALA                  | D      |
| 211            | 453           | ALA                  | D      |
| 212            | 464           | ALA                  | A      |
| 213            | 467           | ARG                  | A      |
| 214            | 468           | ILE                  | A      |
| 215            | 469           | LYS                  | A      |
| 216            | 470           | LEU                  | A      |
| 217            | 471           | LEU                  | A      |
| 218            | 472           | TYR                  | A      |
| 219            | 473           | SER                  | A      |
| 220            | 474           | ILE                  | A      |
| 221            | 475           | ALA                  | A      |
| 222            | 476           | LEU                  | A      |
| 223            | 477           | SER                  | A      |
| 224            | 478           | THR                  | A      |
| 225            | 479           | GLY                  | D      |
| 226            | 480           | GLY                  | D      |
| 227            | 481           | LEU                  | D      |
| 228            | 482           | PRO                  | A      |
| 229            | 483           | LEU                  | D      |
| 230            | 484           | ILE                  | A      |
| 231            | 485           | TYR                  | D      |
| 232            | 486           | LEU                  | C      |
| 233            | 487           | GLY                  | D      |
| 234            | 488           | ASP                  | A      |
| 235            | 514           | PRO                  | C      |
| 236            | 515           | ARG                  | C      |
| 237            | 516           | TYR                  | D      |
| 238            | 517           | ASN                  | D      |
| 239            | 521           | TYR                  | D      |
| 240            | 534           | ILE                  | A      |
| 241            | 535           | TYR                  | A      |
| 242            | 536           | GLN                  | A      |
| 243            | 537           | GLY                  | A      |
| 244            | 538           | LEU                  | A      |
| 245            | 539           | ARG                  | A      |
| 246            | 540           | HIS                  | A      |
| 247            | 541           | MET                  | A      |
| 248            | 542           | ILE                  | A      |
| 249            | 543           | ALA                  | A      |

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Table S60 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 544           | VAL                  | A      |
| 251            | 545           | ARG                  | A      |
| 252            | 546           | GLN                  | A      |
| 253            | 547           | SER                  | A      |
| 254            | 548           | ASN                  | A      |
| 255            | 549           | PRO                  | A      |
| 256            | 553           | GLY                  | A      |
| 257            | 554           | GLY                  | A      |
| 258            | 555           | ARG                  | A      |
| 259            | 556           | LEU                  | A      |
| 260            | 558           | THR                  | A      |
| 261            | 559           | PHE                  | A      |
| 262            | 560           | ASN                  | A      |
| 263            | 561           | THR                  | A      |
| 264            | 563           | ASN                  | A      |
| 265            | 564           | LYS                  | A      |
| 266            | 565           | HIS                  | A      |
| 267            | 566           | ILE                  | A      |
| 268            | 567           | ILE                  | A      |
| 269            | 568           | GLY                  | A      |
| 270            | 569           | TYR                  | A      |
| 271            | 570           | ILE                  | A      |
| 272            | 571           | ARG                  | A      |
| 273            | 573           | ASN                  | A      |
| 274            | 574           | ALA                  | A      |
| 275            | 575           | LEU                  | A      |
| 276            | 576           | LEU                  | A      |
| 277            | 577           | ALA                  | A      |
| 278            | 578           | PHE                  | A      |
| 279            | 579           | GLY                  | A      |
| 280            | 580           | ASN                  | A      |
| 281            | 584           | TYR                  | A      |
| 282            | 585           | PRO                  | A      |
| 283            | 586           | GLN                  | A      |
| 284            | 587           | THR                  | A      |
| 285            | 588           | VAL                  | A      |
| 286            | 589           | THR                  | A      |
| 287            | 590           | ALA                  | A      |
| 288            | 599           | LYS                  | A      |
| 289            | 600           | ALA                  | A      |
| 290            | 601           | HIS                  | A      |
| 291            | 602           | ASP                  | A      |
| 292            | 603           | LEU                  | A      |
| 293            | 604           | ILE                  | A      |
| 294            | 617           | LEU                  | A      |
| 295            | 618           | GLN                  | A      |

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Table S60 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 619           | PRO                  | A      |
| 297            | 621           | GLN                  | A      |
| 298            | 622           | VAL                  | A      |
| 299            | 623           | MET                  | A      |
| 300            | 624           | TRP                  | A      |
| 301            | 625           | LEU                  | A      |
| 302            | 626           | GLU                  | A      |

Table S61: Residues membership for the *T. vulgaris* R47  $\alpha$ -amylase (PDB code 1WZM, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |
| 30             | 192           | PHE                  | C      |

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Table S61 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |
| 76             | 239           | ASP                  | C      |

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Table S61 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |
| 122            | 316           | GLU                  | B      |

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Table S61 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASP                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |
| 168            | 370           | SER                  | B      |

*Continued on next page*

Table S61 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASP                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |
| 214            | 436           | PHE                  | A      |

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Table S61 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |
| 260            | 507           | SER                  | A      |

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Table S61 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 574           | ARG                  | A      |
| 295            | 575           | PRO                  | A      |
| 296            | 576           | TYR                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S62: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 2QMK, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |

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Table S62 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |

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Table S62 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |

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Table S62 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |

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Table S62 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |

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Table S62 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |

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Table S62 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S63: Residues membership for the *A.niger*  $\alpha$ -amylase (PDB code 2AAA, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | GLN                  | A      |
| 1              | 10            | SER                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | TYR                  | B      |
| 4              | 13            | PHE                  | B      |
| 5              | 14            | LEU                  | C      |
| 6              | 15            | LEU                  | C      |
| 7              | 16            | THR                  | C      |
| 8              | 40            | GLY                  | C      |

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Table S63 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 41            | SER                  | C      |
| 10             | 42            | TRP                  | C      |
| 11             | 43            | GLN                  | C      |
| 12             | 44            | GLY                  | C      |
| 13             | 45            | ILE                  | C      |
| 14             | 46            | ILE                  | C      |
| 15             | 47            | ASP                  | C      |
| 16             | 48            | HIS                  | C      |
| 17             | 49            | LEU                  | C      |
| 18             | 50            | ASP                  | C      |
| 19             | 51            | TYR                  | C      |
| 20             | 52            | ILE                  | C      |
| 21             | 53            | GLU                  | C      |
| 22             | 54            | GLY                  | C      |
| 23             | 55            | MET                  | C      |
| 24             | 56            | GLY                  | C      |
| 25             | 57            | PHE                  | C      |
| 26             | 58            | THR                  | C      |
| 27             | 59            | ALA                  | C      |
| 28             | 60            | ILE                  | C      |
| 29             | 61            | TRP                  | C      |
| 30             | 62            | ILE                  | C      |
| 31             | 63            | SER                  | C      |
| 32             | 64            | PRO                  | C      |
| 33             | 65            | ILE                  | C      |
| 34             | 66            | THR                  | C      |
| 35             | 67            | GLU                  | C      |
| 36             | 68            | GLN                  | C      |
| 37             | 69            | LEU                  | C      |
| 38             | 77            | GLU                  | C      |
| 39             | 79            | TYR                  | C      |
| 40             | 80            | HIS                  | C      |
| 41             | 81            | GLY                  | C      |
| 42             | 82            | TYR                  | C      |
| 43             | 83            | TRP                  | C      |
| 44             | 84            | GLN                  | C      |
| 45             | 85            | GLN                  | C      |
| 46             | 86            | LYS                  | C      |
| 47             | 88            | TYR                  | C      |
| 48             | 89            | ASP                  | C      |
| 49             | 90            | VAL                  | C      |
| 50             | 91            | ASN                  | C      |
| 51             | 92            | SER                  | C      |
| 52             | 93            | ASN                  | C      |
| 53             | 94            | PHE                  | C      |
| 54             | 95            | GLY                  | C      |

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Table S63 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 96            | THR                  | C      |
| 56             | 97            | ALA                  | C      |
| 57             | 98            | ASP                  | C      |
| 58             | 99            | ASN                  | C      |
| 59             | 100           | LEU                  | C      |
| 60             | 101           | LYS                  | C      |
| 61             | 102           | SER                  | C      |
| 62             | 103           | LEU                  | C      |
| 63             | 104           | SER                  | C      |
| 64             | 105           | ASP                  | C      |
| 65             | 106           | ALA                  | C      |
| 66             | 107           | LEU                  | C      |
| 67             | 108           | HIS                  | C      |
| 68             | 109           | ALA                  | C      |
| 69             | 110           | ARG                  | C      |
| 70             | 111           | GLY                  | C      |
| 71             | 112           | MET                  | C      |
| 72             | 113           | TYR                  | C      |
| 73             | 114           | LEU                  | C      |
| 74             | 115           | MET                  | C      |
| 75             | 116           | VAL                  | C      |
| 76             | 117           | ASP                  | C      |
| 77             | 118           | VAL                  | C      |
| 78             | 119           | VAL                  | C      |
| 79             | 120           | PRO                  | C      |
| 80             | 121           | ASP                  | C      |
| 81             | 122           | HIS                  | C      |
| 82             | 123           | MET                  | C      |
| 83             | 124           | GLY                  | C      |
| 84             | 125           | TYR                  | C      |
| 85             | 126           | ALA                  | C      |
| 86             | 137           | PHE                  | C      |
| 87             | 139           | PRO                  | C      |
| 88             | 140           | PHE                  | C      |
| 89             | 141           | ASP                  | C      |
| 90             | 143           | SER                  | C      |
| 91             | 144           | SER                  | C      |
| 92             | 145           | TYR                  | C      |
| 93             | 146           | PHE                  | C      |
| 94             | 147           | HIS                  | B      |
| 95             | 164           | CYS                  | B      |
| 96             | 165           | TRP                  | B      |
| 97             | 166           | GLU                  | B      |
| 98             | 167           | GLY                  | B      |
| 99             | 173           | LEU                  | B      |
| 100            | 174           | PRO                  | B      |

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Table S63 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 175           | ASP                  | B      |
| 102            | 176           | LEU                  | B      |
| 103            | 177           | ASP                  | B      |
| 104            | 178           | THR                  | B      |
| 105            | 179           | THR                  | B      |
| 106            | 180           | GLU                  | B      |
| 107            | 181           | THR                  | B      |
| 108            | 182           | ALA                  | B      |
| 109            | 183           | VAL                  | B      |
| 110            | 184           | ARG                  | B      |
| 111            | 185           | THR                  | B      |
| 112            | 186           | ILE                  | B      |
| 113            | 187           | TRP                  | B      |
| 114            | 188           | TYR                  | B      |
| 115            | 189           | ASP                  | B      |
| 116            | 190           | TRP                  | B      |
| 117            | 191           | VAL                  | B      |
| 118            | 192           | ALA                  | B      |
| 119            | 193           | ASP                  | B      |
| 120            | 194           | LEU                  | B      |
| 121            | 195           | VAL                  | B      |
| 122            | 196           | SER                  | B      |
| 123            | 198           | TYR                  | C      |
| 124            | 199           | SER                  | C      |
| 125            | 200           | VAL                  | C      |
| 126            | 201           | ASP                  | C      |
| 127            | 202           | GLY                  | C      |
| 128            | 203           | LEU                  | B      |
| 129            | 204           | ARG                  | D      |
| 130            | 205           | ILE                  | B      |
| 131            | 206           | ASP                  | B      |
| 132            | 207           | SER                  | B      |
| 133            | 208           | VAL                  | B      |
| 134            | 209           | LEU                  | B      |
| 135            | 210           | GLU                  | B      |
| 136            | 211           | VAL                  | B      |
| 137            | 212           | GLN                  | B      |
| 138            | 213           | PRO                  | B      |
| 139            | 214           | ASP                  | B      |
| 140            | 215           | PHE                  | B      |
| 141            | 216           | PHE                  | B      |
| 142            | 217           | PRO                  | B      |
| 143            | 218           | GLY                  | B      |
| 144            | 219           | TYR                  | B      |
| 145            | 220           | ASN                  | B      |
| 146            | 221           | LYS                  | B      |

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Table S63 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 222           | ALA                  | B      |
| 148            | 223           | SER                  | B      |
| 149            | 224           | GLY                  | B      |
| 150            | 225           | VAL                  | B      |
| 151            | 226           | TYR                  | B      |
| 152            | 227           | CYS                  | B      |
| 153            | 228           | VAL                  | C      |
| 154            | 229           | GLY                  | B      |
| 155            | 230           | GLU                  | B      |
| 156            | 231           | ILE                  | B      |
| 157            | 232           | ASP                  | B      |
| 158            | 233           | ASN                  | B      |
| 159            | 234           | GLY                  | B      |
| 160            | 239           | ASP                  | B      |
| 161            | 240           | CYS                  | B      |
| 162            | 241           | PRO                  | B      |
| 163            | 242           | TYR                  | B      |
| 164            | 243           | GLN                  | B      |
| 165            | 244           | LYS                  | B      |
| 166            | 246           | LEU                  | B      |
| 167            | 247           | ASP                  | B      |
| 168            | 248           | GLY                  | B      |
| 169            | 249           | VAL                  | B      |
| 170            | 250           | LEU                  | D      |
| 171            | 251           | ASN                  | D      |
| 172            | 252           | TYR                  | D      |
| 173            | 253           | PRO                  | D      |
| 174            | 255           | TYR                  | D      |
| 175            | 256           | TRP                  | D      |
| 176            | 257           | GLN                  | D      |
| 177            | 258           | LEU                  | D      |
| 178            | 259           | LEU                  | D      |
| 179            | 260           | TYR                  | D      |
| 180            | 261           | ALA                  | D      |
| 181            | 262           | PHE                  | D      |
| 182            | 267           | GLY                  | D      |
| 183            | 268           | SER                  | A      |
| 184            | 269           | ILE                  | A      |
| 185            | 270           | SER                  | A      |
| 186            | 275           | MET                  | A      |
| 187            | 276           | ILE                  | D      |
| 188            | 277           | LYS                  | D      |
| 189            | 278           | SER                  | D      |
| 190            | 279           | VAL                  | D      |
| 191            | 280           | ALA                  | B      |
| 192            | 281           | SER                  | B      |

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Table S63 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 285           | ASP                  | B      |
| 194            | 286           | PRO                  | B      |
| 195            | 287           | THR                  | B      |
| 196            | 288           | LEU                  | B      |
| 197            | 289           | LEU                  | B      |
| 198            | 290           | GLY                  | D      |
| 199            | 291           | ASN                  | D      |
| 200            | 292           | PHE                  | D      |
| 201            | 293           | ILE                  | A      |
| 202            | 294           | GLU                  | D      |
| 203            | 295           | ASN                  | D      |
| 204            | 296           | HIS                  | D      |
| 205            | 297           | ASP                  | D      |
| 206            | 298           | ASN                  | D      |
| 207            | 299           | PRO                  | D      |
| 208            | 300           | ARG                  | D      |
| 209            | 301           | PHE                  | D      |
| 210            | 302           | ALA                  | D      |
| 211            | 303           | LYS                  | D      |
| 212            | 308           | TYR                  | A      |
| 213            | 310           | GLN                  | A      |
| 214            | 311           | ALA                  | A      |
| 215            | 312           | LYS                  | A      |
| 216            | 313           | ASN                  | A      |
| 217            | 314           | VAL                  | A      |
| 218            | 315           | LEU                  | A      |
| 219            | 316           | SER                  | A      |
| 220            | 317           | TYR                  | A      |
| 221            | 318           | ILE                  | A      |
| 222            | 319           | PHE                  | A      |
| 223            | 320           | LEU                  | A      |
| 224            | 321           | SER                  | A      |
| 225            | 322           | ASP                  | D      |
| 226            | 323           | GLY                  | D      |
| 227            | 324           | ILE                  | D      |
| 228            | 325           | PRO                  | A      |
| 229            | 326           | ILE                  | D      |
| 230            | 327           | VAL                  | A      |
| 231            | 328           | TYR                  | D      |
| 232            | 329           | ALA                  | C      |
| 233            | 330           | GLY                  | D      |
| 234            | 331           | GLU                  | A      |
| 235            | 345           | GLU                  | C      |
| 236            | 346           | ALA                  | C      |
| 237            | 347           | THR                  | D      |
| 238            | 348           | TRP                  | D      |

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Table S63 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 352           | TYR                  | D      |
| 240            | 358           | LEU                  | A      |
| 241            | 359           | TYR                  | A      |
| 242            | 360           | THR                  | A      |
| 243            | 361           | TRP                  | A      |
| 244            | 362           | ILE                  | A      |
| 245            | 363           | ALA                  | A      |
| 246            | 364           | THR                  | A      |
| 247            | 365           | THR                  | A      |
| 248            | 366           | ASN                  | A      |
| 249            | 367           | ALA                  | A      |
| 250            | 368           | ILE                  | A      |
| 251            | 373           | ILE                  | A      |
| 252            | 374           | ALA                  | A      |
| 253            | 375           | ALA                  | A      |
| 254            | 376           | ASP                  | A      |
| 255            | 377           | SER                  | A      |
| 256            | 381           | THR                  | A      |
| 257            | 382           | TYR                  | A      |
| 258            | 383           | ALA                  | A      |
| 259            | 384           | ASN                  | A      |
| 260            | 386           | ALA                  | A      |
| 261            | 387           | PHE                  | A      |
| 262            | 388           | TYR                  | A      |
| 263            | 389           | THR                  | A      |
| 264            | 390           | ASP                  | A      |
| 265            | 391           | SER                  | A      |
| 266            | 392           | ASN                  | A      |
| 267            | 393           | THR                  | A      |
| 268            | 394           | ILE                  | A      |
| 269            | 395           | ALA                  | A      |
| 270            | 396           | MET                  | A      |
| 271            | 397           | ALA                  | A      |
| 272            | 398           | LYS                  | A      |
| 273            | 403           | SER                  | A      |
| 274            | 404           | GLN                  | A      |
| 275            | 405           | VAL                  | A      |
| 276            | 406           | ILE                  | A      |
| 277            | 407           | THR                  | A      |
| 278            | 408           | VAL                  | A      |
| 279            | 409           | LEU                  | A      |
| 280            | 410           | SER                  | A      |
| 281            | 416           | GLY                  | A      |
| 282            | 417           | SER                  | A      |
| 283            | 418           | SER                  | A      |
| 284            | 419           | TYR                  | A      |

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Table S63 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 420           | THR                  | A      |
| 286            | 421           | LEU                  | A      |
| 287            | 422           | THR                  | A      |
| 288            | 433           | LYS                  | A      |
| 289            | 434           | LEU                  | A      |
| 290            | 435           | ILE                  | A      |
| 291            | 436           | GLU                  | A      |
| 292            | 437           | ALA                  | A      |
| 293            | 438           | TYR                  | A      |
| 294            | 456           | ALA                  | A      |
| 295            | 457           | SER                  | A      |
| 296            | 458           | GLY                  | A      |
| 297            | 459           | LEU                  | A      |
| 298            | 460           | PRO                  | A      |
| 299            | 461           | ARG                  | A      |
| 300            | 462           | VAL                  | A      |
| 301            | 463           | LEU                  | A      |
| 302            | 464           | LEU                  | A      |

Table S64: Residues membership for the *A. oryzae*  $\alpha$ -amylase (PDB code 2TAA, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | GLN                  | A      |
| 1              | 10            | SER                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | TYR                  | B      |
| 4              | 13            | PHE                  | B      |
| 5              | 14            | LEU                  | C      |
| 6              | 15            | LEU                  | C      |
| 7              | 16            | THR                  | C      |
| 8              | 40            | GLY                  | C      |
| 9              | 41            | THR                  | C      |
| 10             | 42            | TRP                  | C      |
| 11             | 43            | GLN                  | C      |
| 12             | 44            | GLY                  | C      |
| 13             | 45            | ILE                  | C      |
| 14             | 46            | ILE                  | C      |
| 15             | 47            | ASP                  | C      |
| 16             | 48            | LYS                  | C      |
| 17             | 49            | LEU                  | C      |
| 18             | 50            | ASP                  | C      |
| 19             | 51            | TYR                  | C      |

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Table S64 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 52            | ILE                  | C      |
| 21             | 53            | GLN                  | C      |
| 22             | 54            | GLY                  | C      |
| 23             | 55            | MET                  | C      |
| 24             | 56            | GLY                  | C      |
| 25             | 57            | PHE                  | C      |
| 26             | 58            | THR                  | C      |
| 27             | 59            | ALA                  | C      |
| 28             | 60            | ILE                  | C      |
| 29             | 61            | TRP                  | C      |
| 30             | 62            | ILE                  | C      |
| 31             | 63            | THR                  | C      |
| 32             | 64            | PRO                  | C      |
| 33             | 65            | VAL                  | C      |
| 34             | 66            | THR                  | C      |
| 35             | 67            | ALA                  | C      |
| 36             | 68            | GLN                  | C      |
| 37             | 69            | LEU                  | C      |
| 38             | 77            | ASP                  | C      |
| 39             | 79            | TYR                  | C      |
| 40             | 80            | THR                  | C      |
| 41             | 81            | GLY                  | C      |
| 42             | 82            | TYR                  | C      |
| 43             | 83            | TRP                  | C      |
| 44             | 84            | GLN                  | C      |
| 45             | 85            | THR                  | C      |
| 46             | 86            | ASP                  | C      |
| 47             | 88            | TYR                  | C      |
| 48             | 89            | SER                  | C      |
| 49             | 90            | LEU                  | C      |
| 50             | 91            | ASN                  | C      |
| 51             | 92            | GLU                  | C      |
| 52             | 93            | ASN                  | C      |
| 53             | 94            | TYR                  | C      |
| 54             | 95            | GLY                  | C      |
| 55             | 96            | THR                  | C      |
| 56             | 97            | ALA                  | C      |
| 57             | 98            | ASP                  | C      |
| 58             | 99            | ASP                  | C      |
| 59             | 100           | LEU                  | C      |
| 60             | 101           | LYS                  | C      |
| 61             | 102           | ALA                  | C      |
| 62             | 103           | LEU                  | C      |
| 63             | 104           | SER                  | C      |
| 64             | 105           | SER                  | C      |
| 65             | 106           | ALA                  | C      |

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Table S64 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 107           | LEU                  | C      |
| 67             | 108           | HIS                  | C      |
| 68             | 109           | GLU                  | C      |
| 69             | 110           | ARG                  | C      |
| 70             | 111           | GLY                  | C      |
| 71             | 112           | MET                  | C      |
| 72             | 113           | TYR                  | C      |
| 73             | 114           | LEU                  | C      |
| 74             | 115           | MET                  | C      |
| 75             | 116           | VAL                  | C      |
| 76             | 117           | ASP                  | C      |
| 77             | 118           | VAL                  | C      |
| 78             | 119           | VAL                  | C      |
| 79             | 120           | ALA                  | C      |
| 80             | 121           | ASN                  | C      |
| 81             | 122           | HIS                  | C      |
| 82             | 123           | MET                  | C      |
| 83             | 124           | GLY                  | C      |
| 84             | 125           | TYR                  | C      |
| 85             | 126           | ASP                  | C      |
| 86             | 137           | PHE                  | C      |
| 87             | 139           | PRO                  | C      |
| 88             | 140           | PHE                  | C      |
| 89             | 141           | SER                  | C      |
| 90             | 143           | GLN                  | C      |
| 91             | 144           | ASP                  | C      |
| 92             | 145           | TYR                  | C      |
| 93             | 146           | PHE                  | C      |
| 94             | 147           | HIS                  | B      |
| 95             | 164           | CYS                  | B      |
| 96             | 165           | TRP                  | B      |
| 97             | 166           | LEU                  | B      |
| 98             | 167           | GLY                  | B      |
| 99             | 173           | LEU                  | B      |
| 100            | 174           | PRO                  | B      |
| 101            | 175           | ASP                  | B      |
| 102            | 176           | LEU                  | B      |
| 103            | 177           | ASP                  | B      |
| 104            | 178           | THR                  | B      |
| 105            | 179           | THR                  | B      |
| 106            | 180           | LYS                  | B      |
| 107            | 181           | ASP                  | B      |
| 108            | 182           | VAL                  | B      |
| 109            | 183           | VAL                  | B      |
| 110            | 184           | LYS                  | B      |
| 111            | 185           | ASN                  | B      |

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Table S64 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 186           | GLU                  | B      |
| 113            | 187           | TRP                  | B      |
| 114            | 188           | TYR                  | B      |
| 115            | 189           | ASP                  | B      |
| 116            | 190           | TRP                  | B      |
| 117            | 191           | VAL                  | B      |
| 118            | 192           | GLY                  | B      |
| 119            | 193           | SER                  | B      |
| 120            | 194           | LEU                  | B      |
| 121            | 195           | VAL                  | B      |
| 122            | 196           | SER                  | B      |
| 123            | 198           | TYR                  | C      |
| 124            | 199           | SER                  | C      |
| 125            | 200           | ILE                  | C      |
| 126            | 201           | ASP                  | C      |
| 127            | 202           | GLY                  | C      |
| 128            | 203           | LEU                  | B      |
| 129            | 204           | ARG                  | D      |
| 130            | 205           | ILE                  | B      |
| 131            | 206           | ASP                  | B      |
| 132            | 207           | THR                  | B      |
| 133            | 208           | VAL                  | B      |
| 134            | 209           | LYS                  | B      |
| 135            | 210           | HIS                  | B      |
| 136            | 211           | VAL                  | B      |
| 137            | 212           | GLN                  | B      |
| 138            | 213           | LYS                  | B      |
| 139            | 214           | ASP                  | B      |
| 140            | 215           | PHE                  | B      |
| 141            | 216           | TRP                  | B      |
| 142            | 217           | PRO                  | B      |
| 143            | 218           | GLY                  | B      |
| 144            | 219           | TYR                  | B      |
| 145            | 220           | ASN                  | B      |
| 146            | 221           | LYS                  | B      |
| 147            | 222           | ALA                  | B      |
| 148            | 223           | ALA                  | B      |
| 149            | 224           | GLY                  | B      |
| 150            | 225           | VAL                  | B      |
| 151            | 226           | TYR                  | B      |
| 152            | 227           | CYS                  | B      |
| 153            | 228           | ILE                  | C      |
| 154            | 229           | GLY                  | B      |
| 155            | 230           | GLU                  | B      |
| 156            | 231           | VAL                  | B      |
| 157            | 232           | LEU                  | B      |

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Table S64 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 233           | ASP                  | B      |
| 159            | 234           | GLY                  | B      |
| 160            | 239           | THR                  | B      |
| 161            | 240           | CYS                  | B      |
| 162            | 241           | PRO                  | B      |
| 163            | 242           | TYR                  | B      |
| 164            | 243           | GLN                  | B      |
| 165            | 244           | ASN                  | B      |
| 166            | 246           | MET                  | B      |
| 167            | 247           | ASP                  | B      |
| 168            | 248           | GLY                  | B      |
| 169            | 249           | VAL                  | B      |
| 170            | 250           | LEU                  | D      |
| 171            | 251           | ASN                  | D      |
| 172            | 252           | TYR                  | D      |
| 173            | 253           | PRO                  | D      |
| 174            | 255           | TYR                  | D      |
| 175            | 256           | TYR                  | D      |
| 176            | 257           | PRO                  | D      |
| 177            | 258           | LEU                  | D      |
| 178            | 259           | LEU                  | D      |
| 179            | 260           | ASN                  | D      |
| 180            | 261           | ALA                  | D      |
| 181            | 262           | PHE                  | D      |
| 182            | 267           | GLY                  | D      |
| 183            | 268           | SER                  | A      |
| 184            | 269           | MET                  | A      |
| 185            | 270           | ASP                  | A      |
| 186            | 275           | MET                  | A      |
| 187            | 276           | ILE                  | D      |
| 188            | 277           | ASN                  | D      |
| 189            | 278           | THR                  | D      |
| 190            | 279           | VAL                  | D      |
| 191            | 280           | LYS                  | B      |
| 192            | 281           | SER                  | B      |
| 193            | 285           | ASP                  | B      |
| 194            | 286           | SER                  | B      |
| 195            | 287           | THR                  | B      |
| 196            | 288           | LEU                  | B      |
| 197            | 289           | LEU                  | B      |
| 198            | 290           | GLY                  | D      |
| 199            | 291           | THR                  | D      |
| 200            | 292           | PHE                  | D      |
| 201            | 293           | VAL                  | A      |
| 202            | 294           | GLU                  | D      |
| 203            | 295           | ASN                  | D      |

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Table S64 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 296           | HIS                  | D      |
| 205            | 297           | ASP                  | D      |
| 206            | 298           | ASN                  | D      |
| 207            | 299           | PRO                  | D      |
| 208            | 300           | ARG                  | D      |
| 209            | 301           | PHE                  | D      |
| 210            | 302           | ALA                  | D      |
| 211            | 303           | SER                  | D      |
| 212            | 308           | ILE                  | A      |
| 213            | 310           | LEU                  | A      |
| 214            | 311           | ALA                  | A      |
| 215            | 312           | LYS                  | A      |
| 216            | 313           | ASN                  | A      |
| 217            | 314           | VAL                  | A      |
| 218            | 315           | ALA                  | A      |
| 219            | 316           | ALA                  | A      |
| 220            | 317           | PHE                  | A      |
| 221            | 318           | ILE                  | A      |
| 222            | 319           | ILE                  | A      |
| 223            | 320           | LEU                  | A      |
| 224            | 321           | ASN                  | A      |
| 225            | 322           | ASP                  | D      |
| 226            | 323           | GLY                  | D      |
| 227            | 324           | LEU                  | D      |
| 228            | 325           | PRO                  | A      |
| 229            | 326           | ILE                  | D      |
| 230            | 327           | ILE                  | A      |
| 231            | 328           | TYR                  | D      |
| 232            | 329           | ALA                  | C      |
| 233            | 330           | GLY                  | D      |
| 234            | 331           | GLN                  | A      |
| 235            | 345           | GLU                  | C      |
| 236            | 346           | ALA                  | C      |
| 237            | 347           | THR                  | D      |
| 238            | 348           | TRP                  | D      |
| 239            | 352           | TYR                  | D      |
| 240            | 358           | LEU                  | A      |
| 241            | 359           | TYR                  | A      |
| 242            | 360           | LYS                  | A      |
| 243            | 361           | LEU                  | A      |
| 244            | 362           | ILE                  | A      |
| 245            | 363           | ALA                  | A      |
| 246            | 364           | SER                  | A      |
| 247            | 365           | ALA                  | A      |
| 248            | 366           | ASN                  | A      |
| 249            | 367           | ALA                  | A      |

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Table S64 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 368           | ILE                  | A      |
| 251            | 373           | ILE                  | A      |
| 252            | 374           | SER                  | A      |
| 253            | 375           | LYS                  | A      |
| 254            | 376           | ASP                  | A      |
| 255            | 377           | THR                  | A      |
| 256            | 381           | THR                  | A      |
| 257            | 382           | TYR                  | A      |
| 258            | 383           | LYS                  | A      |
| 259            | 384           | ASN                  | A      |
| 260            | 385           | PRO                  | A      |
| 261            | 386           | TYR                  | A      |
| 262            | 387           | ILE                  | A      |
| 263            | 388           | LYS                  | A      |
| 264            | 389           | ASP                  | A      |
| 265            | 390           | ASP                  | A      |
| 266            | 391           | THR                  | A      |
| 267            | 392           | THR                  | A      |
| 268            | 393           | ILE                  | A      |
| 269            | 394           | ALA                  | A      |
| 270            | 395           | MET                  | A      |
| 271            | 396           | ARG                  | A      |
| 272            | 397           | LYS                  | A      |
| 273            | 403           | GLN                  | A      |
| 274            | 404           | ILE                  | A      |
| 275            | 405           | VAL                  | A      |
| 276            | 406           | THR                  | A      |
| 277            | 407           | ILE                  | A      |
| 278            | 408           | LEU                  | A      |
| 279            | 409           | SER                  | A      |
| 280            | 410           | ASN                  | A      |
| 281            | 415           | GLY                  | A      |
| 282            | 416           | ASP                  | A      |
| 283            | 417           | SER                  | A      |
| 284            | 418           | TYR                  | A      |
| 285            | 419           | THR                  | A      |
| 286            | 420           | LEU                  | A      |
| 287            | 421           | SER                  | A      |
| 288            | 431           | GLN                  | A      |
| 289            | 432           | GLN                  | A      |
| 290            | 434           | THR                  | A      |
| 291            | 435           | GLU                  | A      |
| 292            | 436           | VAL                  | A      |
| 293            | 437           | ILE                  | A      |
| 294            | 454           | MET                  | A      |
| 295            | 455           | ALA                  | A      |

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Table S64 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 456           | GLY                  | A      |
| 297            | 458           | LEU                  | A      |
| 298            | 459           | PRO                  | A      |
| 299            | 460           | ARG                  | A      |
| 300            | 461           | VAL                  | A      |
| 301            | 462           | LEU                  | A      |
| 302            | 463           | TYR                  | A      |

Table S65: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 2QV4, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |

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Table S65 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |

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Table S65 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |

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Table S65 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |

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Table S65 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |

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Table S65 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |

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Table S65 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S66: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 3BAJ, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |

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Table S66 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |

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Table S66 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |

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Table S66 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |

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Table S66 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |

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Table S66 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |

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Table S66 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S67: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 3BAI, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |

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Table S67 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |

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Table S67 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |

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Table S67 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |

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Table S67 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |

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Table S67 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |

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Table S67 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |

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Table S67 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S68: Residues membership for the *T. thermosulfurigenes EM1*  $\alpha$ -amylase (PDB code 3BMV, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | VAL                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |

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Table S68 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | PRO                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 96            | THR                  | C      |
| 39             | 98            | TYR                  | C      |
| 40             | 99            | HIS                  | C      |
| 41             | 100           | GLY                  | C      |
| 42             | 101           | TYR                  | C      |
| 43             | 102           | TRP                  | C      |
| 44             | 103           | ALA                  | C      |
| 45             | 104           | ARG                  | C      |
| 46             | 105           | ASP                  | C      |
| 47             | 107           | LYS                  | C      |
| 48             | 108           | ARG                  | C      |
| 49             | 109           | THR                  | C      |
| 50             | 110           | ASN                  | C      |
| 51             | 111           | PRO                  | C      |
| 52             | 112           | TYR                  | C      |
| 53             | 113           | PHE                  | C      |
| 54             | 114           | GLY                  | C      |
| 55             | 115           | SER                  | C      |
| 56             | 116           | PHE                  | C      |
| 57             | 117           | THR                  | C      |
| 58             | 118           | ASP                  | C      |
| 59             | 119           | PHE                  | C      |
| 60             | 120           | GLN                  | C      |
| 61             | 121           | ASN                  | C      |
| 62             | 122           | LEU                  | C      |
| 63             | 123           | ILE                  | C      |
| 64             | 124           | ASN                  | C      |
| 65             | 125           | THR                  | C      |

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Table S68 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 126           | ALA                  | C      |
| 67             | 127           | HIS                  | C      |
| 68             | 128           | ALA                  | C      |
| 69             | 129           | HIS                  | C      |
| 70             | 130           | ASN                  | C      |
| 71             | 131           | ILE                  | C      |
| 72             | 132           | LYS                  | C      |
| 73             | 133           | VAL                  | C      |
| 74             | 134           | ILE                  | C      |
| 75             | 135           | ILE                  | C      |
| 76             | 136           | ASP                  | C      |
| 77             | 137           | PHE                  | C      |
| 78             | 138           | ALA                  | C      |
| 79             | 139           | PRO                  | C      |
| 80             | 140           | ASN                  | C      |
| 81             | 141           | HIS                  | C      |
| 82             | 142           | THR                  | C      |
| 83             | 143           | SER                  | C      |
| 84             | 144           | PRO                  | C      |
| 85             | 145           | ALA                  | C      |
| 86             | 157           | ARG                  | C      |
| 87             | 164           | LEU                  | C      |
| 88             | 165           | LEU                  | C      |
| 89             | 166           | GLY                  | C      |
| 90             | 173           | ASN                  | C      |
| 91             | 174           | GLY                  | C      |
| 92             | 175           | TYR                  | C      |
| 93             | 176           | PHE                  | C      |
| 94             | 177           | HIS                  | B      |
| 95             | 193           | ARG                  | B      |
| 96             | 194           | ASN                  | B      |
| 97             | 195           | LEU                  | B      |
| 98             | 196           | PHE                  | B      |
| 99             | 198           | LEU                  | B      |
| 100            | 199           | ALA                  | B      |
| 101            | 200           | ASP                  | B      |
| 102            | 201           | LEU                  | B      |
| 103            | 202           | ASN                  | B      |
| 104            | 203           | GLN                  | B      |
| 105            | 204           | GLN                  | B      |
| 106            | 205           | ASN                  | B      |
| 107            | 206           | SER                  | B      |
| 108            | 207           | THR                  | B      |
| 109            | 208           | ILE                  | B      |
| 110            | 209           | ASP                  | B      |
| 111            | 210           | SER                  | B      |

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Table S68 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 211           | TYR                  | B      |
| 113            | 212           | LEU                  | B      |
| 114            | 213           | LYS                  | B      |
| 115            | 214           | SER                  | B      |
| 116            | 215           | ALA                  | B      |
| 117            | 216           | ILE                  | B      |
| 118            | 217           | LYS                  | B      |
| 119            | 218           | VAL                  | B      |
| 120            | 219           | TRP                  | B      |
| 121            | 220           | LEU                  | B      |
| 122            | 221           | ASP                  | B      |
| 123            | 222           | MET                  | C      |
| 124            | 223           | GLY                  | C      |
| 125            | 224           | ILE                  | C      |
| 126            | 225           | ASP                  | C      |
| 127            | 226           | GLY                  | C      |
| 128            | 227           | ILE                  | B      |
| 129            | 228           | ARG                  | D      |
| 130            | 229           | LEU                  | B      |
| 131            | 230           | ASP                  | B      |
| 132            | 231           | ALA                  | B      |
| 133            | 232           | VAL                  | B      |
| 134            | 233           | LYS                  | B      |
| 135            | 234           | HIS                  | B      |
| 136            | 235           | MET                  | B      |
| 137            | 236           | PRO                  | B      |
| 138            | 237           | PHE                  | B      |
| 139            | 238           | GLY                  | B      |
| 140            | 239           | TRP                  | B      |
| 141            | 240           | GLN                  | B      |
| 142            | 241           | LYS                  | B      |
| 143            | 242           | ASN                  | B      |
| 144            | 243           | PHE                  | B      |
| 145            | 244           | MET                  | B      |
| 146            | 245           | ASP                  | B      |
| 147            | 246           | SER                  | B      |
| 148            | 247           | ILE                  | B      |
| 149            | 248           | LEU                  | B      |
| 150            | 253           | VAL                  | B      |
| 151            | 254           | PHE                  | B      |
| 152            | 255           | THR                  | B      |
| 153            | 256           | PHE                  | C      |
| 154            | 257           | GLY                  | B      |
| 155            | 258           | GLU                  | B      |
| 156            | 259           | TRP                  | B      |
| 157            | 260           | PHE                  | B      |

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Table S68 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 261           | LEU                  | B      |
| 159            | 262           | GLY                  | B      |
| 160            | 270           | ASN                  | B      |
| 161            | 271           | THR                  | B      |
| 162            | 272           | TYR                  | B      |
| 163            | 273           | PHE                  | B      |
| 164            | 275           | ASN                  | B      |
| 165            | 276           | GLU                  | B      |
| 166            | 278           | GLY                  | B      |
| 167            | 279           | MET                  | B      |
| 168            | 280           | SER                  | B      |
| 169            | 281           | LEU                  | B      |
| 170            | 282           | LEU                  | D      |
| 171            | 283           | ASP                  | D      |
| 172            | 284           | PHE                  | D      |
| 173            | 285           | ARG                  | D      |
| 174            | 287           | SER                  | D      |
| 175            | 288           | GLN                  | D      |
| 176            | 289           | LYS                  | D      |
| 177            | 290           | VAL                  | D      |
| 178            | 291           | ARG                  | D      |
| 179            | 292           | GLN                  | D      |
| 180            | 293           | VAL                  | D      |
| 181            | 294           | PHE                  | D      |
| 182            | 299           | ASP                  | D      |
| 183            | 300           | THR                  | A      |
| 184            | 301           | MET                  | A      |
| 185            | 302           | TYR                  | A      |
| 186            | 307           | MET                  | A      |
| 187            | 308           | ILE                  | D      |
| 188            | 309           | GLN                  | D      |
| 189            | 310           | SER                  | D      |
| 190            | 311           | THR                  | D      |
| 191            | 312           | ALA                  | B      |
| 192            | 313           | SER                  | B      |
| 193            | 317           | PHE                  | B      |
| 194            | 318           | ILE                  | B      |
| 195            | 319           | ASN                  | B      |
| 196            | 320           | ASP                  | B      |
| 197            | 321           | MET                  | B      |
| 198            | 322           | VAL                  | D      |
| 199            | 323           | THR                  | D      |
| 200            | 324           | PHE                  | D      |
| 201            | 325           | ILE                  | A      |
| 202            | 326           | ASP                  | D      |
| 203            | 327           | ASN                  | D      |

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Table S68 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 328           | HIS                  | D      |
| 205            | 329           | ASP                  | D      |
| 206            | 330           | MET                  | D      |
| 207            | 331           | ASP                  | D      |
| 208            | 332           | ARG                  | D      |
| 209            | 333           | PHE                  | D      |
| 210            | 334           | TYR                  | D      |
| 211            | 335           | ASN                  | D      |
| 212            | 339           | THR                  | A      |
| 213            | 341           | PRO                  | A      |
| 214            | 342           | VAL                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | MET                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | THR                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | LYS                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |

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Table S68 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | THR                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | LEU                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | ILE                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | TYR                  | A      |
| 285            | 443           | ASN                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | THR                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | SER                  | A      |
| 295            | 484           | ALA                  | A      |

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Table S68 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLU                  | A      |
| 298            | 487           | VAL                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S69: Residues membership for the *H. sapiens*  $\alpha$ -amylase (PDB code 3BAW, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |

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Table S69 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | VAL                  | C      |
| 38             | 51            | ILE                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASP                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASN                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |

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Table S69 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | ASN                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | GLY                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | ARG                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | THR                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | LYS                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | GLU                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | MET                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | HIS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |

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Table S69 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | LEU                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | ILE                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | TYR                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | ASP                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |

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Table S69 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | ILE                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | VAL                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |

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Table S69 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 322           | LYS                  | A      |
| 216            | 323           | MET                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | ILE                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |

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Table S69 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TYR                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | SER                  | A      |
| 284            | 436           | PHE                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | LEU                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | ALA                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S70: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase  
(PDB code 3CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S70 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S70 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S70 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | ALA                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S70 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S70 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |

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Table S70 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S71: Residues membership for the *T. thermosulfurigenes* EM1  $\alpha$ -amylase (PDB code 3BMW, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | ILE                  | C      |
| 6              | 21            | VAL                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |

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Table S71 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | ILE                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | LEU                  | C      |
| 21             | 67            | THR                  | C      |
| 22             | 68            | GLY                  | C      |
| 23             | 69            | MET                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | ILE                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | PRO                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 96            | THR                  | C      |
| 39             | 98            | TYR                  | C      |
| 40             | 99            | HIS                  | C      |
| 41             | 100           | GLY                  | C      |
| 42             | 101           | TYR                  | C      |
| 43             | 102           | TRP                  | C      |
| 44             | 103           | ALA                  | C      |
| 45             | 104           | ARG                  | C      |
| 46             | 105           | ASP                  | C      |
| 47             | 107           | LYS                  | C      |
| 48             | 108           | ARG                  | C      |
| 49             | 109           | THR                  | C      |
| 50             | 110           | ASN                  | C      |
| 51             | 111           | PRO                  | C      |
| 52             | 112           | TYR                  | C      |
| 53             | 113           | PHE                  | C      |
| 54             | 114           | GLY                  | C      |

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Table S71 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 115           | SER                  | C      |
| 56             | 116           | PHE                  | C      |
| 57             | 117           | THR                  | C      |
| 58             | 118           | ASP                  | C      |
| 59             | 119           | PHE                  | C      |
| 60             | 120           | GLN                  | C      |
| 61             | 121           | ASN                  | C      |
| 62             | 122           | LEU                  | C      |
| 63             | 123           | ILE                  | C      |
| 64             | 124           | ASN                  | C      |
| 65             | 125           | THR                  | C      |
| 66             | 126           | ALA                  | C      |
| 67             | 127           | HIS                  | C      |
| 68             | 128           | ALA                  | C      |
| 69             | 129           | HIS                  | C      |
| 70             | 130           | ASN                  | C      |
| 71             | 131           | ILE                  | C      |
| 72             | 132           | LYS                  | C      |
| 73             | 133           | VAL                  | C      |
| 74             | 134           | ILE                  | C      |
| 75             | 135           | ILE                  | C      |
| 76             | 136           | ASP                  | C      |
| 77             | 137           | PHE                  | C      |
| 78             | 138           | ALA                  | C      |
| 79             | 139           | PRO                  | C      |
| 80             | 140           | ASN                  | C      |
| 81             | 141           | HIS                  | C      |
| 82             | 142           | THR                  | C      |
| 83             | 143           | SER                  | C      |
| 84             | 144           | PRO                  | C      |
| 85             | 145           | ALA                  | C      |
| 86             | 157           | ARG                  | C      |
| 87             | 164           | LEU                  | C      |
| 88             | 165           | LEU                  | C      |
| 89             | 166           | GLY                  | C      |
| 90             | 173           | ASN                  | C      |
| 91             | 174           | GLY                  | C      |
| 92             | 175           | TYR                  | C      |
| 93             | 176           | PHE                  | C      |
| 94             | 177           | HIS                  | B      |
| 95             | 193           | ARG                  | B      |
| 96             | 194           | ASN                  | B      |
| 97             | 195           | LEU                  | B      |
| 98             | 196           | PHE                  | B      |
| 99             | 198           | LEU                  | B      |
| 100            | 199           | ALA                  | B      |

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Table S71 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 200           | ASP                  | B      |
| 102            | 201           | LEU                  | B      |
| 103            | 202           | ASN                  | B      |
| 104            | 203           | GLN                  | B      |
| 105            | 204           | GLN                  | B      |
| 106            | 205           | ASN                  | B      |
| 107            | 206           | SER                  | B      |
| 108            | 207           | THR                  | B      |
| 109            | 208           | ILE                  | B      |
| 110            | 209           | ASP                  | B      |
| 111            | 210           | SER                  | B      |
| 112            | 211           | TYR                  | B      |
| 113            | 212           | LEU                  | B      |
| 114            | 213           | LYS                  | B      |
| 115            | 214           | SER                  | B      |
| 116            | 215           | ALA                  | B      |
| 117            | 216           | ILE                  | B      |
| 118            | 217           | LYS                  | B      |
| 119            | 218           | VAL                  | B      |
| 120            | 219           | TRP                  | B      |
| 121            | 220           | LEU                  | B      |
| 122            | 221           | ASP                  | B      |
| 123            | 222           | MET                  | C      |
| 124            | 223           | GLY                  | C      |
| 125            | 224           | ILE                  | C      |
| 126            | 225           | ASP                  | C      |
| 127            | 226           | GLY                  | C      |
| 128            | 227           | ILE                  | B      |
| 129            | 228           | ARG                  | D      |
| 130            | 229           | LEU                  | B      |
| 131            | 230           | ASP                  | B      |
| 132            | 231           | ALA                  | B      |
| 133            | 232           | VAL                  | B      |
| 134            | 233           | LYS                  | B      |
| 135            | 234           | HIS                  | B      |
| 136            | 235           | MET                  | B      |
| 137            | 236           | PRO                  | B      |
| 138            | 237           | PHE                  | B      |
| 139            | 238           | GLY                  | B      |
| 140            | 239           | TRP                  | B      |
| 141            | 240           | GLN                  | B      |
| 142            | 241           | LYS                  | B      |
| 143            | 242           | ASN                  | B      |
| 144            | 243           | PHE                  | B      |
| 145            | 244           | MET                  | B      |
| 146            | 245           | ASP                  | B      |

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Table S71 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 246           | SER                  | B      |
| 148            | 247           | ILE                  | B      |
| 149            | 248           | LEU                  | B      |
| 150            | 253           | VAL                  | B      |
| 151            | 254           | PHE                  | B      |
| 152            | 255           | THR                  | B      |
| 153            | 256           | PHE                  | C      |
| 154            | 257           | GLY                  | B      |
| 155            | 258           | GLU                  | B      |
| 156            | 259           | TRP                  | B      |
| 157            | 260           | PHE                  | B      |
| 158            | 261           | LEU                  | B      |
| 159            | 262           | GLY                  | B      |
| 160            | 270           | ASN                  | B      |
| 161            | 271           | THR                  | B      |
| 162            | 272           | TYR                  | B      |
| 163            | 273           | PHE                  | B      |
| 164            | 275           | ASN                  | B      |
| 165            | 276           | GLU                  | B      |
| 166            | 278           | GLY                  | B      |
| 167            | 279           | MET                  | B      |
| 168            | 280           | SER                  | B      |
| 169            | 281           | LEU                  | B      |
| 170            | 282           | LEU                  | D      |
| 171            | 283           | ASP                  | D      |
| 172            | 284           | PHE                  | D      |
| 173            | 285           | ARG                  | D      |
| 174            | 287           | SER                  | D      |
| 175            | 288           | GLN                  | D      |
| 176            | 289           | LYS                  | D      |
| 177            | 290           | VAL                  | D      |
| 178            | 291           | ARG                  | D      |
| 179            | 292           | GLN                  | D      |
| 180            | 293           | VAL                  | D      |
| 181            | 294           | PHE                  | D      |
| 182            | 299           | ASP                  | D      |
| 183            | 300           | THR                  | A      |
| 184            | 301           | MET                  | A      |
| 185            | 302           | TYR                  | A      |
| 186            | 307           | MET                  | A      |
| 187            | 308           | ILE                  | D      |
| 188            | 309           | GLN                  | D      |
| 189            | 310           | SER                  | D      |
| 190            | 311           | THR                  | D      |
| 191            | 312           | ALA                  | B      |
| 192            | 313           | SER                  | B      |

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Table S71 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 317           | PHE                  | B      |
| 194            | 318           | ILE                  | B      |
| 195            | 319           | ASN                  | B      |
| 196            | 320           | ASP                  | B      |
| 197            | 321           | MET                  | B      |
| 198            | 322           | VAL                  | D      |
| 199            | 323           | THR                  | D      |
| 200            | 324           | PHE                  | D      |
| 201            | 325           | ILE                  | A      |
| 202            | 326           | ASP                  | D      |
| 203            | 327           | ASN                  | D      |
| 204            | 328           | HIS                  | D      |
| 205            | 329           | ASP                  | D      |
| 206            | 330           | MET                  | D      |
| 207            | 331           | ASP                  | D      |
| 208            | 332           | ARG                  | D      |
| 209            | 333           | PHE                  | D      |
| 210            | 334           | TYR                  | D      |
| 211            | 335           | ASN                  | D      |
| 212            | 339           | THR                  | A      |
| 213            | 341           | PRO                  | A      |
| 214            | 342           | VAL                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | MET                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | THR                  | D      |

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Table S71 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | TYR                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | LYS                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | THR                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | ILE                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | ASN                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | LEU                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | ILE                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | TYR                  | A      |

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Table S71 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 443           | ASN                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | THR                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 483           | SER                  | A      |
| 295            | 484           | ALA                  | A      |
| 296            | 485           | GLY                  | A      |
| 297            | 486           | GLU                  | A      |
| 298            | 487           | VAL                  | A      |
| 299            | 488           | ALA                  | A      |
| 300            | 489           | VAL                  | A      |
| 301            | 490           | TRP                  | A      |
| 302            | 491           | GLN                  | A      |

Table S72: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 3L2M, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |

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Table S72 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | ILE                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |

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Table S72 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |

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Table S72 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |

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Table S72 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |

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Table S72 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |
| 215            | 322           | LYS                  | A      |
| 216            | 323           | VAL                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |

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Table S72 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |

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Table S72 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S73: Residues membership for the *S. scrofa*  $\alpha$ -amylase (PDB code 3L2L, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 11            | THR                  | A      |
| 1              | 12            | SER                  | A      |
| 2              | 13            | ILE                  | B      |
| 3              | 14            | VAL                  | B      |
| 4              | 15            | HIS                  | B      |
| 5              | 16            | LEU                  | C      |
| 6              | 17            | PHE                  | C      |
| 7              | 18            | GLU                  | C      |
| 8              | 19            | TRP                  | C      |
| 9              | 20            | ARG                  | C      |
| 10             | 21            | TRP                  | C      |
| 11             | 22            | VAL                  | C      |
| 12             | 23            | ASP                  | C      |
| 13             | 24            | ILE                  | C      |
| 14             | 25            | ALA                  | C      |
| 15             | 26            | LEU                  | C      |
| 16             | 27            | GLU                  | C      |
| 17             | 28            | CYS                  | C      |
| 18             | 29            | GLU                  | C      |
| 19             | 30            | ARG                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | GLY                  | C      |
| 22             | 34            | PRO                  | C      |
| 23             | 35            | LYS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | PHE                  | C      |
| 26             | 38            | GLY                  | C      |
| 27             | 39            | GLY                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | GLN                  | C      |
| 30             | 42            | VAL                  | C      |

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Table S73 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 43            | SER                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | PRO                  | C      |
| 34             | 46            | ASN                  | C      |
| 35             | 47            | GLU                  | C      |
| 36             | 48            | ASN                  | C      |
| 37             | 49            | ILE                  | C      |
| 38             | 51            | VAL                  | C      |
| 39             | 59            | TRP                  | C      |
| 40             | 60            | GLU                  | C      |
| 41             | 61            | ARG                  | C      |
| 42             | 62            | TYR                  | C      |
| 43             | 63            | GLN                  | C      |
| 44             | 64            | PRO                  | C      |
| 45             | 65            | VAL                  | C      |
| 46             | 66            | SER                  | C      |
| 47             | 67            | TYR                  | C      |
| 48             | 68            | LYS                  | C      |
| 49             | 69            | LEU                  | C      |
| 50             | 70            | CYS                  | C      |
| 51             | 71            | THR                  | C      |
| 52             | 72            | ARG                  | C      |
| 53             | 73            | SER                  | C      |
| 54             | 74            | GLY                  | C      |
| 55             | 75            | ASN                  | C      |
| 56             | 76            | GLU                  | C      |
| 57             | 77            | ASN                  | C      |
| 58             | 78            | GLU                  | C      |
| 59             | 79            | PHE                  | C      |
| 60             | 80            | ARG                  | C      |
| 61             | 81            | ASP                  | C      |
| 62             | 82            | MET                  | C      |
| 63             | 83            | VAL                  | C      |
| 64             | 84            | THR                  | C      |
| 65             | 85            | ARG                  | C      |
| 66             | 86            | CYS                  | C      |
| 67             | 87            | ASN                  | C      |
| 68             | 88            | ASN                  | C      |
| 69             | 89            | VAL                  | C      |
| 70             | 90            | GLY                  | C      |
| 71             | 91            | VAL                  | C      |
| 72             | 92            | ARG                  | C      |
| 73             | 93            | ILE                  | C      |
| 74             | 94            | TYR                  | C      |
| 75             | 95            | VAL                  | C      |
| 76             | 96            | ASP                  | C      |

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Table S73 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 97            | ALA                  | C      |
| 78             | 98            | VAL                  | C      |
| 79             | 99            | ILE                  | C      |
| 80             | 100           | ASN                  | C      |
| 81             | 101           | HIS                  | C      |
| 82             | 102           | MET                  | C      |
| 83             | 103           | CYS                  | C      |
| 84             | 104           | GLY                  | C      |
| 85             | 105           | SER                  | C      |
| 86             | 126           | PHE                  | C      |
| 87             | 130           | PRO                  | C      |
| 88             | 131           | TYR                  | C      |
| 89             | 132           | SER                  | C      |
| 90             | 133           | ALA                  | C      |
| 91             | 134           | TRP                  | C      |
| 92             | 135           | ASP                  | C      |
| 93             | 136           | PHE                  | C      |
| 94             | 137           | ASN                  | B      |
| 95             | 160           | CYS                  | B      |
| 96             | 161           | GLN                  | B      |
| 97             | 162           | LEU                  | B      |
| 98             | 163           | VAL                  | B      |
| 99             | 165           | LEU                  | B      |
| 100            | 166           | LEU                  | B      |
| 101            | 167           | ASP                  | B      |
| 102            | 168           | LEU                  | B      |
| 103            | 169           | ALA                  | B      |
| 104            | 170           | LEU                  | B      |
| 105            | 171           | GLU                  | B      |
| 106            | 172           | LYS                  | B      |
| 107            | 173           | ASP                  | B      |
| 108            | 174           | TYR                  | B      |
| 109            | 175           | VAL                  | B      |
| 110            | 176           | ARG                  | B      |
| 111            | 177           | SER                  | B      |
| 112            | 178           | MET                  | B      |
| 113            | 179           | ILE                  | B      |
| 114            | 180           | ALA                  | B      |
| 115            | 181           | ASP                  | B      |
| 116            | 182           | TYR                  | B      |
| 117            | 183           | LEU                  | B      |
| 118            | 184           | ASN                  | B      |
| 119            | 185           | LYS                  | B      |
| 120            | 186           | LEU                  | B      |
| 121            | 187           | ILE                  | B      |
| 122            | 188           | ASP                  | B      |

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Table S73 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 189           | ILE                  | C      |
| 124            | 190           | GLY                  | C      |
| 125            | 191           | VAL                  | C      |
| 126            | 192           | ALA                  | C      |
| 127            | 193           | GLY                  | C      |
| 128            | 194           | PHE                  | B      |
| 129            | 195           | ARG                  | D      |
| 130            | 196           | ILE                  | B      |
| 131            | 197           | ASP                  | B      |
| 132            | 198           | ALA                  | B      |
| 133            | 199           | SER                  | B      |
| 134            | 200           | LYS                  | B      |
| 135            | 201           | HIS                  | B      |
| 136            | 202           | MET                  | B      |
| 137            | 203           | TRP                  | B      |
| 138            | 204           | PRO                  | B      |
| 139            | 205           | GLY                  | B      |
| 140            | 206           | ASP                  | B      |
| 141            | 207           | ILE                  | B      |
| 142            | 208           | LYS                  | B      |
| 143            | 209           | ALA                  | B      |
| 144            | 210           | VAL                  | B      |
| 145            | 211           | LEU                  | B      |
| 146            | 212           | ASP                  | B      |
| 147            | 213           | LYS                  | B      |
| 148            | 214           | LEU                  | B      |
| 149            | 215           | HIS                  | B      |
| 150            | 228           | PRO                  | B      |
| 151            | 229           | PHE                  | B      |
| 152            | 230           | ILE                  | B      |
| 153            | 231           | PHE                  | C      |
| 154            | 232           | GLN                  | B      |
| 155            | 233           | GLU                  | B      |
| 156            | 234           | VAL                  | B      |
| 157            | 235           | ILE                  | B      |
| 158            | 236           | ASP                  | B      |
| 159            | 237           | LEU                  | B      |
| 160            | 244           | SER                  | B      |
| 161            | 245           | SER                  | B      |
| 162            | 246           | GLU                  | B      |
| 163            | 247           | TYR                  | B      |
| 164            | 248           | PHE                  | B      |
| 165            | 249           | GLY                  | B      |
| 166            | 250           | ASN                  | B      |
| 167            | 251           | GLY                  | B      |
| 168            | 252           | ARG                  | B      |

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Table S73 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 253           | VAL                  | B      |
| 170            | 254           | THR                  | D      |
| 171            | 255           | GLU                  | D      |
| 172            | 256           | PHE                  | D      |
| 173            | 257           | LYS                  | D      |
| 174            | 259           | GLY                  | D      |
| 175            | 260           | ALA                  | D      |
| 176            | 261           | LYS                  | D      |
| 177            | 262           | LEU                  | D      |
| 178            | 263           | GLY                  | D      |
| 179            | 264           | THR                  | D      |
| 180            | 265           | VAL                  | D      |
| 181            | 266           | VAL                  | D      |
| 182            | 272           | GLU                  | D      |
| 183            | 273           | LYS                  | A      |
| 184            | 274           | MET                  | A      |
| 185            | 275           | SER                  | A      |
| 186            | 280           | TRP                  | A      |
| 187            | 281           | GLY                  | D      |
| 188            | 282           | GLU                  | D      |
| 189            | 283           | GLY                  | D      |
| 190            | 285           | GLY                  | D      |
| 191            | 286           | PHE                  | B      |
| 192            | 287           | MET                  | B      |
| 193            | 288           | PRO                  | B      |
| 194            | 289           | SER                  | B      |
| 195            | 290           | ASP                  | B      |
| 196            | 291           | ARG                  | B      |
| 197            | 292           | ALA                  | B      |
| 198            | 293           | LEU                  | D      |
| 199            | 294           | VAL                  | D      |
| 200            | 295           | PHE                  | D      |
| 201            | 296           | VAL                  | A      |
| 202            | 297           | ASP                  | D      |
| 203            | 298           | ASN                  | D      |
| 204            | 299           | HIS                  | D      |
| 205            | 300           | ASP                  | D      |
| 206            | 301           | ASN                  | D      |
| 207            | 302           | GLN                  | D      |
| 208            | 314           | THR                  | D      |
| 209            | 315           | PHE                  | D      |
| 210            | 316           | TRP                  | D      |
| 211            | 317           | ASP                  | D      |
| 212            | 319           | ARG                  | A      |
| 213            | 320           | LEU                  | A      |
| 214            | 321           | TYR                  | A      |

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Table S73 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 322           | LYS                  | A      |
| 216            | 323           | VAL                  | A      |
| 217            | 324           | ALA                  | A      |
| 218            | 325           | VAL                  | A      |
| 219            | 326           | GLY                  | A      |
| 220            | 327           | PHE                  | A      |
| 221            | 328           | MET                  | A      |
| 222            | 329           | LEU                  | A      |
| 223            | 330           | ALA                  | A      |
| 224            | 331           | HIS                  | A      |
| 225            | 333           | TYR                  | D      |
| 226            | 334           | GLY                  | D      |
| 227            | 335           | PHE                  | D      |
| 228            | 336           | THR                  | A      |
| 229            | 337           | ARG                  | D      |
| 230            | 338           | VAL                  | A      |
| 231            | 339           | MET                  | D      |
| 232            | 340           | SER                  | C      |
| 233            | 341           | SER                  | D      |
| 234            | 342           | TYR                  | A      |
| 235            | 343           | ARG                  | C      |
| 236            | 381           | ASP                  | C      |
| 237            | 382           | TRP                  | D      |
| 238            | 383           | VAL                  | D      |
| 239            | 384           | CYS                  | D      |
| 240            | 387           | ARG                  | A      |
| 241            | 388           | TRP                  | A      |
| 242            | 389           | ARG                  | A      |
| 243            | 390           | GLN                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | ARG                  | A      |
| 246            | 393           | ASN                  | A      |
| 247            | 394           | MET                  | A      |
| 248            | 395           | VAL                  | A      |
| 249            | 396           | TRP                  | A      |
| 250            | 397           | PHE                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | ASN                  | A      |
| 253            | 400           | VAL                  | A      |
| 254            | 401           | VAL                  | A      |
| 255            | 402           | ASP                  | A      |
| 256            | 403           | GLY                  | A      |
| 257            | 404           | GLN                  | A      |
| 258            | 405           | PRO                  | A      |
| 259            | 406           | PHE                  | A      |
| 260            | 408           | ASN                  | A      |

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Table S73 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 409           | TRP                  | A      |
| 262            | 410           | TRP                  | A      |
| 263            | 411           | ASP                  | A      |
| 264            | 413           | GLY                  | A      |
| 265            | 414           | SER                  | A      |
| 266            | 415           | ASN                  | A      |
| 267            | 416           | GLN                  | A      |
| 268            | 417           | VAL                  | A      |
| 269            | 418           | ALA                  | A      |
| 270            | 419           | PHE                  | A      |
| 271            | 420           | GLY                  | A      |
| 272            | 421           | ARG                  | A      |
| 273            | 422           | GLY                  | A      |
| 274            | 423           | ASN                  | A      |
| 275            | 425           | GLY                  | A      |
| 276            | 426           | PHE                  | A      |
| 277            | 427           | ILE                  | A      |
| 278            | 428           | VAL                  | A      |
| 279            | 429           | PHE                  | A      |
| 280            | 430           | ASN                  | A      |
| 281            | 433           | ASP                  | A      |
| 282            | 434           | TRP                  | A      |
| 283            | 435           | GLN                  | A      |
| 284            | 436           | LEU                  | A      |
| 285            | 437           | SER                  | A      |
| 286            | 438           | SER                  | A      |
| 287            | 439           | THR                  | A      |
| 288            | 445           | PRO                  | A      |
| 289            | 446           | GLY                  | A      |
| 290            | 449           | TYR                  | A      |
| 291            | 450           | CYS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | VAL                  | A      |
| 294            | 479           | ILE                  | A      |
| 295            | 480           | SER                  | A      |
| 296            | 481           | ASN                  | A      |
| 297            | 486           | PRO                  | A      |
| 298            | 487           | PHE                  | A      |
| 299            | 488           | ILE                  | A      |
| 300            | 489           | ALA                  | A      |
| 301            | 490           | ILE                  | A      |
| 302            | 491           | HIS                  | A      |

Table S74: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase  
(PDB code 4CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S74 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S74 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S74 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S74 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S74 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |

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Table S74 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S75: Residues membership for the *N. polysaccharea*  $\alpha$ -amylase (PDB code 3UEQ, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 98            | GLN                  | A      |
| 1              | 99            | VAL                  | A      |
| 2              | 100           | GLY                  | B      |
| 3              | 101           | GLY                  | B      |
| 4              | 102           | VAL                  | B      |
| 5              | 103           | CYS                  | C      |
| 6              | 104           | TYR                  | C      |
| 7              | 105           | VAL                  | C      |
| 8              | 110           | GLY                  | C      |

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Table S75 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 111           | ASP                  | C      |
| 10             | 112           | LEU                  | C      |
| 11             | 113           | LYS                  | C      |
| 12             | 114           | GLY                  | C      |
| 13             | 115           | LEU                  | C      |
| 14             | 116           | LYS                  | C      |
| 15             | 117           | ASP                  | C      |
| 16             | 118           | LYS                  | C      |
| 17             | 119           | ILE                  | C      |
| 18             | 120           | PRO                  | C      |
| 19             | 121           | TYR                  | C      |
| 20             | 122           | PHE                  | C      |
| 21             | 123           | GLN                  | C      |
| 22             | 124           | GLU                  | C      |
| 23             | 125           | LEU                  | C      |
| 24             | 126           | GLY                  | C      |
| 25             | 127           | LEU                  | C      |
| 26             | 128           | THR                  | C      |
| 27             | 129           | TYR                  | C      |
| 28             | 130           | LEU                  | C      |
| 29             | 131           | HIS                  | C      |
| 30             | 132           | LEU                  | C      |
| 31             | 133           | MET                  | C      |
| 32             | 134           | PRO                  | C      |
| 33             | 135           | LEU                  | C      |
| 34             | 136           | PHE                  | C      |
| 35             | 137           | LYS                  | C      |
| 36             | 138           | CYS                  | C      |
| 37             | 139           | PRO                  | C      |
| 38             | 141           | GLY                  | C      |
| 39             | 144           | ASP                  | C      |
| 40             | 145           | GLY                  | C      |
| 41             | 146           | GLY                  | C      |
| 42             | 147           | TYR                  | C      |
| 43             | 148           | ALA                  | C      |
| 44             | 149           | VAL                  | C      |
| 45             | 150           | SER                  | C      |
| 46             | 151           | SER                  | C      |
| 47             | 153           | ARG                  | C      |
| 48             | 154           | ASP                  | C      |
| 49             | 155           | VAL                  | C      |
| 50             | 156           | ASN                  | C      |
| 51             | 157           | PRO                  | C      |
| 52             | 158           | ALA                  | C      |
| 53             | 159           | LEU                  | C      |
| 54             | 160           | GLY                  | C      |

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Table S75 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 161           | THR                  | C      |
| 56             | 162           | ILE                  | C      |
| 57             | 163           | GLY                  | C      |
| 58             | 164           | ASP                  | C      |
| 59             | 165           | LEU                  | C      |
| 60             | 166           | ARG                  | C      |
| 61             | 167           | GLU                  | C      |
| 62             | 168           | VAL                  | C      |
| 63             | 169           | ILE                  | C      |
| 64             | 170           | ALA                  | C      |
| 65             | 171           | ALA                  | C      |
| 66             | 172           | LEU                  | C      |
| 67             | 173           | HIS                  | C      |
| 68             | 174           | GLU                  | C      |
| 69             | 175           | ALA                  | C      |
| 70             | 176           | GLY                  | C      |
| 71             | 177           | ILE                  | C      |
| 72             | 178           | SER                  | C      |
| 73             | 179           | ALA                  | C      |
| 74             | 180           | VAL                  | C      |
| 75             | 181           | VAL                  | C      |
| 76             | 182           | ASP                  | C      |
| 77             | 183           | PHE                  | C      |
| 78             | 184           | ILE                  | C      |
| 79             | 185           | PHE                  | C      |
| 80             | 186           | ASN                  | C      |
| 81             | 187           | HIS                  | C      |
| 82             | 188           | THR                  | C      |
| 83             | 189           | SER                  | C      |
| 84             | 190           | ASN                  | C      |
| 85             | 191           | GLU                  | C      |
| 86             | 192           | HIS                  | C      |
| 87             | 193           | GLU                  | C      |
| 88             | 194           | TRP                  | C      |
| 89             | 195           | ALA                  | C      |
| 90             | 206           | ASP                  | C      |
| 91             | 207           | ASN                  | C      |
| 92             | 208           | PHE                  | C      |
| 93             | 209           | TYR                  | C      |
| 94             | 210           | TYR                  | B      |
| 95             | 247           | TRP                  | B      |
| 96             | 248           | THR                  | B      |
| 97             | 249           | THR                  | B      |
| 98             | 250           | PHE                  | B      |
| 99             | 254           | GLN                  | B      |
| 100            | 255           | TRP                  | B      |

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Table S75 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 256           | ASP                  | B      |
| 102            | 257           | LEU                  | B      |
| 103            | 258           | ASN                  | B      |
| 104            | 259           | TYR                  | B      |
| 105            | 260           | SER                  | B      |
| 106            | 261           | ASN                  | B      |
| 107            | 262           | PRO                  | B      |
| 108            | 263           | TRP                  | B      |
| 109            | 264           | VAL                  | B      |
| 110            | 265           | PHE                  | B      |
| 111            | 266           | ARG                  | B      |
| 112            | 267           | ALA                  | B      |
| 113            | 268           | MET                  | B      |
| 114            | 269           | ALA                  | B      |
| 115            | 270           | GLY                  | B      |
| 116            | 271           | GLU                  | B      |
| 117            | 272           | MET                  | B      |
| 118            | 273           | LEU                  | B      |
| 119            | 274           | PHE                  | B      |
| 120            | 275           | LEU                  | B      |
| 121            | 276           | ALA                  | B      |
| 122            | 277           | ASN                  | B      |
| 123            | 278           | LEU                  | C      |
| 124            | 279           | GLY                  | C      |
| 125            | 280           | VAL                  | C      |
| 126            | 281           | ASP                  | C      |
| 127            | 282           | ILE                  | C      |
| 128            | 283           | LEU                  | B      |
| 129            | 284           | ARG                  | D      |
| 130            | 285           | MET                  | B      |
| 131            | 286           | ASP                  | B      |
| 132            | 287           | ALA                  | B      |
| 133            | 288           | VAL                  | B      |
| 134            | 289           | ALA                  | B      |
| 135            | 290           | PHE                  | B      |
| 136            | 291           | ILE                  | B      |
| 137            | 292           | TRP                  | B      |
| 138            | 306           | HIS                  | B      |
| 139            | 307           | ALA                  | B      |
| 140            | 308           | LEU                  | B      |
| 141            | 309           | ILE                  | B      |
| 142            | 310           | ARG                  | B      |
| 143            | 311           | ALA                  | B      |
| 144            | 312           | PHE                  | B      |
| 145            | 313           | ASN                  | B      |
| 146            | 314           | ALA                  | B      |

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Table S75 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 315           | VAL                  | B      |
| 148            | 316           | MET                  | B      |
| 149            | 317           | ARG                  | B      |
| 150            | 323           | VAL                  | B      |
| 151            | 324           | PHE                  | B      |
| 152            | 325           | PHE                  | B      |
| 153            | 326           | LYS                  | C      |
| 154            | 327           | SER                  | B      |
| 155            | 328           | GLU                  | B      |
| 156            | 329           | ALA                  | B      |
| 157            | 330           | ILE                  | B      |
| 158            | 331           | VAL                  | B      |
| 159            | 332           | HIS                  | B      |
| 160            | 336           | VAL                  | B      |
| 161            | 337           | VAL                  | B      |
| 162            | 338           | GLN                  | B      |
| 163            | 339           | TYR                  | B      |
| 164            | 340           | ILE                  | B      |
| 165            | 341           | GLY                  | B      |
| 166            | 345           | CYS                  | B      |
| 167            | 346           | GLN                  | B      |
| 168            | 347           | ILE                  | B      |
| 169            | 348           | GLY                  | B      |
| 170            | 349           | TYR                  | D      |
| 171            | 350           | ASN                  | D      |
| 172            | 351           | PRO                  | D      |
| 173            | 352           | LEU                  | D      |
| 174            | 354           | MET                  | D      |
| 175            | 355           | ALA                  | D      |
| 176            | 356           | LEU                  | D      |
| 177            | 357           | LEU                  | D      |
| 178            | 358           | TRP                  | D      |
| 179            | 359           | ASN                  | D      |
| 180            | 360           | THR                  | D      |
| 181            | 361           | LEU                  | D      |
| 182            | 364           | ARG                  | D      |
| 183            | 365           | GLU                  | A      |
| 184            | 366           | VAL                  | A      |
| 185            | 367           | ASN                  | A      |
| 186            | 372           | ALA                  | A      |
| 187            | 373           | LEU                  | D      |
| 188            | 374           | THR                  | D      |
| 189            | 375           | TYR                  | D      |
| 190            | 376           | ARG                  | D      |
| 191            | 377           | HIS                  | B      |
| 192            | 378           | ASN                  | B      |

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Table S75 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 381           | GLU                  | B      |
| 194            | 382           | HIS                  | B      |
| 195            | 383           | THR                  | B      |
| 196            | 384           | ALA                  | B      |
| 197            | 385           | TRP                  | B      |
| 198            | 386           | VAL                  | D      |
| 199            | 387           | ASN                  | D      |
| 200            | 388           | TYR                  | D      |
| 201            | 389           | VAL                  | A      |
| 202            | 390           | ARG                  | D      |
| 203            | 391           | SER                  | D      |
| 204            | 392           | HIS                  | D      |
| 205            | 393           | ASP                  | D      |
| 206            | 394           | ASP                  | D      |
| 207            | 448           | SER                  | D      |
| 208            | 450           | THR                  | D      |
| 209            | 451           | ALA                  | D      |
| 210            | 452           | ALA                  | D      |
| 211            | 453           | ALA                  | D      |
| 212            | 464           | ALA                  | A      |
| 213            | 467           | ARG                  | A      |
| 214            | 468           | ILE                  | A      |
| 215            | 469           | LYS                  | A      |
| 216            | 470           | LEU                  | A      |
| 217            | 471           | LEU                  | A      |
| 218            | 472           | TYR                  | A      |
| 219            | 473           | SER                  | A      |
| 220            | 474           | ILE                  | A      |
| 221            | 475           | ALA                  | A      |
| 222            | 476           | LEU                  | A      |
| 223            | 477           | SER                  | A      |
| 224            | 478           | THR                  | A      |
| 225            | 479           | GLY                  | D      |
| 226            | 480           | GLY                  | D      |
| 227            | 481           | LEU                  | D      |
| 228            | 482           | PRO                  | A      |
| 229            | 483           | LEU                  | D      |
| 230            | 484           | ILE                  | A      |
| 231            | 485           | TYR                  | D      |
| 232            | 486           | LEU                  | C      |
| 233            | 487           | GLY                  | D      |
| 234            | 488           | ASP                  | A      |
| 235            | 514           | PRO                  | C      |
| 236            | 515           | ARG                  | C      |
| 237            | 516           | TYR                  | D      |
| 238            | 517           | ASN                  | D      |

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Table S75 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 521           | TYR                  | D      |
| 240            | 534           | ILE                  | A      |
| 241            | 535           | TYR                  | A      |
| 242            | 536           | GLN                  | A      |
| 243            | 537           | ASP                  | A      |
| 244            | 538           | LEU                  | A      |
| 245            | 539           | ARG                  | A      |
| 246            | 540           | HIS                  | A      |
| 247            | 541           | MET                  | A      |
| 248            | 542           | ILE                  | A      |
| 249            | 543           | ALA                  | A      |
| 250            | 544           | VAL                  | A      |
| 251            | 545           | ARG                  | A      |
| 252            | 546           | GLN                  | A      |
| 253            | 547           | SER                  | A      |
| 254            | 548           | ASN                  | A      |
| 255            | 549           | PRO                  | A      |
| 256            | 553           | GLY                  | A      |
| 257            | 554           | GLY                  | A      |
| 258            | 555           | ARG                  | A      |
| 259            | 556           | LEU                  | A      |
| 260            | 558           | THR                  | A      |
| 261            | 559           | PHE                  | A      |
| 262            | 560           | ASN                  | A      |
| 263            | 561           | THR                  | A      |
| 264            | 563           | ASN                  | A      |
| 265            | 564           | LYS                  | A      |
| 266            | 565           | HIS                  | A      |
| 267            | 566           | ILE                  | A      |
| 268            | 567           | ILE                  | A      |
| 269            | 568           | GLY                  | A      |
| 270            | 569           | TYR                  | A      |
| 271            | 570           | ILE                  | A      |
| 272            | 571           | ARG                  | A      |
| 273            | 573           | ASN                  | A      |
| 274            | 574           | ALA                  | A      |
| 275            | 575           | LEU                  | A      |
| 276            | 576           | LEU                  | A      |
| 277            | 577           | ALA                  | A      |
| 278            | 578           | PHE                  | A      |
| 279            | 579           | GLY                  | A      |
| 280            | 580           | ASN                  | A      |
| 281            | 584           | TYR                  | A      |
| 282            | 585           | PRO                  | A      |
| 283            | 586           | GLN                  | A      |
| 284            | 587           | THR                  | A      |

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Table S75 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 588           | VAL                  | A      |
| 286            | 589           | THR                  | A      |
| 287            | 590           | ALA                  | A      |
| 288            | 599           | LYS                  | A      |
| 289            | 600           | ALA                  | A      |
| 290            | 601           | HIS                  | A      |
| 291            | 602           | ASP                  | A      |
| 292            | 603           | LEU                  | A      |
| 293            | 604           | ILE                  | A      |
| 294            | 617           | LEU                  | A      |
| 295            | 618           | GLN                  | A      |
| 296            | 619           | PRO                  | A      |
| 297            | 621           | GLN                  | A      |
| 298            | 622           | VAL                  | A      |
| 299            | 623           | MET                  | A      |
| 300            | 624           | TRP                  | A      |
| 301            | 625           | LEU                  | A      |
| 302            | 626           | GLU                  | A      |

Table S76: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase (PDB code 6CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |

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Table S76 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |

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Table S76 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | THR                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |

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Table S76 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |

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Table S76 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |

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Table S76 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |

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Table S76 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |

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Table S76 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S77: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase (PDB code 5CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |

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Table S77 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |

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Table S77 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |

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Table S77 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ALA                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |

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Table S77 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |

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Table S77 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |

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Table S77 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S78: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase  
(PDB code 7CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S78 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S78 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ALA                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S78 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | GLU                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S78 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S78 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |

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Table S78 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S79: Residues membership for the *A. oryzae*  $\alpha$ -amylase (PDB code 6TAA, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | GLN                  | A      |
| 1              | 10            | SER                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | TYR                  | B      |
| 4              | 13            | PHE                  | B      |
| 5              | 14            | LEU                  | C      |
| 6              | 15            | LEU                  | C      |
| 7              | 16            | THR                  | C      |
| 8              | 40            | GLY                  | C      |

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Table S79 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 41            | THR                  | C      |
| 10             | 42            | TRP                  | C      |
| 11             | 43            | GLN                  | C      |
| 12             | 44            | GLY                  | C      |
| 13             | 45            | ILE                  | C      |
| 14             | 46            | ILE                  | C      |
| 15             | 47            | ASP                  | C      |
| 16             | 48            | LYS                  | C      |
| 17             | 49            | LEU                  | C      |
| 18             | 50            | ASP                  | C      |
| 19             | 51            | TYR                  | C      |
| 20             | 52            | ILE                  | C      |
| 21             | 53            | GLN                  | C      |
| 22             | 54            | GLY                  | C      |
| 23             | 55            | MET                  | C      |
| 24             | 56            | GLY                  | C      |
| 25             | 57            | PHE                  | C      |
| 26             | 58            | THR                  | C      |
| 27             | 59            | ALA                  | C      |
| 28             | 60            | ILE                  | C      |
| 29             | 61            | TRP                  | C      |
| 30             | 62            | ILE                  | C      |
| 31             | 63            | THR                  | C      |
| 32             | 64            | PRO                  | C      |
| 33             | 65            | VAL                  | C      |
| 34             | 66            | THR                  | C      |
| 35             | 67            | ALA                  | C      |
| 36             | 68            | GLN                  | C      |
| 37             | 69            | LEU                  | C      |
| 38             | 77            | ASP                  | C      |
| 39             | 79            | TYR                  | C      |
| 40             | 80            | HIS                  | C      |
| 41             | 81            | GLY                  | C      |
| 42             | 82            | TYR                  | C      |
| 43             | 83            | TRP                  | C      |
| 44             | 84            | GLN                  | C      |
| 45             | 85            | GLN                  | C      |
| 46             | 86            | ASP                  | C      |
| 47             | 88            | TYR                  | C      |
| 48             | 89            | SER                  | C      |
| 49             | 90            | LEU                  | C      |
| 50             | 91            | ASN                  | C      |
| 51             | 92            | GLU                  | C      |
| 52             | 93            | ASN                  | C      |
| 53             | 94            | TYR                  | C      |
| 54             | 95            | GLY                  | C      |

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Table S79 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 96            | THR                  | C      |
| 56             | 97            | ALA                  | C      |
| 57             | 98            | ASP                  | C      |
| 58             | 99            | ASP                  | C      |
| 59             | 100           | LEU                  | C      |
| 60             | 101           | LYS                  | C      |
| 61             | 102           | ALA                  | C      |
| 62             | 103           | LEU                  | C      |
| 63             | 104           | SER                  | C      |
| 64             | 105           | SER                  | C      |
| 65             | 106           | ALA                  | C      |
| 66             | 107           | LEU                  | C      |
| 67             | 108           | HIS                  | C      |
| 68             | 109           | GLU                  | C      |
| 69             | 110           | ARG                  | C      |
| 70             | 111           | GLY                  | C      |
| 71             | 112           | MET                  | C      |
| 72             | 113           | TYR                  | C      |
| 73             | 114           | LEU                  | C      |
| 74             | 115           | MET                  | C      |
| 75             | 116           | VAL                  | C      |
| 76             | 117           | ASP                  | C      |
| 77             | 118           | VAL                  | C      |
| 78             | 119           | VAL                  | C      |
| 79             | 120           | ALA                  | C      |
| 80             | 121           | ASN                  | C      |
| 81             | 122           | HIS                  | C      |
| 82             | 123           | MET                  | C      |
| 83             | 124           | GLY                  | C      |
| 84             | 125           | TYR                  | C      |
| 85             | 126           | ASP                  | C      |
| 86             | 137           | PHE                  | C      |
| 87             | 139           | PRO                  | C      |
| 88             | 140           | PHE                  | C      |
| 89             | 141           | SER                  | C      |
| 90             | 143           | GLN                  | C      |
| 91             | 144           | ASP                  | C      |
| 92             | 145           | TYR                  | C      |
| 93             | 146           | PHE                  | C      |
| 94             | 147           | HIS                  | B      |
| 95             | 164           | CYS                  | B      |
| 96             | 165           | TRP                  | B      |
| 97             | 166           | LEU                  | B      |
| 98             | 167           | GLY                  | B      |
| 99             | 173           | LEU                  | B      |
| 100            | 174           | PRO                  | B      |

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Table S79 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 175           | ASP                  | B      |
| 102            | 176           | LEU                  | B      |
| 103            | 177           | ASP                  | B      |
| 104            | 178           | THR                  | B      |
| 105            | 179           | THR                  | B      |
| 106            | 180           | LYS                  | B      |
| 107            | 181           | ASP                  | B      |
| 108            | 182           | VAL                  | B      |
| 109            | 183           | VAL                  | B      |
| 110            | 184           | LYS                  | B      |
| 111            | 185           | ASN                  | B      |
| 112            | 186           | GLU                  | B      |
| 113            | 187           | TRP                  | B      |
| 114            | 188           | TYR                  | B      |
| 115            | 189           | ASP                  | B      |
| 116            | 190           | TRP                  | B      |
| 117            | 191           | VAL                  | B      |
| 118            | 192           | GLY                  | B      |
| 119            | 193           | SER                  | B      |
| 120            | 194           | LEU                  | B      |
| 121            | 195           | VAL                  | B      |
| 122            | 196           | SER                  | B      |
| 123            | 198           | TYR                  | C      |
| 124            | 199           | SER                  | C      |
| 125            | 200           | ILE                  | C      |
| 126            | 201           | ASP                  | C      |
| 127            | 202           | GLY                  | C      |
| 128            | 203           | LEU                  | B      |
| 129            | 204           | ARG                  | D      |
| 130            | 205           | ILE                  | B      |
| 131            | 206           | ASP                  | B      |
| 132            | 207           | THR                  | B      |
| 133            | 208           | VAL                  | B      |
| 134            | 209           | LYS                  | B      |
| 135            | 210           | HIS                  | B      |
| 136            | 211           | VAL                  | B      |
| 137            | 212           | GLN                  | B      |
| 138            | 213           | LYS                  | B      |
| 139            | 214           | ASP                  | B      |
| 140            | 215           | PHE                  | B      |
| 141            | 216           | TRP                  | B      |
| 142            | 217           | PRO                  | B      |
| 143            | 218           | GLY                  | B      |
| 144            | 219           | TYR                  | B      |
| 145            | 220           | ASN                  | B      |
| 146            | 221           | LYS                  | B      |

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Table S79 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 222           | ALA                  | B      |
| 148            | 223           | ALA                  | B      |
| 149            | 224           | GLY                  | B      |
| 150            | 225           | VAL                  | B      |
| 151            | 226           | TYR                  | B      |
| 152            | 227           | CYS                  | B      |
| 153            | 228           | ILE                  | C      |
| 154            | 229           | GLY                  | B      |
| 155            | 230           | GLU                  | B      |
| 156            | 231           | VAL                  | B      |
| 157            | 232           | LEU                  | B      |
| 158            | 233           | ASP                  | B      |
| 159            | 234           | GLY                  | B      |
| 160            | 239           | THR                  | B      |
| 161            | 240           | CYS                  | B      |
| 162            | 241           | PRO                  | B      |
| 163            | 242           | TYR                  | B      |
| 164            | 243           | GLN                  | B      |
| 165            | 244           | ASN                  | B      |
| 166            | 246           | MET                  | B      |
| 167            | 247           | ASP                  | B      |
| 168            | 248           | GLY                  | B      |
| 169            | 249           | VAL                  | B      |
| 170            | 250           | LEU                  | D      |
| 171            | 251           | ASN                  | D      |
| 172            | 252           | TYR                  | D      |
| 173            | 253           | PRO                  | D      |
| 174            | 255           | TYR                  | D      |
| 175            | 256           | TYR                  | D      |
| 176            | 257           | PRO                  | D      |
| 177            | 258           | LEU                  | D      |
| 178            | 259           | LEU                  | D      |
| 179            | 260           | ASN                  | D      |
| 180            | 261           | ALA                  | D      |
| 181            | 262           | PHE                  | D      |
| 182            | 267           | GLY                  | D      |
| 183            | 268           | SER                  | A      |
| 184            | 269           | MET                  | A      |
| 185            | 270           | ASP                  | A      |
| 186            | 275           | MET                  | A      |
| 187            | 276           | ILE                  | D      |
| 188            | 277           | ASN                  | D      |
| 189            | 278           | THR                  | D      |
| 190            | 279           | VAL                  | D      |
| 191            | 280           | LYS                  | B      |
| 192            | 281           | SER                  | B      |

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Table S79 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 285           | ASP                  | B      |
| 194            | 286           | SER                  | B      |
| 195            | 287           | THR                  | B      |
| 196            | 288           | LEU                  | B      |
| 197            | 289           | LEU                  | B      |
| 198            | 290           | GLY                  | D      |
| 199            | 291           | THR                  | D      |
| 200            | 292           | PHE                  | D      |
| 201            | 293           | VAL                  | A      |
| 202            | 294           | GLU                  | D      |
| 203            | 295           | ASN                  | D      |
| 204            | 296           | HIS                  | D      |
| 205            | 297           | ASP                  | D      |
| 206            | 298           | ASN                  | D      |
| 207            | 299           | PRO                  | D      |
| 208            | 300           | ARG                  | D      |
| 209            | 301           | PHE                  | D      |
| 210            | 302           | ALA                  | D      |
| 211            | 303           | SER                  | D      |
| 212            | 308           | ILE                  | A      |
| 213            | 310           | LEU                  | A      |
| 214            | 311           | ALA                  | A      |
| 215            | 312           | LYS                  | A      |
| 216            | 313           | ASN                  | A      |
| 217            | 314           | VAL                  | A      |
| 218            | 315           | ALA                  | A      |
| 219            | 316           | ALA                  | A      |
| 220            | 317           | PHE                  | A      |
| 221            | 318           | ILE                  | A      |
| 222            | 319           | ILE                  | A      |
| 223            | 320           | LEU                  | A      |
| 224            | 321           | ASN                  | A      |
| 225            | 322           | ASP                  | D      |
| 226            | 323           | GLY                  | D      |
| 227            | 324           | ILE                  | D      |
| 228            | 325           | PRO                  | A      |
| 229            | 326           | ILE                  | D      |
| 230            | 327           | ILE                  | A      |
| 231            | 328           | TYR                  | D      |
| 232            | 329           | ALA                  | C      |
| 233            | 330           | GLY                  | D      |
| 234            | 331           | GLN                  | A      |
| 235            | 345           | GLU                  | C      |
| 236            | 346           | ALA                  | C      |
| 237            | 347           | THR                  | D      |
| 238            | 348           | TRP                  | D      |

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Table S79 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 352           | TYR                  | D      |
| 240            | 358           | LEU                  | A      |
| 241            | 359           | TYR                  | A      |
| 242            | 360           | LYS                  | A      |
| 243            | 361           | LEU                  | A      |
| 244            | 362           | ILE                  | A      |
| 245            | 363           | ALA                  | A      |
| 246            | 364           | SER                  | A      |
| 247            | 365           | ALA                  | A      |
| 248            | 366           | ASN                  | A      |
| 249            | 367           | ALA                  | A      |
| 250            | 368           | ILE                  | A      |
| 251            | 373           | ILE                  | A      |
| 252            | 374           | SER                  | A      |
| 253            | 375           | LYS                  | A      |
| 254            | 376           | ASP                  | A      |
| 255            | 377           | THR                  | A      |
| 256            | 381           | THR                  | A      |
| 257            | 382           | TYR                  | A      |
| 258            | 383           | LYS                  | A      |
| 259            | 384           | ASN                  | A      |
| 260            | 386           | PRO                  | A      |
| 261            | 387           | ILE                  | A      |
| 262            | 388           | TYR                  | A      |
| 263            | 389           | LYS                  | A      |
| 264            | 390           | ASP                  | A      |
| 265            | 391           | ASP                  | A      |
| 266            | 392           | THR                  | A      |
| 267            | 393           | THR                  | A      |
| 268            | 394           | ILE                  | A      |
| 269            | 395           | ALA                  | A      |
| 270            | 396           | MET                  | A      |
| 271            | 397           | ARG                  | A      |
| 272            | 398           | LYS                  | A      |
| 273            | 403           | SER                  | A      |
| 274            | 404           | GLN                  | A      |
| 275            | 405           | ILE                  | A      |
| 276            | 406           | VAL                  | A      |
| 277            | 407           | THR                  | A      |
| 278            | 408           | ILE                  | A      |
| 279            | 409           | LEU                  | A      |
| 280            | 410           | SER                  | A      |
| 281            | 416           | GLY                  | A      |
| 282            | 417           | ASP                  | A      |
| 283            | 418           | SER                  | A      |
| 284            | 419           | TYR                  | A      |

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Table S79 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 420           | THR                  | A      |
| 286            | 421           | LEU                  | A      |
| 287            | 422           | SER                  | A      |
| 288            | 432           | GLN                  | A      |
| 289            | 433           | GLN                  | A      |
| 290            | 435           | THR                  | A      |
| 291            | 436           | GLU                  | A      |
| 292            | 437           | VAL                  | A      |
| 293            | 438           | ILE                  | A      |
| 294            | 456           | ALA                  | A      |
| 295            | 457           | GLY                  | A      |
| 296            | 458           | GLY                  | A      |
| 297            | 459           | LEU                  | A      |
| 298            | 460           | PRO                  | A      |
| 299            | 461           | ARG                  | A      |
| 300            | 462           | VAL                  | A      |
| 301            | 463           | LEU                  | A      |
| 302            | 464           | TYR                  | A      |

Table S80: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase (PDB code 8CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |

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Table S80 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |

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Table S80 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |

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Table S80 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | ALA                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |

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Table S80 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |

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Table S80 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |

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Table S80 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |

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Table S80 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S81: Residues membership for the *A. oryzae*  $\alpha$ -amylase (PDB code 7TAA, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 9             | GLN                  | A      |
| 1              | 10            | SER                  | A      |
| 2              | 11            | ILE                  | B      |
| 3              | 12            | TYR                  | B      |
| 4              | 13            | PHE                  | B      |
| 5              | 14            | LEU                  | C      |
| 6              | 15            | LEU                  | C      |
| 7              | 16            | THR                  | C      |
| 8              | 40            | GLY                  | C      |
| 9              | 41            | THR                  | C      |
| 10             | 42            | TRP                  | C      |
| 11             | 43            | GLN                  | C      |
| 12             | 44            | GLY                  | C      |
| 13             | 45            | ILE                  | C      |
| 14             | 46            | ILE                  | C      |
| 15             | 47            | ASP                  | C      |
| 16             | 48            | LYS                  | C      |
| 17             | 49            | LEU                  | C      |
| 18             | 50            | ASP                  | C      |
| 19             | 51            | TYR                  | C      |
| 20             | 52            | ILE                  | C      |
| 21             | 53            | GLN                  | C      |
| 22             | 54            | GLY                  | C      |
| 23             | 55            | MET                  | C      |
| 24             | 56            | GLY                  | C      |
| 25             | 57            | PHE                  | C      |
| 26             | 58            | THR                  | C      |
| 27             | 59            | ALA                  | C      |
| 28             | 60            | ILE                  | C      |
| 29             | 61            | TRP                  | C      |
| 30             | 62            | ILE                  | C      |

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Table S81 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 63            | THR                  | C      |
| 32             | 64            | PRO                  | C      |
| 33             | 65            | VAL                  | C      |
| 34             | 66            | THR                  | C      |
| 35             | 67            | ALA                  | C      |
| 36             | 68            | GLN                  | C      |
| 37             | 69            | LEU                  | C      |
| 38             | 77            | ASP                  | C      |
| 39             | 79            | TYR                  | C      |
| 40             | 80            | HIS                  | C      |
| 41             | 81            | GLY                  | C      |
| 42             | 82            | TYR                  | C      |
| 43             | 83            | TRP                  | C      |
| 44             | 84            | GLN                  | C      |
| 45             | 85            | GLN                  | C      |
| 46             | 86            | ASP                  | C      |
| 47             | 88            | TYR                  | C      |
| 48             | 89            | SER                  | C      |
| 49             | 90            | LEU                  | C      |
| 50             | 91            | ASN                  | C      |
| 51             | 92            | GLU                  | C      |
| 52             | 93            | ASN                  | C      |
| 53             | 94            | TYR                  | C      |
| 54             | 95            | GLY                  | C      |
| 55             | 96            | THR                  | C      |
| 56             | 97            | ALA                  | C      |
| 57             | 98            | ASP                  | C      |
| 58             | 99            | ASP                  | C      |
| 59             | 100           | LEU                  | C      |
| 60             | 101           | LYS                  | C      |
| 61             | 102           | ALA                  | C      |
| 62             | 103           | LEU                  | C      |
| 63             | 104           | SER                  | C      |
| 64             | 105           | SER                  | C      |
| 65             | 106           | ALA                  | C      |
| 66             | 107           | LEU                  | C      |
| 67             | 108           | HIS                  | C      |
| 68             | 109           | GLU                  | C      |
| 69             | 110           | ARG                  | C      |
| 70             | 111           | GLY                  | C      |
| 71             | 112           | MET                  | C      |
| 72             | 113           | TYR                  | C      |
| 73             | 114           | LEU                  | C      |
| 74             | 115           | MET                  | C      |
| 75             | 116           | VAL                  | C      |
| 76             | 117           | ASP                  | C      |

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Table S81 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 118           | VAL                  | C      |
| 78             | 119           | VAL                  | C      |
| 79             | 120           | ALA                  | C      |
| 80             | 121           | ASN                  | C      |
| 81             | 122           | HIS                  | C      |
| 82             | 123           | MET                  | C      |
| 83             | 124           | GLY                  | C      |
| 84             | 125           | TYR                  | C      |
| 85             | 126           | ASP                  | C      |
| 86             | 137           | PHE                  | C      |
| 87             | 139           | PRO                  | C      |
| 88             | 140           | PHE                  | C      |
| 89             | 141           | SER                  | C      |
| 90             | 143           | GLN                  | C      |
| 91             | 144           | ASP                  | C      |
| 92             | 145           | TYR                  | C      |
| 93             | 146           | PHE                  | C      |
| 94             | 147           | HIS                  | B      |
| 95             | 164           | CYS                  | B      |
| 96             | 165           | TRP                  | B      |
| 97             | 166           | LEU                  | B      |
| 98             | 167           | GLY                  | B      |
| 99             | 173           | LEU                  | B      |
| 100            | 174           | PRO                  | B      |
| 101            | 175           | ASP                  | B      |
| 102            | 176           | LEU                  | B      |
| 103            | 177           | ASP                  | B      |
| 104            | 178           | THR                  | B      |
| 105            | 179           | THR                  | B      |
| 106            | 180           | LYS                  | B      |
| 107            | 181           | ASP                  | B      |
| 108            | 182           | VAL                  | B      |
| 109            | 183           | VAL                  | B      |
| 110            | 184           | LYS                  | B      |
| 111            | 185           | ASN                  | B      |
| 112            | 186           | GLU                  | B      |
| 113            | 187           | TRP                  | B      |
| 114            | 188           | TYR                  | B      |
| 115            | 189           | ASP                  | B      |
| 116            | 190           | TRP                  | B      |
| 117            | 191           | VAL                  | B      |
| 118            | 192           | GLY                  | B      |
| 119            | 193           | SER                  | B      |
| 120            | 194           | LEU                  | B      |
| 121            | 195           | VAL                  | B      |
| 122            | 196           | SER                  | B      |

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Table S81 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 198           | TYR                  | C      |
| 124            | 199           | SER                  | C      |
| 125            | 200           | ILE                  | C      |
| 126            | 201           | ASP                  | C      |
| 127            | 202           | GLY                  | C      |
| 128            | 203           | LEU                  | B      |
| 129            | 204           | ARG                  | D      |
| 130            | 205           | ILE                  | B      |
| 131            | 206           | ASP                  | B      |
| 132            | 207           | THR                  | B      |
| 133            | 208           | VAL                  | B      |
| 134            | 209           | LYS                  | B      |
| 135            | 210           | HIS                  | B      |
| 136            | 211           | VAL                  | B      |
| 137            | 212           | GLN                  | B      |
| 138            | 213           | LYS                  | B      |
| 139            | 214           | ASP                  | B      |
| 140            | 215           | PHE                  | B      |
| 141            | 216           | TRP                  | B      |
| 142            | 217           | PRO                  | B      |
| 143            | 218           | GLY                  | B      |
| 144            | 219           | TYR                  | B      |
| 145            | 220           | ASN                  | B      |
| 146            | 221           | LYS                  | B      |
| 147            | 222           | ALA                  | B      |
| 148            | 223           | ALA                  | B      |
| 149            | 224           | GLY                  | B      |
| 150            | 225           | VAL                  | B      |
| 151            | 226           | TYR                  | B      |
| 152            | 227           | CYS                  | B      |
| 153            | 228           | ILE                  | C      |
| 154            | 229           | GLY                  | B      |
| 155            | 230           | GLU                  | B      |
| 156            | 231           | VAL                  | B      |
| 157            | 232           | LEU                  | B      |
| 158            | 233           | ASP                  | B      |
| 159            | 234           | GLY                  | B      |
| 160            | 239           | THR                  | B      |
| 161            | 240           | CYS                  | B      |
| 162            | 241           | PRO                  | B      |
| 163            | 242           | TYR                  | B      |
| 164            | 243           | GLN                  | B      |
| 165            | 244           | ASN                  | B      |
| 166            | 246           | MET                  | B      |
| 167            | 247           | ASP                  | B      |
| 168            | 248           | GLY                  | B      |

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Table S81 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 249           | VAL                  | B      |
| 170            | 250           | LEU                  | D      |
| 171            | 251           | ASN                  | D      |
| 172            | 252           | TYR                  | D      |
| 173            | 253           | PRO                  | D      |
| 174            | 255           | TYR                  | D      |
| 175            | 256           | TYR                  | D      |
| 176            | 257           | PRO                  | D      |
| 177            | 258           | LEU                  | D      |
| 178            | 259           | LEU                  | D      |
| 179            | 260           | ASN                  | D      |
| 180            | 261           | ALA                  | D      |
| 181            | 262           | PHE                  | D      |
| 182            | 267           | GLY                  | D      |
| 183            | 268           | SER                  | A      |
| 184            | 269           | MET                  | A      |
| 185            | 270           | ASP                  | A      |
| 186            | 275           | MET                  | A      |
| 187            | 276           | ILE                  | D      |
| 188            | 277           | ASN                  | D      |
| 189            | 278           | THR                  | D      |
| 190            | 279           | VAL                  | D      |
| 191            | 280           | LYS                  | B      |
| 192            | 281           | SER                  | B      |
| 193            | 285           | ASP                  | B      |
| 194            | 286           | SER                  | B      |
| 195            | 287           | THR                  | B      |
| 196            | 288           | LEU                  | B      |
| 197            | 289           | LEU                  | B      |
| 198            | 290           | GLY                  | D      |
| 199            | 291           | THR                  | D      |
| 200            | 292           | PHE                  | D      |
| 201            | 293           | VAL                  | A      |
| 202            | 294           | GLU                  | D      |
| 203            | 295           | ASN                  | D      |
| 204            | 296           | HIS                  | D      |
| 205            | 297           | ASP                  | D      |
| 206            | 298           | ASN                  | D      |
| 207            | 299           | PRO                  | D      |
| 208            | 300           | ARG                  | D      |
| 209            | 301           | PHE                  | D      |
| 210            | 302           | ALA                  | D      |
| 211            | 303           | SER                  | D      |
| 212            | 308           | ILE                  | A      |
| 213            | 310           | LEU                  | A      |
| 214            | 311           | ALA                  | A      |

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Table S81 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 312           | LYS                  | A      |
| 216            | 313           | ASN                  | A      |
| 217            | 314           | VAL                  | A      |
| 218            | 315           | ALA                  | A      |
| 219            | 316           | ALA                  | A      |
| 220            | 317           | PHE                  | A      |
| 221            | 318           | ILE                  | A      |
| 222            | 319           | ILE                  | A      |
| 223            | 320           | LEU                  | A      |
| 224            | 321           | ASN                  | A      |
| 225            | 322           | ASP                  | D      |
| 226            | 323           | GLY                  | D      |
| 227            | 324           | ILE                  | D      |
| 228            | 325           | PRO                  | A      |
| 229            | 326           | ILE                  | D      |
| 230            | 327           | ILE                  | A      |
| 231            | 328           | TYR                  | D      |
| 232            | 329           | ALA                  | C      |
| 233            | 330           | GLY                  | D      |
| 234            | 331           | GLN                  | A      |
| 235            | 345           | GLU                  | C      |
| 236            | 346           | ALA                  | C      |
| 237            | 347           | THR                  | D      |
| 238            | 348           | TRP                  | D      |
| 239            | 352           | TYR                  | D      |
| 240            | 358           | LEU                  | A      |
| 241            | 359           | TYR                  | A      |
| 242            | 360           | LYS                  | A      |
| 243            | 361           | LEU                  | A      |
| 244            | 362           | ILE                  | A      |
| 245            | 363           | ALA                  | A      |
| 246            | 364           | SER                  | A      |
| 247            | 365           | ALA                  | A      |
| 248            | 366           | ASN                  | A      |
| 249            | 367           | ALA                  | A      |
| 250            | 368           | ILE                  | A      |
| 251            | 373           | ILE                  | A      |
| 252            | 374           | SER                  | A      |
| 253            | 375           | LYS                  | A      |
| 254            | 376           | ASP                  | A      |
| 255            | 377           | THR                  | A      |
| 256            | 381           | THR                  | A      |
| 257            | 382           | TYR                  | A      |
| 258            | 383           | LYS                  | A      |
| 259            | 384           | ASN                  | A      |
| 260            | 386           | PRO                  | A      |

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Table S81 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 387           | ILE                  | A      |
| 262            | 388           | TYR                  | A      |
| 263            | 389           | LYS                  | A      |
| 264            | 390           | ASP                  | A      |
| 265            | 391           | ASP                  | A      |
| 266            | 392           | THR                  | A      |
| 267            | 393           | THR                  | A      |
| 268            | 394           | ILE                  | A      |
| 269            | 395           | ALA                  | A      |
| 270            | 396           | MET                  | A      |
| 271            | 397           | ARG                  | A      |
| 272            | 398           | LYS                  | A      |
| 273            | 403           | SER                  | A      |
| 274            | 404           | GLN                  | A      |
| 275            | 405           | ILE                  | A      |
| 276            | 406           | VAL                  | A      |
| 277            | 407           | THR                  | A      |
| 278            | 408           | ILE                  | A      |
| 279            | 409           | LEU                  | A      |
| 280            | 410           | SER                  | A      |
| 281            | 416           | GLY                  | A      |
| 282            | 417           | ASP                  | A      |
| 283            | 418           | SER                  | A      |
| 284            | 419           | TYR                  | A      |
| 285            | 420           | THR                  | A      |
| 286            | 421           | LEU                  | A      |
| 287            | 422           | SER                  | A      |
| 288            | 432           | GLN                  | A      |
| 289            | 433           | GLN                  | A      |
| 290            | 435           | THR                  | A      |
| 291            | 436           | GLU                  | A      |
| 292            | 437           | VAL                  | A      |
| 293            | 438           | ILE                  | A      |
| 294            | 456           | ALA                  | A      |
| 295            | 457           | GLY                  | A      |
| 296            | 458           | GLY                  | A      |
| 297            | 459           | LEU                  | A      |
| 298            | 460           | PRO                  | A      |
| 299            | 461           | ARG                  | A      |
| 300            | 462           | VAL                  | A      |
| 301            | 463           | LEU                  | A      |
| 302            | 464           | TYR                  | A      |

Table S82: Residues membership for the *B. circulans,s8*  $\alpha$ -amylase  
(PDB code 9CGT, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 15            | ASP                  | A      |
| 1              | 16            | VAL                  | A      |
| 2              | 17            | ILE                  | B      |
| 3              | 18            | TYR                  | B      |
| 4              | 19            | GLN                  | B      |
| 5              | 20            | VAL                  | C      |
| 6              | 21            | PHE                  | C      |
| 7              | 22            | THR                  | C      |
| 8              | 52            | GLY                  | C      |
| 9              | 53            | ASP                  | C      |
| 10             | 54            | TRP                  | C      |
| 11             | 55            | GLN                  | C      |
| 12             | 56            | GLY                  | C      |
| 13             | 57            | LEU                  | C      |
| 14             | 58            | ILE                  | C      |
| 15             | 59            | ASN                  | C      |
| 16             | 60            | LYS                  | C      |
| 17             | 61            | ILE                  | C      |
| 18             | 62            | ASN                  | C      |
| 19             | 63            | ASP                  | C      |
| 20             | 66            | PHE                  | C      |
| 21             | 67            | SER                  | C      |
| 22             | 68            | ASP                  | C      |
| 23             | 69            | LEU                  | C      |
| 24             | 70            | GLY                  | C      |
| 25             | 71            | VAL                  | C      |
| 26             | 72            | THR                  | C      |
| 27             | 73            | ALA                  | C      |
| 28             | 74            | LEU                  | C      |
| 29             | 75            | TRP                  | C      |
| 30             | 76            | ILE                  | C      |
| 31             | 77            | SER                  | C      |
| 32             | 78            | GLN                  | C      |
| 33             | 79            | PRO                  | C      |
| 34             | 80            | VAL                  | C      |
| 35             | 81            | GLU                  | C      |
| 36             | 82            | ASN                  | C      |
| 37             | 83            | ILE                  | C      |
| 38             | 95            | THR                  | C      |
| 39             | 97            | TYR                  | C      |
| 40             | 98            | HIS                  | C      |
| 41             | 99            | GLY                  | C      |
| 42             | 100           | TYR                  | C      |
| 43             | 101           | TRP                  | C      |

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Table S82 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 102           | ALA                  | C      |
| 45             | 103           | ARG                  | C      |
| 46             | 104           | ASP                  | C      |
| 47             | 106           | LYS                  | C      |
| 48             | 107           | LYS                  | C      |
| 49             | 108           | THR                  | C      |
| 50             | 109           | ASN                  | C      |
| 51             | 110           | PRO                  | C      |
| 52             | 111           | TYR                  | C      |
| 53             | 112           | PHE                  | C      |
| 54             | 113           | GLY                  | C      |
| 55             | 114           | THR                  | C      |
| 56             | 115           | MET                  | C      |
| 57             | 116           | ALA                  | C      |
| 58             | 117           | ASP                  | C      |
| 59             | 118           | PHE                  | C      |
| 60             | 119           | GLN                  | C      |
| 61             | 120           | ASN                  | C      |
| 62             | 121           | LEU                  | C      |
| 63             | 122           | ILE                  | C      |
| 64             | 123           | THR                  | C      |
| 65             | 124           | THR                  | C      |
| 66             | 125           | ALA                  | C      |
| 67             | 126           | HIS                  | C      |
| 68             | 127           | ALA                  | C      |
| 69             | 128           | LYS                  | C      |
| 70             | 129           | GLY                  | C      |
| 71             | 130           | ILE                  | C      |
| 72             | 131           | LYS                  | C      |
| 73             | 132           | ILE                  | C      |
| 74             | 133           | VAL                  | C      |
| 75             | 134           | ILE                  | C      |
| 76             | 135           | ASP                  | C      |
| 77             | 136           | PHE                  | C      |
| 78             | 137           | ALA                  | C      |
| 79             | 138           | PRO                  | C      |
| 80             | 139           | ASN                  | C      |
| 81             | 140           | HIS                  | C      |
| 82             | 141           | THR                  | C      |
| 83             | 142           | SER                  | C      |
| 84             | 143           | PRO                  | C      |
| 85             | 144           | ALA                  | C      |
| 86             | 156           | ARG                  | C      |
| 87             | 163           | LEU                  | C      |
| 88             | 164           | VAL                  | C      |
| 89             | 165           | GLY                  | C      |

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Table S82 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 172           | ASN                  | C      |
| 91             | 173           | GLY                  | C      |
| 92             | 174           | TYR                  | C      |
| 93             | 175           | PHE                  | C      |
| 94             | 176           | HIS                  | B      |
| 95             | 192           | LYS                  | B      |
| 96             | 193           | ASN                  | B      |
| 97             | 194           | LEU                  | B      |
| 98             | 195           | TYR                  | B      |
| 99             | 197           | LEU                  | B      |
| 100            | 198           | ALA                  | B      |
| 101            | 199           | ASP                  | B      |
| 102            | 200           | PHE                  | B      |
| 103            | 201           | ASN                  | B      |
| 104            | 202           | HIS                  | B      |
| 105            | 203           | ASN                  | B      |
| 106            | 204           | ASN                  | B      |
| 107            | 205           | ALA                  | B      |
| 108            | 206           | THR                  | B      |
| 109            | 207           | ILE                  | B      |
| 110            | 208           | ASP                  | B      |
| 111            | 209           | LYS                  | B      |
| 112            | 210           | TYR                  | B      |
| 113            | 211           | PHE                  | B      |
| 114            | 212           | LYS                  | B      |
| 115            | 213           | ASP                  | B      |
| 116            | 214           | ALA                  | B      |
| 117            | 215           | ILE                  | B      |
| 118            | 216           | LYS                  | B      |
| 119            | 217           | LEU                  | B      |
| 120            | 218           | TRP                  | B      |
| 121            | 219           | LEU                  | B      |
| 122            | 220           | ASP                  | B      |
| 123            | 221           | MET                  | C      |
| 124            | 222           | GLY                  | C      |
| 125            | 223           | VAL                  | C      |
| 126            | 224           | ASP                  | C      |
| 127            | 225           | GLY                  | C      |
| 128            | 226           | ILE                  | B      |
| 129            | 227           | ARG                  | D      |
| 130            | 228           | VAL                  | B      |
| 131            | 229           | ASP                  | B      |
| 132            | 230           | ALA                  | B      |
| 133            | 231           | VAL                  | B      |
| 134            | 232           | LYS                  | B      |
| 135            | 233           | HIS                  | B      |

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Table S82 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 234           | MET                  | B      |
| 137            | 235           | PRO                  | B      |
| 138            | 236           | LEU                  | B      |
| 139            | 237           | GLY                  | B      |
| 140            | 238           | TRP                  | B      |
| 141            | 239           | GLN                  | B      |
| 142            | 240           | LYS                  | B      |
| 143            | 241           | SER                  | B      |
| 144            | 242           | TRP                  | B      |
| 145            | 243           | MET                  | B      |
| 146            | 244           | SER                  | B      |
| 147            | 245           | SER                  | B      |
| 148            | 246           | ILE                  | B      |
| 149            | 247           | TYR                  | B      |
| 150            | 252           | VAL                  | B      |
| 151            | 253           | PHE                  | B      |
| 152            | 254           | THR                  | B      |
| 153            | 255           | PHE                  | C      |
| 154            | 256           | GLY                  | B      |
| 155            | 257           | ALA                  | B      |
| 156            | 258           | TRP                  | B      |
| 157            | 259           | PHE                  | B      |
| 158            | 260           | LEU                  | B      |
| 159            | 261           | GLY                  | B      |
| 160            | 269           | ASN                  | B      |
| 161            | 270           | THR                  | B      |
| 162            | 271           | ASP                  | B      |
| 163            | 272           | PHE                  | B      |
| 164            | 274           | ASN                  | B      |
| 165            | 275           | LYS                  | B      |
| 166            | 277           | GLY                  | B      |
| 167            | 278           | MET                  | B      |
| 168            | 279           | SER                  | B      |
| 169            | 280           | LEU                  | B      |
| 170            | 281           | LEU                  | D      |
| 171            | 282           | ASP                  | D      |
| 172            | 283           | PHE                  | D      |
| 173            | 284           | ARG                  | D      |
| 174            | 286           | ASN                  | D      |
| 175            | 287           | SER                  | D      |
| 176            | 288           | ALA                  | D      |
| 177            | 289           | VAL                  | D      |
| 178            | 290           | ARG                  | D      |
| 179            | 291           | ASN                  | D      |
| 180            | 292           | VAL                  | D      |
| 181            | 293           | PHE                  | D      |

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Table S82 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 298           | SER                  | D      |
| 183            | 299           | ASN                  | A      |
| 184            | 300           | MET                  | A      |
| 185            | 301           | TYR                  | A      |
| 186            | 306           | MET                  | A      |
| 187            | 307           | ILE                  | D      |
| 188            | 308           | ASN                  | D      |
| 189            | 309           | SER                  | D      |
| 190            | 310           | THR                  | D      |
| 191            | 311           | ALA                  | B      |
| 192            | 312           | THR                  | B      |
| 193            | 316           | GLN                  | B      |
| 194            | 317           | VAL                  | B      |
| 195            | 318           | ASN                  | B      |
| 196            | 319           | ASP                  | B      |
| 197            | 320           | GLN                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | ILE                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | MET                  | D      |
| 207            | 330           | ASP                  | D      |
| 208            | 331           | ARG                  | D      |
| 209            | 332           | PHE                  | D      |
| 210            | 333           | LYS                  | D      |
| 211            | 334           | THR                  | D      |
| 212            | 339           | ASN                  | A      |
| 213            | 341           | ARG                  | A      |
| 214            | 342           | LEU                  | A      |
| 215            | 343           | GLU                  | A      |
| 216            | 344           | GLN                  | A      |
| 217            | 345           | ALA                  | A      |
| 218            | 346           | LEU                  | A      |
| 219            | 347           | ALA                  | A      |
| 220            | 348           | PHE                  | A      |
| 221            | 349           | THR                  | A      |
| 222            | 350           | LEU                  | A      |
| 223            | 351           | THR                  | A      |
| 224            | 352           | SER                  | A      |
| 225            | 353           | ARG                  | D      |
| 226            | 354           | GLY                  | D      |
| 227            | 355           | VAL                  | D      |

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Table S82 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 228            | 356           | PRO                  | A      |
| 229            | 357           | ALA                  | D      |
| 230            | 358           | ILE                  | A      |
| 231            | 359           | TYR                  | D      |
| 232            | 360           | TYR                  | C      |
| 233            | 361           | GLY                  | D      |
| 234            | 362           | THR                  | A      |
| 235            | 376           | ALA                  | C      |
| 236            | 377           | LYS                  | C      |
| 237            | 378           | MET                  | D      |
| 238            | 379           | PRO                  | D      |
| 239            | 381           | PHE                  | D      |
| 240            | 387           | ALA                  | A      |
| 241            | 388           | PHE                  | A      |
| 242            | 389           | ASN                  | A      |
| 243            | 390           | VAL                  | A      |
| 244            | 391           | ILE                  | A      |
| 245            | 392           | SER                  | A      |
| 246            | 393           | LYS                  | A      |
| 247            | 394           | LEU                  | A      |
| 248            | 395           | ALA                  | A      |
| 249            | 396           | PRO                  | A      |
| 250            | 397           | LEU                  | A      |
| 251            | 398           | ARG                  | A      |
| 252            | 399           | LYS                  | A      |
| 253            | 400           | SER                  | A      |
| 254            | 401           | ASN                  | A      |
| 255            | 402           | PRO                  | A      |
| 256            | 406           | TYR                  | A      |
| 257            | 407           | GLY                  | A      |
| 258            | 408           | SER                  | A      |
| 259            | 409           | THR                  | A      |
| 260            | 411           | GLN                  | A      |
| 261            | 412           | ARG                  | A      |
| 262            | 413           | TRP                  | A      |
| 263            | 414           | ILE                  | A      |
| 264            | 415           | ASN                  | A      |
| 265            | 416           | ASN                  | A      |
| 266            | 417           | ASP                  | A      |
| 267            | 418           | VAL                  | A      |
| 268            | 419           | TYR                  | A      |
| 269            | 420           | VAL                  | A      |
| 270            | 421           | TYR                  | A      |
| 271            | 422           | GLU                  | A      |
| 272            | 423           | ARG                  | A      |
| 273            | 428           | SER                  | A      |

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Table S82 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 274            | 429           | VAL                  | A      |
| 275            | 430           | ALA                  | A      |
| 276            | 431           | VAL                  | A      |
| 277            | 432           | VAL                  | A      |
| 278            | 433           | ALA                  | A      |
| 279            | 434           | VAL                  | A      |
| 280            | 435           | ASN                  | A      |
| 281            | 439           | SER                  | A      |
| 282            | 440           | THR                  | A      |
| 283            | 441           | SER                  | A      |
| 284            | 442           | ALA                  | A      |
| 285            | 443           | SER                  | A      |
| 286            | 444           | ILE                  | A      |
| 287            | 445           | THR                  | A      |
| 288            | 454           | GLY                  | A      |
| 289            | 455           | SER                  | A      |
| 290            | 457           | THR                  | A      |
| 291            | 458           | ASP                  | A      |
| 292            | 459           | VAL                  | A      |
| 293            | 460           | LEU                  | A      |
| 294            | 482           | ALA                  | A      |
| 295            | 483           | ALA                  | A      |
| 296            | 484           | GLY                  | A      |
| 297            | 485           | ALA                  | A      |
| 298            | 486           | THR                  | A      |
| 299            | 487           | ALA                  | A      |
| 300            | 488           | VAL                  | A      |
| 301            | 489           | TRP                  | A      |
| 302            | 490           | GLN                  | A      |

Table S83: Residues membership for the *B. licheniformis*  $\alpha$ -amylase (PDB code 1VJS, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 5             | GLY                  | A      |
| 1              | 6             | THR                  | A      |
| 2              | 7             | LEU                  | B      |
| 3              | 8             | MET                  | B      |
| 4              | 9             | GLN                  | B      |
| 5              | 10            | TYR                  | C      |
| 6              | 11            | PHE                  | C      |
| 7              | 15            | MET                  | C      |
| 8              | 20            | GLN                  | C      |

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Table S83 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 9              | 21            | HIS                  | C      |
| 10             | 22            | TRP                  | C      |
| 11             | 23            | LYS                  | C      |
| 12             | 24            | ARG                  | C      |
| 13             | 25            | LEU                  | C      |
| 14             | 26            | GLN                  | C      |
| 15             | 27            | ASN                  | C      |
| 16             | 28            | ASP                  | C      |
| 17             | 29            | SER                  | C      |
| 18             | 30            | ALA                  | C      |
| 19             | 31            | TYR                  | C      |
| 20             | 32            | LEU                  | C      |
| 21             | 33            | ALA                  | C      |
| 22             | 34            | GLU                  | C      |
| 23             | 35            | HIS                  | C      |
| 24             | 36            | GLY                  | C      |
| 25             | 37            | ILE                  | C      |
| 26             | 38            | THR                  | C      |
| 27             | 39            | ALA                  | C      |
| 28             | 40            | VAL                  | C      |
| 29             | 41            | TRP                  | C      |
| 30             | 42            | ILE                  | C      |
| 31             | 43            | PRO                  | C      |
| 32             | 44            | PRO                  | C      |
| 33             | 45            | ALA                  | C      |
| 34             | 46            | TYR                  | C      |
| 35             | 47            | LYS                  | C      |
| 36             | 48            | GLY                  | C      |
| 37             | 49            | THR                  | C      |
| 38             | 50            | SER                  | C      |
| 39             | 53            | ASP                  | C      |
| 40             | 54            | VAL                  | C      |
| 41             | 55            | GLY                  | C      |
| 42             | 56            | TYR                  | C      |
| 43             | 57            | GLY                  | C      |
| 44             | 58            | ALA                  | C      |
| 45             | 59            | TYR                  | C      |
| 46             | 60            | ASP                  | C      |
| 47             | 62            | TYR                  | C      |
| 48             | 63            | ASP                  | C      |
| 49             | 64            | LEU                  | C      |
| 50             | 65            | GLY                  | C      |
| 51             | 75            | THR                  | C      |
| 52             | 76            | LYS                  | C      |
| 53             | 77            | TYR                  | C      |
| 54             | 78            | GLY                  | C      |

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Table S83 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 55             | 79            | THR                  | C      |
| 56             | 80            | LYS                  | C      |
| 57             | 81            | GLY                  | C      |
| 58             | 82            | GLU                  | C      |
| 59             | 83            | LEU                  | C      |
| 60             | 84            | GLN                  | C      |
| 61             | 85            | SER                  | C      |
| 62             | 86            | ALA                  | C      |
| 63             | 87            | ILE                  | C      |
| 64             | 88            | LYS                  | C      |
| 65             | 89            | SER                  | C      |
| 66             | 90            | LEU                  | C      |
| 67             | 91            | HIS                  | C      |
| 68             | 92            | SER                  | C      |
| 69             | 93            | ARG                  | C      |
| 70             | 94            | ASP                  | C      |
| 71             | 95            | ILE                  | C      |
| 72             | 96            | ASN                  | C      |
| 73             | 97            | VAL                  | C      |
| 74             | 98            | TYR                  | C      |
| 75             | 99            | GLY                  | C      |
| 76             | 100           | ASP                  | C      |
| 77             | 101           | VAL                  | C      |
| 78             | 102           | VAL                  | C      |
| 79             | 103           | ILE                  | C      |
| 80             | 104           | ASN                  | C      |
| 81             | 105           | HIS                  | C      |
| 82             | 106           | LYS                  | C      |
| 83             | 107           | GLY                  | C      |
| 84             | 108           | GLY                  | C      |
| 85             | 109           | ALA                  | C      |
| 86             | 141           | PHE                  | C      |
| 87             | 154           | LYS                  | C      |
| 88             | 155           | TRP                  | C      |
| 89             | 156           | HIS                  | C      |
| 90             | 157           | TRP                  | C      |
| 91             | 158           | TYR                  | C      |
| 92             | 159           | HIS                  | C      |
| 93             | 160           | PHE                  | C      |
| 94             | 161           | ASP                  | B      |
| 95             | 162           | GLY                  | B      |
| 96             | 163           | THR                  | B      |
| 97             | 164           | ASP                  | B      |
| 98             | 165           | TRP                  | B      |
| 99             | 198           | TYR                  | B      |
| 100            | 199           | ALA                  | B      |

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Table S83 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 101            | 200           | ASP                  | B      |
| 102            | 201           | ILE                  | B      |
| 103            | 202           | ASP                  | B      |
| 104            | 203           | TYR                  | B      |
| 105            | 204           | ASP                  | B      |
| 106            | 205           | HIS                  | B      |
| 107            | 206           | PRO                  | B      |
| 108            | 207           | ASP                  | B      |
| 109            | 208           | VAL                  | B      |
| 110            | 209           | ALA                  | B      |
| 111            | 210           | ALA                  | B      |
| 112            | 211           | GLU                  | B      |
| 113            | 212           | ILE                  | B      |
| 114            | 213           | LYS                  | B      |
| 115            | 214           | ARG                  | B      |
| 116            | 215           | TRP                  | B      |
| 117            | 216           | GLY                  | B      |
| 118            | 217           | THR                  | B      |
| 119            | 218           | TRP                  | B      |
| 120            | 219           | TYR                  | B      |
| 121            | 220           | ALA                  | B      |
| 122            | 221           | ASN                  | B      |
| 123            | 223           | LEU                  | C      |
| 124            | 224           | GLN                  | C      |
| 125            | 225           | LEU                  | C      |
| 126            | 226           | ASP                  | C      |
| 127            | 227           | GLY                  | C      |
| 128            | 228           | PHE                  | B      |
| 129            | 229           | ARG                  | D      |
| 130            | 230           | LEU                  | B      |
| 131            | 231           | ASP                  | B      |
| 132            | 232           | ALA                  | B      |
| 133            | 233           | VAL                  | B      |
| 134            | 234           | LYS                  | B      |
| 135            | 235           | HIS                  | B      |
| 136            | 236           | ILE                  | B      |
| 137            | 237           | LYS                  | B      |
| 138            | 238           | PHE                  | B      |
| 139            | 239           | SER                  | B      |
| 140            | 240           | PHE                  | B      |
| 141            | 241           | LEU                  | B      |
| 142            | 242           | ARG                  | B      |
| 143            | 243           | ASP                  | B      |
| 144            | 244           | TRP                  | B      |
| 145            | 245           | VAL                  | B      |
| 146            | 246           | ASN                  | B      |

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Table S83 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 147            | 247           | HIS                  | B      |
| 148            | 248           | VAL                  | B      |
| 149            | 249           | ARG                  | B      |
| 150            | 256           | MET                  | B      |
| 151            | 257           | PHE                  | B      |
| 152            | 258           | THR                  | B      |
| 153            | 259           | VAL                  | C      |
| 154            | 260           | ALA                  | B      |
| 155            | 261           | GLU                  | B      |
| 156            | 262           | TYR                  | B      |
| 157            | 263           | TRP                  | B      |
| 158            | 264           | GLN                  | B      |
| 159            | 265           | ASN                  | B      |
| 160            | 270           | LEU                  | B      |
| 161            | 271           | GLU                  | B      |
| 162            | 272           | ASN                  | B      |
| 163            | 273           | TYR                  | B      |
| 164            | 274           | LEU                  | B      |
| 165            | 275           | ASN                  | B      |
| 166            | 280           | ASN                  | B      |
| 167            | 281           | HIS                  | B      |
| 168            | 282           | SER                  | B      |
| 169            | 283           | VAL                  | B      |
| 170            | 284           | PHE                  | D      |
| 171            | 285           | ASP                  | D      |
| 172            | 286           | VAL                  | D      |
| 173            | 287           | PRO                  | D      |
| 174            | 289           | HIS                  | D      |
| 175            | 290           | TYR                  | D      |
| 176            | 291           | GLN                  | D      |
| 177            | 292           | PHE                  | D      |
| 178            | 293           | HIS                  | D      |
| 179            | 294           | ALA                  | D      |
| 180            | 295           | ALA                  | D      |
| 181            | 296           | SER                  | D      |
| 182            | 302           | TYR                  | D      |
| 183            | 303           | ASP                  | A      |
| 184            | 304           | MET                  | A      |
| 185            | 305           | ARG                  | A      |
| 186            | 307           | LEU                  | A      |
| 187            | 308           | LEU                  | D      |
| 188            | 309           | ASN                  | D      |
| 189            | 310           | SER                  | D      |
| 190            | 313           | VAL                  | D      |
| 191            | 314           | SER                  | B      |
| 192            | 315           | LYS                  | B      |

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Table S83 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 193            | 316           | HIS                  | B      |
| 194            | 317           | PRO                  | B      |
| 195            | 318           | LEU                  | B      |
| 196            | 319           | LYS                  | B      |
| 197            | 320           | ALA                  | B      |
| 198            | 321           | VAL                  | D      |
| 199            | 322           | THR                  | D      |
| 200            | 323           | PHE                  | D      |
| 201            | 324           | VAL                  | A      |
| 202            | 325           | ASP                  | D      |
| 203            | 326           | ASN                  | D      |
| 204            | 327           | HIS                  | D      |
| 205            | 328           | ASP                  | D      |
| 206            | 329           | THR                  | D      |
| 207            | 330           | GLN                  | D      |
| 208            | 338           | THR                  | D      |
| 209            | 339           | VAL                  | D      |
| 210            | 340           | GLN                  | D      |
| 211            | 341           | THR                  | D      |
| 212            | 342           | TRP                  | A      |
| 213            | 343           | PHE                  | A      |
| 214            | 344           | LYS                  | A      |
| 215            | 345           | PRO                  | A      |
| 216            | 346           | LEU                  | A      |
| 217            | 347           | ALA                  | A      |
| 218            | 348           | TYR                  | A      |
| 219            | 349           | ALA                  | A      |
| 220            | 350           | PHE                  | A      |
| 221            | 351           | ILE                  | A      |
| 222            | 352           | LEU                  | A      |
| 223            | 353           | THR                  | A      |
| 224            | 354           | ARG                  | A      |
| 225            | 356           | SER                  | D      |
| 226            | 357           | GLY                  | D      |
| 227            | 358           | TYR                  | D      |
| 228            | 359           | PRO                  | A      |
| 229            | 360           | GLN                  | D      |
| 230            | 361           | VAL                  | A      |
| 231            | 362           | PHE                  | D      |
| 232            | 363           | TYR                  | C      |
| 233            | 364           | GLY                  | D      |
| 234            | 365           | ASP                  | A      |
| 235            | 366           | MET                  | C      |
| 236            | 367           | TYR                  | C      |
| 237            | 368           | GLY                  | D      |
| 238            | 369           | THR                  | D      |

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Table S83 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 239            | 379           | ALA                  | D      |
| 240            | 380           | LEU                  | A      |
| 241            | 381           | LYS                  | A      |
| 242            | 382           | HIS                  | A      |
| 243            | 383           | LYS                  | A      |
| 244            | 384           | ILE                  | A      |
| 245            | 385           | GLU                  | A      |
| 246            | 386           | PRO                  | A      |
| 247            | 387           | ILE                  | A      |
| 248            | 388           | LEU                  | A      |
| 249            | 389           | LYS                  | A      |
| 250            | 390           | ALA                  | A      |
| 251            | 391           | ARG                  | A      |
| 252            | 392           | LYS                  | A      |
| 253            | 393           | GLN                  | A      |
| 254            | 394           | TYR                  | A      |
| 255            | 395           | ALA                  | A      |
| 256            | 397           | GLY                  | A      |
| 257            | 398           | ALA                  | A      |
| 258            | 399           | GLN                  | A      |
| 259            | 400           | HIS                  | A      |
| 260            | 401           | ASP                  | A      |
| 261            | 402           | TYR                  | A      |
| 262            | 403           | PHE                  | A      |
| 263            | 404           | ASP                  | A      |
| 264            | 405           | HIS                  | A      |
| 265            | 406           | HIS                  | A      |
| 266            | 407           | ASP                  | A      |
| 267            | 408           | ILE                  | A      |
| 268            | 409           | VAL                  | A      |
| 269            | 410           | GLY                  | A      |
| 270            | 411           | TRP                  | A      |
| 271            | 412           | THR                  | A      |
| 272            | 413           | ARG                  | A      |
| 273            | 414           | GLU                  | A      |
| 274            | 415           | GLY                  | A      |
| 275            | 424           | LEU                  | A      |
| 276            | 425           | ALA                  | A      |
| 277            | 426           | ALA                  | A      |
| 278            | 427           | LEU                  | A      |
| 279            | 428           | ILE                  | A      |
| 280            | 429           | THR                  | A      |
| 281            | 431           | GLY                  | A      |
| 282            | 432           | PRO                  | A      |
| 283            | 433           | GLY                  | A      |
| 284            | 434           | GLY                  | A      |

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Table S83 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 285            | 435           | ALA                  | A      |
| 286            | 436           | LYS                  | A      |
| 287            | 437           | ARG                  | A      |
| 288            | 446           | GLY                  | A      |
| 289            | 447           | GLU                  | A      |
| 290            | 449           | TRP                  | A      |
| 291            | 450           | HIS                  | A      |
| 292            | 451           | ASP                  | A      |
| 293            | 452           | ILE                  | A      |
| 294            | 472           | VAL                  | A      |
| 295            | 473           | ASN                  | A      |
| 296            | 474           | GLY                  | A      |
| 297            | 476           | SER                  | A      |
| 298            | 477           | VAL                  | A      |
| 299            | 478           | SER                  | A      |
| 300            | 479           | ILE                  | A      |
| 301            | 480           | TYR                  | A      |
| 302            | 481           | VAL                  | A      |

Table S84: Residues membership for the *T. vulgaris* R47  $\alpha$ -amylase (PDB code 1WZK, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 131           | ALA                  | A      |
| 1              | 132           | VAL                  | A      |
| 2              | 133           | ILE                  | B      |
| 3              | 134           | TYR                  | B      |
| 4              | 135           | GLN                  | B      |
| 5              | 136           | ILE                  | C      |
| 6              | 137           | PHE                  | C      |
| 7              | 138           | PRO                  | C      |
| 8              | 170           | GLY                  | C      |
| 9              | 171           | ASP                  | C      |
| 10             | 172           | LEU                  | C      |
| 11             | 173           | LYS                  | C      |
| 12             | 174           | GLY                  | C      |
| 13             | 175           | VAL                  | C      |
| 14             | 176           | ILE                  | C      |
| 15             | 177           | ASP                  | C      |
| 16             | 178           | ARG                  | C      |
| 17             | 179           | LEU                  | C      |
| 18             | 180           | PRO                  | C      |
| 19             | 181           | TYR                  | C      |

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Table S84 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 20             | 182           | LEU                  | C      |
| 21             | 183           | GLU                  | C      |
| 22             | 184           | GLU                  | C      |
| 23             | 185           | LEU                  | C      |
| 24             | 186           | GLY                  | C      |
| 25             | 187           | VAL                  | C      |
| 26             | 188           | THR                  | C      |
| 27             | 189           | ALA                  | C      |
| 28             | 190           | LEU                  | C      |
| 29             | 191           | TYR                  | C      |
| 30             | 192           | PHE                  | C      |
| 31             | 193           | THR                  | C      |
| 32             | 194           | PRO                  | C      |
| 33             | 195           | ILE                  | C      |
| 34             | 196           | PHE                  | C      |
| 35             | 197           | ALA                  | C      |
| 36             | 198           | SER                  | C      |
| 37             | 199           | PRO                  | C      |
| 38             | 200           | SER                  | C      |
| 39             | 201           | HIS                  | C      |
| 40             | 202           | HIS                  | C      |
| 41             | 203           | LYS                  | C      |
| 42             | 204           | TYR                  | C      |
| 43             | 205           | ASP                  | C      |
| 44             | 206           | THR                  | C      |
| 45             | 207           | ALA                  | C      |
| 46             | 208           | ASP                  | C      |
| 47             | 210           | LEU                  | C      |
| 48             | 211           | ALA                  | C      |
| 49             | 212           | ILE                  | C      |
| 50             | 213           | ASP                  | C      |
| 51             | 214           | PRO                  | C      |
| 52             | 215           | GLN                  | C      |
| 53             | 216           | PHE                  | C      |
| 54             | 217           | GLY                  | C      |
| 55             | 218           | ASP                  | C      |
| 56             | 219           | LEU                  | C      |
| 57             | 220           | PRO                  | C      |
| 58             | 221           | THR                  | C      |
| 59             | 222           | PHE                  | C      |
| 60             | 223           | ARG                  | C      |
| 61             | 224           | ARG                  | C      |
| 62             | 225           | LEU                  | C      |
| 63             | 226           | VAL                  | C      |
| 64             | 227           | ASP                  | C      |
| 65             | 228           | GLU                  | C      |

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Table S84 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 66             | 229           | ALA                  | C      |
| 67             | 230           | HIS                  | C      |
| 68             | 231           | ARG                  | C      |
| 69             | 232           | ARG                  | C      |
| 70             | 233           | GLY                  | C      |
| 71             | 234           | ILE                  | C      |
| 72             | 235           | LYS                  | C      |
| 73             | 236           | ILE                  | C      |
| 74             | 237           | ILE                  | C      |
| 75             | 238           | LEU                  | C      |
| 76             | 239           | ASP                  | C      |
| 77             | 240           | ALA                  | C      |
| 78             | 241           | VAL                  | C      |
| 79             | 242           | PHE                  | C      |
| 80             | 243           | ASN                  | C      |
| 81             | 244           | HIS                  | C      |
| 82             | 245           | ALA                  | C      |
| 83             | 246           | GLY                  | C      |
| 84             | 247           | ASP                  | C      |
| 85             | 248           | GLN                  | C      |
| 86             | 249           | PHE                  | C      |
| 87             | 250           | PHE                  | C      |
| 88             | 251           | ALA                  | C      |
| 89             | 252           | PHE                  | C      |
| 90             | 265           | LYS                  | C      |
| 91             | 266           | ASP                  | C      |
| 92             | 267           | TRP                  | C      |
| 93             | 268           | PHE                  | C      |
| 94             | 269           | PHE                  | B      |
| 95             | 284           | GLU                  | B      |
| 96             | 285           | THR                  | B      |
| 97             | 286           | PHE                  | B      |
| 98             | 287           | ALA                  | B      |
| 99             | 293           | MET                  | B      |
| 100            | 294           | PRO                  | B      |
| 101            | 295           | LYS                  | B      |
| 102            | 296           | LEU                  | B      |
| 103            | 297           | ARG                  | B      |
| 104            | 298           | THR                  | B      |
| 105            | 299           | GLU                  | B      |
| 106            | 300           | ASN                  | B      |
| 107            | 301           | PRO                  | B      |
| 108            | 302           | GLU                  | B      |
| 109            | 303           | VAL                  | B      |
| 110            | 304           | LYS                  | B      |
| 111            | 305           | GLU                  | B      |

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Table S84 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 112            | 306           | TYR                  | B      |
| 113            | 307           | LEU                  | B      |
| 114            | 308           | PHE                  | B      |
| 115            | 309           | ASP                  | B      |
| 116            | 310           | VAL                  | B      |
| 117            | 311           | ALA                  | B      |
| 118            | 312           | ARG                  | B      |
| 119            | 313           | PHE                  | B      |
| 120            | 314           | TRP                  | B      |
| 121            | 315           | MET                  | B      |
| 122            | 316           | GLU                  | B      |
| 123            | 317           | GLN                  | C      |
| 124            | 318           | GLY                  | C      |
| 125            | 319           | ILE                  | C      |
| 126            | 320           | ASP                  | C      |
| 127            | 321           | GLY                  | C      |
| 128            | 322           | TRP                  | B      |
| 129            | 323           | ARG                  | D      |
| 130            | 324           | LEU                  | B      |
| 131            | 325           | ASP                  | B      |
| 132            | 326           | VAL                  | B      |
| 133            | 327           | ALA                  | B      |
| 134            | 328           | ASN                  | B      |
| 135            | 329           | GLU                  | B      |
| 136            | 330           | VAL                  | B      |
| 137            | 331           | ASP                  | B      |
| 138            | 332           | HIS                  | B      |
| 139            | 333           | ALA                  | B      |
| 140            | 334           | PHE                  | B      |
| 141            | 335           | TRP                  | B      |
| 142            | 336           | ARG                  | B      |
| 143            | 337           | GLU                  | B      |
| 144            | 338           | PHE                  | B      |
| 145            | 339           | ARG                  | B      |
| 146            | 340           | ARG                  | B      |
| 147            | 341           | LEU                  | B      |
| 148            | 342           | VAL                  | B      |
| 149            | 343           | LYS                  | B      |
| 150            | 349           | ALA                  | B      |
| 151            | 350           | LEU                  | B      |
| 152            | 351           | ILE                  | B      |
| 153            | 352           | VAL                  | C      |
| 154            | 353           | GLY                  | B      |
| 155            | 354           | GLU                  | B      |
| 156            | 355           | ILE                  | B      |
| 157            | 356           | TRP                  | B      |

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Table S84 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 158            | 357           | HIS                  | B      |
| 159            | 358           | ASP                  | B      |
| 160            | 359           | ALA                  | B      |
| 161            | 360           | SER                  | B      |
| 162            | 361           | GLY                  | B      |
| 163            | 362           | TRP                  | B      |
| 164            | 363           | LEU                  | B      |
| 165            | 364           | MET                  | B      |
| 166            | 368           | PHE                  | B      |
| 167            | 369           | ASP                  | B      |
| 168            | 370           | SER                  | B      |
| 169            | 371           | VAL                  | B      |
| 170            | 372           | MET                  | D      |
| 171            | 373           | ASN                  | D      |
| 172            | 374           | TYR                  | D      |
| 173            | 375           | LEU                  | D      |
| 174            | 377           | ARG                  | D      |
| 175            | 378           | GLU                  | D      |
| 176            | 379           | SER                  | D      |
| 177            | 380           | VAL                  | D      |
| 178            | 381           | ILE                  | D      |
| 179            | 382           | ARG                  | D      |
| 180            | 383           | PHE                  | D      |
| 181            | 384           | PHE                  | D      |
| 182            | 389           | ILE                  | D      |
| 183            | 390           | HIS                  | A      |
| 184            | 391           | ALA                  | A      |
| 185            | 392           | GLU                  | A      |
| 186            | 397           | GLU                  | A      |
| 187            | 398           | LEU                  | D      |
| 188            | 399           | THR                  | D      |
| 189            | 400           | ARG                  | D      |
| 190            | 401           | ALA                  | D      |
| 191            | 402           | ARG                  | B      |
| 192            | 403           | MET                  | B      |
| 193            | 409           | ALA                  | B      |
| 194            | 410           | ALA                  | B      |
| 195            | 411           | GLN                  | B      |
| 196            | 412           | GLY                  | B      |
| 197            | 413           | LEU                  | B      |
| 198            | 414           | TRP                  | D      |
| 199            | 415           | ASN                  | D      |
| 200            | 416           | LEU                  | D      |
| 201            | 417           | LEU                  | A      |
| 202            | 418           | ASP                  | D      |
| 203            | 419           | SER                  | D      |

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Table S84 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 204            | 420           | HIS                  | D      |
| 205            | 421           | ASP                  | D      |
| 206            | 422           | THR                  | D      |
| 207            | 423           | GLU                  | D      |
| 208            | 424           | ARG                  | D      |
| 209            | 425           | PHE                  | D      |
| 210            | 426           | LEU                  | D      |
| 211            | 427           | THR                  | D      |
| 212            | 433           | GLU                  | A      |
| 213            | 435           | LYS                  | A      |
| 214            | 436           | PHE                  | A      |
| 215            | 437           | ARG                  | A      |
| 216            | 438           | LEU                  | A      |
| 217            | 439           | ALA                  | A      |
| 218            | 440           | VAL                  | A      |
| 219            | 441           | LEU                  | A      |
| 220            | 442           | PHE                  | A      |
| 221            | 443           | GLN                  | A      |
| 222            | 444           | MET                  | A      |
| 223            | 445           | THR                  | A      |
| 224            | 446           | TYR                  | A      |
| 225            | 447           | LEU                  | D      |
| 226            | 448           | GLY                  | D      |
| 227            | 449           | THR                  | D      |
| 228            | 450           | PRO                  | A      |
| 229            | 451           | LEU                  | D      |
| 230            | 452           | ILE                  | A      |
| 231            | 453           | TYR                  | D      |
| 232            | 454           | TYR                  | C      |
| 233            | 455           | GLY                  | D      |
| 234            | 456           | ASP                  | A      |
| 235            | 470           | ARG                  | C      |
| 236            | 471           | PRO                  | C      |
| 237            | 472           | MET                  | D      |
| 238            | 473           | ILE                  | D      |
| 239            | 474           | TRP                  | D      |
| 240            | 483           | LEU                  | A      |
| 241            | 484           | PHE                  | A      |
| 242            | 485           | GLU                  | A      |
| 243            | 486           | PHE                  | A      |
| 244            | 487           | TYR                  | A      |
| 245            | 488           | LYS                  | A      |
| 246            | 489           | GLU                  | A      |
| 247            | 490           | LEU                  | A      |
| 248            | 491           | ILE                  | A      |
| 249            | 492           | ARG                  | A      |

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Table S84 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 250            | 493           | LEU                  | A      |
| 251            | 494           | ARG                  | A      |
| 252            | 495           | HIS                  | A      |
| 253            | 496           | ARG                  | A      |
| 254            | 497           | LEU                  | A      |
| 255            | 498           | ALA                  | A      |
| 256            | 502           | ARG                  | A      |
| 257            | 503           | GLY                  | A      |
| 258            | 504           | ASN                  | A      |
| 259            | 505           | VAL                  | A      |
| 260            | 507           | SER                  | A      |
| 261            | 508           | TRP                  | A      |
| 262            | 509           | HIS                  | A      |
| 263            | 510           | ALA                  | A      |
| 264            | 513           | GLN                  | A      |
| 265            | 514           | ALA                  | A      |
| 266            | 515           | ASN                  | A      |
| 267            | 516           | LEU                  | A      |
| 268            | 517           | TYR                  | A      |
| 269            | 518           | ALA                  | A      |
| 270            | 519           | PHE                  | A      |
| 271            | 520           | VAL                  | A      |
| 272            | 521           | ARG                  | A      |
| 273            | 526           | GLN                  | A      |
| 274            | 527           | HIS                  | A      |
| 275            | 528           | VAL                  | A      |
| 276            | 529           | GLY                  | A      |
| 277            | 530           | VAL                  | A      |
| 278            | 531           | VAL                  | A      |
| 279            | 532           | LEU                  | A      |
| 280            | 533           | ASN                  | A      |
| 281            | 536           | GLY                  | A      |
| 282            | 537           | GLU                  | A      |
| 283            | 538           | LYS                  | A      |
| 284            | 539           | GLN                  | A      |
| 285            | 540           | THR                  | A      |
| 286            | 541           | VAL                  | A      |
| 287            | 542           | LEU                  | A      |
| 288            | 552           | THR                  | A      |
| 289            | 553           | TRP                  | A      |
| 290            | 554           | LEU                  | A      |
| 291            | 555           | ASP                  | A      |
| 292            | 556           | CYS                  | A      |
| 293            | 557           | LEU                  | A      |
| 294            | 574           | ARG                  | A      |
| 295            | 575           | PRO                  | A      |

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Table S84 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 296            | 576           | TYR                  | A      |
| 297            | 577           | GLN                  | A      |
| 298            | 578           | GLY                  | A      |
| 299            | 579           | MET                  | A      |
| 300            | 580           | ILE                  | A      |
| 301            | 581           | LEU                  | A      |
| 302            | 582           | TRP                  | A      |

Table S85: Residues membership for the *N. polysaccharea*  $\alpha$ -amylase (PDB code 1JGI, chain A)

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 98            | GLN                  | A      |
| 1              | 99            | VAL                  | A      |
| 2              | 100           | GLY                  | B      |
| 3              | 101           | GLY                  | B      |
| 4              | 102           | VAL                  | B      |
| 5              | 103           | CYS                  | C      |
| 6              | 104           | TYR                  | C      |
| 7              | 105           | VAL                  | C      |
| 8              | 110           | GLY                  | C      |
| 9              | 111           | ASP                  | C      |
| 10             | 112           | LEU                  | C      |
| 11             | 113           | LYS                  | C      |
| 12             | 114           | GLY                  | C      |
| 13             | 115           | LEU                  | C      |
| 14             | 116           | LYS                  | C      |
| 15             | 117           | ASP                  | C      |
| 16             | 118           | LYS                  | C      |
| 17             | 119           | ILE                  | C      |
| 18             | 120           | PRO                  | C      |
| 19             | 121           | TYR                  | C      |
| 20             | 122           | PHE                  | C      |
| 21             | 123           | GLN                  | C      |
| 22             | 124           | GLU                  | C      |
| 23             | 125           | LEU                  | C      |
| 24             | 126           | GLY                  | C      |
| 25             | 127           | LEU                  | C      |
| 26             | 128           | THR                  | C      |
| 27             | 129           | TYR                  | C      |
| 28             | 130           | LEU                  | C      |
| 29             | 131           | TYR                  | C      |
| 30             | 132           | LEU                  | C      |

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Table S85 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 31             | 133           | MET                  | C      |
| 32             | 134           | PRO                  | C      |
| 33             | 135           | LEU                  | C      |
| 34             | 136           | PHE                  | C      |
| 35             | 137           | LYS                  | C      |
| 36             | 138           | CYS                  | C      |
| 37             | 139           | PRO                  | C      |
| 38             | 141           | GLY                  | C      |
| 39             | 144           | ASP                  | C      |
| 40             | 145           | GLY                  | C      |
| 41             | 146           | GLY                  | C      |
| 42             | 147           | TYR                  | C      |
| 43             | 148           | ALA                  | C      |
| 44             | 149           | VAL                  | C      |
| 45             | 150           | SER                  | C      |
| 46             | 151           | SER                  | C      |
| 47             | 153           | ARG                  | C      |
| 48             | 154           | ASP                  | C      |
| 49             | 155           | VAL                  | C      |
| 50             | 156           | ASN                  | C      |
| 51             | 157           | PRO                  | C      |
| 52             | 158           | ALA                  | C      |
| 53             | 159           | LEU                  | C      |
| 54             | 160           | GLY                  | C      |
| 55             | 161           | THR                  | C      |
| 56             | 162           | ILE                  | C      |
| 57             | 163           | GLY                  | C      |
| 58             | 164           | ASP                  | C      |
| 59             | 165           | LEU                  | C      |
| 60             | 166           | ARG                  | C      |
| 61             | 167           | GLU                  | C      |
| 62             | 168           | VAL                  | C      |
| 63             | 169           | ILE                  | C      |
| 64             | 170           | ALA                  | C      |
| 65             | 171           | ALA                  | C      |
| 66             | 172           | LEU                  | C      |
| 67             | 173           | HIS                  | C      |
| 68             | 174           | GLU                  | C      |
| 69             | 175           | ALA                  | C      |
| 70             | 176           | GLY                  | C      |
| 71             | 177           | ILE                  | C      |
| 72             | 178           | SER                  | C      |
| 73             | 179           | ALA                  | C      |
| 74             | 180           | VAL                  | C      |
| 75             | 181           | VAL                  | C      |
| 76             | 182           | ASP                  | C      |

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Table S85 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 77             | 183           | PHE                  | C      |
| 78             | 184           | ILE                  | C      |
| 79             | 185           | PHE                  | C      |
| 80             | 186           | ASN                  | C      |
| 81             | 187           | HIS                  | C      |
| 82             | 188           | THR                  | C      |
| 83             | 189           | SER                  | C      |
| 84             | 190           | ASN                  | C      |
| 85             | 191           | GLU                  | C      |
| 86             | 192           | HIS                  | C      |
| 87             | 193           | GLU                  | C      |
| 88             | 194           | TRP                  | C      |
| 89             | 195           | ALA                  | C      |
| 90             | 206           | ASP                  | C      |
| 91             | 207           | ASN                  | C      |
| 92             | 208           | PHE                  | C      |
| 93             | 209           | TYR                  | C      |
| 94             | 210           | TYR                  | B      |
| 95             | 247           | TRP                  | B      |
| 96             | 248           | THR                  | B      |
| 97             | 249           | THR                  | B      |
| 98             | 250           | PHE                  | B      |
| 99             | 254           | GLN                  | B      |
| 100            | 255           | TRP                  | B      |
| 101            | 256           | ASP                  | B      |
| 102            | 257           | LEU                  | B      |
| 103            | 258           | ASN                  | B      |
| 104            | 259           | TYR                  | B      |
| 105            | 260           | SER                  | B      |
| 106            | 261           | ASN                  | B      |
| 107            | 262           | PRO                  | B      |
| 108            | 263           | TRP                  | B      |
| 109            | 264           | VAL                  | B      |
| 110            | 265           | PHE                  | B      |
| 111            | 266           | ARG                  | B      |
| 112            | 267           | ALA                  | B      |
| 113            | 268           | MET                  | B      |
| 114            | 269           | ALA                  | B      |
| 115            | 270           | GLY                  | B      |
| 116            | 271           | GLU                  | B      |
| 117            | 272           | MET                  | B      |
| 118            | 273           | LEU                  | B      |
| 119            | 274           | PHE                  | B      |
| 120            | 275           | LEU                  | B      |
| 121            | 276           | ALA                  | B      |
| 122            | 277           | ASN                  | B      |

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Table S85 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 123            | 278           | LEU                  | C      |
| 124            | 279           | GLY                  | C      |
| 125            | 280           | VAL                  | C      |
| 126            | 281           | ASP                  | C      |
| 127            | 282           | ILE                  | C      |
| 128            | 283           | LEU                  | B      |
| 129            | 284           | ARG                  | D      |
| 130            | 285           | MET                  | B      |
| 131            | 286           | ASP                  | B      |
| 132            | 287           | ALA                  | B      |
| 133            | 288           | VAL                  | B      |
| 134            | 289           | ALA                  | B      |
| 135            | 290           | PHE                  | B      |
| 136            | 291           | ILE                  | B      |
| 137            | 292           | TRP                  | B      |
| 138            | 306           | HIS                  | B      |
| 139            | 307           | ALA                  | B      |
| 140            | 308           | LEU                  | B      |
| 141            | 309           | ILE                  | B      |
| 142            | 310           | ARG                  | B      |
| 143            | 311           | ALA                  | B      |
| 144            | 312           | PHE                  | B      |
| 145            | 313           | ASN                  | B      |
| 146            | 314           | ALA                  | B      |
| 147            | 315           | VAL                  | B      |
| 148            | 316           | MET                  | B      |
| 149            | 317           | ARG                  | B      |
| 150            | 323           | VAL                  | B      |
| 151            | 324           | PHE                  | B      |
| 152            | 325           | PHE                  | B      |
| 153            | 326           | LYS                  | C      |
| 154            | 327           | SER                  | B      |
| 155            | 328           | GLN                  | B      |
| 156            | 329           | ALA                  | B      |
| 157            | 330           | ILE                  | B      |
| 158            | 331           | VAL                  | B      |
| 159            | 332           | HIS                  | B      |
| 160            | 336           | VAL                  | B      |
| 161            | 337           | VAL                  | B      |
| 162            | 338           | GLN                  | B      |
| 163            | 339           | TYR                  | B      |
| 164            | 340           | ILE                  | B      |
| 165            | 341           | GLY                  | B      |
| 166            | 345           | CYS                  | B      |
| 167            | 346           | GLN                  | B      |
| 168            | 347           | ILE                  | B      |

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Table S85 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 169            | 348           | GLY                  | B      |
| 170            | 349           | TYR                  | D      |
| 171            | 350           | ASN                  | D      |
| 172            | 351           | PRO                  | D      |
| 173            | 352           | LEU                  | D      |
| 174            | 354           | MET                  | D      |
| 175            | 355           | ALA                  | D      |
| 176            | 356           | LEU                  | D      |
| 177            | 357           | LEU                  | D      |
| 178            | 358           | TRP                  | D      |
| 179            | 359           | ASN                  | D      |
| 180            | 360           | THR                  | D      |
| 181            | 361           | LEU                  | D      |
| 182            | 364           | ARG                  | D      |
| 183            | 365           | GLU                  | A      |
| 184            | 366           | VAL                  | A      |
| 185            | 367           | ASN                  | A      |
| 186            | 372           | ALA                  | A      |
| 187            | 373           | LEU                  | D      |
| 188            | 374           | THR                  | D      |
| 189            | 375           | TYR                  | D      |
| 190            | 376           | ARG                  | D      |
| 191            | 377           | HIS                  | B      |
| 192            | 378           | ASN                  | B      |
| 193            | 381           | GLU                  | B      |
| 194            | 382           | HIS                  | B      |
| 195            | 383           | THR                  | B      |
| 196            | 384           | ALA                  | B      |
| 197            | 385           | TRP                  | B      |
| 198            | 386           | VAL                  | D      |
| 199            | 387           | ASN                  | D      |
| 200            | 388           | TYR                  | D      |
| 201            | 389           | VAL                  | A      |
| 202            | 390           | ARG                  | D      |
| 203            | 391           | SER                  | D      |
| 204            | 392           | HIS                  | D      |
| 205            | 393           | ASP                  | D      |
| 206            | 394           | ASP                  | D      |
| 207            | 448           | SER                  | D      |
| 208            | 450           | THR                  | D      |
| 209            | 451           | ALA                  | D      |
| 210            | 452           | ALA                  | D      |
| 211            | 453           | ALA                  | D      |
| 212            | 464           | ALA                  | A      |
| 213            | 467           | ARG                  | A      |
| 214            | 468           | ILE                  | A      |

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Table S85 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 215            | 469           | LYS                  | A      |
| 216            | 470           | LEU                  | A      |
| 217            | 471           | LEU                  | A      |
| 218            | 472           | TYR                  | A      |
| 219            | 473           | SER                  | A      |
| 220            | 474           | ILE                  | A      |
| 221            | 475           | ALA                  | A      |
| 222            | 476           | LEU                  | A      |
| 223            | 477           | SER                  | A      |
| 224            | 478           | THR                  | A      |
| 225            | 479           | GLY                  | D      |
| 226            | 480           | GLY                  | D      |
| 227            | 481           | LEU                  | D      |
| 228            | 482           | PRO                  | A      |
| 229            | 483           | LEU                  | D      |
| 230            | 484           | ILE                  | A      |
| 231            | 485           | TYR                  | D      |
| 232            | 486           | LEU                  | C      |
| 233            | 487           | GLY                  | D      |
| 234            | 488           | ASP                  | A      |
| 235            | 514           | PRO                  | C      |
| 236            | 515           | ARG                  | C      |
| 237            | 516           | TYR                  | D      |
| 238            | 517           | ASN                  | D      |
| 239            | 521           | TYR                  | D      |
| 240            | 534           | ILE                  | A      |
| 241            | 535           | TYR                  | A      |
| 242            | 536           | GLN                  | A      |
| 243            | 537           | ASP                  | A      |
| 244            | 538           | LEU                  | A      |
| 245            | 539           | ARG                  | A      |
| 246            | 540           | HIS                  | A      |
| 247            | 541           | MET                  | A      |
| 248            | 542           | ILE                  | A      |
| 249            | 543           | ALA                  | A      |
| 250            | 544           | VAL                  | A      |
| 251            | 545           | ARG                  | A      |
| 252            | 546           | GLN                  | A      |
| 253            | 547           | SER                  | A      |
| 254            | 548           | ASN                  | A      |
| 255            | 549           | PRO                  | A      |
| 256            | 553           | GLY                  | A      |
| 257            | 554           | GLY                  | A      |
| 258            | 555           | ARG                  | A      |
| 259            | 556           | LEU                  | A      |
| 260            | 558           | THR                  | A      |

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Table S85 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 261            | 559           | PHE                  | A      |
| 262            | 560           | ASN                  | A      |
| 263            | 561           | THR                  | A      |
| 264            | 563           | ASN                  | A      |
| 265            | 564           | LYS                  | A      |
| 266            | 565           | HIS                  | A      |
| 267            | 566           | ILE                  | A      |
| 268            | 567           | ILE                  | A      |
| 269            | 568           | GLY                  | A      |
| 270            | 569           | TYR                  | A      |
| 271            | 570           | ILE                  | A      |
| 272            | 571           | ARG                  | A      |
| 273            | 573           | ASN                  | A      |
| 274            | 574           | ALA                  | A      |
| 275            | 575           | LEU                  | A      |
| 276            | 576           | LEU                  | A      |
| 277            | 577           | ALA                  | A      |
| 278            | 578           | PHE                  | A      |
| 279            | 579           | GLY                  | A      |
| 280            | 580           | ASN                  | A      |
| 281            | 584           | TYR                  | A      |
| 282            | 585           | PRO                  | A      |
| 283            | 586           | GLN                  | A      |
| 284            | 587           | THR                  | A      |
| 285            | 588           | VAL                  | A      |
| 286            | 589           | THR                  | A      |
| 287            | 590           | ALA                  | A      |
| 288            | 599           | LYS                  | A      |
| 289            | 600           | ALA                  | A      |
| 290            | 601           | HIS                  | A      |
| 291            | 602           | ASP                  | A      |
| 292            | 603           | LEU                  | A      |
| 293            | 604           | ILE                  | A      |
| 294            | 617           | LEU                  | A      |
| 295            | 618           | GLN                  | A      |
| 296            | 619           | PRO                  | A      |
| 297            | 621           | GLN                  | A      |
| 298            | 622           | VAL                  | A      |
| 299            | 623           | MET                  | A      |
| 300            | 624           | TRP                  | A      |
| 301            | 625           | LEU                  | A      |
| 302            | 626           | GLU                  | A      |

Table S86: Residues membership for the *H. sapiens* NPC1 (PDB code 3GKH, chain A)protein

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 0              | 23            | GLN                  | A      |
| 1              | 24            | SER                  | A      |
| 2              | 25            | CYS                  | A      |
| 3              | 26            | VAL                  | A      |
| 4              | 27            | TRP                  | A      |
| 5              | 28            | TYR                  | A      |
| 6              | 29            | GLY                  | A      |
| 7              | 30            | GLU                  | A      |
| 8              | 31            | CYS                  | A      |
| 9              | 32            | GLY                  | B      |
| 10             | 33            | ILE                  | B      |
| 11             | 34            | ALA                  | B      |
| 12             | 35            | TYR                  | B      |
| 13             | 36            | GLY                  | B      |
| 14             | 37            | ASP                  | B      |
| 15             | 38            | LYS                  | B      |
| 16             | 39            | ARG                  | B      |
| 17             | 40            | TYR                  | B      |
| 18             | 41            | ASN                  | A      |
| 19             | 42            | CYS                  | A      |
| 20             | 43            | GLU                  | B      |
| 21             | 44            | TYR                  | A      |
| 22             | 45            | SER                  | A      |
| 23             | 46            | GLY                  | A      |
| 24             | 47            | PRO                  | A      |
| 25             | 48            | PRO                  | A      |
| 26             | 49            | LYS                  | A      |
| 27             | 50            | PRO                  | A      |
| 28             | 51            | LEU                  | A      |
| 29             | 52            | PRO                  | A      |
| 30             | 53            | LYS                  | A      |
| 31             | 54            | ASP                  | A      |
| 32             | 55            | GLY                  | A      |
| 33             | 56            | TYR                  | A      |
| 34             | 57            | ASP                  | A      |
| 35             | 58            | LEU                  | A      |
| 36             | 59            | VAL                  | A      |
| 37             | 60            | GLN                  | A      |
| 38             | 61            | GLU                  | A      |
| 39             | 62            | LEU                  | A      |
| 40             | 63            | CYS                  | A      |
| 41             | 64            | PRO                  | A      |
| 42             | 65            | GLY                  | A      |
| 43             | 66            | PHE                  | A      |

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Table S86 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 44             | 67            | PHE                  | A      |
| 45             | 68            | PHE                  | A      |
| 46             | 69            | GLY                  | A      |
| 47             | 70            | GLN                  | A      |
| 48             | 71            | VAL                  | A      |
| 49             | 72            | SER                  | A      |
| 50             | 73            | LEU                  | A      |
| 51             | 74            | CYS                  | A      |
| 52             | 75            | CYS                  | A      |
| 53             | 76            | ASP                  | A      |
| 54             | 77            | VAL                  | A      |
| 55             | 78            | ARG                  | A      |
| 56             | 79            | GLN                  | A      |
| 57             | 80            | LEU                  | A      |
| 58             | 81            | GLN                  | A      |
| 59             | 82            | THR                  | A      |
| 60             | 83            | LEU                  | A      |
| 61             | 84            | LYS                  | A      |
| 62             | 85            | ASP                  | A      |
| 63             | 86            | ASN                  | B      |
| 64             | 87            | LEU                  | B      |
| 65             | 88            | GLN                  | B      |
| 66             | 89            | LEU                  | B      |
| 67             | 90            | PRO                  | B      |
| 68             | 91            | LEU                  | B      |
| 69             | 92            | GLN                  | B      |
| 70             | 93            | PHE                  | E      |
| 71             | 94            | LEU                  | E      |
| 72             | 95            | SER                  | E      |
| 73             | 96            | ARG                  | E      |
| 74             | 97            | CYS                  | E      |
| 75             | 98            | PRO                  | E      |
| 76             | 99            | SER                  | E      |
| 77             | 100           | CYS                  | E      |
| 78             | 101           | PHE                  | E      |
| 79             | 102           | TYR                  | E      |
| 80             | 103           | ASN                  | E      |
| 81             | 104           | LEU                  | E      |
| 82             | 105           | LEU                  | E      |
| 83             | 106           | ASN                  | E      |
| 84             | 107           | LEU                  | F      |
| 85             | 108           | PHE                  | F      |
| 86             | 109           | CYS                  | A      |
| 87             | 110           | GLU                  | F      |
| 88             | 111           | LEU                  | F      |
| 89             | 112           | THR                  | A      |

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Table S86 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 90             | 113           | CYS                  | A      |
| 91             | 114           | SER                  | A      |
| 92             | 115           | PRO                  | A      |
| 93             | 116           | ARG                  | A      |
| 94             | 117           | GLN                  | A      |
| 95             | 118           | SER                  | A      |
| 96             | 119           | GLN                  | A      |
| 97             | 120           | PHE                  | F      |
| 98             | 121           | LEU                  | F      |
| 99             | 122           | GLN                  | F      |
| 100            | 123           | VAL                  | F      |
| 101            | 124           | THR                  | F      |
| 102            | 125           | ALA                  | B      |
| 103            | 126           | THR                  | B      |
| 104            | 127           | GLU                  | B      |
| 105            | 128           | ASP                  | B      |
| 106            | 129           | TYR                  | B      |
| 107            | 130           | VAL                  | B      |
| 108            | 131           | ASP                  | B      |
| 109            | 132           | PRO                  | B      |
| 110            | 133           | VAL                  | B      |
| 111            | 134           | THR                  | B      |
| 112            | 135           | ASN                  | B      |
| 113            | 136           | GLN                  | B      |
| 114            | 137           | THR                  | B      |
| 115            | 138           | LYS                  | A      |
| 116            | 139           | THR                  | B      |
| 117            | 140           | ASN                  | B      |
| 118            | 141           | VAL                  | B      |
| 119            | 142           | LYS                  | B      |
| 120            | 143           | GLU                  | F      |
| 121            | 144           | LEU                  | F      |
| 122            | 145           | GLN                  | F      |
| 123            | 146           | TYR                  | F      |
| 124            | 147           | TYR                  | F      |
| 125            | 148           | VAL                  | F      |
| 126            | 149           | GLY                  | F      |
| 127            | 150           | GLN                  | F      |
| 128            | 151           | SER                  | F      |
| 129            | 152           | PHE                  | F      |
| 130            | 153           | ALA                  | F      |
| 131            | 154           | ASN                  | F      |
| 132            | 155           | ALA                  | E      |
| 133            | 156           | MET                  | E      |
| 134            | 157           | TYR                  | E      |
| 135            | 158           | ASN                  | E      |

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Table S86 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 136            | 159           | ALA                  | E      |
| 137            | 160           | CYS                  | E      |
| 138            | 161           | ARG                  | E      |
| 139            | 162           | ASP                  | E      |
| 140            | 163           | VAL                  | E      |
| 141            | 164           | GLU                  | E      |
| 142            | 165           | ALA                  | E      |
| 143            | 166           | PRO                  | E      |
| 144            | 167           | SER                  | E      |
| 145            | 168           | SER                  | E      |
| 146            | 169           | ASN                  | E      |
| 147            | 170           | ASP                  | E      |
| 148            | 171           | LYS                  | E      |
| 149            | 172           | ALA                  | E      |
| 150            | 173           | LEU                  | E      |
| 151            | 174           | GLY                  | E      |
| 152            | 175           | LEU                  | E      |
| 153            | 176           | LEU                  | E      |
| 154            | 177           | CYS                  | E      |
| 155            | 178           | GLY                  | E      |
| 156            | 179           | LYS                  | E      |
| 157            | 180           | ASP                  | E      |
| 158            | 181           | ALA                  | E      |
| 159            | 182           | ASP                  | E      |
| 160            | 183           | ALA                  | E      |
| 161            | 184           | CYS                  | E      |
| 162            | 185           | GLN                  | E      |
| 163            | 186           | ALA                  | E      |
| 164            | 187           | THR                  | E      |
| 165            | 188           | ASN                  | E      |
| 166            | 189           | TRP                  | D      |
| 167            | 190           | ILE                  | F      |
| 168            | 191           | GLU                  | E      |
| 169            | 192           | TYR                  | E      |
| 170            | 193           | MET                  | D      |
| 171            | 194           | PHE                  | F      |
| 172            | 195           | ASN                  | E      |
| 173            | 196           | LYS                  | B      |
| 174            | 197           | ASP                  | C      |
| 175            | 198           | ASN                  | C      |
| 176            | 199           | GLY                  | C      |
| 177            | 200           | GLN                  | C      |
| 178            | 201           | ALA                  | C      |
| 179            | 202           | PRO                  | C      |
| 180            | 203           | PHE                  | F      |
| 181            | 204           | THR                  | F      |

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Table S86 – *Continued from previous page*

| Homology index | Residue Index | Residue abbreviation | Module |
|----------------|---------------|----------------------|--------|
| 182            | 205           | ILE                  | F      |
| 183            | 206           | THR                  | F      |
| 184            | 207           | PRO                  | F      |
| 185            | 208           | VAL                  | F      |
| 186            | 209           | PHE                  | F      |
| 187            | 210           | SER                  | F      |
| 188            | 211           | ASP                  | F      |
| 189            | 212           | PHE                  | F      |
| 190            | 213           | PRO                  | F      |
| 191            | 214           | VAL                  | F      |
| 192            | 215           | HIS                  | F      |
| 193            | 216           | GLY                  | F      |
| 194            | 217           | MET                  | F      |
| 195            | 218           | GLU                  | F      |
| 196            | 219           | PRO                  | F      |
| 197            | 220           | MET                  | F      |
| 198            | 221           | ASN                  | F      |
| 199            | 222           | ASN                  | F      |
| 200            | 223           | ALA                  | F      |
| 201            | 224           | THR                  | D      |
| 202            | 225           | LYS                  | D      |
| 203            | 226           | GLY                  | D      |
| 204            | 227           | CYS                  | D      |
| 205            | 228           | ASP                  | D      |
| 206            | 229           | GLU                  | D      |
| 207            | 230           | SER                  | D      |
| 208            | 231           | VAL                  | D      |
| 209            | 232           | ASP                  | D      |
| 210            | 233           | GLU                  | D      |
| 211            | 234           | VAL                  | D      |
| 212            | 235           | THR                  | D      |
| 213            | 236           | ALA                  | D      |
| 214            | 237           | PRO                  | D      |
| 215            | 238           | CYS                  | D      |
| 216            | 239           | SER                  | D      |
| 217            | 240           | CYS                  | D      |
| 218            | 241           | GLN                  | D      |
| 219            | 242           | ASP                  | D      |
| 220            | 243           | CYS                  | D      |
| 221            | 244           | SER                  | D      |
| 222            | 245           | ILE                  | D      |
| 223            | 246           | VAL                  | D      |