
Supplementary information

**Autoimmunity-associated T cell receptors
recognize HLA-B27-bound peptides**

In the format provided by the
authors and unedited

Supplementary Information

Supplementary Table 1.

Top table: Top clonotypes for each sorted HLA-B*27:05⁺ patient PBMC sample. Frequencies within each sample are listed as number and percentage of barcodes within each library. Bottom table: AS-associated CDR3 β -like sequences detected in HLA-B*27:05⁺ AS PBMC samples and their corresponding TCR α chain pairings. Frequencies within each sample are listed as number and percentage of barcodes within each library.

Supplementary Table 2.

CD3⁺CD8⁺TRBV9⁺ TCR alpha-beta pairing information isolated from patient 3 synovial fluid, and putative AS-related TCR sequences identified in three other patient SF samples by 10x Chromium VDJ SCS.

Supplementary Table 3.

Top enriched synthetic peptides from AS3.1, AS4.1, AS4.2, AS4.3 and AS4.4 selections, their sequence and activation status by these AS TCRs.

Supplementary Table 4.

Predicted natural peptides, sequence, and their activation status by AS3.1, AS4.1, AS4.2, AS4.3 and AS4.4 TCRs. The peptides predicted from human proteome are in black. The peptides predicted from microbial proteomes are in red.

Supplementary Table 5.

Comparison of natural peptides EC₅₀ via *in vitro* activation assay and their equilibrium dissociation constant, K_D, as determined by SPR.

Supplementary Table 6.

Data collection and structure refinement statistics for x-ray crystallography.

Supplementary Table 1

Sample	Freq.	TRBV	CDR3β	TRBJ	TRAV	CDR3α	TRAJ
AS1311	338/2275 14.8%	TRBV9	CASSVGTGGTRLYEQYF	TRBJ2-7	TRAV1-2	CAVRSGQNFVF	TRAJ26
AS1541	276/4868 5.67%	TRBV9	CASSEAGDTHNEQFF	TRBJ2-1	TRAV20	CAVRHSNNAGNMLTF	TRAJ39
AS1802	47/6069 0.774%	TRBV5-5	CASSYSGTGGTDTQYF	TRBJ2-3	TRAV29	CAASAPRLMF	TRAJ31
AS1455	260/10736 2.42%	TRBV9	CASSVGATGVNGYTF	TRBJ1-2	TRAV12-1	CVVKRDDKIIF	TRAJ30
AS1567	63/1462 4.31%	TRBV9	CASSPWDSSSYGYTF	TRBJ1-2	TRAV21	CAVNSGAGSYQLTF	TRAJ28
AS1661	364/7679 4.74%	TRBV9	CASSPGTSYEQYF	TRBJ2-7	TRAV25	CAGPFLGSNYQLIW	TRAJ33
AS1803	4367/6255 69.8%	TRBV9	CASSVEDQVAGDFLNEQFF	TRBJ2-1	TRAV1-2	CAVTNDYKLSF	TRAJ20

Sample	Freq.	TRBV	CDR3β	TRBJ	TRAV	CDR3α	TRAJ
AS1541 (AS2)	1/4868 0.021%	TRBV9	CASSVGLYSTDTQY F	TRBJ2-3	TRAV21; TRAV8-6	CAALGGDSGGGADGL TF; CAVIESNYQLIW	TRAJ45; TRAJ33
AS1455 (AS4.1)	4/10736 0.037%	TRBV9	CASSVGLYSTDTQY F	TRBJ2-3	TRAV21	CAVSSPQGGSEKLVF	TRAJ57
AS1455 (AS4.2)	1/10736 0.009%	TRBV9	CASSVGLFSTDTQY F	TRBJ2-3	TRAV21	CAVLSPVQETSGSRLT F	TRAJ58
AS1455 (AS4.3)	1/10736 0.009%	TRBV9	CASSVATYSTDTQY F	TRBJ2-3	TRAV21	CAVSNFNKFYF	TRAJ21
AS1455 (AS4.4)	3/10736 0.028%	TRBV9	CASSVGLYSTGELFF	TRBJ2-2	TRAV21; TRAV4	CAVSFFDKLIF; CLVGEARGWELPTHF	TRAJ34; TRAJ28
AS1455 (AS4.4)	1/10736 0.009%	TRBV9	CASSVGLYSTGELFF	TRBJ2-2	TRAV21; TRAV38	CAVSFFDKLIF; CAYTNAGKSTF	TRAJ34; TRAJ27
AS1455 (AS4.4)	1/10736 0.009%	TRBV9	CASSVGLYSTGELFF	TRBJ2-2	TRAV21	CAVSFFDKLIF	TRAJ34

Supplementary Table 2

Frequency-based TRA-TRB pairing data (Patient P)									
	Freq. (clonotype cDNA count)	TRAV	CDR3b	TRAJ		Freq. (clonotype cDNA count)	TRBV	CDR3a	TRBJ
Replicate 1 (85% TRBV9+ of CD3+CD8+)									
TRB	<u>20.6% (116/564)</u>	<u>TRBV9</u>	<u>CASSVGLYSTDTQ</u>	<u>TRBJ2-3</u>	TRA	<u>39.5% (217/550)</u>	<u>TRAV21</u>	<u>CAVSLGTGAGSYQL</u>	<u>TRAJ28</u>
	7.8% (44/564)	TRBV9	CASSPDGGNTGEL	TRBJ2-2		4.0% (22/550)	TRAV30	CGTVAH_DSNYQL	TRAJ33
	5.3% (30/564)	TRBV9	CASSVAGEAYNEQ	TRBJ2-1		3.1% (17/550)	TRAV12-1	CVVESGGSYIP	TRAJ6
	4.3% (24/564)	TRBV9	CASSVEGHSPYEQ	TRBJ2-7		2.4% (13/550)	TRAV41	CAVGINFGNEKL	TRAJ48
	2.7% (15/564)	TRBV9	CASSVEAYNEQ	TRBJ2-1		2.0% (11/550)	TRAV38-2DV8	CAYLNMNRDDKI	TRAJ30
	2.5% (14/564)	TRBV9	CASSGGLVADTQ	TRBJ2-3		1.8% (10/550)	TRAV30	CGTEILNDYKL	TRAJ20
	2.3% (13/564)	TRBV9	CASSEDGNYEQ	TRBJ2-7		1.8% (10/550)	TRAV1-2	CAVTDSNYQL	TRAJ33
	1.6% (9/564)	TRBV9	CASSVVTGVHTGEL	TRBJ2-2		1.6% (9/550)	TRAV41	CAAPGGYGGSGQNL	TRAJ42
	1.2% (7/564)	TRBV9	CASSVGISDNEQ	TRBJ2-1		1.6% (9/550)	TRAV13-1	CAVEGGANNL	TRAJ36
1.2% (7/564)	TRBV9	CASSVEAYNEQ	TRBJ2-1		1.1% (6/550)	TRAV12-1	CVVNNYGGSQGNL	TRAJ42	
Replicate 2 (90% TRBV9+ of CD3+CD8+)									
TRB	<u>26.9% (215/800)</u>	<u>TRBV9</u>	<u>CASSVGLYSTDTQ</u>	<u>TRBJ2-3</u>	TRA	<u>41.7% (287/688)</u>	<u>TRAV21</u>	<u>CAVSLGTGAGSYQL</u>	<u>TRAJ28</u>
	5.4% (43/800)	TRBV9	CASSPDGGNTGEL	TRBJ2-2		3.8% (26/688)	TRAV30	CGTVAH_DSNYQL	TRAJ33
	4.1% (33/800)	TRBV9	CASSVAGEAYNEQ	TRBJ2-1		3.6% (25/688)	TRAV38-2DV8	CAYLNMNRDDKI	TRAJ30
	3.4% (27/800)	TRBV9	CASSVEGHSPYEQ	TRBJ2-7		2.6% (18/688)	TRAV13-1	CAVEGGANNL	TRAJ36
	2.6% (21/800)	TRBV9	CASSVDREGLDEQ	TRBJ2-7		2.3% (16/688)	TRAV30	CGTEILNDYKL	TRAJ20
	2.6% (21/800)	TRBV9	CASSPRLAHEQ	TRBJ2-1		1.9% (13/688)	TRAV1-2	CAVTDSNYQL	TRAJ33
	1.8% (14/800)	TRBV9	CASSAGQGQETQ	TRBJ2-5		1.6% (11/688)	TRAV27	CAGAETMIKAAGNKL	TRAJ17
	1.6% (13/800)	TRBV9	CASSGGLVADTQ	TRBJ2-3		1.6% (11/688)	TRAV12-1	CVVESGGSYIP	TRAJ6
	1.5% (12/800)	TRBV5-1	CATPPLGV_RGTSSYEQ	TRBJ2-7		1.5% (10/688)	TRAV13-2	CAETGQGGKL	TRAJ23
	1.5% (12/800)	TRBV9	CASSTGQLSSGNTI	TRBJ1-3		1.2% (8/688)	TRAV4	CLVGVPYSSASKI	TRAJ3

Single-cell VDJ-paring data (Patient P)							
Sample	Freq.	TRBV	CDR3b	TRBJ	TRAV	CDR3a	TRAJ
AS3.1	15.241%	TRBV9	CASSVGLYSTDTQYF	TRBJ2-3	TRAV21	CAVSLGTGAGSYQLTF	TRAJ28

Single-cell VDJ-paring data (Patient K)							
Sample	Freq.	TRBV	CDR3b	TRBJ	TRAV	CDR3a	TRAJ
AS8.2	3.181%	TRBV9	CASSVGLYSTDTQYF	TRBJ2-3	TRAV21	CAVPNQAGTALIF	TRAJ15
AS8.3	1.438%	TRBV9	CASSVGLYSTDTQYF	TRBJ2-3	TRAV21	CAATSPRRQGGSEKLVF	TRAJ57
AS8.4	1.787%	TRBV9	CASSVGTYSTDTQYF	TRBJ2-3	TRAV21	CAVNSPGSGAGSYQLTF	TRAJ28
AS8.5	0.872%	TRBV9	CASSVATYSTDTQYF	TRBJ2-3	TRAV21	CAVMDQDGANSKLTF	TRAJ56

Single-cell VDJ-paring data (Patient N)							
Sample	Freq.	TRBV	CDR3b	TRBJ	TRAV	CDR3a	TRAJ
AS9.1	2.436%	TRBV9	CASSGGLYSTDTQYF	TRBJ2-3	TRAV21	CAVSFPAGANSKLTF	TRAJ56
AS9.2	0.244%	TRBV9	CASSVGLYSTDTQYF	TRBJ2-3	TRAV21	CAVLMEYGNKLVF	TRAJ47

Single-cell VDJ-paring data (Patient S)							
Sample	Freq.	TRBV	CDR3b	TRBJ	TRAV	CDR3a	TRAJ
AS10.1	1.956%	TRBV9	CASSVATYSTDTQYF	TRBJ2-3	TRAV21	CAADSGSARQLTF	TRAJ22
AS10.2	0.775%	TRBV9	CASSLGLYSTDTQYF	TRBJ2-3	TRAV21	CAAYSGGGADGLTF	TRAJ45
AS10.3	0.443%	TRBV9	CASSVATYSTDTQYF	TRBJ2-3	TRAV21	CAVSSGGSGAGSYQLTF	TRAJ28
AS10.4	0.037%	TRBV9	CASSVGLYSTDTQYF	TRBJ2-3	TRAV21	CAVSTIIQGAQKLVF	TRAJ54

Supplementary Table 3

Name	Sequence	Activated TCR	Name	Sequence	Activated TCR
AS 9mer 1	SRIMLLAPK	AS3.1 AS4.1 AS4.2 AS4.3 AS4.4	AS 10mer 1	YRNGHVYPAR	None
AS 9mer 2	GRIMLLAPK	AS3.1 AS4.1 AS4.2 AS4.3 AS4.5	AS 10mer 2	RRDWSYVQPK	None
AS 9mer 3	SRVMLLAPK	AS3.1 AS4.1 AS4.2 AS4.3 AS4.6	AS 10mer 3	YRLGHVYPAK	None
AS 9mer 4	DRVMLIAPR	AS3.1 AS4.1 AS4.2 AS4.3	AS 10mer 4	HRQPRISWVR	None
AS 9mer 5	GRLMLIAPK	AS3.1 AS4.1 AS4.2 AS4.3	AS 10mer 5	YRDGHTWIVR	None
AS 9mer 6	NRLMMIAPR	AS3.1 AS4.1 AS4.2 AS4.3	AS 10mer 6	IRLPGFP LRK	None
AS 9mer 7	GRVMLVAPK	AS3.1 AS4.1 AS4.2 AS4.3 AS4.6	AS 10mer 7	ERSSYWARRR	AS4.1
AS 9mer 8	TRVMLISPK	AS3.1 AS4.1 AS4.2 AS4.3	AS 10mer 8	GRVMLLNPMR	AS3.1 AS4.2 AS4.3
AS 9mer 9	ARVMLVAPR	AS3.1 AS4.1 AS4.2 AS4.3	AS 10mer 9	IRLPGFP LRR	None
AS 9mer 10	SRVMLLAPR	AS3.1 AS4.1 AS4.2 AS4.3	AS 10mer 10	GRLPGFP LRK	None
AS 9mer 11	GRQVPV LWR	AS3.1 AS4.1 AS4.2	AS 10mer 11	NRIMLQLDPK	None
AS 9mer 12	SRVMLLNPK	AS3.1 AS4.1 AS4.2 AS4.3	AS 10mer 12	ARRVMLVAPK	AS4.2 AS4.3
AS 9mer 13	GRMPLVAPK	AS3.1 AS4.1 AS4.2 AS4.3 AS4.4	AS 10mer 13	TRLMLITDPK	AS4.2
AS 9mer 14	DRMMLHAPK	AS4.3	AS 10mer 14	TRQMLVARLK	None
AS 9mer 15	ARPQLVAPK	AS4.3	AS 10mer 15	SRNMLVARLK	None
AS 9mer 16	NRVQIIISP K	AS3.1 AS4.3	AS 10mer 16	GRVMLLAPLR	AS3.1 AS4.2 AS4.3 AS4.4
AS 9mer 17	GRVMLRAPK	AS4.1 AS4.3 AS4.4	AS 10mer 17	DRLMLNPMR	None
AS 9mer 18	GRPMFYSVK	AS4.2 AS4.4	AS 10mer 18	VRVMLENPMR	None
AS 9mer 19	GRVPLRAPK	AS4.1 AS4.2 AS4.3 AS4.4	AS 10mer 19	GRLMLVSPKG	AS4.2 AS4.3
			AS 10mer 20	ERLMLIAPLR	AS4.2 AS4.3

Supplementary Table 4

Name	Sequence	Activated TCR	Name	Sequence	Activated TCR
NPDC1	GRVVVISPR	None	PLEKHA7	DRAVLIPPK	None
MRPL52	SRKMLLNPK	None	CCDC61	GRPGSLAPR	None
ACSM5	DRMMLVLPR	None	TMTC4	GRRLHLAPR	None
PLEKHA7	SRSMLEVPR	None	ZNF286B	GRVELVAWK	None
SH3PXD2B	GRALLVPPK	None	PLEKHJ1	GRVPGWAPR	None
LIRC47	NRLMLPEPR	None	ZBTB5	SRVMIGSPR	None
WDR73	GRLCLLDPR	None	LINC00346	ARVGLSSPR	None
DYNC1H1	GRTMAITPR	None	SEC14L2	GRVGDLSPR	AS4.3 AS4.4
ACD	GRGLLLRPR	None	SEC14L3	GRVGDLSPK	None
PRKACA	GRVMLVKHK	None	KIF26B	SRLLLASPR	None
ZNF469	GRPLLRPPK	None	ITPKC	ARMGLEAPR	None
SERPINH1	GREELRSPK	None	CPT1C	SRNSLLSPR	None
ANKRD24	GRRLLLEPR	None	KIF26B	SRLLLASPR	None
LOC102723971	ARRMLEDPK	None	DICER1	SRLNLLTPR	None
WNK3	GRHPLPSPK	None	KMT5C	SRQGLLGPR	None
DCAF10	GRVSLYQPK	None	PKD1	SRPRLVLP	None
COL20A1	GRVGLQGPK	None	RFX5	ARLPLLLPR	None
FBXL21	GRVGLNCPR	None	UMODL1	SRLLLGLPR	None
C11orf96	GRGRLRRPR	None	PIF1	ARAQLLGPR	None
GAS2L2	GRRTLRKPK	None	PACS2	ARSQLQIPR	None
SYNGR3	GRRGLREPR	None	NOS1	SRQNLSQPK	None
PKHD1	GRFSLRQPR	None	CCDC177	SRVVLTPR	None
NUP214	GRLLLMRPK	None	ROBO4	SRRGLSSPR	None
WNT2B	GRVMLRSSR	None	BSN	SRAPLQKPR	None
MCAT	GRGLLNYP	None	UBQLN1	MQNMLSAPY	None
CCND3	GRSLLPSPR	None	GPER1	GQMWLLAPR	AS3.1 AS4.1 AS4.2
KCNN1	GRVMLLSHK	None	UBQLN2	IQNMLSAPY	None
KAT6A	GRIALPKPR	None	TTC13	TKVMLNDPL	None
SPEG	GRQLLSIPR	None	HELQ	RRVILRAPY	AS4.2 AS4.3
RNF130	GRYGLDSPK	None	IPO9	TQMPLVAPV	AS4.3
ARHGAP33	GRCLLPKPR	None	RANBP3	GRGQLAAPV	None
SGSM1	GRSMLVVAR	None	PIEZO2	GRNNLTAPV	None
RP11	GRMVLEPPR	None	CNNM4	GRLLLAAPV	None
C1QTNF5	GRPGLPGPR	None	GLRB	VQVMLNNPK	AS4.3
MEGF8	GRDGLQGPR	None	SYMPK	TKVVLEAPL	None
VWF F8VWF	GRCELNCPK	None	UBE2U	LQVMSNPV	None
ATR FRP1	GRAMLLVGR	None	AOX1	TQSMLVVPK	None
SHISAL1	GRWMKQDPR	None	ETV4	GREPLPAPY	None
CHD9	GRRMKSKPK	None	ZC3H7B	RKDMLLCPR	None
C20orf203	GRAMGGMPR	None	MICU3	GRGMLPIPV	None
TRIL	GRVCPVAPR	None	EXPH5	QRVSLNAPM	None
MKI67	SRRVLRAPK	None	TTC17	ERVNLSAPL	None
USP4	GRDAHVAPR	None	VRTN	SKVMLQAVR	None
GAS2L1	ARLGLLAPR	None	ICMT	TQVMLCNP I	None
GAREM2	ARLCLPAPR	None	TTC13	TKVMLNDPL	None
IL23R	RRILLIIPK	None	DCAF10	GRVSLYQPK	None
ACSM3	DRVILILPR	None	SRCAP	TQTMLPAPV	None
TRPM4	NRDTLINPK	None	RNASEH2B	GQVMVAPR	AS4.2 AS4.3
PRPF3	TRLALIAPK	AS3.1 AS4.3	DAB2IP	GRPQLLAPL	None
JAK3	DRQQLPAPK	AS4.3	HPS6	GKVMVAAPR	None
JAK2	DRHQLPAPK	None	CBFB	GKVYLKAPM	None
CBL	DRVSLLLPR	None	MICU3	GRGMLPIPV	None
EFNB3	DRLDLLCPR	None	CATSPERB	GRVPLQSPY	None
KCNQ3	DRVRLSNPR	None	CHPF	RRVQLLRPL	None
KLHL5	RRPMLQSPR	None	IQCN	VQGMVLVPPM	None
MUC5B	NRVVLLDPK	None	RPL13A	GKSLLVAPL	None
C10orf143	SRGCLPAPR	None	NAGK	GRNPLVMAR	None
GON4L	SRYPLLLPK	None	OPRT	GRVMLVDDV	None
ARHGEF3	SRPDILAPR	None	PBP-1b	GRVMLVDAL	None
TP53TG5	TRIHLAPR	None	UvrABC	KRLMLLAPI	AS4.2
CDKAL1	SRMVLPMPR	None	UPF0324 YeiH	LRVMMLAPF	AS3.1 AS4.1 AS4.2 AS4.3
SF3A1	MRIGLLDPR	None	ITOCD	SRIMLLVLI	None
BSN	TRVPMIAPR	None	gspD	GKTELLAPF	AS4.3
MPP4	LRQMLQAPH	AS4.3			

Supplementary Table 5

Protein name	Peptide sequence	EC ₅₀ (uM)						K _D (uM)					
		AS3.1	AS4.1	AS4.2	AS4.3	AS4.4	AS8.4	AS3.1	AS4.1	AS4.2	AS4.3	AS4.4	AS8.4
PRPF3	TRLALIAPK	7.8			2.8		4.47	42.9	50	157	17.6		
JAK3	DRQQLPAPK				375								
GPB1	GQMWLLAPR	2	38.4	29.3			<0.001	118	82	50	>200		15
HELQ	RRVILRAPY			60.6	36								
IPO9	TQMPLVAPV				43								
GLRB	VQVMLNNPK				6.7								
RNASEH2B	GQVMVVAPR			12.7	0.08					36	15		
SEC14L2	GRVGDLSPR				>1000	>1000							
MPP4	LRQMLQAPH				1.1								
UvrABC	KRLMLLAPI			0.3									
YEIH	LRVVMLAPF	2.2		0.9	0.3		<0.001	14.4	26	19	4.1		1.2

Supplementary Table 6. Data collection and refinement statistics (molecular replacement)

	AS3.1-PRPF3-B27	AS4.2-PRPF3-B27	AS4.2-YEIH-B27	AS4.3-PRPF3-B27	AS4.3-RNASEH2B-B27	AS4.3-YEIH-B27	AS8.4-YEIH-B27
Data collection							
Space group	P 1 21 1	P 1 21 1	P 21 21 21	P21 21 21	P21 21 21	P 1 21 1	P 1 21 1
Cell dimensions <i>a</i> , <i>b</i> , <i>c</i> (Å)	83.211, 52.789, 106.291	83.109, 53.154, 106.818	54.832, 95.999, 180.481	54.68, 94.423, 178.522	54.925, 93.992, 177.774	54.977, 97.412, 175.484	83.226, 51.731, 98.411
α , β , γ (°)	90, 98.278, 90	90, 98.485, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 92.325, 90	90, 96.995, 90
Resolution (Å)	42.13 - 2.37 (2.455 - 2.37)	42.35 - 2.3 (2.382 - 2.3)	42.38 - 2.303 (2.385 - 2.303)	36.99 - 2.284 (2.366 - 2.284)	47 - 2.5 (2.589 - 2.5)	46.58 - 2.7 (2.796 - 2.7)	39.82 - 2.2 (2.279 - 2.2)
Ellipsoidal ^a Resolution Limit (Å) (direction) ^b	2.398 (0.969 a* + 0.245 c*) 2.366 (b*) 4.148 (-0.262 a* + 0.968 c*)						
<i>R</i> _{merge}	0.270	0.0883	0.122	0.293	0.2445	0.1261	0.213
<i>I</i> / σ <i>I</i>	4.9	9.79	7.0	7.6	5.88	2.69	6.8
Completeness (%)	50.56 (2.25)	96.30 (98.05)	99.12 (93.06)	99.20 (95.94)	99.12 (97.94)	96.99 (96.10)	92.97 (92.38)
Completeness (ellipsoidal) ^c (%)	88.5 (48.6)						
Redundancy	3.4	3.4	3.4	13.1	4.4	2.0	7.3
Refinement							
Resolution (Å)	42.13 - 2.37 (2.455 - 2.37)	42.35 - 2.3 (2.382 - 2.3)	42.38 - 2.303 (2.385 - 2.303)	36.99 - 2.284 (2.366 - 2.284)	47 - 2.5 (2.589 - 2.5)	46.58 - 2.7 (2.796 - 2.7)	39.82 - 2.2 (2.279 - 2.2)
No. reflections	18996 (84)	39924 (4022)	42680 (3929)	42521 (4062)	32459 (3131)	49470 (4879)	39685 (3915)
<i>R</i> _{work} / <i>R</i> _{free}	0.250/0.309	0.248/0.291	0.221/0.267	0.248/0.289	0.230/0.288	0.213/0.264	0.220/0.264
No. atoms	6464	6715	6738	6612	6624	13413	6706
Protein	6439	6563	6624	6460	6467	13221	6637
Ligand/ion	20	75	54	89	97	122	6
Water	5	77	60	63	60	70	63
<i>B</i> -factors							
Protein	46.25	48.32	60.39	88.07	65.76	77.20	59.63
Ligand/ion	54.93	60.63	74.78	101.98	72.40	88.88	68.73
Water	28.47	30.00	49.41	64.13	40.88	55.38	51.12
R.m.s. deviations							
Bond lengths (Å)	0.002	0.002	0.002	0.002	0.002	0.002	0.003
Bond angles (°)	0.43	0.46	0.46	0.48	0.46	0.51	0.58
PDB	7N2S	7N2N	7N2O	7N2R	7N2P	7N2Q	8CX4

Values in parentheses are for highest-resolution shell.

^a These statistics are for data that were truncated by STARANISO to remove poorly measured reflections affected by anisotropy.

^b The resolution limits for three directions in reciprocal space are indicated here. To accomplish this, STARANISO computed an ellipsoid postfitted by least squares to the cutoff surface, removing points where the fit was poor. Note that the cutoff surface is unlikely to be perfectly ellipsoidal, so this is only an estimate.

^c The anisotropic completeness was obtained by least squares fitting an ellipsoid to the reciprocal lattice points at the cutoff surface defined by a local mean *I*/ σ *I* threshold of 1.0, rejecting outliers in the fit due to spurious deviations (including any cusp), and calculating the fraction of observed data lying inside the ellipsoid so defined. Note that the cutoff surface is unlikely to be perfectly ellipsoidal, so this is only an estimate.