



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:11 AM UTC

PDB ID : 6OMF / pdb_00006omf
EMDB ID : EMD-20090
Title : CryoEM structure of SigmaS-transcription initiation complex with activator CrI
Authors : Jaramillo Cartagena, A.; Darst, S.A.; Campbell, E.A.
Deposited on : 2019-04-18
Resolution : 3.26 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

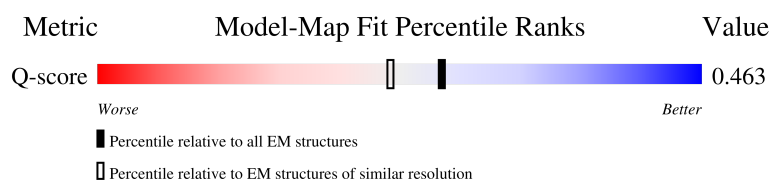
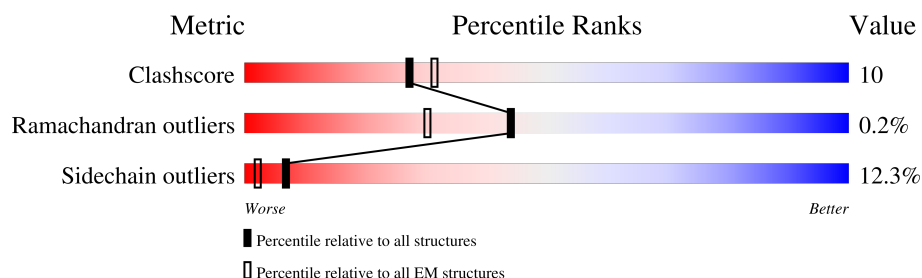
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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.



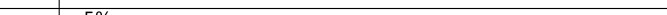
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	239	7% 63% 29% 5% .
1	B	239	. 61% 29% 7%
2	C	1342	6% 69% 26% .
3	D	1407	10% 66% 25% 5%

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Mol	Chain	Length	Quality of chain
4	E	91	
5	F	331	
6	J	136	
7	T	66	
8	N	66	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 30251 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	233	Total	C	N	O	S	0	0
			1806	1127	317	356	6		
1	B	223	Total	C	N	O	S	0	0
			1714	1070	302	336	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z6
A	236	VAL	-	expression tag	UNP P0A7Z6
A	237	LEU	-	expression tag	UNP P0A7Z6
A	238	PHE	-	expression tag	UNP P0A7Z6
A	239	GLN	-	expression tag	UNP P0A7Z6
B	235	GLU	-	expression tag	UNP P0A7Z6
B	236	VAL	-	expression tag	UNP P0A7Z6
B	237	LEU	-	expression tag	UNP P0A7Z6
B	238	PHE	-	expression tag	UNP P0A7Z6
B	239	GLN	-	expression tag	UNP P0A7Z6

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1336	Total	C	N	O	S	0	0
			10382	6522	1851	1960	49		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoS.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	278	Total	C	N	O	S	0	0
			2244	1406	415	419	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP S5ZIY8

- Molecule 6 is a protein called Sigma factor-binding protein Crl.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	127	Total	C	N	O	S	0	0
			1024	667	166	187	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP A0A0F7J6B7
J	-1	PRO	-	expression tag	UNP A0A0F7J6B7
J	0	HIS	-	expression tag	UNP A0A0F7J6B7

- Molecule 7 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	43	Total	C	N	O	P	0	0
			876	418	155	260	43		

- Molecule 8 is a DNA chain called Non-template DNA strand.

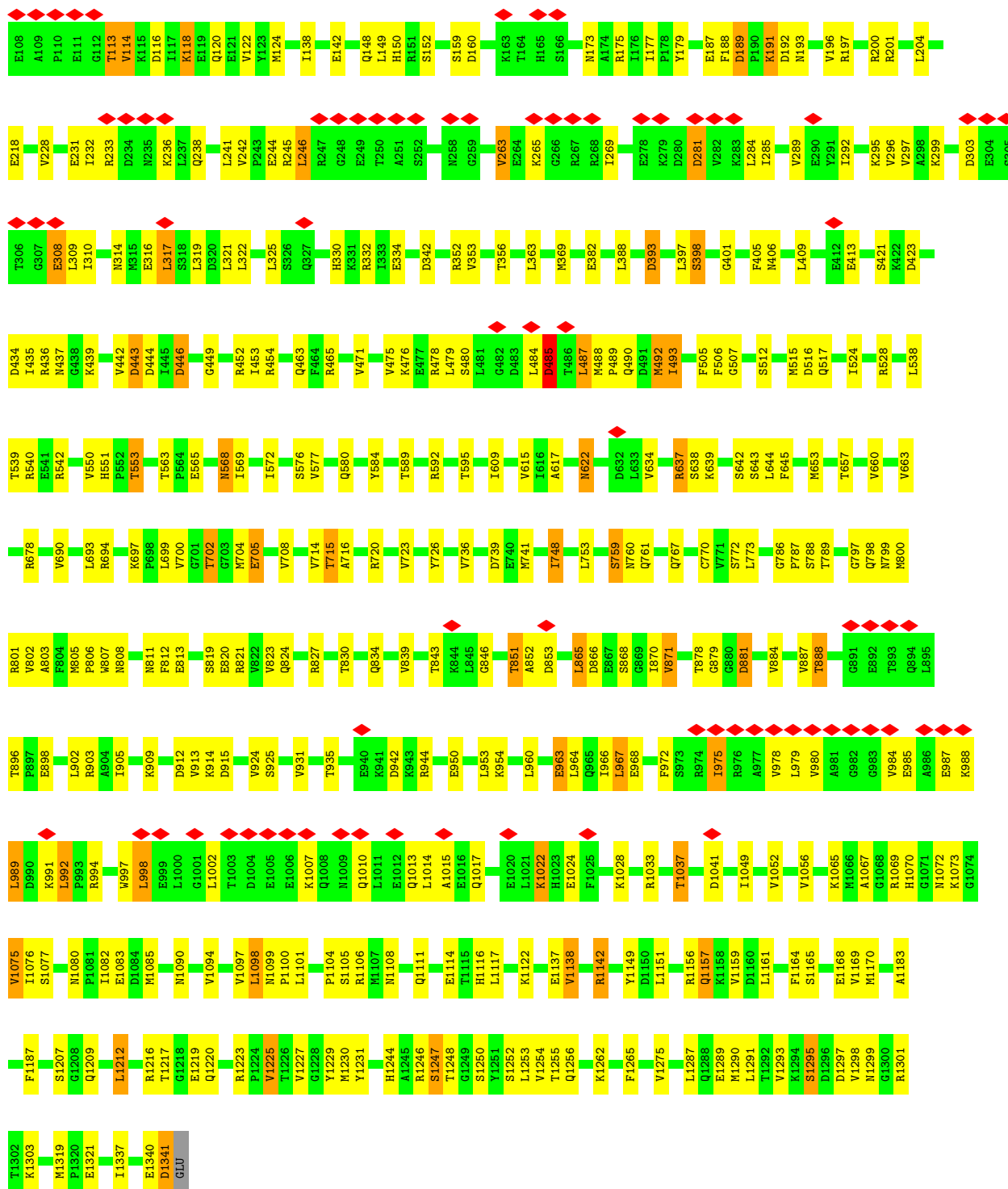
Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	49	Total	C	N	O	P	0	0
			1008	481	191	288	48		

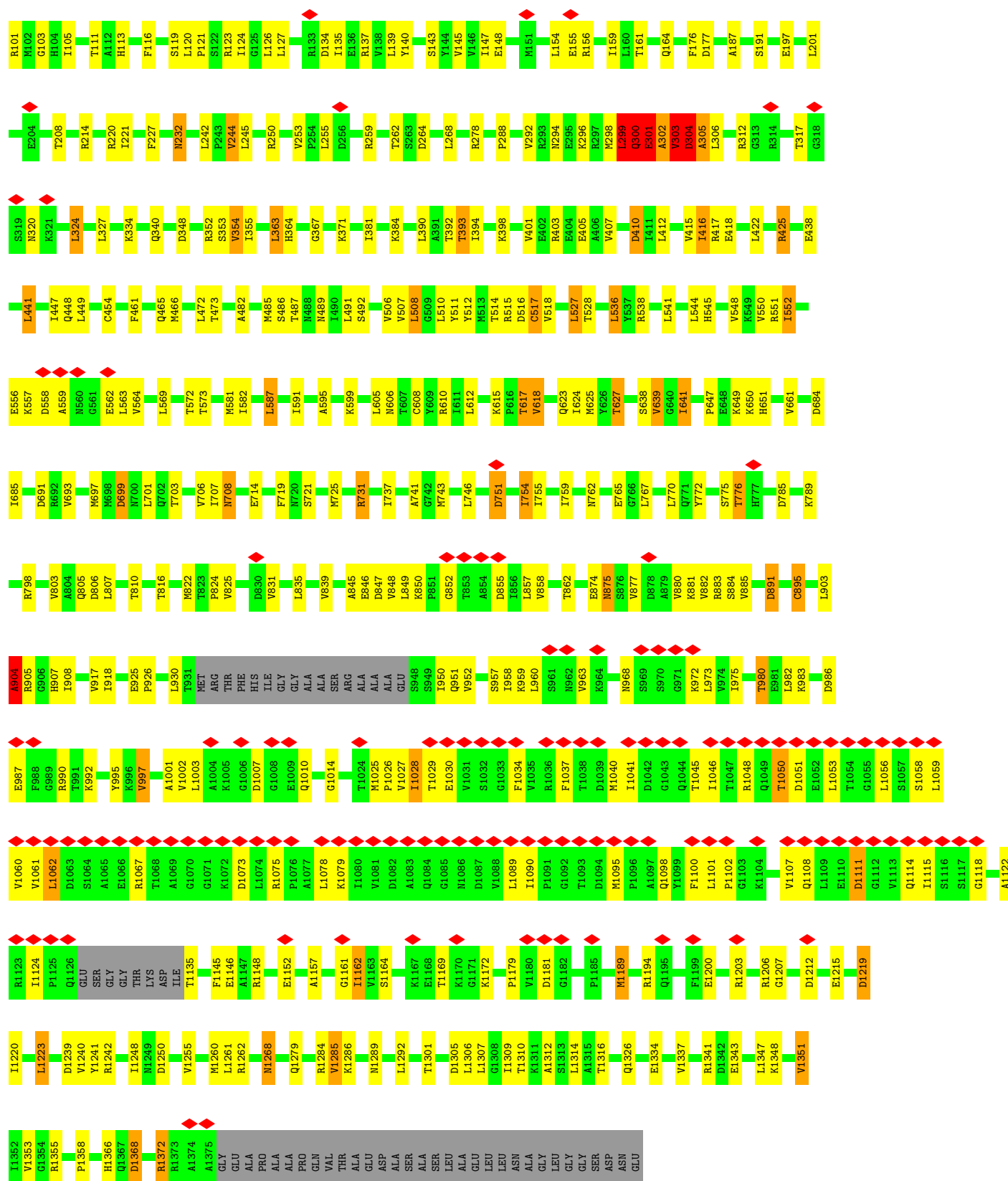
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total 1	Mg 1	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total 2	Zn 2	0

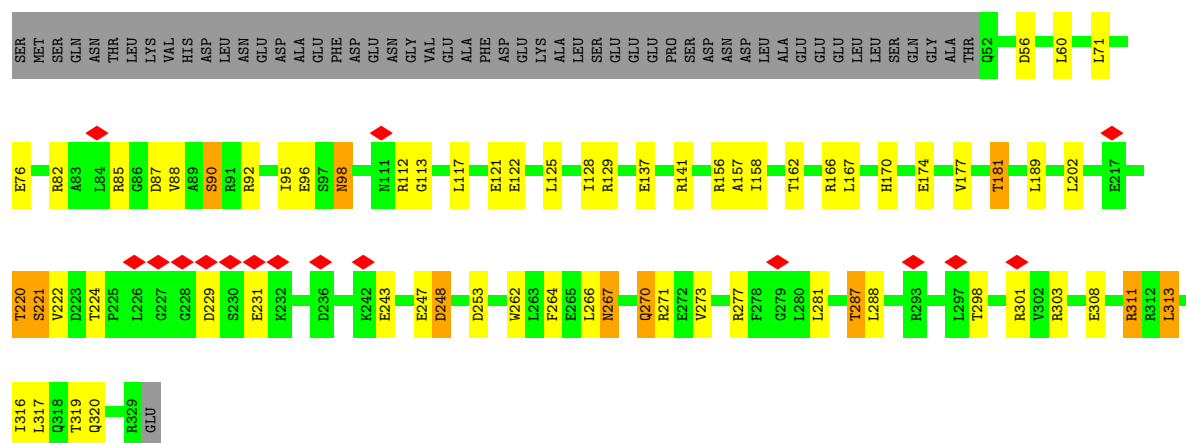




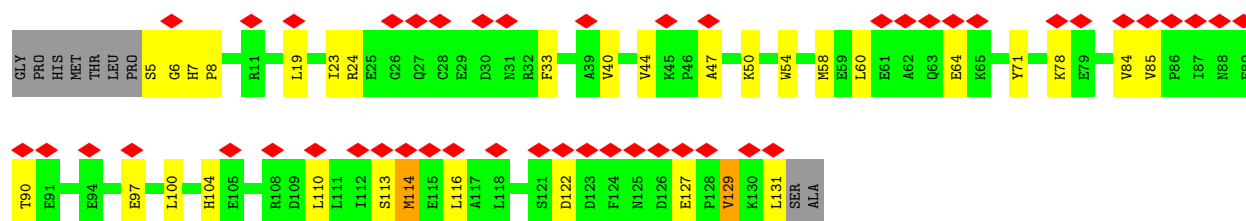
• Molecule 4: DNA-directed RNA polymerase subunit omega



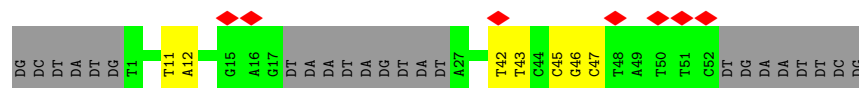
Chain F: 5% 64% 17% 16%



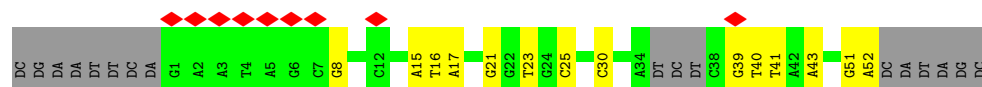
Chain J: 35% 70% 22% 7%



Chain T:



Chain N:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	292000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.935	Depositor
Minimum map value	-2.803	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.55	0/1828	0.67	2/2479 (0.1%)
1	B	0.46	0/1734	0.64	2/2349 (0.1%)
2	C	0.55	0/10736	0.61	6/14487 (0.0%)
3	D	0.63	17/10539 (0.2%)	0.65	7/14232 (0.0%)
4	E	0.48	0/629	0.64	0/847
5	F	0.40	0/2273	0.56	0/3065
6	J	0.25	0/1054	0.52	0/1433
7	T	0.42	0/979	0.56	0/1505
8	N	0.42	0/1132	0.60	0/1744
All	All	0.55	17/30904 (0.1%)	0.62	17/42141 (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	1
1	B	0	1
2	C	0	2
3	D	0	3
All	All	0	7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	300	GLN	CA-C	-11.35	1.37	1.52
3	D	305	ALA	CA-C	-8.93	1.43	1.52
3	D	302	ALA	C-O	-8.64	1.13	1.24
3	D	302	ALA	CA-CB	-8.25	1.40	1.53
3	D	304	ASP	C-O	-8.15	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	ALA	CA-C	-7.92	1.42	1.52
3	D	301	GLU	N-CA	-7.11	1.36	1.46
3	D	301	GLU	CA-CB	-6.84	1.44	1.53
3	D	299	LEU	CB-CG	-6.62	1.40	1.53
3	D	305	ALA	C-N	-6.17	1.25	1.33
3	D	300	GLN	CA-CB	-6.04	1.43	1.53
3	D	305	ALA	C-O	-6.00	1.15	1.23
3	D	299	LEU	CA-C	-5.92	1.44	1.52
3	D	303	VAL	C-O	-5.88	1.17	1.24
3	D	303	VAL	CA-C	-5.73	1.45	1.52
3	D	303	VAL	CA-CB	-5.28	1.47	1.54
3	D	300	GLN	CG-CD	-5.18	1.39	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	305	ALA	N-CA-C	-7.60	102.82	112.93
3	D	301	GLU	N-CA-C	-6.98	105.30	113.88
3	D	903	LEU	CA-C-N	6.71	134.35	121.54
3	D	903	LEU	C-N-CA	6.71	134.35	121.54
3	D	300	GLN	CB-CA-C	-6.39	97.69	110.42
3	D	1240	VAL	N-CA-C	-6.16	106.91	111.90
2	C	485	ASP	CA-C-N	5.68	132.38	121.54
2	C	485	ASP	C-N-CA	5.68	132.38	121.54
2	C	484	LEU	CA-C-N	5.56	131.71	121.70
2	C	484	LEU	C-N-CA	5.56	131.71	121.70
1	B	168	ILE	CA-C-N	5.42	131.45	121.70
1	B	168	ILE	C-N-CA	5.42	131.45	121.70
1	A	7	GLU	CA-C-N	5.26	131.58	121.54
1	A	7	GLU	C-N-CA	5.26	131.58	121.54
3	D	299	LEU	CB-CG-CD1	-5.23	95.02	110.70
2	C	233	ARG	CA-C-N	5.19	131.45	121.54
2	C	233	ARG	C-N-CA	5.19	131.45	121.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	GLU	Peptide
1	B	19	VAL	Peptide
2	C	398	SER	Peptide
2	C	485	ASP	Peptide

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Mol	Chain	Res	Type	Group
3	D	119	SER	Peptide
3	D	1326	GLN	Peptide
3	D	904	ALA	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	1806	0	1835	48	0
1	B	1714	0	1748	44	0
2	C	10567	0	10585	214	0
3	D	10382	0	10594	238	0
4	E	627	0	634	11	0
5	F	2244	0	2279	46	0
6	J	1024	0	949	16	0
7	T	876	0	487	7	0
8	N	1008	0	554	11	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	30251	0	29665	588	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 10.

All (588) 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:236:VAL:HG13	1:B:16:ILE:CG2	1.79	1.13
3:D:300:GLN:NE2	3:D:304:ASP:OD2	1.85	1.08
3:D:299:LEU:O	3:D:302:ALA:N	1.85	1.06
3:D:300:GLN:NE2	3:D:300:GLN:O	1.90	1.05
1:A:233:ASP:O	1:A:235:GLU:OE1	1.80	1.00
3:D:299:LEU:O	3:D:301:GLU:N	2.04	0.89
1:A:236:VAL:HG13	1:B:16:ILE:HG21	1.55	0.86
2:C:963:GLU:O	2:C:967:LEU:HB2	1.79	0.83
3:D:303:VAL:O	3:D:305:ALA:N	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:299:LEU:C	3:D:301:GLU:H	1.85	0.81
1:A:236:VAL:CG1	1:B:16:ILE:CG2	2.58	0.81
5:F:273:VAL:O	5:F:277:ARG:HB2	1.89	0.72
1:A:237:LEU:HD23	1:B:15:ASP:HA	1.70	0.72
3:D:70:CYS:SG	3:D:71:LEU:N	2.64	0.71
1:A:45:ARG:O	1:A:49:SER:HB2	1.92	0.70
3:D:963:VAL:HG11	3:D:980:THR:HA	1.72	0.70
1:A:45:ARG:HE	1:B:38:THR:HG22	1.57	0.68
2:C:398:SER:HB2	2:C:401:GLY:H	1.58	0.67
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	1.77	0.66
1:A:236:VAL:HG13	1:B:16:ILE:HG23	1.73	0.65
3:D:885:VAL:HG11	3:D:1255:VAL:HG12	1.76	0.65
1:A:236:VAL:CG1	1:B:16:ILE:HG23	2.26	0.64
3:D:85:CYS:SG	3:D:86:GLU:N	2.70	0.64
3:D:393:THR:OG1	3:D:394:ILE:N	2.31	0.64
1:A:233:ASP:C	1:A:235:GLU:OE1	2.41	0.64
5:F:92:ARG:O	5:F:96:GLU:HB2	1.98	0.63
2:C:1341:ASP:N	2:C:1341:ASP:OD1	2.31	0.63
3:D:1285:VAL:O	3:D:1289:ASN:ND2	2.31	0.63
1:A:95:LYS:NZ	1:A:120:ASP:OD2	2.32	0.63
6:J:47:ALA:HB3	6:J:50:LYS:HG3	1.79	0.63
2:C:528:ARG:NH2	2:C:576:SER:O	2.32	0.63
3:D:849:LEU:HA	3:D:857:LEU:H	1.62	0.62
3:D:959:LYS:HB3	3:D:983:LYS:HB2	1.80	0.62
2:C:1341:ASP:HB3	3:D:17:PHE:HA	1.82	0.62
3:D:303:VAL:C	3:D:305:ALA:H	2.08	0.62
1:A:182:ARG:NH1	2:C:1090:ASN:O	2.33	0.62
2:C:1223:ARG:NH2	3:D:721:SER:OG	2.34	0.61
5:F:156:ARG:HH12	8:N:23:DT:H72	1.65	0.61
1:A:11:PRO:HA	1:A:30:PRO:HD2	1.83	0.61
1:A:125:LYS:HE2	1:A:128:HIS:HB2	1.83	0.61
2:C:985:GLU:HB3	2:C:988:LYS:HB3	1.82	0.60
3:D:121:PRO:O	3:D:123:ARG:NH1	2.34	0.60
4:E:4:VAL:HG22	4:E:5:THR:HG23	1.83	0.60
3:D:1219:ASP:N	3:D:1219:ASP:OD1	2.34	0.60
2:C:452:ARG:NH2	2:C:584:TYR:O	2.35	0.60
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.84	0.60
3:D:582:ILE:HD12	3:D:623:GLN:HB3	1.84	0.60
3:D:708:ASN:OD1	3:D:708:ASN:N	2.34	0.59
2:C:159:SER:OG	2:C:160:ASP:N	2.34	0.59
2:C:191:LYS:H	2:C:191:LYS:HZ2	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:565:GLU:HA	2:C:569:ILE:HG12	1.84	0.59
2:C:642:SER:OG	2:C:643:SER:N	2.35	0.59
2:C:699:LEU:HB2	2:C:799:ASN:HD22	1.67	0.59
5:F:267:ASN:OD1	5:F:267:ASN:N	2.35	0.59
1:A:222:THR:HA	1:B:232:VAL:HG23	1.85	0.59
5:F:311:ARG:HA	5:F:311:ARG:HH11	1.68	0.59
2:C:446:ASP:N	2:C:446:ASP:OD1	2.37	0.58
2:C:989:LEU:O	2:C:997:TRP:NE1	2.36	0.58
5:F:122:GLU:HG2	5:F:157:ALA:HB2	1.85	0.58
3:D:111:THR:HG21	3:D:300:GLN:HA	1.86	0.58
1:A:70:THR:OG1	1:A:71:LYS:N	2.35	0.58
2:C:992:LEU:O	2:C:997:TRP:NE1	2.33	0.58
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.86	0.58
2:C:998:LEU:HD22	2:C:1015:ALA:HA	1.86	0.58
3:D:850:LYS:NZ	3:D:852:GLY:O	2.37	0.58
3:D:232:ASN:N	3:D:232:ASN:OD1	2.36	0.58
3:D:846:GLU:HG2	3:D:881:LYS:HB3	1.86	0.58
1:A:29:GLU:HA	1:A:200:LYS:HG3	1.86	0.58
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.86	0.58
2:C:60:GLN:HA	2:C:67:GLU:HA	1.86	0.57
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.36	0.57
3:D:111:THR:HG22	3:D:300:GLN:HG2	1.86	0.57
3:D:294:ASN:ND2	5:F:121:GLU:OE2	2.35	0.57
3:D:973:LEU:HB3	3:D:1003:LEU:HB2	1.85	0.57
2:C:120:GLN:NE2	2:C:490:GLN:OE1	2.36	0.57
3:D:27:PRO:O	3:D:31:ARG:NH1	2.37	0.57
6:J:33:PHE:H	6:J:60:LEU:HB2	1.70	0.57
3:D:352:ARG:NH1	3:D:465:GLN:OE1	2.36	0.57
3:D:398:LYS:NZ	5:F:247:GLU:OE1	2.38	0.57
2:C:998:LEU:HB2	2:C:1015:ALA:HB2	1.86	0.57
2:C:122:VAL:HG23	2:C:490:GLN:HG3	1.86	0.57
2:C:714:VAL:O	2:C:767:GLN:NE2	2.38	0.57
2:C:1142:ARG:NH2	2:C:1164:PHE:O	2.32	0.56
3:D:559:ALA:HB3	3:D:562:GLU:HB2	1.87	0.56
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.36	0.56
2:C:972:PHE:HA	2:C:975:ILE:HB	1.87	0.56
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.86	0.56
5:F:262:TRP:NE1	5:F:320:GLN:OE1	2.37	0.56
2:C:576:SER:OG	2:C:577:VAL:N	2.36	0.56
2:C:748:ILE:HD13	2:C:966:ILE:HG22	1.88	0.56
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:33:PHE:HB2	6:J:60:LEU:HD12	1.86	0.56
2:C:113:THR:OG1	2:C:114:VAL:N	2.39	0.56
2:C:720:ARG:HH21	2:C:736:VAL:HG21	1.71	0.56
3:D:482:ALA:O	4:E:16:ARG:NH2	2.39	0.56
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.87	0.56
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.86	0.56
4:E:3:ARG:NH1	4:E:5:THR:O	2.39	0.56
2:C:91:THR:OG1	2:C:92:TYR:N	2.39	0.56
7:T:42:DT:H4'	7:T:43:DT:OP1	2.04	0.56
2:C:478:ARG:O	2:C:478:ARG:NH1	2.39	0.56
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.39	0.56
3:D:847:ASP:N	3:D:847:ASP:OD1	2.36	0.56
3:D:177:ASP:N	3:D:177:ASP:OD1	2.37	0.55
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.72	0.55
3:D:299:LEU:C	3:D:301:GLU:N	2.40	0.55
1:B:111:THR:HG23	1:B:113:ALA:H	1.71	0.55
2:C:317:LEU:HA	2:C:321:LEU:HD23	1.88	0.55
5:F:266:LEU:O	5:F:271:ARG:NH1	2.38	0.55
1:A:50:SER:HB2	1:A:150:ARG:HD2	1.89	0.55
2:C:423:ASP:OD1	2:C:423:ASP:N	2.38	0.55
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.86	0.55
2:C:694:ARG:O	2:C:798:GLN:NE2	2.39	0.55
3:D:54:ASP:N	3:D:54:ASP:OD1	2.39	0.55
3:D:1026:PRO:HB2	3:D:1028:ILE:HG23	1.87	0.55
1:A:33:ARG:HE	1:A:197:ASP:HB2	1.71	0.55
3:D:1152:GLU:OE1	3:D:1194:ARG:NH1	2.40	0.55
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.88	0.55
3:D:1111:ASP:OD1	3:D:1111:ASP:N	2.36	0.55
2:C:978:VAL:HG13	2:C:1007:LYS:HB2	1.89	0.54
3:D:1161:GLY:HA3	3:D:1179:PRO:HA	1.89	0.54
3:D:699:ASP:OD1	3:D:699:ASP:N	2.40	0.54
3:D:1307:LEU:HB2	3:D:1312:ALA:HB2	1.90	0.54
1:A:120:ASP:OD1	1:A:120:ASP:N	2.40	0.54
3:D:111:THR:CG2	3:D:300:GLN:HG2	2.38	0.54
3:D:638:SER:OG	3:D:639:VAL:N	2.40	0.54
3:D:1148:ARG:HH21	8:N:43:DA:H4'	1.73	0.54
5:F:98:ASN:OD1	5:F:98:ASN:N	2.37	0.54
1:B:44:ARG:NH2	2:C:1219:GLU:OE2	2.41	0.54
1:B:120:ASP:OD1	1:B:120:ASP:N	2.38	0.54
2:C:820:GLU:OE1	2:C:824:GLN:NE2	2.40	0.54
3:D:1041:ILE:O	3:D:1045:THR:OG1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:GLN:O	2:C:476:LYS:NZ	2.39	0.54
2:C:18:ARG:O	2:C:1156:ARG:NH1	2.40	0.54
2:C:960:LEU:HD21	2:C:1028:LYS:HB3	1.89	0.54
2:C:516:ASP:OD1	2:C:516:ASP:O	2.25	0.54
2:C:798:GLN:OE1	2:C:827:ARG:NH2	2.40	0.54
2:C:942:ASP:OD1	2:C:942:ASP:N	2.35	0.54
3:D:587:LEU:HD21	3:D:608:CYS:HB2	1.90	0.54
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.89	0.54
2:C:159:SER:HB2	2:C:442:VAL:HG11	1.90	0.53
3:D:785:ASP:O	3:D:789:LYS:HB2	2.07	0.53
3:D:1212:ASP:OD1	3:D:1212:ASP:N	2.41	0.53
1:A:20:SER:OG	1:A:21:SER:N	2.41	0.53
1:B:71:LYS:HB2	1:B:78:ILE:HD11	1.90	0.53
1:B:168:ILE:H	1:B:169:GLY:HA2	1.74	0.53
2:C:406:ASN:ND2	2:C:413:GLU:OE2	2.42	0.53
3:D:697:MET:HE2	3:D:741:ALA:HB3	1.89	0.53
3:D:58:CYS:O	3:D:98:ARG:NH2	2.41	0.53
2:C:903:ARG:NH1	2:C:909:LYS:O	2.42	0.53
1:B:12:ARG:HG3	1:B:13:LEU:HD23	1.89	0.53
2:C:715:THR:OG1	2:C:716:ALA:N	2.41	0.53
2:C:912:ASP:OD1	2:C:912:ASP:N	2.39	0.53
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.89	0.53
3:D:1279:GLN:NE2	3:D:1305:ASP:OD2	2.41	0.53
3:D:907:HIS:ND1	3:D:908:ILE:O	2.41	0.53
6:J:47:ALA:H	6:J:50:LYS:HZ3	1.55	0.53
2:C:434:ASP:HB3	2:C:439:LYS:HG3	1.90	0.53
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.91	0.53
1:B:197:ASP:OD1	1:B:197:ASP:N	2.40	0.52
2:C:325:LEU:HG	2:C:330:HIS:HB2	1.91	0.52
2:C:739:ASP:OD1	2:C:739:ASP:N	2.41	0.52
2:C:81:ASP:OD1	2:C:81:ASP:N	2.36	0.52
2:C:193:ASN:HD21	2:C:353:VAL:HG21	1.74	0.52
2:C:568:ASN:OD1	2:C:568:ASN:N	2.39	0.52
1:A:95:LYS:O	1:A:148:ARG:NH1	2.42	0.52
3:D:1034:PHE:HA	3:D:1114:GLN:HA	1.90	0.52
6:J:127:GLU:HG3	6:J:129:VAL:H	1.73	0.52
2:C:363:LEU:HD13	2:C:382:GLU:HB3	1.92	0.52
2:C:1244:HIS:HB2	2:C:1262:LYS:HG3	1.90	0.52
3:D:572:THR:OG1	3:D:573:THR:N	2.41	0.52
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.92	0.52
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:303:VAL:O	3:D:306:LEU:N	2.43	0.52
2:C:515:MET:HE3	2:C:517:GLN:HG3	1.91	0.52
2:C:1010:GLN:NE2	2:C:1013:GLN:OE1	2.42	0.52
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.92	0.52
3:D:1101:LEU:HD13	3:D:1102:PRO:HD2	1.92	0.52
2:C:421:SER:OG	2:C:423:ASP:OD1	2.26	0.52
2:C:485:ASP:HB3	2:C:487:LEU:HB3	1.90	0.52
2:C:931:VAL:HG22	2:C:1052:VAL:HG22	1.92	0.52
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.91	0.52
5:F:113:GLY:HA3	5:F:162:THR:HG23	1.90	0.52
1:B:111:THR:HA	1:B:129:VAL:HA	1.92	0.52
5:F:248:ASP:OD1	5:F:248:ASP:N	2.43	0.52
6:J:40:VAL:HB	6:J:54:TRP:HB2	1.92	0.52
3:D:516:ASP:HA	3:D:545:HIS:HB3	1.92	0.52
3:D:875:ASN:N	3:D:875:ASN:OD1	2.41	0.52
3:D:982:LEU:HB3	3:D:995:TYR:HB2	1.91	0.52
3:D:91:GLU:OE1	3:D:101:ARG:NH2	2.39	0.51
3:D:148:GLU:OE2	3:D:156:ARG:NE	2.38	0.51
3:D:208:THR:HG23	3:D:214:ARG:HE	1.76	0.51
3:D:334:LYS:O	3:D:340:GLN:NE2	2.44	0.51
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.92	0.51
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.43	0.51
3:D:123:ARG:HG3	3:D:1337:VAL:HG11	1.93	0.51
3:D:1062:LEU:O	3:D:1067:ARG:NH2	2.42	0.51
2:C:812:PHE:O	2:C:1099:ASN:ND2	2.43	0.51
3:D:73:GLY:O	3:D:76:LYS:NZ	2.39	0.51
3:D:245:LEU:HD23	3:D:250:ARG:HG2	1.93	0.51
3:D:845:ALA:HB3	3:D:881:LYS:HG2	1.92	0.51
3:D:208:THR:O	3:D:214:ARG:NH2	2.39	0.51
3:D:806:ASP:OD1	3:D:806:ASP:N	2.44	0.51
2:C:242:VAL:HB	2:C:245:ARG:HG2	1.93	0.51
3:D:417:ARG:HG2	3:D:418:GLU:HG2	1.92	0.51
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.91	0.51
2:C:189:ASP:N	2:C:193:ASN:O	2.43	0.51
5:F:85:ARG:HH12	6:J:78:LYS:HA	1.76	0.51
2:C:714:VAL:HB	2:C:787:PRO:HD2	1.93	0.51
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.93	0.51
2:C:622:ASN:N	2:C:622:ASN:OD1	2.41	0.51
2:C:866:ASP:OD2	2:C:944:ARG:NH1	2.42	0.51
3:D:558:ASP:N	3:D:558:ASP:OD1	2.44	0.51
5:F:141:ARG:NH1	8:N:30:DC:OP1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:303:ASP:N	2:C:308:GLU:O	2.44	0.50
2:C:881:ASP:N	2:C:881:ASP:OD1	2.44	0.50
2:C:197:ARG:NH1	2:C:201:ARG:O	2.44	0.50
3:D:1181:ASP:OD1	3:D:1181:ASP:N	2.42	0.50
3:D:201:LEU:HD13	3:D:220:ARG:HG2	1.93	0.50
3:D:693:VAL:HG11	3:D:743:MET:H	1.76	0.50
3:D:891:ASP:OD1	3:D:891:ASP:N	2.44	0.50
1:B:82:LEU:HD11	1:B:171:LEU:HG	1.94	0.50
2:C:905:ILE:HG21	5:F:317:LEU:HD12	1.94	0.50
3:D:608:CYS:SG	3:D:617:THR:OG1	2.63	0.50
3:D:775:SER:O	3:D:775:SER:OG	2.26	0.50
2:C:173:ASN:OD1	2:C:173:ASN:N	2.45	0.50
3:D:187:ALA:O	3:D:191:SER:HB3	2.11	0.50
3:D:296:LYS:O	3:D:300:GLN:HB2	2.11	0.50
3:D:363:LEU:HD21	3:D:618:VAL:HG22	1.94	0.50
3:D:528:THR:O	3:D:528:THR:OG1	2.28	0.50
1:B:4:SER:OG	1:B:5:VAL:N	2.44	0.50
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.94	0.50
3:D:1027:VAL:HG11	3:D:1101:LEU:HD11	1.93	0.50
2:C:1247:SER:OG	2:C:1248:THR:N	2.44	0.49
3:D:1341:ARG:NH1	3:D:1343:GLU:OE1	2.44	0.49
2:C:1299:ASN:O	2:C:1303:LYS:NZ	2.44	0.49
3:D:197:GLU:OE2	3:D:220:ARG:NH2	2.45	0.49
3:D:410:ASP:OD1	3:D:410:ASP:N	2.42	0.49
3:D:527:LEU:HD22	3:D:548:VAL:HG11	1.94	0.49
5:F:298:THR:HG22	5:F:301:ARG:H	1.77	0.49
2:C:1246:ARG:NH1	2:C:1265:PHE:O	2.45	0.49
3:D:137:ARG:NH2	3:D:143:SER:OG	2.45	0.49
2:C:55:SER:OG	2:C:465:ARG:NH1	2.46	0.49
2:C:197:ARG:HD3	2:C:200:ARG:HA	1.95	0.49
6:J:100:LEU:HD22	6:J:129:VAL:HG21	1.95	0.49
1:A:71:LYS:HB2	1:A:78:ILE:HD11	1.94	0.49
1:A:207:THR:OG1	1:A:209:GLY:N	2.45	0.49
1:B:212:ASP:OD1	1:B:212:ASP:N	2.41	0.49
1:A:234:LEU:C	1:A:235:GLU:OE1	2.56	0.49
3:D:353:SER:OG	3:D:354:VAL:N	2.46	0.49
5:F:229:ASP:OD1	5:F:229:ASP:N	2.40	0.49
1:B:28:LEU:HD21	1:B:201:LEU:HD23	1.95	0.49
2:C:1105:SER:OG	3:D:731:ARG:NH1	2.45	0.49
3:D:245:LEU:O	3:D:250:ARG:NH2	2.45	0.49
3:D:951:GLN:NE2	3:D:1014:GLY:O	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:29:GLN:HB3	4:E:35:LYS:HG3	1.93	0.49
2:C:11:ILE:O	2:C:1149:TYR:OH	2.28	0.49
2:C:56:VAL:HG13	2:C:57:PHE:HD1	1.78	0.49
2:C:148:GLN:O	2:C:454:ARG:N	2.44	0.49
2:C:488:MET:HE3	2:C:489:PRO:HD2	1.94	0.49
2:C:808:ASN:OD1	2:C:1216:ARG:NH1	2.42	0.49
3:D:123:ARG:O	3:D:127:LEU:HB3	2.12	0.49
2:C:150:HIS:CD2	2:C:452:ARG:HB2	2.48	0.49
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.45	0.49
2:C:968:GLU:OE2	2:C:994:ARG:NH1	2.45	0.49
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.94	0.48
5:F:170:HIS:HE1	8:N:21:DG:H2'	1.78	0.48
2:C:50:GLU:OE1	2:C:54:ARG:NE	2.43	0.48
2:C:878:THR:OG1	2:C:879:GLY:N	2.38	0.48
3:D:42:GLU:HG3	3:D:52:GLU:HG2	1.95	0.48
5:F:71:LEU:HB2	5:F:76:GLU:HG3	1.94	0.48
5:F:129:ARG:NH2	8:N:25:DC:OP2	2.41	0.48
2:C:393:ASP:OD1	2:C:393:ASP:N	2.44	0.48
2:C:979:LEU:HD23	2:C:1002:LEU:HD21	1.95	0.48
1:A:188:GLU:OE2	1:A:200:LYS:NZ	2.36	0.48
2:C:231:GLU:N	2:C:238:GLN:O	2.47	0.48
2:C:772:SER:OG	2:C:773:LEU:N	2.47	0.48
2:C:807:TRP:HB2	2:C:1097:VAL:HG11	1.95	0.48
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.43	0.48
3:D:264:ASP:HB3	3:D:324:LEU:HB3	1.94	0.48
3:D:975:ILE:HD12	3:D:1001:ALA:HB3	1.95	0.48
1:B:91:ARG:HB3	1:B:122:GLU:HB3	1.96	0.48
3:D:968:ASN:HA	3:D:1118:GLY:HA3	1.95	0.48
2:C:851:THR:OG1	2:C:852:ALA:N	2.46	0.48
3:D:403:ARG:NH1	3:D:405:GLU:OE2	2.38	0.48
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.96	0.48
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.78	0.48
2:C:1295:SER:O	2:C:1301:ARG:NH1	2.47	0.48
3:D:986:ASP:OD1	3:D:990:ARG:N	2.43	0.48
3:D:1037:PHE:HB3	3:D:1040:MET:HB3	1.96	0.48
2:C:138:ILE:HG21	2:C:507:GLY:HA2	1.95	0.47
3:D:512:TYR:O	3:D:545:HIS:NE2	2.42	0.47
3:D:516:ASP:OD1	3:D:516:ASP:N	2.46	0.47
5:F:177:VAL:O	5:F:181:THR:OG1	2.31	0.47
2:C:865:LEU:HA	2:C:871:VAL:HA	1.96	0.47
3:D:156:ARG:NH2	3:D:191:SER:OG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:952:VAL:O	3:D:1014:GLY:N	2.44	0.47
3:D:255:LEU:HB2	3:D:259:ARG:HB3	1.97	0.47
2:C:759:SER:OG	2:C:760:ASN:N	2.45	0.47
3:D:772:TYR:O	3:D:776:THR:OG1	2.31	0.47
1:B:193:GLU:HG2	1:B:194:GLN:HG2	1.97	0.47
2:C:231:GLU:O	2:C:238:GLN:N	2.48	0.47
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.95	0.47
3:D:623:GLN:O	3:D:627:THR:OG1	2.29	0.47
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.97	0.47
5:F:277:ARG:NH2	7:T:46:DG:OP1	2.48	0.47
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.97	0.47
2:C:726:TYR:HA	2:C:773:LEU:HD12	1.95	0.47
3:D:1046:ILE:HD12	3:D:1059:LEU:HB3	1.95	0.47
6:J:6:GLY:O	6:J:7:HIS:ND1	2.48	0.47
6:J:122:ASP:N	6:J:122:ASP:OD1	2.47	0.47
8:N:8:DG:OP2	8:N:8:DG:H8	1.98	0.47
1:A:207:THR:OG1	1:A:208:ASN:N	2.45	0.47
3:D:425:ARG:HG3	3:D:466:MET:HG2	1.96	0.47
3:D:1050:THR:OG1	3:D:1051:ASP:N	2.46	0.47
1:B:80:GLU:OE2	3:D:551:ARG:NH2	2.40	0.47
2:C:868:SER:O	2:C:868:SER:OG	2.31	0.47
3:D:641:ILE:HD12	3:D:641:ILE:HA	1.81	0.47
3:D:1051:ASP:OD1	3:D:1058:SER:OG	2.33	0.47
3:D:305:ALA:O	3:D:306:LEU:C	2.52	0.46
3:D:950:ILE:HD12	3:D:997:VAL:HG13	1.97	0.46
2:C:1072:ASN:ND2	2:C:1230:MET:SD	2.88	0.46
1:B:203:ILE:HG21	1:B:217:ILE:HD11	1.97	0.46
3:D:1268:ASN:HD22	3:D:1301:THR:HG23	1.80	0.46
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.98	0.46
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.97	0.46
2:C:980:VAL:HA	2:C:984:VAL:HG13	1.98	0.46
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.98	0.46
3:D:53:ARG:HA	3:D:54:ASP:HA	1.60	0.46
3:D:1037:PHE:H	3:D:1111:ASP:HB3	1.80	0.46
3:D:1115:ILE:HD12	3:D:1115:ILE:HA	1.82	0.46
5:F:56:ASP:N	5:F:56:ASP:OD1	2.48	0.46
5:F:288:LEU:N	7:T:46:DG:OP2	2.49	0.46
2:C:444:ASP:N	2:C:444:ASP:OD1	2.47	0.46
2:C:637:ARG:HA	2:C:642:SER:HA	1.98	0.46
2:C:805:MET:HE3	2:C:805:MET:HB2	1.66	0.46
2:C:820:GLU:N	2:C:1080:ASN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:ALA:O	3:D:191:SER:CB	2.64	0.46
3:D:416:ILE:HD13	3:D:441:LEU:HD21	1.97	0.46
1:B:31:LEU:HB2	1:B:199:ASP:HB2	1.98	0.46
2:C:29:SER:O	2:C:33:ASP:HB2	2.16	0.46
2:C:281:ASP:OD1	2:C:281:ASP:N	2.49	0.46
7:T:42:DT:H2''	7:T:43:DT:H2'	1.98	0.46
2:C:1287:LEU:HD21	3:D:1351:VAL:HG22	1.97	0.45
3:D:647:PRO:HG2	3:D:650:LYS:HB2	1.98	0.45
4:E:43:ASN:N	4:E:43:ASN:OD1	2.49	0.45
3:D:105:ILE:HD12	3:D:242:LEU:HD23	1.97	0.45
1:A:124:VAL:HG21	1:A:209:GLY:HA3	1.99	0.45
2:C:175:ARG:HE	2:C:175:ARG:HB2	1.55	0.45
3:D:438:GLU:HG3	3:D:485:MET:HE1	1.98	0.45
1:B:27:THR:HA	1:B:202:VAL:HA	1.98	0.45
1:B:62:ASP:N	1:B:62:ASP:OD1	2.48	0.45
2:C:642:SER:HB2	3:D:770:LEU:HD21	1.99	0.45
2:C:878:THR:HA	2:C:925:SER:HA	1.97	0.45
6:J:8:PRO:HG2	6:J:114:MET:HE1	1.98	0.45
2:C:118:LYS:HE2	2:C:118:LYS:HB3	1.71	0.45
2:C:314:ASN:OD1	2:C:352:ARG:NH1	2.49	0.45
2:C:539:THR:OG1	2:C:540:ARG:N	2.50	0.45
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.97	0.45
2:C:843:THR:OG1	2:C:846:GLY:O	2.29	0.45
2:C:953:LEU:HD13	2:C:1033:ARG:HG3	1.98	0.45
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.98	0.45
2:C:49:LEU:HD23	2:C:49:LEU:HA	1.82	0.45
2:C:1340:GLU:OE2	3:D:1341:ARG:NE	2.36	0.45
3:D:649:LYS:HA	3:D:649:LYS:HD3	1.75	0.45
6:J:7:HIS:ND1	6:J:64:GLU:OE2	2.50	0.45
1:A:234:LEU:HD12	1:B:218:ARG:HE	1.82	0.45
3:D:1262:ARG:HH22	3:D:1316:THR:HG23	1.81	0.45
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.99	0.45
2:C:950:GLU:HG3	2:C:954:LYS:HE2	1.99	0.45
2:C:975:ILE:HG13	2:C:1014:LEU:HD12	1.99	0.45
2:C:1157:GLN:NE2	2:C:1157:GLN:O	2.50	0.45
3:D:18:ASP:OD1	3:D:18:ASP:N	2.50	0.45
3:D:300:GLN:NE2	3:D:300:GLN:C	2.69	0.45
3:D:1058:SER:OG	3:D:1108:GLN:OE1	2.29	0.45
1:B:51:MET:HA	1:B:52:PRO:HD3	1.88	0.45
2:C:870:ILE:HD12	2:C:944:ARG:HG2	1.99	0.45
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1033:ARG:O	2:C:1037:THR:OG1	2.32	0.44
3:D:85:CYS:SG	3:D:87:LYS:N	2.90	0.44
5:F:303:ARG:HH12	7:T:47:DC:H2'	1.82	0.44
2:C:142:GLU:HG2	2:C:515:MET:HE2	1.99	0.44
3:D:124:ILE:HG22	3:D:135:ILE:HD13	1.99	0.44
3:D:511:TYR:CZ	3:D:515:ARG:HD2	2.52	0.44
1:A:77:ASP:OD1	1:A:77:ASP:N	2.48	0.44
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.98	0.44
2:C:232:ILE:H	2:C:332:ARG:HH12	1.65	0.44
1:A:114:ASP:OD1	1:A:114:ASP:N	2.51	0.44
2:C:21:VAL:HG11	2:C:592:ARG:HD3	1.99	0.44
2:C:296:VAL:HA	2:C:316:GLU:HA	1.98	0.44
2:C:506:PHE:O	2:C:512:SER:OG	2.33	0.44
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	1.99	0.44
5:F:95:ILE:HD13	5:F:128:ILE:HG12	1.99	0.44
1:A:161:SER:O	1:A:161:SER:OG	2.32	0.44
3:D:384:LYS:HE3	3:D:415:VAL:HG12	2.00	0.44
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.44
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.53	0.44
6:J:110:LEU:O	6:J:113:SER:OG	2.30	0.44
3:D:514:THR:OG1	3:D:595:ALA:O	2.35	0.44
3:D:1025:MET:HB3	3:D:1124:ILE:HB	2.00	0.44
2:C:443:ASP:OD1	2:C:443:ASP:N	2.50	0.44
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.98	0.44
3:D:538:ARG:HA	3:D:538:ARG:HD2	1.82	0.44
3:D:707:ILE:O	3:D:714:GLU:N	2.50	0.44
3:D:891:ASP:OD1	3:D:1286:LYS:NZ	2.51	0.44
3:D:1286:LYS:HB3	3:D:1286:LYS:HE3	1.76	0.44
1:A:16:ILE:HG23	1:A:26:VAL:HG13	2.00	0.43
1:B:11:PRO:HB3	1:B:28:LEU:HD12	2.00	0.43
1:B:188:GLU:HG2	1:B:200:LYS:HB3	1.99	0.43
3:D:1189:MET:H	3:D:1189:MET:HG2	1.61	0.43
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.82	0.43
3:D:140:TYR:OH	3:D:312:ARG:NE	2.48	0.43
3:D:884:SER:OG	3:D:885:VAL:N	2.51	0.43
3:D:925:GLU:HG3	3:D:926:PRO:HD3	2.00	0.43
5:F:287:THR:HB	7:T:45:DC:H3'	2.00	0.43
3:D:103:GLY:H	3:D:244:VAL:HG22	1.83	0.43
3:D:751:ASP:OD1	3:D:751:ASP:N	2.51	0.43
2:C:1256:GLN:HG2	2:C:1321:GLU:HG2	2.00	0.43
3:D:278:ARG:HG3	5:F:125:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1172:LYS:HA	3:D:1172:LYS:HD3	1.78	0.43
3:D:1172:LYS:HD2	3:D:1189:MET:HB2	2.00	0.43
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.82	0.43
3:D:661:VAL:HB	3:D:685:ILE:HD11	2.01	0.43
3:D:1157:ALA:O	3:D:1207:GLY:N	2.47	0.43
5:F:112:ARG:HD2	5:F:158:ILE:HG21	2.01	0.43
2:C:303:ASP:HA	2:C:310:ILE:HD11	2.00	0.43
2:C:813:GLU:HB2	3:D:461:PHE:CD2	2.54	0.43
2:C:1297:ASP:OD2	2:C:1319:MET:N	2.52	0.43
3:D:288:PRO:HA	5:F:92:ARG:HE	1.83	0.43
3:D:957:SER:HA	3:D:1010:GLN:HA	1.99	0.43
2:C:342:ASP:O	2:C:437:ASN:ND2	2.51	0.43
3:D:1050:THR:OG1	3:D:1056:LEU:O	2.30	0.43
4:E:38:LEU:HD12	4:E:58:LEU:HD13	2.00	0.43
2:C:401:GLY:O	2:C:405:PHE:HB2	2.18	0.43
3:D:848:VAL:HG21	3:D:880:VAL:HG13	2.00	0.43
2:C:104:ILE:HD12	2:C:116:ASP:HB2	2.00	0.43
2:C:449:GLY:HA3	2:C:609:ILE:HG23	2.01	0.43
2:C:870:ILE:HG23	2:C:884:VAL:HG22	2.01	0.43
3:D:221:ILE:HD13	3:D:221:ILE:HA	1.90	0.43
3:D:746:LEU:HD22	3:D:754:ILE:HD11	2.00	0.43
8:N:40:DT:C6	8:N:41:DT:H72	2.54	0.43
3:D:569:LEU:HD12	3:D:569:LEU:HA	1.84	0.43
3:D:581:MET:H	3:D:581:MET:HG3	1.65	0.43
3:D:1046:ILE:HA	3:D:1061:VAL:HA	2.00	0.43
3:D:1046:ILE:HG22	3:D:1061:VAL:HG22	2.01	0.43
3:D:1260:MET:HE2	3:D:1306:LEU:HD21	2.00	0.43
3:D:883:ARG:NH2	3:D:895:CYS:SG	2.92	0.42
3:D:930:LEU:HD11	3:D:1241:TYR:HE1	1.85	0.42
3:D:968:ASN:HD21	3:D:972:LYS:HB2	1.84	0.42
3:D:1090:ILE:HD12	3:D:1095:MET:HB2	2.01	0.42
3:D:1206:ARG:HE	3:D:1223:LEU:HD12	1.84	0.42
5:F:311:ARG:HA	5:F:311:ARG:HD3	1.69	0.42
1:A:205:MET:HE2	1:A:205:MET:HB3	1.84	0.42
1:B:134:THR:HG23	1:B:136:GLU:HB2	2.01	0.42
2:C:524:ILE:HD12	2:C:708:VAL:HG13	2.01	0.42
2:C:741:MET:HE2	2:C:741:MET:HB3	1.87	0.42
3:D:805:GLN:HG3	3:D:1347:LEU:HB2	2.02	0.42
5:F:137:GLU:HB3	6:J:44:VAL:HG13	2.01	0.42
1:A:84:ASN:ND2	1:A:130:ILE:O	2.53	0.42
3:D:113:HIS:HB3	3:D:116:PHE:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:ARG:HH21	3:D:1334:GLU:HB2	1.84	0.42
3:D:1250:ASP:N	3:D:1250:ASP:OD1	2.52	0.42
1:A:134:THR:O	1:A:134:THR:OG1	2.35	0.42
2:C:786:GLY:N	2:C:789:THR:OG1	2.53	0.42
3:D:111:THR:HB	3:D:300:GLN:HG2	2.00	0.42
5:F:221:SER:OG	5:F:222:VAL:N	2.51	0.42
1:A:185:TYR:HB2	1:A:201:LEU:HD11	2.02	0.42
1:B:64:VAL:HG23	1:B:71:LYS:HD3	2.02	0.42
2:C:3:TYR:HB3	2:C:7:GLU:HB2	2.00	0.42
2:C:59:ILE:O	2:C:68:LEU:N	2.44	0.42
2:C:638:SER:OG	2:C:639:LYS:NZ	2.49	0.42
2:C:1104:PRO:HG3	3:D:725:MET:HE3	2.01	0.42
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.40	0.42
3:D:552:ILE:H	3:D:552:ILE:HG13	1.64	0.42
4:E:30:MET:HE1	4:E:49:ILE:HB	2.01	0.42
5:F:82:ARG:CZ	6:J:24:ARG:HE	2.32	0.42
5:F:220:THR:OG1	5:F:221:SER:N	2.52	0.42
2:C:453:ILE:HD13	2:C:453:ILE:HA	1.91	0.42
2:C:489:PRO:HA	2:C:492:MET:HG3	2.01	0.42
2:C:702:THR:N	2:C:705:GLU:OE2	2.47	0.42
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.55	0.42
7:T:11:DT:H2'	7:T:12:DA:C8	2.54	0.42
2:C:369:MET:HB3	2:C:369:MET:HE3	1.77	0.42
2:C:1138:VAL:HG22	2:C:1170:MET:HE3	2.00	0.42
3:D:1037:PHE:HE2	3:D:1059:LEU:HD13	1.85	0.42
5:F:141:ARG:HD3	5:F:141:ARG:HA	1.85	0.42
6:J:5:SER:OG	6:J:6:GLY:N	2.53	0.42
2:C:478:ARG:HA	2:C:478:ARG:HD2	1.89	0.42
3:D:599:LYS:HE2	3:D:599:LYS:HB2	1.82	0.42
1:B:77:ASP:OD1	1:B:78:ILE:N	2.53	0.42
2:C:187:GLU:OE2	2:C:197:ARG:NE	2.36	0.42
2:C:704:MET:HE3	2:C:704:MET:HB3	1.76	0.42
3:D:489:ASN:OD1	3:D:489:ASN:N	2.53	0.42
3:D:625:MET:HE2	3:D:625:MET:HB3	1.75	0.42
3:D:1029:THR:OG1	3:D:1030:GLU:N	2.53	0.42
3:D:1050:THR:HA	3:D:1058:SER:HB2	2.02	0.42
1:A:44:ARG:O	1:A:48:LEU:HB2	2.19	0.42
1:B:18:GLN:HA	1:B:24:ALA:HA	2.02	0.42
2:C:50:GLU:OE2	2:C:70:TYR:OH	2.35	0.42
2:C:542:ARG:HB2	8:N:39:DG:C6	2.54	0.42
2:C:1014:LEU:HA	2:C:1017:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1065:LYS:HA	2:C:1075:VAL:HA	2.01	0.42
3:D:120:LEU:HA	3:D:120:LEU:HD23	1.82	0.42
3:D:139:LEU:HD23	3:D:139:LEU:HA	1.90	0.42
3:D:145:VAL:HA	3:D:159:ILE:HA	2.02	0.42
3:D:268:LEU:HD22	3:D:306:LEU:HA	2.02	0.42
3:D:340:GLN:HE21	3:D:340:GLN:HB2	1.61	0.42
3:D:591:ILE:HD12	3:D:591:ILE:HA	1.86	0.42
2:C:797:GLY:H	2:C:1231:TYR:HH	1.62	0.41
2:C:1290:MET:HE3	2:C:1290:MET:HB2	1.70	0.41
3:D:544:LEU:HD12	3:D:544:LEU:HA	1.87	0.41
3:D:968:ASN:OD1	3:D:972:LYS:N	2.52	0.41
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	2.02	0.41
4:E:10:VAL:HG21	4:E:16:ARG:HD2	2.02	0.41
1:A:20:SER:HB3	1:A:23:HIS:HB2	2.02	0.41
1:A:24:ALA:HB3	1:A:205:MET:HG2	2.02	0.41
2:C:638:SER:HB2	2:C:645:PHE:HE2	1.85	0.41
2:C:693:LEU:HD12	2:C:693:LEU:HA	1.91	0.41
3:D:303:VAL:HG12	3:D:304:ASP:N	2.35	0.41
3:D:1048:ARG:HA	3:D:1048:ARG:HD3	1.85	0.41
1:A:35:PHE:HE1	1:B:46:ILE:HG12	1.86	0.41
2:C:263:VAL:HG21	2:C:269:ILE:HG23	2.00	0.41
3:D:557:LYS:HB3	3:D:563:LEU:HD12	2.02	0.41
3:D:1107:VAL:HG22	3:D:1122:ALA:HB2	2.02	0.41
5:F:316:ILE:O	5:F:319:THR:OG1	2.39	0.41
2:C:1067:ALA:HA	2:C:1073:LYS:HA	2.02	0.41
2:C:1165:SER:OG	2:C:1168:GLU:OE1	2.35	0.41
3:D:1075:ARG:HB2	3:D:1100:PHE:HB3	2.03	0.41
5:F:117:LEU:HD23	5:F:117:LEU:HA	1.93	0.41
5:F:298:THR:HB	5:F:301:ARG:HB2	2.02	0.41
1:A:194:GLN:H	1:A:194:GLN:HG2	1.64	0.41
2:C:62:TYR:H	2:C:480:SER:HB3	1.86	0.41
2:C:759:SER:OG	2:C:761:GLN:N	2.47	0.41
2:C:888:THR:O	2:C:914:LYS:N	2.48	0.41
2:C:1022:LYS:HB3	2:C:1022:LYS:HE3	1.77	0.41
3:D:517:CYS:HB3	3:D:719:PHE:HE2	1.86	0.41
3:D:29:MET:HB2	3:D:29:MET:HE2	1.75	0.41
3:D:762:ASN:ND2	3:D:765:GLU:OE1	2.54	0.41
3:D:1314:LEU:HD12	3:D:1314:LEU:HA	1.86	0.41
4:E:64:LEU:HD23	4:E:64:LEU:HA	1.86	0.41
5:F:253:ASP:OD1	5:F:253:ASP:N	2.52	0.41
1:A:100:LEU:HD21	1:A:121:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:CB	1:A:235:GLU:OE2	2.68	0.41
2:C:241:LEU:HD11	2:C:246:LEU:HD21	2.02	0.41
2:C:295:LYS:HD3	2:C:295:LYS:HA	1.93	0.41
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.67	0.41
3:D:40:LYS:HE2	3:D:40:LYS:HB2	1.93	0.41
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.03	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.96	0.41
2:C:18:ARG:HA	2:C:18:ARG:HD3	1.84	0.41
2:C:228:VAL:HG22	2:C:245:ARG:HH12	1.84	0.41
2:C:1106:ARG:HH21	3:D:731:ARG:HH22	1.69	0.41
3:D:1355:ARG:HE	3:D:1355:ARG:HB3	1.57	0.41
5:F:313:LEU:HD12	5:F:313:LEU:HA	1.87	0.41
1:A:181:GLU:O	2:C:821:ARG:NH1	2.47	0.41
2:C:299:LYS:HE3	2:C:299:LYS:HB2	1.83	0.41
3:D:134:ASP:N	3:D:134:ASP:OD1	2.53	0.41
3:D:536:LEU:HD13	3:D:541:LEU:HB2	2.02	0.41
8:N:15:DA:H1'	8:N:16:DT:H5'	2.03	0.41
1:A:107:ILE:HD11	1:A:136:GLU:HG2	2.02	0.40
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.73	0.40
2:C:1098:LEU:HD12	2:C:1098:LEU:HA	1.83	0.40
3:D:510:LEU:HD23	3:D:510:LEU:HA	1.90	0.40
3:D:1051:ASP:HB2	3:D:1056:LEU:H	1.86	0.40
3:D:1073:ASP:OD1	3:D:1073:ASP:N	2.48	0.40
3:D:1079:LYS:HD2	3:D:1098:GLN:HB3	2.03	0.40
2:C:60:GLN:H	2:C:60:GLN:HG2	1.71	0.40
2:C:236:LYS:HB2	2:C:236:LYS:HE3	1.89	0.40
3:D:582:ILE:HD13	3:D:582:ILE:HA	1.89	0.40
5:F:270:GLN:NE2	5:F:308:GLU:OE2	2.52	0.40
3:D:327:LEU:HA	3:D:327:LEU:HD23	1.84	0.40
5:F:87:ASP:O	5:F:90:SER:OG	2.36	0.40
8:N:16:DT:H2''	8:N:17:DA:C8	2.56	0.40
8:N:51:DG:H2''	8:N:52:DA:C8	2.56	0.40
1:A:166:ARG:HA	1:A:166:ARG:HD2	1.88	0.40
2:C:388:LEU:HD23	2:C:388:LEU:HA	1.90	0.40
2:C:657:THR:HB	2:C:1187:PHE:HB2	2.04	0.40
3:D:1368:ASP:OD2	3:D:1372:ARG:NH1	2.55	0.40
5:F:264:PHE:HD1	5:F:264:PHE:HA	1.78	0.40
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.86	0.40
1:B:45:ARG:O	1:B:49:SER:OG	2.36	0.40
1:B:111:THR:OG1	1:B:112:ALA:N	2.54	0.40
2:C:84:GLU:O	2:C:88:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:987:GLU:O	2:C:991:LYS:N	2.55	0.40
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.54	0.40
3:D:958:ILE:HD12	3:D:982:LEU:HD11	2.03	0.40
4:E:8:ASP:OD1	4:E:8:ASP:N	2.53	0.40
5:F:202:LEU:HD23	5:F:202:LEU:HA	1.91	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	231/239 (97%)	208 (90%)	22 (10%)	1 (0%)	30	59
1	B	219/239 (92%)	203 (93%)	16 (7%)	0	100	100
2	C	1338/1342 (100%)	1234 (92%)	104 (8%)	0	100	100
3	D	1330/1407 (94%)	1233 (93%)	92 (7%)	5 (0%)	30	59
4	E	77/91 (85%)	69 (90%)	8 (10%)	0	100	100
5	F	276/331 (83%)	266 (96%)	10 (4%)	0	100	100
6	J	125/136 (92%)	118 (94%)	7 (6%)	0	100	100
All	All	3596/3785 (95%)	3331 (93%)	259 (7%)	6 (0%)	44	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	300	GLN
3	D	304	ASP
3	D	904	ALA
1	A	8	PHE
3	D	299	LEU
3	D	303	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	201/206 (98%)	162 (81%)	39 (19%)	1	6
1	B	190/206 (92%)	165 (87%)	25 (13%)	4	17
2	C	1155/1157 (100%)	1012 (88%)	143 (12%)	4	19
3	D	1118/1168 (96%)	983 (88%)	135 (12%)	5	20
4	E	67/75 (89%)	64 (96%)	3 (4%)	24	52
5	F	236/287 (82%)	215 (91%)	21 (9%)	9	30
6	J	104/123 (85%)	91 (88%)	13 (12%)	4	19
All	All	3071/3222 (95%)	2692 (88%)	379 (12%)	7	19

All (379) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	THR
1	A	7	GLU
1	A	13	LEU
1	A	19	VAL
1	A	23	HIS
1	A	26	VAL
1	A	48	LEU
1	A	49	SER
1	A	56	VAL
1	A	57	THR
1	A	65	LEU
1	A	69	SER
1	A	70	THR
1	A	74	VAL
1	A	77	ASP
1	A	90	VAL
1	A	97	GLU
1	A	107	ILE
1	A	114	ASP

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Mol	Chain	Res	Type
1	A	115	ILE
1	A	118	ASP
1	A	120	ASP
1	A	124	VAL
1	A	137	ASN
1	A	140	ILE
1	A	159	ILE
1	A	173	VAL
1	A	177	TYR
1	A	178	SER
1	A	192	VAL
1	A	194	GLN
1	A	207	THR
1	A	212	ASP
1	A	215	GLU
1	A	217	ILE
1	A	223	ILE
1	A	227	GLN
1	A	234	LEU
1	B	7	GLU
1	B	13	LEU
1	B	14	VAL
1	B	17	GLU
1	B	27	THR
1	B	31	LEU
1	B	38	THR
1	B	43	LEU
1	B	60	GLU
1	B	61	ILE
1	B	98	VAL
1	B	102	LEU
1	B	110	VAL
1	B	140	ILE
1	B	144	ILE
1	B	168	ILE
1	B	171	LEU
1	B	173	VAL
1	B	183	ILE
1	B	188	GLU
1	B	192	VAL
1	B	196	THR
1	B	206	GLU

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Mol	Chain	Res	Type
1	B	207	THR
1	B	217	ILE
2	C	11	ILE
2	C	21	VAL
2	C	30	ILE
2	C	39	ILE
2	C	60	GLN
2	C	62	TYR
2	C	65	ASN
2	C	66	SER
2	C	75	LEU
2	C	91	THR
2	C	96	LEU
2	C	103	VAL
2	C	113	THR
2	C	114	VAL
2	C	118	LYS
2	C	149	LEU
2	C	152	SER
2	C	177	ILE
2	C	179	TYR
2	C	188	PHE
2	C	189	ASP
2	C	191	LYS
2	C	196	VAL
2	C	204	LEU
2	C	218	GLU
2	C	244	GLU
2	C	246	LEU
2	C	263	VAL
2	C	265	LYS
2	C	281	ASP
2	C	289	VAL
2	C	292	ILE
2	C	297	VAL
2	C	308	GLU
2	C	309	LEU
2	C	317	LEU
2	C	319	LEU
2	C	322	LEU
2	C	334	GLU
2	C	356	THR

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Mol	Chain	Res	Type
2	C	393	ASP
2	C	397	LEU
2	C	409	LEU
2	C	435	ILE
2	C	443	ASP
2	C	446	ASP
2	C	471	VAL
2	C	475	VAL
2	C	487	LEU
2	C	492	MET
2	C	493	ILE
2	C	538	LEU
2	C	550	VAL
2	C	553	THR
2	C	563	THR
2	C	568	ASN
2	C	572	ILE
2	C	580	GLN
2	C	589	THR
2	C	595	THR
2	C	615	VAL
2	C	622	ASN
2	C	634	VAL
2	C	637	ARG
2	C	644	LEU
2	C	660	VAL
2	C	663	VAL
2	C	690	VAL
2	C	697	LYS
2	C	702	THR
2	C	705	GLU
2	C	715	THR
2	C	723	VAL
2	C	748	ILE
2	C	753	LEU
2	C	759	SER
2	C	770	CYS
2	C	788	SER
2	C	800	MET
2	C	802	VAL
2	C	823	VAL
2	C	830	THR

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Mol	Chain	Res	Type
2	C	834	GLN
2	C	851	THR
2	C	853	ASP
2	C	865	LEU
2	C	871	VAL
2	C	881	ASP
2	C	887	VAL
2	C	888	THR
2	C	896	THR
2	C	898	GLU
2	C	902	LEU
2	C	913	VAL
2	C	915	ASP
2	C	924	VAL
2	C	935	THR
2	C	963	GLU
2	C	964	LEU
2	C	967	LEU
2	C	975	ILE
2	C	989	LEU
2	C	992	LEU
2	C	998	LEU
2	C	1022	LYS
2	C	1024	GLU
2	C	1037	THR
2	C	1041	ASP
2	C	1056	VAL
2	C	1075	VAL
2	C	1076	ILE
2	C	1077	SER
2	C	1082	ILE
2	C	1083	GLU
2	C	1098	LEU
2	C	1137	GLU
2	C	1138	VAL
2	C	1142	ARG
2	C	1151	LEU
2	C	1157	GLN
2	C	1159	VAL
2	C	1161	LEU
2	C	1169	VAL
2	C	1207	SER

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Mol	Chain	Res	Type
2	C	1209	GLN
2	C	1212	LEU
2	C	1217	THR
2	C	1220	GLN
2	C	1225	VAL
2	C	1227	VAL
2	C	1247	SER
2	C	1250	SER
2	C	1252	SER
2	C	1253	LEU
2	C	1254	VAL
2	C	1255	THR
2	C	1289	GLU
2	C	1291	LEU
2	C	1293	VAL
2	C	1295	SER
2	C	1298	VAL
2	C	1337	ILE
2	C	1341	ASP
3	D	18	ASP
3	D	24	LEU
3	D	26	SER
3	D	40	LYS
3	D	65	VAL
3	D	83	VAL
3	D	92	VAL
3	D	126	LEU
3	D	147	ILE
3	D	154	LEU
3	D	155	GLU
3	D	176	PHE
3	D	227	PHE
3	D	232	ASN
3	D	244	VAL
3	D	253	VAL
3	D	262	THR
3	D	292	VAL
3	D	298	MET
3	D	300	GLN
3	D	301	GLU
3	D	317	THR
3	D	320	ASN

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Mol	Chain	Res	Type
3	D	324	LEU
3	D	354	VAL
3	D	363	LEU
3	D	371	LYS
3	D	390	LEU
3	D	392	THR
3	D	393	THR
3	D	401	VAL
3	D	407	VAL
3	D	410	ASP
3	D	416	ILE
3	D	422	LEU
3	D	425	ARG
3	D	441	LEU
3	D	449	LEU
3	D	454	CYS
3	D	472	LEU
3	D	473	THR
3	D	486	SER
3	D	492	SER
3	D	506	VAL
3	D	507	VAL
3	D	508	LEU
3	D	517	CYS
3	D	518	VAL
3	D	527	LEU
3	D	536	LEU
3	D	550	VAL
3	D	552	ILE
3	D	556	GLU
3	D	564	VAL
3	D	587	LEU
3	D	605	LEU
3	D	612	LEU
3	D	615	LYS
3	D	617	THR
3	D	618	VAL
3	D	624	ILE
3	D	627	THR
3	D	639	VAL
3	D	641	ILE
3	D	651	HIS

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Mol	Chain	Res	Type
3	D	684	ASP
3	D	691	ASP
3	D	699	ASP
3	D	701	LEU
3	D	703	THR
3	D	706	VAL
3	D	708	ASN
3	D	731	ARG
3	D	751	ASP
3	D	754	ILE
3	D	755	ILE
3	D	759	ILE
3	D	767	LEU
3	D	776	THR
3	D	798	ARG
3	D	803	VAL
3	D	807	LEU
3	D	810	THR
3	D	816	THR
3	D	822	MET
3	D	825	VAL
3	D	831	VAL
3	D	839	VAL
3	D	855	ASP
3	D	858	VAL
3	D	862	THR
3	D	874	GLU
3	D	875	ASN
3	D	877	VAL
3	D	882	VAL
3	D	891	ASP
3	D	895	CYS
3	D	905	ARG
3	D	917	VAL
3	D	918	ILE
3	D	960	LEU
3	D	980	THR
3	D	987	GLU
3	D	992	LYS
3	D	997	VAL
3	D	1002	VAL
3	D	1007	ASP

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Mol	Chain	Res	Type
3	D	1028	ILE
3	D	1050	THR
3	D	1053	LEU
3	D	1060	VAL
3	D	1062	LEU
3	D	1078	LEU
3	D	1089	LEU
3	D	1111	ASP
3	D	1135	THR
3	D	1146	GLU
3	D	1162	ILE
3	D	1164	SER
3	D	1169	THR
3	D	1189	MET
3	D	1200	GLU
3	D	1219	ASP
3	D	1223	LEU
3	D	1261	LEU
3	D	1268	ASN
3	D	1284	ARG
3	D	1285	VAL
3	D	1292	LEU
3	D	1310	THR
3	D	1348	LYS
3	D	1351	VAL
3	D	1353	VAL
3	D	1368	ASP
3	D	1372	ARG
4	E	4	VAL
4	E	43	ASN
4	E	58	LEU
5	F	60	LEU
5	F	88	VAL
5	F	90	SER
5	F	98	ASN
5	F	166	ARG
5	F	167	LEU
5	F	174	GLU
5	F	181	THR
5	F	189	LEU
5	F	220	THR
5	F	221	SER

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Mol	Chain	Res	Type
5	F	224	THR
5	F	231	GLU
5	F	243	GLU
5	F	248	ASP
5	F	267	ASN
5	F	270	GLN
5	F	281	LEU
5	F	287	THR
5	F	311	ARG
5	F	313	LEU
6	J	19	LEU
6	J	23	ILE
6	J	58	MET
6	J	71	TYR
6	J	84	VAL
6	J	85	VAL
6	J	90	THR
6	J	97	GLU
6	J	104	HIS
6	J	114	MET
6	J	116	LEU
6	J	129	VAL
6	J	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	B	84	ASN
1	B	137	ASN
1	B	186	ASN
2	C	31	GLN
2	C	120	GLN
2	C	219	GLN
2	C	276	GLN
2	C	387	ASN
2	C	510	GLN
2	C	618	GLN
2	C	620	ASN
2	C	649	GLN
2	C	684	ASN
2	C	752	ASN

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Mol	Chain	Res	Type
2	C	766	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1157	GLN
2	C	1312	ASN
2	C	1324	ASN
3	D	206	ASN
3	D	340	GLN
3	D	365	GLN
3	D	424	ASN
3	D	560	ASN
3	D	623	GLN
3	D	667	GLN
3	D	669	GLN
3	D	720	ASN
3	D	771	GLN
3	D	910	ASN
3	D	1019	ASN
3	D	1195	GLN
3	D	1227	HIS
3	D	1235	ASN
3	D	1238	GLN
3	D	1252	HIS
3	D	1268	ASN
3	D	1289	ASN
4	E	31	GLN
5	F	160	ASN
5	F	244	ASN
5	F	251	GLN
6	J	63	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

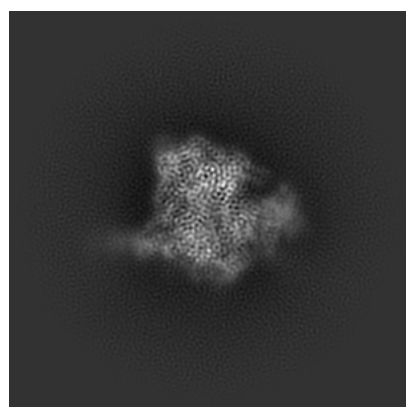
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20090. These allow visual inspection of the internal detail of the map and identification of artifacts.

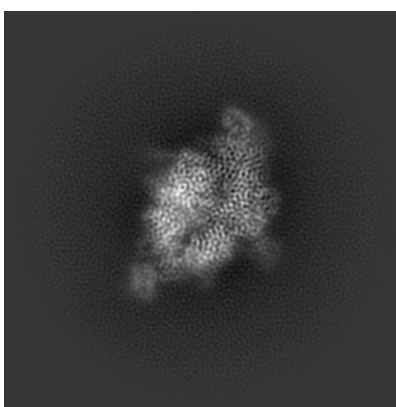
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

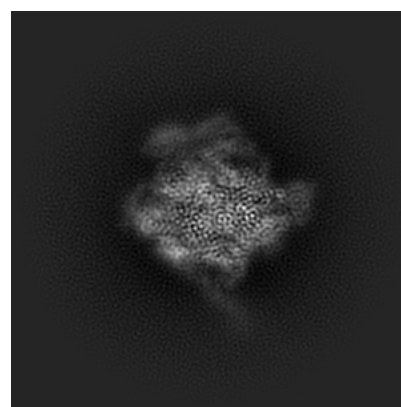
6.1.1 Primary map



X



Y

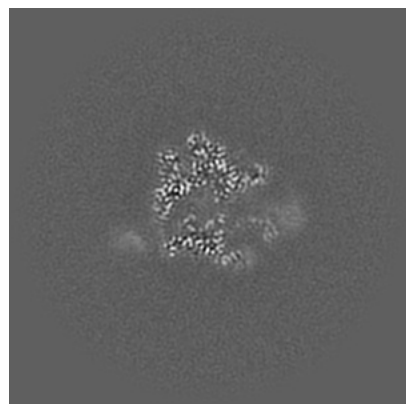


Z

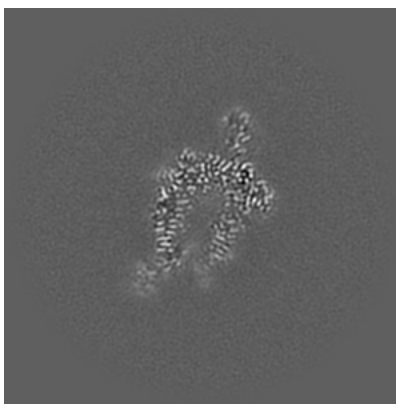
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

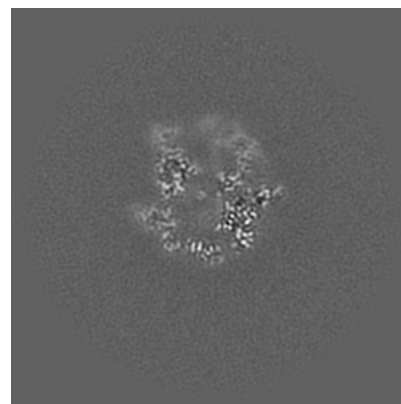
6.2.1 Primary map



X Index: 128



Y Index: 128

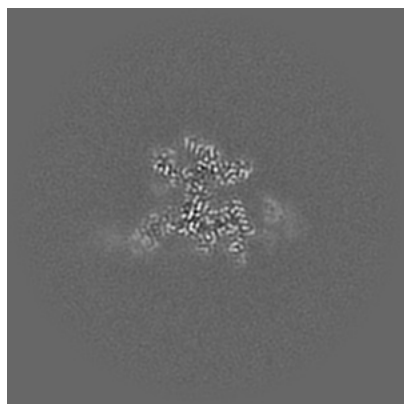


Z Index: 128

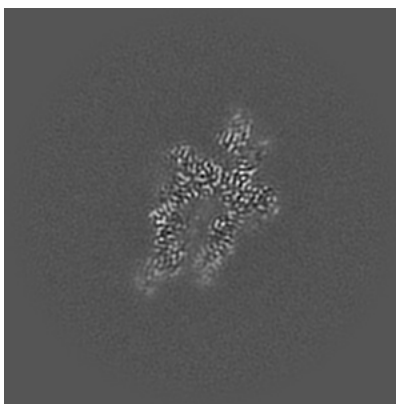
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

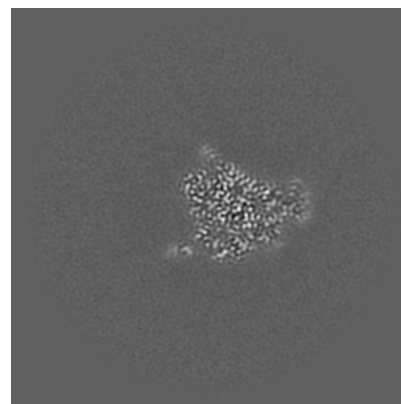
6.3.1 Primary map



X Index: 141



Y Index: 123

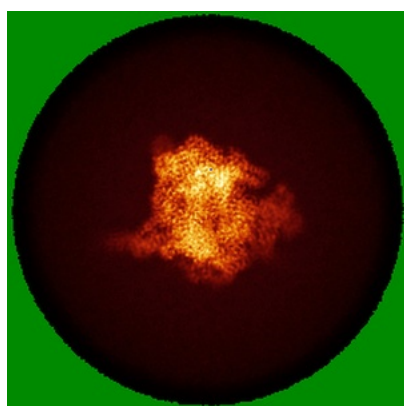


Z Index: 151

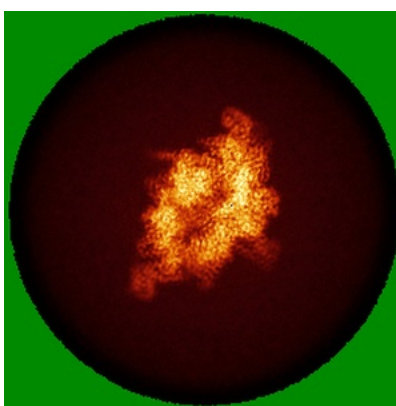
The images above show the largest variance slices of the map in three orthogonal directions.

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

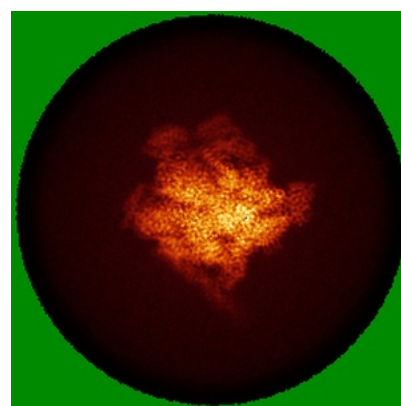
6.4.1 Primary map



X



Y



Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

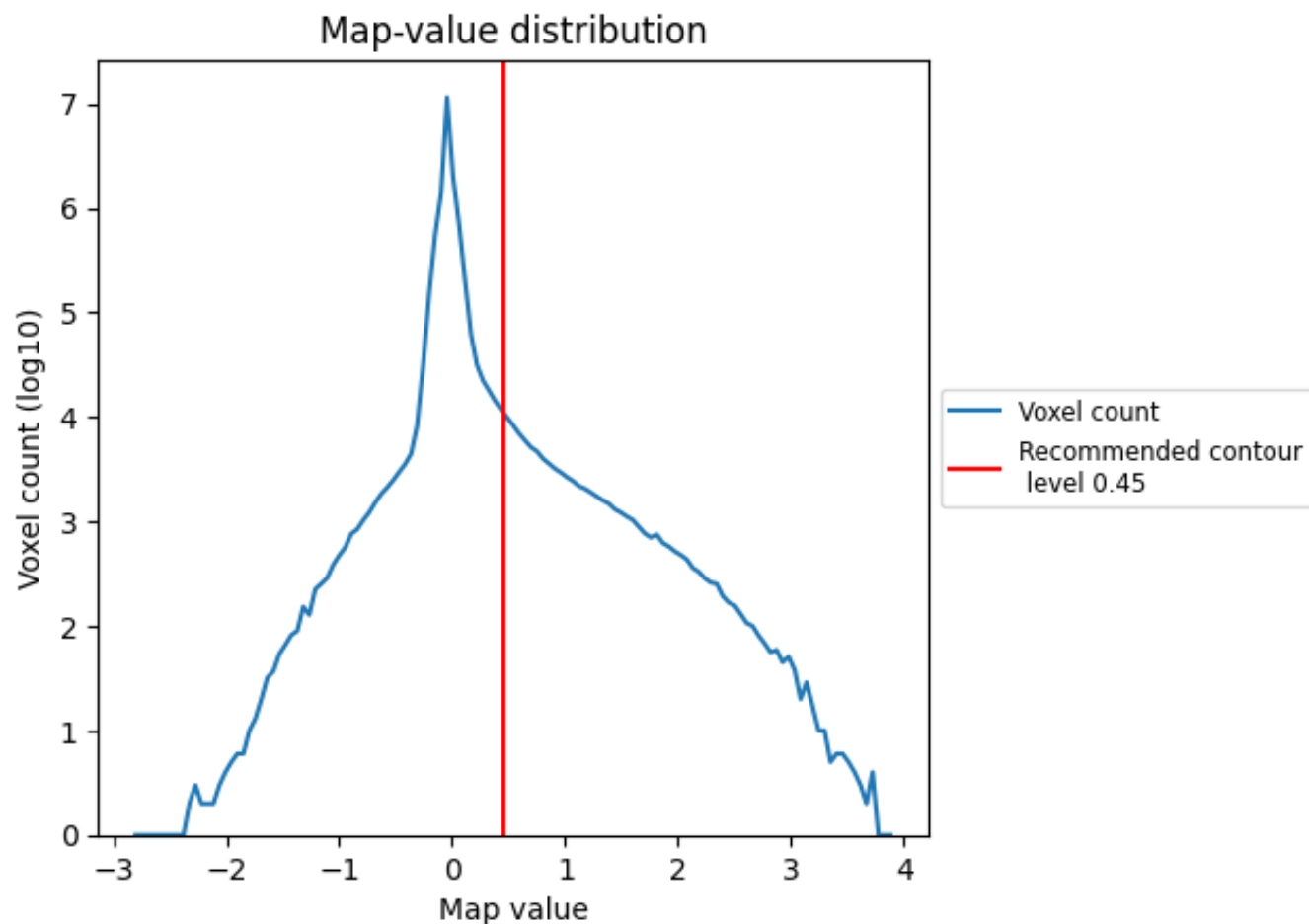
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

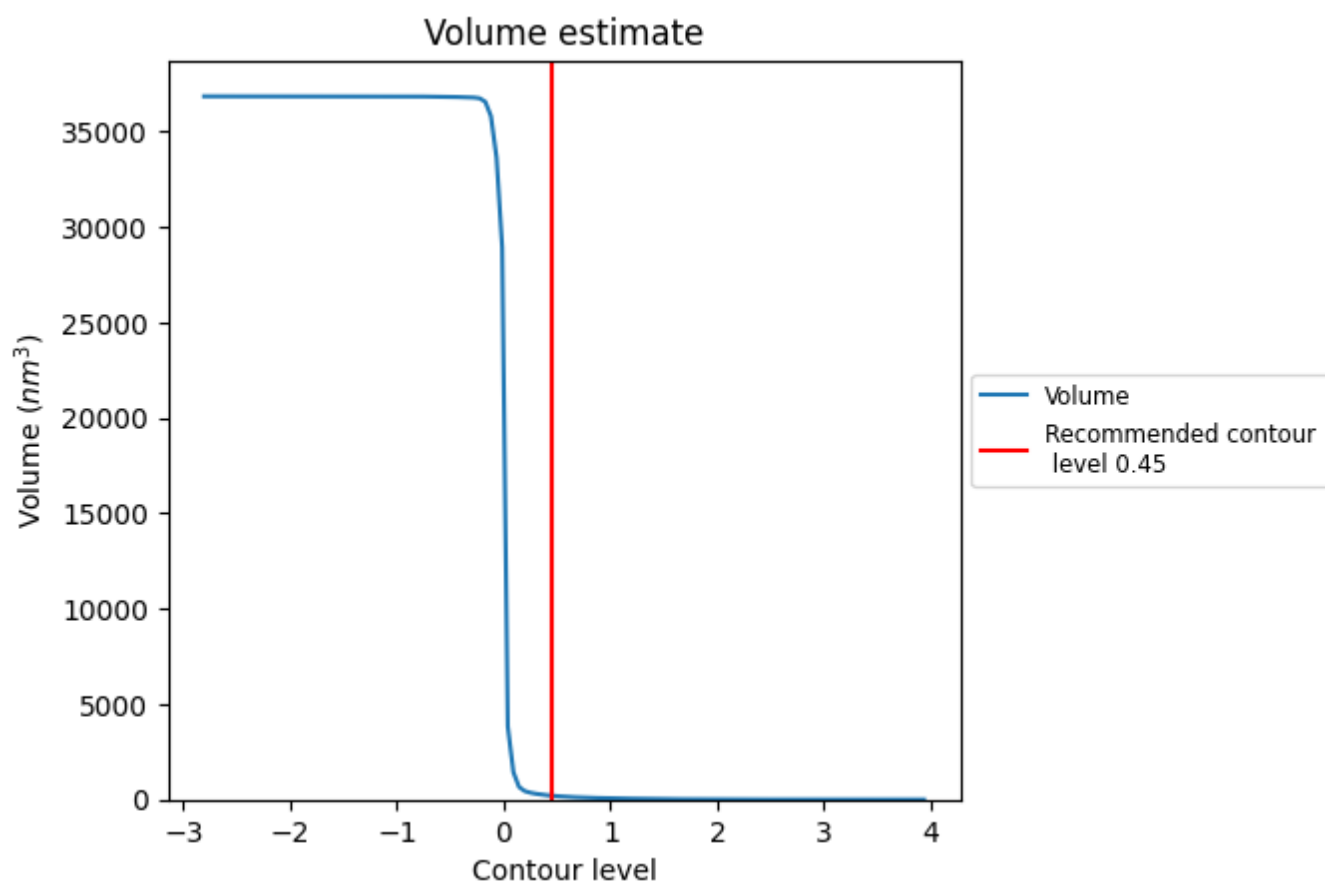
This section contains the results of statistical analysis of the map.

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.

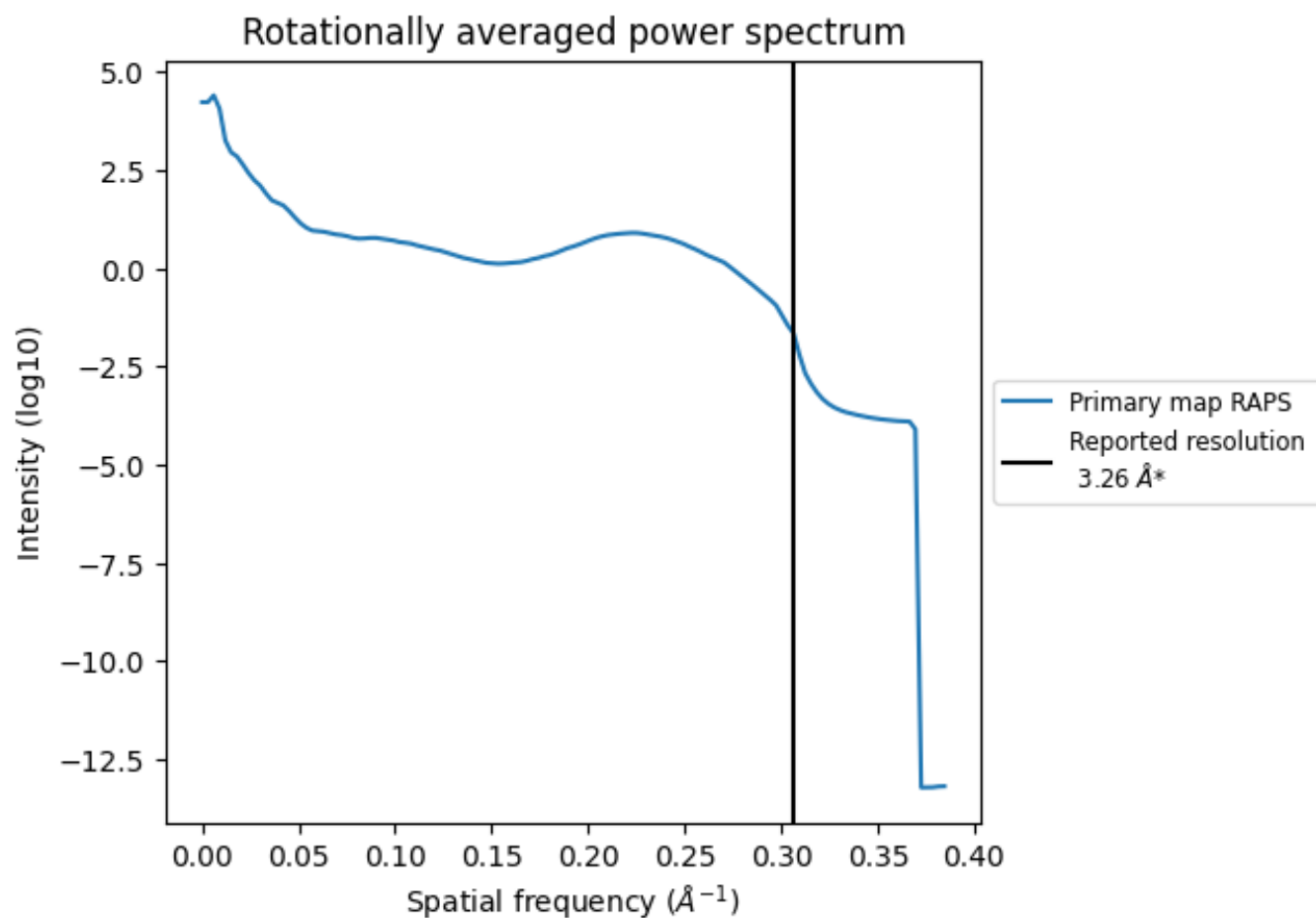
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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 0.307 Å⁻¹

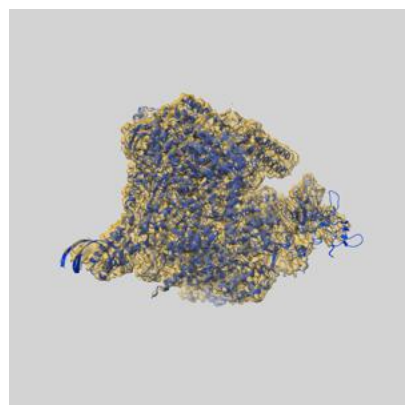
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

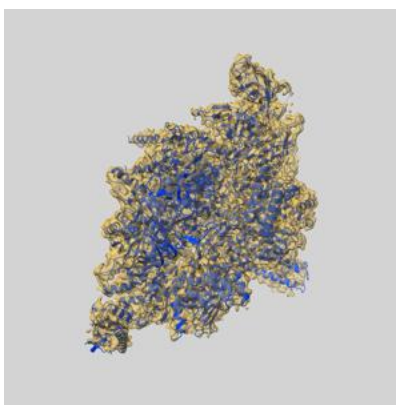
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20090 and PDB model 6OMF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

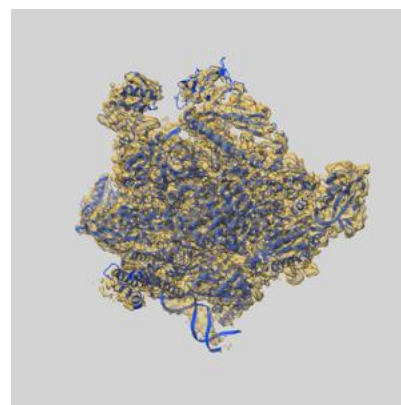
9.1 Map-model overlay [i](#)



X



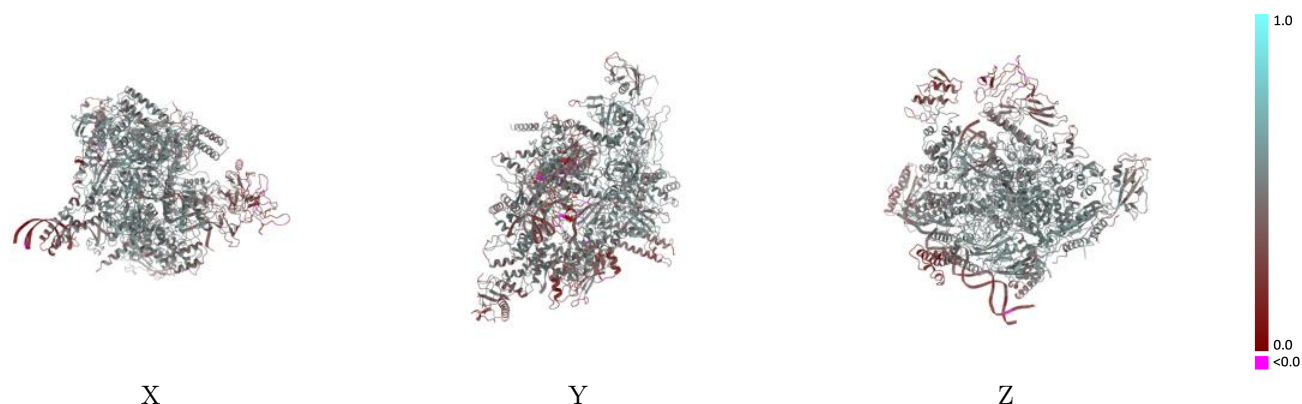
Y



Z

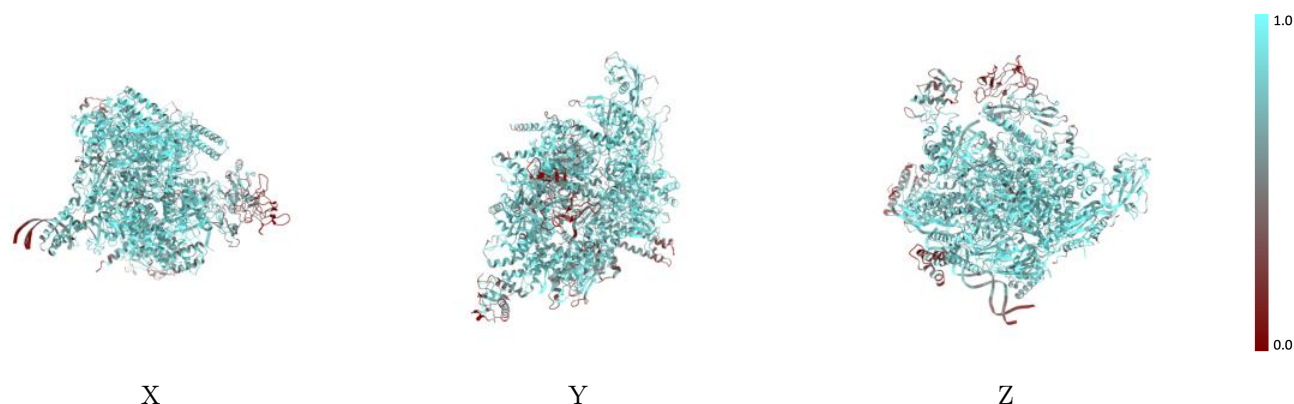
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



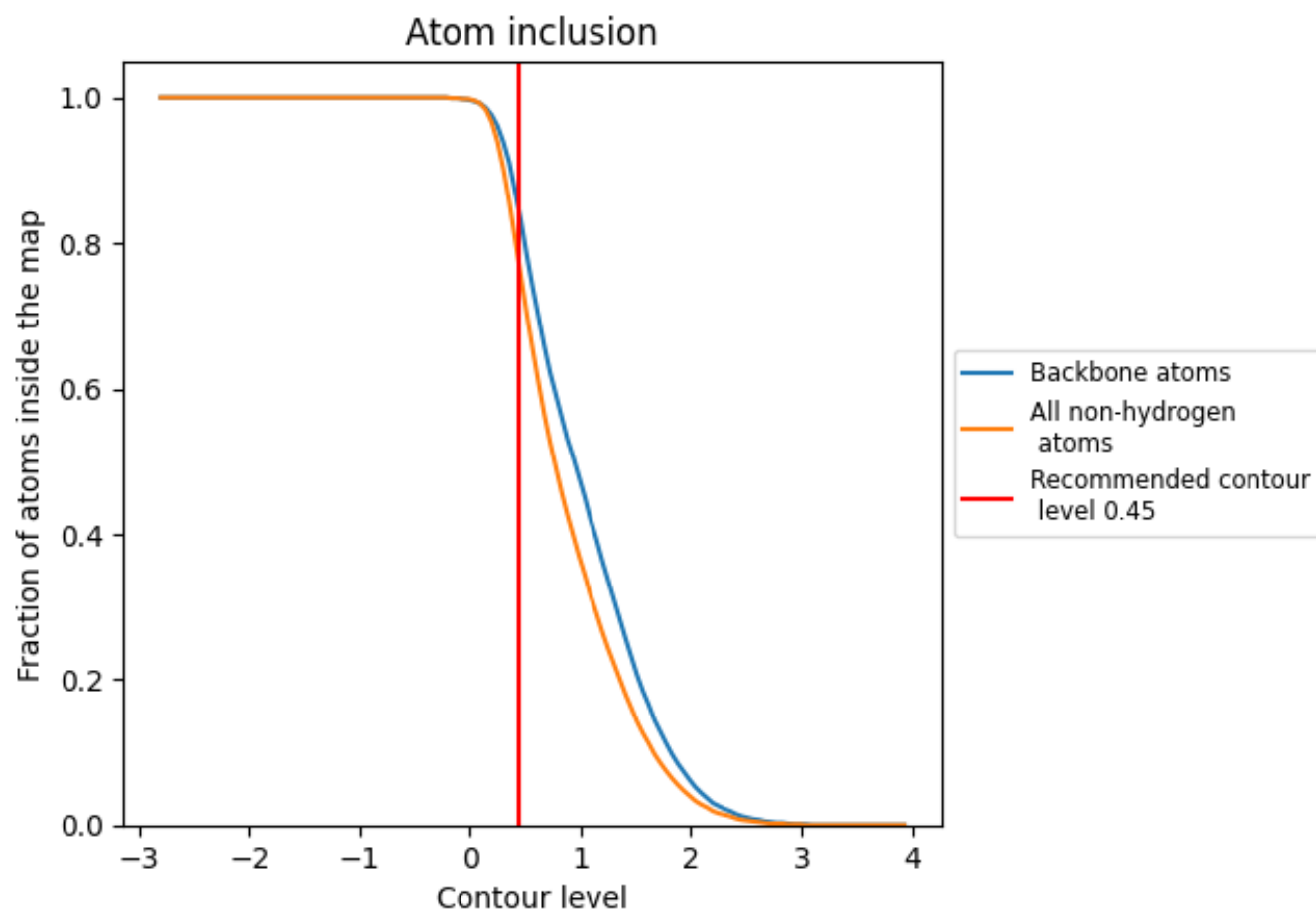
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.4630
A	0.8210	0.5020
B	0.7810	0.4680
C	0.7880	0.4830
D	0.7680	0.4740
E	0.7640	0.4840
F	0.7680	0.4560
J	0.5190	0.3690
N	0.6740	0.3060
T	0.7020	0.3110

1.0

0.0

<0.0