



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:57 PM UTC

PDB ID : 6C05 / pdb_00006c05
EMDB ID : EMD-7322
Title : Mycobacterium tuberculosis RNAP Holo/RbpA in relaxed state
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.; Lilic, M.
Deposited on : 2017-12-27
Resolution : 5.15 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

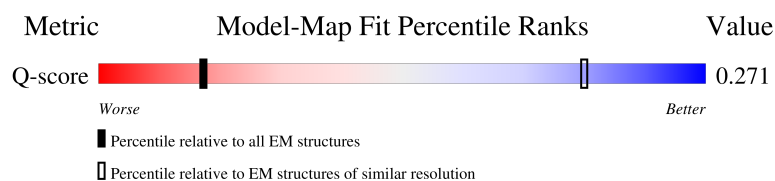
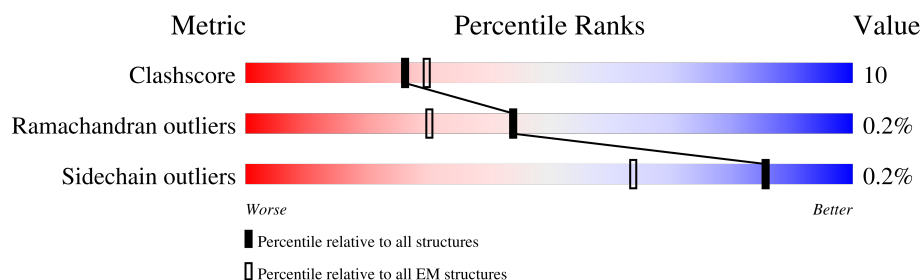
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.15 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	694 (4.65 - 5.65)

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	347	55% 10% 35%
1	B	347	52% 16% 32%
2	C	1181	70% 24% 6%
3	D	1324	70% 25% 5%

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	531	
6	J	111	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26024 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	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8556	5361	1504	1652	39		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879
C	1186	GLY	-	expression tag	UNP V9Z879
C	1187	ALA	-	expression tag	UNP V9Z879

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1263	Total	C	N	O	S	0	0
			9857	6175	1791	1850	41		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A0A045J9E2
D	1318	HIS	-	expression tag	UNP A0A045J9E2
D	1319	HIS	-	expression tag	UNP A0A045J9E2
D	1320	HIS	-	expression tag	UNP A0A045J9E2
D	1321	HIS	-	expression tag	UNP A0A045J9E2
D	1322	HIS	-	expression tag	UNP A0A045J9E2
D	1323	HIS	-	expression tag	UNP A0A045J9E2
D	1324	HIS	-	expression tag	UNP A0A045J9E2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	326	Total	C	N	O	S	0	0
			2588	1617	467	495	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A045HD00
F	-1	PRO	-	expression tag	UNP A0A045HD00
F	0	HIS	-	expression tag	UNP A0A045HD00

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	107	Total	C	N	O	S	0	0
			872	539	162	168	3		

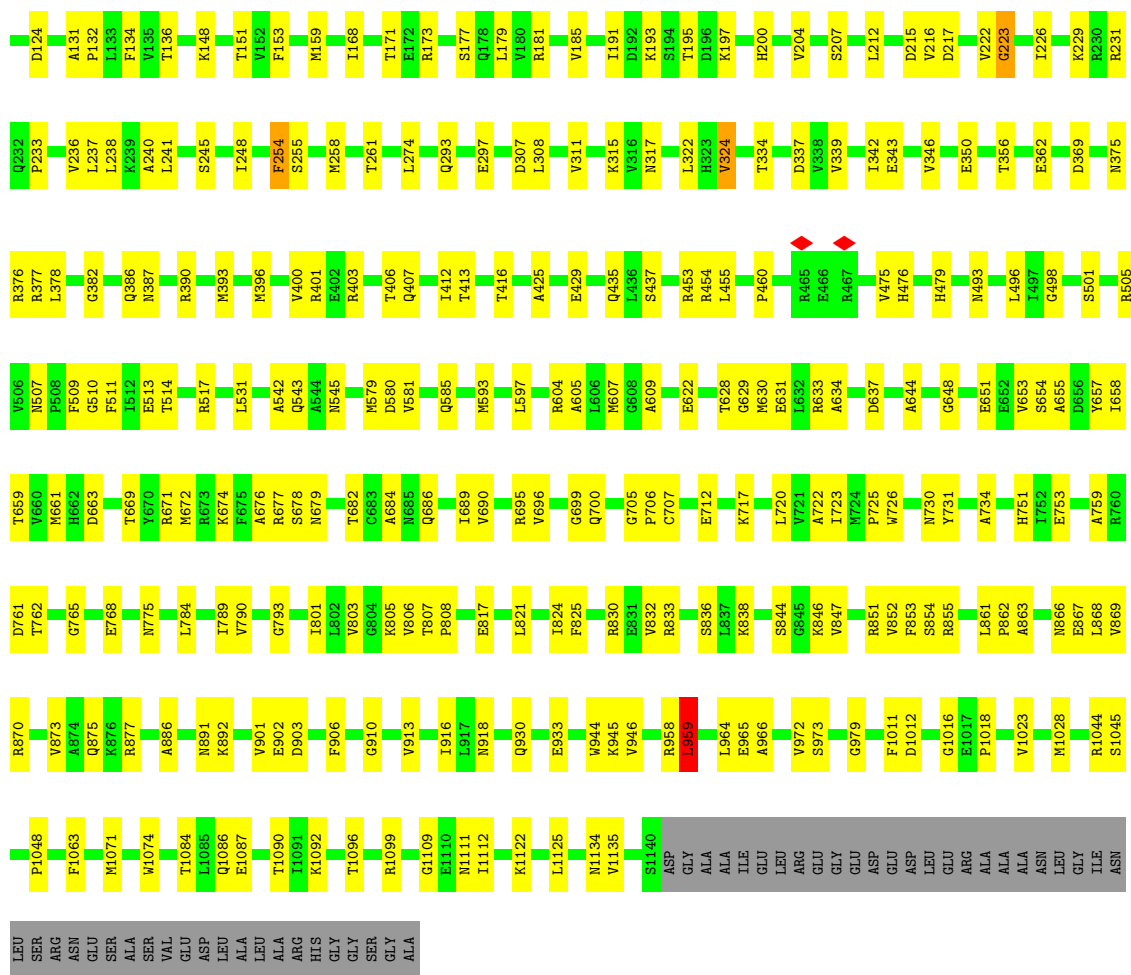
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

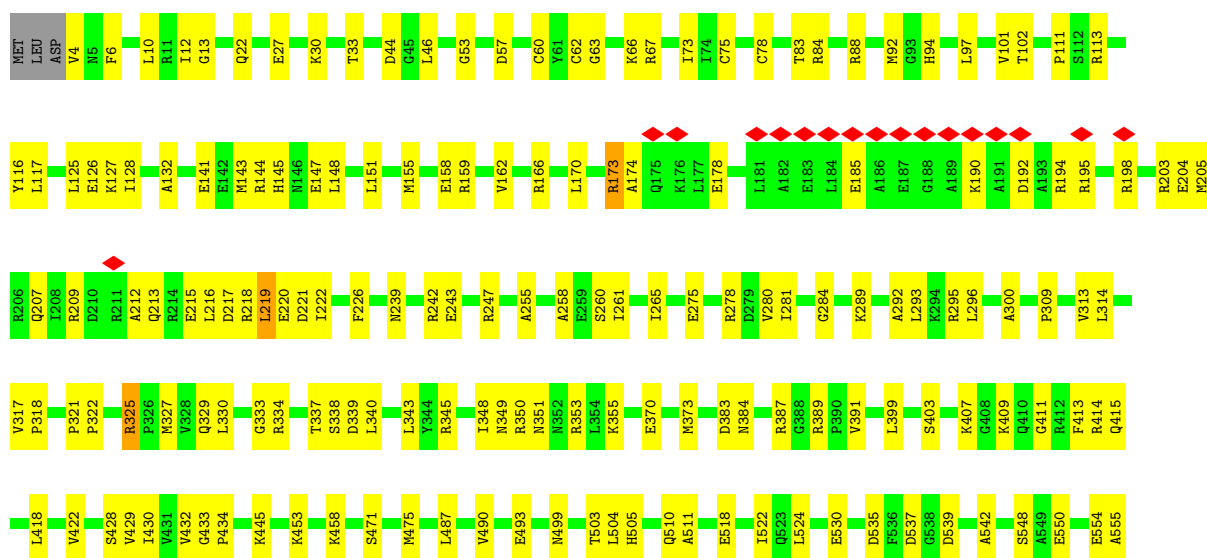
Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

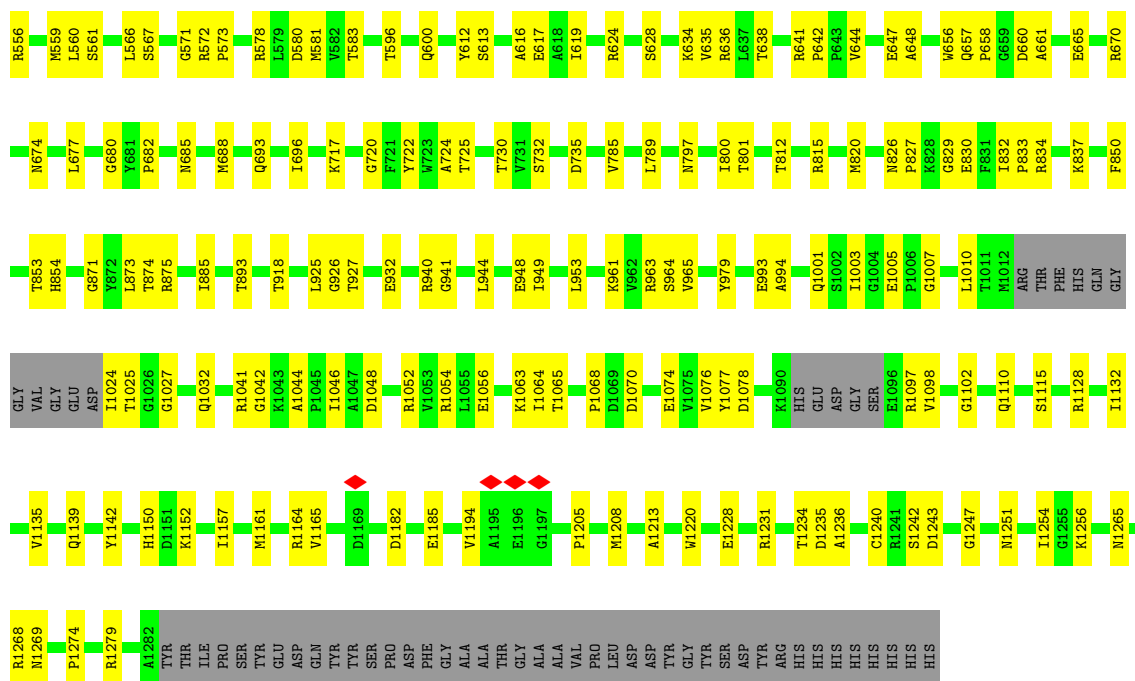




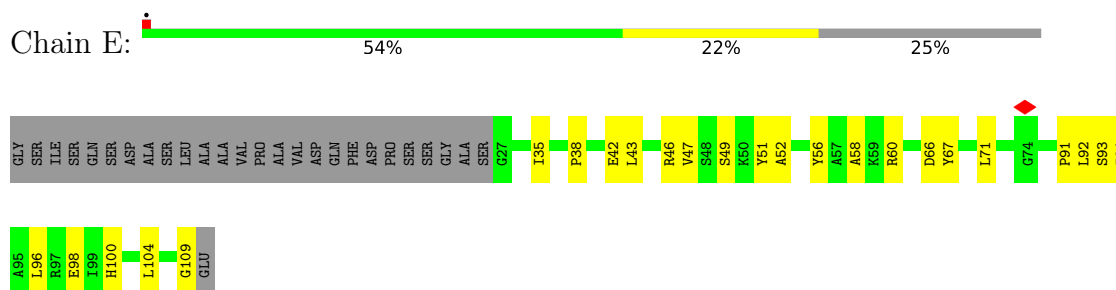
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 70% 25% 5%

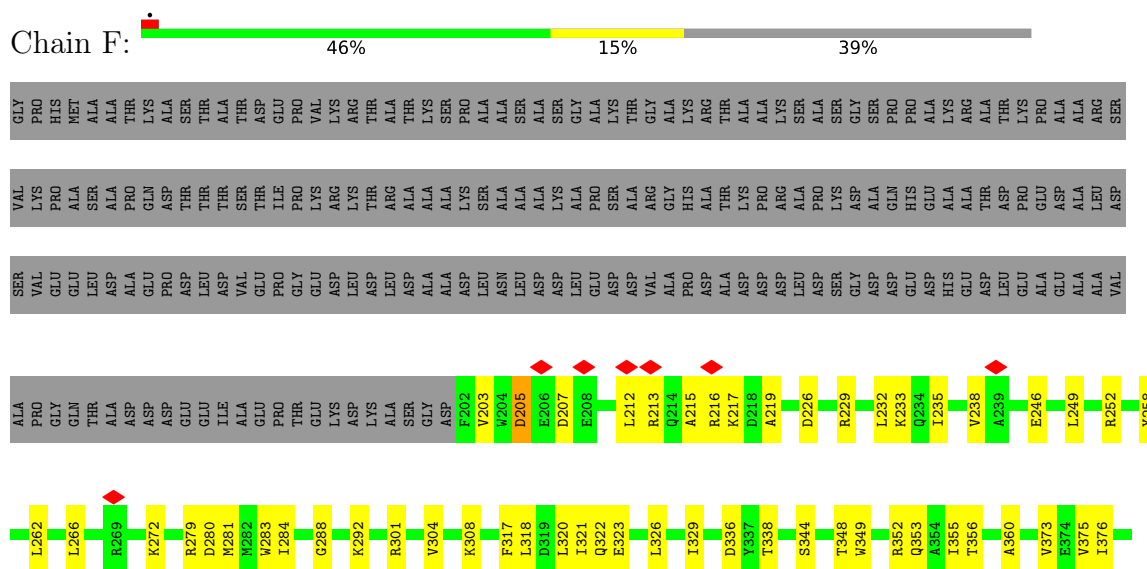


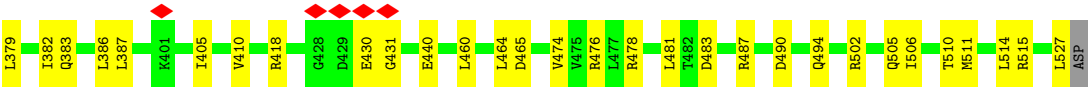


• Molecule 4: DNA-directed RNA polymerase subunit omega

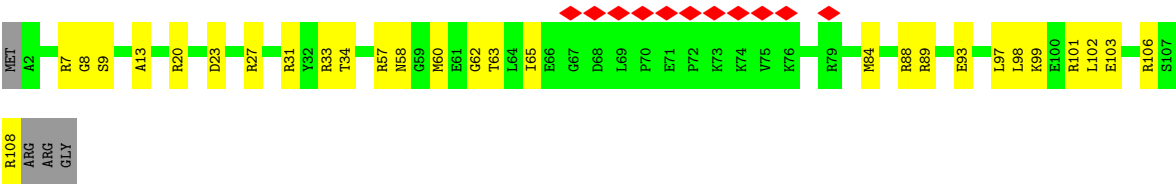


• Molecule 5: RNA polymerase sigma factor SigA





• Molecule 6: RNA polymerase-binding protein RbpA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	6.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0189	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	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	0.29	0/1750	0.63	1/2380 (0.0%)
1	B	0.30	0/1802	0.66	0/2454
2	C	0.34	0/8714	0.74	11/11824 (0.1%)
3	D	0.31	0/10021	0.69	5/13549 (0.0%)
4	E	0.32	0/662	0.68	0/901
5	F	0.24	0/2622	0.61	2/3538 (0.1%)
6	J	0.26	0/888	0.63	0/1199
All	All	0.31	0/26459	0.69	19/35845 (0.1%)

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
2	C	0	4
3	D	0	3
All	All	0	7

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	475	VAL	CA-C-N	8.79	147.87	122.38
2	C	475	VAL	C-N-CA	8.79	147.87	122.38
2	C	350	GLU	N-CA-C	-8.53	104.00	114.75
2	C	254	PHE	CA-C-N	8.15	136.36	121.70
2	C	254	PHE	C-N-CA	8.15	136.36	121.70
2	C	229	LYS	CA-C-N	6.11	133.22	121.54
2	C	229	LYS	C-N-CA	6.11	133.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1070	ASP	CA-C-N	6.06	132.61	121.70
3	D	1070	ASP	C-N-CA	6.06	132.61	121.70
3	D	834	ARG	CA-C-N	5.66	140.59	127.00
3	D	834	ARG	C-N-CA	5.66	140.59	127.00
2	C	723	ILE	CA-C-N	-5.58	110.70	123.15
2	C	723	ILE	C-N-CA	-5.58	110.70	123.15
2	C	597	LEU	CA-C-N	5.48	132.01	121.54
2	C	597	LEU	C-N-CA	5.48	132.01	121.54
1	A	2	LEU	CA-CB-CG	5.31	134.88	116.30
3	D	834	ARG	C-N-CD	-5.27	109.00	120.60
5	F	205	ASP	CA-C-N	5.21	131.49	121.54
5	F	205	ASP	C-N-CA	5.21	131.49	121.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	223	GLY	Peptide
2	C	61	PHE	Peptide
2	C	958	ARG	Peptide
2	C	959	LEU	Peptide
3	D	1194	VAL	Peptide
3	D	600	GLN	Peptide
3	D	932	GLU	Peptide

5.2 Too-close contacts [i](#)

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	1724	0	1768	23	0
1	B	1775	0	1809	33	0
2	C	8556	0	8459	180	0
3	D	9857	0	9920	222	0
4	E	649	0	645	18	0
5	F	2588	0	2602	69	0
6	J	872	0	852	26	0
7	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	1	0	0	0	0
All	All	26024	0	26055	527	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 (527) 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)
3:D:75:CYS:HB3	3:D:78:CYS:SG	2.07	0.94
3:D:144:ARG:O	3:D:148:LEU:HB2	1.77	0.84
2:C:97:GLU:H	2:C:401:ARG:HH21	1.28	0.81
3:D:292:ALA:O	3:D:296:LEU:HB2	1.80	0.81
5:F:460:LEU:O	5:F:464:LEU:HB2	1.80	0.80
3:D:537:ASP:OD1	3:D:539:ASP:OD1	1.99	0.79
3:D:143:MET:O	3:D:147:GLU:HB2	1.82	0.79
2:C:237:LEU:O	2:C:241:LEU:HB2	1.83	0.78
3:D:1001:GLN:O	3:D:1005:GLU:HB2	1.84	0.78
4:E:52:ALA:O	4:E:56:TYR:HB2	1.84	0.77
3:D:351:ASN:O	3:D:355:LYS:HB2	1.85	0.77
3:D:217:ASP:O	3:D:221:ASP:HB2	1.85	0.76
2:C:425:ALA:O	2:C:429:GLU:HB2	1.86	0.75
3:D:162:VAL:O	3:D:166:ARG:HB2	1.87	0.74
5:F:383:GLN:O	5:F:387:LEU:HB2	1.87	0.73
5:F:348:THR:HG22	5:F:352:ARG:HE	1.54	0.73
2:C:507:ASN:HB3	2:C:511:PHE:H	1.54	0.72
2:C:236:VAL:O	2:C:240:ALA:HB3	1.90	0.72
2:C:382:GLY:O	2:C:386:GLN:HB2	1.89	0.71
3:D:113:ARG:O	3:D:117:LEU:HB2	1.90	0.71
3:D:330:LEU:HB2	3:D:334:ARG:HB3	1.71	0.70
3:D:329:GLN:HE21	3:D:333:GLY:HA2	1.57	0.70
2:C:759:ALA:HB3	2:C:867:GLU:HB3	1.75	0.68
2:C:435:GLN:HE21	2:C:460:PRO:HD3	1.59	0.67
2:C:254:PHE:H	2:C:255:SER:HB2	1.60	0.67
3:D:871:GLY:O	3:D:875:ARG:HB2	1.95	0.67
2:C:891:ASN:HD21	2:C:1028:MET:HE1	1.60	0.66
2:C:853:PHE:HB2	2:C:868:LEU:HB3	1.78	0.66
2:C:854:SER:HA	2:C:867:GLU:HA	1.77	0.66
5:F:215:ALA:O	5:F:219:ALA:HB2	1.96	0.66
5:F:349:TRP:O	5:F:353:GLN:HB2	1.95	0.66
1:B:78:LEU:HA	1:B:81:LYS:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:686:GLN:HA	2:C:705:GLY:HA2	1.78	0.65
2:C:1012:ASP:HB3	2:C:1016:GLY:H	1.62	0.65
2:C:215:ASP:HB2	2:C:223:GLY:HA3	1.78	0.64
2:C:476:HIS:H	2:C:479:HIS:HD2	1.45	0.64
3:D:578:ARG:H	3:D:581:MET:HE2	1.63	0.63
2:C:847:VAL:HG22	2:C:873:VAL:HG22	1.79	0.63
6:J:99:LYS:O	6:J:103:GLU:HB2	1.97	0.63
2:C:96:ILE:HB	2:C:105:LEU:HB3	1.79	0.63
2:C:217:ASP:OD1	2:C:231:ARG:NH1	2.32	0.63
3:D:203:ARG:O	3:D:207:GLN:HB2	1.98	0.63
3:D:215:GLU:O	3:D:219:LEU:HB2	1.97	0.63
2:C:207:SER:H	2:C:308:LEU:HA	1.64	0.62
5:F:490:ASP:O	5:F:494:GLN:HB2	1.99	0.62
2:C:38:ARG:NH1	2:C:972:VAL:O	2.32	0.62
2:C:1111:ASN:ND2	4:E:66:ASP:OD1	2.32	0.62
1:B:2:LEU:HD23	1:B:4:SER:H	1.64	0.62
2:C:604:ARG:NH1	2:C:607:MET:SD	2.73	0.61
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.33	0.61
3:D:53:GLY:O	3:D:88:ARG:NH1	2.33	0.61
1:B:180:ALA:HA	1:B:190:ASP:HA	1.82	0.60
2:C:1112:ILE:HG13	3:D:548:SER:HA	1.83	0.60
6:J:89:ARG:HD2	6:J:93:GLU:HG2	1.82	0.60
3:D:1046:ILE:HA	3:D:1110:GLN:HA	1.82	0.60
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.65	0.60
2:C:695:ARG:NH1	2:C:696:VAL:O	2.35	0.60
1:B:146:TYR:O	3:D:624:ARG:NH2	2.35	0.60
2:C:946:VAL:HB	2:C:964:LEU:HB3	1.84	0.60
3:D:1274:PRO:HA	4:E:104:LEU:HB2	1.84	0.60
2:C:517:ARG:HG3	2:C:581:VAL:HG12	1.82	0.60
3:D:885:ILE:HA	3:D:994:ALA:HA	1.83	0.60
2:C:233:PRO:HB3	5:F:203:VAL:HG11	1.83	0.59
1:A:179:ASP:HB2	1:A:191:LYS:HB3	1.82	0.59
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.35	0.59
6:J:20:ARG:NH2	6:J:23:ASP:O	2.35	0.59
6:J:93:GLU:O	6:J:97:LEU:HB2	2.02	0.59
1:B:100:GLN:HA	1:B:133:LYS:HA	1.84	0.59
1:A:6:ARG:NH2	1:B:217:GLU:O	2.36	0.59
3:D:190:LYS:HE2	3:D:192:ASP:HB3	1.85	0.59
3:D:322:PRO:HA	3:D:325:ARG:HE	1.66	0.59
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.35	0.59
1:B:17:ASN:HB2	1:B:198:THR:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:677:ARG:HH21	2:C:753:GLU:HA	1.68	0.59
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.35	0.59
2:C:120:ASP:O	2:C:124:ASP:HB2	2.02	0.58
2:C:181:ARG:HA	2:C:376:ARG:HA	1.84	0.58
3:D:720:GLY:O	3:D:724:ALA:HB2	2.03	0.58
2:C:71:ARG:O	2:C:75:ALA:HB2	2.02	0.58
2:C:945:LYS:HA	2:C:965:GLU:HA	1.85	0.58
3:D:159:ARG:NH2	3:D:220:GLU:OE1	2.36	0.58
3:D:292:ALA:O	3:D:296:LEU:CB	2.50	0.58
5:F:465:ASP:OD1	5:F:476:ARG:NH2	2.37	0.57
6:J:102:LEU:O	6:J:106:ARG:HB2	2.03	0.57
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.85	0.57
2:C:593:MET:HE3	2:C:631:GLU:HG3	1.85	0.57
3:D:185:GLU:HG2	3:D:194:ARG:HH11	1.69	0.57
2:C:689:ILE:HG13	2:C:690:VAL:HG13	1.87	0.57
2:C:1044:ARG:NH2	2:C:1048:PRO:O	2.36	0.57
3:D:1254:ILE:HG13	3:D:1256:LYS:H	1.69	0.57
1:B:1:MET:HB2	1:B:232:ILE:HG12	1.87	0.56
2:C:855:ARG:NH1	2:C:862:PRO:O	2.38	0.56
3:D:330:LEU:HA	6:J:8:GLY:HA2	1.87	0.56
5:F:375:VAL:O	5:F:379:LEU:HB2	2.05	0.56
3:D:4:VAL:HG12	3:D:6:PHE:H	1.70	0.56
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.86	0.56
3:D:1251:ASN:HA	3:D:1254:ILE:HG12	1.87	0.56
2:C:672:MET:HG3	2:C:674:LYS:HD3	1.87	0.56
3:D:1097:ARG:HG2	3:D:1098:VAL:HG12	1.86	0.56
3:D:1164:ARG:HD2	3:D:1208:MET:HE1	1.88	0.56
3:D:612:TYR:HB2	3:D:635:VAL:HG12	1.88	0.56
3:D:674:ASN:HA	3:D:677:LEU:HD13	1.86	0.56
2:C:659:THR:HG22	2:C:669:THR:HG22	1.87	0.56
5:F:212:LEU:O	5:F:216:ARG:CB	2.54	0.56
3:D:166:ARG:HG3	3:D:212:ALA:HB1	1.86	0.56
3:D:413:PHE:O	3:D:418:LEU:N	2.39	0.56
3:D:926:GLY:O	3:D:940:ARG:NH2	2.39	0.56
5:F:375:VAL:O	5:F:379:LEU:CB	2.53	0.56
6:J:31:ARG:HB2	6:J:65:ILE:HD12	1.87	0.56
3:D:1044:ALA:HB3	3:D:1110:GLN:HE21	1.70	0.56
2:C:678:SER:HB3	2:C:682:THR:H	1.71	0.55
5:F:511:MET:HB3	5:F:515:ARG:HH12	1.71	0.55
6:J:84:MET:O	6:J:88:ARG:NH1	2.40	0.55
5:F:229:ARG:O	5:F:233:LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:676:ALA:HB3	2:C:684:ALA:HB3	1.89	0.55
3:D:333:GLY:O	5:F:418:ARG:NH1	2.39	0.55
3:D:820:MET:HE3	3:D:837:LYS:HA	1.88	0.55
6:J:58:ASN:ND2	6:J:60:MET:SD	2.79	0.55
2:C:805:LYS:HB3	2:C:836:SER:HA	1.89	0.55
2:C:425:ALA:O	2:C:429:GLU:CB	2.55	0.55
3:D:434:PRO:O	3:D:717:LYS:NZ	2.40	0.55
2:C:89:VAL:O	2:C:93:LEU:HB2	2.07	0.54
2:C:855:ARG:HH11	2:C:861:LEU:HD12	1.72	0.54
3:D:116:TYR:O	3:D:295:ARG:NE	2.40	0.54
2:C:191:ILE:O	2:C:193:LYS:NZ	2.41	0.54
3:D:173:ARG:NH2	3:D:204:GLU:OE1	2.39	0.54
3:D:389:ARG:NH2	5:F:226:ASP:OD1	2.39	0.54
2:C:648:GLY:O	2:C:695:ARG:NH1	2.40	0.54
2:C:906:PHE:HD2	2:C:910:GLY:HA2	1.72	0.54
2:C:43:LYS:NZ	2:C:979:GLY:O	2.39	0.54
3:D:471:SER:O	3:D:475:MET:HB2	2.07	0.54
3:D:218:ARG:NH1	3:D:243:GLU:OE2	2.41	0.54
3:D:893:THR:O	3:D:963:ARG:NH2	2.41	0.54
3:D:62:CYS:H	3:D:78:CYS:HB3	1.72	0.54
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.90	0.54
1:A:43:LEU:HD23	2:C:901:VAL:HG13	1.90	0.53
2:C:493:ASN:HA	2:C:496:LEU:HD12	1.89	0.53
3:D:203:ARG:O	3:D:207:GLN:CB	2.55	0.53
3:D:555:ALA:HA	3:D:559:MET:HB2	1.90	0.53
3:D:566:LEU:HA	3:D:573:PRO:HA	1.90	0.53
3:D:797:ASN:HB3	3:D:800:ILE:HG22	1.90	0.53
5:F:502:ARG:HD2	5:F:505:GLN:HE21	1.73	0.53
1:A:12:ASP:HB2	1:A:20:GLN:HB2	1.89	0.53
2:C:61:PHE:O	2:C:63:TRP:N	2.38	0.53
3:D:636:ARG:HH21	3:D:661:ALA:HB3	1.74	0.53
6:J:93:GLU:O	6:J:97:LEU:CB	2.57	0.53
6:J:106:ARG:O	6:J:108:ARG:NH2	2.41	0.53
1:B:34:LEU:HA	1:B:37:SER:HB2	1.90	0.53
1:A:151:GLN:HG3	1:A:154:ALA:H	1.72	0.53
3:D:530:GLU:OE1	3:D:578:ARG:NH1	2.42	0.53
2:C:644:ALA:O	2:C:699:GLY:N	2.39	0.53
3:D:10:LEU:N	3:D:1243:ASP:OD1	2.42	0.53
5:F:382:ILE:O	5:F:386:LEU:CB	2.57	0.53
3:D:102:THR:HG22	3:D:313:VAL:HG12	1.90	0.53
3:D:111:PRO:O	3:D:113:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HB2	1:A:138:LEU:HB2	1.91	0.53
2:C:678:SER:OG	2:C:679:ASN:N	2.40	0.53
3:D:83:THR:OG1	3:D:84:ARG:N	2.42	0.53
3:D:873:LEU:HD13	3:D:1032:GLN:HG3	1.90	0.53
5:F:352:ARG:HA	5:F:355:ILE:HD12	1.91	0.53
2:C:38:ARG:HD3	2:C:973:SER:HB3	1.90	0.53
3:D:1052:ARG:HH21	3:D:1102:GLY:HA2	1.74	0.53
1:B:74:THR:HA	1:B:77:ILE:HD12	1.91	0.53
3:D:826:ASN:HB3	3:D:829:GLY:H	1.73	0.53
3:D:213:GLN:HA	3:D:216:LEU:HD12	1.92	0.52
3:D:339:ASP:HB3	3:D:399:LEU:HD23	1.91	0.52
3:D:350:ARG:NH1	3:D:373:MET:O	2.41	0.52
3:D:567:SER:N	3:D:572:ARG:O	2.41	0.52
2:C:238:LEU:HD23	2:C:248:ILE:HG12	1.90	0.52
6:J:98:LEU:O	6:J:102:LEU:CB	2.57	0.52
2:C:803:VAL:O	2:C:836:SER:OG	2.27	0.52
3:D:826:ASN:N	3:D:830:GLU:O	2.42	0.52
1:B:95:MET:HB2	1:B:138:LEU:HB2	1.91	0.52
3:D:125:LEU:HA	3:D:128:ILE:HD12	1.91	0.52
3:D:535:ASP:N	3:D:535:ASP:OD1	2.43	0.52
3:D:927:THR:OG1	3:D:961:LYS:O	2.28	0.52
1:B:55:ARG:HH21	1:B:60:LEU:HD11	1.75	0.52
2:C:71:ARG:HH11	2:C:82:PRO:HG2	1.73	0.52
2:C:1045:SER:OG	3:D:453:LYS:NZ	2.41	0.52
2:C:387:ASN:OD1	2:C:390:ARG:NH1	2.43	0.52
3:D:641:ARG:HB3	3:D:682:PRO:HA	1.91	0.52
2:C:377:ARG:HH21	2:C:510:GLY:HA3	1.75	0.52
2:C:622:GLU:H	2:C:717:LYS:HE2	1.75	0.52
2:C:830:ARG:HB3	2:C:832:VAL:HG22	1.92	0.52
2:C:944:TRP:H	2:C:966:ALA:HB3	1.74	0.52
3:D:944:LEU:HD23	3:D:948:GLU:HG2	1.91	0.51
1:B:34:LEU:HB2	1:B:38:LEU:HD23	1.92	0.51
1:A:40:ARG:HG3	2:C:902:GLU:HG3	1.91	0.51
3:D:732:SER:N	3:D:735:ASP:OD2	2.42	0.51
2:C:605:ALA:O	2:C:609:ALA:CB	2.58	0.51
3:D:101:VAL:O	3:D:314:LEU:N	2.41	0.51
3:D:162:VAL:O	3:D:166:ARG:CB	2.57	0.51
1:B:11:GLU:OE1	1:B:205:ARG:NH1	2.44	0.51
2:C:1096:THR:HA	2:C:1099:ARG:HE	1.74	0.51
3:D:1063:LYS:NZ	3:D:1078:ASP:OD1	2.41	0.51
3:D:22:GLN:O	6:J:57:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:656:TRP:HE3	3:D:658:PRO:HD2	1.76	0.51
1:A:226:ASN:HD22	1:B:9:LEU:HG	1.76	0.51
2:C:245:SER:HA	2:C:248:ILE:HD12	1.93	0.51
3:D:550:GLU:HG3	4:E:58:ALA:HB1	1.92	0.51
1:B:54:ILE:O	1:B:162:ILE:N	2.41	0.50
2:C:356:THR:HA	2:C:362:GLU:HA	1.92	0.50
2:C:762:THR:HG23	2:C:765:GLY:H	1.75	0.50
3:D:964:SER:OG	3:D:965:VAL:N	2.44	0.50
3:D:1025:THR:HG22	3:D:1027:GLY:H	1.76	0.50
3:D:1242:SER:OG	3:D:1243:ASP:N	2.44	0.50
2:C:1011:PHE:HA	2:C:1018:PRO:HA	1.93	0.50
4:E:60:ARG:NE	4:E:98:GLU:OE1	2.44	0.50
3:D:510:GLN:HB3	3:D:561:SER:HB2	1.93	0.50
3:D:797:ASN:O	3:D:801:THR:OG1	2.26	0.50
5:F:379:LEU:HD11	5:F:410:VAL:HG23	1.94	0.50
5:F:474:VAL:O	5:F:478:ARG:CB	2.59	0.50
5:F:506:ILE:O	5:F:510:THR:OG1	2.22	0.50
2:C:1122:LYS:HA	2:C:1125:LEU:HD13	1.93	0.50
3:D:949:ILE:O	3:D:953:LEU:CB	2.59	0.50
2:C:393:MET:HA	2:C:396:MET:HB3	1.94	0.50
3:D:949:ILE:O	3:D:953:LEU:HB2	2.12	0.50
3:D:1024:ILE:O	3:D:1041:ARG:NH2	2.44	0.50
1:A:97:LEU:HD13	1:A:110:ILE:HA	1.94	0.50
2:C:69:ARG:O	2:C:73:SER:CB	2.60	0.50
2:C:400:VAL:HA	2:C:403:ARG:HG2	1.93	0.50
2:C:343:GLU:HA	2:C:346:VAL:HG12	1.94	0.50
2:C:542:ALA:HB3	2:C:579:MET:HA	1.93	0.49
2:C:654:SER:OG	2:C:655:ALA:N	2.44	0.49
2:C:654:SER:HB3	2:C:657:TYR:H	1.77	0.49
6:J:98:LEU:O	6:J:102:LEU:HB3	2.12	0.49
2:C:633:ARG:NH1	2:C:637:ASP:OD2	2.37	0.49
2:C:653:VAL:HG12	2:C:658:ILE:HG23	1.94	0.49
5:F:344:SER:O	5:F:348:THR:OG1	2.26	0.49
2:C:1084:THR:OG1	3:D:554:GLU:OE1	2.26	0.49
3:D:511:ALA:HB3	3:D:560:LEU:HA	1.94	0.49
2:C:403:ARG:HA	2:C:406:THR:HG22	1.94	0.49
5:F:258:TYR:O	5:F:262:LEU:HB2	2.12	0.49
2:C:69:ARG:O	2:C:73:SER:HB2	2.12	0.49
3:D:280:VAL:O	3:D:284:GLY:N	2.44	0.49
5:F:212:LEU:O	5:F:216:ARG:HB3	2.13	0.49
2:C:148:LYS:NZ	2:C:412:ILE:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:HA	1:A:140:VAL:HA	1.94	0.49
1:A:171:VAL:HA	1:A:198:THR:HA	1.95	0.49
2:C:1135:VAL:HG12	3:D:12:ILE:HG12	1.95	0.49
3:D:255:ALA:HB3	3:D:260:SER:HB3	1.94	0.49
3:D:504:LEU:HB3	3:D:1005:GLU:HG2	1.94	0.49
2:C:177:SER:OG	2:C:454:ARG:O	2.29	0.49
3:D:499:ASN:HB3	3:D:542:ALA:HB3	1.95	0.49
6:J:58:ASN:HB3	6:J:60:MET:HG2	1.94	0.48
3:D:827:PRO:HD3	3:D:854:HIS:HB3	1.95	0.48
2:C:90:LEU:O	2:C:94:SER:N	2.45	0.48
2:C:317:ASN:HB3	2:C:324:VAL:HG12	1.94	0.48
2:C:903:ASP:OD1	2:C:903:ASP:N	2.45	0.48
3:D:567:SER:HB2	3:D:571:GLY:H	1.77	0.48
2:C:855:ARG:HH12	2:C:863:ALA:HA	1.79	0.48
3:D:141:GLU:O	3:D:145:HIS:CB	2.61	0.48
3:D:289:LYS:O	3:D:293:LEU:N	2.46	0.48
3:D:1048:ASP:OD2	3:D:1077:TYR:OH	2.30	0.48
5:F:288:GLY:O	5:F:292:LYS:HB2	2.13	0.48
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.57	0.48
1:A:223:ARG:HD2	1:A:224:GLU:H	1.79	0.48
2:C:886:ALA:HA	2:C:892:LYS:HA	1.94	0.48
3:D:657:GLN:NE2	3:D:660:ASP:O	2.43	0.48
3:D:1025:THR:OG1	3:D:1041:ARG:NH2	2.46	0.48
1:B:21:PHE:HB2	1:B:194:LEU:HB2	1.96	0.48
3:D:411:GLY:O	3:D:415:GLN:N	2.45	0.48
2:C:71:ARG:O	2:C:75:ALA:CB	2.62	0.48
2:C:657:TYR:HB3	2:C:671:ARG:HD2	1.95	0.48
2:C:959:LEU:H	2:C:959:LEU:HG	1.47	0.48
3:D:205:MET:O	3:D:209:ARG:HB2	2.13	0.48
3:D:638:THR:HG22	3:D:661:ALA:HB2	1.94	0.48
5:F:338:THR:HG23	6:J:89:ARG:HH22	1.78	0.48
1:A:95:MET:N	1:A:138:LEU:O	2.47	0.48
3:D:258:ALA:HA	3:D:261:ILE:HD12	1.95	0.48
3:D:642:PRO:HG2	3:D:647:GLU:HB3	1.95	0.48
3:D:60:CYS:SG	3:D:63:GLY:N	2.86	0.47
3:D:151:LEU:O	3:D:155:MET:HB2	2.14	0.47
1:B:39:ARG:HA	1:B:174:VAL:HG11	1.96	0.47
3:D:1128:ARG:HH12	3:D:1132:ILE:HD11	1.79	0.47
2:C:674:LYS:NZ	2:C:686:GLN:O	2.40	0.47
3:D:127:LYS:HB3	3:D:132:ALA:HB3	1.95	0.47
3:D:720:GLY:O	3:D:724:ALA:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:ND2	1:B:125:ILE:O	2.47	0.47
1:B:105:VAL:N	1:B:126:ALA:O	2.45	0.47
3:D:1135:VAL:O	3:D:1139:GLN:HB3	2.15	0.47
2:C:1092:LYS:HB3	3:D:422:VAL:HB	1.97	0.47
3:D:613:SER:N	3:D:617:GLU:OE1	2.47	0.47
5:F:483:ASP:OD1	5:F:483:ASP:N	2.47	0.47
2:C:179:LEU:HD11	2:C:455:LEU:HB3	1.96	0.47
3:D:92:MET:HG2	3:D:321:PRO:HD3	1.97	0.47
5:F:382:ILE:O	5:F:386:LEU:HB2	2.15	0.47
1:A:204:PRO:O	1:A:208:LEU:CB	2.63	0.47
1:B:6:ARG:NE	1:B:236:PRO:O	2.48	0.47
1:B:17:ASN:ND2	1:B:198:THR:O	2.48	0.47
2:C:236:VAL:O	2:C:240:ALA:CB	2.62	0.47
2:C:768:GLU:HB3	2:C:806:VAL:HG13	1.96	0.47
2:C:1109:GLY:HA3	3:D:458:LYS:HE3	1.96	0.47
3:D:918:THR:HB	3:D:1150:HIS:HA	1.96	0.47
3:D:1231:ARG:HA	3:D:1234:THR:HG22	1.96	0.47
4:E:42:GLU:O	4:E:46:ARG:NH1	2.48	0.47
5:F:238:VAL:HB	5:F:301:ARG:HH22	1.80	0.47
5:F:318:LEU:HD23	5:F:321:ILE:HD12	1.96	0.47
3:D:432:VAL:HG13	3:D:434:PRO:HD3	1.96	0.47
1:A:97:LEU:HD22	1:A:110:ILE:HG12	1.97	0.47
2:C:722:ALA:HB3	2:C:916:ILE:HG12	1.97	0.47
2:C:177:SER:HB2	2:C:378:LEU:HD11	1.96	0.47
2:C:207:SER:OG	2:C:307:ASP:O	2.32	0.47
2:C:369:ASP:O	2:C:375:ASN:ND2	2.48	0.47
3:D:265:ILE:HG23	3:D:309:PRO:HG2	1.97	0.47
3:D:340:LEU:HA	3:D:343:LEU:HD12	1.95	0.47
3:D:634:LYS:HG2	3:D:665:GLU:HB3	1.97	0.47
3:D:1274:PRO:O	3:D:1279:ARG:NH2	2.48	0.47
4:E:52:ALA:O	4:E:56:TYR:CB	2.60	0.47
5:F:356:THR:O	5:F:360:ALA:HB2	2.15	0.47
1:B:108:GLY:N	1:B:121:PRO:O	2.48	0.46
3:D:349:ASN:O	3:D:353:ARG:HB2	2.15	0.46
3:D:1042:GLY:O	3:D:1115:SER:N	2.46	0.46
1:A:46:ILE:HD11	1:A:211:ALA:HB2	1.96	0.46
1:A:78:LEU:HA	1:A:81:LYS:HD3	1.96	0.46
1:A:204:PRO:O	1:A:208:LEU:HB2	2.15	0.46
4:E:38:PRO:HG2	4:E:43:LEU:HD11	1.97	0.46
2:C:173:ARG:NH2	2:C:437:SER:O	2.49	0.46
3:D:239:ASN:OD1	3:D:242:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:353:ARG:NE	5:F:323:GLU:OE2	2.44	0.46
3:D:660:ASP:OD1	3:D:660:ASP:N	2.46	0.46
1:A:186:ARG:NH1	1:B:149:ALA:O	2.46	0.46
2:C:817:GLU:HG3	5:F:481:LEU:HD22	1.98	0.46
4:E:47:VAL:HG12	4:E:49:SER:H	1.81	0.46
2:C:453:ARG:NH2	2:C:501:SER:O	2.45	0.46
3:D:66:LYS:HB3	3:D:67:ARG:HH21	1.80	0.46
3:D:345:ARG:HA	3:D:348:ILE:HG22	1.98	0.46
3:D:383:ASP:OD1	3:D:403:SER:OG	2.27	0.46
2:C:726:TRP:HA	3:D:725:THR:HG22	1.98	0.46
2:C:825:PHE:HD2	5:F:527:LEU:HD12	1.81	0.46
3:D:281:ILE:HG22	3:D:289:LYS:HG3	1.98	0.46
3:D:641:ARG:NH1	3:D:680:GLY:O	2.47	0.46
3:D:925:LEU:HB2	3:D:941:GLY:H	1.80	0.46
1:B:107:ALA:N	1:B:123:MET:O	2.47	0.46
2:C:311:VAL:HG22	2:C:509:PHE:HD1	1.81	0.46
2:C:630:MET:O	2:C:634:ALA:N	2.49	0.46
2:C:851:ARG:HB2	2:C:870:ARG:HB2	1.98	0.46
2:C:793:GLY:O	2:C:846:LYS:NZ	2.47	0.46
3:D:1135:VAL:O	3:D:1139:GLN:CB	2.64	0.46
6:J:34:THR:HA	6:J:62:GLY:HA3	1.98	0.46
1:A:108:GLY:N	1:A:121:PRO:O	2.48	0.46
3:D:116:TYR:HB3	3:D:295:ARG:HG3	1.98	0.46
3:D:1064:ILE:HB	3:D:1077:TYR:HB2	1.97	0.46
1:B:213:LYS:NZ	1:B:217:GLU:OE2	2.48	0.46
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.49	0.46
2:C:56:VAL:HG13	2:C:57:GLN:HG2	1.97	0.45
3:D:322:PRO:HA	3:D:325:ARG:NE	2.32	0.45
3:D:487:LEU:HA	3:D:490:VAL:HG22	1.97	0.45
5:F:483:ASP:OD2	5:F:487:ARG:NH2	2.50	0.45
3:D:493:GLU:HA	4:E:35:ILE:HD11	1.97	0.45
3:D:205:MET:O	3:D:209:ARG:CB	2.65	0.45
5:F:379:LEU:O	5:F:383:GLN:HB2	2.16	0.45
3:D:126:GLU:OE2	3:D:387:ARG:NH2	2.49	0.45
3:D:215:GLU:O	3:D:219:LEU:CB	2.63	0.45
2:C:200:HIS:H	2:C:216:VAL:HB	1.80	0.45
2:C:476:HIS:H	2:C:479:HIS:CD2	2.28	0.45
3:D:334:ARG:HA	5:F:418:ARG:HH11	1.81	0.45
2:C:311:VAL:O	2:C:315:LYS:N	2.46	0.45
2:C:334:THR:HG23	2:C:337:ASP:H	1.81	0.45
2:C:382:GLY:O	2:C:386:GLN:CB	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:654:SER:N	2:C:657:TYR:O	2.50	0.45
2:C:844:SER:OG	2:C:875:GLN:NE2	2.50	0.45
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.50	0.45
5:F:279:ARG:O	5:F:283:TRP:HB2	2.15	0.45
2:C:1134:ASN:N	3:D:13:GLY:O	2.50	0.45
1:B:149:ALA:N	1:B:165:ASP:OD1	2.50	0.45
2:C:455:LEU:O	2:C:498:GLY:N	2.43	0.45
2:C:808:PRO:HA	2:C:832:VAL:HA	1.98	0.45
2:C:1086:GLN:O	2:C:1090:THR:OG1	2.29	0.45
3:D:97:LEU:HD11	3:D:317:VAL:HG23	1.98	0.45
3:D:428:SER:OG	3:D:429:VAL:N	2.50	0.45
5:F:212:LEU:O	5:F:216:ARG:HB2	2.15	0.45
2:C:131:ALA:HB3	2:C:159:MET:HE3	1.99	0.45
2:C:339:VAL:HA	2:C:342:ILE:HD12	1.98	0.45
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.99	0.45
2:C:222:VAL:O	2:C:231:ARG:NH1	2.46	0.45
2:C:644:ALA:HB3	2:C:700:GLN:H	1.82	0.45
3:D:30:LYS:N	3:D:44:ASP:O	2.49	0.45
3:D:275:GLU:HA	3:D:278:ARG:HB2	1.97	0.45
3:D:409:LYS:H	3:D:409:LYS:HD2	1.82	0.45
5:F:326:LEU:HD23	5:F:329:ILE:HD12	1.99	0.45
3:D:144:ARG:NH2	3:D:226:PHE:O	2.50	0.44
3:D:812:THR:HB	3:D:815:ARG:HH21	1.82	0.44
3:D:1157:ILE:HG22	3:D:1161:MET:HE3	1.99	0.44
4:E:91:PRO:HA	4:E:94:ILE:HD12	2.00	0.44
5:F:246:GLU:HA	5:F:249:LEU:HB2	1.99	0.44
3:D:850:PHE:O	3:D:853:THR:OG1	2.27	0.44
5:F:379:LEU:O	5:F:383:GLN:CB	2.64	0.44
2:C:317:ASN:HA	2:C:322:LEU:HD12	1.99	0.44
2:C:240:ALA:HB1	2:C:274:LEU:HD13	2.00	0.44
3:D:337:THR:OG1	3:D:338:SER:N	2.49	0.44
5:F:318:LEU:HA	5:F:321:ILE:HD12	2.00	0.44
5:F:440:GLU:HB3	6:J:7:ARG:HA	1.99	0.44
3:D:1056:GLU:HB2	3:D:1063:LYS:HB3	1.98	0.44
2:C:1023:VAL:HA	3:D:730:THR:HG21	2.00	0.44
3:D:505:HIS:HB3	3:D:1005:GLU:HG3	2.00	0.44
3:D:616:ALA:HA	3:D:619:ILE:HD12	2.00	0.44
1:B:56:ILE:HG12	1:B:136:VAL:HG22	1.99	0.44
2:C:237:LEU:O	2:C:241:LEU:CB	2.62	0.44
2:C:730:ASN:HB2	2:C:918:ASN:HB2	1.99	0.44
3:D:993:GLU:OE2	4:E:51:TYR:OH	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:67:TYR:O	4:E:71:LEU:N	2.48	0.44
3:D:1269:ASN:HB2	4:E:109:GLY:HA3	2.00	0.43
1:B:46:ILE:HD11	1:B:211:ALA:HB2	1.99	0.43
3:D:351:ASN:O	3:D:355:LYS:CB	2.63	0.43
3:D:556:ARG:HE	4:E:35:ILE:HG23	1.82	0.43
3:D:644:VAL:O	3:D:648:ALA:HB2	2.17	0.43
3:D:1208:MET:HG3	3:D:1213:ALA:HB2	1.99	0.43
3:D:1265:ASN:HA	3:D:1268:ARG:HG3	2.01	0.43
5:F:258:TYR:HD2	6:J:98:LEU:HD13	1.83	0.43
3:D:281:ILE:HB	3:D:289:LYS:HE3	2.00	0.43
2:C:111:ARG:HE	2:C:134:PHE:HB2	1.83	0.43
2:C:725:PRO:HA	2:C:730:ASN:HD21	1.82	0.43
2:C:891:ASN:OD1	2:C:891:ASN:N	2.51	0.43
3:D:158:GLU:OE2	3:D:247:ARG:NH1	2.51	0.43
3:D:433:GLY:N	3:D:524:LEU:O	2.43	0.43
5:F:205:ASP:OD1	5:F:205:ASP:N	2.43	0.43
5:F:382:ILE:O	5:F:386:LEU:HB3	2.18	0.43
6:J:99:LYS:O	6:J:103:GLU:CB	2.66	0.43
5:F:280:ASP:OD1	5:F:281:MET:N	2.50	0.43
2:C:413:THR:HG23	2:C:416:THR:H	1.84	0.43
2:C:543:GLN:NE2	2:C:545:ASN:OD1	2.47	0.43
3:D:148:LEU:HA	3:D:151:LEU:HB2	2.01	0.43
5:F:288:GLY:O	5:F:292:LYS:CB	2.67	0.43
5:F:304:VAL:O	5:F:308:LYS:HB3	2.19	0.43
5:F:474:VAL:O	5:F:478:ARG:HB3	2.19	0.43
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.84	0.43
3:D:174:ALA:O	3:D:178:GLU:HB2	2.19	0.43
3:D:384:ASN:ND2	3:D:391:VAL:O	2.44	0.43
3:D:693:GLN:HA	3:D:696:ILE:HD12	2.00	0.43
2:C:784:LEU:HA	2:C:790:VAL:HA	2.00	0.43
3:D:871:GLY:HA2	3:D:874:THR:HB	2.01	0.43
2:C:168:ILE:O	2:C:171:THR:OG1	2.31	0.43
2:C:514:THR:O	2:C:531:LEU:N	2.48	0.43
2:C:580:ASP:HB3	2:C:585:GLN:HE22	1.83	0.43
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.54	0.43
3:D:222:ILE:HG21	3:D:247:ARG:HH21	1.84	0.43
3:D:722:TYR:O	3:D:725:THR:OG1	2.37	0.43
1:B:179:ASP:O	1:B:191:LYS:N	2.50	0.43
2:C:801:ILE:HG13	2:C:838:LYS:HG2	2.00	0.43
2:C:852:VAL:HA	2:C:869:VAL:HA	2.01	0.43
2:C:62:GLU:HG3	2:C:70:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:832:ILE:HA	3:D:833:PRO:HD3	1.74	0.42
4:E:93:SER:HA	4:E:96:LEU:HD12	2.01	0.42
5:F:252:ARG:HG2	6:J:101:ARG:CZ	2.49	0.42
2:C:185:VAL:HG12	2:C:204:VAL:HG22	2.01	0.42
2:C:517:ARG:O	2:C:579:MET:N	2.38	0.42
3:D:329:GLN:O	6:J:9:SER:N	2.52	0.42
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	2.00	0.42
5:F:511:MET:HE3	5:F:515:ARG:HH12	1.84	0.42
3:D:73:ILE:HG22	6:J:27:ARG:HG2	2.01	0.42
3:D:370:GLU:OE1	5:F:322:GLN:NE2	2.51	0.42
5:F:213:ARG:O	5:F:217:LYS:HB2	2.18	0.42
5:F:232:LEU:HA	5:F:235:ILE:HG12	2.01	0.42
3:D:170:LEU:O	3:D:174:ALA:HB2	2.20	0.42
3:D:596:THR:HB	3:D:628:SER:HB2	2.01	0.42
5:F:317:PHE:HA	5:F:320:LEU:HD12	2.01	0.42
5:F:349:TRP:O	5:F:353:GLN:CB	2.65	0.42
2:C:663:ASP:OD2	2:C:695:ARG:NH2	2.52	0.42
3:D:1007:GLY:HA2	3:D:1010:LEU:HD13	2.02	0.42
1:B:40:ARG:HD3	1:B:43:LEU:HD23	2.00	0.42
2:C:212:LEU:HB2	2:C:226:ILE:HG22	2.01	0.42
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	2.01	0.42
5:F:373:VAL:HA	5:F:376:ILE:HD12	2.01	0.42
3:D:871:GLY:O	3:D:875:ARG:CB	2.65	0.42
2:C:258:MET:HA	2:C:261:THR:HG23	2.00	0.42
3:D:1236:ALA:O	3:D:1240:CYS:N	2.53	0.42
2:C:1071:MET:HB2	3:D:503:THR:HB	2.02	0.42
3:D:102:THR:HA	3:D:313:VAL:HA	2.02	0.42
5:F:281:MET:HA	5:F:284:ILE:HG22	2.00	0.42
6:J:33:ARG:O	6:J:63:THR:N	2.52	0.42
5:F:229:ARG:O	5:F:233:LYS:CB	2.67	0.42
2:C:644:ALA:N	2:C:700:GLN:O	2.47	0.41
2:C:1074:TRP:HH2	3:D:875:ARG:HG3	1.84	0.41
3:D:785:VAL:O	3:D:789:LEU:HB2	2.20	0.41
3:D:1235:ASP:OD1	3:D:1235:ASP:N	2.52	0.41
2:C:731:TYR:H	2:C:734:ALA:HB3	1.85	0.41
2:C:136:THR:HA	2:C:151:THR:HA	2.01	0.41
2:C:775:ASN:OD1	2:C:775:ASN:N	2.54	0.41
3:D:141:GLU:O	3:D:145:HIS:HB2	2.20	0.41
3:D:979:TYR:O	3:D:1152:LYS:NZ	2.43	0.41
3:D:1003:ILE:O	3:D:1142:TYR:OH	2.37	0.41
2:C:807:THR:O	2:C:833:ARG:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:944:TRP:O	2:C:966:ALA:N	2.44	0.41
5:F:375:VAL:O	5:F:379:LEU:HB3	2.19	0.41
2:C:195:THR:HG23	2:C:197:LYS:HG2	2.03	0.41
2:C:761:ASP:OD1	2:C:866:ASN:ND2	2.38	0.41
2:C:1087:GLU:HG2	2:C:1092:LYS:HE3	2.02	0.41
3:D:27:GLU:HB2	3:D:94:HIS:CE1	2.54	0.41
3:D:445:LYS:NZ	3:D:518:GLU:OE2	2.53	0.41
2:C:403:ARG:HB2	2:C:407:GLN:HG2	2.01	0.41
3:D:57:ASP:H	6:J:13:ALA:HB3	1.86	0.41
3:D:430:ILE:HG22	3:D:522:ILE:HB	2.02	0.41
3:D:927:THR:HG21	3:D:961:LYS:HB3	2.02	0.41
1:A:97:LEU:HB2	1:A:110:ILE:HG23	2.02	0.41
2:C:1044:ARG:HD2	2:C:1063:PHE:HB2	2.01	0.41
3:D:94:HIS:HA	3:D:318:PRO:HA	2.02	0.41
3:D:219:LEU:HD22	3:D:222:ILE:HD12	2.02	0.41
3:D:1182:ASP:OD2	3:D:1185:GLU:N	2.46	0.41
5:F:262:LEU:O	5:F:266:LEU:HB2	2.20	0.41
5:F:405:ILE:HD11	5:F:410:VAL:HB	2.03	0.41
3:D:33:THR:HG22	3:D:46:LEU:HD12	2.02	0.41
3:D:556:ARG:HH11	4:E:92:LEU:HD12	1.86	0.41
3:D:1065:THR:HG23	3:D:1076:VAL:HG22	2.02	0.41
5:F:266:LEU:HD11	5:F:272:LYS:HA	2.02	0.41
2:C:322:LEU:HD23	2:C:322:LEU:HA	1.91	0.41
2:C:651:GLU:HB2	2:C:661:MET:HB2	2.02	0.41
2:C:821:LEU:HA	2:C:824:ILE:HD12	2.03	0.41
2:C:930:GLN:HA	2:C:933:GLU:HG2	2.02	0.41
3:D:428:SER:HB3	3:D:522:ILE:HD11	2.03	0.41
3:D:580:ASP:HA	3:D:583:THR:HG22	2.03	0.41
5:F:430:GLU:HA	5:F:431:GLY:HA3	1.77	0.41
2:C:628:THR:OG1	2:C:629:GLY:N	2.54	0.41
2:C:824:ILE:HG12	5:F:514:LEU:HD13	2.03	0.41
3:D:407:LYS:HE2	3:D:407:LYS:HB3	1.91	0.41
3:D:414:ARG:HA	3:D:418:LEU:HB2	2.02	0.41
3:D:296:LEU:O	3:D:300:ALA:CB	2.70	0.40
3:D:327:MET:HG3	3:D:337:THR:HB	2.03	0.40
1:B:51:VAL:HA	1:B:140:VAL:HG22	2.04	0.40
2:C:293:GLN:NE2	2:C:297:GLU:OE2	2.46	0.40
3:D:1228:GLU:OE2	3:D:1231:ARG:NH2	2.39	0.40
2:C:38:ARG:NH2	2:C:712:GLU:OE2	2.53	0.40
5:F:474:VAL:O	5:F:478:ARG:HB2	2.20	0.40
1:A:80:LEU:HD22	1:A:83:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLY:N	1:A:168:TYR:HB2	2.36	0.40
2:C:238:LEU:HD12	2:C:241:LEU:HD23	2.04	0.40
3:D:195:ARG:HD3	3:D:198:ARG:HE	1.86	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	224/347 (65%)	205 (92%)	19 (8%)	0	100	100
1	B	235/347 (68%)	215 (92%)	20 (8%)	0	100	100
2	C	1109/1181 (94%)	986 (89%)	117 (11%)	6 (0%)	24	62
3	D	1257/1324 (95%)	1169 (93%)	87 (7%)	1 (0%)	48	83
4	E	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
5	F	324/531 (61%)	306 (94%)	17 (5%)	1 (0%)	36	71
6	J	105/111 (95%)	92 (88%)	13 (12%)	0	100	100
All	All	3335/3951 (84%)	3048 (91%)	279 (8%)	8 (0%)	44	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	GLU
2	C	707	CYS
2	C	61	PHE
2	C	959	LEU
5	F	207	ASP
3	D	1220	TRP
2	C	706	PRO
2	C	324	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	195/297 (66%)	195 (100%)	0	100	100
1	B	197/297 (66%)	195 (99%)	2 (1%)	68	77
2	C	924/997 (93%)	923 (100%)	1 (0%)	88	88
3	D	1041/1103 (94%)	1038 (100%)	3 (0%)	86	84
4	E	69/89 (78%)	69 (100%)	0	100	100
5	F	272/429 (63%)	272 (100%)	0	100	100
6	J	93/97 (96%)	93 (100%)	0	100	100
All	All	2791/3309 (84%)	2785 (100%)	6 (0%)	85	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	LEU
1	B	202	ILE
2	C	959	LEU
3	D	173	ARG
3	D	219	LEU
3	D	325	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	20	GLN
1	A	79	ASN
1	A	100	GLN
1	A	226	ASN
1	B	79	ASN
1	B	185	GLN
2	C	232	GLN
2	C	317	ASN

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Mol	Chain	Res	Type
2	C	375	ASN
2	C	435	GLN
2	C	479	HIS
2	C	585	GLN
2	C	875	GLN
2	C	891	ASN
2	C	981	GLN
2	C	1042	HIS
3	D	207	GLN
3	D	213	GLN
3	D	307	ASN
3	D	329	GLN
3	D	465	HIS
3	D	494	HIS
3	D	552	GLN
3	D	563	ASN
3	D	564	ASN
3	D	600	GLN
3	D	693	GLN
3	D	854	HIS
3	D	889	HIS
3	D	1032	GLN
3	D	1145	GLN
3	D	1239	ASN
3	D	1251	ASN
4	E	65	ASN
4	E	70	GLN
5	F	234	GLN
5	F	325	ASN
5	F	353	GLN
5	F	415	GLN
5	F	505	GLN
6	J	28	GLN
6	J	58	ASN

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.

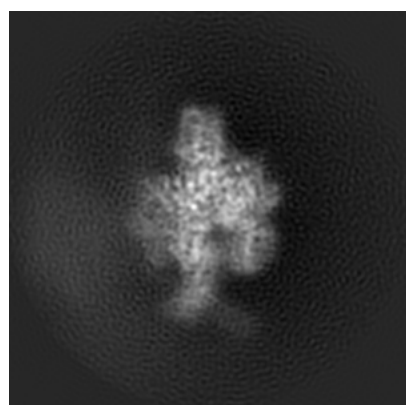
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7322. These allow visual inspection of the internal detail of the map and identification of artifacts.

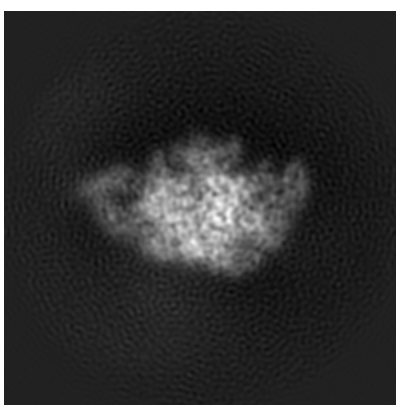
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

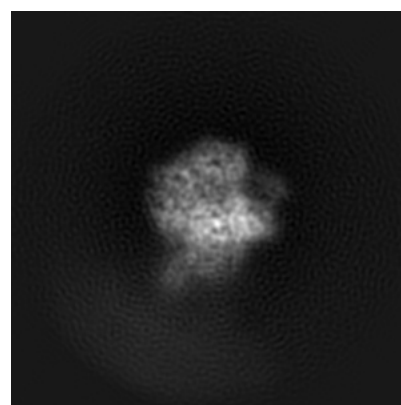
6.1.1 Primary map



X



Y

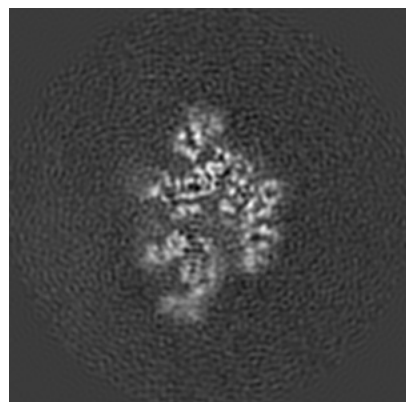


Z

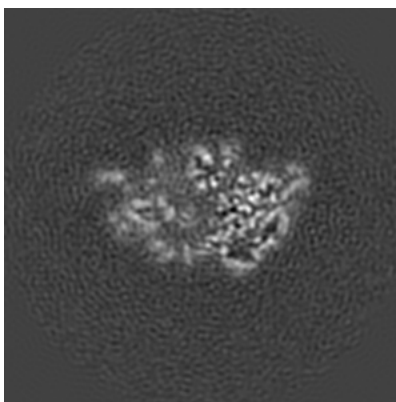
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

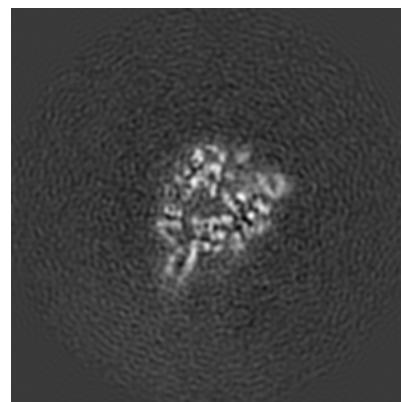
6.2.1 Primary map



X Index: 110



Y Index: 110

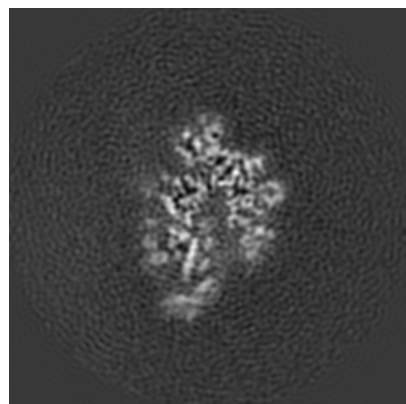


Z Index: 110

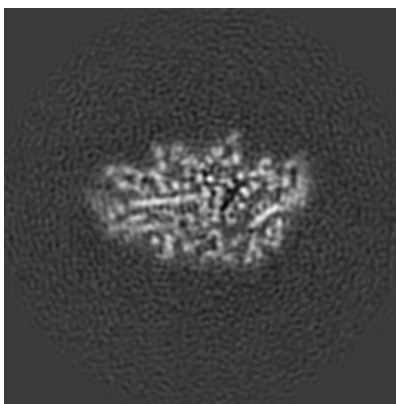
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

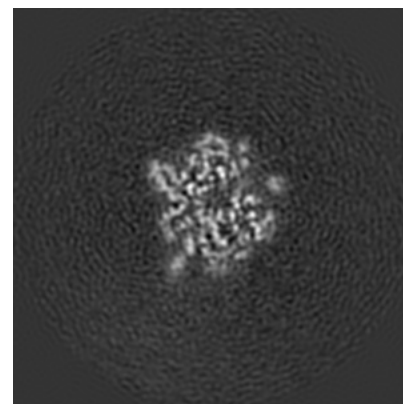
6.3.1 Primary map



X Index: 107



Y Index: 103

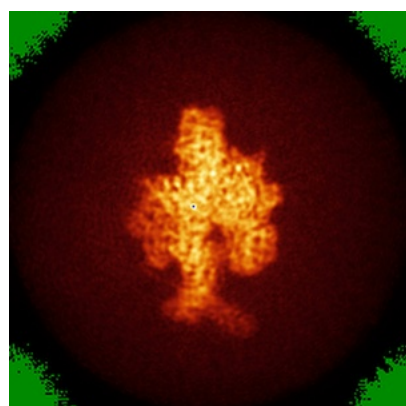


Z Index: 116

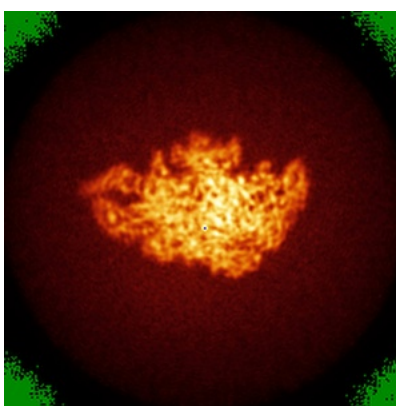
The images above show the largest variance slices of the map in three orthogonal directions.

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

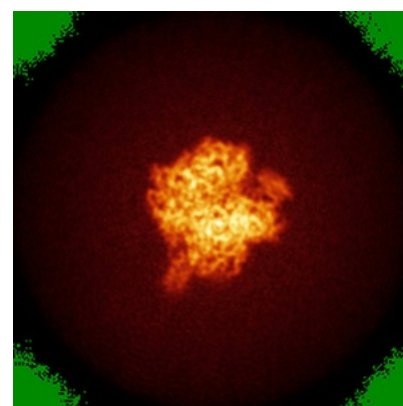
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.0189. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

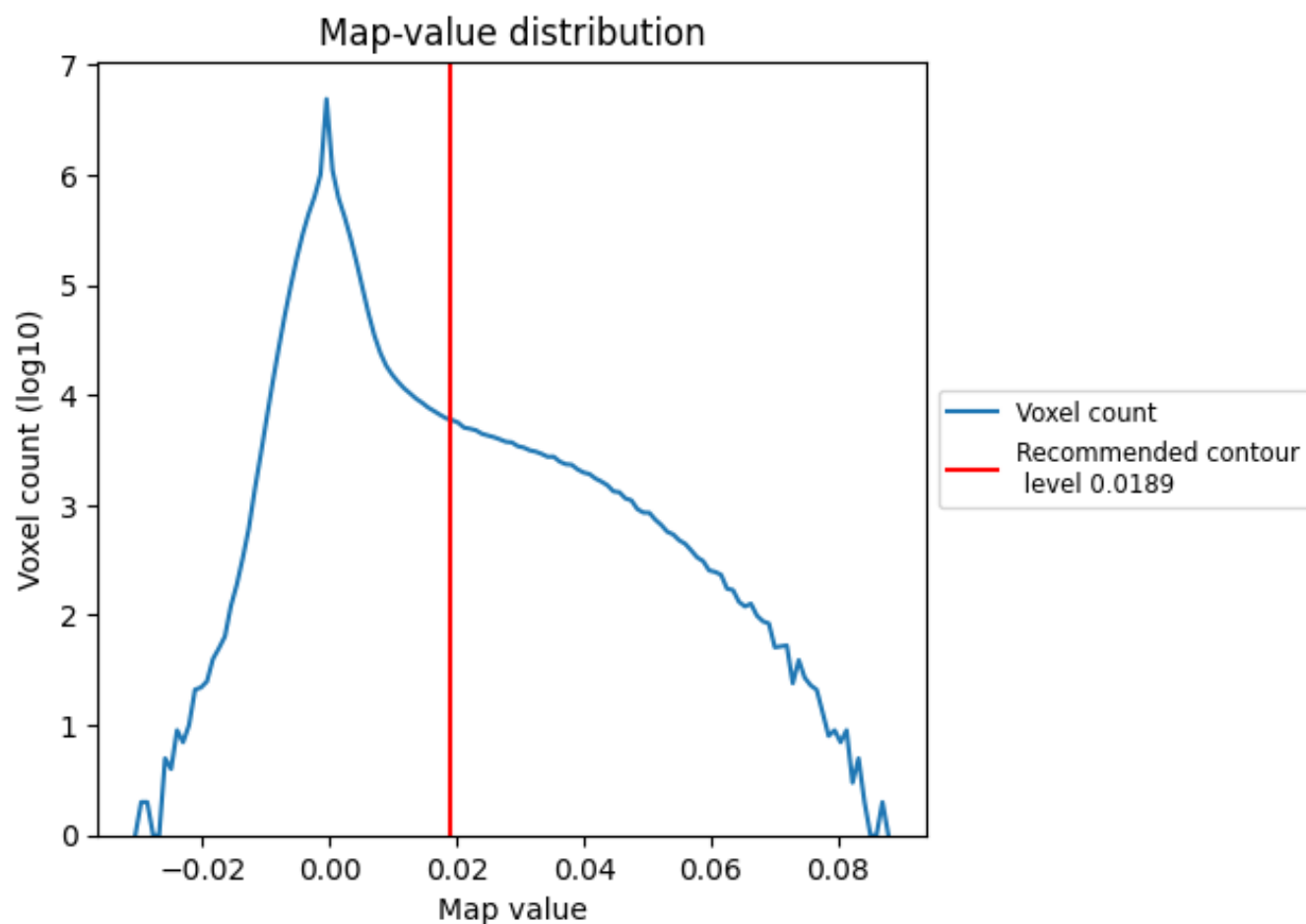
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

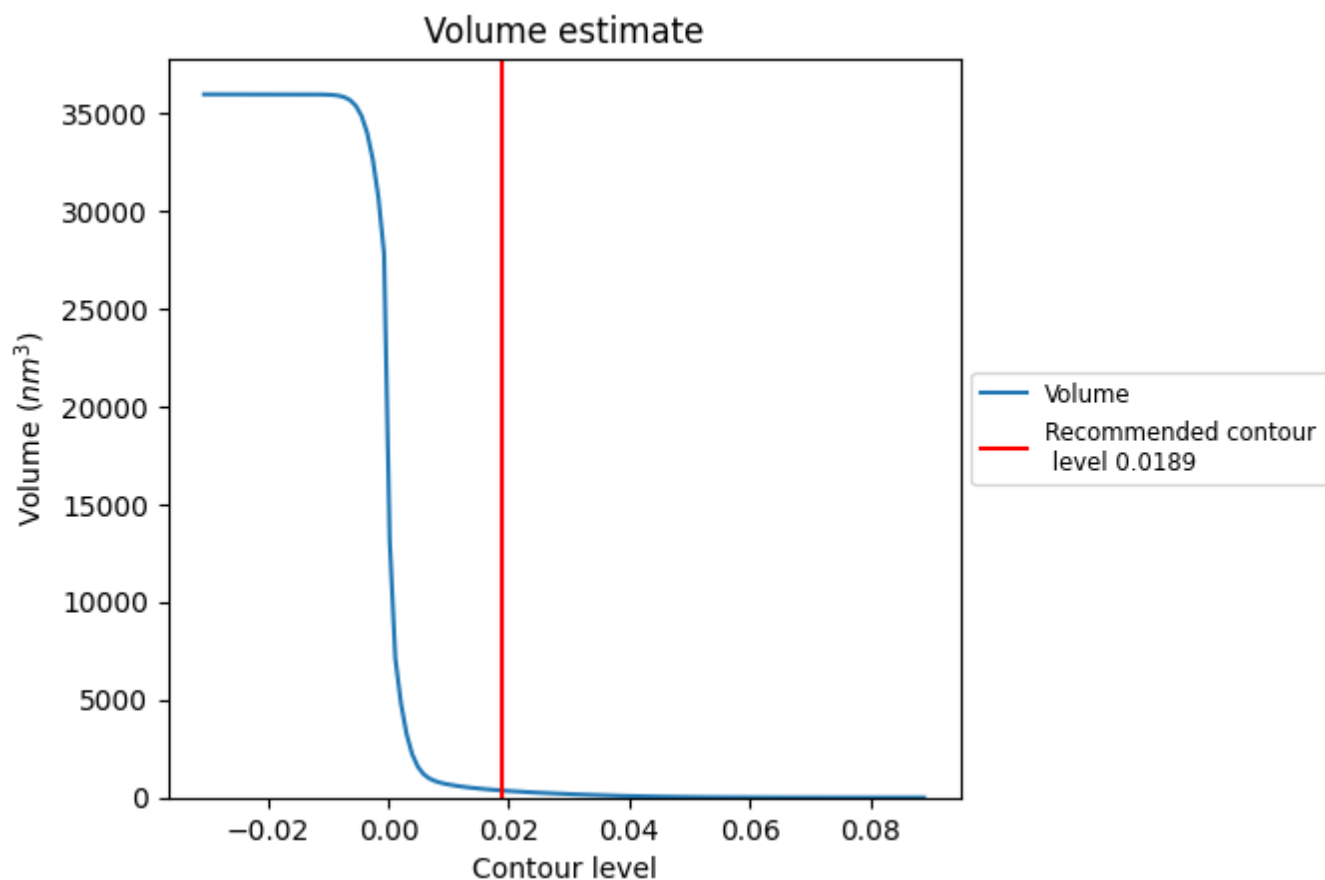
This section contains the results of statistical analysis of the map.

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.

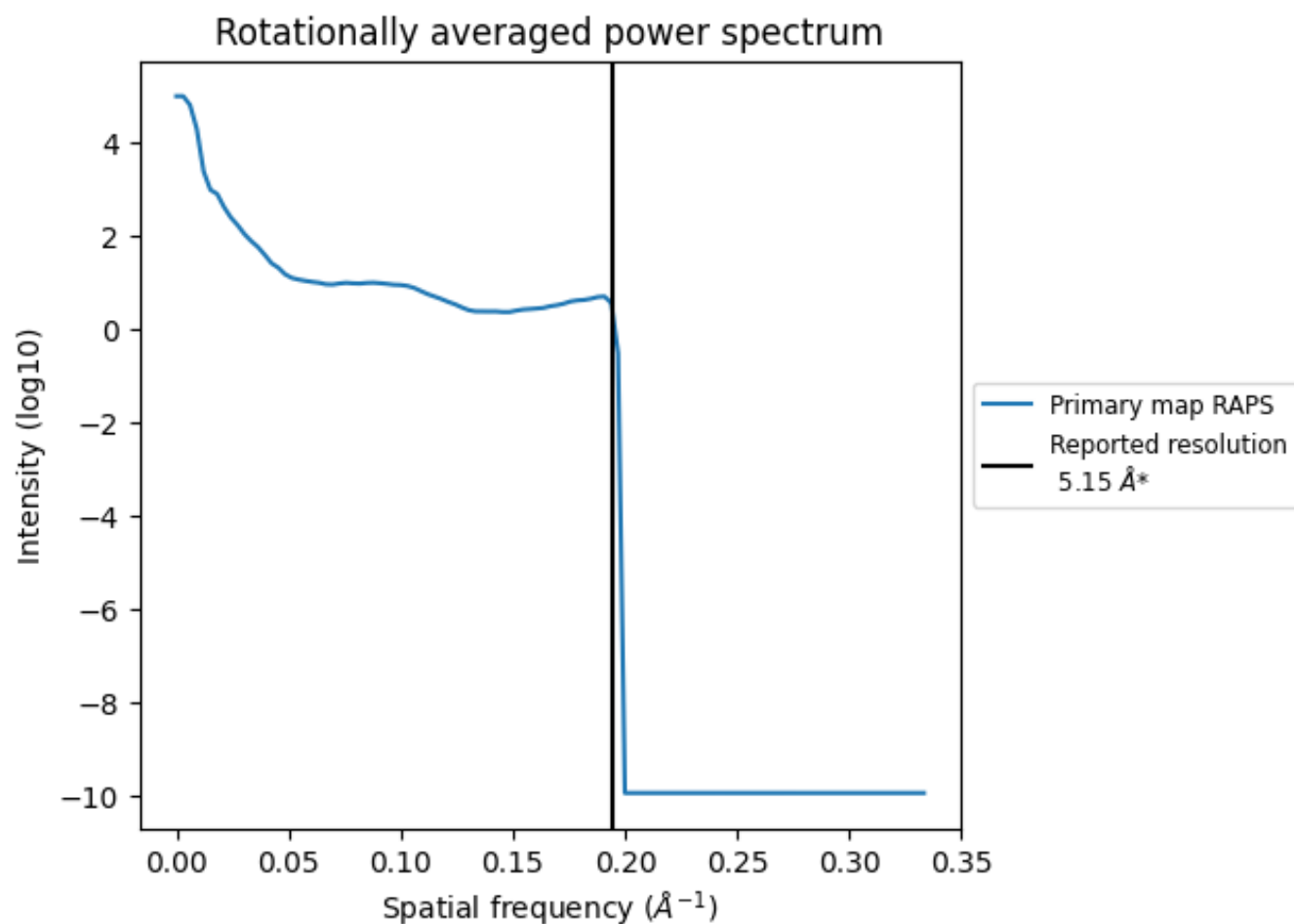
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm³; this corresponds to an approximate mass of 325 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 0.194 Å⁻¹

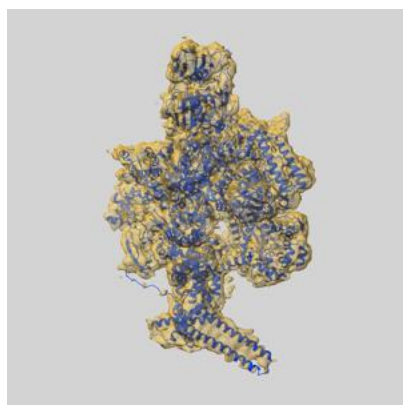
8 Fourier-Shell correlation ⓘ

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

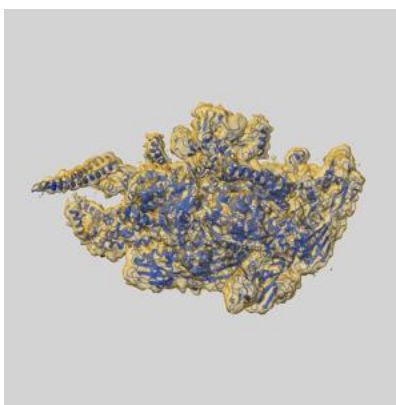
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7322 and PDB model 6C05. Per-residue inclusion information can be found in section [3](#) on page [7](#).

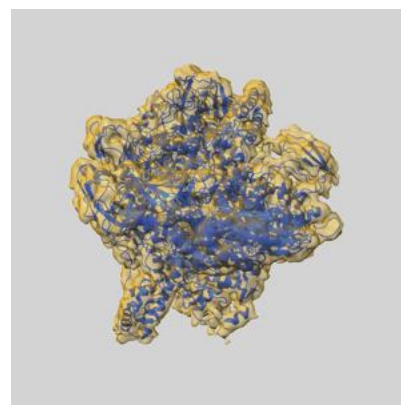
9.1 Map-model overlay [i](#)



X



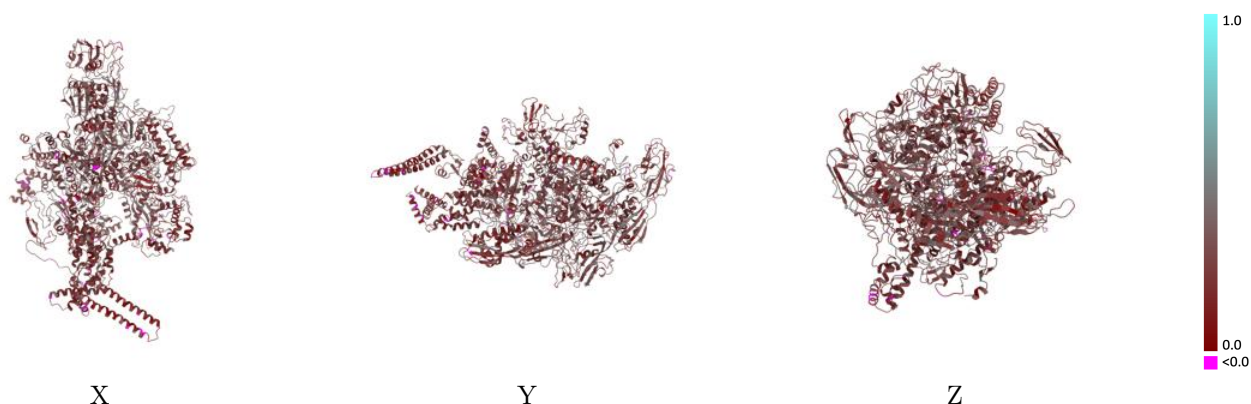
Y



Z

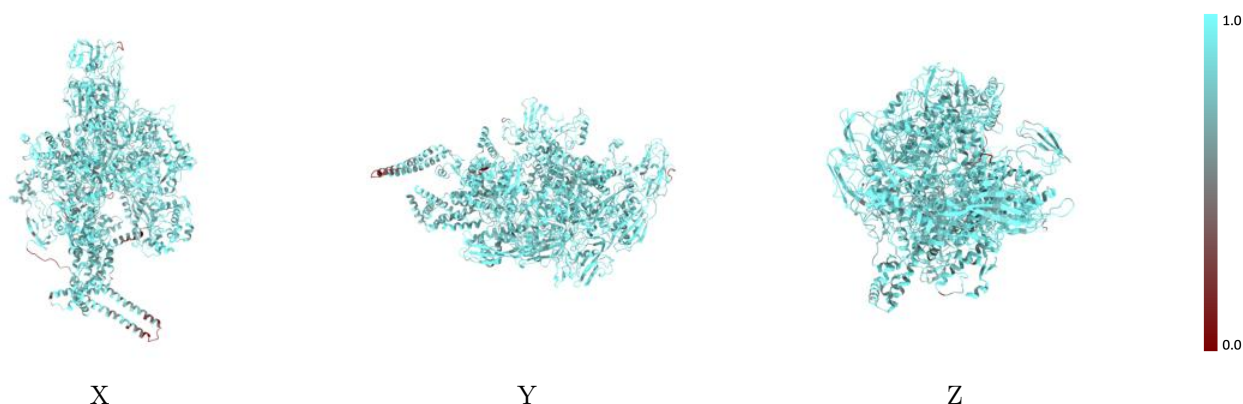
The images above show the 3D surface view of the map at the recommended contour level 0.0189 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



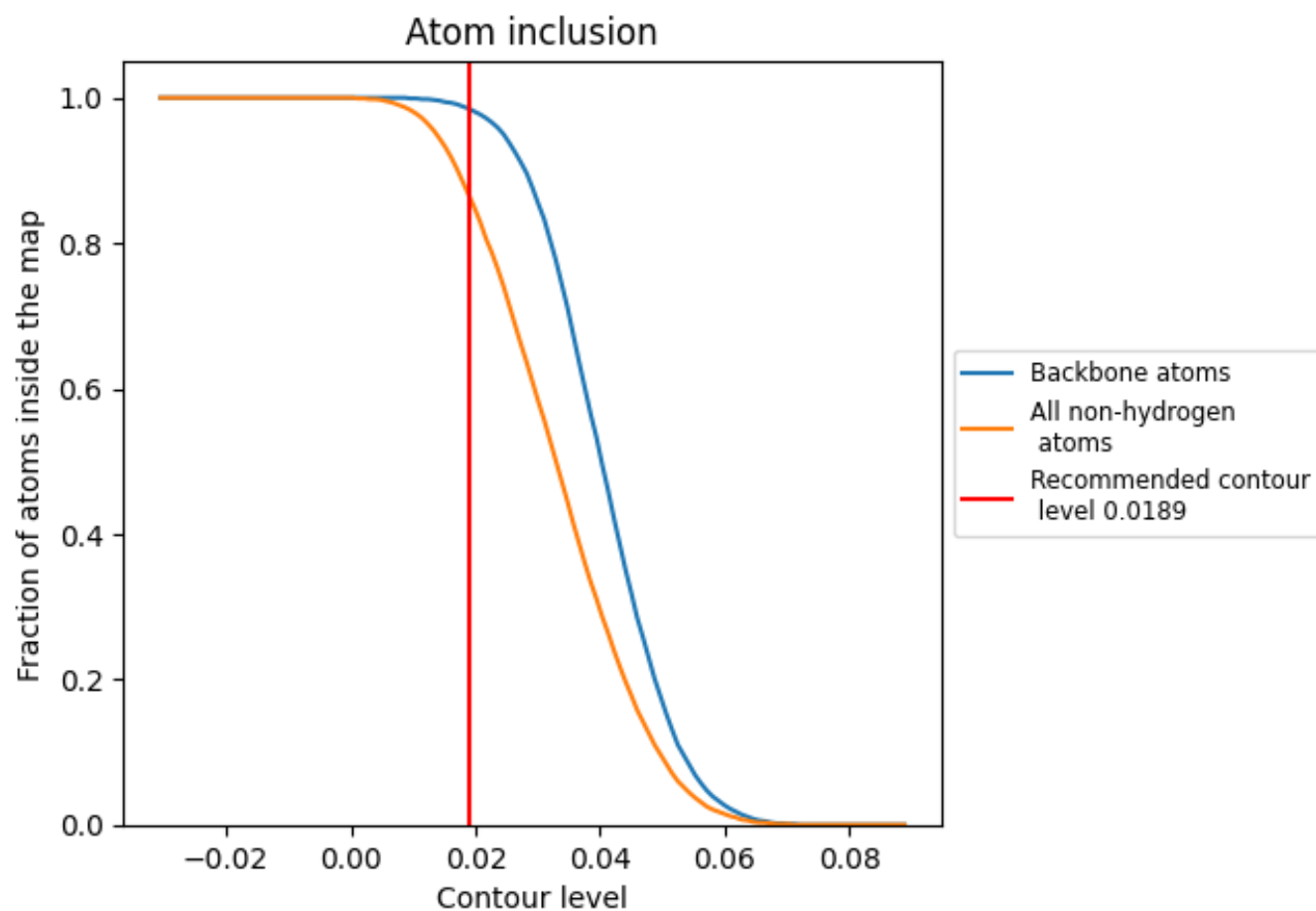
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0189).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 87% 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 (0.0189) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.2710
A	0.8760	0.2960
B	0.8790	0.2770
C	0.8910	0.2830
D	0.8660	0.2690
E	0.8870	0.2880
F	0.8170	0.2260
J	0.7510	0.2440

1.0

0.0

<0.0