



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:56 AM UTC

PDB ID : 6VW0 / pdb_00006vw0
EMDB ID : EMD-21409
Title : Mycobacterium tuberculosis RNAP S456L mutant open promoter complex
Authors : Lilic, M.; Boyaci, H.; Chen, J.; Darst, S.A.; Campbell, E.A.
Deposited on : 2020-02-18
Resolution : 3.59 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

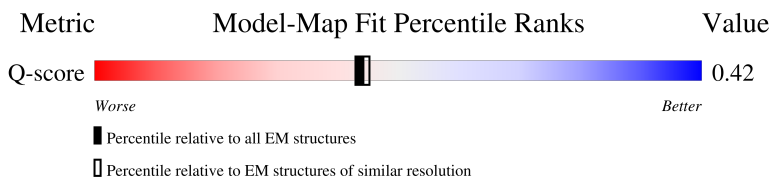
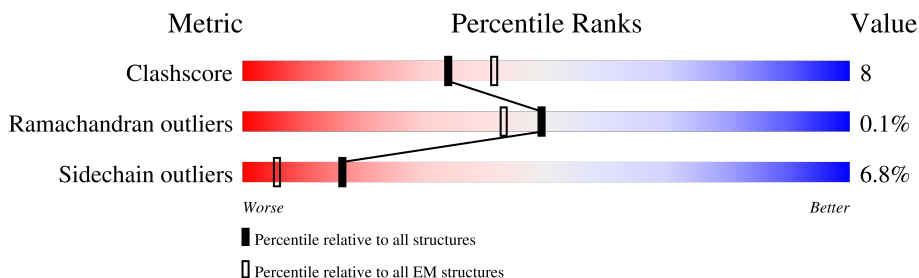
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.59 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	12565 (3.09 - 4.09)

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	
1	B	347	
2	C	1179	
3	D	1326	

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Mol	Chain	Length	Quality of chain
4	E	110	59%15%25%
5	F	531	48%11%39%
6	J	111	71%25%
7	M	162	72%25%
8	O	90	58%14%28%
9	P	90	62%10%28%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 29944 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	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	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
			8584	5382	1504	1659	39		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	456	LEU	SER	engineered mutation	UNP V9Z879
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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9914	6208	1802	1862	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A5U053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ALA	-	expression tag	UNP A5U053
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

- 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	322	Total	C	N	O	S	0	0
			2527	1576	459	483	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	109	Total	C	N	O	S	0	0
			880	543	166	168	3		

- Molecule 7 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

- Molecule 8 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	65	Total	C	N	O	P	0	0
			1336	633	243	395	65		

- Molecule 9 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	65	Total	C	N	O	P	0	0
			1329	629	250	385	65		

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

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

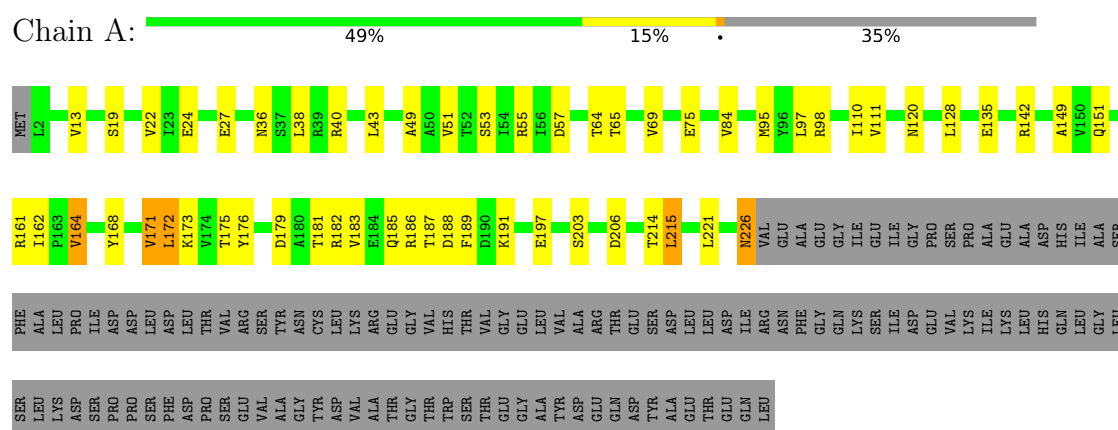
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

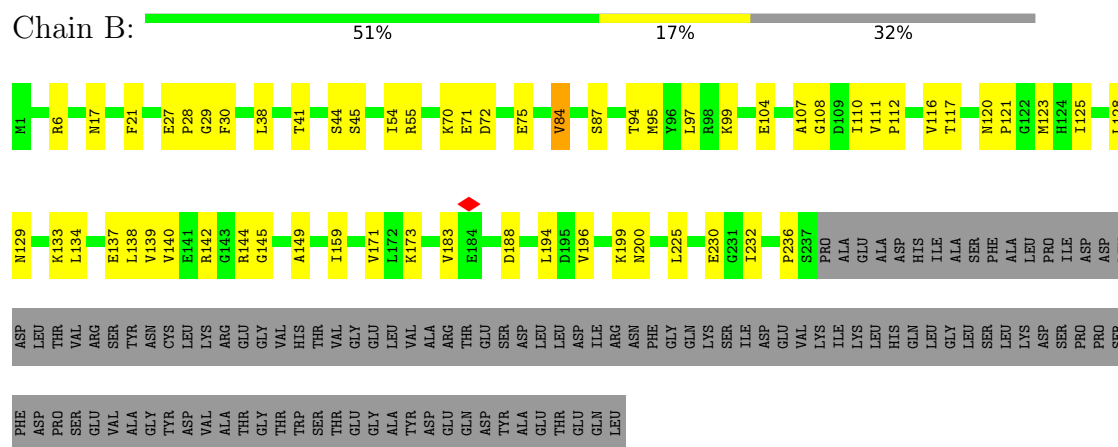
3 Residue-property plots

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

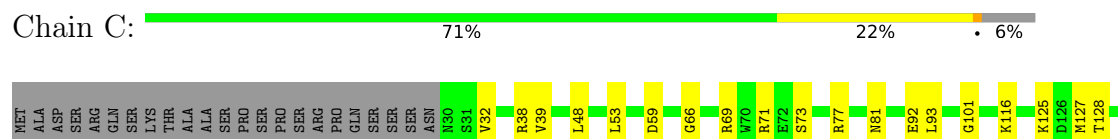
• Molecule 1: DNA-directed RNA polymerase subunit alpha

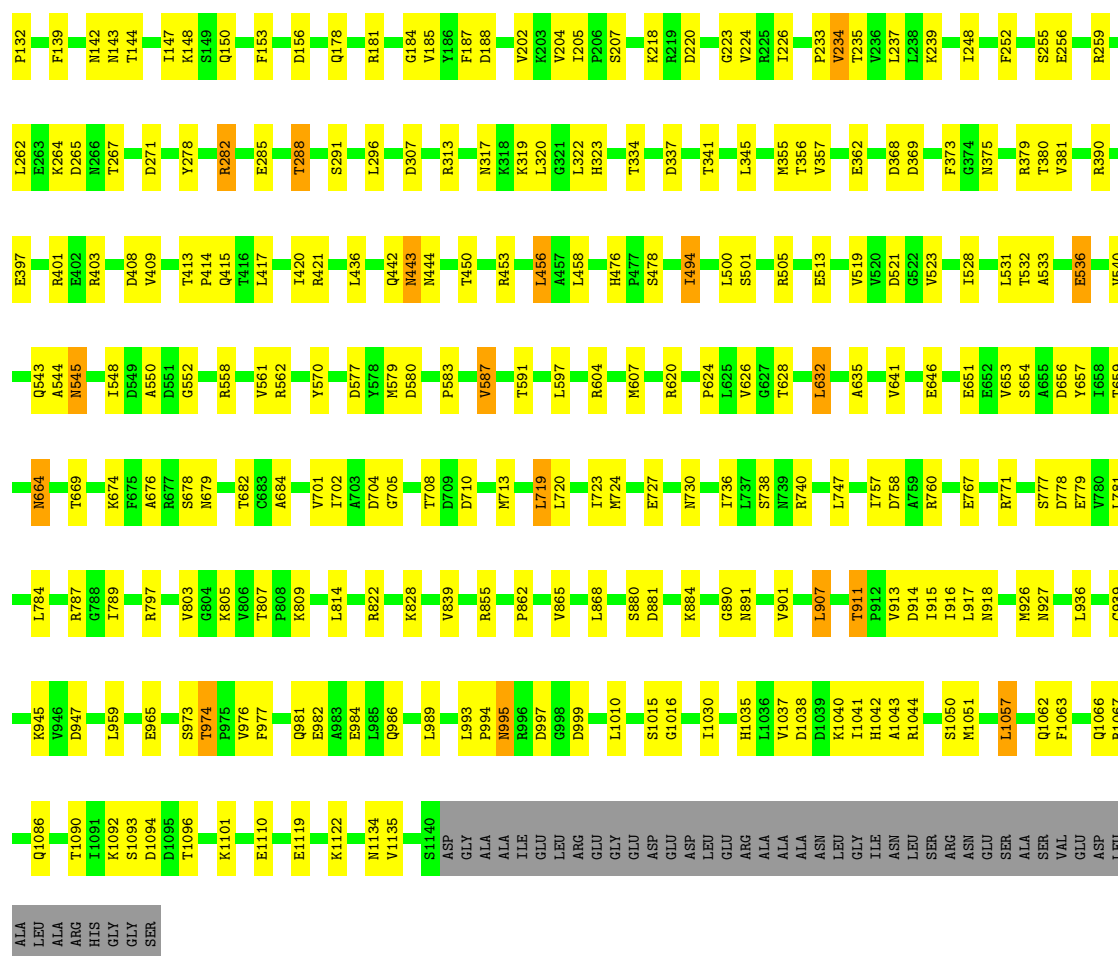


• Molecule 1: DNA-directed RNA polymerase subunit alpha



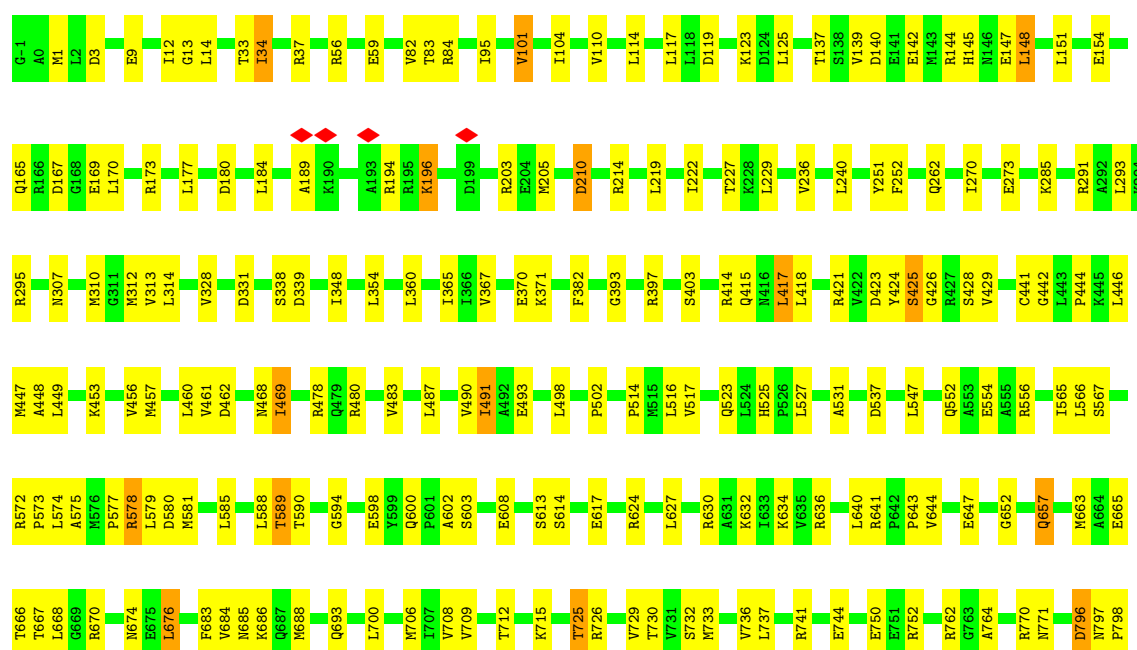
• Molecule 2: DNA-directed RNA polymerase subunit beta

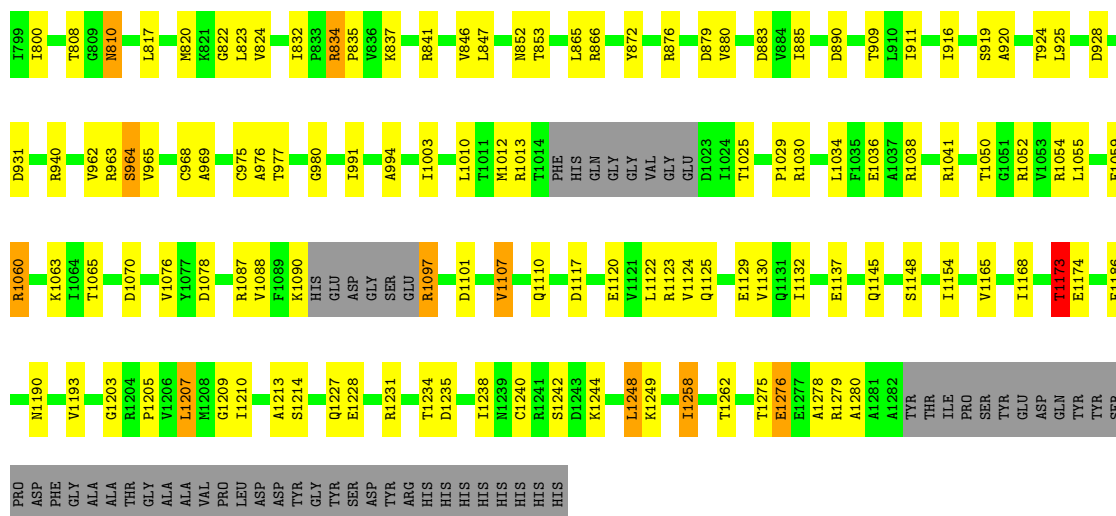




• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 71% 23%





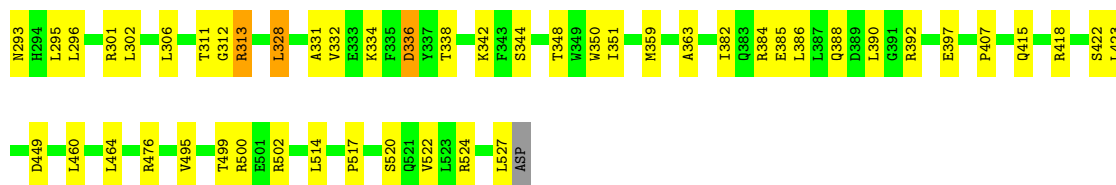
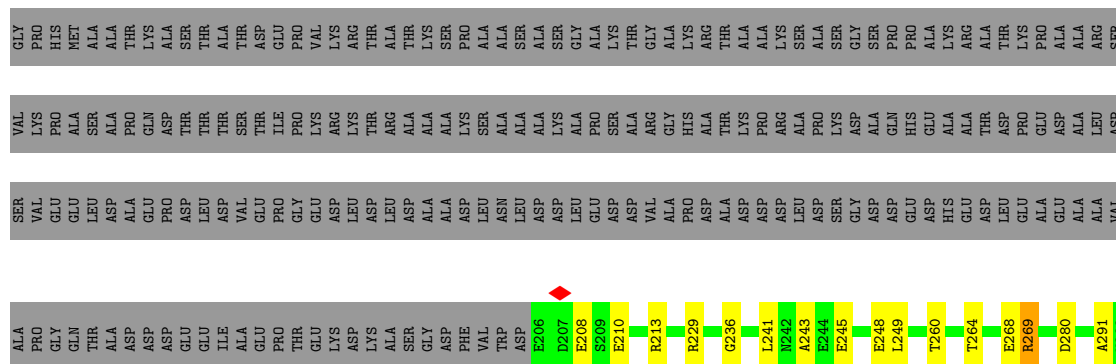
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 59% 15% 25%



- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 48% 11% 39%



- Molecule 6: RNA polymerase-binding protein RbpA

Chain J: 71% 25% 4%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55833	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 ($e^-/\text{\AA}^2$)	71	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	2.591	Depositor
Minimum map value	-1.047	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.387	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, ZN

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	0.46	0/1742	0.56	2/2370 (0.1%)
1	B	0.43	0/1792	0.54	0/2442
2	C	0.48	0/8743	0.59	0/11860
3	D	0.48	0/10078	0.58	6/13624 (0.0%)
4	E	0.46	0/662	0.51	0/901
5	F	0.34	0/2558	0.48	0/3451
6	J	0.31	0/896	0.50	0/1210
7	M	0.27	0/1257	0.53	0/1700
8	O	0.40	0/1497	0.55	0/2310
9	P	0.39	0/1491	0.54	0/2297
All	All	0.45	0/30716	0.56	8/42165 (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
2	C	0	1
3	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	834	ARG	CA-C-N	6.26	142.01	127.00
3	D	834	ARG	C-N-CA	6.26	142.01	127.00
1	A	168	TYR	CA-C-N	-6.23	115.41	122.26
1	A	168	TYR	C-N-CA	-6.23	115.41	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1070	ASP	CA-C-N	6.11	132.70	121.70
3	D	1070	ASP	C-N-CA	6.11	132.70	121.70
3	D	834	ARG	C-N-CD	-5.67	108.12	120.60
3	D	657	GLN	N-CA-C	5.24	121.39	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	282	ARG	Peptide
3	D	1173	THR	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	1716	0	1756	34	0
1	B	1765	0	1794	32	0
2	C	8584	0	8509	163	0
3	D	9914	0	9986	185	0
4	E	649	0	645	10	0
5	F	2527	0	2535	40	0
6	J	880	0	852	19	0
7	M	1241	0	1259	26	0
8	O	1336	0	732	10	0
9	P	1329	0	727	7	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	29944	0	28795	480	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 8.

All (480) 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:144:ARG:O	3:D:148:LEU:HB2	1.79	0.82
7:M:112:TRP:O	7:M:116:GLN:HB2	1.88	0.74
3:D:880:VAL:HG21	3:D:1210:ILE:HB	1.71	0.73
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.70	0.72
5:F:386:LEU:O	5:F:390:LEU:HB3	1.94	0.68
3:D:147:GLU:O	3:D:151:LEU:HB2	1.94	0.67
2:C:771:ARG:NH2	2:C:781:LEU:O	2.28	0.66
1:B:55:ARG:HB3	1:B:137:GLU:HB2	1.77	0.66
5:F:384:ARG:HG2	5:F:388:GLN:HE22	1.58	0.66
3:D:676:LEU:HD12	3:D:715:LYS:HB3	1.78	0.65
2:C:453:ARG:NH2	2:C:501:SER:O	2.31	0.63
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.81	0.63
1:A:183:VAL:HG13	1:A:185:GLN:H	1.63	0.62
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.80	0.62
5:F:328:LEU:HD23	5:F:351:ILE:HD11	1.82	0.62
3:D:1:MET:SD	3:D:1:MET:N	2.72	0.62
3:D:83:THR:OG1	3:D:84:ARG:N	2.33	0.62
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.81	0.62
7:M:121:SER:O	7:M:125:LYS:HB2	1.99	0.61
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.33	0.61
2:C:224:VAL:HG11	2:C:237:LEU:HD13	1.82	0.61
1:A:24:GLU:HB3	1:A:191:LYS:HG3	1.83	0.61
1:A:182:ARG:HH12	3:D:624:ARG:HG2	1.66	0.60
3:D:210:ASP:HB3	3:D:214:ARG:HH21	1.66	0.60
3:D:752:ARG:O	3:D:752:ARG:NH1	2.34	0.60
1:A:64:THR:OG1	1:A:65:THR:N	2.34	0.60
2:C:558:ARG:HB3	2:C:570:TYR:HB3	1.84	0.60
3:D:307:ASN:HD21	3:D:1240:CYS:HB2	1.66	0.60
3:D:425:SER:OG	3:D:426:GLY:N	2.35	0.60
3:D:1276:GLU:HB3	3:D:1279:ARG:HH21	1.67	0.60
3:D:1052:ARG:HH12	3:D:1054:ARG:HH12	1.48	0.60
2:C:1041:ILE:HG13	3:D:428:SER:HB2	1.84	0.59
5:F:248:GLU:OE2	6:J:101:ARG:NH1	2.35	0.59
1:A:75:GLU:OE2	2:C:620:ARG:NH1	2.36	0.59
3:D:1025:THR:OG1	3:D:1041:ARG:NH2	2.35	0.59
5:F:517:PRO:HA	5:F:520:SER:HB3	1.83	0.59
2:C:150:GLN:HG3	7:M:44:LEU:HB3	1.84	0.59
3:D:144:ARG:HH12	3:D:229:LEU:HB3	1.68	0.59
2:C:380:THR:OG1	2:C:381:VAL:N	2.36	0.59
2:C:184:GLY:H	2:C:205:ILE:HG13	1.68	0.59
3:D:866:ARG:NH1	3:D:1010:LEU:O	2.35	0.59
5:F:415:GLN:HG2	5:F:418:ARG:HH22	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1066:GLN:NE2	3:D:425:SER:HG	2.00	0.58
2:C:604:ARG:NH1	2:C:607:MET:SD	2.76	0.58
7:M:115:ASP:HA	7:M:119:GLY:H	1.68	0.58
3:D:173:ARG:HG2	3:D:205:MET:HB2	1.85	0.58
1:A:149:ALA:O	1:A:151:GLN:NE2	2.36	0.58
3:D:762:ARG:HH12	3:D:764:ALA:HB2	1.68	0.58
3:D:810:ASN:N	3:D:810:ASN:OD1	2.34	0.58
5:F:500:ARG:NH2	9:P:126:DG:N7	2.52	0.58
1:B:97:LEU:HB3	1:B:110:ILE:HG13	1.86	0.58
2:C:73:SER:O	2:C:77:ARG:NH2	2.37	0.58
2:C:116:LYS:NZ	2:C:156:ASP:OD2	2.37	0.58
2:C:881:ASP:N	2:C:881:ASP:OD1	2.33	0.57
2:C:181:ARG:NH2	8:O:62:DT:O2	2.38	0.57
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.24	0.57
2:C:1094:ASP:HB3	2:C:1119:GLU:H	1.69	0.57
2:C:1066:GLN:NE2	3:D:425:SER:OG	2.36	0.57
3:D:1090:LYS:O	3:D:1097:ARG:N	2.38	0.57
5:F:311:THR:OG1	5:F:312:GLY:N	2.38	0.57
2:C:995:ASN:N	2:C:995:ASN:OD1	2.38	0.57
5:F:500:ARG:NH1	9:P:127:DT:O4	2.38	0.57
2:C:66:GLY:O	2:C:71:ARG:NH2	2.39	0.56
2:C:730:ASN:ND2	2:C:917:LEU:O	2.38	0.56
6:J:20:ARG:NH1	6:J:23:ASP:OD1	2.38	0.56
6:J:33:ARG:NH1	6:J:34:THR:O	2.39	0.56
1:A:97:LEU:HB2	1:A:110:ILE:HG12	1.87	0.56
3:D:37:ARG:NH2	8:O:44:DT:OP1	2.39	0.56
3:D:1065:THR:HG23	3:D:1076:VAL:HG22	1.88	0.56
5:F:268:GLU:O	5:F:269:ARG:NH1	2.34	0.56
1:A:57:ASP:OD1	1:A:57:ASP:N	2.38	0.56
1:A:175:THR:OG1	1:A:176:TYR:N	2.38	0.56
1:B:6:ARG:NH1	1:B:236:PRO:O	2.39	0.55
3:D:331:ASP:OD1	3:D:331:ASP:N	2.39	0.55
4:E:39:PRO:HG2	4:E:42:GLU:HB2	1.88	0.55
1:A:36:ASN:ND2	2:C:1015:SER:O	2.40	0.55
2:C:313:ARG:O	2:C:317:ASN:ND2	2.40	0.55
1:B:99:LYS:NZ	1:B:104:GLU:O	2.37	0.55
3:D:184:LEU:O	3:D:194:ARG:NH1	2.39	0.55
7:M:68:ASP:HA	7:M:71:PHE:HB2	1.88	0.55
3:D:585:LEU:O	3:D:589:THR:OG1	2.24	0.55
3:D:144:ARG:NH2	3:D:227:THR:O	2.40	0.55
3:D:339:ASP:OD2	3:D:397:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.36	0.55
3:D:461:VAL:HG21	3:D:469:ILE:HG22	1.89	0.55
2:C:577:ASP:OD1	2:C:577:ASP:N	2.37	0.54
3:D:203:ARG:O	3:D:203:ARG:NH1	2.40	0.54
3:D:414:ARG:HA	3:D:418:LEU:HD12	1.88	0.54
3:D:1036:GLU:HG2	3:D:1038:ARG:HE	1.72	0.54
2:C:150:GLN:HE22	2:C:415:GLN:HB2	1.72	0.54
2:C:545:ASN:OD1	2:C:545:ASN:N	2.39	0.54
3:D:1190:ASN:HA	3:D:1193:VAL:HG12	1.88	0.54
6:J:20:ARG:NH1	6:J:23:ASP:O	2.41	0.54
7:M:59:ARG:NH2	7:M:99:GLY:O	2.39	0.54
4:E:48:SER:OG	4:E:49:SER:N	2.40	0.54
4:E:84:GLU:O	4:E:97:ARG:NH2	2.41	0.54
2:C:654:SER:HG	2:C:657:TYR:H	1.54	0.54
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.88	0.54
2:C:101:GLY:O	2:C:142:ASN:ND2	2.41	0.54
7:M:147:ASP:OD1	7:M:147:ASP:N	2.38	0.54
2:C:543:GLN:NE2	2:C:580:ASP:OD2	2.41	0.54
1:B:200:ASN:OD1	1:B:200:ASN:N	2.39	0.53
2:C:505:ARG:HB3	2:C:513:GLU:HB2	1.90	0.53
3:D:1120:GLU:OE2	3:D:1123:ARG:NH2	2.40	0.53
3:D:382:PHE:O	3:D:403:SER:OG	2.26	0.53
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.73	0.53
3:D:1117:ASP:OD1	3:D:1117:ASP:N	2.40	0.53
5:F:344:SER:O	5:F:348:THR:OG1	2.25	0.53
2:C:986:GLN:HB2	3:D:733:MET:HE1	1.91	0.53
5:F:464:LEU:HD23	5:F:476:ARG:HE	1.72	0.53
8:O:43:DT:H2"	8:O:44:DT:H71	1.88	0.53
2:C:271:ASP:OD1	2:C:271:ASP:N	2.39	0.53
2:C:456:LEU:HD23	2:C:458:LEU:H	1.74	0.53
2:C:443:ASN:OD1	2:C:443:ASN:N	2.41	0.53
2:C:1043:ALA:HB2	3:D:447:MET:HG3	1.90	0.53
3:D:33:THR:HG22	3:D:34:ILE:HD12	1.90	0.53
3:D:674:ASN:HD21	3:D:684:VAL:H	1.57	0.53
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.90	0.53
5:F:210:GLU:OE1	5:F:213:ARG:NH2	2.39	0.53
6:J:79:ARG:NH2	6:J:87:GLU:OE2	2.42	0.53
3:D:627:LEU:HD13	3:D:668:LEU:HD12	1.90	0.52
3:D:151:LEU:HA	3:D:154:GLU:HB3	1.90	0.52
3:D:1025:THR:HG21	3:D:1029:PRO:HB2	1.91	0.52
3:D:203:ARG:NH2	5:F:208:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1030:ARG:NH2	3:D:1137:GLU:OE2	2.42	0.52
2:C:604:ARG:NH2	2:C:890:GLY:O	2.42	0.52
2:C:678:SER:OG	2:C:679:ASN:N	2.42	0.52
2:C:855:ARG:NH1	2:C:862:PRO:O	2.43	0.52
3:D:632:LYS:NZ	3:D:665:GLU:OE1	2.43	0.52
1:B:70:LYS:HD3	1:B:71:GLU:HG3	1.92	0.52
2:C:139:PHE:HB3	2:C:148:LYS:HB2	1.92	0.52
3:D:1063:LYS:NZ	3:D:1078:ASP:OD1	2.40	0.52
2:C:822:ARG:NH1	2:C:828:LYS:O	2.42	0.52
2:C:945:LYS:HG3	2:C:965:GLU:HB3	1.91	0.52
1:B:45:SER:O	1:B:144:ARG:NH1	2.43	0.52
2:C:397:GLU:OE2	2:C:401:ARG:NE	2.42	0.52
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.90	0.51
3:D:1003:ILE:HD11	3:D:1154:ILE:HA	1.93	0.51
1:A:226:ASN:OD1	1:A:226:ASN:N	2.43	0.51
3:D:531:ALA:HA	3:D:574:LEU:HD23	1.91	0.51
3:D:1228:GLU:HB2	3:D:1231:ARG:HB3	1.93	0.51
6:J:35:ASP:OD1	6:J:35:ASP:N	2.43	0.51
7:M:88:ARG:O	7:M:92:ASN:ND2	2.44	0.51
1:B:70:LYS:HB2	1:B:129:ASN:HD21	1.76	0.51
2:C:320:LEU:HB2	2:C:322:LEU:HG	1.93	0.51
2:C:408:ASP:OD1	2:C:408:ASP:N	2.43	0.51
2:C:421:ARG:HH22	9:P:103:DT:H5''	1.74	0.51
3:D:556:ARG:NH2	4:E:37:ASN:O	2.44	0.51
3:D:1276:GLU:HA	3:D:1279:ARG:HB2	1.93	0.51
1:B:72:ASP:OD1	1:B:72:ASP:N	2.43	0.50
2:C:664:ASN:OD1	2:C:664:ASN:N	2.39	0.50
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.93	0.50
2:C:730:ASN:O	2:C:918:ASN:ND2	2.45	0.50
3:D:502:PRO:HB3	9:P:94:DC:H1'	1.94	0.50
3:D:491:ILE:HG23	3:D:514:PRO:HG2	1.92	0.50
1:B:128:LEU:HD11	1:B:134:LEU:HB2	1.92	0.50
2:C:544:ALA:HA	2:C:579:MET:HE3	1.92	0.50
3:D:567:SER:OG	3:D:572:ARG:O	2.27	0.50
3:D:975:CYS:SG	3:D:976:ALA:N	2.84	0.50
2:C:38:ARG:HG2	2:C:973:SER:HB3	1.91	0.50
2:C:188:ASP:OD1	2:C:188:ASP:N	2.42	0.50
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.77	0.50
3:D:820:MET:HE2	3:D:822:GLY:HA2	1.93	0.50
7:M:59:ARG:HH22	7:M:100:ASP:HA	1.75	0.50
7:M:95:LYS:O	7:M:98:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:SER:OG	2:C:307:ASP:O	2.26	0.50
2:C:536:GLU:OE2	2:C:562:ARG:NH1	2.43	0.50
5:F:384:ARG:NH2	5:F:385:GLU:OE2	2.44	0.50
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.45	0.50
3:D:1122:LEU:HD22	3:D:1207:LEU:HB2	1.94	0.50
8:O:21:DG:H2'	8:O:22:DG:C8	2.47	0.50
2:C:53:LEU:O	2:C:453:ARG:NH1	2.43	0.50
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.92	0.50
6:J:34:THR:HA	6:J:62:GLY:HA2	1.94	0.50
2:C:523:VAL:HA	2:C:552:GLY:HA3	1.93	0.50
3:D:487:LEU:HD23	3:D:516:LEU:HD11	1.94	0.50
3:D:148:LEU:HD21	3:D:227:THR:HG22	1.94	0.49
2:C:322:LEU:O	2:C:323:HIS:ND1	2.44	0.49
3:D:444:PRO:HG2	3:D:447:MET:HB3	1.93	0.49
3:D:931:ASP:N	3:D:931:ASP:OD1	2.45	0.49
1:A:179:ASP:OD2	1:A:191:LYS:NZ	2.39	0.49
2:C:736:ILE:HG12	2:C:916:ILE:HB	1.94	0.49
3:D:670:ARG:HD3	3:D:685:ASN:HA	1.94	0.49
3:D:750:GLU:OE2	3:D:837:LYS:NZ	2.45	0.49
2:C:48:LEU:HB2	2:C:528:ILE:HD13	1.94	0.49
2:C:334:THR:HG23	2:C:337:ASP:H	1.76	0.49
3:D:307:ASN:ND2	3:D:1238:ILE:O	2.45	0.49
3:D:872:TYR:OH	3:D:1227:GLN:NE2	2.45	0.49
3:D:1231:ARG:NH1	3:D:1235:ASP:OD2	2.44	0.49
3:D:453:LYS:HG2	3:D:457:MET:HE2	1.94	0.49
3:D:1235:ASP:HA	3:D:1238:ILE:HD12	1.93	0.49
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.94	0.49
7:M:87:ARG:NH1	8:O:51:DG:OP2	2.44	0.49
1:A:181:THR:OG1	1:A:189:PHE:O	2.31	0.49
3:D:641:ARG:O	3:D:683:PHE:N	2.45	0.49
3:D:167:ASP:HA	3:D:170:LEU:HB2	1.94	0.49
2:C:781:LEU:HA	2:C:784:LEU:HD13	1.94	0.49
3:D:196:LYS:HD2	3:D:196:LYS:HA	1.58	0.49
5:F:249:LEU:HD22	5:F:291:ALA:HB1	1.95	0.48
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.95	0.48
2:C:38:ARG:NH2	2:C:624:PRO:O	2.41	0.48
2:C:223:GLY:HA2	2:C:233:PRO:HA	1.95	0.48
2:C:727:GLU:H	3:D:725:THR:HG22	1.79	0.48
6:J:109:ARG:HH22	6:J:110:ARG:HH21	1.61	0.48
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.78	0.48
2:C:256:GLU:OE1	2:C:259:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:444:ASN:N	2:C:444:ASN:OD1	2.47	0.48
1:A:186:ARG:NH1	1:B:149:ALA:O	2.46	0.48
1:B:87:SER:O	1:B:142:ARG:NH1	2.46	0.48
3:D:602:ALA:H	3:D:608:GLU:HA	1.79	0.48
5:F:524:ARG:HH22	5:F:527:LEU:HD12	1.77	0.48
7:M:23:GLU:N	7:M:34:TYR:O	2.47	0.48
2:C:562:ARG:HG2	3:D:847:LEU:HD21	1.96	0.48
5:F:241:LEU:HD22	5:F:245:GLU:HG2	1.95	0.48
5:F:499:THR:HG1	5:F:502:ARG:H	1.60	0.48
2:C:548:ILE:HG22	2:C:550:ALA:H	1.79	0.48
1:B:183:VAL:HA	1:B:188:ASP:H	1.79	0.47
2:C:239:LYS:NZ	2:C:267:THR:O	2.40	0.47
2:C:1050:SER:OG	2:C:1051:MET:N	2.47	0.47
3:D:1059:GLU:O	3:D:1060:ARG:NH1	2.47	0.47
3:D:517:VAL:HG11	3:D:523:GLN:HG3	1.95	0.47
3:D:796:ASP:OD1	3:D:796:ASP:N	2.44	0.47
2:C:235:THR:HG22	2:C:248:ILE:HD13	1.96	0.47
2:C:505:ARG:O	2:C:513:GLU:N	2.47	0.47
4:E:52:ALA:O	4:E:56:TYR:HB2	2.14	0.47
3:D:890:ASP:OD1	3:D:977:THR:OG1	2.30	0.47
1:B:95:MET:O	1:B:138:LEU:N	2.47	0.47
1:B:183:VAL:HG12	1:B:188:ASP:HA	1.96	0.47
3:D:140:ASP:N	3:D:251:TYR:O	2.41	0.47
1:A:120:ASN:OD1	1:A:120:ASN:N	2.47	0.47
2:C:994:PRO:HB3	2:C:999:ASP:H	1.79	0.47
3:D:125:LEU:HD12	3:D:125:LEU:HA	1.79	0.47
3:D:189:ALA:O	3:D:194:ARG:NH2	2.48	0.47
3:D:700:LEU:HD23	3:D:709:VAL:HG22	1.97	0.47
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.48	0.47
2:C:278:TYR:O	2:C:282:ARG:HB2	2.15	0.47
2:C:337:ASP:O	2:C:341:THR:OG1	2.32	0.47
3:D:643:PRO:HD3	3:D:683:PHE:HB3	1.96	0.47
3:D:940:ARG:HH11	3:D:963:ARG:HH21	1.62	0.47
7:M:146:ASP:HB3	7:M:149:LYS:HB3	1.97	0.47
1:B:108:GLY:N	1:B:121:PRO:O	2.46	0.47
7:M:41:GLN:OE1	7:M:133:GLN:NE2	2.47	0.47
9:P:122:DT:H2'	9:P:123:DG:C8	2.49	0.47
2:C:587:VAL:HG22	2:C:591:THR:HB	1.96	0.47
2:C:654:SER:OG	2:C:657:TYR:N	2.41	0.47
2:C:1067:ARG:NH1	3:D:415:GLN:O	2.48	0.47
3:D:393:GLY:N	3:D:397:ARG:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:31:ARG:NH1	6:J:41:GLU:OE2	2.46	0.47
3:D:547:LEU:O	3:D:552:GLN:NE2	2.48	0.46
2:C:828:LYS:HD2	2:C:828:LYS:HA	1.76	0.46
3:D:1276:GLU:O	3:D:1280:ALA:N	2.47	0.46
1:B:21:PHE:O	1:B:194:LEU:N	2.48	0.46
1:B:107:ALA:N	1:B:123:MET:O	2.48	0.46
1:B:27:GLU:O	1:B:30:PHE:N	2.47	0.46
2:C:583:PRO:HB2	2:C:977:PHE:HB2	1.97	0.46
2:C:704:ASP:OD2	2:C:710:ASP:N	2.47	0.46
3:D:56:ARG:HB2	3:D:59:GLU:HB2	1.98	0.46
3:D:725:THR:OG1	3:D:726:ARG:NH1	2.49	0.46
3:D:741:ARG:HG2	3:D:744:GLU:HB2	1.98	0.46
3:D:968:CYS:SG	3:D:969:ALA:N	2.88	0.46
5:F:336:ASP:OD1	5:F:338:THR:OG1	2.34	0.46
1:B:94:THR:HG22	1:B:139:VAL:HG22	1.97	0.46
2:C:945:LYS:HA	2:C:965:GLU:HA	1.97	0.46
3:D:114:LEU:HG	3:D:312:MET:HE2	1.98	0.46
3:D:338:SER:O	3:D:338:SER:OG	2.30	0.46
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.47	0.46
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.34	0.46
7:M:95:LYS:HG2	7:M:103:LYS:HD3	1.97	0.46
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.80	0.46
3:D:1050:THR:HG23	3:D:1107:VAL:HG22	1.97	0.46
6:J:28:GLN:N	6:J:44:PHE:O	2.49	0.46
1:A:43:LEU:HA	1:A:171:VAL:HG11	1.97	0.46
2:C:143:ASN:OD1	2:C:143:ASN:N	2.49	0.46
2:C:1086:GLN:O	2:C:1090:THR:OG1	2.27	0.46
2:C:1092:LYS:HD3	3:D:424:TYR:HD2	1.80	0.46
1:A:179:ASP:HB2	1:A:191:LYS:HB3	1.97	0.46
2:C:187:PHE:N	2:C:368:ASP:OD2	2.45	0.46
3:D:589:THR:HG21	3:D:688:MET:HG2	1.97	0.46
7:M:128:LEU:O	7:M:132:ARG:HB2	2.16	0.46
2:C:947:ASP:OD1	2:C:947:ASP:N	2.38	0.46
3:D:1186:PHE:O	3:D:1190:ASN:ND2	2.49	0.46
1:A:55:ARG:HG3	1:A:161:ARG:HA	1.98	0.45
2:C:494:ILE:H	2:C:494:ILE:HG13	1.58	0.45
3:D:736:VAL:O	3:D:841:ARG:NE	2.49	0.45
2:C:235:THR:HG21	2:C:262:LEU:HA	1.97	0.45
3:D:554:GLU:HG3	4:E:54:VAL:HG11	1.98	0.45
3:D:832:ILE:HG22	3:D:834:ARG:H	1.81	0.45
3:D:1012:MET:HG3	3:D:1013:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:301:ARG:NH1	8:O:55:DG:N7	2.64	0.45
5:F:331:ALA:HB2	5:F:350:TRP:HB2	1.97	0.45
1:A:95:MET:HE2	1:A:95:MET:HB3	1.82	0.45
2:C:369:ASP:O	2:C:375:ASN:ND2	2.48	0.45
2:C:674:LYS:HD3	2:C:674:LYS:HA	1.79	0.45
2:C:757:ILE:HD12	2:C:757:ILE:HA	1.85	0.45
3:D:273:GLU:OE2	3:D:295:ARG:NH2	2.41	0.45
2:C:1010:LEU:HD23	2:C:1010:LEU:HA	1.85	0.45
3:D:119:ASP:OD1	3:D:291:ARG:NH2	2.48	0.45
3:D:666:THR:OG1	3:D:667:THR:O	2.33	0.45
3:D:1262:THR:HB	4:E:55:ILE:HD11	1.97	0.45
1:B:84:VAL:HB	1:B:199:LYS:HD3	1.98	0.45
2:C:178:GLN:OE1	2:C:379:ARG:NH2	2.45	0.45
2:C:476:HIS:O	2:C:478:SER:N	2.46	0.45
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.97	0.45
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.55	0.45
2:C:767:GLU:HG2	2:C:807:THR:HG22	1.98	0.45
2:C:777:SER:OG	2:C:778:ASP:N	2.50	0.45
3:D:101:VAL:O	3:D:314:LEU:N	2.49	0.45
7:M:52:ASN:OD1	7:M:52:ASN:N	2.39	0.45
1:B:17:ASN:OD1	1:B:17:ASN:N	2.50	0.45
2:C:974:THR:O	2:C:974:THR:OG1	2.32	0.45
3:D:823:LEU:HD23	3:D:835:PRO:HB3	1.99	0.45
3:D:919:SER:OG	3:D:920:ALA:N	2.50	0.45
2:C:981:GLN:O	2:C:984:GLU:N	2.50	0.45
7:M:121:SER:HB3	7:M:124:GLU:HB2	1.99	0.45
1:A:206:ASP:OD1	1:A:206:ASP:N	2.49	0.45
2:C:150:GLN:HB2	2:C:414:PRO:HG2	1.98	0.45
2:C:403:ARG:HD2	2:C:417:LEU:HA	1.98	0.45
2:C:659:THR:HA	2:C:669:THR:HA	1.99	0.44
2:C:705:GLY:N	2:C:708:THR:OG1	2.50	0.44
2:C:760:ARG:HA	2:C:865:VAL:HA	1.98	0.44
3:D:9:GLU:OE2	3:D:1244:LYS:NZ	2.43	0.44
3:D:348:ILE:HD13	3:D:348:ILE:HA	1.85	0.44
3:D:614:SER:HG	3:D:617:GLU:H	1.64	0.44
2:C:891:ASN:OD1	2:C:891:ASN:N	2.46	0.44
3:D:879:ASP:OD1	3:D:1249:LYS:NZ	2.37	0.44
5:F:397:GLU:HA	5:F:407:PRO:HG3	2.00	0.44
7:M:12:PRO:HA	7:M:13:HIS:HA	1.65	0.44
9:P:97:DT:H2"	9:P:98:DG:C8	2.53	0.44
3:D:590:THR:HG23	3:D:630:ARG:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:594:GLY:N	3:D:598:GLU:OE2	2.50	0.44
7:M:111:LEU:HB3	7:M:128:LEU:HD12	2.00	0.44
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.98	0.44
7:M:28:LYS:HD2	7:M:28:LYS:HA	1.79	0.44
6:J:90:SER:OG	6:J:92:GLU:OE1	2.35	0.44
7:M:112:TRP:O	7:M:116:GLN:CB	2.63	0.44
1:B:120:ASN:OD1	1:B:120:ASN:N	2.51	0.44
2:C:442:GLN:O	2:C:678:SER:OG	2.27	0.44
3:D:338:SER:HA	5:F:423:LEU:HB2	1.99	0.44
2:C:915:ILE:HD13	2:C:1030:ILE:HD13	2.00	0.44
3:D:468:ASN:OD1	3:D:468:ASN:N	2.50	0.44
1:B:112:PRO:HB2	1:B:116:VAL:HG23	2.00	0.44
2:C:532:THR:OG1	2:C:533:ALA:N	2.47	0.44
2:C:738:SER:N	2:C:914:ASP:O	2.51	0.44
2:C:880:SER:OG	2:C:881:ASP:N	2.50	0.44
2:C:1044:ARG:NE	3:D:423:ASP:OD1	2.50	0.44
3:D:537:ASP:OD1	3:D:537:ASP:N	2.47	0.44
3:D:1275:THR:O	3:D:1278:ALA:N	2.40	0.44
2:C:562:ARG:HD2	3:D:847:LEU:HD11	1.98	0.43
3:D:1010:LEU:HA	3:D:1145:GLN:HG3	1.98	0.43
1:A:172:LEU:HB3	1:A:197:GLU:HG2	2.00	0.43
3:D:147:GLU:HB3	3:D:151:LEU:HD12	2.00	0.43
3:D:354:LEU:HB2	3:D:370:GLU:HG3	1.99	0.43
7:M:5:VAL:HG22	7:M:21:ALA:HA	2.00	0.43
1:A:182:ARG:HA	1:A:188:ASP:HB3	2.00	0.43
2:C:288:THR:HG23	2:C:291:SER:HB3	2.00	0.43
2:C:1101:LYS:HA	2:C:1101:LYS:HD3	1.69	0.43
3:D:708:VAL:O	3:D:712:THR:OG1	2.29	0.43
2:C:285:GLU:OE1	5:F:229:ARG:NH1	2.46	0.43
2:C:758:ASP:OD1	2:C:758:ASP:N	2.49	0.43
2:C:125:LYS:HB2	2:C:127:MET:HE2	2.01	0.43
3:D:577:PRO:HB3	3:D:581:MET:HG3	2.01	0.43
7:M:100:ASP:OD2	7:M:103:LYS:N	2.45	0.43
1:B:75:GLU:OE2	3:D:636:ARG:NH2	2.46	0.43
6:J:108:ARG:HE	6:J:108:ARG:HB3	1.57	0.43
7:M:149:LYS:HE2	7:M:149:LYS:HB2	1.74	0.43
2:C:178:GLN:HB2	2:C:436:LEU:HD21	2.00	0.43
2:C:907:LEU:HD12	2:C:911:THR:HB	2.00	0.43
2:C:927:ASN:OD1	2:C:927:ASN:N	2.51	0.43
2:C:1110:GLU:HA	4:E:69:ASN:HD21	1.84	0.43
3:D:647:GLU:O	3:D:652:GLY:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HD13	1:A:162:ILE:HA	1.81	0.43
2:C:319:LYS:NZ	2:C:368:ASP:OD1	2.49	0.43
3:D:797:ASN:HD22	3:D:798:PRO:HD2	1.83	0.43
5:F:464:LEU:HB3	5:F:476:ARG:HH21	1.84	0.43
8:O:33:DA:H2''	8:O:34:DT:H2'	2.01	0.43
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.82	0.43
2:C:758:ASP:O	2:C:805:LYS:NZ	2.52	0.43
3:D:177:LEU:HD12	3:D:177:LEU:HA	1.90	0.43
3:D:1055:LEU:N	3:D:1101:ASP:OD1	2.47	0.43
1:B:95:MET:HE2	1:B:140:VAL:HG21	2.01	0.42
2:C:777:SER:OG	2:C:779:GLU:OE1	2.31	0.42
3:D:165:GLN:NE2	3:D:169:GLU:OE2	2.52	0.42
3:D:1034:LEU:HD21	3:D:1137:GLU:HB3	2.00	0.42
5:F:260:THR:O	5:F:264:THR:OG1	2.31	0.42
1:B:38:LEU:HA	1:B:38:LEU:HD12	1.82	0.42
1:B:225:LEU:HD23	1:B:225:LEU:HA	1.89	0.42
3:D:634:LYS:HG2	3:D:665:GLU:HB3	2.01	0.42
3:D:1248:LEU:HD21	3:D:1258:ILE:HD12	2.01	0.42
2:C:252:PHE:HB3	2:C:255:SER:HB2	2.01	0.42
1:A:13:VAL:HA	1:A:19:SER:HB2	2.02	0.42
1:A:214:THR:HG23	1:B:232:ILE:HB	2.01	0.42
2:C:356:THR:HA	2:C:362:GLU:HA	2.01	0.42
3:D:663:MET:HE2	3:D:663:MET:HB3	1.89	0.42
8:O:36:DG:H2''	8:O:37:DC:H5''	1.99	0.42
2:C:224:VAL:HG23	2:C:234:VAL:HG12	2.01	0.42
5:F:236:GLY:HA2	5:F:301:ARG:HH21	1.83	0.42
6:J:60:MET:HE2	6:J:60:MET:HB3	1.84	0.42
2:C:926:MET:HB3	2:C:926:MET:HE3	1.80	0.42
2:C:278:TYR:HE2	2:C:285:GLU:HB3	1.85	0.42
2:C:1057:LEU:HD23	2:C:1062:GLN:HG2	2.02	0.42
3:D:310:MET:HE2	3:D:310:MET:HB2	1.89	0.42
3:D:1055:LEU:HB3	3:D:1101:ASP:HA	2.01	0.42
6:J:34:THR:OG1	6:J:36:ASN:OD1	2.29	0.42
2:C:92:GLU:OE2	2:C:390:ARG:NE	2.44	0.42
5:F:293:ASN:HA	5:F:296:LEU:HD12	2.02	0.42
2:C:59:ASP:OD1	2:C:69:ARG:NH1	2.53	0.42
2:C:322:LEU:HD23	2:C:357:VAL:HG11	2.02	0.42
5:F:382:ILE:HD13	5:F:382:ILE:HA	1.94	0.42
5:F:449:ASP:OD1	5:F:449:ASP:N	2.51	0.42
2:C:740:ARG:NH2	2:C:914:ASP:OD2	2.37	0.41
3:D:880:VAL:HG22	3:D:1214:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:46:ARG:NE	4:E:102:ASP:OD1	2.52	0.41
2:C:32:VAL:HG11	2:C:632:LEU:HD11	2.01	0.41
2:C:724:MET:HB2	2:C:724:MET:HE3	1.77	0.41
3:D:262:GLN:HG3	3:D:313:VAL:HG21	2.02	0.41
3:D:797:ASN:HB3	3:D:800:ILE:HG22	2.01	0.41
3:D:817:LEU:HD23	3:D:817:LEU:HA	1.81	0.41
2:C:81:ASN:OD1	2:C:81:ASN:N	2.54	0.41
2:C:413:THR:HG23	2:C:415:GLN:H	1.85	0.41
2:C:676:ALA:HB3	2:C:684:ALA:HB3	2.01	0.41
2:C:1093:SER:OG	3:D:421:ARG:O	2.31	0.41
3:D:733:MET:H	3:D:733:MET:HG3	1.69	0.41
3:D:142:GLU:O	3:D:145:HIS:ND1	2.53	0.41
3:D:516:LEU:HD23	3:D:516:LEU:HA	1.81	0.41
3:D:928:ASP:OD1	3:D:940:ARG:N	2.54	0.41
6:J:32:TYR:OH	6:J:51:PRO:O	2.27	0.41
1:A:49:ALA:HB2	1:A:142:ARG:HD2	2.01	0.41
2:C:278:TYR:CZ	2:C:282:ARG:HG3	2.56	0.41
3:D:173:ARG:NH2	3:D:180:ASP:OD2	2.54	0.41
3:D:448:ALA:HB1	3:D:491:ILE:HD11	2.03	0.41
3:D:640:LEU:HD23	3:D:640:LEU:HA	1.92	0.41
3:D:824:VAL:HG11	3:D:852:ASN:HA	2.01	0.41
6:J:99:LYS:HD2	6:J:99:LYS:HA	1.93	0.41
2:C:641:VAL:HG11	2:C:701:VAL:HG22	2.01	0.41
2:C:797:ARG:HH22	3:D:478:ARG:HA	1.85	0.41
2:C:884:LYS:HD3	2:C:1035:HIS:HD2	1.84	0.41
3:D:1168:ILE:HG12	3:D:1203:GLY:HA2	2.03	0.41
5:F:243:ALA:HB2	5:F:342:LYS:HE2	2.00	0.41
2:C:218:LYS:HE3	2:C:218:LYS:HB2	1.88	0.41
2:C:747:LEU:HD23	2:C:747:LEU:HA	1.91	0.41
2:C:1015:SER:OG	2:C:1016:GLY:N	2.53	0.41
3:D:139:VAL:HA	3:D:252:PHE:HA	2.01	0.41
3:D:417:LEU:HD13	3:D:417:LEU:HA	1.87	0.41
3:D:566:LEU:HA	3:D:573:PRO:HA	2.03	0.41
7:M:121:SER:OG	7:M:122:ALA:N	2.54	0.41
1:A:27:GLU:H	1:A:27:GLU:HG2	1.69	0.41
3:D:916:ILE:HG23	3:D:920:ALA:HB3	2.01	0.41
1:A:40:ARG:HE	1:A:40:ARG:HB3	1.68	0.41
2:C:264:LYS:HA	2:C:264:LYS:HD2	1.76	0.41
2:C:1040:LYS:HA	2:C:1040:LYS:HD3	1.83	0.41
5:F:342:LYS:N	8:O:52:DA:OP2	2.50	0.41
5:F:390:LEU:HD11	5:F:392:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD13	1:A:215:LEU:HA	1.86	0.41
1:B:44:SER:HA	1:B:145:GLY:HA2	2.03	0.41
2:C:500:LEU:HA	2:C:500:LEU:HD23	1.86	0.41
2:C:1134:ASN:N	3:D:13:GLY:O	2.52	0.41
5:F:334:LYS:NZ	8:O:49:DT:OP2	2.38	0.41
1:A:98:ARG:HG2	1:A:135:GLU:HG2	2.03	0.40
2:C:545:ASN:HD21	3:D:846:VAL:HG23	1.85	0.40
2:C:597:LEU:HB3	2:C:976:VAL:HG13	2.03	0.40
3:D:706:MET:HB3	4:E:40:ILE:HD11	2.03	0.40
5:F:359:MET:O	5:F:363:ALA:HB2	2.21	0.40
2:C:531:LEU:HD23	2:C:531:LEU:HA	1.86	0.40
3:D:525:HIS:CE1	3:D:527:LEU:HD12	2.55	0.40
5:F:280:ASP:HB2	6:J:105:ILE:HG21	2.02	0.40
2:C:319:LYS:HA	2:C:319:LYS:HD2	1.88	0.40
3:D:95:ILE:HG12	3:D:348:ILE:HD11	2.04	0.40
3:D:453:LYS:HA	3:D:456:VAL:HG12	2.02	0.40
5:F:313:ARG:NH1	9:P:104:DC:O5'	2.55	0.40
1:A:53:SER:HA	1:A:164:VAL:HG23	2.04	0.40
3:D:670:ARG:NE	3:D:686:LYS:O	2.54	0.40
3:D:924:THR:HG23	3:D:980:GLY:HA2	2.03	0.40
3:D:1173:THR:HG21	3:D:1193:VAL:HG11	2.04	0.40
3:D:1209:GLY:O	3:D:1213:ALA:N	2.53	0.40
6:J:89:ARG:HA	6:J:89:ARG:HD3	1.77	0.40
2:C:1057:LEU:HD12	2:C:1057:LEU:HA	1.79	0.40
3:D:367:VAL:HG12	3:D:371:LYS:HE3	2.03	0.40
3:D:578:ARG:HB2	3:D:579:LEU:H	1.60	0.40
3:D:964:SER:OG	3:D:965:VAL:N	2.53	0.40
3:D:1124:VAL:HG12	3:D:1125:GLN:HG3	2.03	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	223/347 (64%)	202 (91%)	21 (9%)	0	100	100
1	B	235/347 (68%)	204 (87%)	31 (13%)	0	100	100
2	C	1109/1179 (94%)	1007 (91%)	101 (9%)	1 (0%)	48	79
3	D	1264/1326 (95%)	1174 (93%)	89 (7%)	1 (0%)	48	79
4	E	81/110 (74%)	78 (96%)	3 (4%)	0	100	100
5	F	320/531 (60%)	309 (97%)	11 (3%)	0	100	100
6	J	107/111 (96%)	96 (90%)	11 (10%)	0	100	100
7	M	157/162 (97%)	148 (94%)	9 (6%)	0	100	100
All	All	3496/4113 (85%)	3218 (92%)	276 (8%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1276	GLU
2	C	982	GLU

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	194/297 (65%)	180 (93%)	14 (7%)	13	40
1	B	195/297 (66%)	184 (94%)	11 (6%)	19	47
2	C	932/997 (94%)	872 (94%)	60 (6%)	16	43
3	D	1048/1103 (95%)	968 (92%)	80 (8%)	12	39
4	E	69/89 (78%)	65 (94%)	4 (6%)	18	46
5	F	262/429 (61%)	250 (95%)	12 (5%)	24	51
6	J	92/97 (95%)	85 (92%)	7 (8%)	12	39
7	M	129/131 (98%)	119 (92%)	10 (8%)	11	38
All	All	2921/3440 (85%)	2723 (93%)	198 (7%)	16	42

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	51	VAL
1	A	69	VAL
1	A	84	VAL
1	A	111	VAL
1	A	128	LEU
1	A	164	VAL
1	A	171	VAL
1	A	172	LEU
1	A	187	THR
1	A	203	SER
1	A	215	LEU
1	A	221	LEU
1	A	226	ASN
1	B	41	THR
1	B	54	ILE
1	B	84	VAL
1	B	111	VAL
1	B	117	THR
1	B	125	ILE
1	B	133	LYS
1	B	159	ILE
1	B	171	VAL
1	B	173	LYS
1	B	196	VAL
2	C	39	VAL
2	C	93	LEU
2	C	128	THR
2	C	144	THR
2	C	147	ILE
2	C	202	VAL
2	C	220	ASP
2	C	226	ILE
2	C	234	VAL
2	C	288	THR
2	C	296	LEU
2	C	345	LEU
2	C	355	MET
2	C	373	PHE
2	C	409	VAL
2	C	420	ILE
2	C	443	ASN
2	C	450	THR

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Mol	Chain	Res	Type
2	C	456	LEU
2	C	494	ILE
2	C	519	VAL
2	C	521	ASP
2	C	536	GLU
2	C	540	VAL
2	C	545	ASN
2	C	561	VAL
2	C	587	VAL
2	C	626	VAL
2	C	628	THR
2	C	632	LEU
2	C	646	GLU
2	C	651	GLU
2	C	653	VAL
2	C	656	ASP
2	C	664	ASN
2	C	682	THR
2	C	702	ILE
2	C	719	LEU
2	C	723	ILE
2	C	787	ARG
2	C	809	LYS
2	C	814	LEU
2	C	839	VAL
2	C	868	LEU
2	C	901	VAL
2	C	907	LEU
2	C	911	THR
2	C	936	LEU
2	C	939	CYS
2	C	959	LEU
2	C	974	THR
2	C	989	LEU
2	C	993	LEU
2	C	995	ASN
2	C	997	ASP
2	C	1037	VAL
2	C	1038	ASP
2	C	1057	LEU
2	C	1096	THR
2	C	1122	LYS

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Mol	Chain	Res	Type
3	D	3	ASP
3	D	14	LEU
3	D	34	ILE
3	D	82	VAL
3	D	101	VAL
3	D	104	ILE
3	D	110	VAL
3	D	117	LEU
3	D	123	LYS
3	D	137	THR
3	D	148	LEU
3	D	196	LYS
3	D	210	ASP
3	D	219	LEU
3	D	222	ILE
3	D	236	VAL
3	D	240	LEU
3	D	270	ILE
3	D	285	LYS
3	D	293	LEU
3	D	328	VAL
3	D	360	LEU
3	D	365	ILE
3	D	417	LEU
3	D	425	SER
3	D	429	VAL
3	D	441	CYS
3	D	446	LEU
3	D	449	LEU
3	D	460	LEU
3	D	462	ASP
3	D	469	ILE
3	D	480	ARG
3	D	483	VAL
3	D	490	VAL
3	D	491	ILE
3	D	493	GLU
3	D	498	LEU
3	D	578	ARG
3	D	580	ASP
3	D	588	LEU
3	D	589	THR

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Mol	Chain	Res	Type
3	D	600	GLN
3	D	603	SER
3	D	613	SER
3	D	644	VAL
3	D	676	LEU
3	D	725	THR
3	D	729	VAL
3	D	730	THR
3	D	732	SER
3	D	737	LEU
3	D	796	ASP
3	D	808	THR
3	D	810	ASN
3	D	853	THR
3	D	865	LEU
3	D	876	ARG
3	D	883	ASP
3	D	909	THR
3	D	911	ILE
3	D	925	LEU
3	D	962	VAL
3	D	964	SER
3	D	991	ILE
3	D	1060	ARG
3	D	1088	VAL
3	D	1097	ARG
3	D	1107	VAL
3	D	1129	GLU
3	D	1130	VAL
3	D	1132	ILE
3	D	1148	SER
3	D	1173	THR
3	D	1174	GLU
3	D	1207	LEU
3	D	1234	THR
3	D	1242	SER
3	D	1248	LEU
3	D	1258	ILE
4	E	33	LEU
4	E	49	SER
4	E	53	LEU
4	E	92	LEU

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Mol	Chain	Res	Type
5	F	269	ARG
5	F	295	LEU
5	F	302	LEU
5	F	313	ARG
5	F	328	LEU
5	F	332	VAL
5	F	336	ASP
5	F	422	SER
5	F	460	LEU
5	F	495	VAL
5	F	514	LEU
5	F	522	VAL
6	J	57	ARG
6	J	60	MET
6	J	61	GLU
6	J	64	LEU
6	J	86	LEU
6	J	97	LEU
6	J	105	ILE
7	M	35	LEU
7	M	36	VAL
7	M	44	LEU
7	M	52	ASN
7	M	56	VAL
7	M	62	VAL
7	M	85	TRP
7	M	96	LEU
7	M	111	LEU
7	M	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	61	HIS
1	A	100	GLN
1	A	151	GLN
1	B	61	HIS
1	B	129	ASN
1	B	151	GLN
1	B	185	GLN
2	C	57	GLN

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Mol	Chain	Res	Type
2	C	141	ASN
2	C	142	ASN
2	C	232	GLN
2	C	247	GLN
2	C	293	GLN
2	C	407	GLN
2	C	419	ASN
2	C	1062	GLN
2	C	1066	GLN
2	C	1134	ASN
3	D	146	ASN
3	D	213	GLN
3	D	287	GLN
3	D	307	ASN
3	D	329	GLN
3	D	351	ASN
3	D	368	ASN
3	D	369	ASN
3	D	396	ASN
3	D	416	ASN
3	D	482	GLN
3	D	494	HIS
3	D	499	ASN
3	D	525	HIS
3	D	552	GLN
3	D	564	ASN
3	D	693	GLN
3	D	797	ASN
3	D	1160	GLN
3	D	1227	GLN
3	D	1251	ASN
5	F	325	ASN
5	F	353	GLN
5	F	388	GLN
5	F	459	GLN
7	M	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

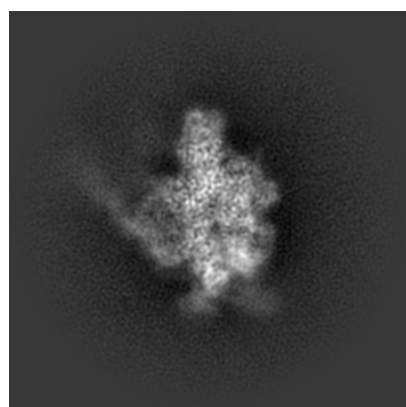
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21409. These allow visual inspection of the internal detail of the map and identification of artifacts.

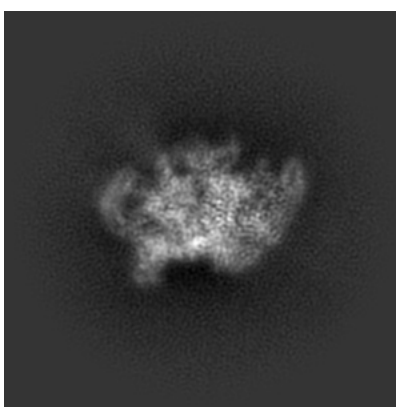
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

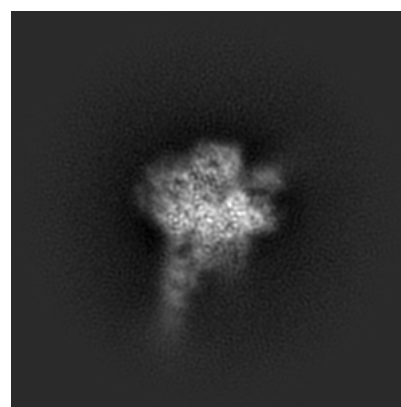
6.1.1 Primary map



X



Y

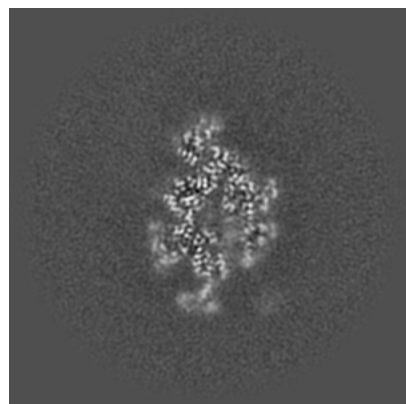


Z

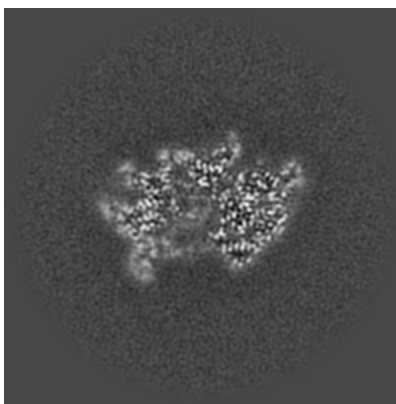
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

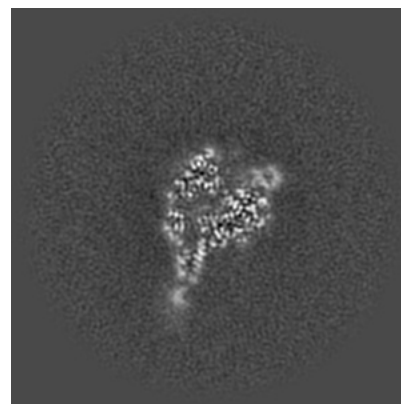
6.2.1 Primary map



X Index: 128



Y Index: 128

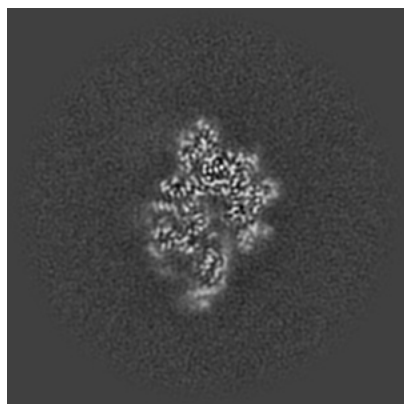


Z Index: 128

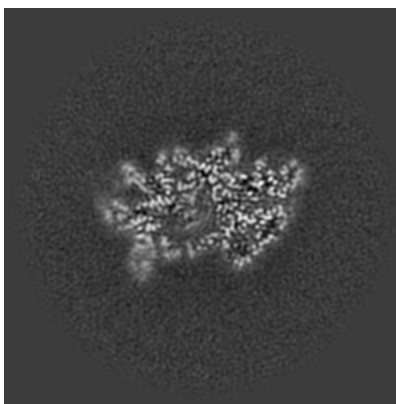
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

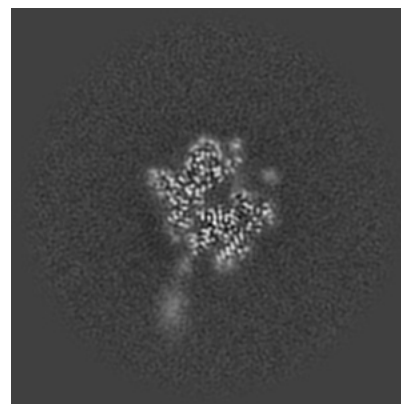
6.3.1 Primary map



X Index: 122



Y Index: 126

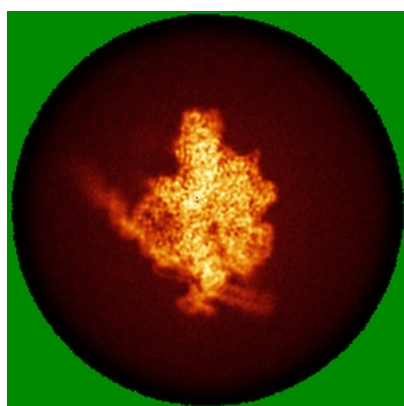


Z Index: 137

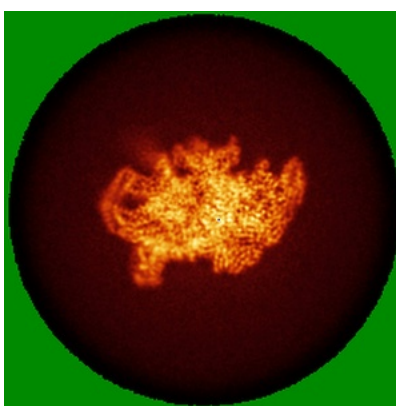
The images above show the largest variance slices of the map in three orthogonal directions.

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

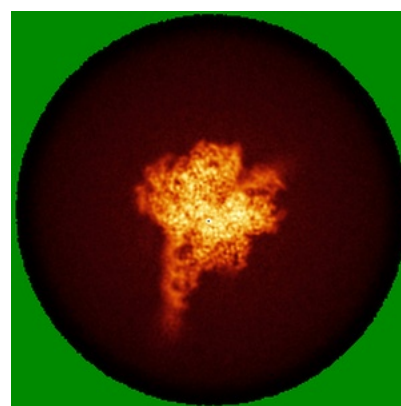
6.4.1 Primary map



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 0.387. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

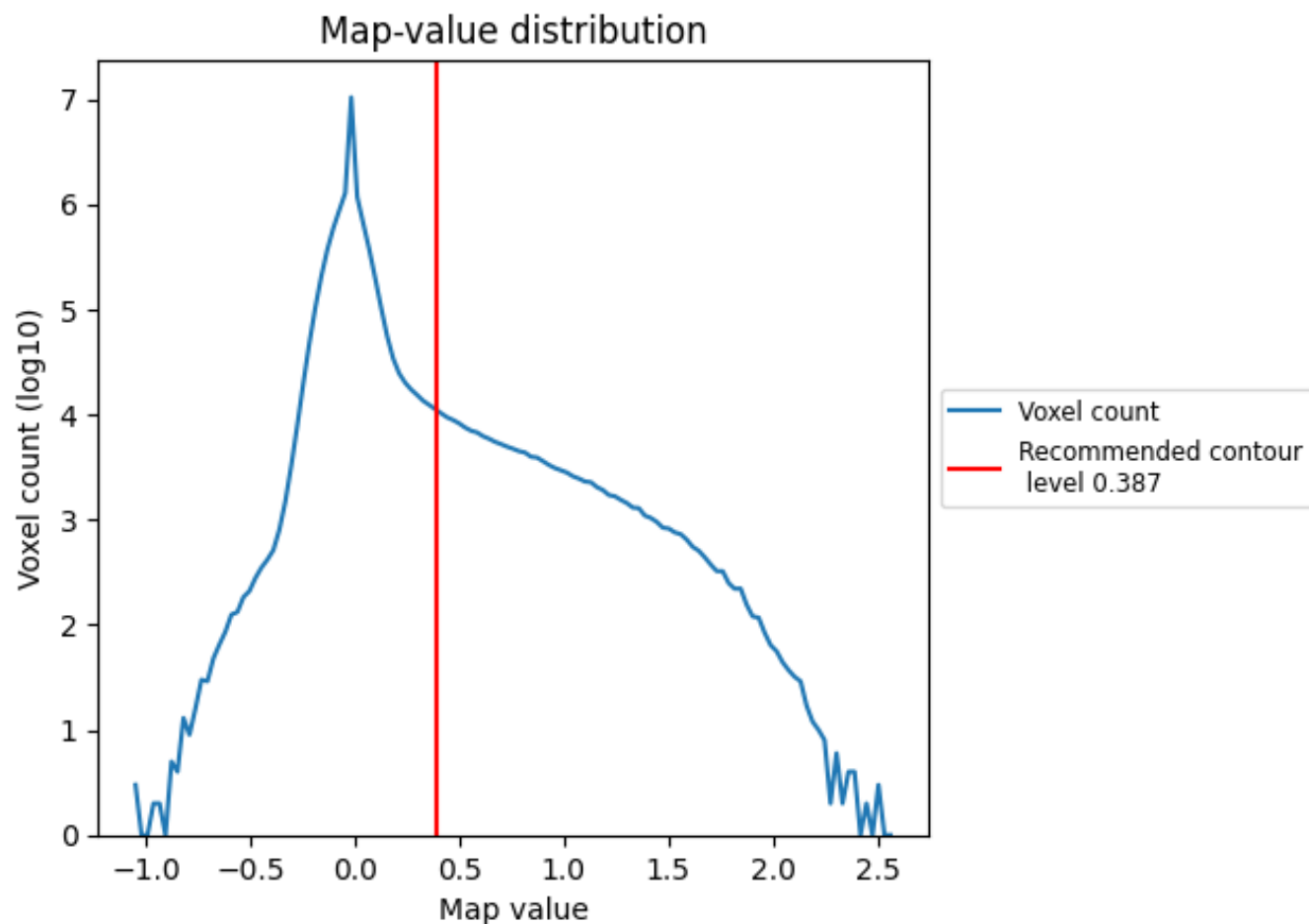
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

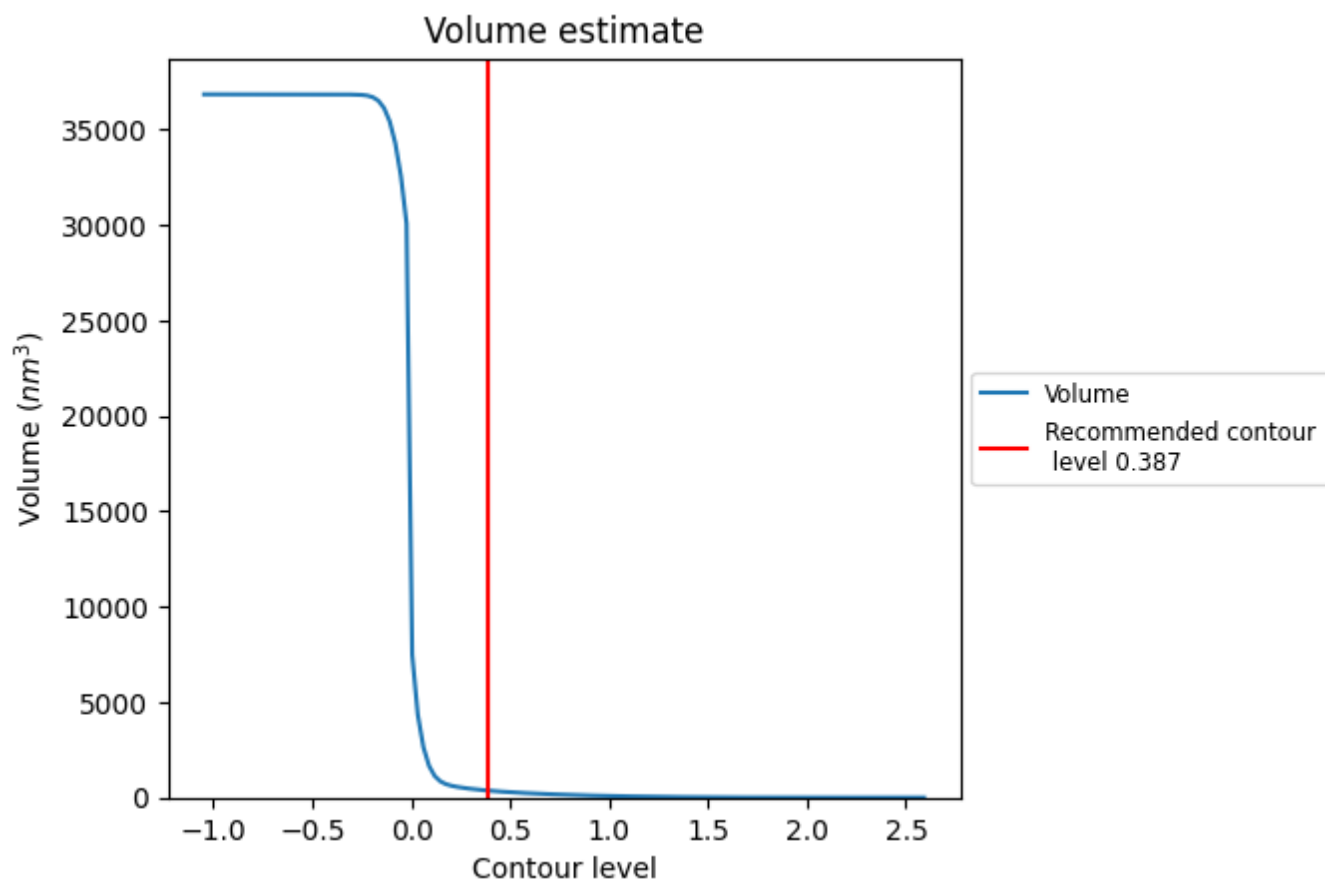
This section contains the results of statistical analysis of the map.

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.

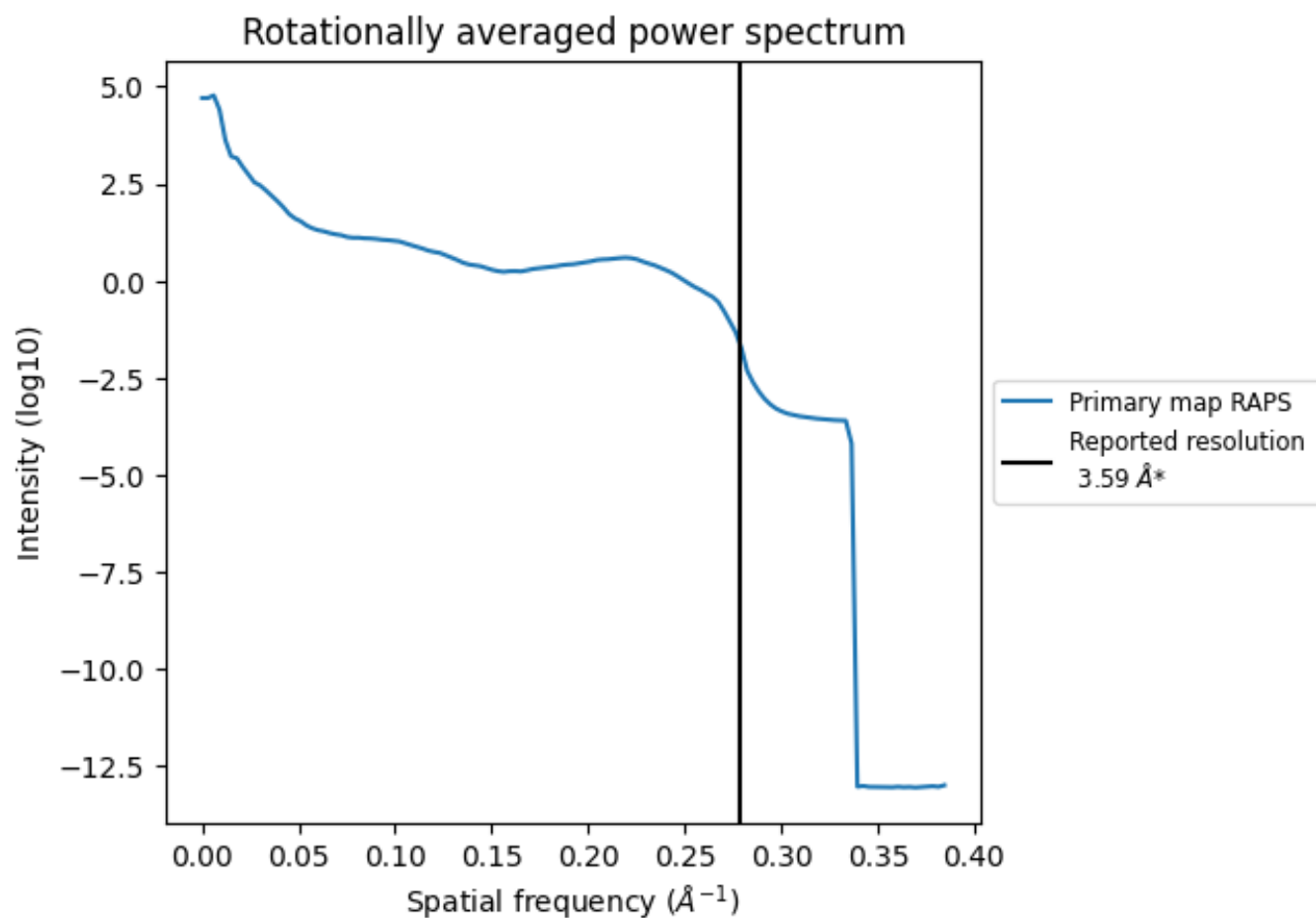
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 367 nm³; this corresponds to an approximate mass of 332 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 0.279 Å⁻¹

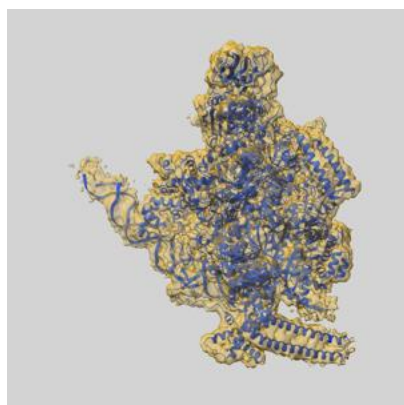
8 Fourier-Shell correlation ⓘ

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

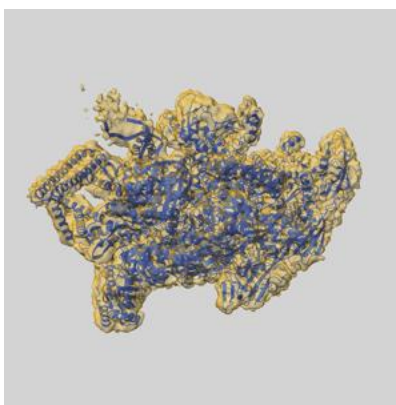
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21409 and PDB model 6VW0. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

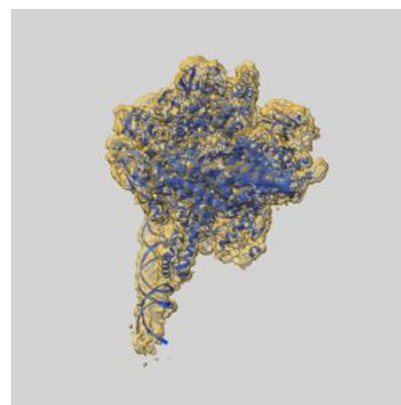
9.1 Map-model overlay [i](#)



X



Y



Z

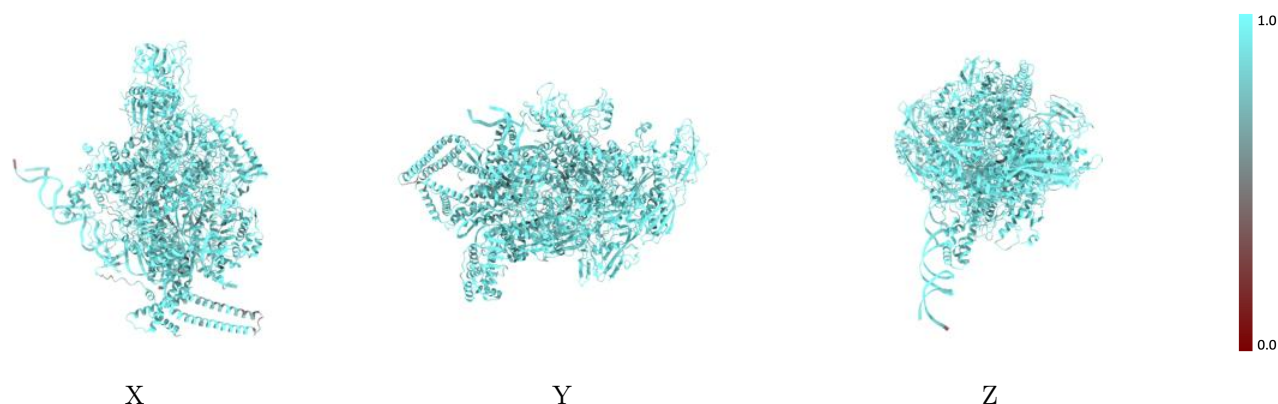
The images above show the 3D surface view of the map at the recommended contour level 0.387 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



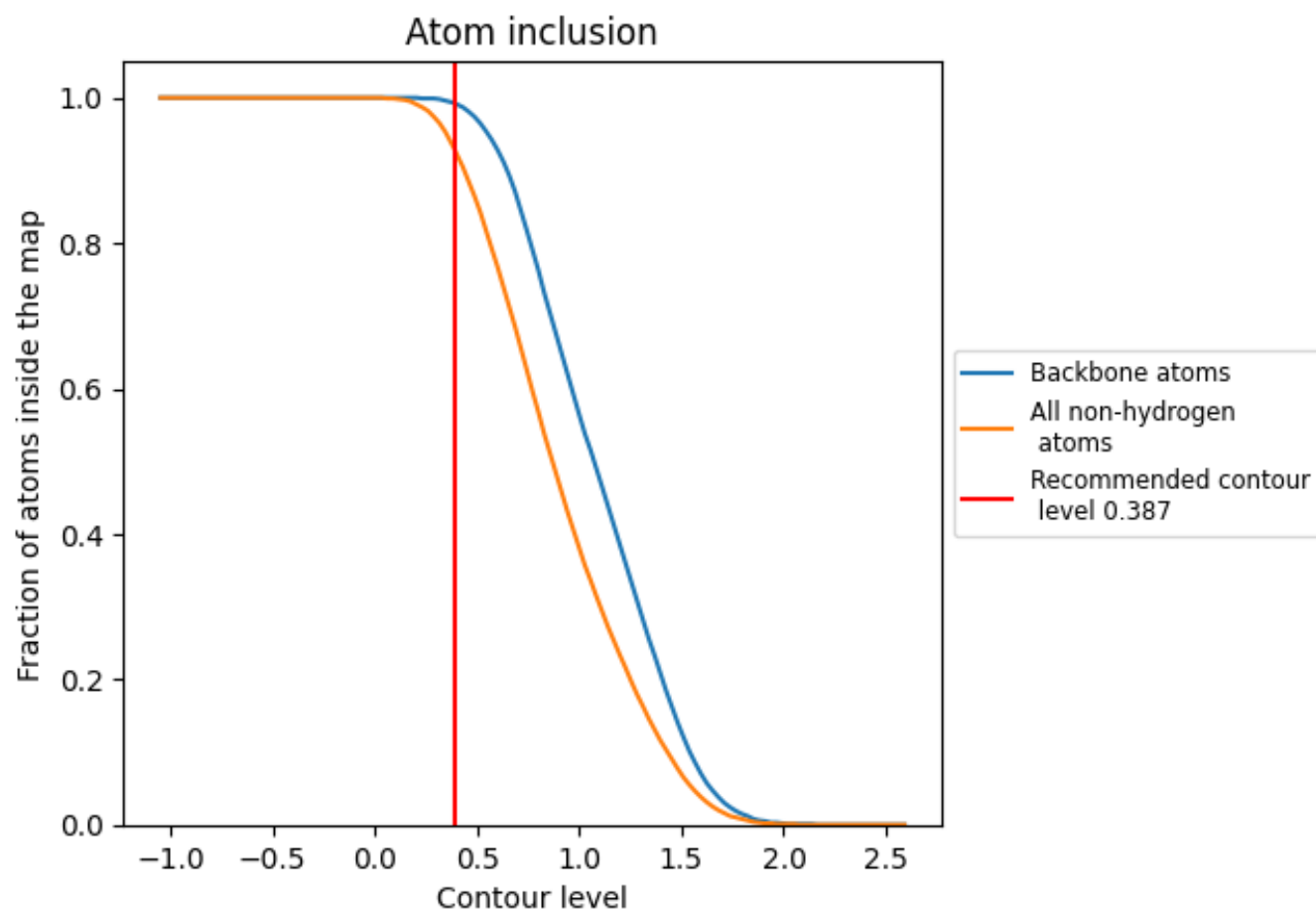
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.387).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.387) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.4200
A	0.9580	0.4650
B	0.9400	0.4320
C	0.9420	0.4560
D	0.9290	0.4360
E	0.9430	0.4620
F	0.9100	0.3720
J	0.8630	0.3690
M	0.8980	0.3230
O	0.9520	0.3080
P	0.9030	0.3050

1.0

0.0

<0.0