



Full wwPDB EM Validation Report ⓘ

Nov 25, 2025 – 03:03 PM EST

PDB ID : 9EFM / pdb_00009efm
EMDB ID : EMD-47976
Title : Cryo-EM structure of COP9 signalosome precatalytic state with neddylated cullin-1
Authors : Shi, H.; Zheng, N.
Deposited on : 2024-11-20
Resolution : 3.16 Å (reported)
Based on initial models : 1LDJ, 4D10

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:

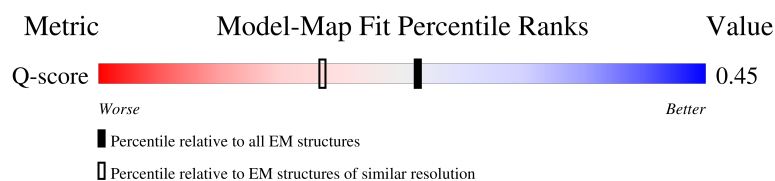
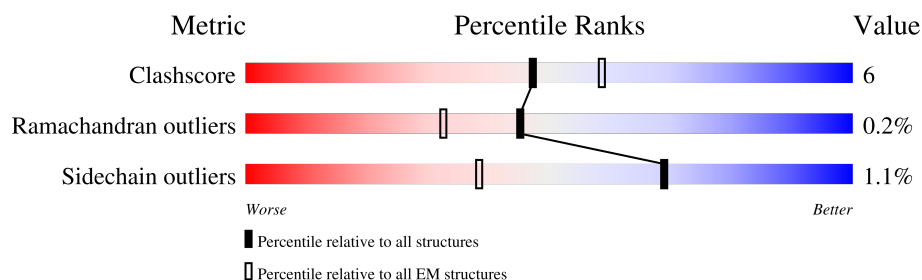
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.16 Å.

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





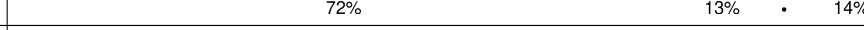

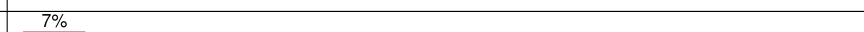


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	491	
2	B	443	
3	C	423	
4	D	406	

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Mol	Chain	Length	Quality of chain
5	E	334	
6	F	327	
7	G	264	
8	H	209	
9	I	81	
10	J	776	
11	K	108	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 24951 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	409	Total	C	N	O	S	0	0
			3271	2066	573	610	22		

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	408	Total	C	N	O	S	0	0
			3342	2126	574	627	15		

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	404	Total	C	N	O	S	0	0
			3216	2048	540	602	26		

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	405	Total	C	N	O	S	0	0
			3241	2042	564	619	16		

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	306	Total	C	N	O	S	0	0
			2433	1552	409	458	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	76	ALA	GLU	engineered mutation	UNP Q92905
E	151	ASN	ASP	engineered mutation	UNP Q92905

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	280	Total	C	N	O	S	0	0
			2227	1421	371	422	13		

- Molecule 7 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	213	Total	C	N	O	S	0	0
			1687	1070	287	324	6		

- Molecule 8 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	172	Total	C	N	O	S	0	0
			1374	880	239	251	4		

- Molecule 9 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	76	Total	C	N	O	S	0	0
			599	378	104	115	2		

- Molecule 10 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	345	Total	C	N	O	S	0	0
			2813	1797	473	529	14		

- Molecule 11 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			745	472	137	127	9		

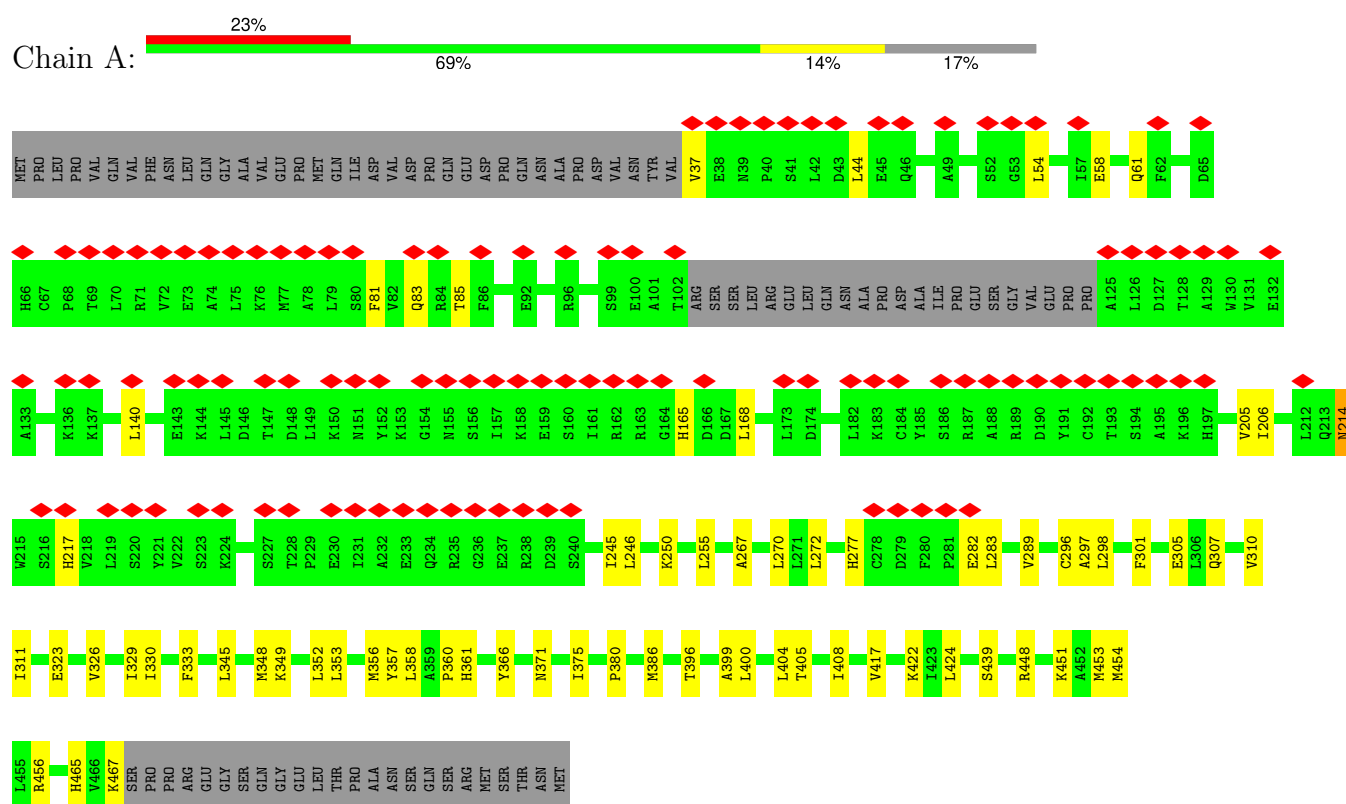
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	K	3	Total	Zn	0
			3	3	

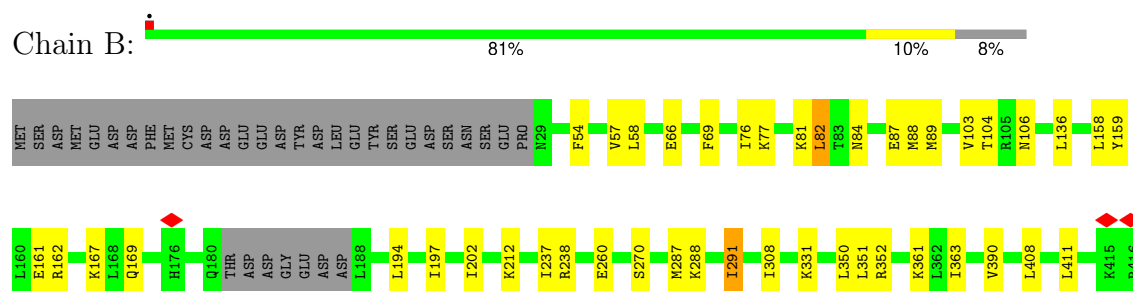
3 Residue-property plots

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: COP9 signalosome complex subunit 1

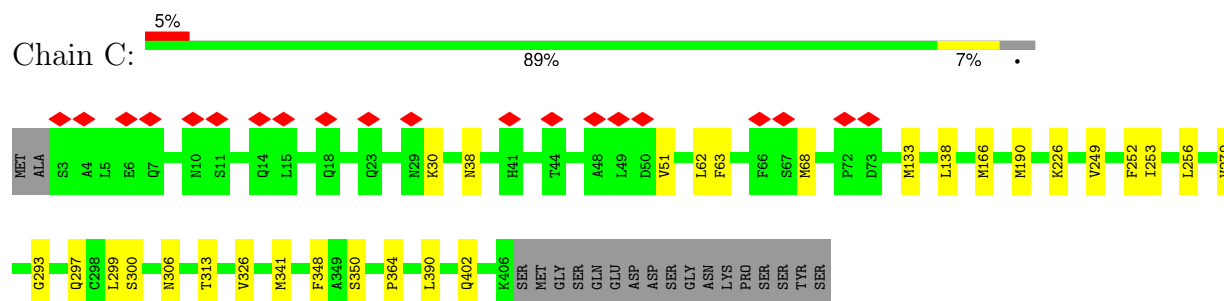


• Molecule 2: COP9 signalosome complex subunit 2

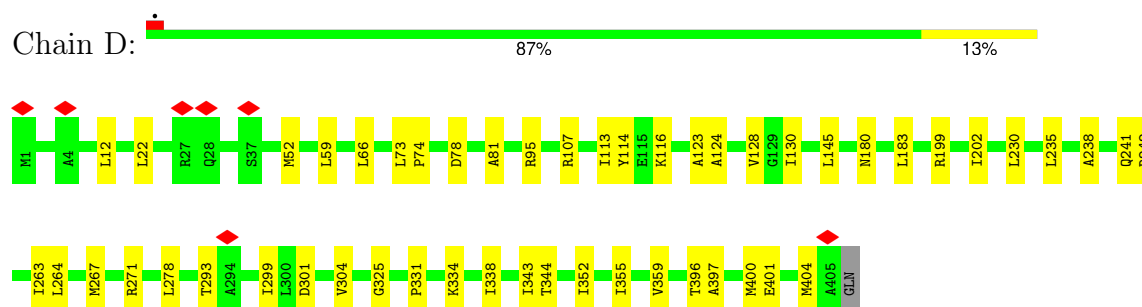




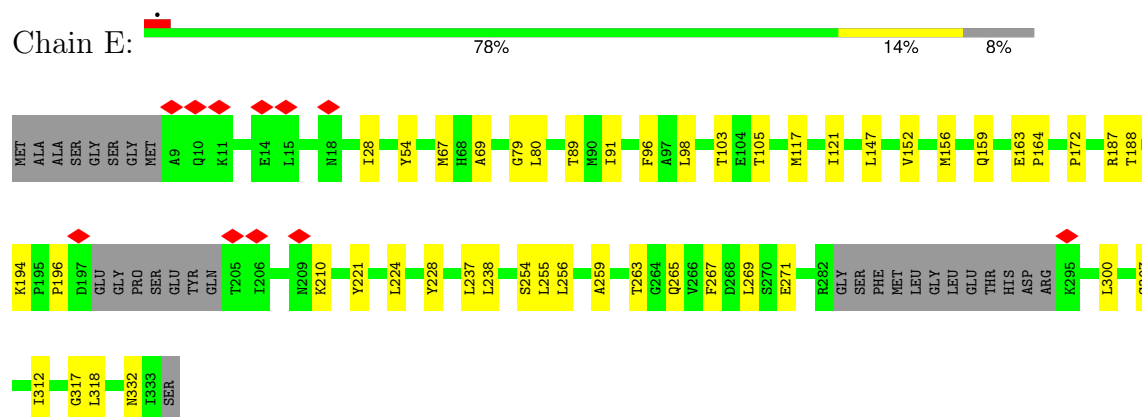
- Molecule 3: COP9 signalosome complex subunit 3



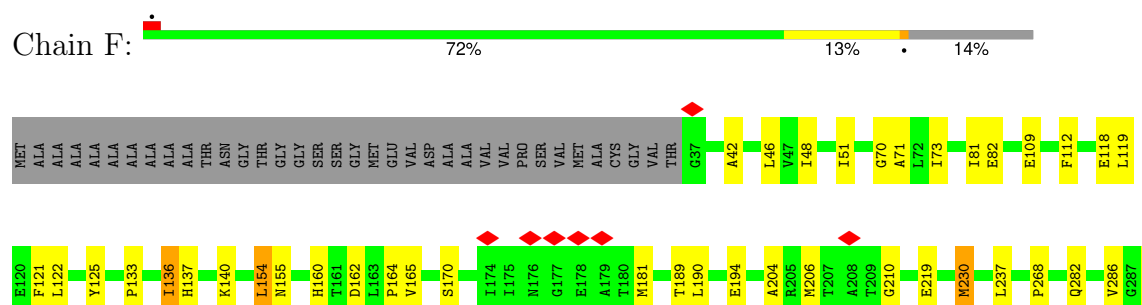
- Molecule 4: COP9 signalosome complex subunit 4

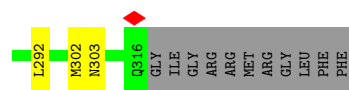


- Molecule 5: COP9 signalosome complex subunit 5

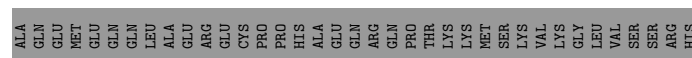


- Molecule 6: COP9 signalosome complex subunit 6

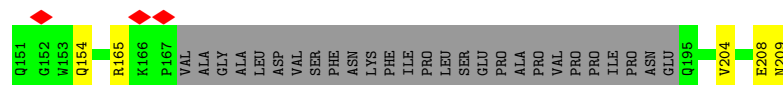




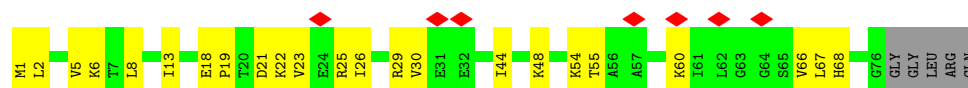
• Molecule 7: COP9 signalosome complex subunit 7b



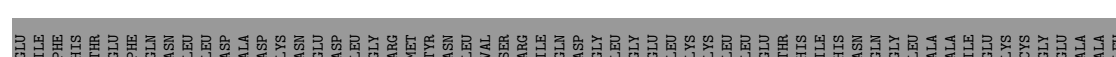
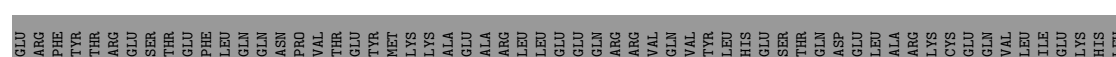
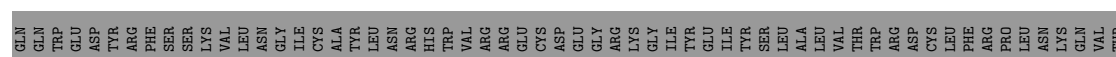
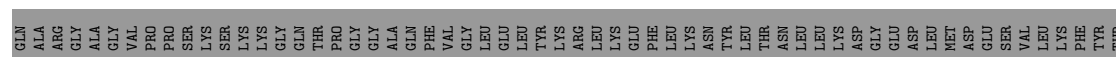
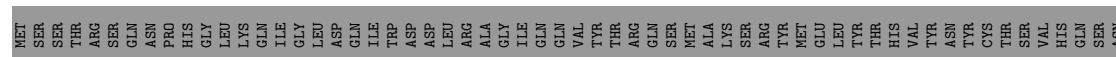
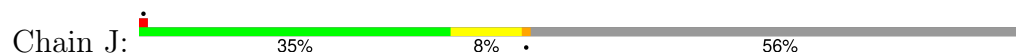
• Molecule 8: COP9 signalosome complex subunit 8

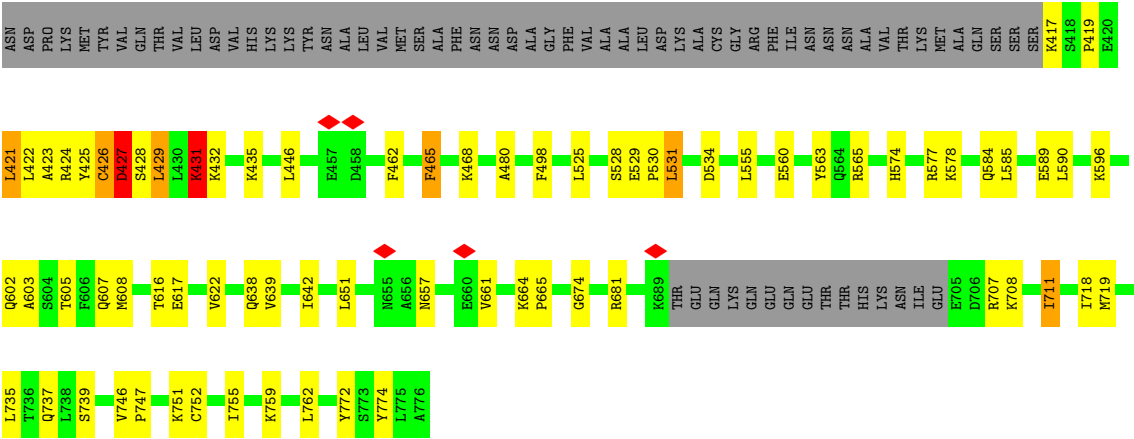


• Molecule 9: NEDD8

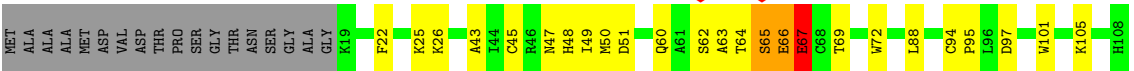


• Molecule 10: Cullin-1





● Molecule 11: E3 ubiquitin-protein ligase RBX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	177066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.031	Depositor
Minimum map value	-0.452	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	335.6, 335.6, 335.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.839, 0.839, 0.839	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.11	0/3324	0.34	0/4478
2	B	0.13	0/3399	0.35	0/4571
3	C	0.12	0/3275	0.34	0/4423
4	D	0.11	0/3293	0.33	0/4448
5	E	0.14	0/2483	0.38	0/3353
6	F	0.13	0/2274	0.34	0/3082
7	G	0.09	0/1707	0.27	0/2309
8	H	0.12	0/1407	0.39	1/1912 (0.1%)
9	I	0.16	0/604	0.45	0/808
10	J	0.21	1/2857 (0.0%)	0.40	0/3840
11	K	0.22	0/767	0.49	2/1040 (0.2%)
All	All	0.14	1/25390 (0.0%)	0.36	3/34264 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	427	ASP	C-O	-5.29	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	65	SER	N-CA-C	-5.39	105.10	110.97
11	K	66	GLU	N-CA-C	-5.18	105.06	111.33
8	H	102	VAL	N-CA-C	-5.12	108.30	113.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3271	0	3309	49	0
2	B	3342	0	3397	34	0
3	C	3216	0	3238	19	0
4	D	3241	0	3245	30	0
5	E	2433	0	2419	33	0
6	F	2227	0	2206	35	0
7	G	1687	0	1730	15	0
8	H	1374	0	1360	16	0
9	I	599	0	638	17	0
10	J	2813	0	2890	51	0
11	K	745	0	699	18	0
12	K	3	0	0	0	0
All	All	24951	0	25131	288	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 6.

All (288) 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:C:138:LEU:HB2	3:C:166:MET:HG3	1.69	0.74
11:K:94:CYS:HB3	11:K:97:ASP:OD1	1.91	0.71
10:J:429:LEU:HD21	10:J:446:LEU:HD21	1.74	0.70
10:J:622:VAL:HB	10:J:665:PRO:HA	1.74	0.70
2:B:202:ILE:HD12	2:B:237:ILE:HG22	1.74	0.69
10:J:465:PHE:HA	10:J:468:LYS:HE2	1.74	0.69
1:A:307:GLN:HA	1:A:311:ILE:HB	1.73	0.68
9:I:5:VAL:HG12	9:I:67:LEU:HB2	1.75	0.68
1:A:454:MET:HE2	3:C:390:LEU:HD13	1.74	0.68
5:E:69:ALA:HB1	5:E:172:PRO:HG3	1.78	0.66
6:F:48:ILE:HD12	6:F:165:VAL:HG21	1.78	0.65
10:J:560:GLU:O	10:J:563:TYR:HB3	1.97	0.65
2:B:76:ILE:HG23	2:B:88:MET:HG3	1.78	0.64
10:J:616:THR:HG23	10:J:617:GLU:HG2	1.78	0.64
10:J:664:LYS:HE3	10:J:665:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:HA	1:A:451:LYS:HE2	1.81	0.62
8:H:50:MET:HE2	8:H:50:MET:HA	1.82	0.61
1:A:467:LYS:HE2	1:A:467:LYS:HA	1.83	0.61
9:I:26:ILE:O	9:I:30:VAL:HG23	2.02	0.59
3:C:279:VAL:HG21	3:C:299:LEU:HD21	1.85	0.58
6:F:42:ALA:HB3	6:F:82:GLU:HG3	1.86	0.58
4:D:113:ILE:HA	4:D:116:LYS:HE3	1.86	0.58
1:A:245:ILE:HG13	1:A:246:LEU:HD22	1.86	0.58
1:A:255:LEU:HD11	1:A:357:TYR:HD2	1.69	0.58
5:E:269:LEU:HD11	5:E:307:SER:HA	1.86	0.57
4:D:352:ILE:HG12	4:D:359:VAL:HG13	1.86	0.57
1:A:255:LEU:HD11	1:A:357:TYR:CD2	2.40	0.57
4:D:230:LEU:HD11	4:D:264:LEU:HB2	1.86	0.57
6:F:170:SER:HB2	6:F:181:MET:HE2	1.85	0.56
2:B:408:LEU:HD21	4:D:355:ILE:HG13	1.88	0.56
6:F:189:THR:HG22	6:F:190:LEU:H	1.68	0.56
8:H:111:ASP:HB3	8:H:115:ARG:HH12	1.69	0.56
1:A:386:MET:HG3	1:A:422:LYS:C	2.31	0.56
5:E:103:THR:HG23	5:E:105:THR:H	1.70	0.55
1:A:250:LYS:HE3	1:A:272:LEU:HB2	1.88	0.55
5:E:237:LEU:HD13	6:F:48:ILE:HG22	1.87	0.55
8:H:154:GLN:H	8:H:165:ARG:HH21	1.54	0.55
7:G:17:LEU:HD23	7:G:18:LEU:HD12	1.89	0.55
3:C:190:MET:HE3	3:C:226:LYS:HE3	1.88	0.55
1:A:348:MET:HG2	1:A:352:LEU:HD11	1.88	0.54
4:D:199:ARG:HH12	4:D:293:THR:HG22	1.72	0.54
4:D:278:LEU:HD11	4:D:304:VAL:HG21	1.88	0.54
4:D:12:LEU:HD21	4:D:22:LEU:HD13	1.88	0.54
5:E:159:GLN:NE2	5:E:188:THR:HG22	2.22	0.54
11:K:48:HIS:HB3	11:K:51:ASP:OD1	2.08	0.54
7:G:66:LEU:HD11	7:G:88:LEU:HD21	1.90	0.53
10:J:431:LYS:O	10:J:480:ALA:CB	2.56	0.53
1:A:360:PRO:HG2	1:A:361:HIS:CE1	2.43	0.53
1:A:396:THR:HG23	1:A:399:ALA:H	1.74	0.53
10:J:603:ALA:HB1	10:J:607:GLN:HB2	1.91	0.53
6:F:137:HIS:HA	6:F:140:LYS:HD2	1.90	0.52
10:J:421:LEU:HA	10:J:424:ARG:HG2	1.90	0.52
8:H:101:THR:HG23	8:H:102:VAL:HG23	1.90	0.52
10:J:718:ILE:HD11	10:J:737:GLN:HG3	1.90	0.52
4:D:180:ASN:HB3	4:D:183:LEU:HB2	1.91	0.52
4:D:235:LEU:HD22	4:D:299:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:238:ALA:HA	4:D:242:ARG:HD2	1.91	0.52
10:J:707:ARG:O	10:J:711:ILE:HD12	2.09	0.52
5:E:187:ARG:HG3	5:E:224:LEU:HD11	1.91	0.52
1:A:297:ALA:HA	1:A:301:PHE:CE1	2.44	0.52
9:I:5:VAL:HG22	9:I:13:ILE:HB	1.92	0.51
2:B:106:ASN:HD21	10:J:480:ALA:HA	1.76	0.51
1:A:386:MET:HE2	1:A:400:LEU:HD23	1.93	0.51
9:I:6:LYS:NZ	9:I:66:VAL:HG13	2.25	0.51
1:A:456:ARG:HH21	2:B:443:ALA:HB1	1.76	0.51
6:F:109:GLU:HA	6:F:112:PHE:CD2	2.46	0.50
1:A:298:LEU:HD11	1:A:333:PHE:CG	2.47	0.50
5:E:194:LYS:O	5:E:196:PRO:HD3	2.11	0.50
11:K:65:SER:O	11:K:66:GLU:C	2.55	0.50
8:H:87:PRO:HB3	8:H:135:ALA:HB1	1.94	0.50
4:D:334:LYS:HE2	4:D:338:ILE:HD11	1.92	0.50
5:E:79:GLY:HA2	5:E:98:LEU:HG	1.93	0.50
7:G:122:MET:HE3	7:G:131:LEU:HD22	1.94	0.50
5:E:67:MET:HE1	6:F:46:LEU:HD22	1.93	0.50
7:G:28:THR:HB	7:G:63:TYR:HD2	1.77	0.50
2:B:194:LEU:HD23	2:B:197:ILE:HD11	1.95	0.49
5:E:267:PHE:O	5:E:271:GLU:HG2	2.12	0.49
7:G:123:ARG:HG2	7:G:123:ARG:HH11	1.78	0.49
10:J:735:LEU:HA	10:J:739:SER:HB2	1.94	0.49
10:J:423:ALA:HB2	10:J:462:PHE:HE1	1.77	0.49
10:J:525:LEU:HD11	10:J:531:LEU:HD22	1.94	0.49
11:K:67:GLU:O	11:K:67:GLU:HG2	2.12	0.49
4:D:145:LEU:HD23	4:D:183:LEU:HD23	1.94	0.49
5:E:300:LEU:HD23	6:F:303:ASN:HD22	1.78	0.49
10:J:584:GLN:HG3	10:J:585:LEU:HG	1.94	0.49
1:A:439:SER:HB3	6:F:292:LEU:HD21	1.94	0.48
1:A:282:GLU:CD	1:A:282:GLU:H	2.20	0.48
4:D:52:MET:HG2	4:D:66:LEU:HD13	1.95	0.48
5:E:117:MET:HB3	9:I:8:LEU:HD11	1.93	0.48
1:A:83:GLN:CD	1:A:83:GLN:H	2.21	0.48
2:B:291:ILE:HG13	11:K:95:PRO:HB3	1.94	0.48
1:A:356:MET:HE3	1:A:356:MET:HA	1.95	0.48
6:F:73:ILE:HG22	6:F:119:LEU:HD23	1.96	0.48
10:J:755:ILE:HD11	10:J:759:LYS:HZ3	1.78	0.48
4:D:114:TYR:HB3	4:D:123:ALA:HB2	1.96	0.48
5:E:259:ALA:O	5:E:263:THR:HG23	2.14	0.48
5:E:318:LEU:HD22	6:F:286:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:154:GLN:H	8:H:165:ARG:NH2	2.10	0.48
1:A:453:MET:HB2	2:B:439:VAL:HG13	1.94	0.48
9:I:22:LYS:HD2	9:I:23:VAL:N	2.29	0.48
4:D:107:ARG:HD3	4:D:130:ILE:HG13	1.96	0.48
6:F:109:GLU:HA	6:F:112:PHE:HD2	1.79	0.48
1:A:439:SER:HB2	6:F:288:LEU:HD11	1.96	0.48
2:B:84:ASN:OD1	2:B:87:GLU:HB2	2.14	0.48
7:G:124:ASN:HB3	7:G:127:GLU:HG2	1.94	0.48
9:I:22:LYS:HD2	9:I:23:VAL:H	1.78	0.48
10:J:607:GLN:HG2	10:J:639:VAL:HG13	1.96	0.48
6:F:71:ALA:HB1	6:F:121:PHE:HE1	1.79	0.47
5:E:228:TYR:HB2	6:F:206:MET:HE3	1.95	0.47
2:B:158:LEU:O	2:B:162:ARG:HG3	2.14	0.47
3:C:249:VAL:HA	3:C:253:ILE:HB	1.95	0.47
4:D:124:ALA:O	4:D:128:VAL:HG23	2.15	0.47
4:D:396:THR:O	4:D:400:MET:HG3	2.14	0.47
10:J:719:MET:HB3	10:J:774:TYR:HB2	1.96	0.47
5:E:121:ILE:HD12	9:I:8:LEU:HD22	1.96	0.47
5:E:238:LEU:HD22	6:F:204:ALA:HB2	1.96	0.47
10:J:555:LEU:HD21	10:J:560:GLU:HA	1.97	0.47
11:K:72:TRP:HB2	11:K:105:LYS:HB3	1.97	0.47
7:G:14:GLN:O	7:G:18:LEU:HD13	2.15	0.47
8:H:50:MET:HG3	8:H:82:TRP:HE3	1.80	0.47
10:J:427:ASP:O	10:J:428:SER:C	2.54	0.47
11:K:49:ILE:HG22	11:K:50:MET:SD	2.54	0.47
1:A:408:ILE:HB	3:C:313:THR:HG23	1.95	0.47
6:F:154:LEU:HD12	6:F:165:VAL:HG22	1.95	0.47
2:B:82:LEU:HG	2:B:82:LEU:O	2.14	0.47
10:J:531:LEU:HD11	10:J:565:ARG:HG3	1.95	0.47
1:A:54:LEU:HA	1:A:81:PHE:HZ	1.79	0.47
6:F:109:GLU:HG3	6:F:112:PHE:HE2	1.80	0.47
11:K:88:LEU:HD11	11:K:101:TRP:CD1	2.50	0.47
5:E:265:GLN:O	5:E:269:LEU:HB2	2.15	0.47
7:G:129:GLU:HG2	7:G:145:LEU:HD22	1.97	0.47
1:A:310:VAL:HG11	1:A:330:ILE:HD13	1.97	0.46
7:G:163:ARG:HG3	7:G:165:LYS:HG2	1.96	0.46
10:J:423:ALA:HB2	10:J:462:PHE:CE1	2.50	0.46
7:G:117:LEU:HD23	7:G:122:MET:HB2	1.96	0.46
1:A:81:PHE:HE1	1:A:85:THR:HG21	1.79	0.46
3:C:402:GLN:H	3:C:402:GLN:HG2	1.60	0.46
8:H:26:GLU:O	8:H:26:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:44:ILE:HB	9:I:68:HIS:HB2	1.97	0.46
1:A:417:VAL:HG22	1:A:424:LEU:HD13	1.98	0.46
6:F:155:ASN:HB3	6:F:164:PRO:HB3	1.96	0.46
10:J:426:CYS:O	10:J:429:LEU:HD23	2.16	0.46
10:J:528:SER:HB3	10:J:565:ARG:HH22	1.79	0.46
10:J:638:GLN:O	10:J:642:ILE:HG22	2.15	0.46
10:J:762:LEU:HD13	10:J:772:TYR:HB3	1.98	0.46
4:D:73:LEU:N	4:D:74:PRO:HD2	2.30	0.46
4:D:271:ARG:HB2	4:D:271:ARG:HH11	1.81	0.46
10:J:431:LYS:O	10:J:432:LYS:HB2	2.15	0.46
2:B:331:LYS:HB3	2:B:331:LYS:HE2	1.71	0.45
6:F:133:PRO:O	6:F:136:ILE:HG22	2.16	0.45
1:A:323:GLU:HB3	1:A:326:VAL:HG12	1.98	0.45
10:J:435:LYS:HE2	10:J:435:LYS:HB3	1.75	0.45
2:B:54:PHE:HA	2:B:57:VAL:HG23	1.98	0.45
2:B:350:LEU:C	2:B:352:ARG:H	2.25	0.45
10:J:751:LYS:O	10:J:755:ILE:HG22	2.16	0.45
3:C:133:MET:HE3	3:C:133:MET:HA	1.99	0.45
4:D:404:MET:N	4:D:404:MET:HE2	2.31	0.45
6:F:230:MET:HE3	6:F:230:MET:HB2	1.92	0.45
6:F:81:ILE:HG23	6:F:122:LEU:HD13	1.97	0.45
11:K:62:SER:C	11:K:64:THR:H	2.22	0.45
1:A:205:VAL:HG13	1:A:206:ILE:HD13	1.99	0.45
2:B:291:ILE:HD12	11:K:43:ALA:O	2.17	0.45
4:D:301:ASP:HA	4:D:304:VAL:HG12	1.97	0.45
1:A:297:ALA:HA	1:A:301:PHE:CD1	2.51	0.45
2:B:104:THR:HG21	10:J:432:LYS:HE2	1.99	0.45
8:H:74:ILE:HD13	8:H:106:MET:HE2	1.99	0.45
1:A:272:LEU:HD12	1:A:272:LEU:H	1.82	0.45
4:D:202:ILE:HG12	4:D:241:GLN:HG3	1.99	0.45
5:E:255:LEU:HD11	5:E:317:GLY:C	2.42	0.45
6:F:160:HIS:CE1	6:F:162:ASP:HB3	2.52	0.45
11:K:62:SER:O	11:K:64:THR:N	2.44	0.44
3:C:390:LEU:HD21	6:F:302:MET:HA	1.99	0.44
5:E:28:ILE:HD11	5:E:91:ILE:HG12	1.99	0.44
5:E:210:LYS:HA	5:E:210:LYS:HD3	1.85	0.44
9:I:54:LYS:HD3	9:I:55:THR:N	2.32	0.44
1:A:165:HIS:HA	1:A:168:LEU:HD23	1.99	0.44
1:A:404:LEU:HD13	1:A:424:LEU:HD22	1.98	0.44
6:F:210:GLY:HA3	6:F:219:GLU:HG3	1.98	0.44
10:J:498:PHE:HD1	10:J:498:PHE:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:51:ILE:HG12	6:F:125:TYR:CE1	2.52	0.44
3:C:62:LEU:HD12	3:C:63:PHE:CD1	2.53	0.44
8:H:41:LEU:HD13	8:H:56:LEU:HD22	1.99	0.44
2:B:169:GLN:CD	2:B:169:GLN:H	2.26	0.44
2:B:66:GLU:OE1	2:B:66:GLU:N	2.50	0.44
10:J:498:PHE:CD1	10:J:498:PHE:C	2.96	0.44
6:F:282:GLN:O	6:F:286:VAL:HG23	2.18	0.44
9:I:1:MET:HE3	9:I:2:LEU:H	1.83	0.44
10:J:657:ASN:O	10:J:661:VAL:HG23	2.17	0.44
5:E:159:GLN:HE22	5:E:188:THR:H	1.66	0.43
2:B:212:LYS:HE2	2:B:212:LYS:HA	2.00	0.43
10:J:534:ASP:HB2	11:K:26:LYS:HG2	1.99	0.43
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.86	0.43
2:B:54:PHE:O	2:B:58:LEU:HG	2.18	0.43
3:C:30:LYS:HB3	3:C:30:LYS:HE3	1.87	0.43
4:D:343:ILE:HG22	4:D:344:THR:H	1.84	0.43
8:H:208:GLU:HG3	8:H:209:ASN:ND2	2.33	0.43
10:J:596:LYS:NZ	10:J:674:GLY:HA2	2.33	0.43
11:K:25:LYS:HE3	11:K:25:LYS:HB3	1.71	0.43
4:D:59:LEU:HD21	4:D:95:ARG:NH2	2.33	0.43
1:A:301:PHE:HB3	1:A:305:GLU:HB2	2.00	0.43
1:A:352:LEU:HD22	1:A:358:LEU:HD23	2.00	0.43
10:J:574:HIS:HB3	10:J:577:ARG:HD2	2.01	0.43
2:B:77:LYS:HE2	2:B:77:LYS:HB2	1.73	0.43
2:B:351:LEU:HD23	2:B:351:LEU:HA	1.81	0.43
11:K:45:CYS:SG	11:K:47:ASN:HB2	2.58	0.43
11:K:63:ALA:C	11:K:65:SER:N	2.74	0.43
1:A:329:ILE:HD12	1:A:345:LEU:HG	2.00	0.43
5:E:254:SER:C	5:E:255:LEU:HD12	2.43	0.43
8:H:40:LEU:HD12	8:H:40:LEU:HA	1.86	0.43
9:I:18:GLU:HG2	9:I:19:PRO:HD2	2.01	0.43
2:B:81:LYS:HD2	2:B:81:LYS:HA	1.71	0.43
2:B:136:LEU:HD23	2:B:136:LEU:HA	1.81	0.43
10:J:589:GLU:HG3	10:J:602:GLN:HG2	2.01	0.43
1:A:380:PRO:HG2	2:B:390:VAL:HG13	2.00	0.42
10:J:431:LYS:O	10:J:480:ALA:HB3	2.18	0.42
3:C:293:GLY:O	3:C:297:GLN:HG3	2.19	0.42
5:E:159:GLN:HE21	5:E:188:THR:HG22	1.83	0.42
1:A:349:LYS:HB2	1:A:366:TYR:CE2	2.54	0.42
2:B:238:ARG:HE	2:B:260:GLU:HG2	1.85	0.42
2:B:287:MET:O	2:B:288:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:271:ARG:HH21	7:G:137:TYR:HB3	1.84	0.42
5:E:332:ASN:HB3	6:F:268:PRO:HG3	2.02	0.42
1:A:267:ALA:HB2	1:A:296:CYS:HB2	2.01	0.42
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.92	0.42
8:H:31:ILE:HD13	8:H:61:PRO:HG2	2.02	0.42
3:C:68:MET:HA	3:C:68:MET:HE2	2.02	0.42
10:J:424:ARG:HG3	10:J:425:TYR:N	2.33	0.42
1:A:44:LEU:HD12	1:A:44:LEU:H	1.84	0.42
4:D:325:GLY:HA3	4:D:331:PRO:O	2.19	0.42
1:A:270:LEU:HD21	1:A:289:VAL:HG13	2.02	0.42
1:A:405:THR:HA	3:C:313:THR:HG21	2.01	0.42
2:B:363:ILE:HD12	2:B:411:LEU:HD11	2.01	0.42
5:E:54:TYR:HB2	5:E:89:THR:HG23	2.01	0.42
10:J:590:LEU:HD21	11:K:22:PHE:CD2	2.55	0.42
6:F:118:GLU:O	6:F:119:LEU:HD12	2.20	0.42
10:J:421:LEU:HA	10:J:421:LEU:HD12	1.74	0.42
10:J:498:PHE:HD1	10:J:498:PHE:C	2.28	0.42
3:C:306:ASN:HB3	3:C:326:VAL:HG12	2.01	0.42
5:E:152:VAL:HG12	5:E:156:MET:HE3	2.02	0.42
5:E:312:ILE:HG12	8:H:204:VAL:HG13	2.02	0.42
9:I:48:LYS:HD2	9:I:48:LYS:HA	1.89	0.42
11:K:67:GLU:O	11:K:69:THR:N	2.47	0.41
9:I:25:ARG:HH21	9:I:29:ARG:NH1	2.19	0.41
2:B:435:ASN:O	2:B:439:VAL:HG23	2.19	0.41
3:C:341:MET:HE3	3:C:341:MET:HB3	1.85	0.41
6:F:194:GLU:H	6:F:194:GLU:HG2	1.66	0.41
9:I:60:LYS:HD2	9:I:60:LYS:HA	1.87	0.41
11:K:65:SER:C	11:K:67:GLU:N	2.74	0.41
5:E:80:LEU:HB2	5:E:96:PHE:CE2	2.55	0.41
1:A:58:GLU:HA	1:A:61:GLN:HG2	2.01	0.41
6:F:109:GLU:HG3	6:F:112:PHE:CE2	2.56	0.41
8:H:25:LEU:HD23	8:H:25:LEU:HA	1.93	0.41
9:I:6:LYS:HZ2	9:I:66:VAL:HG13	1.85	0.41
2:B:159:TYR:CE2	2:B:167:LYS:HG3	2.55	0.41
2:B:361:LYS:HB3	2:B:361:LYS:HE2	1.79	0.41
3:C:350:SER:HB3	8:H:126:THR:HG23	2.03	0.41
4:D:263:ILE:O	4:D:267:MET:HG3	2.20	0.41
5:E:163:GLU:HB2	5:E:164:PRO:HD3	2.03	0.41
5:E:254:SER:C	5:E:256:LEU:H	2.29	0.41
10:J:428:SER:O	10:J:429:LEU:C	2.62	0.41
1:A:214:ASN:HB2	1:A:217:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:397:ALA:O	4:D:401:GLU:HG2	2.21	0.41
10:J:708:LYS:HG3	10:J:752:CYS:SG	2.61	0.41
1:A:371:ASN:O	1:A:375:ILE:HG13	2.21	0.41
6:F:70:GLY:HA3	6:F:125:TYR:CE2	2.56	0.41
6:F:189:THR:HG22	6:F:190:LEU:N	2.35	0.41
5:E:255:LEU:HD13	6:F:282:GLN:NE2	2.36	0.41
1:A:329:ILE:HD13	1:A:329:ILE:HA	1.91	0.40
2:B:411:LEU:HD13	2:B:411:LEU:HA	1.91	0.40
4:D:12:LEU:O	4:D:12:LEU:HD23	2.21	0.40
7:G:55:LEU:HD23	7:G:55:LEU:HA	1.89	0.40
7:G:221:LYS:HD3	7:G:221:LYS:HA	1.91	0.40
10:J:419:PRO:HB2	10:J:465:PHE:HZ	1.86	0.40
2:B:69:PHE:HD2	2:B:103:VAL:HG11	1.86	0.40
7:G:30:LEU:HD12	7:G:30:LEU:HA	1.86	0.40
10:J:529:GLU:HA	10:J:530:PRO:HD3	1.98	0.40
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.89	0.40
3:C:252:PHE:O	3:C:256:LEU:HD12	2.21	0.40
5:E:147:LEU:HB2	5:E:221:TYR:CZ	2.57	0.40
7:G:165:LYS:HG3	7:G:166:ASP:OD1	2.21	0.40
9:I:21:ASP:OD1	9:I:21:ASP:N	2.54	0.40
10:J:746:VAL:N	10:J:747:PRO:HD2	2.36	0.40
3:C:348:PHE:CZ	3:C:364:PRO:HB3	2.56	0.40
4:D:78:ASP:HA	4:D:81:ALA:HB3	2.03	0.40
10:J:651:LEU:HD12	10:J:651:LEU:HA	1.90	0.40
2:B:158:LEU:HA	2:B:161:GLU:OE2	2.22	0.40
10:J:578:LYS:HB3	10:J:578:LYS:HE2	1.79	0.40
10:J:605:THR:HA	10:J:608:MET:HE3	2.04	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	405/491 (82%)	392 (97%)	13 (3%)	0	100	100
2	B	404/443 (91%)	372 (92%)	30 (7%)	2 (0%)	25	57
3	C	402/423 (95%)	364 (90%)	37 (9%)	1 (0%)	44	72
4	D	403/406 (99%)	386 (96%)	17 (4%)	0	100	100
5	E	300/334 (90%)	283 (94%)	17 (6%)	0	100	100
6	F	278/327 (85%)	267 (96%)	11 (4%)	0	100	100
7	G	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
8	H	168/209 (80%)	165 (98%)	3 (2%)	0	100	100
9	I	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
10	J	341/776 (44%)	328 (96%)	12 (4%)	1 (0%)	37	66
11	K	88/108 (82%)	75 (85%)	12 (14%)	1 (1%)	12	40
All	All	3074/3862 (80%)	2905 (94%)	164 (5%)	5 (0%)	45	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	51	VAL
10	J	431	LYS
2	B	270	SER
11	K	67	GLU
2	B	291	ILE

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	356/429 (83%)	352 (99%)	4 (1%)	70	84
2	B	371/405 (92%)	367 (99%)	4 (1%)	70	84
3	C	361/377 (96%)	359 (99%)	2 (1%)	84	91
4	D	346/347 (100%)	346 (100%)	0	100	100
5	E	261/282 (93%)	261 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	248/276 (90%)	244 (98%)	4 (2%)	58	77
7	G	185/229 (81%)	184 (100%)	1 (0%)	86	92
8	H	143/173 (83%)	142 (99%)	1 (1%)	81	90
9	I	66/69 (96%)	66 (100%)	0	100	100
10	J	318/698 (46%)	307 (96%)	11 (4%)	31	59
11	K	79/90 (88%)	77 (98%)	2 (2%)	42	67
All	All	2734/3375 (81%)	2705 (99%)	29 (1%)	69	84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	214	ASN
1	A	277	HIS
1	A	465	HIS
2	B	82	LEU
2	B	89	MET
2	B	308	ILE
2	B	426	LYS
3	C	38	ASN
3	C	300	SER
6	F	136	ILE
6	F	154	LEU
6	F	230	MET
6	F	237	LEU
7	G	161	ASP
8	H	139	LEU
10	J	417	LYS
10	J	421	LEU
10	J	422	LEU
10	J	426	CYS
10	J	427	ASP
10	J	429	LEU
10	J	431	LYS
10	J	465	PHE
10	J	531	LEU
10	J	681	ARG
10	J	711	ILE
11	K	60	GLN
11	K	67	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	151	ASN
1	A	351	ASN
1	A	368	GLN
2	B	94	GLN
2	B	169	GLN
2	B	208	GLN
2	B	319	GLN
2	B	333	ASN
2	B	336	ASN
2	B	391	GLN
3	C	132	GLN
3	C	180	HIS
3	C	400	ASN
4	D	184	GLN
5	E	10	GLN
5	E	17	ASN
5	E	126	GLN
5	E	151	ASN
5	E	158	ASN
5	E	159	GLN
5	E	162	GLN
5	E	321	GLN
5	E	329	ASN
6	F	111	GLN
6	F	282	GLN
6	F	300	ASN
7	G	10	ASN
7	G	33	GLN
7	G	168	ASN
8	H	51	ASN
8	H	103	GLN
8	H	209	ASN
10	J	624	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.

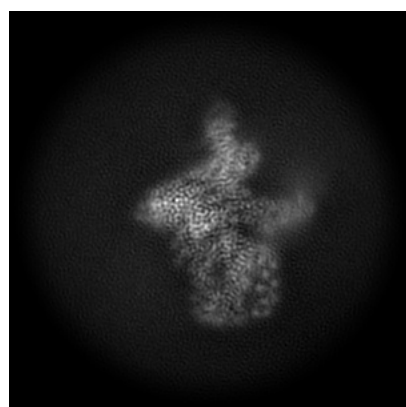
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47976. These allow visual inspection of the internal detail of the map and identification of artifacts.

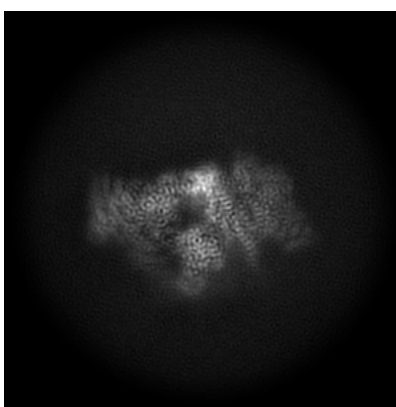
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

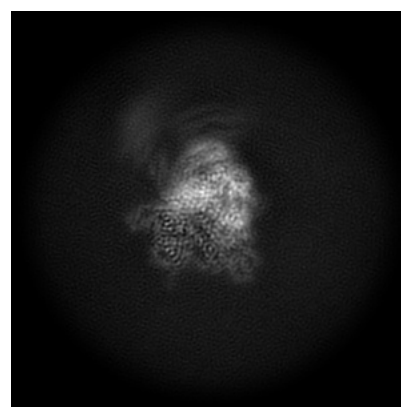
6.1.1 Primary map



X



Y

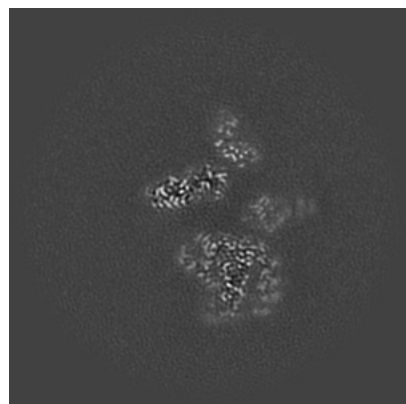


Z

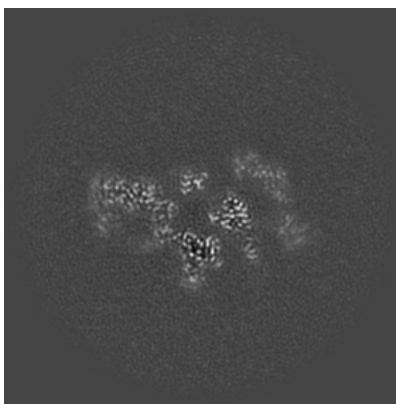
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

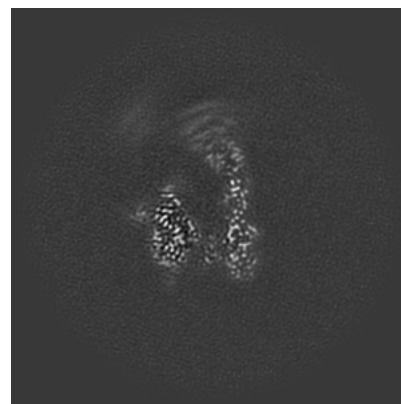
6.2.1 Primary map



X Index: 200



Y Index: 200

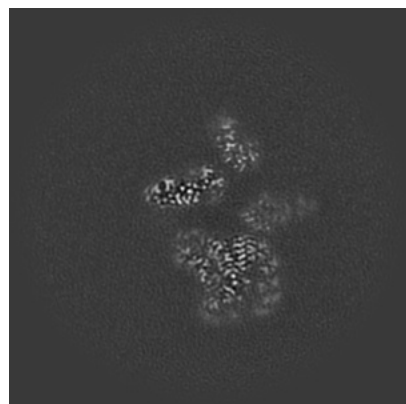


Z Index: 200

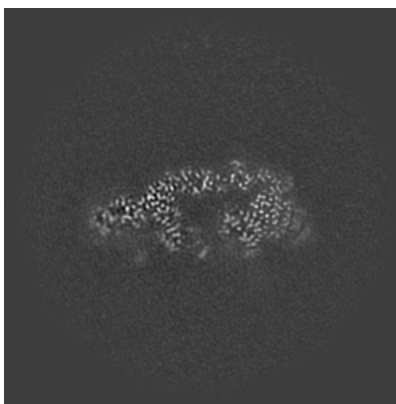
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

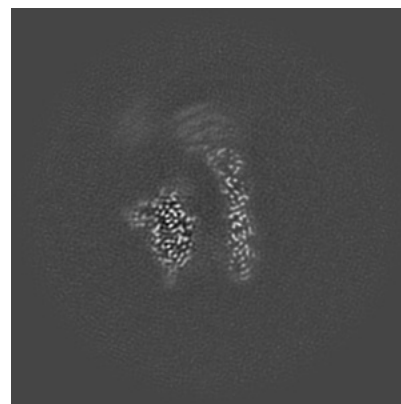
6.3.1 Primary map



X Index: 204



Y Index: 218

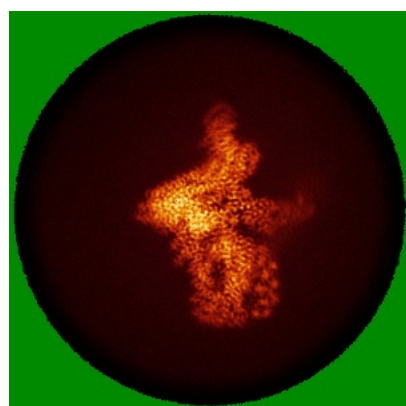


Z Index: 195

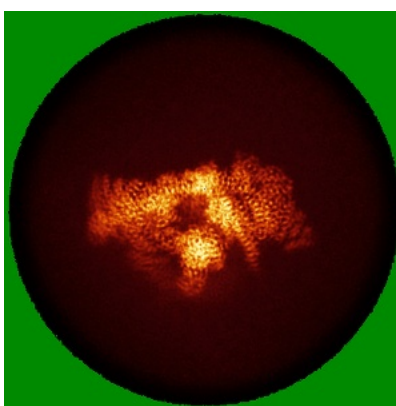
The images above show the largest variance slices of the map in three orthogonal directions.

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

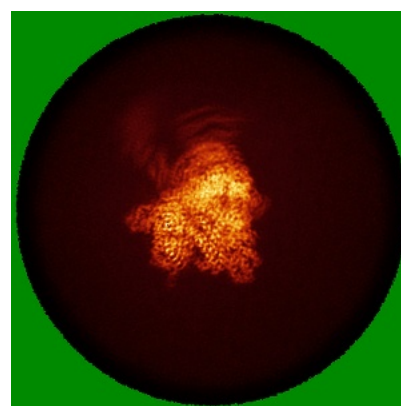
6.4.1 Primary map



X



Y

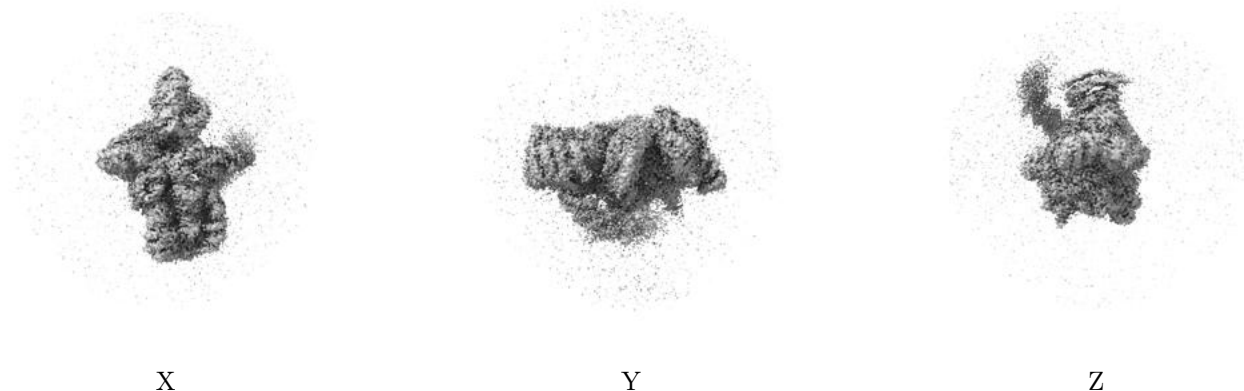


Z

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

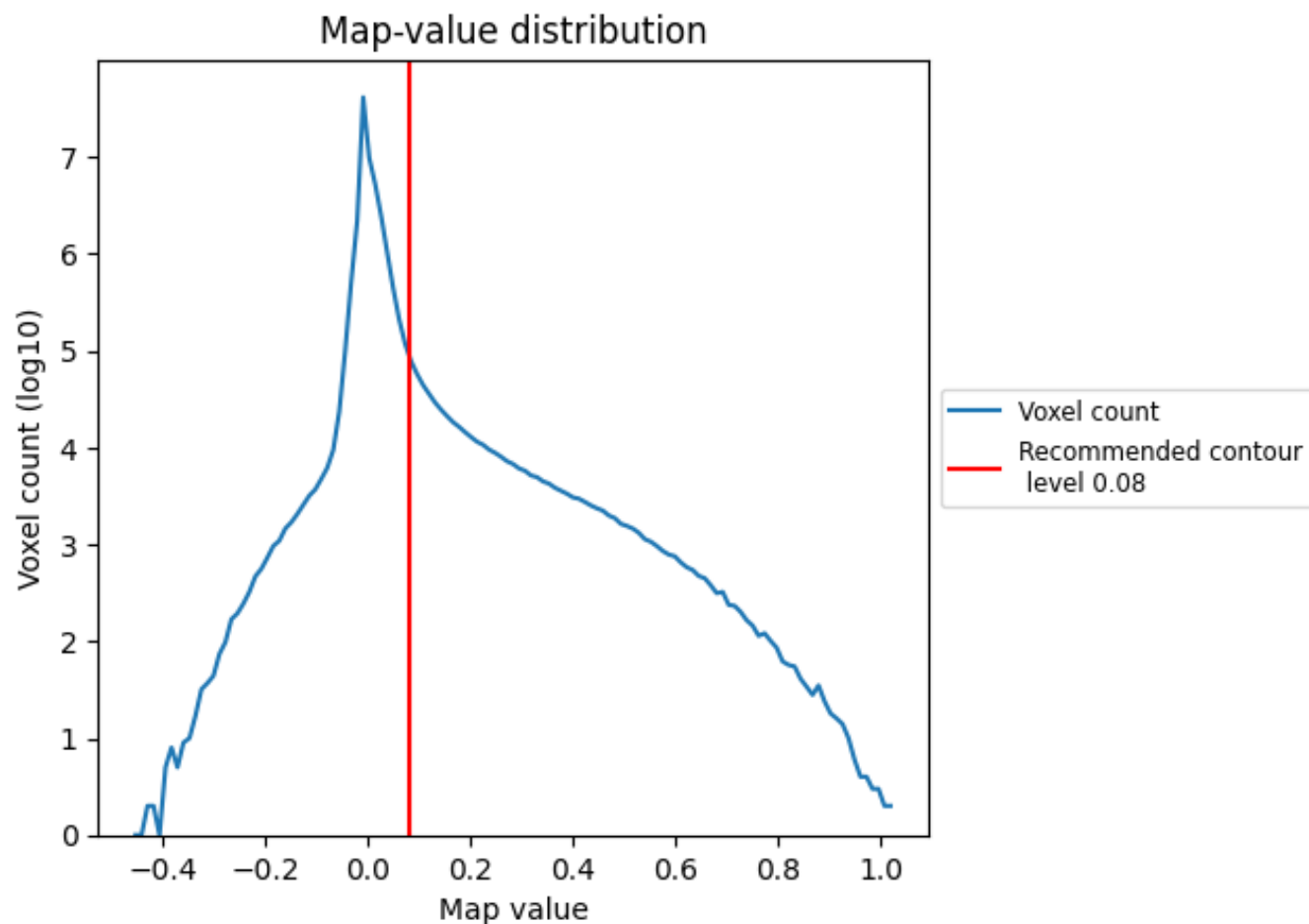
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

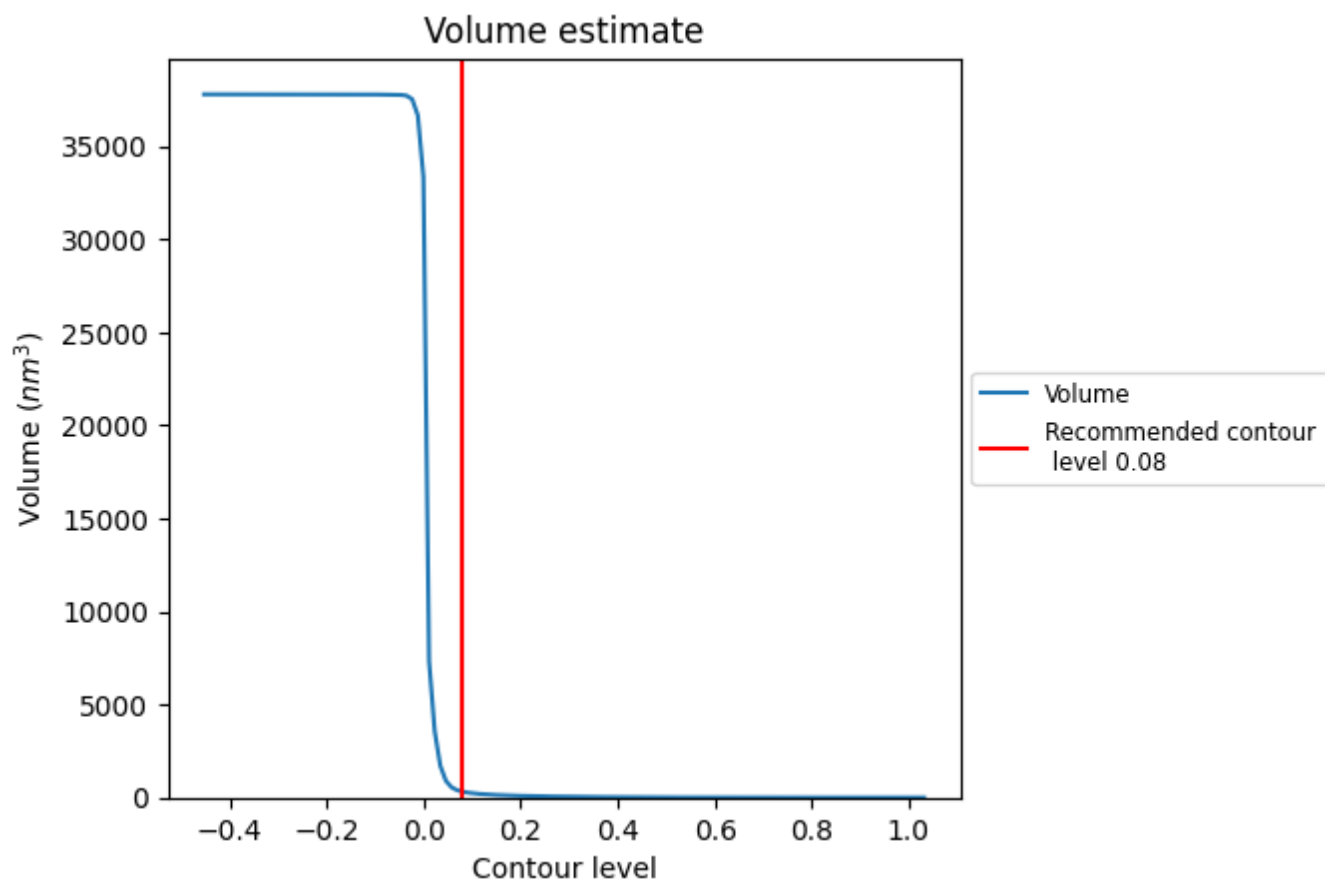
This section contains the results of statistical analysis of the map.

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.

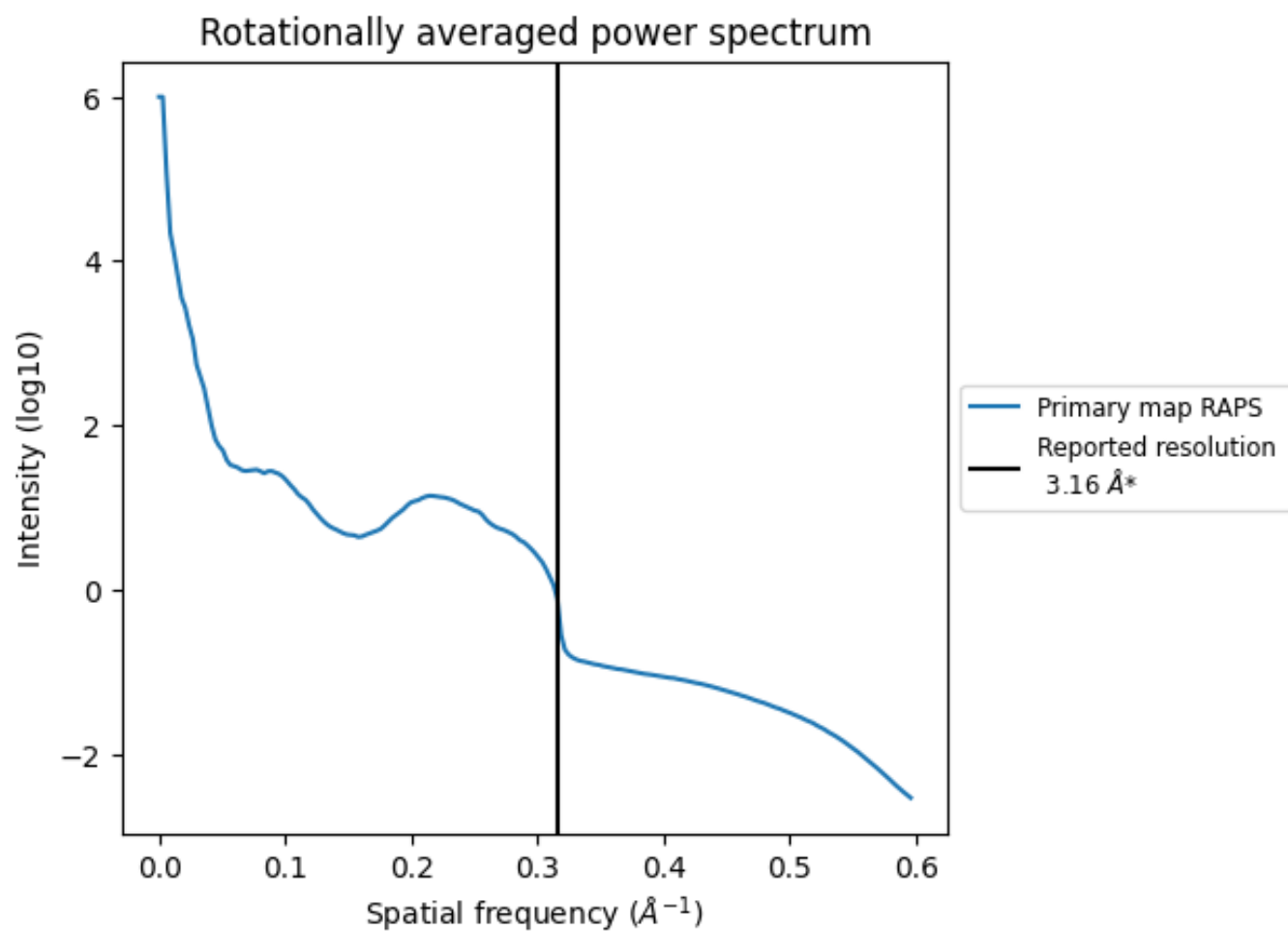
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm³; this corresponds to an approximate mass of 287 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 0.316 Å⁻¹

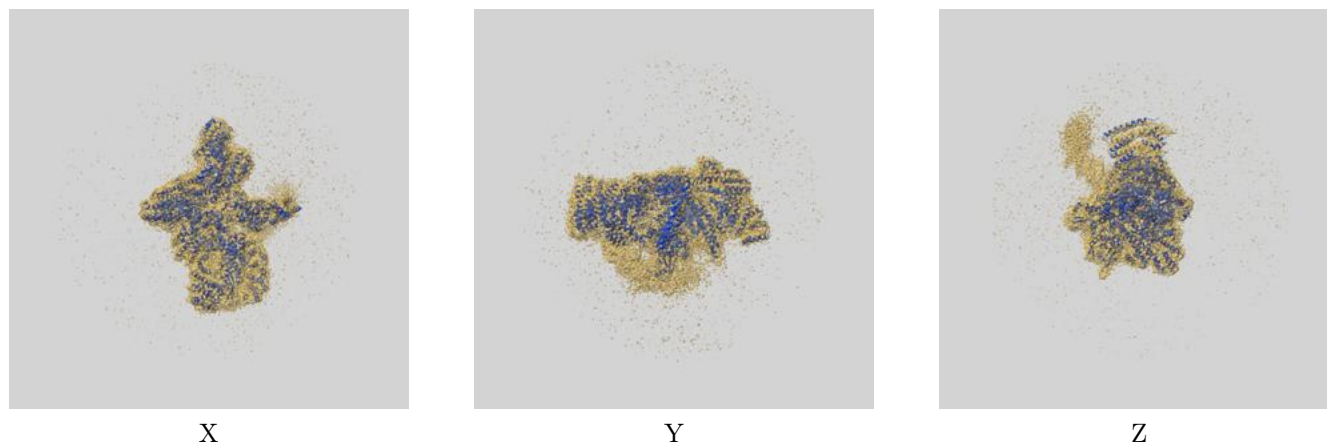
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

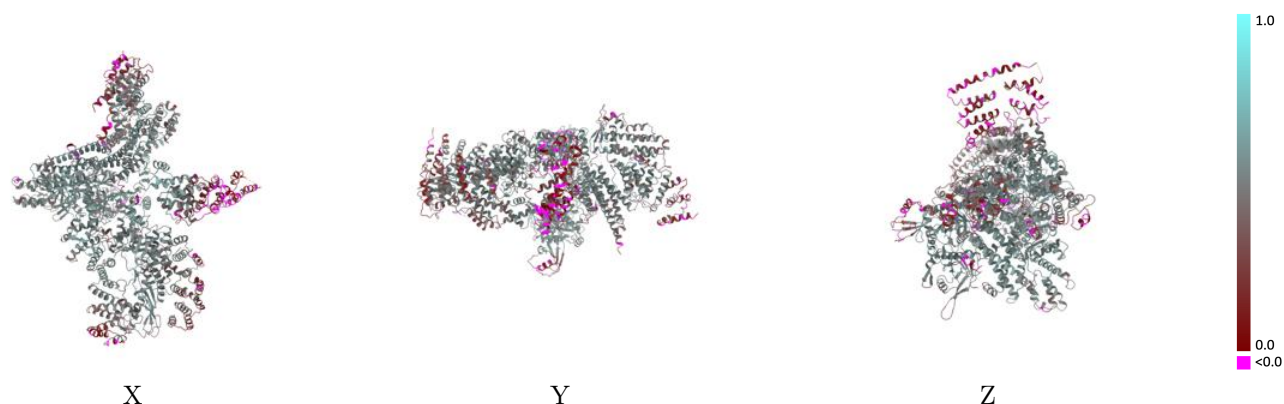
This section contains information regarding the fit between EMDB map EMD-47976 and PDB model 9EFM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



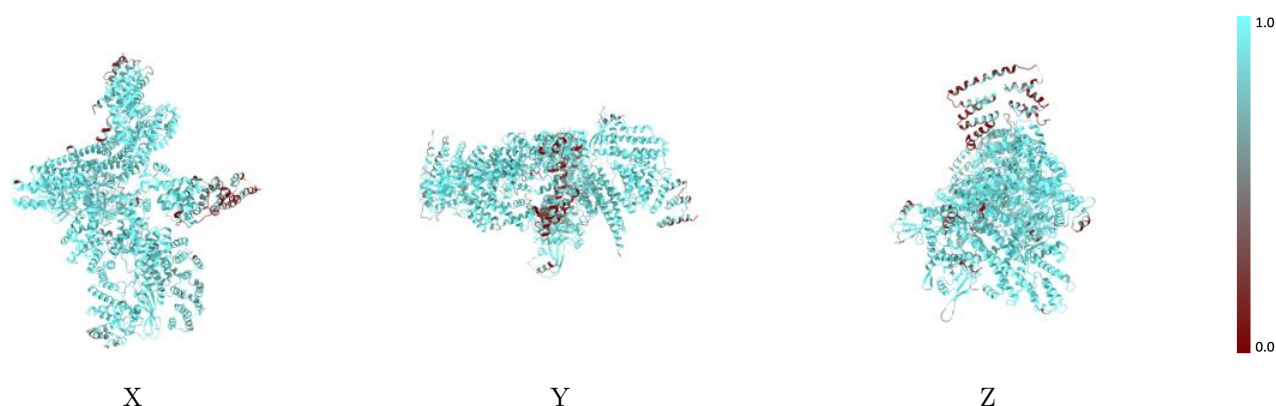
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



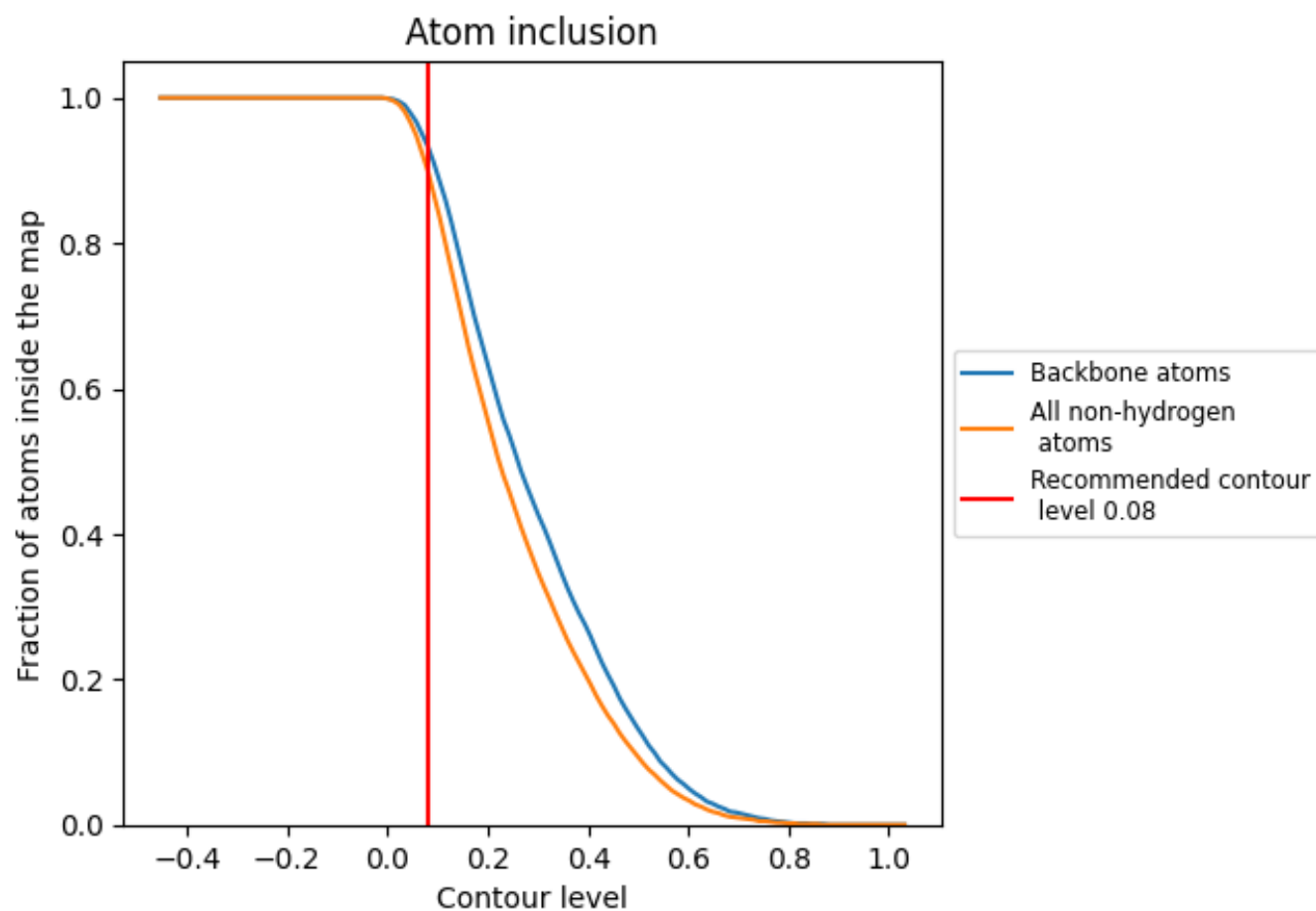
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

























9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.4500
A	 0.6980	 0.3130
B	 0.9300	 0.4480
C	 0.9060	 0.4460
D	 0.9440	 0.4810
E	 0.9370	 0.5120
F	 0.9590	 0.5180
G	 0.9660	 0.5120
H	 0.8860	 0.4090
I	 0.8390	 0.3280
J	 0.9370	 0.4660
K	 0.9430	 0.5100

