



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 07:47 PM EDT

PDB ID : 9ZOH / pdb_00009zoh
EMDB ID : EMD-74496
Title : Cryo-EM structure of the complete *Sulfolobus acidocaldarius* RNA polymerase in open clamp conformation
Authors : Fordjour, G.N.R.; Armache, J.-P.; Murakami, K.S.
Deposited on : 2025-12-15
Resolution : 3.87 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:

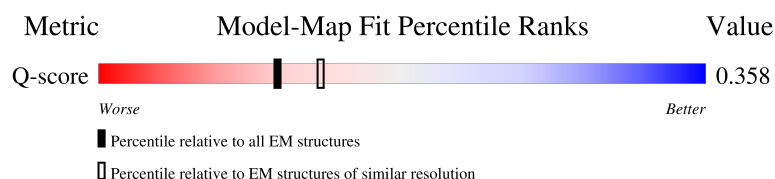
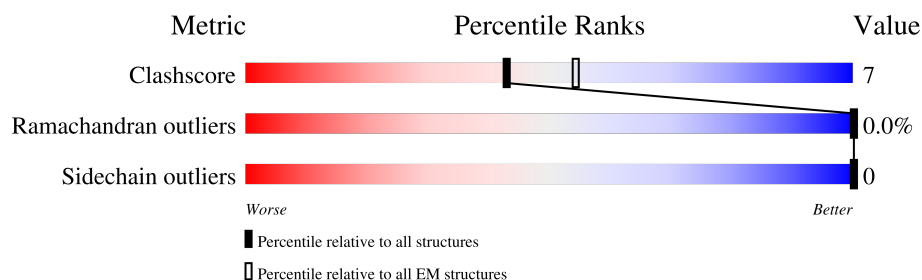
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.87 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	8831 (3.37 - 4.37)

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	880	 84% 15%
2	B	1126	 84% 15%
3	C	393	 13% 79% 17%
4	E	183	 11% 74% 21%

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Mol	Chain	Length	Quality of chain
5	G	124	
6	H	84	
7	K	89	
8	L	90	
9	N	66	
10	Y	105	
11	D	264	
12	P	48	
13	F	114	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 27273 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 Rpo1N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	874	Total	C	N	O	S	0	0
			6982	4443	1230	1279	30		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit Rpo2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1109	Total	C	N	O	S	0	0
			8725	5531	1533	1628	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ILE	VAL	conflict	UNP P11513

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit Rpo1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	377	Total	C	N	O	S	0	0
			2954	1856	508	577	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit Rpo7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	178	Total	C	N	O	S	0	0
			1405	901	236	262	6		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit Rpo8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	122	Total	C	N	O	S	0	0
			991	637	155	190	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP Q4JAY4
G	2	LYS	-	expression tag	UNP Q4JAY4
G	3	GLU	-	expression tag	UNP Q4JAY4

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit Rpo5.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	78	Total	C	N	O	0	0
			617	399	104	114		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit Rpo6.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	86	Total	C	N	O	S	0
			690	441	120	127	2	0

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit Rpo11.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	90	Total	C	N	O	S	0
			707	459	112	134	2	0

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit Rpo10.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	66	Total	C	N	O	S	0
			534	339	97	91	7	0

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit Rpo13.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	44	Total	C	N	O	S	0
			357	226	57	72	2	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit Rpo3.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	D	261	Total	C	N	O	S	0
			2066	1318	342	392	14	0

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit Rpo12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	47	Total	C	N	O	S	0	0
			376	241	67	63	5		

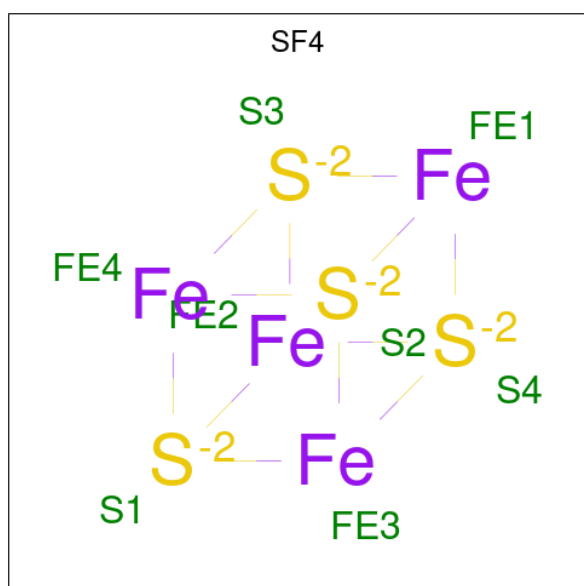
- Molecule 13 is a protein called DNA-directed RNA polymerase subunit Rpo4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	109	Total	C	N	O	S	0	0
			856	543	136	174	3		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	A	2	Total	Zn	0
			2	2	
14	B	1	Total	Zn	0
			1	1	
14	N	1	Total	Zn	0
			1	1	
14	P	1	Total	Zn	0
			1	1	

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

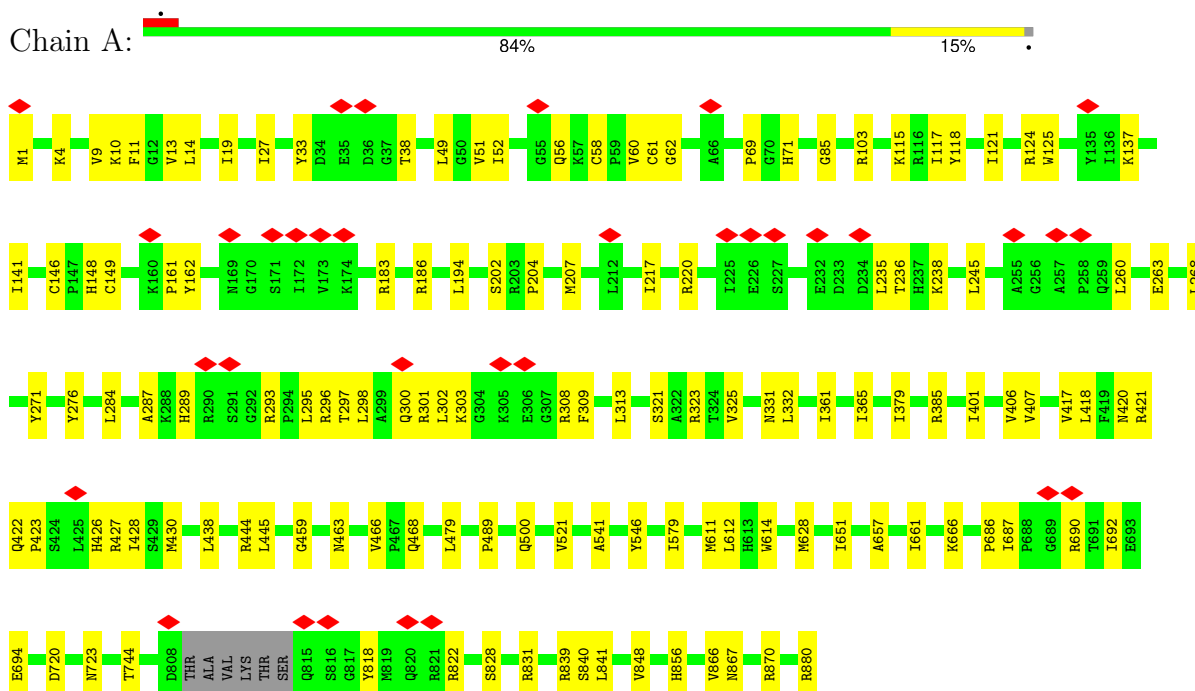


Mol	Chain	Residues	Atoms			AltConf
15	D	1	Total	Fe	S	0
			8	4	4	

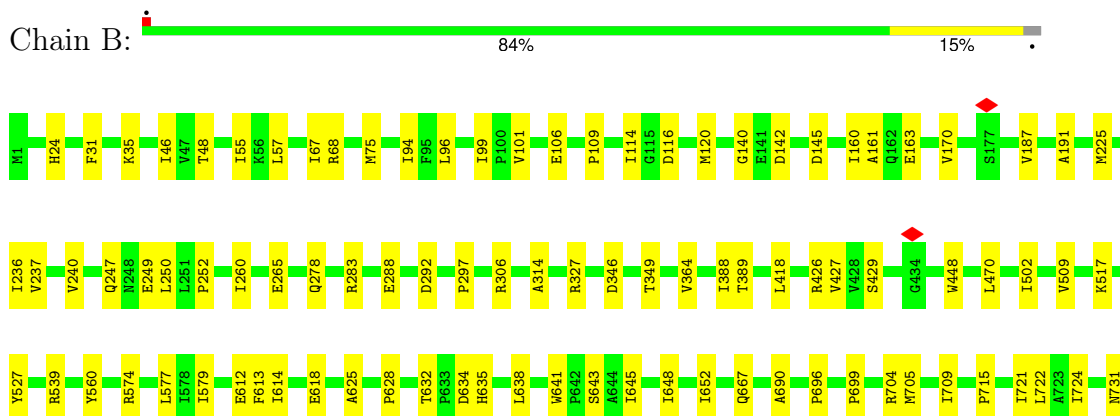
3 Residue-property plots

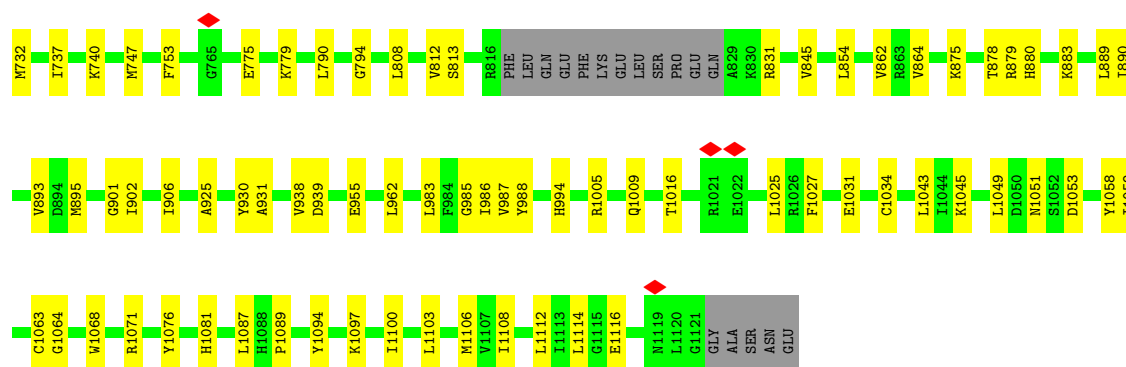
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 Rpo1N

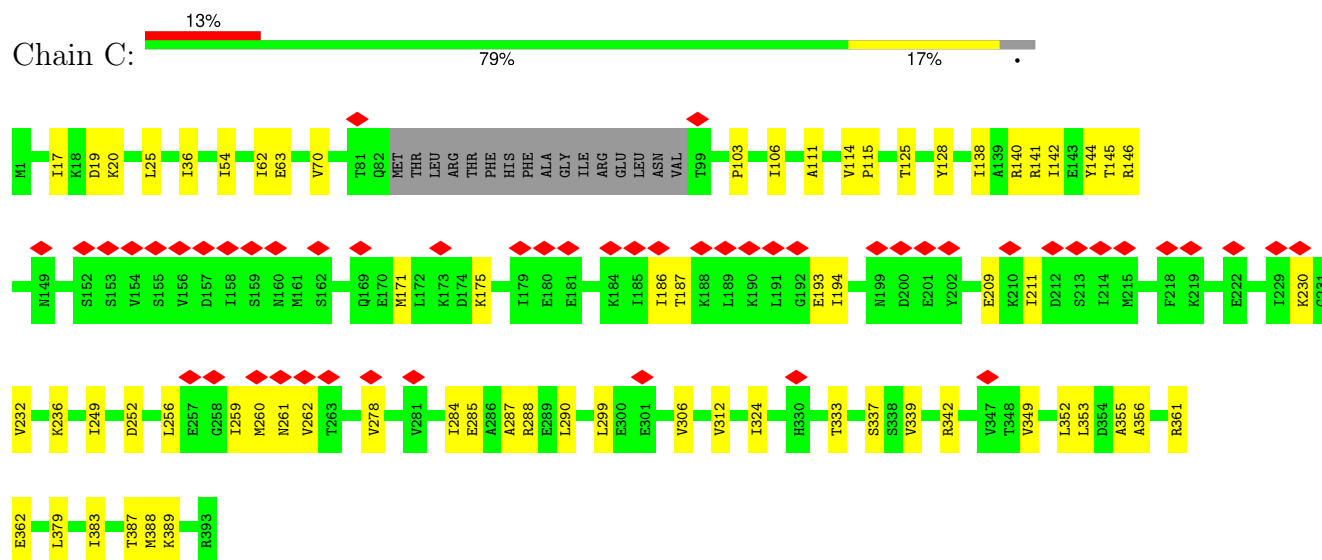


• Molecule 2: DNA-directed RNA polymerase subunit Rpo2

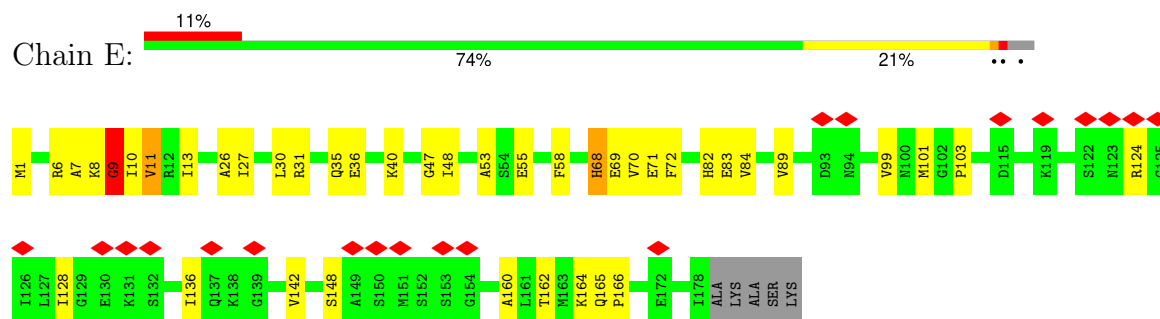




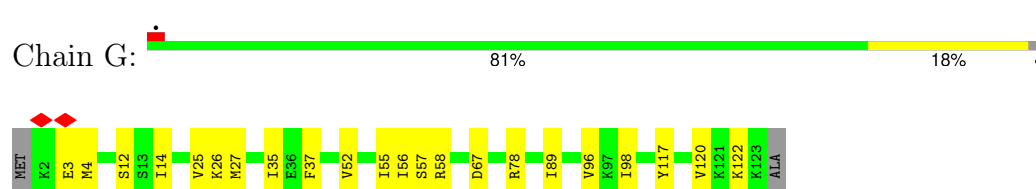
• Molecule 3: DNA-directed RNA polymerase subunit Rpo1C



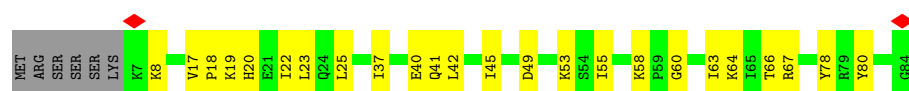
• Molecule 4: DNA-directed RNA polymerase subunit Rpo7



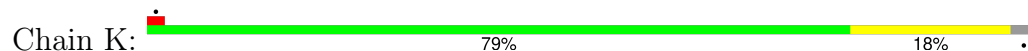
• Molecule 5: DNA-directed RNA polymerase subunit Rpo8



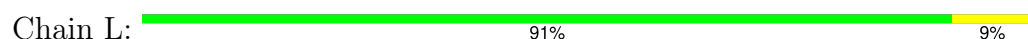
• Molecule 6: DNA-directed RNA polymerase subunit Rpo5



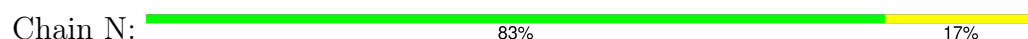
- Molecule 7: DNA-directed RNA polymerase subunit Rpo6



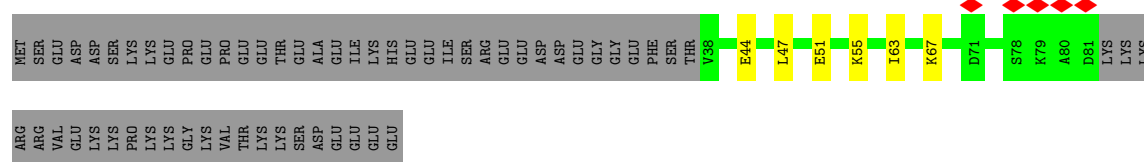
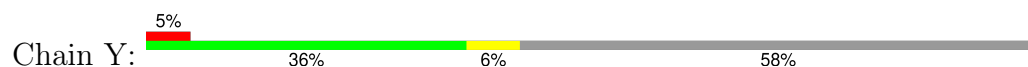
- Molecule 8: DNA-directed RNA polymerase subunit Rpo11



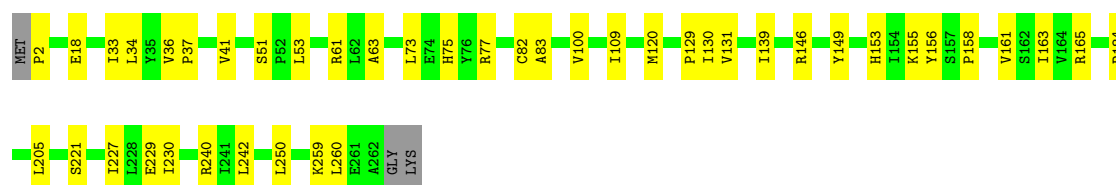
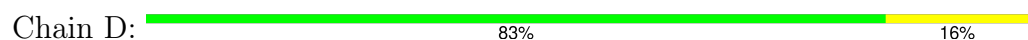
- Molecule 9: DNA-directed RNA polymerase subunit Rpo10



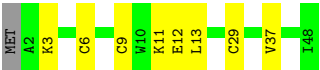
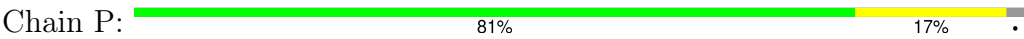
- Molecule 10: DNA-directed RNA polymerase subunit Rpo13



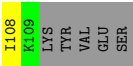
- Molecule 11: DNA-directed RNA polymerase subunit Rpo3



- Molecule 12: DNA-directed RNA polymerase subunit Rpo12



● Molecule 13: DNA-directed RNA polymerase subunit Rpo4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81025	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.163	Depositor
Minimum map value	-1.275	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	377.6, 377.6, 377.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.944, 0.944, 0.944	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, SF4

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	0.19	0/7131	0.35	0/9640
2	B	0.21	0/8885	0.35	2/12016 (0.0%)
3	C	0.16	0/2979	0.36	0/4007
4	E	0.20	0/1428	0.52	1/1923 (0.1%)
5	G	0.23	0/1006	0.44	0/1342
6	H	0.15	0/630	0.33	0/851
7	K	0.19	0/697	0.36	0/938
8	L	0.21	0/716	0.29	0/964
9	N	0.28	0/545	0.42	0/735
10	Y	0.10	0/360	0.27	0/482
11	D	0.26	0/2100	0.41	0/2839
12	P	0.21	0/382	0.43	0/510
13	F	0.23	0/866	0.69	2/1172 (0.2%)
All	All	0.20	0/27725	0.38	5/37419 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	E	0	4
13	F	0	1
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	5	LEU	N-CA-C	7.58	119.78	110.91
4	E	9	GLY	N-CA-C	6.93	129.61	113.18
13	F	3	TYR	CA-CB-CG	5.30	123.45	113.90
2	B	1064	GLY	CA-C-N	5.10	131.58	122.09
2	B	1064	GLY	C-N-CA	5.10	131.58	122.09

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	ALA	Peptide
4	E	11	VAL	Peptide
4	E	68	HIS	Peptide
4	E	9	GLY	Mainchain,Peptide
13	F	5	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6982	0	7063	95	0
2	B	8725	0	8862	100	0
3	C	2954	0	3053	53	0
4	E	1405	0	1443	51	0
5	G	991	0	996	13	0
6	H	617	0	644	18	0
7	K	690	0	745	11	0
8	L	707	0	751	6	0
9	N	534	0	545	9	0
10	Y	357	0	360	5	0
11	D	2066	0	2117	28	0
12	P	376	0	398	6	0
13	F	856	0	869	49	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
15	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27273	0	27846	366	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 7.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:CYS:SG	1:A:71:HIS:NE2	2.03	1.29
12:P:6:CYS:HB3	12:P:9:CYS:SG	1.95	1.05
4:E:9:GLY:HA2	13:F:5:LEU:H	1.31	0.95
4:E:8:LYS:HB2	13:F:4:SER:HB2	1.50	0.94
1:A:61:CYS:SG	1:A:71:HIS:CE1	2.64	0.91
2:B:878:THR:HG23	2:B:880:HIS:H	1.43	0.82
4:E:8:LYS:HE2	13:F:6:LYS:HB3	1.65	0.77
1:A:427:ARG:HD3	1:A:489:PRO:HG2	1.67	0.77
4:E:8:LYS:HG3	13:F:6:LYS:H	1.50	0.77
4:E:10:ILE:H	13:F:5:LEU:HD23	1.51	0.75
4:E:9:GLY:HA2	13:F:5:LEU:N	2.02	0.75
13:F:90:ILE:HG22	13:F:92:PRO:HD2	1.69	0.75
1:A:421:ARG:HG3	1:A:423:PRO:HD2	1.68	0.74
3:C:278:VAL:HB	3:C:287:ALA:HB3	1.71	0.73
1:A:438:LEU:HB2	1:A:444:ARG:HH21	1.54	0.72
1:A:183:ARG:HA	1:A:186:ARG:HH21	1.54	0.71
3:C:145:THR:HG23	3:C:175:LYS:HD2	1.72	0.70
2:B:142:ASP:HB3	2:B:145:ASP:HB2	1.73	0.70
7:K:26:ILE:HD11	7:K:69:ILE:HD11	1.74	0.70
2:B:901:GLY:HA3	11:D:161:VAL:HG13	1.74	0.70
1:A:117:ILE:HG23	10:Y:47:LEU:HD11	1.75	0.69
2:B:116:ASP:H	2:B:389:THR:HG22	1.56	0.69
12:P:9:CYS:HB3	12:P:29:CYS:SG	2.33	0.69
4:E:6:ARG:HB2	13:F:9:GLU:HB3	1.74	0.68
2:B:925:ALA:HB1	2:B:985:GLY:HA3	1.76	0.68
4:E:70:VAL:N	13:F:3:TYR:HB2	2.08	0.68
2:B:292:ASP:HB2	2:B:306:ARG:HH21	1.58	0.67
2:B:724:ILE:HD12	2:B:983:LEU:HD23	1.78	0.66
2:B:893:VAL:HG21	11:D:34:LEU:HD11	1.77	0.66
1:A:687:ILE:HD11	1:A:690:ARG:HD2	1.78	0.66
3:C:140:ARG:HH21	3:C:175:LYS:HA	1.60	0.66
1:A:379:ILE:HB	1:A:406:VAL:HB	1.78	0.66
2:B:696:PRO:HB2	2:B:715:PRO:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLN:HG3	2:B:1051:ASN:HD21	1.62	0.65
1:A:298:LEU:HD22	2:B:1106:MET:HE3	1.79	0.65
1:A:58:CYS:SG	1:A:61:CYS:HB2	2.36	0.64
2:B:632:THR:HG22	2:B:634:ASP:H	1.62	0.64
2:B:163:GLU:HB3	2:B:429:SER:HA	1.80	0.64
4:E:6:ARG:HH22	13:F:11:HIS:HB2	1.63	0.64
4:E:10:ILE:HA	13:F:3:TYR:O	1.98	0.64
11:D:83:ALA:HA	11:D:146:ARG:HD2	1.80	0.63
2:B:140:GLY:HA2	9:N:62:TYR:HE1	1.64	0.63
1:A:848:VAL:HB	7:K:3:ILE:HD12	1.79	0.63
11:D:130:ILE:HG22	11:D:131:VAL:HG23	1.79	0.62
1:A:422:GLN:HG3	1:A:463:ASN:HD21	1.62	0.62
1:A:124:ARG:HG3	1:A:125:TRP:H	1.65	0.62
3:C:260:MET:HA	6:H:8:LYS:HZ2	1.65	0.62
11:D:37:PRO:HG3	11:D:149:TYR:HE1	1.65	0.62
4:E:69:GLU:HA	13:F:3:TYR:O	2.00	0.62
1:A:121:ILE:HD12	1:A:124:ARG:HB3	1.81	0.62
13:F:69:VAL:HA	13:F:72:VAL:HG12	1.82	0.62
2:B:101:VAL:HG22	2:B:106:GLU:HA	1.83	0.61
2:B:740:LYS:HB2	2:B:889:LEU:HB3	1.82	0.61
4:E:53:ALA:HA	4:E:70:VAL:HG12	1.83	0.61
6:H:18:PRO:HD2	6:H:20:HIS:HE1	1.65	0.60
11:D:100:VAL:HG21	11:D:109:ILE:HD12	1.82	0.60
10:Y:63:ILE:HG23	10:Y:67:LYS:HZ3	1.65	0.60
3:C:284:ILE:HD13	6:H:45:ILE:HD12	1.83	0.60
2:B:1045:LYS:O	2:B:1049:LEU:HB3	2.02	0.59
4:E:148:SER:HB3	4:E:160:ALA:HB3	1.83	0.59
1:A:500:GLN:HG2	2:B:732:MET:HE3	1.84	0.59
4:E:30:LEU:HD13	4:E:48:ILE:HG21	1.83	0.58
1:A:309:PHE:HA	1:A:313:LEU:HD12	1.84	0.58
1:A:332:LEU:HD21	1:A:438:LEU:HD11	1.86	0.58
2:B:779:LYS:HG2	2:B:831:ARG:HA	1.85	0.58
1:A:60:VAL:HB	1:A:71:HIS:HE1	1.69	0.58
2:B:1059:ILE:HB	2:B:1114:LEU:HD11	1.85	0.58
3:C:19:ASP:HA	7:K:5:LYS:HD2	1.85	0.57
4:E:136:ILE:HG22	4:E:142:VAL:HG11	1.86	0.57
2:B:31:PHE:HA	2:B:35:LYS:HB2	1.86	0.57
4:E:9:GLY:N	13:F:4:SER:H	2.02	0.57
3:C:285:GLU:HG2	3:C:288:ARG:HG2	1.84	0.57
11:D:205:LEU:HD21	11:D:221:SER:HB3	1.87	0.57
1:A:62:GLY:HA3	2:B:1071:ARG:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:63:ILE:HG22	13:F:64:VAL:HG23	1.85	0.57
3:C:278:VAL:HG12	3:C:290:LEU:HD23	1.85	0.57
11:D:163:ILE:HB	11:D:229:GLU:HB2	1.87	0.57
11:D:36:VAL:HB	11:D:158:PRO:HG3	1.87	0.57
1:A:245:LEU:HD11	1:A:268:LEU:HD23	1.86	0.56
4:E:8:LYS:HD3	4:E:71:GLU:HG3	1.85	0.56
9:N:40:VAL:HG13	9:N:45:CYS:HB2	1.87	0.56
1:A:579:ILE:HD11	5:G:78:ARG:HG3	1.85	0.56
2:B:161:ALA:HB3	2:B:427:VAL:HG22	1.87	0.56
5:G:12:SER:HB3	5:G:26:LYS:HB2	1.87	0.56
11:D:51:SER:HB3	11:D:139:ILE:HD11	1.87	0.56
1:A:271:TYR:HD1	1:A:284:LEU:HD13	1.70	0.56
1:A:51:VAL:HG21	1:A:56:GLN:HB3	1.87	0.56
3:C:141:ARG:HG3	3:C:230:LYS:HE3	1.88	0.56
2:B:893:VAL:HG12	11:D:33:ILE:HD12	1.86	0.55
11:D:53:LEU:HD12	11:D:131:VAL:HG22	1.87	0.55
1:A:866:VAL:HG22	3:C:25:LEU:HD11	1.87	0.55
3:C:193:GLU:HB3	3:C:209:GLU:HG2	1.87	0.55
2:B:962:LEU:HD23	11:D:184:PRO:HG2	1.89	0.55
1:A:4:LYS:HD3	2:B:1116:GLU:HA	1.88	0.55
2:B:327:ARG:HD3	2:B:560:TYR:HB3	1.86	0.55
2:B:1053:ASP:HB2	2:B:1094:TYR:HB3	1.88	0.54
13:F:25:LEU:HD22	13:F:35:ILE:HG21	1.88	0.54
2:B:160:ILE:HD11	2:B:426:ARG:HD2	1.88	0.54
2:B:648:ILE:HD11	2:B:709:ILE:HG21	1.89	0.54
9:N:63:THR:HG23	12:P:11:LYS:HE3	1.90	0.54
2:B:288:GLU:HG3	2:B:306:ARG:HH22	1.72	0.54
4:E:10:ILE:HG12	13:F:5:LEU:HD23	1.89	0.53
1:A:831:ARG:HD2	3:C:383:ILE:HD12	1.90	0.53
1:A:426:HIS:HD2	1:A:428:ILE:HG12	1.72	0.53
1:A:828:SER:HB2	3:C:70:VAL:HG22	1.90	0.53
2:B:67:ILE:HD12	2:B:854:LEU:HD13	1.90	0.53
4:E:8:LYS:HB3	4:E:71:GLU:HA	1.91	0.53
7:K:71:ARG:HB2	7:K:79:GLU:HB3	1.89	0.53
2:B:690:ALA:HB3	2:B:753:PHE:HB2	1.91	0.53
6:H:18:PRO:HB3	6:H:67:ARG:HA	1.91	0.53
2:B:240:VAL:HA	2:B:314:ALA:HB1	1.91	0.53
1:A:11:PHE:HB3	3:C:356:ALA:HA	1.92	0.53
4:E:1:MET:HE3	4:E:83:GLU:HG3	1.91	0.53
11:D:41:VAL:HB	11:D:63:ALA:HA	1.91	0.53
4:E:11:VAL:HG13	13:F:2:SER:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:52:VAL:HG12	5:G:122:LYS:HA	1.91	0.52
2:B:574:ARG:HD3	2:B:613:PHE:HB3	1.91	0.52
2:B:845:VAL:HG12	2:B:864:VAL:HG22	1.91	0.52
2:B:278:GLN:HB2	2:B:283:ARG:HG3	1.92	0.52
3:C:17:ILE:HG23	3:C:20:LYS:HB2	1.90	0.52
4:E:26:ALA:HA	13:F:3:TYR:OH	2.10	0.52
2:B:237:VAL:HB	2:B:247:GLN:HG2	1.91	0.52
4:E:30:LEU:HB3	4:E:48:ILE:HD13	1.91	0.52
5:G:3:GLU:H	5:G:58:ARG:HH21	1.56	0.52
1:A:52:ILE:HG23	1:A:217:ILE:HG22	1.92	0.51
2:B:722:LEU:HA	2:B:906:ILE:HG13	1.92	0.51
2:B:747:MET:HG3	9:N:8:PHE:CD2	2.44	0.51
4:E:35:GLN:HG2	4:E:36:GLU:HG3	1.91	0.51
6:H:19:LYS:HB3	6:H:66:THR:HB	1.93	0.51
1:A:289:HIS:CE1	1:A:293:ARG:HB3	2.46	0.51
3:C:284:ILE:HG12	3:C:285:GLU:H	1.75	0.51
9:N:15:ALA:HB1	11:D:129:PRO:HD2	1.91	0.51
3:C:141:ARG:HD2	3:C:262:VAL:HG23	1.93	0.51
4:E:68:HIS:O	13:F:3:TYR:HB3	2.10	0.51
3:C:236:LYS:HB2	3:C:252:ASP:HB3	1.92	0.51
11:D:230:ILE:HG13	11:D:242:LEU:HD21	1.92	0.51
4:E:68:HIS:C	13:F:3:TYR:HB3	2.37	0.50
9:N:35:LEU:HD13	9:N:46:ARG:HG2	1.94	0.50
1:A:430:MET:HE1	2:B:1027:PHE:HE1	1.76	0.50
13:F:60:LEU:HB3	13:F:70:ARG:HG3	1.92	0.50
1:A:220:ARG:HH11	1:A:236:THR:HG22	1.76	0.50
1:A:298:LEU:HG	1:A:302:LEU:HD13	1.92	0.50
3:C:186:ILE:HG22	3:C:194:ILE:HG21	1.93	0.50
4:E:70:VAL:H	13:F:3:TYR:HB2	1.76	0.50
5:G:56:ILE:HA	5:G:117:TYR:O	2.11	0.50
1:A:60:VAL:HB	1:A:71:HIS:CE1	2.45	0.50
4:E:124:ARG:HH21	4:E:128:ILE:HG12	1.76	0.50
3:C:339:VAL:HG22	3:C:342:ARG:HH21	1.77	0.50
4:E:10:ILE:HA	13:F:3:TYR:C	2.37	0.50
6:H:22:ILE:HD11	6:H:55:ILE:HG23	1.93	0.49
2:B:1009:GLN:HG3	2:B:1016:THR:HG22	1.94	0.49
13:F:2:SER:O	13:F:3:TYR:HD1	1.94	0.49
4:E:7:ALA:HB3	4:E:72:PHE:CZ	2.48	0.49
9:N:65:PRO:HA	12:P:11:LYS:HE2	1.94	0.49
1:A:125:TRP:HE1	6:H:40:GLU:HG2	1.77	0.49
1:A:204:PRO:HA	1:A:207:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:HIS:HB2	3:C:62:ILE:HG13	1.94	0.49
3:C:299:LEU:HD13	3:C:306:VAL:HB	1.94	0.49
3:C:256:LEU:HA	3:C:259:ILE:HG12	1.95	0.49
4:E:47:GLY:HA3	13:F:25:LEU:HD11	1.94	0.49
2:B:577:LEU:HD12	2:B:614:ILE:HG13	1.94	0.49
11:D:73:LEU:HD12	11:D:240:ARG:HE	1.77	0.49
2:B:1076:TYR:HB3	2:B:1087:LEU:HD12	1.95	0.49
3:C:389:LYS:HD2	4:E:55:GLU:HB3	1.94	0.49
1:A:880:ARG:HH22	3:C:36:ILE:HD12	1.78	0.48
3:C:232:VAL:HG22	3:C:261:ASN:HB2	1.94	0.48
4:E:82:HIS:HB2	13:F:89:VAL:HG21	1.95	0.48
4:E:162:THR:HG22	4:E:164:LYS:H	1.78	0.48
2:B:808:LEU:HD23	2:B:862:VAL:HG11	1.95	0.48
2:B:931:ALA:HB2	2:B:938:VAL:HG23	1.96	0.48
8:L:1:MET:HG3	11:D:259:LYS:HE3	1.95	0.48
2:B:775:GLU:HB3	2:B:812:VAL:HG12	1.96	0.48
3:C:285:GLU:HA	3:C:288:ARG:HB3	1.96	0.48
1:A:420:ASN:HD22	2:B:1031:GLU:HG2	1.79	0.48
2:B:539:ARG:HH21	2:B:618:GLU:HG3	1.79	0.47
2:B:699:PRO:HG3	2:B:988:TYR:CZ	2.49	0.47
3:C:144:TYR:CE2	3:C:146:ARG:HB2	2.49	0.47
3:C:387:THR:HA	4:E:58:PHE:HA	1.96	0.47
2:B:641:TRP:CD1	2:B:643:SER:HG	2.32	0.47
2:B:813:SER:HB2	2:B:831:ARG:HB3	1.96	0.47
13:F:84:VAL:HG21	13:F:102:GLN:HE22	1.80	0.47
2:B:790:LEU:HD23	2:B:794:GLY:HA2	1.96	0.47
3:C:187:THR:HA	3:C:194:ILE:HB	1.95	0.47
3:C:111:ALA:HB1	3:C:324:ILE:HD12	1.96	0.47
4:E:9:GLY:CA	13:F:5:LEU:H	2.12	0.47
2:B:99:ILE:HG12	2:B:109:PRO:HG3	1.96	0.47
8:L:21:GLU:HG2	8:L:23:THR:H	1.80	0.47
11:D:77:ARG:HB2	11:D:82:CYS:HB2	1.97	0.47
2:B:240:VAL:HG11	2:B:250:LEU:HD11	1.97	0.47
2:B:902:ILE:HD11	9:N:42:ARG:HB3	1.97	0.47
3:C:17:ILE:HG21	3:C:54:ILE:HD11	1.97	0.47
1:A:115:LYS:HG3	1:A:194:LEU:HD22	1.98	0.46
4:E:103:PRO:HA	13:F:34:LEU:HD21	1.97	0.46
1:A:49:LEU:HA	1:A:71:HIS:HB2	1.97	0.46
2:B:418:LEU:HD23	2:B:418:LEU:HA	1.80	0.46
2:B:625:ALA:HB2	2:B:635:HIS:CD2	2.50	0.46
2:B:1058:TYR:HB3	2:B:1087:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:58:LYS:HA	6:H:58:LYS:HD3	1.73	0.46
1:A:10:LYS:HD2	3:C:361:ARG:NH1	2.30	0.46
2:B:574:ARG:HH11	2:B:613:PHE:HB3	1.79	0.46
5:G:4:MET:SD	5:G:55:ILE:HD11	2.56	0.46
4:E:10:ILE:N	13:F:5:LEU:HD23	2.26	0.46
1:A:238:LYS:HZ3	1:A:287:ALA:HB1	1.81	0.46
2:B:731:ASN:HB3	2:B:737:ILE:HG13	1.98	0.46
2:B:470:LEU:HD13	2:B:705:MET:HE3	1.97	0.46
6:H:64:LYS:HG2	6:H:78:TYR:CE1	2.51	0.46
6:H:25:LEU:HB2	10:Y:67:LYS:NZ	2.31	0.46
1:A:331:ASN:O	1:A:331:ASN:ND2	2.48	0.45
1:A:137:LYS:O	1:A:141:ILE:HG12	2.16	0.45
2:B:1063:CYS:HB2	2:B:1081:HIS:CE1	2.51	0.45
13:F:52:SER:HB2	13:F:108:ILE:HG23	1.98	0.45
5:G:14:ILE:HG12	5:G:25:VAL:HG22	1.99	0.45
3:C:333:THR:HG22	3:C:342:ARG:HD3	1.99	0.45
11:D:153:HIS:ND1	11:D:155:LYS:HE3	2.30	0.45
2:B:878:THR:HG23	2:B:880:HIS:N	2.23	0.45
4:E:99:VAL:HG12	4:E:101:MET:HG3	1.99	0.45
10:Y:51:GLU:O	10:Y:55:LYS:HG2	2.17	0.45
1:A:612:LEU:HD21	1:A:628:MET:HE2	1.99	0.45
3:C:337:SER:HB3	3:C:362:GLU:HG2	1.98	0.45
6:H:22:ILE:HG12	6:H:63:ILE:HD12	1.99	0.45
8:L:57:ILE:HD11	8:L:69:LEU:HD13	1.98	0.45
2:B:1097:LYS:HA	2:B:1100:ILE:HG22	1.98	0.45
3:C:142:ILE:HD11	3:C:249:ILE:HG21	1.98	0.45
11:D:75:HIS:ND1	11:D:120:MET:HE1	2.32	0.45
2:B:46:ILE:HB	2:B:55:ILE:HB	1.99	0.45
2:B:191:ALA:HB3	2:B:297:PRO:HB2	1.99	0.45
9:N:49:LEU:HD23	9:N:49:LEU:HA	1.82	0.44
2:B:170:VAL:HA	2:B:187:VAL:HG22	1.98	0.44
7:K:30:ARG:HH22	7:K:41:LEU:HD23	1.83	0.44
13:F:2:SER:C	13:F:3:TYR:HD1	2.25	0.44
13:F:91:ASP:OD1	13:F:92:PRO:HD3	2.17	0.44
2:B:94:ILE:HG13	2:B:114:ILE:HB	1.99	0.44
2:B:517:LYS:HG2	2:B:527:TYR:CE2	2.52	0.44
1:A:146:CYS:HB3	1:A:149:CYS:SG	2.56	0.44
1:A:296:ARG:HA	1:A:300:GLN:HG2	1.99	0.44
1:A:867:ASN:HB3	1:A:870:ARG:HB3	1.99	0.44
1:A:33:TYR:HD1	1:A:38:THR:HA	1.83	0.44
11:D:165:ARG:HH21	11:D:227:ILE:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PRO:HG2	1:A:162:TYR:CD1	2.53	0.44
1:A:417:VAL:HG12	1:A:466:VAL:HG22	2.00	0.44
1:A:611:MET:HB3	1:A:611:MET:HE3	1.88	0.44
1:A:14:LEU:HD11	1:A:19:ILE:HD11	1.98	0.44
1:A:361:ILE:HD12	1:A:407:VAL:HG11	1.99	0.44
1:A:686:PRO:HB3	1:A:692:ILE:HD13	1.98	0.44
1:A:720:ASP:HB3	1:A:723:ASN:HD22	1.83	0.44
3:C:288:ARG:NH2	6:H:67:ARG:HH21	2.15	0.44
5:G:37:PHE:HB3	5:G:96:VAL:HG13	2.00	0.44
11:D:2:PRO:HB2	11:D:18:GLU:HG3	1.99	0.44
4:E:40:LYS:HB2	4:E:40:LYS:HE2	1.76	0.43
13:F:56:ILE:HB	13:F:108:ILE:HG21	1.99	0.43
1:A:9:VAL:HG22	2:B:1112:LEU:HD13	1.99	0.43
1:A:614:TRP:CZ3	1:A:870:ARG:HG2	2.54	0.43
2:B:448:TRP:CZ2	2:B:645:ILE:HD11	2.53	0.43
2:B:579:ILE:HD11	2:B:612:GLU:HB3	1.99	0.43
4:E:11:VAL:HG12	13:F:1:MET:HB2	2.00	0.43
8:L:71:LYS:HE2	8:L:71:LYS:HB2	1.91	0.43
1:A:839:ARG:HG2	1:A:840:SER:O	2.18	0.43
2:B:667:GLN:HG3	2:B:879:ARG:C	2.44	0.43
4:E:70:VAL:HG22	13:F:3:TYR:HB2	2.00	0.43
10:Y:44:GLU:HA	10:Y:47:LEU:HG	2.00	0.43
1:A:161:PRO:HG2	1:A:162:TYR:HD1	1.83	0.43
1:A:235:LEU:HB2	1:A:276:TYR:HE1	1.84	0.43
3:C:138:ILE:HD13	3:C:141:ARG:HH12	1.82	0.43
4:E:27:ILE:O	4:E:31:ARG:HG2	2.19	0.43
1:A:301:ARG:HG3	1:A:308:ARG:HH22	1.84	0.43
2:B:48:THR:HG22	2:B:364:VAL:HG23	2.01	0.43
6:H:23:LEU:HD21	6:H:64:LYS:HE3	2.00	0.43
11:D:155:LYS:HD2	11:D:156:TYR:CZ	2.54	0.43
13:F:47:ARG:HA	13:F:47:ARG:HD2	1.82	0.43
1:A:1:MET:O	1:A:4:LYS:HE3	2.19	0.43
1:A:13:VAL:HG22	1:A:202:SER:HA	2.00	0.43
1:A:666:LYS:HA	1:A:666:LYS:HD3	1.72	0.43
5:G:4:MET:HG3	5:G:57:SER:HB3	2.00	0.43
2:B:346:ASP:O	2:B:349:THR:HG22	2.19	0.43
2:B:225:MET:HE2	2:B:236:ILE:HG23	2.01	0.42
3:C:333:THR:HA	3:C:342:ARG:HH11	1.85	0.42
1:A:418:LEU:HD13	1:A:430:MET:HE2	2.00	0.42
3:C:103:PRO:HA	3:C:106:ILE:HD12	2.01	0.42
4:E:13:ILE:HD11	13:F:3:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:256:LEU:HD12	3:C:259:ILE:HG13	2.01	0.42
5:G:89:ILE:HB	5:G:96:VAL:HB	2.01	0.42
13:F:15:TYR:HB2	13:F:75:SER:HB2	2.00	0.42
1:A:103:ARG:HD2	1:A:148:HIS:CG	2.54	0.42
1:A:365:ILE:HD12	1:A:401:ILE:HD13	2.02	0.42
1:A:385:ARG:NH1	2:B:1005:ARG:HH12	2.17	0.42
2:B:930:TYR:HE1	2:B:955:GLU:HG2	1.84	0.42
3:C:114:VAL:HA	3:C:115:PRO:HD3	1.90	0.42
3:C:288:ARG:HH12	3:C:312:VAL:HG22	1.85	0.42
7:K:27:ILE:HD13	7:K:57:GLU:HG2	2.02	0.42
11:D:61:ARG:HH21	11:D:130:ILE:HA	1.84	0.42
1:A:323:ARG:HD3	1:A:463:ASN:OD1	2.20	0.42
2:B:1058:TYR:CE1	2:B:1089:PRO:HG3	2.55	0.42
1:A:303:LYS:HG3	1:A:309:PHE:CZ	2.55	0.42
5:G:67:ASP:HB2	5:G:120:VAL:O	2.20	0.42
1:A:69:PRO:HG2	2:B:1068:TRP:HB3	2.02	0.42
3:C:125:THR:HB	3:C:128:TYR:HD2	1.85	0.42
3:C:171:MET:O	3:C:175:LYS:HG2	2.20	0.42
4:E:165:GLN:HG2	4:E:166:PRO:HD2	2.01	0.42
7:K:13:ASN:C	7:K:13:ASN:HD22	2.28	0.42
13:F:16:SER:O	13:F:19:LYS:HG2	2.20	0.42
2:B:875:LYS:HD3	2:B:994:HIS:HB2	2.02	0.42
2:B:1103:LEU:HD22	2:B:1108:ILE:HD11	2.02	0.42
4:E:70:VAL:HG22	13:F:3:TYR:CB	2.49	0.42
1:A:657:ALA:O	1:A:661:ILE:HG12	2.19	0.41
1:A:690:ARG:HB3	1:A:694:GLU:HG3	2.02	0.41
2:B:704:ARG:HG3	2:B:939:ASP:OD1	2.20	0.41
3:C:209:GLU:C	3:C:211:ILE:H	2.28	0.41
5:G:96:VAL:O	5:G:98:ILE:HG13	2.20	0.41
13:F:19:LYS:HD3	13:F:42:LEU:HB3	2.01	0.41
1:A:85:GLY:HA2	3:C:353:LEU:HD13	2.01	0.41
1:A:124:ARG:HG3	1:A:125:TRP:HD1	1.85	0.41
2:B:502:ILE:HD13	2:B:509:VAL:HG23	2.02	0.41
3:C:339:VAL:HG11	3:C:355:ALA:HB2	2.01	0.41
8:L:28:LEU:HD23	8:L:28:LEU:HA	1.82	0.41
1:A:295:LEU:HB3	1:A:297:THR:HG23	2.03	0.41
1:A:841:LEU:HD11	3:C:379:LEU:HD22	2.02	0.41
2:B:24:HIS:HB3	2:B:120:MET:HE1	2.02	0.41
2:B:628:PRO:HG3	2:B:638:LEU:HD21	2.02	0.41
4:E:89:VAL:HG21	4:E:136:ILE:HB	2.02	0.41
6:H:37:ILE:HB	6:H:41:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:VAL:HG21	1:A:546:TYR:HB2	2.03	0.41
2:B:875:LYS:HE3	2:B:883:LYS:HE3	2.03	0.41
4:E:84:VAL:HG21	13:F:87:VAL:HG13	2.01	0.41
6:H:49:ASP:O	6:H:53:LYS:HG2	2.21	0.41
13:F:56:ILE:HB	13:F:108:ILE:HG13	2.03	0.41
1:A:479:LEU:HD23	7:K:20:LYS:HE2	2.03	0.41
2:B:57:LEU:HD22	2:B:96:LEU:HD21	2.03	0.41
2:B:249:GLU:O	2:B:252:PRO:HD2	2.21	0.41
2:B:722:LEU:HD13	2:B:987:VAL:HG21	2.02	0.41
2:B:890:ILE:HB	2:B:895:MET:HE2	2.02	0.41
1:A:260:LEU:O	1:A:263:GLU:HG3	2.21	0.41
1:A:361:ILE:HG23	1:A:407:VAL:HG11	2.03	0.41
2:B:418:LEU:HD11	2:B:652:ILE:HG21	2.03	0.41
3:C:388:MET:HB3	7:K:67:ILE:HG12	2.02	0.41
6:H:42:LEU:HD23	6:H:42:LEU:HA	1.93	0.41
6:H:60:GLY:HA2	6:H:80:TYR:OH	2.20	0.41
8:L:3:ILE:HG23	11:D:259:LYS:HD2	2.02	0.41
12:P:12:GLU:HG3	12:P:13:LEU:H	1.86	0.41
1:A:118:TYR:HA	1:A:121:ILE:HG22	2.02	0.41
2:B:260:ILE:HG23	2:B:265:GLU:HB2	2.03	0.41
7:K:44:THR:HA	7:K:47:LEU:HD23	2.02	0.41
13:F:56:ILE:HG13	13:F:104:ILE:HG22	2.02	0.41
3:C:36:ILE:HD13	3:C:36:ILE:HA	1.92	0.41
4:E:8:LYS:HD3	4:E:71:GLU:CG	2.51	0.41
11:D:250:LEU:HD23	11:D:250:LEU:HA	1.96	0.41
4:E:10:ILE:HG23	13:F:5:LEU:HB2	2.03	0.41
1:A:325:VAL:HG13	1:A:459:GLY:HA2	2.03	0.40
1:A:651:ILE:HG23	1:A:744:THR:HG22	2.03	0.40
1:A:818:TYR:CE1	1:A:822:ARG:HD2	2.56	0.40
2:B:114:ILE:HG22	2:B:388:ILE:HG13	2.04	0.40
3:C:349:VAL:HG12	3:C:352:LEU:HD12	2.02	0.40
12:P:3:LYS:HB2	12:P:37:VAL:HG21	2.03	0.40
1:A:321:SER:HB2	2:B:1025:LEU:HD12	2.02	0.40
5:G:27:MET:HB2	5:G:35:ILE:HB	2.02	0.40
6:H:17:VAL:HA	6:H:18:PRO:HD3	1.95	0.40
11:D:260:LEU:HA	11:D:260:LEU:HD23	1.88	0.40
13:F:14:PRO:HA	13:F:71:ALA:HB1	2.03	0.40
1:A:445:LEU:HD23	1:A:445:LEU:HA	1.91	0.40
13:F:48:CYS:HB3	13:F:52:SER:OG	2.20	0.40
1:A:303:LYS:HG3	1:A:309:PHE:HZ	1.85	0.40
1:A:418:LEU:HD11	2:B:1043:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ARG:HA	2:B:1034:CYS:SG	2.62	0.40
2:B:721:ILE:HD13	2:B:986:ILE:HG12	2.04	0.40
3:C:63:GLU:HB3	7:K:19:THR:HB	2.03	0.40
4:E:30:LEU:HD22	4:E:48:ILE:HG12	2.04	0.40
2:B:68:ARG:HH21	2:B:75:MET:HE2	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	870/880 (99%)	806 (93%)	63 (7%)	1 (0%)	48	80
2	B	1105/1126 (98%)	1030 (93%)	75 (7%)	0	100	100
3	C	373/393 (95%)	349 (94%)	24 (6%)	0	100	100
4	E	176/183 (96%)	168 (96%)	8 (4%)	0	100	100
5	G	120/124 (97%)	104 (87%)	16 (13%)	0	100	100
6	H	76/84 (90%)	70 (92%)	6 (8%)	0	100	100
7	K	84/89 (94%)	80 (95%)	4 (5%)	0	100	100
8	L	88/90 (98%)	86 (98%)	2 (2%)	0	100	100
9	N	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
10	Y	42/105 (40%)	41 (98%)	1 (2%)	0	100	100
11	D	259/264 (98%)	236 (91%)	23 (9%)	0	100	100
12	P	45/48 (94%)	36 (80%)	9 (20%)	0	100	100
13	F	107/114 (94%)	90 (84%)	17 (16%)	0	100	100
All	All	3409/3566 (96%)	3158 (93%)	250 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	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	762/768 (99%)	762 (100%)	0	100	100
2	B	948/972 (98%)	948 (100%)	0	100	100
3	C	327/348 (94%)	327 (100%)	0	100	100
4	E	154/157 (98%)	154 (100%)	0	100	100
5	G	113/115 (98%)	113 (100%)	0	100	100
6	H	68/75 (91%)	68 (100%)	0	100	100
7	K	78/81 (96%)	78 (100%)	0	100	100
8	L	78/78 (100%)	78 (100%)	0	100	100
9	N	60/60 (100%)	60 (100%)	0	100	100
10	Y	40/98 (41%)	40 (100%)	0	100	100
11	D	237/239 (99%)	237 (100%)	0	100	100
12	P	41/43 (95%)	41 (100%)	0	100	100
13	F	100/109 (92%)	100 (100%)	0	100	100
All	All	3006/3143 (96%)	3006 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	74	HIS
1	A	300	GLN
1	A	500	GLN
2	B	544	GLN
2	B	627	ASN

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Mol	Chain	Res	Type
2	B	842	ASN
2	B	892	GLN
2	B	1101	GLN
3	C	271	GLN
4	E	68	HIS
4	E	82	HIS
4	E	94	ASN
5	G	79	GLN
5	G	80	GLN
10	Y	59	ASN
11	D	94	ASN
11	D	192	ASN
11	D	199	ASN

5.3.3 RNA [i](#)

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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	SF4	D	1001	11	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	D	1001	11	-	-	0/6/5/5

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.

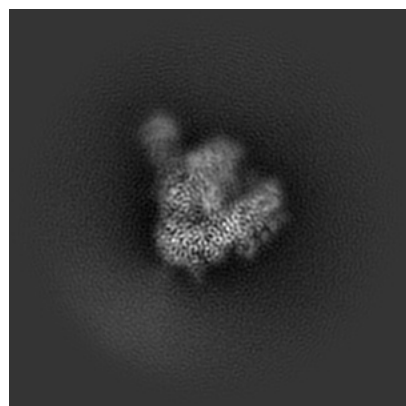
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74496. These allow visual inspection of the internal detail of the map and identification of artifacts.

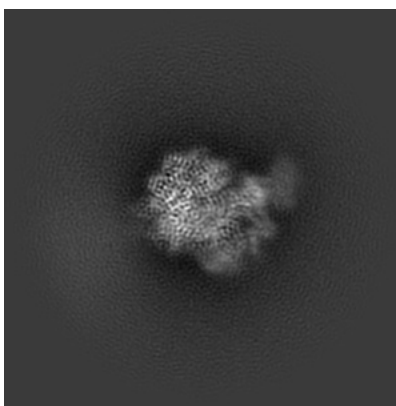
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

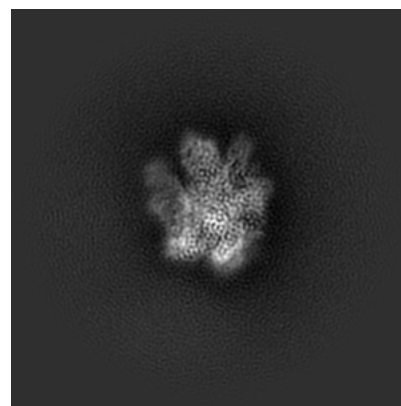
6.1.1 Primary map



X

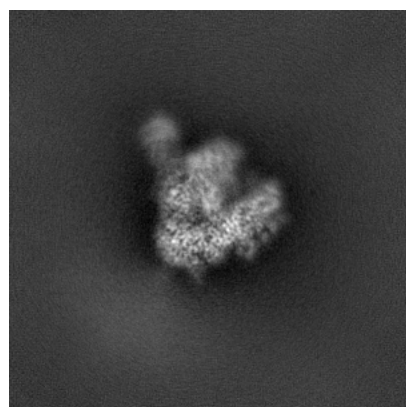


Y

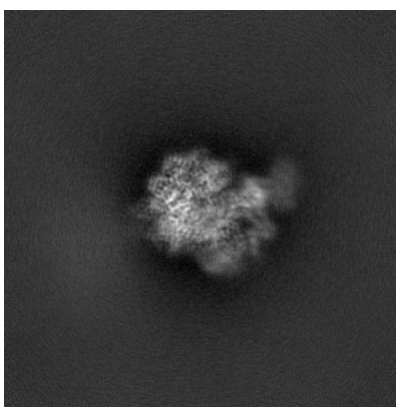


Z

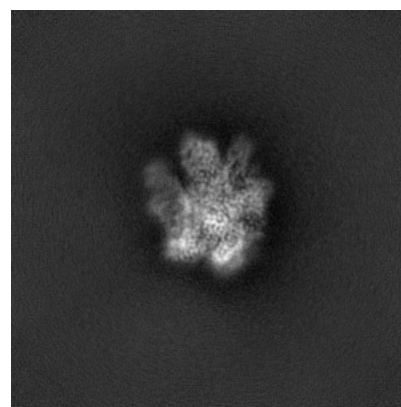
6.1.2 Raw map



X



Y

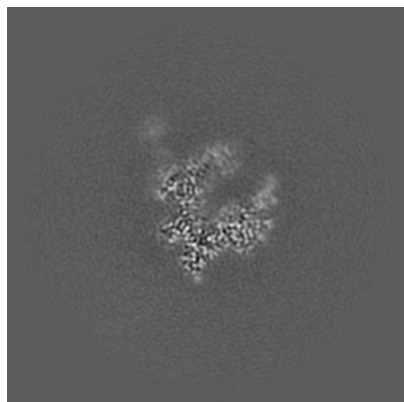


Z

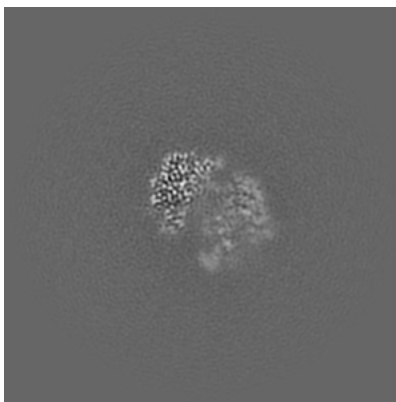
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

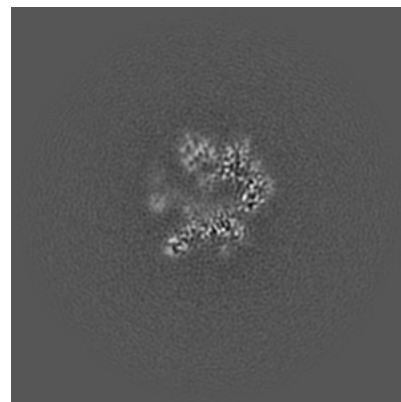
6.2.1 Primary map



X Index: 200

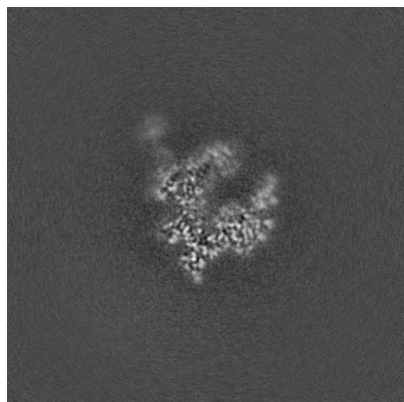


Y Index: 200

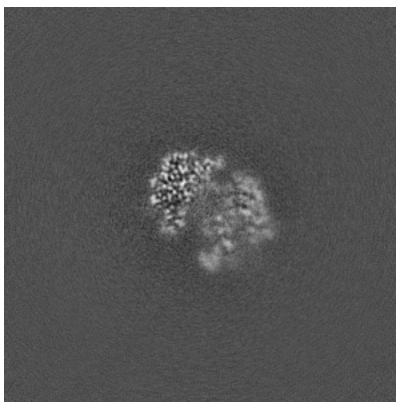


Z Index: 200

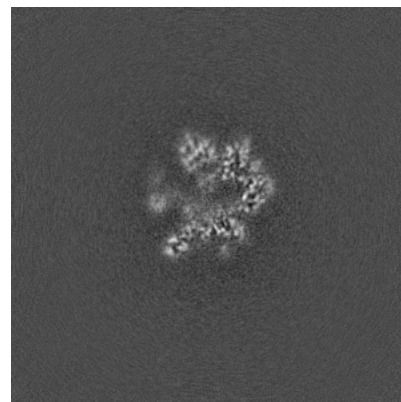
6.2.2 Raw map



X Index: 200



Y Index: 200

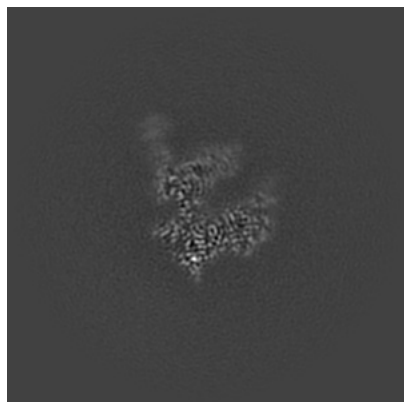


Z Index: 200

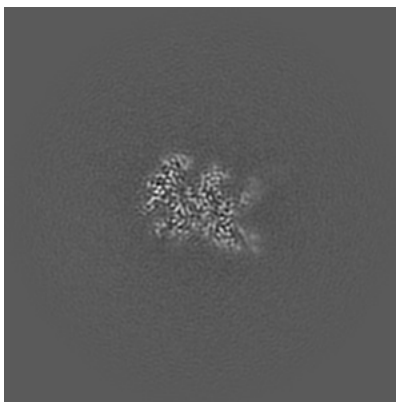
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

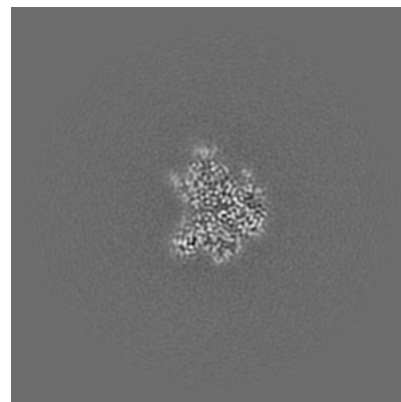
6.3.1 Primary map



X Index: 203

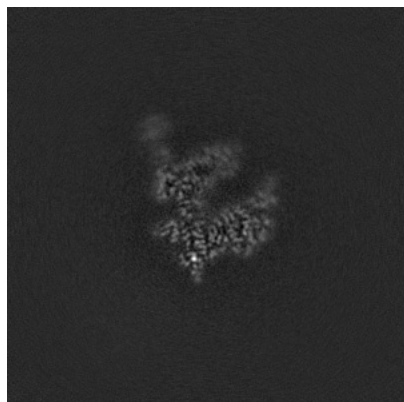


Y Index: 177

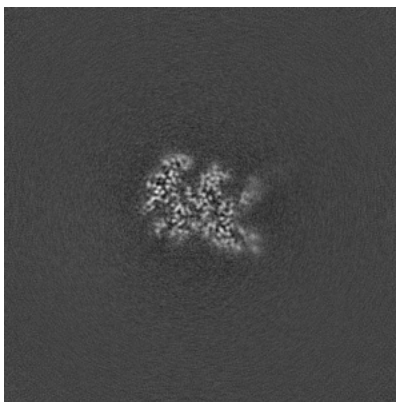


Z Index: 173

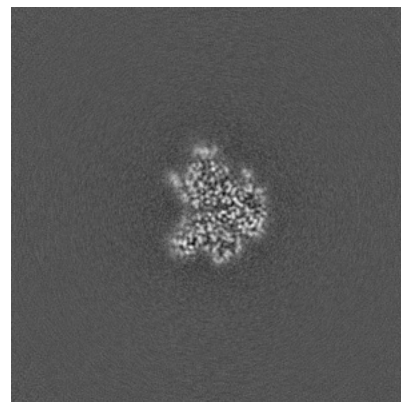
6.3.2 Raw map



X Index: 202



Y Index: 177

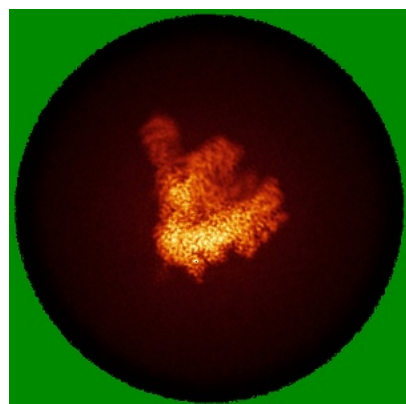


Z Index: 173

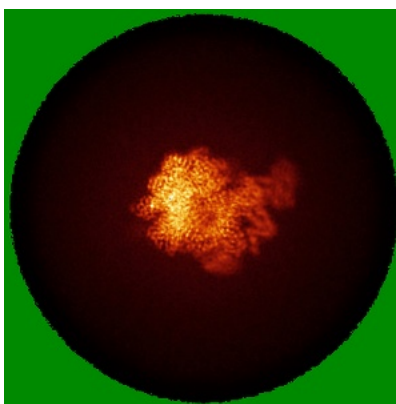
The images above show the largest variance slices of the map in three orthogonal directions.

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

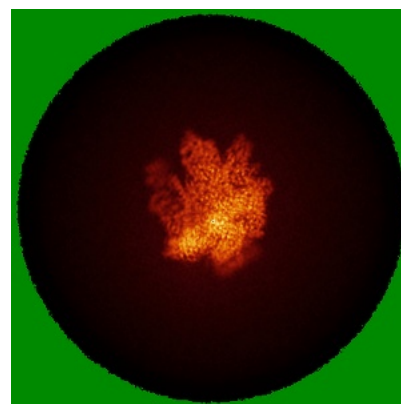
6.4.1 Primary map



X

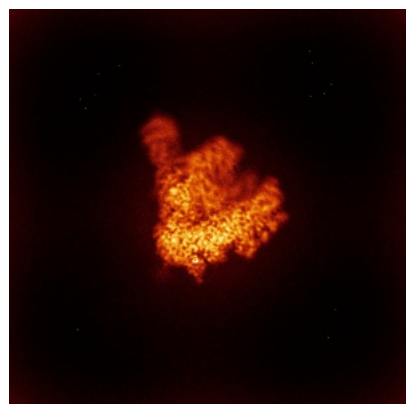


Y

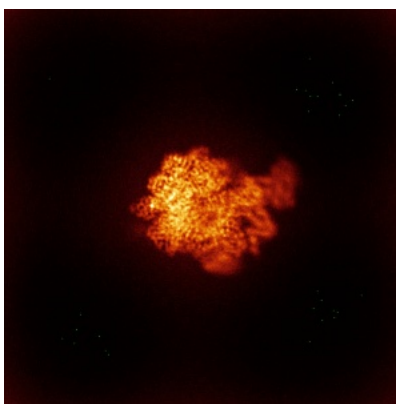


Z

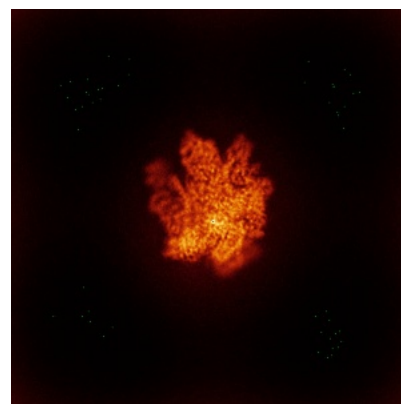
6.4.2 Raw map



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.

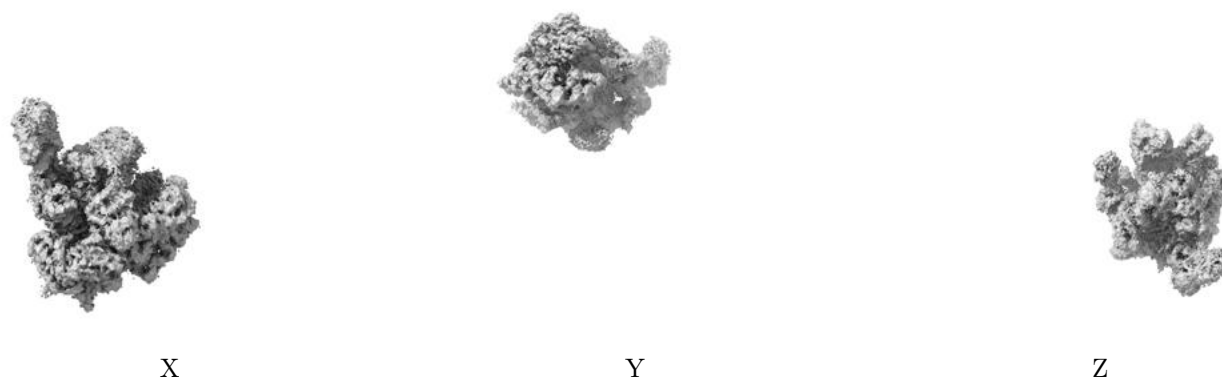
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

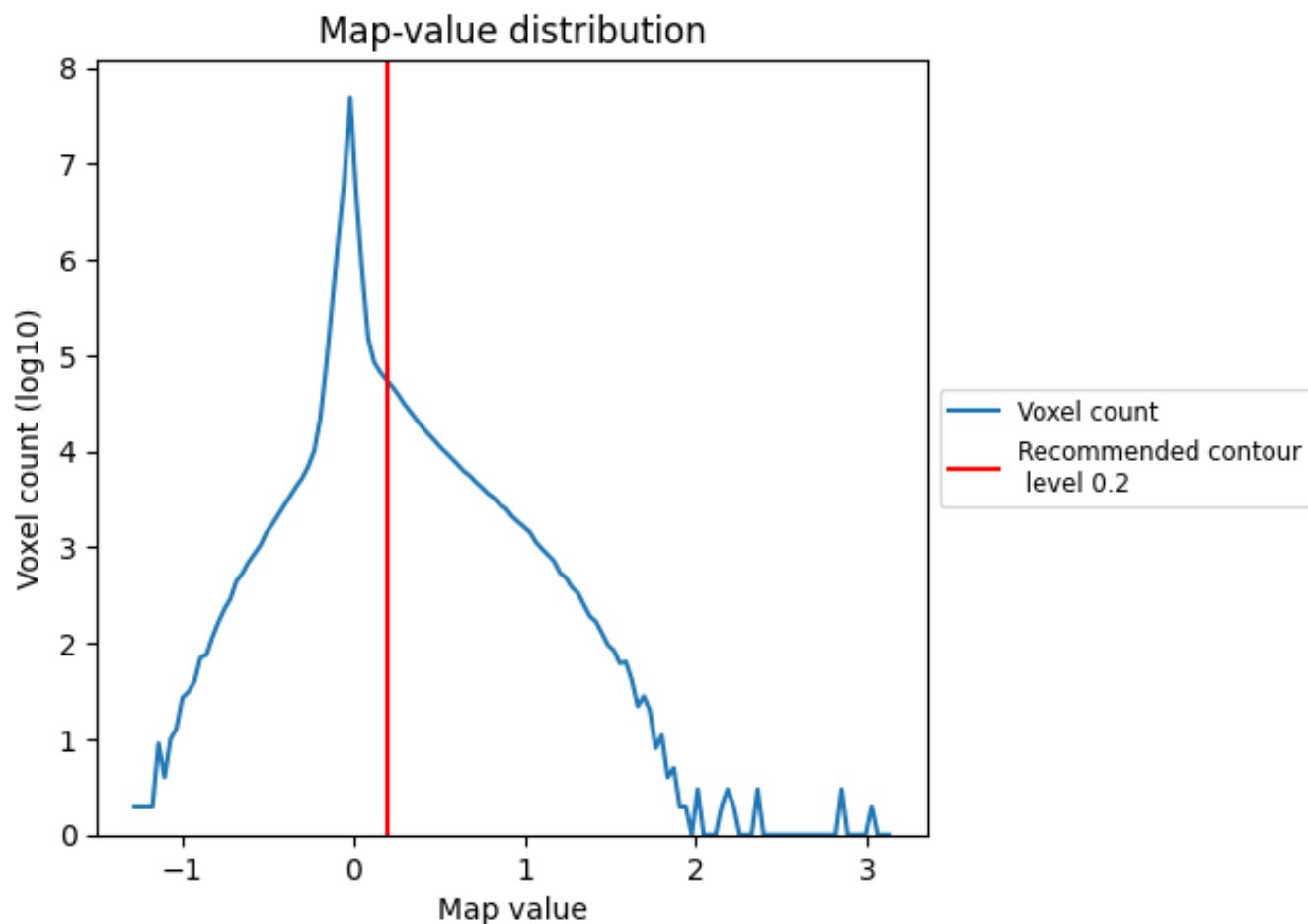
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

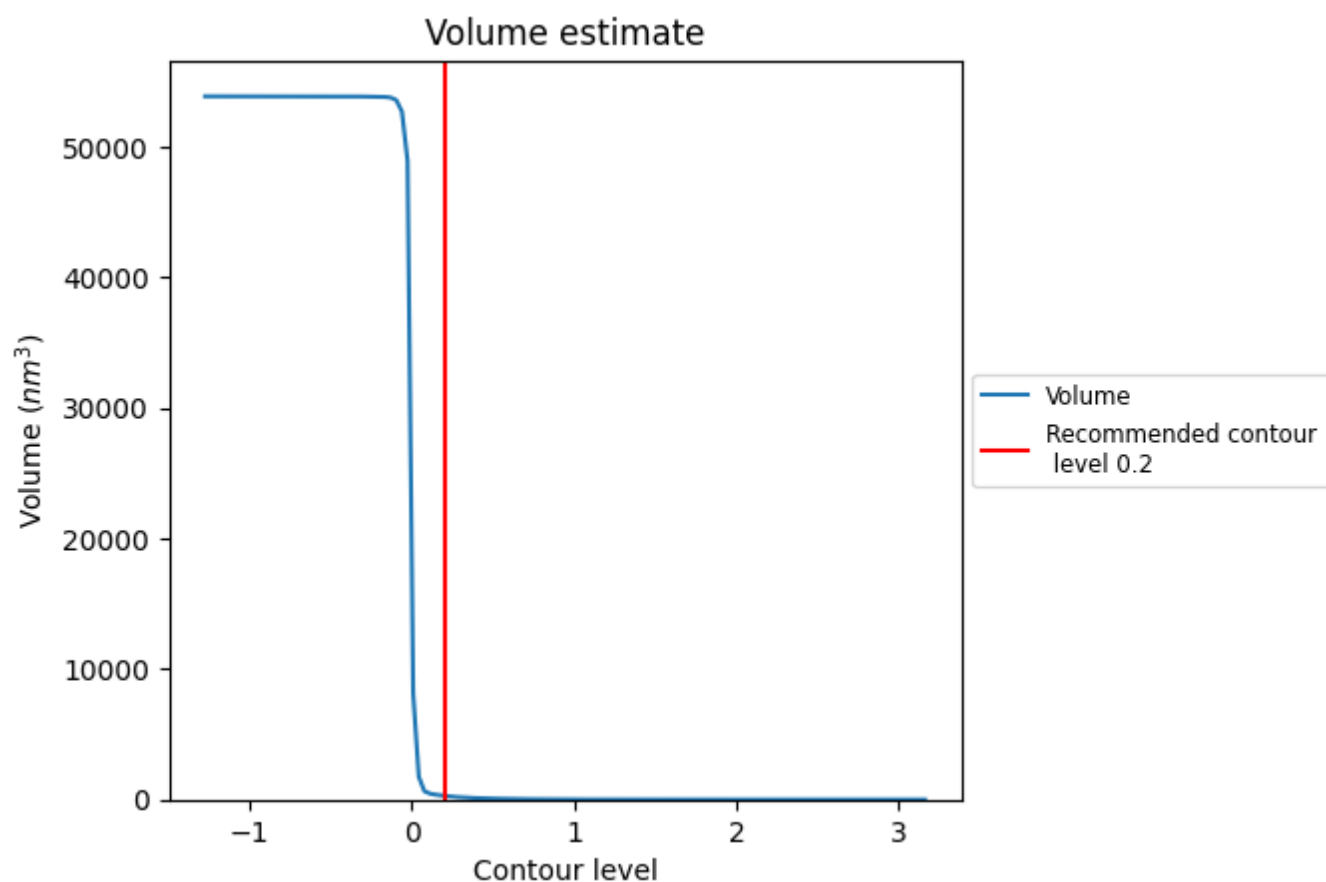
This section contains the results of statistical analysis of the map.

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.

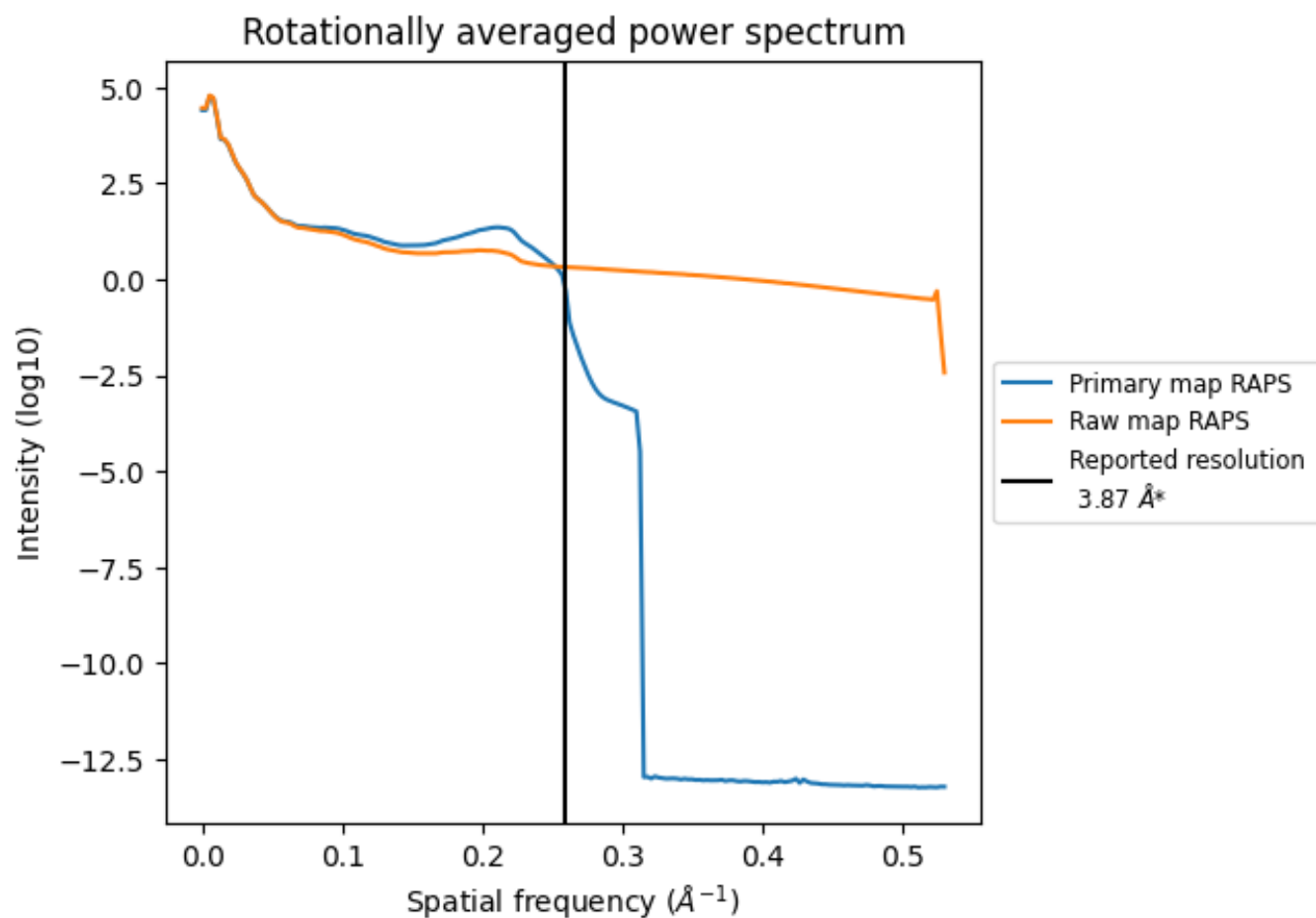
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm³; this corresponds to an approximate mass of 259 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 ⓘ

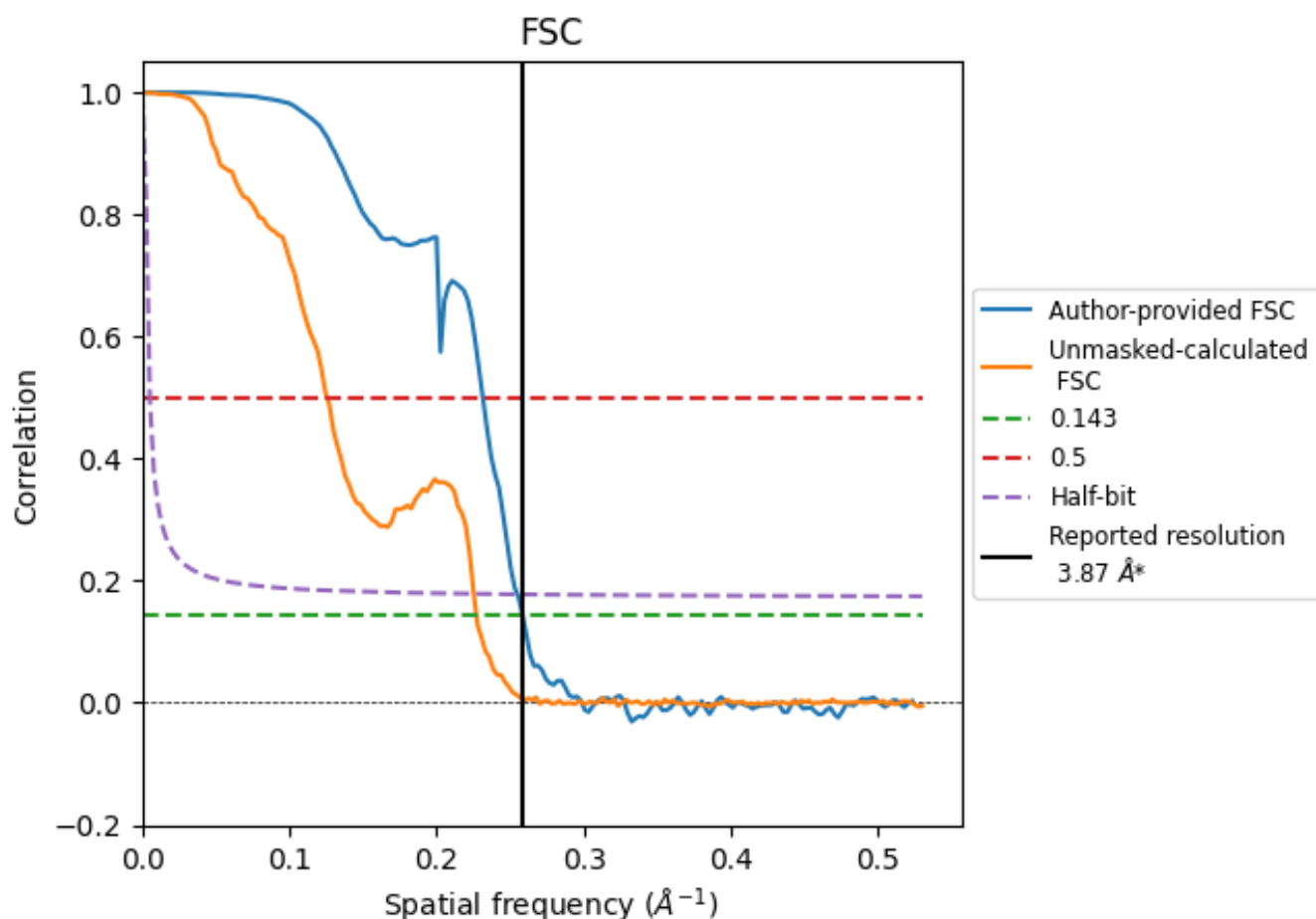


*Reported resolution corresponds to spatial frequency of 0.258 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.258 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

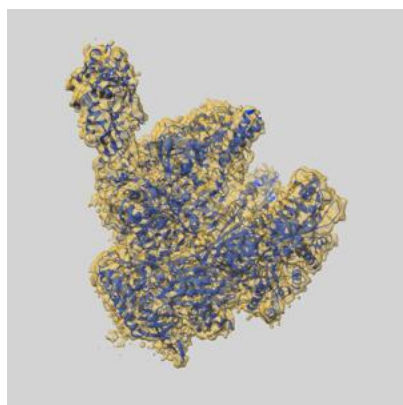
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.87	-	-
Author-provided FSC curve	3.87	4.32	3.92
Unmasked-calculated*	4.41	7.97	4.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.41 differs from the reported value 3.87 by more than 10 %

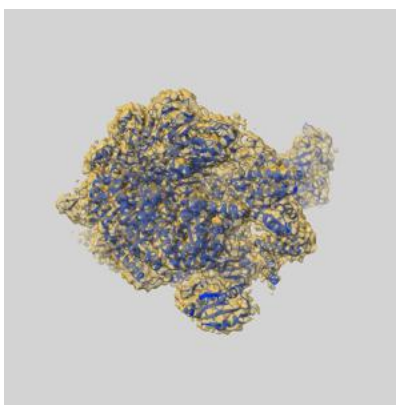
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74496 and PDB model 9ZOH. Per-residue inclusion information can be found in section [3](#) on page [7](#).

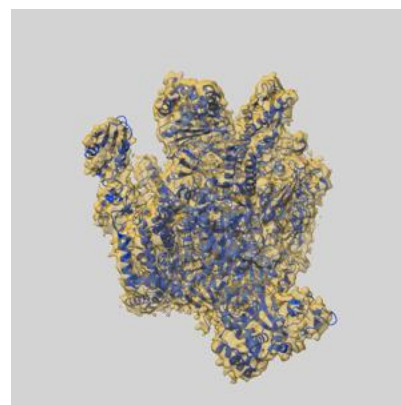
9.1 Map-model overlay [i](#)



X



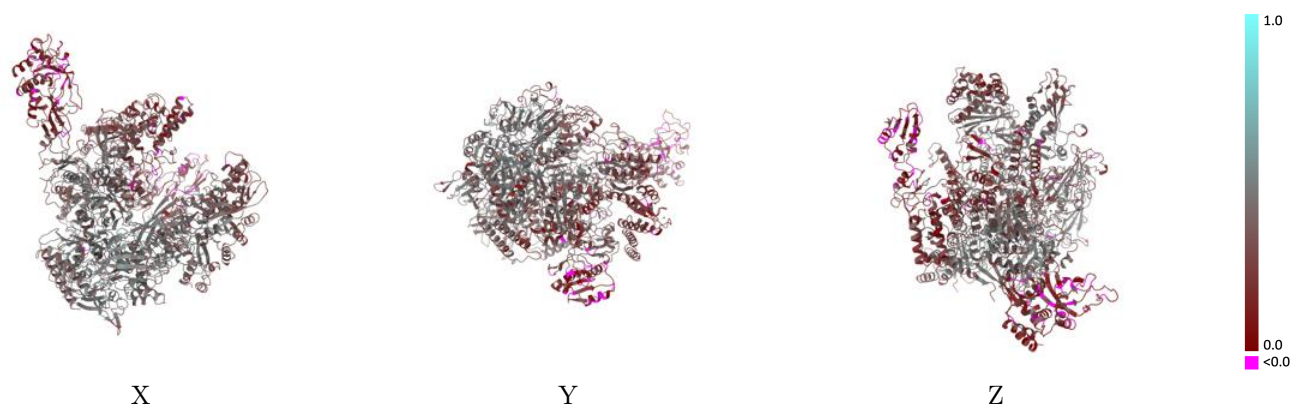
Y



Z

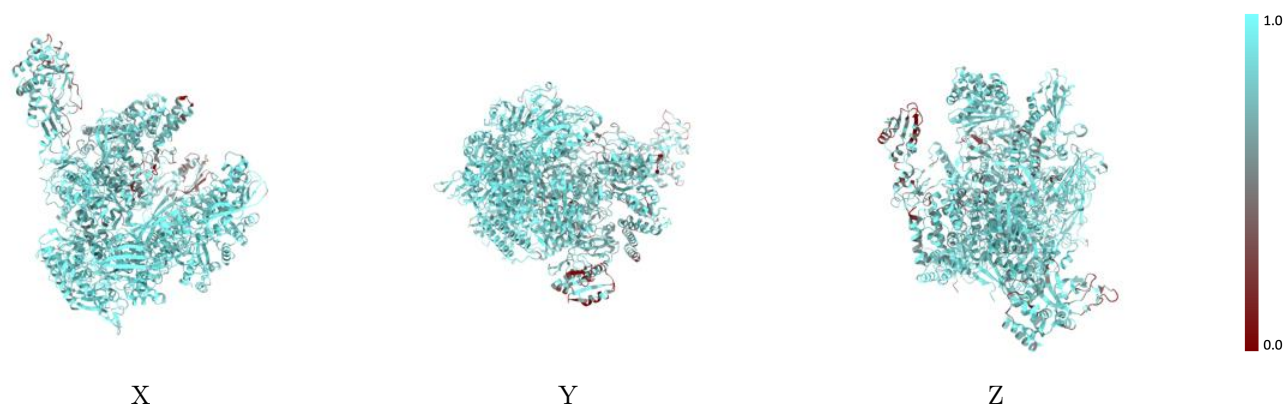
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



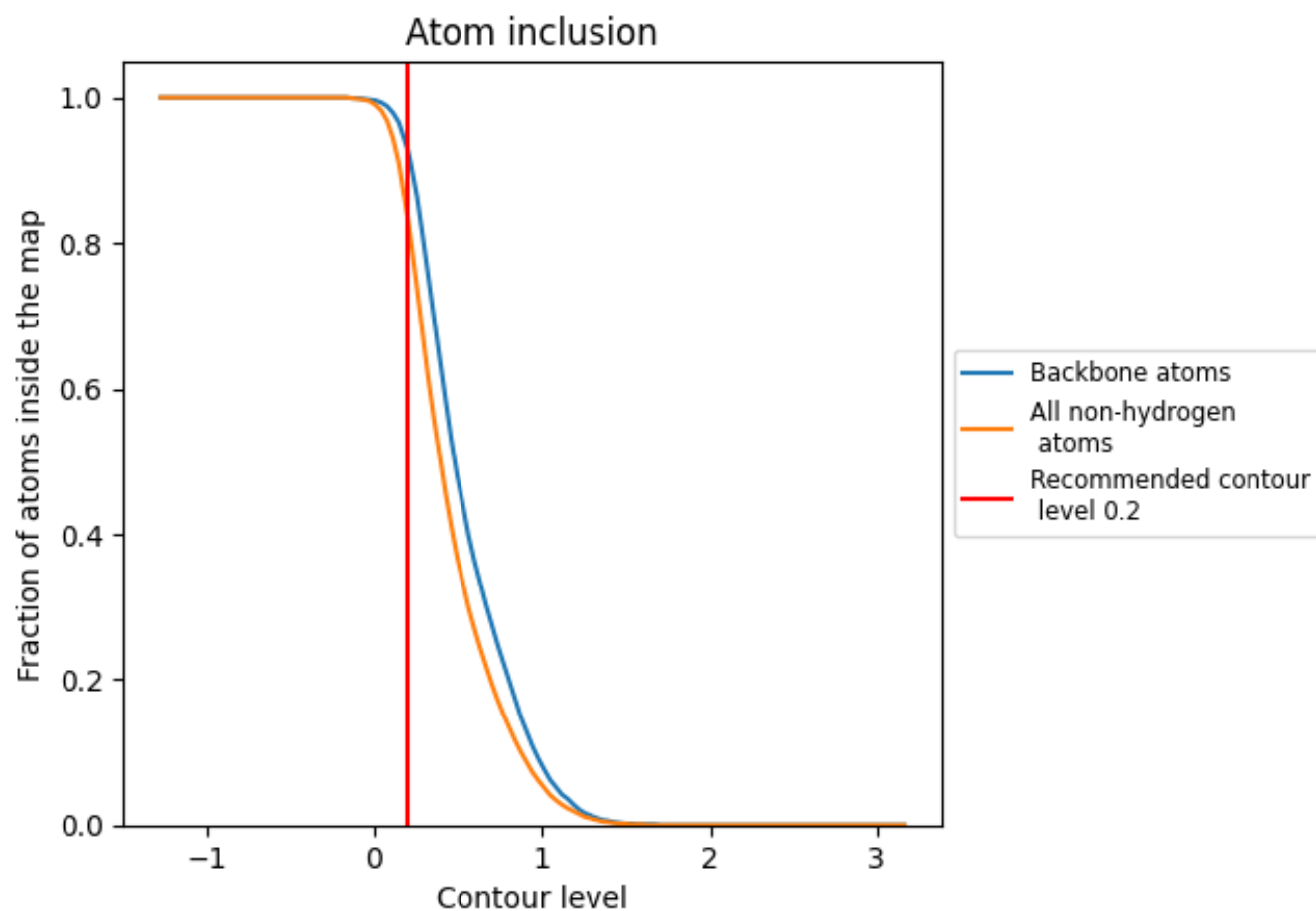
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 83% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.3580
A	 0.8300	 0.3610
B	 0.8790	 0.3990
C	 0.7120	 0.2590
D	 0.8980	 0.4480
E	 0.7180	 0.1920
F	 0.7370	 0.1660
G	 0.8760	 0.4230
H	 0.8160	 0.3220
K	 0.8500	 0.3980
L	 0.8990	 0.4430
N	 0.9230	 0.4530
P	 0.8740	 0.3770
Y	 0.6550	 0.1990

