



Full wwPDB EM Validation Report ⓘ

Nov 26, 2025 – 03:36 PM JST

PDB ID : 9XSB / pdb_00009xsb
EMDB ID : EMD-67169
Title : CCHFV-FL-RNA-bound state
Deposited on : 2025-11-20
Resolution : 3.76 Å(reported)
Based on initial model : .

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

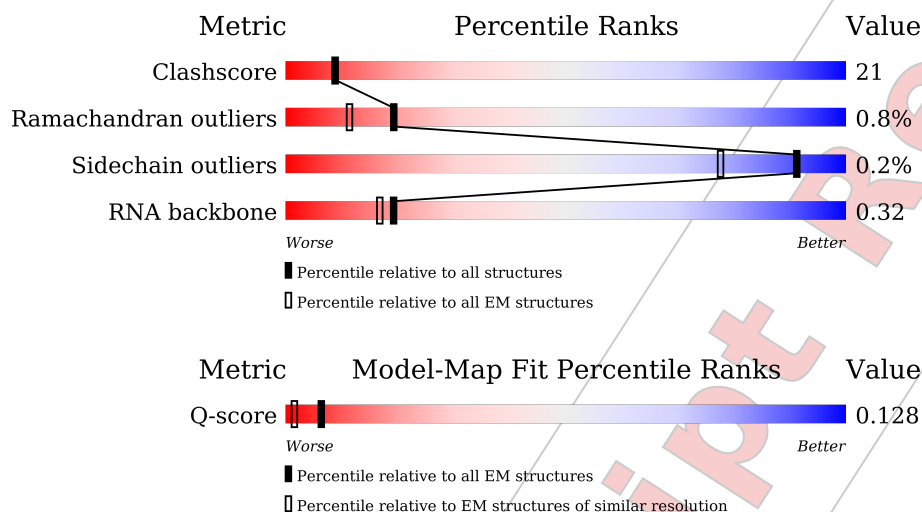
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	10214 (3.26 - 4.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3982	14% 32% 21% 47%
2	C	18	17% 11% 28% 17% 44%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17243 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2128	17029	10795	2918	3205	111	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP A0A1S6XXC8
A	-7	HIS	-	expression tag	UNP A0A1S6XXC8
A	-6	HIS	-	expression tag	UNP A0A1S6XXC8
A	-5	HIS	-	expression tag	UNP A0A1S6XXC8
A	-4	HIS	-	expression tag	UNP A0A1S6XXC8
A	-3	HIS	-	expression tag	UNP A0A1S6XXC8
A	-2	HIS	-	expression tag	UNP A0A1S6XXC8
A	-1	GLY	-	expression tag	UNP A0A1S6XXC8
A	0	THR	-	expression tag	UNP A0A1S6XXC8
A	3946	TRP	-	expression tag	UNP A0A1S6XXC8
A	3947	SER	-	expression tag	UNP A0A1S6XXC8
A	3948	HIS	-	expression tag	UNP A0A1S6XXC8
A	3949	PRO	-	expression tag	UNP A0A1S6XXC8
A	3950	GLN	-	expression tag	UNP A0A1S6XXC8
A	3951	PHE	-	expression tag	UNP A0A1S6XXC8
A	3952	GLU	-	expression tag	UNP A0A1S6XXC8
A	3953	LYS	-	expression tag	UNP A0A1S6XXC8
A	3954	GLY	-	expression tag	UNP A0A1S6XXC8
A	3955	GLY	-	expression tag	UNP A0A1S6XXC8
A	3956	GLY	-	expression tag	UNP A0A1S6XXC8
A	3957	SER	-	expression tag	UNP A0A1S6XXC8
A	3958	GLY	-	expression tag	UNP A0A1S6XXC8
A	3959	GLY	-	expression tag	UNP A0A1S6XXC8
A	3960	GLY	-	expression tag	UNP A0A1S6XXC8
A	3961	SER	-	expression tag	UNP A0A1S6XXC8
A	3962	GLY	-	expression tag	UNP A0A1S6XXC8
A	3963	GLY	-	expression tag	UNP A0A1S6XXC8
A	3964	SER	-	expression tag	UNP A0A1S6XXC8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3965	ALA	-	expression tag	UNP A0A1S6XXC8
A	3966	TRP	-	expression tag	UNP A0A1S6XXC8
A	3967	SER	-	expression tag	UNP A0A1S6XXC8
A	3968	HIS	-	expression tag	UNP A0A1S6XXC8
A	3969	PRO	-	expression tag	UNP A0A1S6XXC8
A	3970	GLN	-	expression tag	UNP A0A1S6XXC8
A	3971	PHE	-	expression tag	UNP A0A1S6XXC8
A	3972	GLU	-	expression tag	UNP A0A1S6XXC8
A	3973	LYS	-	expression tag	UNP A0A1S6XXC8

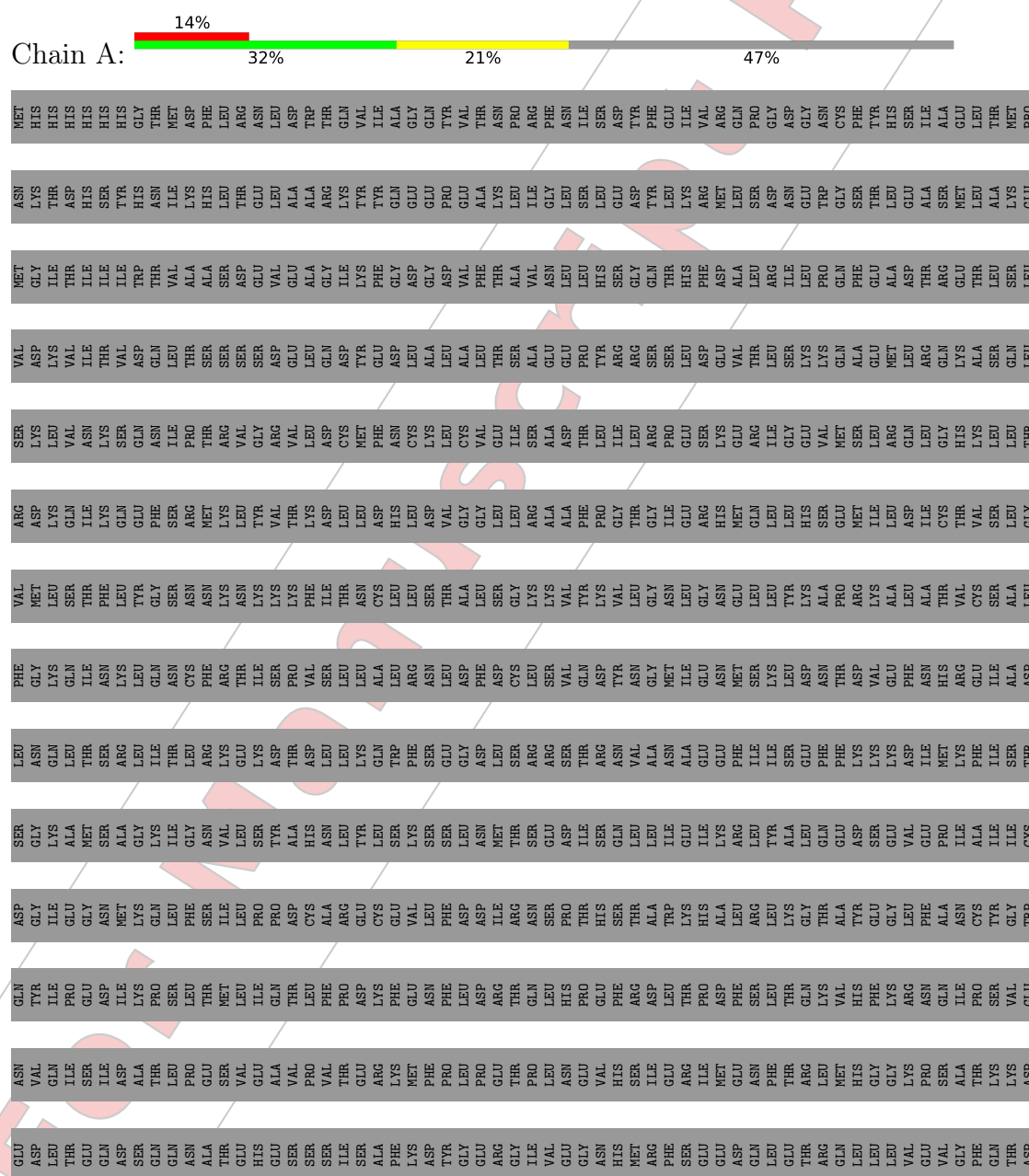
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*CP*UP*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*GP*UP*UP*CP*C)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	10	Total	C	N	O	P	
			214	96	40	68	10	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA-directed RNA polymerase L









ASP
GLU
LEU
MET
SER
LEU
LEU
MET
PRO
GLU
LEU
LEU
LYS
SER
SER
LEU
ALA
VAL
LYS
ASN
CYS
LYS
MET
GLY
SER
LEU
GLU
GLN
GLY
GLU
CYS
PHE
GLU
PHE
THR
ILE
LEU
LYS
ASP
ASN
SER
THR
MET
ARG
LEU
ASP
TYR
ASN
LYS
LEU
ILE
ASP
HIS
ASP
CYS
VAL
ASP
MET
GLU
LYS
ARG
THR
ASP
ALA
VAL
ARG
GLY
ALA
VAL

GLU
ASP
LEU
ILE
SER
ASP
ASP
TRP
SER
HIS
PRO
PHE
GLN
GLU
LYS
VAL
LYS
PRO
SER
CYS
ASN
GLY
VAL
THR
GLN
ILE
ALA
ARG
GLY
GLU
ASP
GLU
CYS
PHE
GLN
CYS
GLU
PHE
THR
GLN
ILE
PHE
GLU
LYS

ASN
TRP
ASP
SER
ASP
TRP
SER
HIS
PRO
PHE
GLN
GLU
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GLY
SER
GLY
GLY
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

- Molecule 2: RNA (5'-R(P*UP*CP*UP*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*GP*UP*U
P*CP*C)-3')



U1
C2
U3
C4
A5
A6
A7
G8
A9
A10
A
U
C
G
U
U
U
C
C

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.180	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/17317	0.47	8/23345 (0.0%)
2	C	0.16	0/239	0.39	0/368
All	All	0.17	0/17556	0.47	8/23713 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1668	PRO	CA-N-CD	-12.50	94.50	112.00
1	A	2751	PRO	CA-N-CD	-10.09	97.87	112.00
1	A	1592	PRO	N-CD-CG	-6.96	92.76	103.20
1	A	1592	PRO	CA-N-CD	-6.82	102.45	112.00
1	A	1668	PRO	N-CD-CG	-6.36	93.66	103.20
1	A	1838	ILE	N-CA-C	-5.84	106.62	112.17
1	A	1118	THR	CB-CA-C	-5.55	108.56	115.89
1	A	3118	ILE	N-CA-C	-5.07	107.61	111.62

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1196	SER	Peptide,Mainchain
1	A	1198	TYR	Peptide
1	A	2473	GLN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17029	0	17299	707	0
2	C	214	0	109	16	0
All	All	17243	0	17408	712	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (712) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:SER:O	1:A:1198:TYR:N	1.73	1.20
1:A:1765:ASP:O	1:A:1768:GLN:HB3	1.71	0.90
1:A:1536:LEU:HB2	1:A:2569:VAL:HB	1.56	0.86
1:A:2282:LEU:HA	1:A:2473:GLN:HA	1.57	0.83
1:A:2549:LYS:NZ	1:A:2563:ASP:OD2	2.11	0.83
1:A:1403:ARG:HA	1:A:1618:ASN:HD22	1.41	0.82
1:A:2654:ILE:O	1:A:2825:GLN:NE2	2.11	0.82
1:A:3061:SER:O	1:A:3065:ARG:HB3	1.80	0.82
1:A:1239:GLU:HA	1:A:1243:ILE:HD11	1.61	0.81
1:A:944:HIS:O	1:A:947:ASN:ND2	2.13	0.81
1:A:3088:VAL:HG22	1:A:3089:LYS:HG2	1.64	0.80
1:A:2414:VAL:HB	2:C:8:G:N3	1.97	0.80
1:A:1056:LEU:HD13	1:A:1264:ILE:HG21	1.65	0.79
1:A:1001:LYS:HE2	1:A:1003:GLU:HG3	1.66	0.78
1:A:1426:TYR:HD2	1:A:1495:ILE:HG13	1.48	0.77
1:A:3055:ASN:HA	1:A:3058:LEU:HD23	1.66	0.76
1:A:1582:GLN:OE1	1:A:1582:GLN:N	2.17	0.76
1:A:2636:LEU:O	1:A:2640:ILE:HD12	1.85	0.76
1:A:2419:LEU:O	1:A:2422:LYS:NZ	2.19	0.76
1:A:3061:SER:O	1:A:3065:ARG:CB	2.34	0.76
1:A:3080:LEU:H	1:A:3216:GLY:HA2	1.52	0.75
1:A:2329:LEU:HD12	1:A:2583:GLY:HA2	1.67	0.74
1:A:1190:THR:HA	1:A:1193:LYS:HB2	1.70	0.73
1:A:2282:LEU:HB2	1:A:2473:GLN:HG2	1.70	0.73
1:A:2374:MET:HG2	1:A:2483:LEU:HD21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ARG:NH1	1:A:1031:CYS:SG	2.61	0.73
1:A:2675:VAL:HG11	1:A:3064:ASN:HB3	1.71	0.72
1:A:2285:GLN:HB3	1:A:2289:THR:HG23	1.71	0.72
1:A:2511:GLU:N	1:A:2511:GLU:OE2	2.23	0.72
1:A:2750:ARG:NH1	1:A:2751:PRO:O	2.22	0.72
1:A:1121:GLU:OE1	1:A:1122:ARG:NH2	2.23	0.72
1:A:1605:ARG:NH1	1:A:2587:THR:OG1	2.20	0.72
1:A:2907:LEU:HD22	1:A:2910:LEU:HD11	1.72	0.72
1:A:3089:LYS:HB3	1:A:3199:LYS:HE2	1.72	0.72
1:A:2410:LYS:HD2	2:C:7:A:H1'	1.72	0.71
1:A:2409:LYS:O	1:A:2413:ASN:ND2	2.24	0.71
1:A:2616:SER:HB3	1:A:2637:ARG:HH12	1.55	0.71
1:A:1241:VAL:HG13	1:A:1242:LEU:HD23	1.74	0.70
1:A:1809:ASN:OD1	1:A:2302:ASN:ND2	2.24	0.70
1:A:947:ASN:OD1	1:A:2466:ASN:ND2	2.26	0.69
1:A:2317:LEU:HA	1:A:2320:THR:HG22	1.74	0.69
1:A:1197:THR:C	1:A:1200:LYS:HB3	2.18	0.69
1:A:1316:ILE:HD11	1:A:2628:ILE:HA	1.74	0.69
1:A:2593:PHE:HE2	1:A:2623:ASN:HD22	1.40	0.68
1:A:2273:LYS:HA	1:A:2282:LEU:HD23	1.74	0.68
1:A:2748:LEU:HD22	1:A:3058:LEU:HD22	1.76	0.68
1:A:1197:THR:HA	1:A:1200:LYS:HB3	1.74	0.68
1:A:2813:LYS:HG3	1:A:2820:LEU:HD22	1.76	0.68
1:A:1081:ARG:HH21	1:A:1400:LEU:HB2	1.59	0.68
1:A:2952:PHE:O	1:A:2993:LYS:NZ	2.25	0.68
1:A:2410:LYS:HA	2:C:8:G:O2'	1.94	0.68
1:A:1354:ASN:O	1:A:1378:LYS:NZ	2.27	0.67
1:A:2671:TYR:HB3	1:A:3068:LEU:HD13	1.74	0.67
1:A:1124:VAL:O	1:A:1128:VAL:HG13	1.93	0.67
1:A:1300:VAL:HG13	1:A:2666:LEU:HD21	1.76	0.67
1:A:1810:TRP:HE1	1:A:3124:THR:HG21	1.59	0.67
1:A:2404:PRO:O	1:A:2406:GLY:N	2.27	0.67
1:A:1551:ARG:NH2	2:C:5:A:N7	2.42	0.67
1:A:1337:VAL:HA	1:A:1412:LEU:HD22	1.76	0.67
1:A:1647:MET:SD	1:A:1648:ASN:ND2	2.67	0.67
1:A:1196:SER:C	1:A:1198:TYR:N	2.53	0.67
1:A:3019:LEU:HA	1:A:3024:ILE:HD11	1.77	0.67
1:A:1264:ILE:HD12	1:A:1559:ARG:HH21	1.58	0.67
1:A:2697:ASN:OD1	1:A:2808:TRP:NE1	2.28	0.66
1:A:1018:TRP:NE1	1:A:1563:GLN:HE21	1.93	0.66
1:A:2291:VAL:O	1:A:2295:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3125:LYS:HD3	1:A:3126:VAL:H	1.60	0.66
1:A:3064:ASN:O	1:A:3068:LEU:HG	1.95	0.66
1:A:1128:VAL:O	1:A:1132:ILE:HG12	1.96	0.65
1:A:2305:LYS:HD3	1:A:2306:THR:HG23	1.77	0.65
1:A:1777:THR:OG1	1:A:2365:ILE:O	2.12	0.65
1:A:3086:VAL:HA	1:A:3198:LEU:HD21	1.78	0.65
1:A:2660:LEU:HD11	1:A:2687:ILE:HD11	1.79	0.65
1:A:2503:LEU:HD11	1:A:2536:GLN:HE22	1.62	0.65
1:A:2804:ASP:HB2	1:A:2810:ARG:HH21	1.62	0.65
1:A:3169:GLN:O	1:A:3171:VAL:N	2.30	0.65
1:A:1473:ARG:HH12	1:A:1561:TYR:HE1	1.45	0.64
1:A:1108:ARG:HG2	1:A:1111:ARG:HH22	1.62	0.64
1:A:1257:ARG:NH1	1:A:1258:ASN:O	2.31	0.64
1:A:1344:GLU:OE1	1:A:2643:ASN:ND2	2.29	0.64
1:A:2283:LEU:HD12	1:A:2472:GLY:HA2	1.79	0.64
1:A:1381:ASN:OD1	1:A:1399:PHE:HB3	1.97	0.63
1:A:1468:GLU:HA	1:A:1471:LYS:HE2	1.80	0.63
1:A:1649:SER:HB3	1:A:1661:ALA:HB3	1.79	0.63
1:A:1643:GLU:OE2	1:A:1643:GLU:N	2.31	0.63
1:A:2592:LYS:HB3	1:A:2593:PHE:CD1	2.34	0.63
1:A:2687:ILE:HD13	1:A:2833:ALA:HB2	1.80	0.63
1:A:2837:ARG:HE	1:A:3019:LEU:HB3	1.63	0.63
1:A:1197:THR:CA	1:A:1200:LYS:HB3	2.29	0.63
1:A:1381:ASN:OD1	1:A:1382:MET:N	2.30	0.63
1:A:1775:SER:O	1:A:2562:LYS:NZ	2.31	0.63
1:A:2410:LYS:HB3	2:C:8:G:C8	2.34	0.63
1:A:1627:GLY:O	1:A:1630:SER:HB2	1.98	0.63
1:A:1332:TRP:O	1:A:1336:VAL:HG23	1.98	0.62
1:A:2512:HIS:HE1	1:A:2519:TYR:HB2	1.63	0.62
1:A:1130:TYR:O	1:A:1134:LEU:HD22	1.99	0.62
1:A:2828:LEU:O	1:A:2832:ILE:HD12	1.99	0.62
1:A:2250:ILE:HB	1:A:2253:GLN:HB2	1.80	0.62
1:A:2325:GLY:O	1:A:2329:LEU:HG	1.99	0.62
1:A:2488:ALA:HB2	1:A:2512:HIS:HD2	1.63	0.62
1:A:2901:GLN:HA	1:A:2905:LYS:HE3	1.81	0.62
1:A:1383:LEU:HD12	1:A:1399:PHE:HE1	1.65	0.62
1:A:1200:LYS:HA	1:A:1203:ILE:HG22	1.82	0.62
1:A:3066:GLN:O	1:A:3070:ILE:HG12	1.99	0.62
1:A:3074:ARG:HH21	1:A:3227:ASP:HB2	1.64	0.62
1:A:2889:LEU:HD21	1:A:2922:SER:HB2	1.81	0.62
1:A:1794:LYS:NZ	1:A:2309:ASP:OD1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1136:MET:SD	1:A:1141:ILE:HB	2.40	0.61
1:A:1325:ASN:HB3	1:A:1329:ARG:HH21	1.64	0.61
1:A:2390:LYS:HG3	1:A:2392:THR:H	1.65	0.61
1:A:1005:THR:HG22	1:A:1573:VAL:HG11	1.81	0.61
1:A:1429:LEU:HD21	1:A:2628:ILE:HD13	1.83	0.61
1:A:1789:GLU:CD	1:A:1790:PHE:H	2.08	0.61
1:A:1649:SER:O	1:A:1656:LYS:NZ	2.32	0.61
1:A:3193:THR:HG22	1:A:3194:VAL:HG23	1.82	0.61
1:A:1580:TRP:CD1	1:A:2572:CYS:HG	2.19	0.61
1:A:1007:ASN:O	1:A:1009:ILE:N	2.24	0.61
1:A:1236:THR:HA	1:A:1246:ARG:HH22	1.65	0.61
1:A:2631:THR:HA	1:A:2669:PRO:HG2	1.82	0.61
1:A:3169:GLN:HG3	1:A:3170:GLN:H	1.66	0.61
1:A:1123:ARG:HA	1:A:1126:ARG:HH21	1.66	0.61
1:A:2911:ASN:HA	1:A:3183:ARG:HH22	1.65	0.61
1:A:1288:VAL:HB	1:A:1334:GLN:HE22	1.66	0.60
1:A:2907:LEU:HD11	1:A:3174:TYR:HB3	1.83	0.60
1:A:1341:LYS:HZ2	1:A:1364:ARG:HH21	1.49	0.60
1:A:1580:TRP:HE3	1:A:1589:VAL:HG11	1.66	0.60
1:A:1260:ASP:HA	1:A:1263:LEU:HD21	1.84	0.60
1:A:1790:PHE:HB3	1:A:2489:VAL:HG11	1.83	0.60
1:A:2857:ASN:ND2	1:A:3183:ARG:O	2.23	0.60
1:A:1808:LYS:O	1:A:1808:LYS:NZ	2.33	0.60
1:A:3214:SER:HA	1:A:3219:GLU:HG3	1.84	0.60
1:A:1542:LEU:O	1:A:1546:PHE:HB2	2.01	0.60
1:A:2376:GLN:HA	1:A:2379:LEU:HD12	1.84	0.60
1:A:1021:GLU:HB2	1:A:1544:LYS:HD3	1.83	0.60
1:A:1322:SER:O	1:A:1326:VAL:HG23	2.02	0.60
1:A:3151:MET:HE1	1:A:3155:GLU:HG3	1.84	0.60
1:A:2322:LEU:HD21	1:A:2574:LEU:HD22	1.83	0.60
1:A:3161:LYS:NZ	1:A:3162:ASN:OD1	2.35	0.59
1:A:1307:ARG:HD2	1:A:2668:VAL:HB	1.83	0.59
1:A:1615:HIS:ND1	1:A:2592:LYS:HA	2.17	0.59
1:A:2744:PHE:HE2	1:A:3148:LEU:HA	1.67	0.59
1:A:1292:VAL:HG22	1:A:1324:ILE:HG22	1.85	0.59
1:A:3114:ASP:OD2	1:A:3114:ASP:N	2.33	0.59
1:A:1955:MET:HE3	1:A:1956:PRO:HD2	1.84	0.59
1:A:3184:MET:HE3	1:A:3184:MET:HA	1.85	0.59
1:A:972:ILE:HG22	1:A:973:SER:H	1.67	0.59
1:A:1352:GLU:O	1:A:1378:LYS:NZ	2.28	0.58
1:A:2751:PRO:O	1:A:2751:PRO:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2839:PHE:HB3	1:A:3180:LEU:HD13	1.84	0.58
1:A:2406:GLY:HA2	1:A:2409:LYS:HE2	1.85	0.58
1:A:3029:LEU:HD11	1:A:3037:ARG:HB2	1.85	0.58
1:A:1403:ARG:NH1	1:A:1620:GLU:O	2.36	0.58
1:A:2476:HIS:O	1:A:2480:SER:N	2.36	0.58
1:A:1204:SER:O	1:A:1208:LYS:HG2	2.03	0.58
1:A:1646:LEU:HD13	1:A:1664:LEU:HD22	1.84	0.58
1:A:2332:MET:HE3	1:A:2352:VAL:HG12	1.84	0.58
1:A:2611:GLN:O	1:A:2615:VAL:HG13	2.04	0.58
1:A:1312:PRO:HG3	1:A:3074:ARG:HB2	1.85	0.58
1:A:2571:ASP:OD1	1:A:2571:ASP:N	2.34	0.58
1:A:1940:LEU:HD13	1:A:2082:PRO:HB3	1.86	0.58
1:A:1577:ILE:O	1:A:1581:LYS:HG2	2.03	0.58
1:A:985:LYS:NZ	1:A:2493:GLU:OE2	2.33	0.58
1:A:1636:ALA:O	1:A:1639:HIS:N	2.34	0.58
1:A:2411:ILE:O	1:A:2415:LEU:HB2	2.04	0.58
1:A:3042:ILE:HG22	1:A:3045:HIS:H	1.68	0.58
1:A:967:VAL:HG13	1:A:968:GLU:HG3	1.86	0.57
1:A:3173:ARG:HA	1:A:3176:ASN:ND2	2.20	0.57
1:A:1022:ASP:OD1	1:A:1547:SER:OG	2.23	0.57
1:A:1194:ASP:C	1:A:1199:ALA:HB3	2.30	0.57
1:A:1248:SER:HA	1:A:1250:LYS:HZ2	1.68	0.57
1:A:3066:GLN:HG3	1:A:3067:LYS:HD3	1.86	0.57
1:A:1184:ARG:HA	1:A:1187:LEU:HD12	1.86	0.57
1:A:1642:TRP:NE1	1:A:1777:THR:HB	2.20	0.57
1:A:2434:ARG:O	1:A:2438:VAL:HG23	2.05	0.57
1:A:1788:SER:OG	1:A:2377:GLN:HG2	2.04	0.57
1:A:2120:LYS:HA	1:A:2123:VAL:HB	1.86	0.57
1:A:1323:LEU:HG	1:A:1432:ILE:HG21	1.86	0.56
1:A:1308:TYR:O	1:A:1311:THR:OG1	2.21	0.56
1:A:2355:ILE:HG22	1:A:2569:VAL:HG13	1.86	0.56
1:A:1413:TYR:CD1	1:A:2636:LEU:HB3	2.40	0.56
1:A:3146:PHE:CG	1:A:3147:THR:N	2.72	0.56
1:A:1798:GLU:O	1:A:1801:ASP:HB3	2.05	0.56
1:A:2993:LYS:O	1:A:2997:TRP:N	2.35	0.56
1:A:1407:LEU:HD22	1:A:1617:TYR:HA	1.87	0.56
1:A:1440:LEU:O	1:A:1443:ILE:HG22	2.06	0.56
1:A:1773:ASN:OD1	1:A:1775:SER:OG	2.22	0.56
1:A:1808:LYS:O	1:A:2252:GLN:NE2	2.38	0.56
1:A:1491:HIS:O	1:A:1495:ILE:HG12	2.06	0.56
1:A:1556:ASN:O	1:A:1560:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1777:THR:HG23	1:A:2560:GLN:HE21	1.70	0.56
1:A:1850:MET:HE3	1:A:1850:MET:O	2.06	0.56
1:A:1258:ASN:OD1	1:A:1259:ASN:N	2.39	0.55
1:A:1467:GLU:OE2	1:A:1571:ARG:NH2	2.38	0.55
1:A:1633:GLU:O	1:A:1637:GLU:N	2.35	0.55
1:A:3016:GLU:OE1	1:A:3021:ASN:ND2	2.39	0.55
1:A:2993:LYS:HB3	1:A:2996:HIS:HB3	1.88	0.55
1:A:3098:GLN:HB2	1:A:3100:ARG:HG2	1.89	0.55
1:A:2403:ILE:HD11	1:A:2465:LEU:HD23	1.87	0.55
1:A:1380:GLU:HG3	1:A:1381:ASN:H	1.71	0.55
1:A:2659:THR:OG1	1:A:2663:PHE:O	2.24	0.55
1:A:1562:LEU:O	1:A:1566:ILE:HB	2.07	0.55
1:A:1378:LYS:O	1:A:1402:ARG:NH1	2.40	0.55
1:A:1774:PRO:HG2	1:A:2557:ARG:NH1	2.22	0.55
1:A:2862:ASP:N	1:A:2862:ASP:OD2	2.40	0.55
1:A:2642:PHE:HA	1:A:2645:VAL:HG22	1.89	0.54
1:A:3145:VAL:O	1:A:3146:PHE:HB3	2.07	0.54
1:A:1325:ASN:HB3	1:A:1329:ARG:NH2	2.22	0.54
1:A:1769:ILE:HG23	1:A:1778:MET:HB3	1.89	0.54
1:A:2358:ASP:H	1:A:2567:THR:HG22	1.70	0.54
1:A:1763:LEU:O	1:A:1766:CYS:HB2	2.06	0.54
1:A:2960:ASP:OD2	1:A:2992:THR:OG1	2.19	0.54
1:A:1111:ARG:HA	1:A:1147:PRO:HG3	1.88	0.54
1:A:1466:PHE:HB3	1:A:1567:TYR:CE2	2.43	0.54
1:A:1340:GLY:HA3	1:A:1412:LEU:HD23	1.90	0.54
1:A:2255:ALA:HB1	1:A:2295:THR:HG22	1.90	0.54
1:A:1568:CYS:HB2	1:A:1592:PRO:HG3	1.90	0.54
1:A:987:ASN:O	1:A:991:ILE:HG13	2.08	0.54
1:A:3212:LEU:HB3	1:A:3218:LYS:HB3	1.89	0.54
1:A:1292:VAL:HG13	1:A:1324:ILE:HG21	1.90	0.54
1:A:1510:ASN:ND2	1:A:1518:GLN:OE1	2.41	0.54
1:A:3125:LYS:HD3	1:A:3126:VAL:HG12	1.89	0.54
1:A:1187:LEU:HB3	1:A:1191:LYS:HD2	1.90	0.53
1:A:3080:LEU:HD13	1:A:3219:GLU:HB3	1.90	0.53
1:A:1085:ILE:HG23	1:A:1289:PRO:HG3	1.89	0.53
1:A:1141:ILE:HG22	1:A:1142:ASP:H	1.74	0.53
1:A:2447:ASN:ND2	2:C:7:A:OP2	2.40	0.53
1:A:2820:LEU:O	1:A:2824:ILE:HG22	2.09	0.53
1:A:1081:ARG:NH2	1:A:1400:LEU:HB2	2.22	0.53
1:A:2655:LEU:O	1:A:2659:THR:HG23	2.08	0.53
1:A:2689:ARG:NH2	1:A:2826:SER:OG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:CYS:HA	1:A:983:MET:HG3	1.90	0.53
1:A:1311:THR:HG22	1:A:3072:GLU:HB3	1.89	0.53
1:A:1421:GLN:O	1:A:1425:GLN:HG3	2.09	0.53
1:A:1808:LYS:HE3	1:A:2298:MET:HE1	1.90	0.53
1:A:1066:HIS:HB3	1:A:1070:VAL:HG23	1.90	0.53
1:A:2506:THR:HG22	1:A:2527:GLY:HA3	1.89	0.53
1:A:1418:LEU:HD11	1:A:1503:TYR:CE1	2.44	0.53
1:A:1638:ARG:NH2	1:A:2364:PRO:O	2.42	0.53
1:A:2406:GLY:HA2	1:A:2409:LYS:HG2	1.90	0.53
1:A:1075:THR:HG21	1:A:1080:LYS:HZ1	1.74	0.53
1:A:1200:LYS:O	1:A:1203:ILE:HG22	2.09	0.53
1:A:1436:ASN:O	1:A:1439:THR:OG1	2.27	0.53
1:A:1854:LYS:HG3	1:A:1855:LEU:HG	1.91	0.53
1:A:1291:GLN:HG2	1:A:2786:SER:HA	1.90	0.53
1:A:3142:PHE:HA	1:A:3146:PHE:HE2	1.74	0.53
1:A:3179:THR:O	1:A:3183:ARG:HG2	2.09	0.53
1:A:1003:GLU:OE1	1:A:1539:PRO:HD2	2.09	0.53
1:A:1114:LEU:HD13	1:A:1125:LYS:HG2	1.90	0.53
1:A:1143:CYS:O	1:A:1220:VAL:N	2.41	0.53
1:A:1840:LEU:HD22	1:A:2416:ARG:HG3	1.91	0.53
1:A:2115:ASP:OD1	1:A:2196:ASN:ND2	2.42	0.53
1:A:2375:MET:HE3	1:A:2379:LEU:HG	1.91	0.52
1:A:2849:LYS:HA	1:A:2852:LEU:HG	1.91	0.52
1:A:1190:THR:O	1:A:1194:ASP:HB2	2.09	0.52
1:A:1195:TYR:O	1:A:1196:SER:O	2.27	0.52
1:A:1584:ASP:OD2	1:A:1584:ASP:N	2.39	0.52
1:A:2300:SER:N	1:A:2389:TYR:OH	2.43	0.52
1:A:2547:ARG:HH21	1:A:2550:ASN:HD22	1.56	0.52
1:A:3137:LYS:O	1:A:3141:PHE:N	2.42	0.52
1:A:985:LYS:O	1:A:988:LEU:HD22	2.08	0.52
1:A:2617:SER:HA	1:A:2633:PHE:HZ	1.74	0.52
1:A:2817:ASN:O	1:A:2820:LEU:HG	2.09	0.52
1:A:1195:TYR:O	1:A:1196:SER:OG	2.21	0.52
1:A:1264:ILE:HD12	1:A:1559:ARG:NH2	2.25	0.52
1:A:1078:VAL:HA	1:A:1081:ARG:HG2	1.91	0.52
1:A:3081:GLU:CD	1:A:3082:ALA:H	2.16	0.52
1:A:1332:TRP:O	1:A:1335:GLU:HG2	2.09	0.52
1:A:1792:MET:SD	1:A:1792:MET:N	2.79	0.52
1:A:3108:VAL:O	1:A:3110:GLY:N	2.42	0.52
1:A:1787:ILE:HD11	1:A:2487:ALA:HA	1.92	0.52
1:A:2329:LEU:HD22	1:A:2352:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2360:THR:HG22	1:A:2564:SER:HB2	1.91	0.52
1:A:2431:GLU:HA	1:A:2434:ARG:HG2	1.92	0.51
1:A:1370:LEU:HD11	1:A:1384:CYS:HB3	1.92	0.51
1:A:1843:GLU:OE2	1:A:2413:ASN:ND2	2.43	0.51
1:A:2336:ASP:OD1	1:A:2336:ASP:N	2.43	0.51
1:A:2683:ASP:O	1:A:2687:ILE:HG13	2.10	0.51
1:A:995:PHE:CD2	1:A:2554:ALA:HB2	2.45	0.51
1:A:1044:ASN:O	1:A:1048:LYS:HG3	2.09	0.51
1:A:938:TRP:O	1:A:942:LYS:HB3	2.11	0.51
1:A:1654:GLU:HG2	1:A:1655:ARG:HG2	1.91	0.51
1:A:2416:ARG:HG2	1:A:2425:VAL:HG21	1.91	0.51
1:A:1018:TRP:NE1	1:A:1563:GLN:NE2	2.59	0.51
1:A:1130:TYR:CZ	1:A:1134:LEU:HD21	2.46	0.51
1:A:2756:GLU:O	1:A:2760:ILE:HG12	2.10	0.51
1:A:1413:TYR:HA	1:A:1416:ILE:HG22	1.93	0.51
1:A:1633:GLU:HG3	2:C:7:A:C8	2.46	0.51
1:A:3067:LYS:HD3	1:A:3067:LYS:N	2.26	0.51
1:A:1194:ASP:HB3	1:A:1200:LYS:N	2.26	0.51
1:A:1416:ILE:O	1:A:1420:ILE:HD12	2.10	0.51
1:A:1556:ASN:C	1:A:1556:ASN:HD22	2.17	0.51
1:A:2453:LEU:O	1:A:2458:ILE:HG22	2.11	0.51
1:A:1429:LEU:HB3	1:A:3215:TYR:CZ	2.46	0.50
1:A:2467:SER:OG	1:A:2469:ASN:OD1	2.29	0.50
1:A:3024:ILE:HA	1:A:3045:HIS:CE1	2.45	0.50
1:A:2410:LYS:HE3	2:C:7:A:N3	2.26	0.50
1:A:2585:ARG:HD2	1:A:2585:ARG:C	2.36	0.50
1:A:1006:GLN:OE1	1:A:1010:THR:OG1	2.29	0.50
1:A:1228:ILE:HG23	1:A:1232:LEU:HD13	1.92	0.50
1:A:1629:ILE:O	1:A:1633:GLU:N	2.42	0.50
1:A:2993:LYS:HG3	1:A:2996:HIS:H	1.77	0.50
1:A:1117:LYS:HD2	1:A:1118:THR:HG23	1.93	0.50
1:A:2588:PRO:HD3	1:A:3196:TYR:CZ	2.47	0.50
1:A:970:VAL:HG11	1:A:1781:PHE:HE2	1.76	0.50
1:A:1003:GLU:OE1	1:A:1003:GLU:N	2.45	0.50
1:A:1411:TYR:HD1	1:A:1414:ILE:HD11	1.76	0.50
1:A:2389:TYR:O	1:A:2390:LYS:HG2	2.11	0.50
1:A:2449:THR:O	1:A:2453:LEU:HG	2.12	0.50
1:A:2592:LYS:C	1:A:2593:PHE:HD1	2.18	0.50
1:A:1038:THR:O	1:A:1042:THR:OG1	2.29	0.50
1:A:1659:ARG:HA	1:A:1662:ARG:HB3	1.93	0.50
1:A:2408:ILE:HD12	1:A:2411:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2623:ASN:OD1	1:A:2623:ASN:N	2.45	0.50
1:A:972:ILE:HD13	1:A:1755:TYR:HE1	1.76	0.50
1:A:1194:ASP:O	1:A:1199:ALA:HB3	2.12	0.50
1:A:1262:LEU:HD11	1:A:1264:ILE:HD11	1.94	0.50
1:A:1542:LEU:HA	1:A:2566:LYS:HZ3	1.77	0.50
1:A:1626:GLU:O	1:A:1628:CYS:N	2.44	0.50
1:A:1183:VAL:O	1:A:1187:LEU:HG	2.12	0.50
1:A:1661:ALA:HA	1:A:1664:LEU:HD13	1.94	0.50
1:A:2499:LEU:HD21	1:A:2548:LEU:HD22	1.94	0.50
1:A:988:LEU:HD13	1:A:2497:PHE:HE2	1.77	0.50
1:A:1077:ASN:OD1	1:A:1078:VAL:N	2.45	0.50
1:A:1534:SER:HA	1:A:2570:SER:HB2	1.94	0.50
1:A:2203:THR:HA	1:A:2206:MET:HE3	1.93	0.50
1:A:2744:PHE:HB3	1:A:3020:PHE:CE2	2.46	0.50
1:A:1383:LEU:HD12	1:A:1399:PHE:CE1	2.45	0.49
1:A:1659:ARG:NH1	1:A:1765:ASP:OD2	2.45	0.49
1:A:1018:TRP:CD1	1:A:1563:GLN:HE21	2.30	0.49
1:A:1605:ARG:HD3	1:A:3087:ILE:HG21	1.94	0.49
1:A:2023:LEU:HD11	1:A:2143:PHE:HE2	1.76	0.49
1:A:2355:ILE:HG13	1:A:2355:ILE:O	2.11	0.49
1:A:2382:VAL:HG11	1:A:2385:TRP:HD1	1.77	0.49
1:A:2434:ARG:HH22	1:A:2437:LEU:HD13	1.76	0.49
1:A:2759:PHE:CE1	1:A:3069:ARG:HG2	2.47	0.49
1:A:2912:VAL:HG13	1:A:3183:ARG:NH1	2.27	0.49
1:A:1383:LEU:HD11	1:A:1397:PRO:HB2	1.94	0.49
1:A:3068:LEU:O	1:A:3072:GLU:HG2	2.12	0.49
1:A:3121:VAL:HG22	1:A:3122:LYS:H	1.76	0.49
1:A:934:VAL:HG22	1:A:2390:LYS:HD2	1.94	0.49
1:A:1024:LYS:HA	1:A:1032:LEU:HD21	1.94	0.49
1:A:1343:CYS:O	1:A:1347:LEU:HG	2.12	0.49
1:A:1352:GLU:HB2	1:A:2944:LEU:HD21	1.95	0.49
1:A:1305:MET:O	1:A:1309:ILE:HG12	2.13	0.49
1:A:1630:SER:O	1:A:1634:GLU:N	2.37	0.49
1:A:2592:LYS:HB3	1:A:2593:PHE:CE1	2.47	0.49
1:A:1306:LYS:HG2	1:A:2775:ILE:HD13	1.93	0.49
1:A:1832:LEU:HD23	1:A:2462:LEU:HA	1.95	0.49
1:A:2903:VAL:HG11	1:A:3155:GLU:HB3	1.95	0.49
1:A:3024:ILE:HG13	1:A:3024:ILE:O	2.12	0.49
1:A:3065:ARG:HD2	1:A:3065:ARG:O	2.12	0.49
1:A:1008:VAL:O	1:A:1012:GLU:HG2	2.12	0.49
1:A:1090:HIS:ND1	1:A:1365:HIS:O	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:VAL:HB	1:A:1334:GLN:NE2	2.28	0.49
1:A:2240:VAL:HA	1:A:2924:LEU:HD13	1.95	0.49
1:A:1414:ILE:HG22	1:A:2595:PHE:CD1	2.48	0.49
1:A:3061:SER:O	1:A:3065:ARG:HB2	2.12	0.49
1:A:988:LEU:HD23	1:A:989:ASP:H	1.77	0.48
1:A:2954:LYS:N	1:A:2993:LYS:HZ1	2.11	0.48
1:A:1352:GLU:HB2	1:A:2944:LEU:HD11	1.96	0.48
1:A:1632:LEU:HA	1:A:1635:THR:HB	1.96	0.48
1:A:2078:ALA:HB1	1:A:2201:ILE:HG12	1.94	0.48
1:A:2083:TRP:HD1	1:A:2083:TRP:O	1.97	0.48
1:A:2355:ILE:HD11	1:A:2521:LYS:HG3	1.95	0.48
1:A:1005:THR:HB	1:A:1535:ARG:HA	1.95	0.48
1:A:1545:LYS:HB2	1:A:2566:LYS:HZ1	1.78	0.48
1:A:2414:VAL:HB	2:C:8:G:C2	2.48	0.48
1:A:2613:CYS:HA	1:A:2637:ARG:NH1	2.27	0.48
1:A:2800:SER:HB3	1:A:3002:LEU:HB2	1.95	0.48
1:A:2925:LYS:O	1:A:2929:THR:HG23	2.14	0.48
1:A:3215:TYR:CE2	1:A:3217:ILE:HG12	2.48	0.48
1:A:2087:TYR:HB2	1:A:2202:TRP:HE1	1.79	0.48
1:A:2389:TYR:O	1:A:2392:THR:OG1	2.32	0.48
1:A:2627:LEU:HD22	1:A:2671:TYR:CZ	2.49	0.48
1:A:983:MET:HA	1:A:986:GLU:HG3	1.94	0.48
1:A:1004:LEU:HA	1:A:1536:LEU:HD23	1.94	0.48
1:A:2543:LYS:HA	1:A:2543:LYS:HE2	1.95	0.48
1:A:959:GLU:OE2	1:A:959:GLU:N	2.41	0.48
1:A:1778:MET:O	1:A:2560:GLN:HG2	2.14	0.48
1:A:2471:MET:HG2	1:A:2472:GLY:N	2.28	0.48
1:A:2826:SER:O	1:A:2830:VAL:HG12	2.13	0.48
1:A:1423:LEU:HD11	1:A:1496:ILE:HD11	1.96	0.48
1:A:2926:GLN:O	1:A:2929:THR:OG1	2.23	0.48
1:A:3215:TYR:CG	1:A:3216:GLY:N	2.82	0.48
1:A:1191:LYS:HG2	1:A:1200:LYS:HG3	1.95	0.48
1:A:1326:VAL:HA	1:A:1329:ARG:NH1	2.28	0.48
1:A:2373:GLY:O	1:A:2376:GLN:HG3	2.13	0.48
1:A:2692:GLN:HB2	1:A:3050:GLU:OE1	2.14	0.48
1:A:1263:LEU:O	1:A:1265:ARG:NH1	2.46	0.48
1:A:2865:ILE:HG12	1:A:2952:PHE:HE2	1.79	0.48
1:A:993:ASP:HA	1:A:996:GLU:OE1	2.13	0.47
1:A:1198:TYR:N	1:A:1200:LYS:H	2.11	0.47
1:A:1351:THR:OG1	1:A:1354:ASN:OD1	2.29	0.47
1:A:2374:MET:O	1:A:2378:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2418:LYS:HD2	1:A:2440:ASN:CG	2.39	0.47
1:A:1200:LYS:O	1:A:1203:ILE:N	2.47	0.47
1:A:2115:ASP:HA	1:A:2196:ASN:HD22	1.79	0.47
1:A:2418:LYS:HD2	1:A:2440:ASN:ND2	2.29	0.47
1:A:2655:LEU:HD13	1:A:2797:ILE:HG12	1.95	0.47
1:A:987:ASN:HD21	1:A:1767:LEU:HD11	1.78	0.47
1:A:1329:ARG:HH11	1:A:1440:LEU:HD21	1.79	0.47
1:A:1410:SER:O	1:A:1414:ILE:HG12	2.14	0.47
1:A:2345:ASN:HA	1:A:2531:LYS:HE2	1.95	0.47
1:A:2955:SER:O	1:A:2993:LYS:NZ	2.34	0.47
2:C:3:U:H2'	2:C:4:C:C6	2.49	0.47
1:A:1991:LEU:HD23	1:A:2116:LEU:HD22	1.97	0.47
1:A:1203:ILE:O	1:A:1207:LEU:HG	2.14	0.47
1:A:1621:MET:HE1	1:A:2272:PRO:HG2	1.94	0.47
1:A:1341:LYS:HA	1:A:1341:LYS:HD3	1.68	0.47
1:A:2609:LEU:HD22	1:A:2641:PHE:CD2	2.50	0.47
1:A:1070:VAL:HG13	1:A:1263:LEU:HD22	1.97	0.47
1:A:1188:SER:HA	1:A:1191:LYS:HD3	1.96	0.47
1:A:1199:ALA:HB2	1:A:2970:TRP:CZ2	2.50	0.47
1:A:1654:GLU:HG2	1:A:1655:ARG:HE	1.80	0.47
1:A:1657:ASP:O	1:A:1659:ARG:N	2.43	0.47
1:A:2474:GLY:O	1:A:2477:HIS:ND1	2.48	0.47
1:A:2622:TYR:O	1:A:3195:PHE:HA	2.14	0.47
1:A:2682:GLU:OE1	1:A:2682:GLU:N	2.46	0.47
1:A:2857:ASN:HB2	1:A:3184:MET:SD	2.55	0.47
1:A:3150:LYS:HB3	1:A:3153:ALA:HA	1.97	0.47
1:A:3177:HIS:O	1:A:3181:LEU:HG	2.14	0.47
1:A:1053:ALA:HA	1:A:1056:LEU:HG	1.97	0.47
1:A:2610:MET:SD	1:A:2667:PHE:HB2	2.55	0.47
1:A:1078:VAL:HG21	1:A:1509:ASP:HA	1.97	0.47
1:A:2915:GLU:O	1:A:2919:ALA:HB3	2.14	0.47
1:A:3160:GLU:HA	1:A:3164:LEU:HD12	1.97	0.47
1:A:1411:TYR:HA	1:A:1414:ILE:CG1	2.45	0.47
1:A:1530:LEU:HD22	1:A:2573:PHE:CD1	2.50	0.47
1:A:1612:TYR:OH	1:A:2592:LYS:HE3	2.15	0.47
1:A:3167:ASP:O	1:A:3168:LEU:HG	2.14	0.47
1:A:929:VAL:HG22	1:A:2260:LEU:HD11	1.97	0.46
1:A:1513:ALA:HB1	1:A:1552:ARG:HH12	1.80	0.46
1:A:1595:THR:HG21	1:A:1609:PHE:HD1	1.80	0.46
1:A:2999:ASP:O	1:A:3002:LEU:HG	2.16	0.46
1:A:2698:SER:OG	1:A:3010:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3067:LYS:O	1:A:3071:VAL:HG22	2.15	0.46
1:A:1348:ARG:HH21	1:A:2644:HIS:HA	1.81	0.46
1:A:1777:THR:HG23	1:A:2560:GLN:NE2	2.31	0.46
1:A:2408:ILE:O	1:A:2412:LEU:HG	2.16	0.46
1:A:2656:THR:O	1:A:2659:THR:OG1	2.34	0.46
1:A:3209:VAL:HG12	1:A:3211:GLU:H	1.80	0.46
1:A:1511:LEU:HD13	1:A:1616:ILE:HD12	1.98	0.46
1:A:1638:ARG:HA	1:A:1641:LEU:HD12	1.97	0.46
1:A:1566:ILE:O	1:A:1570:VAL:HG22	2.15	0.46
1:A:2419:LEU:HG	1:A:2422:LYS:HZ2	1.81	0.46
1:A:996:GLU:OE2	1:A:2547:ARG:NE	2.49	0.46
1:A:1121:GLU:O	1:A:1125:LYS:HG3	2.16	0.46
1:A:2231:VAL:N	1:A:2267:TYR:OH	2.48	0.46
1:A:2494:LEU:HD22	1:A:2551:PHE:HE2	1.81	0.46
1:A:1136:MET:HE3	1:A:1142:ASP:C	2.40	0.46
1:A:1537:VAL:HG23	1:A:1539:PRO:HD3	1.97	0.46
1:A:1516:GLN:O	1:A:1520:LYS:HG2	2.16	0.46
1:A:2280:ARG:HH21	1:A:2362:TRP:HB3	1.81	0.46
1:A:2446:GLY:H	1:A:2451:LYS:HE3	1.81	0.46
1:A:1403:ARG:O	1:A:1514:ASN:ND2	2.49	0.46
1:A:1662:ARG:HD3	1:A:1663:LEU:HG	1.98	0.46
1:A:2665:ARG:HH12	1:A:2686:VAL:HG21	1.80	0.46
1:A:2665:ARG:NH1	1:A:2686:VAL:HG21	2.31	0.46
1:A:2672:SER:O	1:A:3065:ARG:HD3	2.15	0.46
1:A:1116:GLY:HA2	1:A:1121:GLU:OE2	2.15	0.46
1:A:2494:LEU:HD11	1:A:2555:VAL:HG11	1.98	0.46
1:A:1295:ILE:O	1:A:2639:GLN:HG2	2.15	0.45
1:A:1608:ILE:HA	1:A:1611:ILE:HG12	1.97	0.45
1:A:2370:PHE:HD2	1:A:2560:GLN:HG3	1.81	0.45
1:A:2492:GLU:O	1:A:2496:ILE:HG22	2.15	0.45
1:A:1184:ARG:O	1:A:1187:LEU:HB2	2.17	0.45
1:A:1265:ARG:HH12	1:A:1551:ARG:C	2.23	0.45
1:A:1909:ILE:HG23	1:A:2068:MET:HE1	1.97	0.45
1:A:1131:LEU:HA	1:A:1134:LEU:HD23	1.98	0.45
1:A:1420:ILE:HG21	1:A:2628:ILE:HG12	1.98	0.45
1:A:2767:LYS:HD2	1:A:2767:LYS:HA	1.63	0.45
1:A:3221:ARG:HB2	1:A:3225:LEU:HA	1.99	0.45
1:A:1224:TRP:HB3	1:A:1391:MET:HG2	1.98	0.45
1:A:1360:LEU:HD12	1:A:1371:SER:HB2	1.98	0.45
1:A:1768:GLN:HA	1:A:1771:ARG:HB2	1.99	0.45
1:A:2604:THR:OG1	1:A:2932:ASN:OD1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:GLU:HG2	1:A:2657:LEU:HB3	1.99	0.45
1:A:1411:TYR:CE2	1:A:1508:LYS:HG3	2.51	0.45
1:A:2595:PHE:HA	1:A:2598:LEU:HB3	1.98	0.45
1:A:3165:SER:O	1:A:3167:ASP:N	2.49	0.45
1:A:1426:TYR:OH	1:A:1606:GLN:HG2	2.16	0.45
1:A:1535:ARG:HD3	1:A:2542:TRP:CE2	2.51	0.45
1:A:1882:LEU:HD21	1:A:2424:GLY:HA3	1.98	0.45
1:A:2815:ARG:HB2	1:A:2819:GLU:HG2	1.98	0.45
2:C:1:U:H3'	2:C:2:C:C6	2.52	0.45
1:A:988:LEU:HA	1:A:2551:PHE:CE1	2.52	0.45
1:A:1018:TRP:CD1	1:A:1563:GLN:NE2	2.85	0.45
1:A:2869:PRO:HD2	1:A:2872:LEU:HD23	1.97	0.45
1:A:984:LEU:HD11	1:A:2555:VAL:HG22	1.99	0.45
1:A:1011:SER:O	1:A:1014:MET:HB2	2.16	0.45
1:A:1021:GLU:HG3	1:A:1544:LYS:O	2.16	0.45
1:A:1233:LYS:C	1:A:1235:PRO:HD2	2.42	0.45
1:A:2311:GLY:HA3	1:A:2515:SER:HB2	1.97	0.45
1:A:2355:ILE:HG22	1:A:2569:VAL:HG22	1.98	0.45
1:A:1216:SER:OG	1:A:1217:LYS:N	2.50	0.45
1:A:1642:TRP:CD1	1:A:1777:THR:HB	2.52	0.45
1:A:1257:ARG:HD3	1:A:1257:ARG:C	2.42	0.45
1:A:1605:ARG:CD	1:A:3087:ILE:HG21	2.46	0.45
1:A:1952:PRO:HG2	1:A:1954:LEU:HD12	1.99	0.45
2:C:2:C:H2'	2:C:3:U:C5	2.52	0.45
1:A:1179:LYS:O	1:A:1182:ILE:HG13	2.16	0.44
1:A:1235:PRO:HG3	1:A:1242:LEU:HD12	1.98	0.44
1:A:2410:LYS:H	1:A:2410:LYS:HG3	1.57	0.44
1:A:2615:VAL:HG11	1:A:2854:ARG:HG2	1.97	0.44
1:A:2640:ILE:O	1:A:2643:ASN:HB2	2.17	0.44
1:A:1341:LYS:HD2	1:A:1364:ARG:HB2	2.00	0.44
1:A:1412:LEU:HD11	1:A:1413:TYR:CZ	2.52	0.44
1:A:1835:CYS:O	1:A:1839:ILE:HG23	2.16	0.44
1:A:1005:THR:N	1:A:1535:ARG:O	2.42	0.44
1:A:2630:ASN:HA	1:A:2633:PHE:CE2	2.52	0.44
1:A:2636:LEU:O	1:A:2639:GLN:HB3	2.17	0.44
1:A:1187:LEU:O	1:A:1188:SER:C	2.59	0.44
1:A:1604:ASP:OD1	1:A:2582:MET:HB2	2.17	0.44
1:A:2545:ALA:O	1:A:2548:LEU:HG	2.18	0.44
1:A:1440:LEU:HA	1:A:1443:ILE:HG22	2.00	0.44
1:A:2503:LEU:HB2	1:A:2537:TYR:CZ	2.53	0.44
1:A:2592:LYS:HD3	1:A:2593:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2593:PHE:CE2	1:A:2623:ASN:ND2	2.86	0.44
1:A:2750:ARG:HH22	1:A:2756:GLU:HG2	1.81	0.44
1:A:3014:VAL:HG22	1:A:3016:GLU:H	1.83	0.44
1:A:3078:SER:HB3	1:A:3221:ARG:HH21	1.82	0.44
1:A:1130:TYR:CE2	1:A:1134:LEU:HD21	2.53	0.44
1:A:1333:PHE:O	1:A:1337:VAL:HG23	2.17	0.44
1:A:2603:VAL:HG22	1:A:2609:LEU:HA	1.98	0.44
1:A:2911:ASN:ND2	1:A:2913:SER:HB2	2.32	0.44
1:A:934:VAL:HG12	1:A:966:LEU:HD13	2.00	0.44
1:A:1293:ASP:HB3	1:A:2788:GLU:HG3	1.99	0.44
1:A:1373:LYS:CG	1:A:1383:LEU:HB3	2.48	0.44
1:A:1200:LYS:O	1:A:1201:GLY:C	2.61	0.44
1:A:1360:LEU:HD11	1:A:1391:MET:HE1	1.99	0.44
1:A:1420:ILE:HD12	1:A:1420:ILE:H	1.82	0.44
1:A:1595:THR:HG22	1:A:1613:ASN:HD21	1.83	0.44
1:A:2113:LEU:HA	1:A:2116:LEU:HB2	2.00	0.44
1:A:3084:ARG:HD3	1:A:3084:ARG:N	2.33	0.44
2:C:2:C:H2'	2:C:3:U:C6	2.53	0.44
1:A:982:ASN:HA	1:A:985:LYS:HG3	2.00	0.43
1:A:1329:ARG:NH1	1:A:1440:LEU:HD21	2.32	0.43
1:A:1608:ILE:HD11	1:A:2582:MET:CE	2.48	0.43
1:A:2488:ALA:O	1:A:2492:GLU:HG3	2.18	0.43
1:A:2540:THR:O	1:A:2540:THR:OG1	2.35	0.43
1:A:2582:MET:SD	1:A:2582:MET:N	2.91	0.43
1:A:2660:LEU:HD22	1:A:2683:ASP:CG	2.43	0.43
1:A:1077:ASN:O	1:A:1081:ARG:HG2	2.17	0.43
1:A:1271:LYS:HD3	1:A:1455:PHE:CZ	2.53	0.43
1:A:1502:VAL:HA	1:A:1506:LEU:HB2	2.00	0.43
1:A:2335:LEU:HD22	1:A:2350:TYR:CD2	2.53	0.43
1:A:1243:ILE:HG23	1:A:1246:ARG:HD3	2.00	0.43
1:A:1381:ASN:CG	1:A:1399:PHE:HB3	2.43	0.43
1:A:1503:TYR:OH	1:A:1595:THR:HG22	2.18	0.43
1:A:1663:LEU:HD23	1:A:1663:LEU:HA	1.81	0.43
1:A:2873:ARG:NH1	1:A:2877:GLU:OE2	2.51	0.43
1:A:3004:CYS:SG	1:A:3037:ARG:HG3	2.58	0.43
1:A:972:ILE:HG22	1:A:973:SER:N	2.33	0.43
1:A:1493:ILE:HG13	1:A:1494:SER:N	2.34	0.43
1:A:2422:LYS:HG3	1:A:2428:HIS:CE1	2.53	0.43
1:A:2994:TYR:O	1:A:2998:LEU:HD22	2.18	0.43
1:A:1407:LEU:HD21	1:A:1616:ILE:HG22	2.00	0.43
1:A:2510:VAL:CG2	1:A:2523:ILE:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2682:GLU:O	1:A:2686:VAL:HG23	2.18	0.43
2:C:5:A:O2'	2:C:7:A:H5''	2.18	0.43
1:A:1018:TRP:CD1	1:A:1018:TRP:C	2.96	0.43
1:A:1245:ILE:HD12	1:A:1245:ILE:HA	1.90	0.43
1:A:2013:GLN:HE21	1:A:2126:TYR:HD1	1.66	0.43
1:A:2645:VAL:HG23	1:A:2649:ILE:HG12	2.00	0.43
1:A:2839:PHE:N	1:A:2839:PHE:CD2	2.86	0.43
1:A:2379:LEU:HD13	1:A:2386:CYS:HA	2.00	0.43
1:A:1306:LYS:NZ	1:A:2818:LEU:HG	2.34	0.43
1:A:2418:LYS:NZ	1:A:2440:ASN:HA	2.34	0.43
1:A:3111:TYR:N	1:A:3148:LEU:HD12	2.33	0.43
1:A:1479:ALA:HA	1:A:1486:ARG:HH21	1.84	0.43
1:A:1528:GLY:C	1:A:1566:ILE:HD11	2.44	0.43
1:A:1579:HIS:HA	1:A:1582:GLN:HE22	1.83	0.43
1:A:2419:LEU:HG	1:A:2422:LYS:HD3	2.00	0.43
1:A:2694:LEU:HD22	1:A:2827:VAL:HG12	2.01	0.43
1:A:1450:LEU:HD22	1:A:1597:TYR:CE2	2.54	0.43
1:A:1520:LYS:HG2	1:A:1520:LYS:H	1.53	0.43
1:A:1542:LEU:HD13	1:A:2566:LYS:HD3	2.01	0.43
1:A:2761:LYS:HE2	1:A:2761:LYS:HB2	1.90	0.43
1:A:2366:HIS:HA	1:A:2560:GLN:NE2	2.33	0.42
1:A:948:ARG:HH12	1:A:953:THR:HG22	1.84	0.42
1:A:1042:THR:HB	1:A:1048:LYS:HG2	2.01	0.42
1:A:1432:ILE:HA	1:A:1435:VAL:HG23	2.01	0.42
1:A:1628:CYS:O	1:A:1631:VAL:HB	2.20	0.42
1:A:2230:SER:HB3	1:A:2267:TYR:CZ	2.55	0.42
1:A:2449:THR:HB	2:C:7:A:H62	1.84	0.42
1:A:952:LEU:HD11	1:A:1646:LEU:HG	2.02	0.42
1:A:1336:VAL:HG22	1:A:1508:LYS:HD2	2.01	0.42
1:A:1438:LYS:HA	1:A:1441:GLN:OE1	2.19	0.42
1:A:1870:ARG:HA	1:A:1870:ARG:HD3	1.79	0.42
1:A:2696:MET:C	1:A:2696:MET:HE2	2.45	0.42
1:A:936:GLU:O	1:A:939:GLU:HG2	2.19	0.42
1:A:1184:ARG:HH21	1:A:1188:SER:HB3	1.85	0.42
1:A:1323:LEU:HA	1:A:1323:LEU:HD23	1.81	0.42
1:A:1446:HIS:HB3	1:A:1497:SER:OG	2.19	0.42
1:A:1579:HIS:HB2	1:A:1589:VAL:HG12	2.02	0.42
1:A:1991:LEU:HD23	1:A:2116:LEU:HD13	2.01	0.42
1:A:2564:SER:O	1:A:2567:THR:HG23	2.20	0.42
1:A:2689:ARG:NH1	1:A:2693:THR:OG1	2.52	0.42
1:A:2758:GLN:HG2	1:A:3070:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1339:TYR:HE2	1:A:1512:LEU:HD22	1.85	0.42
1:A:1507:ILE:O	1:A:1511:LEU:HG	2.20	0.42
1:A:2512:HIS:ND1	1:A:2521:LYS:HG2	2.34	0.42
1:A:2593:PHE:CD1	1:A:2593:PHE:N	2.87	0.42
1:A:2750:ARG:HB2	1:A:2751:PRO:HD3	2.02	0.42
1:A:2759:PHE:HE1	1:A:2763:LEU:HD21	1.85	0.42
1:A:3120:GLU:O	1:A:3121:VAL:HG12	2.20	0.42
1:A:1027:ARG:HB3	1:A:1031:CYS:HB3	2.01	0.42
1:A:1402:ARG:HB3	1:A:1403:ARG:HH21	1.84	0.42
1:A:1530:LEU:HB3	1:A:2573:PHE:CE1	2.54	0.42
1:A:1972:LEU:HG	1:A:2083:TRP:HH2	1.84	0.42
1:A:2591:ILE:HA	1:A:2594:MET:SD	2.59	0.42
1:A:1207:LEU:O	1:A:1210:LEU:HB3	2.19	0.42
1:A:1478:LYS:HD3	1:A:1478:LYS:HA	1.75	0.42
1:A:1578:LYS:HD2	1:A:1578:LYS:HA	1.72	0.42
1:A:1636:ALA:O	1:A:1638:ARG:N	2.53	0.42
1:A:1761:SER:HA	1:A:1764:LYS:HE3	2.02	0.42
1:A:2322:LEU:HD22	1:A:2581:MET:HB3	2.02	0.42
1:A:1303:GLU:OE2	1:A:1307:ARG:NE	2.53	0.41
1:A:1465:ARG:HA	1:A:1465:ARG:NH1	2.35	0.41
1:A:1656:LYS:HD3	1:A:1656:LYS:HA	1.86	0.41
1:A:2744:PHE:CE2	1:A:3148:LEU:HA	2.51	0.41
1:A:949:PRO:HG2	1:A:952:LEU:HD22	2.02	0.41
1:A:1191:LYS:HE3	1:A:1200:LYS:HE3	2.02	0.41
1:A:1377:ASN:OD1	1:A:1377:ASN:N	2.54	0.41
1:A:1429:LEU:HB3	1:A:3215:TYR:OH	2.20	0.41
1:A:1642:TRP:HD1	1:A:1776:HIS:HB2	1.86	0.41
1:A:2836:TYR:CE2	1:A:2863:PRO:HB3	2.55	0.41
1:A:3150:LYS:HA	1:A:3150:LYS:HD2	1.85	0.41
1:A:1521:GLN:HB2	1:A:1548:THR:OG1	2.19	0.41
1:A:1545:LYS:HB2	1:A:2566:LYS:NZ	2.34	0.41
1:A:1619:LYS:HD2	1:A:2276:LEU:HD21	2.02	0.41
1:A:2362:TRP:O	1:A:2362:TRP:HD1	2.03	0.41
1:A:1846:LYS:NZ	1:A:2226:ARG:HG2	2.35	0.41
1:A:1988:GLN:HA	1:A:2116:LEU:HD11	2.03	0.41
1:A:2379:LEU:HB3	1:A:2386:CYS:SG	2.61	0.41
1:A:2573:PHE:HA	1:A:2581:MET:O	2.21	0.41
1:A:2592:LYS:HB3	1:A:2593:PHE:HD1	1.85	0.41
1:A:2865:ILE:HG12	1:A:2952:PHE:CE2	2.55	0.41
1:A:3067:LYS:HA	1:A:3070:ILE:HG12	2.02	0.41
1:A:1265:ARG:NH1	1:A:1551:ARG:O	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:CYS:SG	1:A:2635:LEU:HD11	2.59	0.41
1:A:1332:TRP:CG	1:A:1333:PHE:N	2.89	0.41
1:A:1808:LYS:HD2	1:A:1808:LYS:HA	1.74	0.41
1:A:2380:LYS:HD3	1:A:2380:LYS:HA	1.93	0.41
1:A:3142:PHE:HA	1:A:3146:PHE:CE2	2.53	0.41
1:A:1467:GLU:CD	1:A:1571:ARG:HH21	2.28	0.41
1:A:2627:LEU:O	1:A:2631:THR:OG1	2.32	0.41
1:A:1058:LEU:HA	1:A:1061:HIS:ND1	2.35	0.41
1:A:2230:SER:HB2	1:A:2269:VAL:HG22	2.02	0.41
1:A:2803:ALA:HA	1:A:2809:LEU:CD2	2.51	0.41
1:A:3146:PHE:CD1	1:A:3148:LEU:HG	2.56	0.41
1:A:1085:ILE:HG12	1:A:1331:THR:HG23	2.02	0.41
1:A:1194:ASP:HB3	1:A:1200:LYS:CA	2.50	0.41
1:A:1204:SER:HA	1:A:1207:LEU:HG	2.03	0.41
1:A:1332:TRP:HA	1:A:1335:GLU:OE2	2.21	0.41
1:A:1466:PHE:HB3	1:A:1567:TYR:CD2	2.55	0.41
1:A:1960:LEU:HD21	1:A:1998:CYS:HA	2.03	0.41
1:A:1018:TRP:CD1	1:A:1547:SER:HB2	2.54	0.41
1:A:1135:MET:HG2	1:A:1210:LEU:HB2	2.03	0.41
1:A:1187:LEU:O	1:A:1190:THR:N	2.54	0.41
1:A:1270:LEU:HD12	1:A:1270:LEU:HA	1.81	0.41
1:A:1362:LYS:NZ	1:A:1367:ASP:HA	2.34	0.41
1:A:1373:LYS:HD3	1:A:1383:LEU:HD22	2.02	0.41
1:A:1443:ILE:HA	1:A:1443:ILE:HD12	1.79	0.41
1:A:1526:ARG:HD2	1:A:2580:PHE:HZ	1.84	0.41
1:A:1975:LEU:HD13	1:A:1980:GLN:HB3	2.03	0.41
1:A:2391:LEU:HD13	1:A:2394:ILE:HD12	2.02	0.41
1:A:2556:GLN:HB3	1:A:2561:MET:SD	2.61	0.41
1:A:3091:LYS:HG3	1:A:3206:GLU:HG2	2.03	0.41
1:A:3134:ASP:HB3	1:A:3137:LYS:HB3	2.01	0.41
1:A:1199:ALA:HB2	1:A:2970:TRP:HZ2	1.86	0.41
1:A:1633:GLU:HG3	2:C:7:A:N7	2.36	0.41
1:A:2374:MET:SD	1:A:2375:MET:N	2.94	0.41
1:A:2436:LEU:O	1:A:2440:ASN:HB2	2.21	0.41
1:A:2936:GLY:HA2	1:A:2942:LYS:HE3	2.03	0.41
1:A:3079:GLU:HA	1:A:3216:GLY:O	2.21	0.41
1:A:937:THR:HG22	1:A:941:MET:HE1	2.03	0.40
1:A:1263:LEU:HD12	1:A:1551:ARG:HG3	2.03	0.40
1:A:1453:ASP:OD2	1:A:1476:ARG:NE	2.48	0.40
1:A:1887:LYS:HA	1:A:1887:LYS:HD3	1.87	0.40
1:A:2961:ASN:HA	1:A:2964:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3173:ARG:HG3	1:A:3177:HIS:CE1	2.56	0.40
1:A:1224:TRP:N	1:A:1224:TRP:CD1	2.87	0.40
1:A:2297:GLU:OE1	1:A:2475:ILE:HD11	2.21	0.40
1:A:2334:ASN:OD1	1:A:2334:ASN:N	2.53	0.40
1:A:2335:LEU:HD22	1:A:2350:TYR:HD2	1.86	0.40
1:A:2359:ASN:OD1	1:A:2563:ASP:HA	2.20	0.40
1:A:2498:TYR:HD2	1:A:2499:LEU:HD22	1.86	0.40
1:A:1136:MET:HE2	1:A:1144:ILE:HG23	2.03	0.40
1:A:1203:ILE:HD13	1:A:1203:ILE:HG21	1.79	0.40
1:A:1396:GLY:HA2	1:A:1398:PHE:HD1	1.86	0.40
1:A:1787:ILE:HG21	1:A:2559:CYS:SG	2.61	0.40
1:A:2332:MET:HE2	1:A:2351:LYS:HA	2.02	0.40
1:A:3058:LEU:HD12	1:A:3058:LEU:O	2.21	0.40
1:A:1152:ILE:HD13	1:A:1152:ILE:HA	1.86	0.40
1:A:1468:GLU:HA	1:A:1471:LYS:CE	2.50	0.40
1:A:1489:ARG:O	1:A:1493:ILE:HG12	2.21	0.40
1:A:2292:MET:HE2	1:A:2393:PHE:HB2	2.04	0.40
1:A:2298:MET:HE2	1:A:2298:MET:HB3	1.90	0.40
1:A:2299:PHE:HB3	1:A:2389:TYR:CE2	2.57	0.40
1:A:2401:VAL:HG22	1:A:2470:HIS:ND1	2.36	0.40
1:A:2761:LYS:O	1:A:2765:SER:HB2	2.22	0.40
1:A:2993:LYS:HB2	1:A:2993:LYS:HE2	1.80	0.40
1:A:3015:LYS:H	1:A:3015:LYS:HG2	1.71	0.40
1:A:3074:ARG:NH2	1:A:3227:ASP:HB2	2.34	0.40
1:A:934:VAL:HG22	1:A:2390:LYS:CD	2.51	0.40
1:A:994:GLU:O	1:A:998:THR:HG23	2.21	0.40
1:A:1121:GLU:HA	1:A:1124:VAL:HG22	2.03	0.40
1:A:1180:ILE:HA	1:A:1183:VAL:HG12	2.03	0.40
1:A:1526:ARG:HG3	1:A:1527:PHE:N	2.36	0.40
1:A:2441:LEU:HD12	1:A:2441:LEU:HA	1.86	0.40
1:A:3026:CYS:SG	1:A:3045:HIS:HB3	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2112/3982 (53%)	1935 (92%)	160 (8%)	17 (1%)	16 49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	972	ILE
1	A	1197	THR
1	A	2405	ALA
1	A	2467	SER
1	A	3109	MET
1	A	3121	VAL
1	A	3146	PHE
1	A	3166	PRO
1	A	1008	VAL
1	A	2401	VAL
1	A	3112	LEU
1	A	3170	GLN
1	A	3085	ALA
1	A	1193	LYS
1	A	3157	THR
1	A	2390	LYS
1	A	3194	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1953/3629 (54%)	1949 (100%)	4 (0%)	92 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1305	MET
1	A	1519	ASN

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Mol	Chain	Res	Type
1	A	2623	ASN
1	A	2902	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1007	ASN
1	A	1174	GLN
1	A	1277	GLN
1	A	1602	ASN
1	A	1669	ASN
1	A	2013	GLN
1	A	2196	ASN
1	A	2209	ASN
1	A	2252	GLN
1	A	2253	GLN
1	A	2302	ASN
1	A	2316	HIS
1	A	2466	ASN
1	A	2473	GLN
1	A	2512	HIS
1	A	2607	GLN
1	A	2764	ASN
1	A	2822	ASN
1	A	2996	HIS
1	A	3083	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/18 (50%)	4 (44%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	U
2	C	6	A
2	C	7	A
2	C	8	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

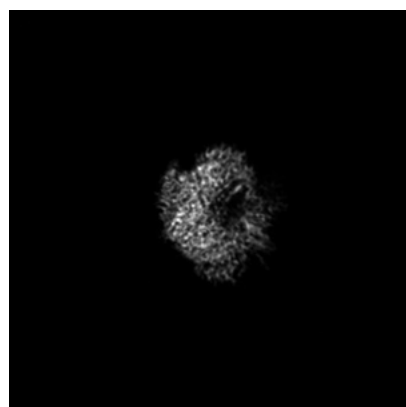
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67169. These allow visual inspection of the internal detail of the map and identification of artifacts.

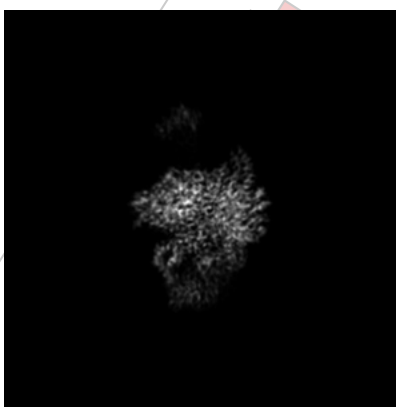
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

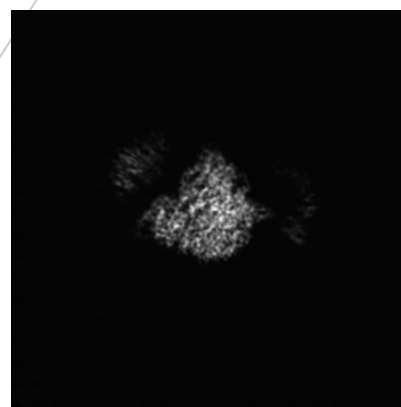
6.1.1 Primary map



X

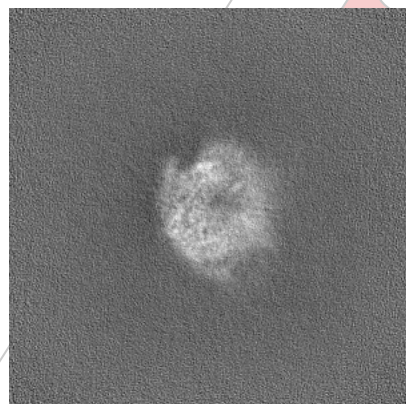


Y

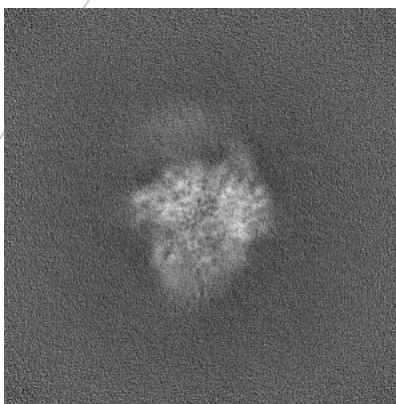


Z

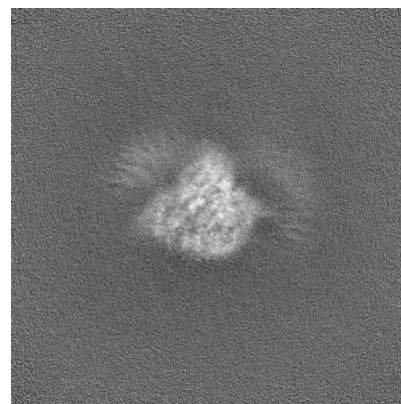
6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

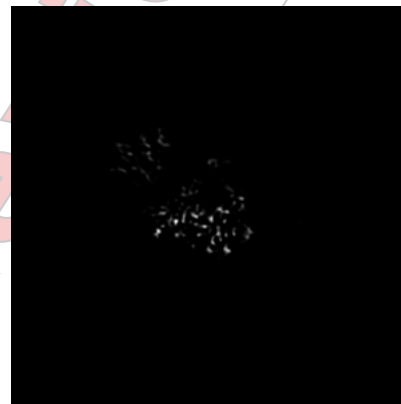
6.2.1 Primary map



X Index: 180

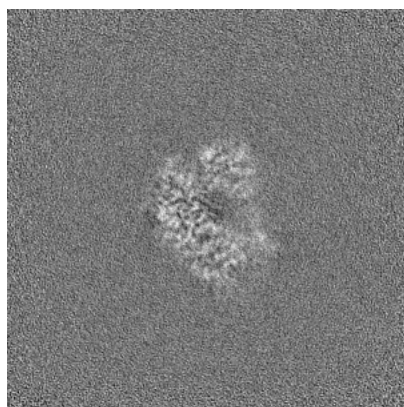


Y Index: 180

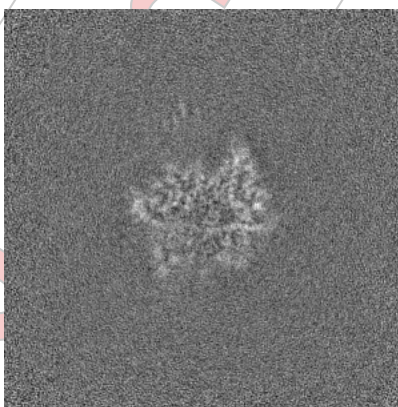


Z Index: 180

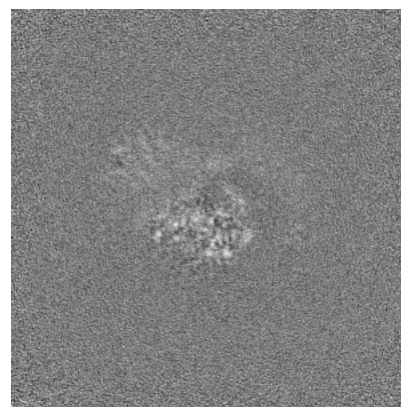
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

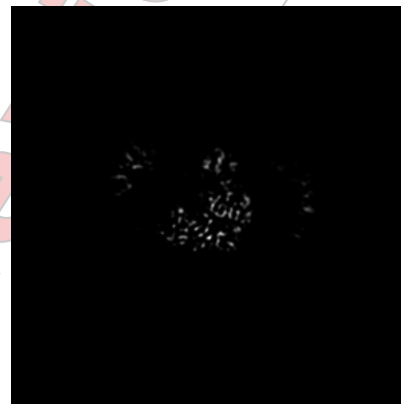
6.3.1 Primary map



X Index: 182

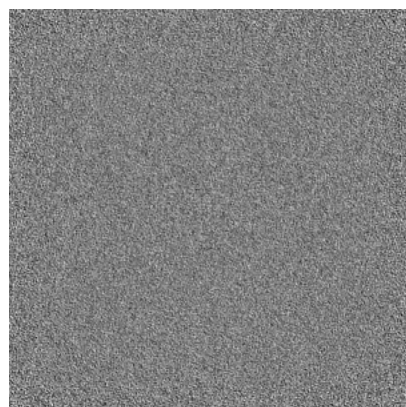


Y Index: 165

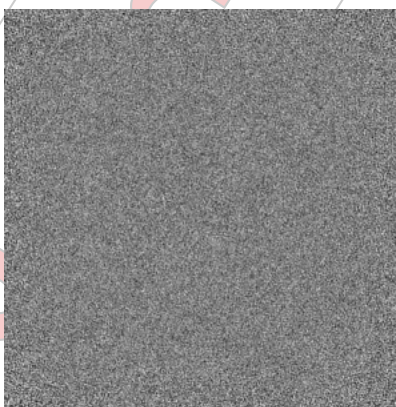


Z Index: 164

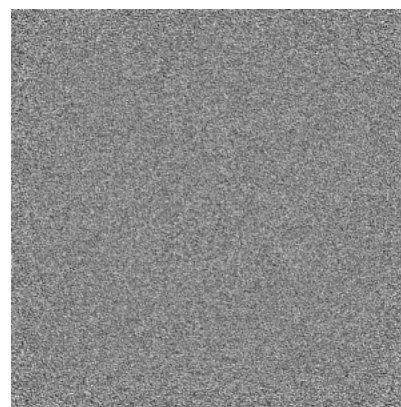
6.3.2 Raw map



X Index: 0



Y Index: 0

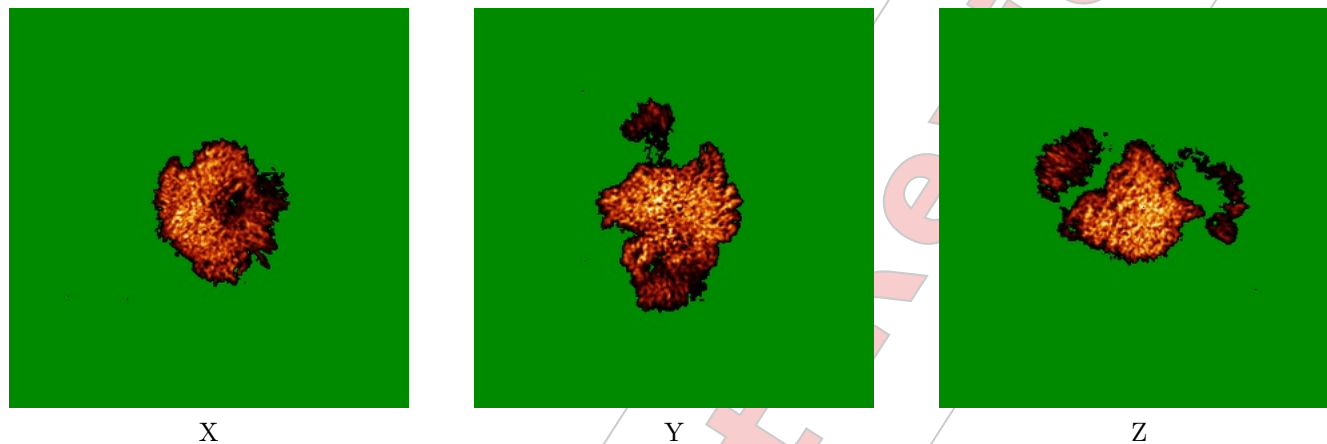


Z Index: 0

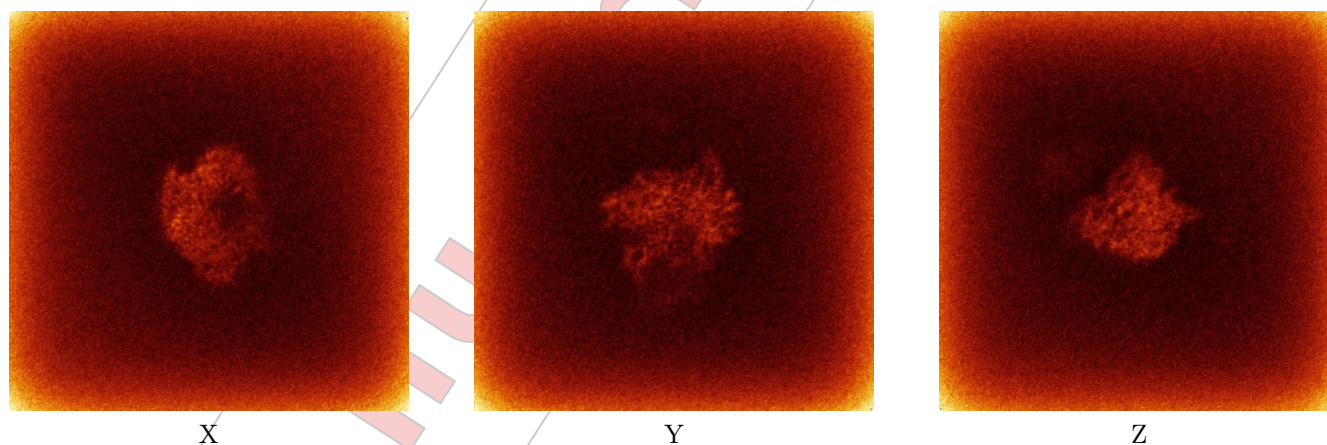
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



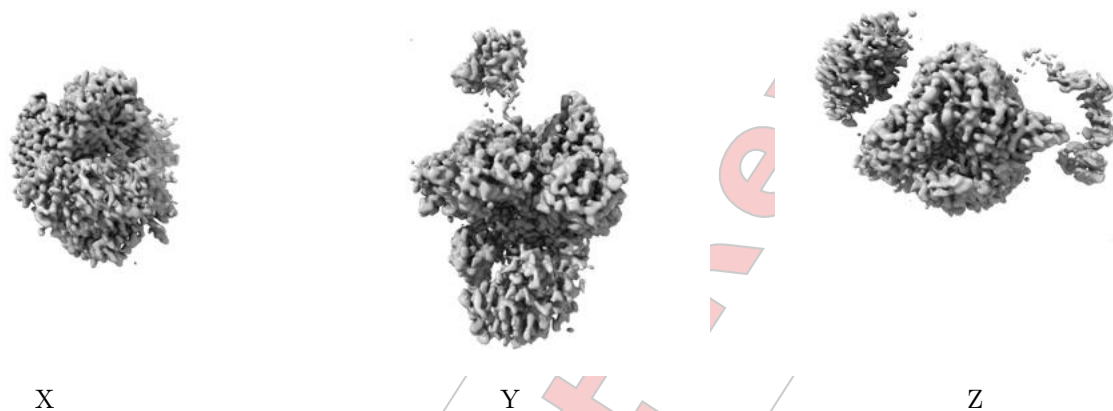
6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

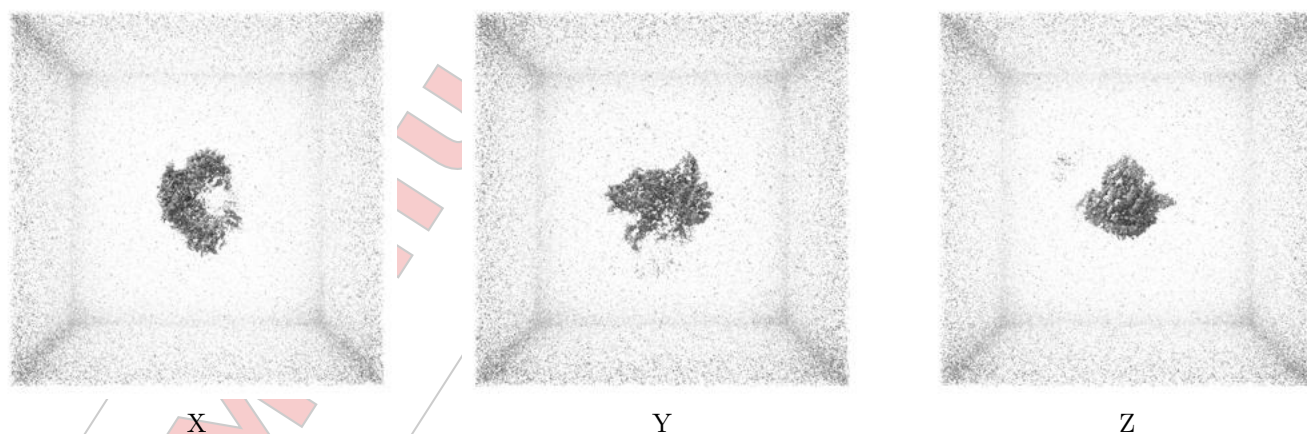
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

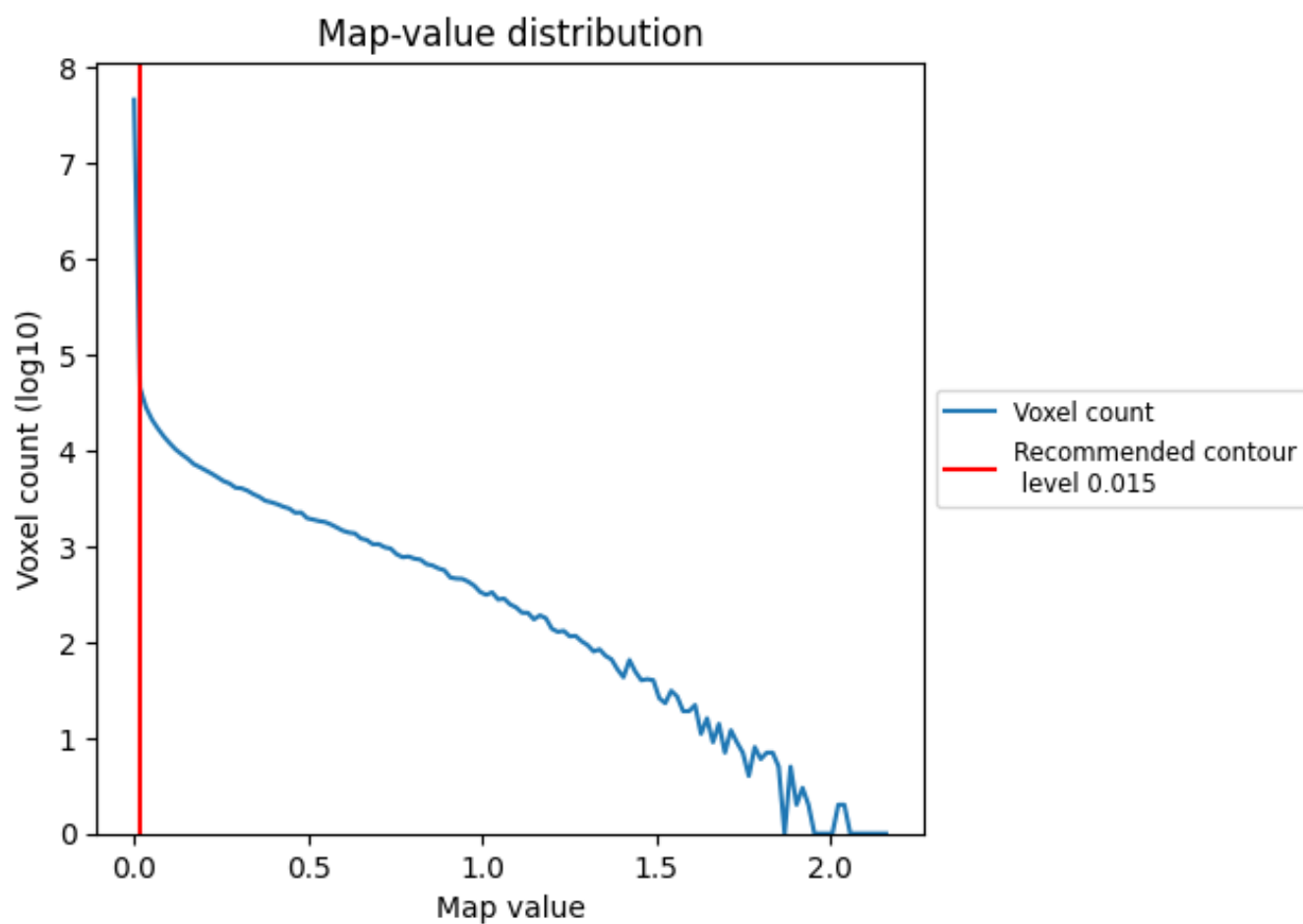
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

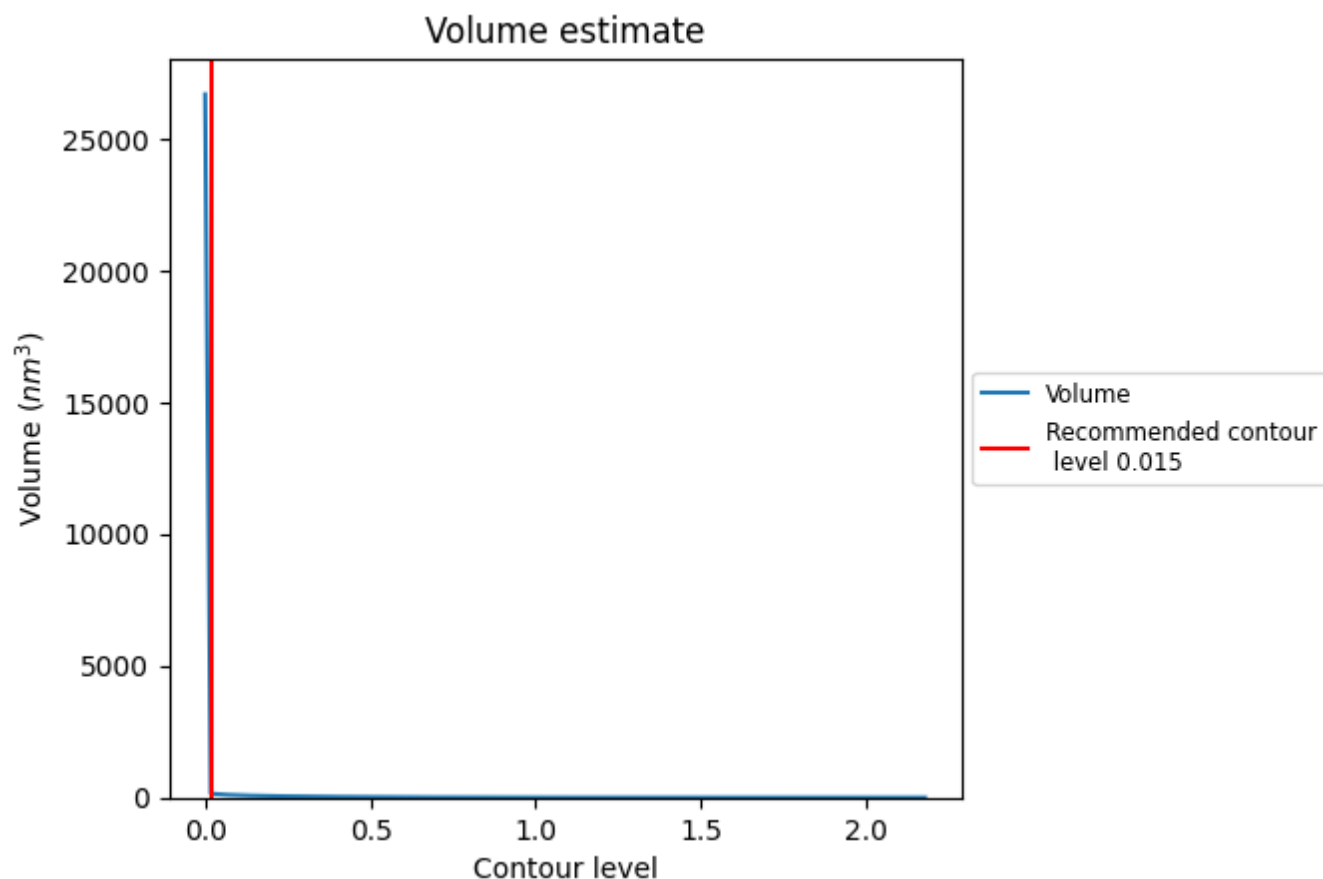
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

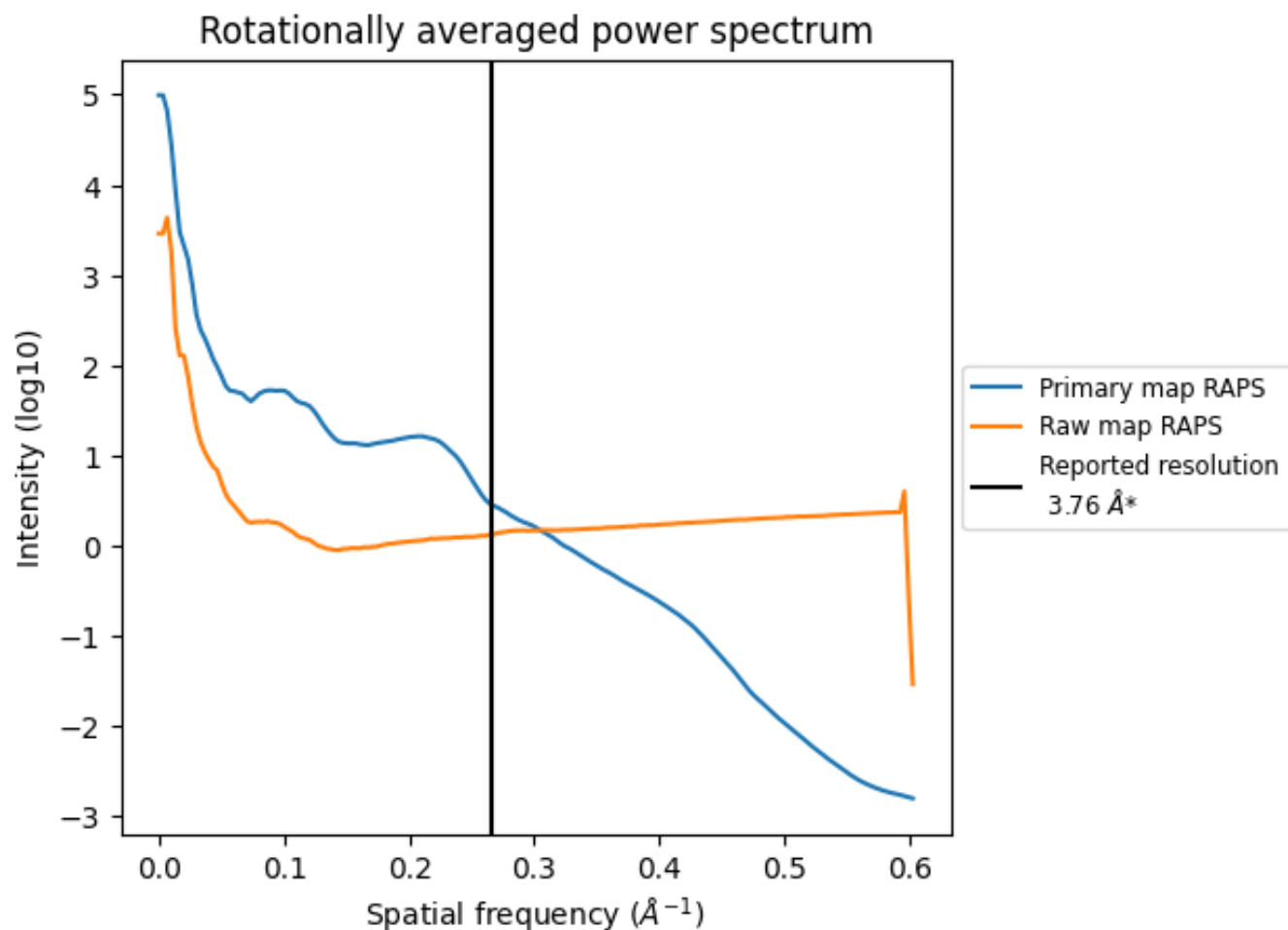
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 603 nm^3 ; this corresponds to an approximate mass of 545 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

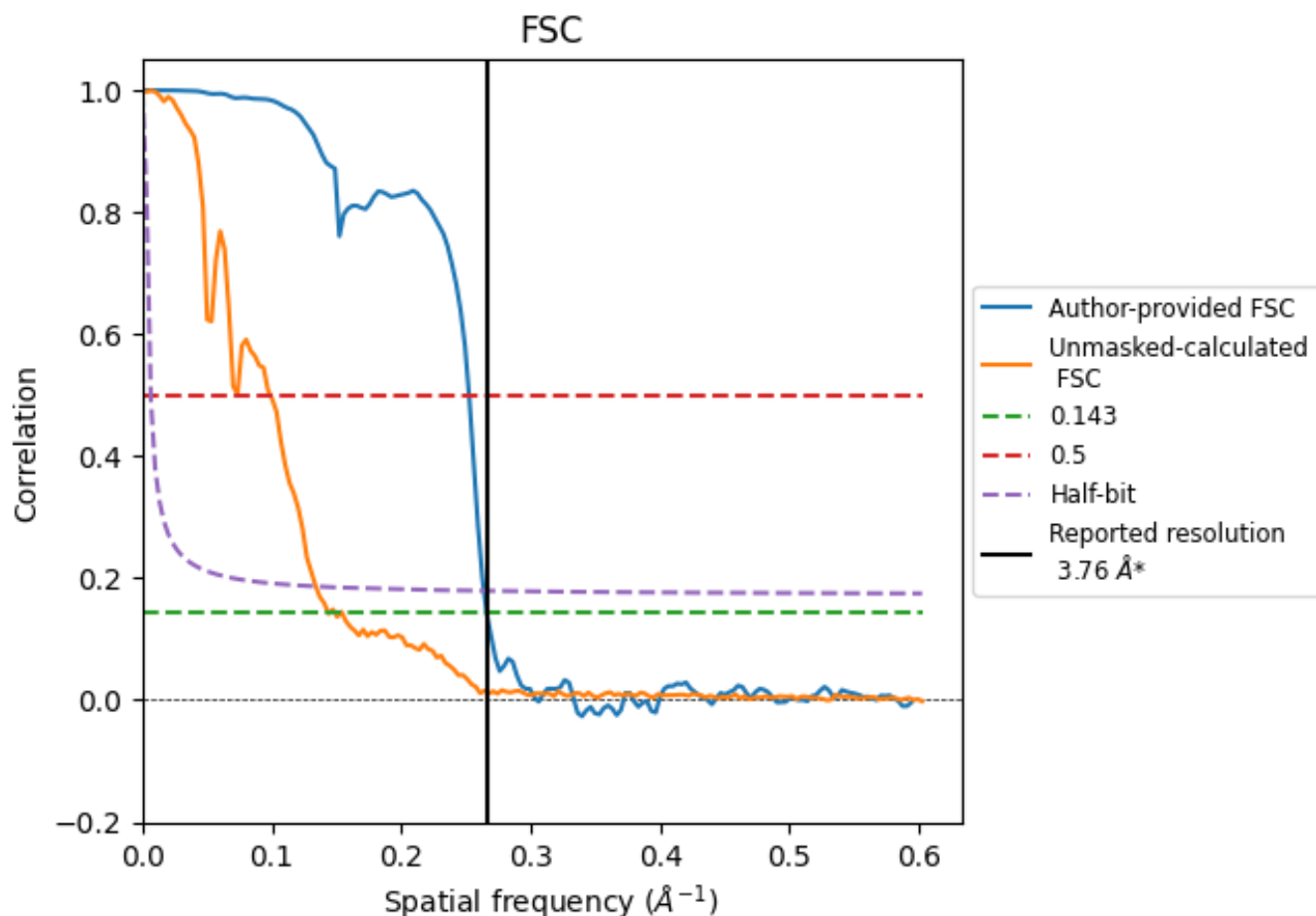


*Reported resolution corresponds to spatial frequency of 0.266 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.266 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

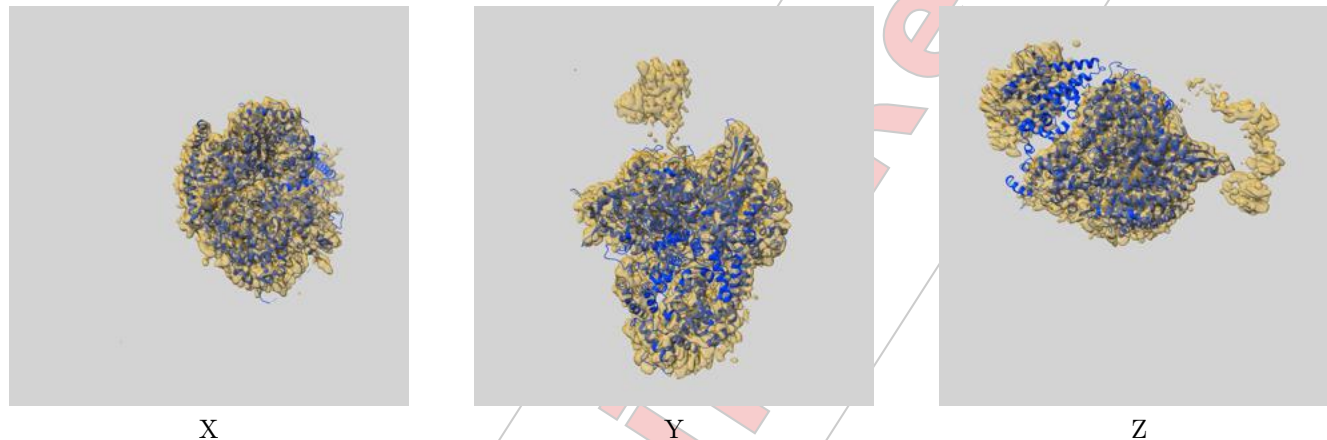
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	3.76	3.96	3.79
Unmasked-calculated*	6.96	10.11	7.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 3.76 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-67169 and PDB model 9XSB. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ



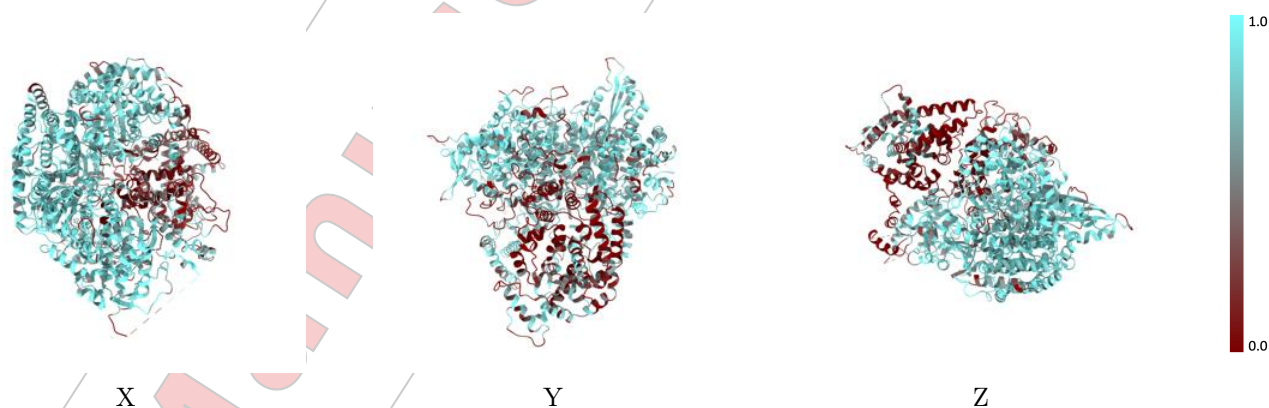
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



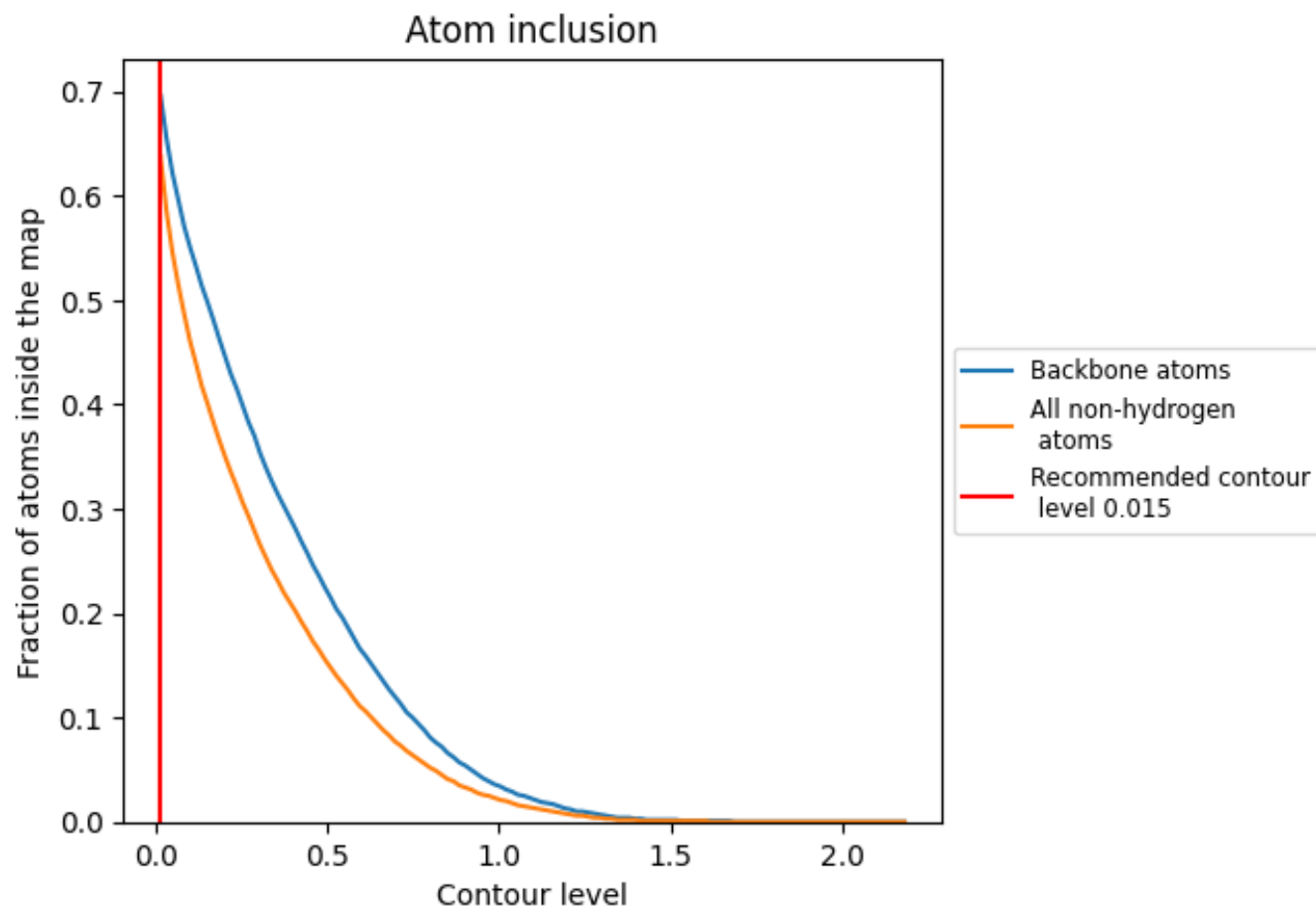
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6380	 0.1280
A	 0.6380	 0.1290
C	 0.6350	 0.0020

