



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:04 PM UTC

PDB ID : 9EX9 / pdb_00009ex9
EMDB ID : EMD-50033
Title : Cryo EM map and model of the vaccinia minimal RNA polymerase
Authors : Grimm, C.; Jungwirth, S.; Fischer, U.
Deposited on : 2024-04-05
Resolution : 2.50 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
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) : 2.49

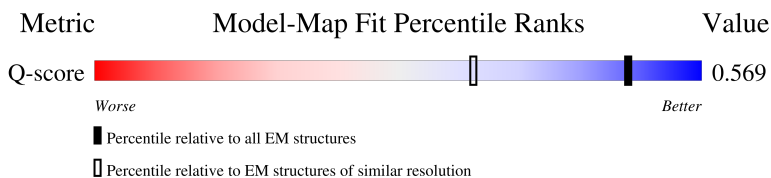
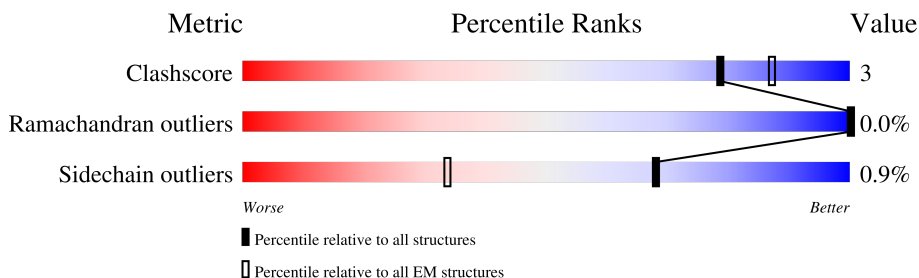
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	1286	 90% 7%
2	B	1164	 91% 5%
3	C	305	 92% 8%
4	E	186	 92% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	164	63%37%
6	G	161	48% 83%12%5%
7	J	63	90%6%
8	S	259	8% 51%7%42%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 54148 atoms, of which 27178 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1260	Total	C	H	N	O	S	0	0
			20363	6511	10242	1669	1896	45		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	THR	SER	variant	UNP P20504
A	489	GLU	LYS	variant	UNP P20504
A	1015	LYS	ARG	variant	UNP P20504

- Molecule 2 is a protein called DNA-directed RNA polymerase 133 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1130	Total	C	H	N	O	S	1	0
			18255	5804	9152	1553	1698	48		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	variant	UNP P68694
B	343	PHE	TYR	variant	UNP P68694

- Molecule 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	304	Total	C	H	N	O	S	0	0
			4954	1608	2470	399	464	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	ASN	ASP	variant	UNP P21087

- Molecule 4 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	185	Total	C	H	N	O	S	0	0
			3038	968	1540	248	277	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ACE	-	acetylation	UNP P68608

- Molecule 5 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	103	Total	C	H	N	O	S	0	0
			1723	545	874	148	153	3		

- Molecule 6 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	153	Total	C	H	N	O	S	0	0
			2373	753	1181	198	235	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	61	Total	C	H	N	O	S	0	0
			1018	310	528	88	88	4		

- Molecule 8 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms							AltConf	Trace
8	S	150	Total	C	H	N	O	P	S	0	0
			2419	768	1191	198	256	2	4		

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

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

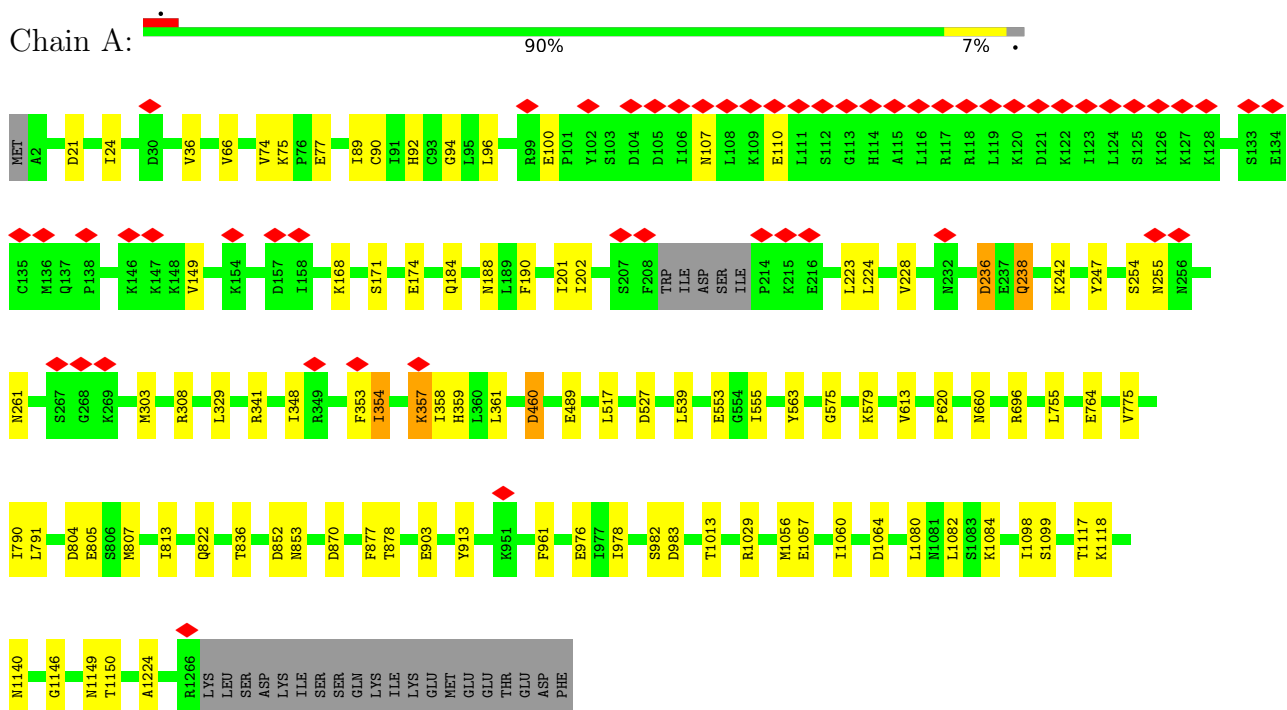
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total 2	Zn 2	0
10	B	1	Total 1	Zn 1	0
10	J	1	Total 1	Zn 1	0

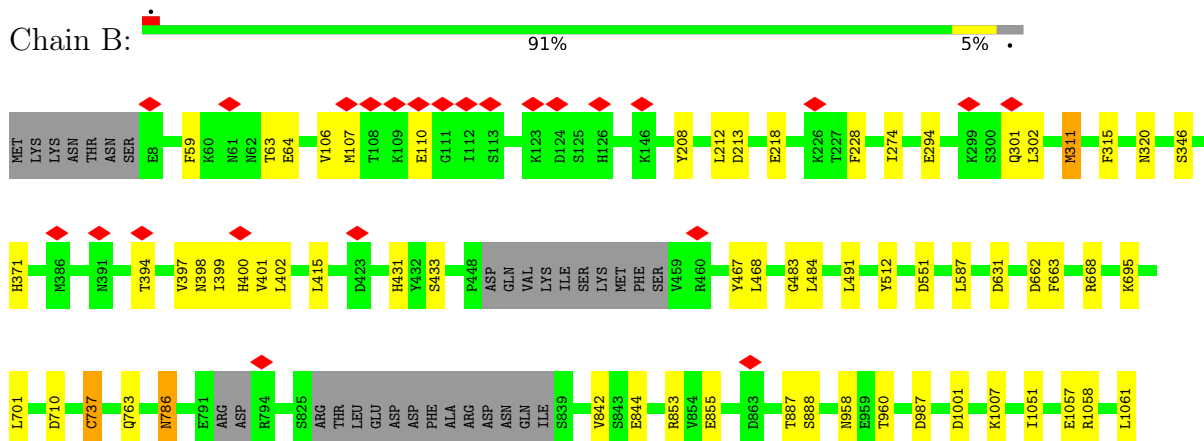
3 Residue-property plots

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 147 kDa polypeptide



- Molecule 2: DNA-directed RNA polymerase 133 kDa polypeptide





- Molecule 3: DNA-directed RNA polymerase 35 kDa subunit

Chain C: 92% 8%



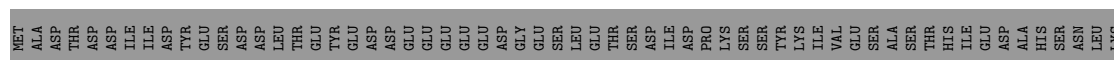
- Molecule 4: DNA-directed RNA polymerase 22 kDa subunit

Chain E: 92% 6% ..



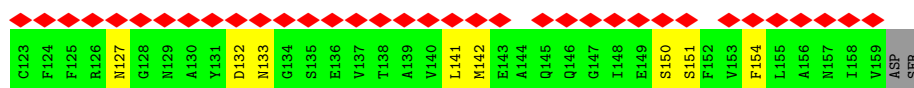
- Molecule 5: DNA-directed RNA polymerase 19 kDa subunit

Chain F: 63% 37%



- Molecule 6: DNA-directed RNA polymerase 18 kDa subunit

Chain G: 48% 83% 12% 5%



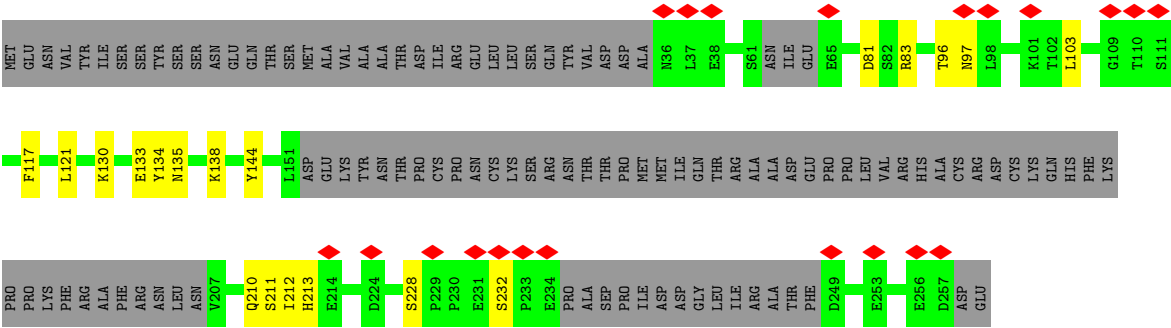
- Molecule 7: DNA-directed RNA polymerase 7 kDa subunit

Chain J: 90% 6% .



- Molecule 8: DNA-directed RNA polymerase 30 kDa polypeptide

Chain S: 8% 51% 7% 42%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	404153	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.256	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	246.784, 246.784, 246.784	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.964, 0.964, 0.964	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: SEP, MG, ACE, 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	0.21	0/10324	0.32	0/13954
2	B	0.20	0/9296	0.29	0/12556
3	C	0.21	0/2540	0.31	0/3440
4	E	0.30	2/1523 (0.1%)	1.00	1/2071 (0.0%)
5	F	0.21	0/863	0.34	0/1158
6	G	0.11	0/1209	0.24	0/1639
7	J	0.23	0/494	0.34	0/663
8	S	0.14	0/1226	0.26	0/1643
All	All	0.21	2/27475 (0.0%)	0.38	1/37124 (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
4	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	MET	C-N	6.36	1.43	1.33
4	E	0	ACE	C-N	6.02	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	MET	O-C-N	-43.13	53.99	123.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	1	MET	Mainchain

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	10121	10242	10242	68	0
2	B	9103	9152	9154	44	0
3	C	2484	2470	2470	14	0
4	E	1498	1540	1549	8	0
5	F	849	874	874	0	0
6	G	1192	1181	1181	13	0
7	J	490	528	528	3	0
8	S	1228	1191	1190	14	0
9	A	1	0	0	0	0
10	A	2	0	0	0	0
10	B	1	0	0	0	0
10	J	1	0	0	0	0
All	All	26970	27178	27188	150	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 3.

All (150) 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:976:GLU:OE1	1:A:1149:ASN:ND2	2.11	0.82
2:B:433:SER:OG	2:B:695:LYS:O	2.01	0.77
1:A:75:LYS:NZ	1:A:188:ASN:O	2.15	0.76
2:B:853:ARG:NH2	2:B:855:GLU:OE1	2.21	0.74
3:C:34:LEU:HD12	3:C:182:VAL:HG12	1.70	0.73
1:A:563:TYR:OH	3:C:272:GLU:OE1	2.06	0.73
2:B:208:TYR:OH	2:B:315:PHE:O	2.05	0.73
1:A:553:GLU:OE1	1:A:553:GLU:N	2.22	0.72
1:A:903:GLU:N	1:A:903:GLU:OE1	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:763:GLN:OE1	2:B:763:GLN:N	2.24	0.71
1:A:764:GLU:OE2	2:B:1058:ARG:NH1	2.24	0.70
3:C:119:GLU:N	3:C:119:GLU:OE1	2.25	0.69
1:A:174:GLU:N	1:A:174:GLU:OE1	2.26	0.69
1:A:527:ASP:O	8:S:210:GLN:NE2	2.27	0.67
6:G:30:ALA:O	6:G:34:THR:HG22	1.95	0.65
6:G:34:THR:HG23	6:G:35:TYR:CD2	2.33	0.64
1:A:575:GLY:O	1:A:660:ASN:ND2	2.32	0.63
2:B:301:GLN:N	2:B:301:GLN:OE1	2.31	0.63
2:B:887:THR:O	2:B:888:SER:OG	2.10	0.62
1:A:870:ASP:OD2	1:A:913:TYR:OH	2.18	0.62
3:C:239:GLU:OE2	3:C:274:TYR:OH	2.17	0.62
1:A:517:LEU:HD11	1:A:539:LEU:HD22	1.82	0.61
1:A:460:ASP:N	1:A:460:ASP:OD1	2.31	0.61
7:J:2:VAL:O	7:J:2:VAL:HG12	2.00	0.60
2:B:987:ASP:OD2	2:B:1007:LYS:NZ	2.35	0.60
6:G:92:GLU:N	6:G:92:GLU:OE1	2.35	0.60
3:C:50:GLU:N	3:C:50:GLU:OE1	2.31	0.59
2:B:218:GLU:HB2	2:B:274:ILE:HD11	1.84	0.59
6:G:127:ASN:O	6:G:127:ASN:ND2	2.35	0.59
1:A:238:GLN:OE1	1:A:238:GLN:N	2.37	0.58
2:B:844:GLU:OE1	2:B:844:GLU:N	2.36	0.58
2:B:431:HIS:HB3	2:B:701:LEU:HD21	1.87	0.57
1:A:807:MET:HE1	1:A:813:ILE:HG21	1.88	0.56
4:E:13:LEU:O	4:E:50:VAL:HG21	2.06	0.56
1:A:74:VAL:HG22	1:A:190:PHE:CE2	2.41	0.56
2:B:59:PHE:N	2:B:64:GLU:O	2.37	0.56
2:B:483:GLY:C	2:B:484:LEU:HD12	2.31	0.56
4:E:71:TYR:OH	4:E:77:ASP:OD2	2.18	0.55
1:A:1057:GLU:OE1	8:S:96:THR:OG1	2.25	0.55
6:G:93:ASP:N	6:G:96:ASN:OD1	2.40	0.55
1:A:77:GLU:OE1	1:A:77:GLU:N	2.39	0.55
6:G:142:MET:HA	6:G:142:MET:HE2	1.89	0.55
2:B:958:ASN:ND2	2:B:960:THR:O	2.40	0.54
6:G:132:ASP:OD1	6:G:133:ASN:N	2.40	0.54
4:E:21:ARG:NH1	4:E:55:ASP:OD2	2.41	0.54
2:B:64:GLU:OE1	2:B:106:VAL:HG22	2.07	0.54
8:S:81:ASP:OD2	8:S:83:ARG:NH1	2.41	0.54
1:A:1064:ASP:N	1:A:1064:ASP:OD1	2.39	0.53
1:A:852:ASP:OD1	1:A:853:ASN:N	2.42	0.53
8:S:97:ASN:CB	8:S:103:LEU:HD11	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:GLU:HG2	2:B:311:MET:HE1	1.91	0.52
8:S:212:ILE:HG22	8:S:213:HIS:CD2	2.43	0.52
1:A:24:ILE:HB	1:A:66:VAL:HG12	1.91	0.52
1:A:341:ARG:NE	1:A:361:LEU:HD13	2.25	0.51
2:B:467:TYR:OH	2:B:668:ARG:NH1	2.43	0.51
1:A:21:ASP:OD1	2:B:1108:LYS:NZ	2.27	0.51
3:C:82:TYR:OH	3:C:140:GLU:OE2	2.19	0.51
1:A:1029:ARG:NH2	8:S:144:TYR:OH	2.43	0.50
1:A:877:PHE:O	1:A:878:THR:OG1	2.21	0.50
1:A:254:SER:OG	1:A:255:ASN:N	2.44	0.50
1:A:92:HIS:O	1:A:168:LYS:NZ	2.44	0.49
2:B:737:CYS:SG	7:J:48:ILE:HD11	2.52	0.49
8:S:211:SER:C	8:S:212:ILE:HD12	2.37	0.49
1:A:223:LEU:HD13	1:A:247:TYR:HA	1.95	0.49
8:S:212:ILE:HD12	8:S:212:ILE:N	2.28	0.49
1:A:36:VAL:HG21	1:A:224:LEU:HB3	1.94	0.48
1:A:89:ILE:HG22	1:A:96:LEU:HD23	1.95	0.48
1:A:354:ILE:HD12	1:A:354:ILE:N	2.28	0.48
1:A:1082:LEU:C	1:A:1082:LEU:HD23	2.38	0.48
4:E:170:VAL:HG23	4:E:171:THR:HG23	1.94	0.48
6:G:141:LEU:HD22	6:G:154:PHE:CB	2.43	0.47
3:C:189:VAL:HG22	3:C:198:PHE:CD2	2.48	0.47
2:B:1001:ASP:OD2	3:C:191:SER:OG	2.29	0.47
4:E:18:GLU:OE1	4:E:35:TYR:OH	2.29	0.47
1:A:804:ASP:OD1	1:A:805:GLU:N	2.47	0.47
2:B:212:LEU:HD23	2:B:213:ASP:N	2.30	0.47
3:C:245:ASN:O	3:C:249:GLY:N	2.48	0.47
2:B:399:ILE:HG22	2:B:400:HIS:N	2.29	0.46
2:B:397:VAL:HG13	2:B:397:VAL:O	2.16	0.46
2:B:662:ASP:OD1	2:B:663:PHE:N	2.48	0.46
1:A:696:ARG:O	2:B:346:SER:O	2.33	0.46
1:A:1080:LEU:HD21	1:A:1084:LYS:HE3	1.98	0.46
6:G:14:LEU:HD13	6:G:68:ILE:HD12	1.98	0.46
1:A:107:ASN:ND2	1:A:110:GLU:OE1	2.49	0.46
3:C:80:LEU:C	3:C:80:LEU:HD12	2.41	0.46
1:A:110:GLU:OE1	1:A:110:GLU:N	2.49	0.46
6:G:141:LEU:HD22	6:G:154:PHE:HB2	1.98	0.46
2:B:1154:ASP:OD1	2:B:1154:ASP:N	2.48	0.46
2:B:394:THR:HG22	2:B:394:THR:O	2.16	0.46
1:A:236:ASP:N	1:A:236:ASP:OD1	2.50	0.45
7:J:2:VAL:HA	7:J:18:ARG:HD3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:GLN:NE2	4:E:167:ASN:OD1	2.47	0.45
3:C:234:VAL:HG12	3:C:234:VAL:O	2.16	0.45
1:A:359:HIS:CE1	1:A:361:LEU:HD12	2.51	0.45
1:A:613:VAL:HG13	1:A:620:PRO:HG3	1.98	0.45
2:B:228:PHE:HA	2:B:311:MET:HE2	1.98	0.45
1:A:201:ILE:HG23	1:A:202:ILE:HG23	1.97	0.45
1:A:1140:ASN:HA	4:E:106:ILE:HD12	1.98	0.45
2:B:786:ASN:N	2:B:786:ASN:OD1	2.49	0.45
8:S:133:GLU:O	8:S:134:TYR:CD2	2.70	0.45
1:A:168:LYS:O	1:A:171:SER:OG	2.34	0.44
1:A:348:ILE:HG23	1:A:353:PHE:CE2	2.53	0.44
1:A:755:LEU:HD23	1:A:961:PHE:HE1	1.82	0.44
8:S:135:ASN:OD1	8:S:138:LYS:N	2.50	0.44
1:A:357:LYS:HG3	1:A:358:ILE:HD12	1.99	0.44
1:A:978:ILE:N	1:A:978:ILE:HD12	2.33	0.44
1:A:1098:ILE:O	1:A:1099:SER:OG	2.31	0.44
3:C:40:VAL:HG23	3:C:53:LEU:HD21	2.00	0.44
1:A:1224:ALA:HB2	2:B:1136:VAL:HG13	1.99	0.44
1:A:1013:THR:O	1:A:1013:THR:HG23	2.18	0.44
2:B:512:TYR:OH	2:B:551:ASP:OD2	2.34	0.44
2:B:483:GLY:O	2:B:484:LEU:HD12	2.17	0.44
1:A:1146:GLY:O	1:A:1150:THR:HG22	2.18	0.43
6:G:39:GLU:OE2	6:G:42:GLY:N	2.50	0.43
1:A:982:SER:OG	1:A:983:ASP:N	2.52	0.43
1:A:1060:ILE:HD12	1:A:1060:ILE:N	2.34	0.43
2:B:1057:GLU:OE1	2:B:1057:GLU:N	2.46	0.43
6:G:150:SER:O	6:G:151:SER:OG	2.35	0.43
1:A:303:MET:O	1:A:308:ARG:NH1	2.52	0.42
1:A:348:ILE:HG23	1:A:353:PHE:CD2	2.54	0.42
2:B:842:VAL:HG22	2:B:842:VAL:O	2.19	0.42
8:S:97:ASN:HB2	8:S:103:LEU:HD11	2.00	0.42
1:A:66:VAL:HG11	1:A:228:VAL:HG22	2.01	0.42
2:B:1051:ILE:N	2:B:1051:ILE:HD12	2.35	0.42
3:C:141:LEU:HD12	3:C:141:LEU:C	2.45	0.42
1:A:90:CYS:O	1:A:94:GLY:N	2.50	0.42
1:A:100:GLU:OE1	1:A:100:GLU:N	2.42	0.42
1:A:149:VAL:HG21	1:A:242:LYS:HB2	2.01	0.42
1:A:489:GLU:OE1	1:A:489:GLU:N	2.51	0.42
1:A:1056:MET:O	8:S:96:THR:HG21	2.20	0.42
1:A:1140:ASN:HA	4:E:106:ILE:CD1	2.50	0.41
2:B:1100:ILE:HD12	2:B:1100:ILE:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:LEU:C	1:A:1080:LEU:HD23	2.45	0.41
6:G:104:LEU:HD21	6:G:141:LEU:HD21	2.01	0.41
2:B:302:LEU:HD12	2:B:302:LEU:N	2.35	0.41
2:B:402:LEU:HD12	2:B:402:LEU:C	2.45	0.41
2:B:398:ASN:O	2:B:401:VAL:HG22	2.19	0.41
8:S:134:TYR:CD1	8:S:134:TYR:O	2.73	0.41
2:B:110:GLU:OE1	2:B:110:GLU:N	2.45	0.41
2:B:399:ILE:HG22	2:B:400:HIS:H	1.85	0.41
1:A:517:LEU:HD12	1:A:517:LEU:H	1.86	0.41
2:B:63:THR:HG22	2:B:107:MET:HB2	2.03	0.41
2:B:467:TYR:O	2:B:468:LEU:HB3	2.21	0.41
3:C:114:VAL:HG12	3:C:115:ASP:N	2.35	0.41
1:A:329:LEU:HD11	1:A:358:ILE:HG21	2.03	0.40
1:A:1117:THR:HG22	1:A:1118:LYS:N	2.37	0.40
1:A:790:ILE:HG22	1:A:791:LEU:N	2.37	0.40
1:A:804:ASP:H	1:A:807:MET:HE2	1.85	0.40
2:B:587:LEU:O	2:B:631:ASP:HA	2.22	0.40
8:S:117:PHE:CZ	8:S:121:LEU:HD11	2.56	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	1256/1286 (98%)	1204 (96%)	52 (4%)	0	100	100
2	B	1123/1164 (96%)	1071 (95%)	51 (4%)	1 (0%)	48	68
3	C	302/305 (99%)	290 (96%)	12 (4%)	0	100	100
4	E	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
5	F	101/164 (62%)	99 (98%)	2 (2%)	0	100	100
6	G	149/161 (92%)	143 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	J	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
8	S	140/259 (54%)	136 (97%)	4 (3%)	0	100	100
All	All	3313/3588 (92%)	3177 (96%)	135 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	737	CYS

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	1131/1157 (98%)	1120 (99%)	11 (1%)	68	86
2	B	1032/1064 (97%)	1022 (99%)	10 (1%)	68	86
3	C	286/287 (100%)	284 (99%)	2 (1%)	76	89
4	E	174/175 (99%)	173 (99%)	1 (1%)	78	91
5	F	94/151 (62%)	94 (100%)	0	100	100
6	G	136/144 (94%)	136 (100%)	0	100	100
7	J	60/62 (97%)	59 (98%)	1 (2%)	53	78
8	S	139/237 (59%)	138 (99%)	1 (1%)	76	89
All	All	3052/3277 (93%)	3026 (99%)	26 (1%)	68	87

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	236	ASP
1	A	238	GLN
1	A	261	ASN
1	A	354	ILE
1	A	357	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	460	ASP
1	A	555	ILE
1	A	579	LYS
1	A	775	VAL
1	A	836	THR
2	B	311	MET
2	B	320	ASN
2	B	371	HIS
2	B	415	LEU
2	B	491	LEU
2	B	710	ASP
2	B	786	ASN
2	B	1061	LEU
2	B	1108	LYS
2	B	1158	LEU
3	C	187	PHE
3	C	286	LEU
4	E	106	ILE
7	J	49	GLU
8	S	130	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	230	ASN
1	A	385	HIS
1	A	413	ASN
1	A	428	ASN
1	A	685	GLN
1	A	686	GLN
2	B	62	ASN
2	B	72	ASN
2	B	380	ASN
2	B	620	GLN
2	B	696	GLN
2	B	1110	ASN
3	C	3	HIS
3	C	260	ASN
6	G	157	ASN
8	S	213	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
8	SEP	S	228	8	8,9,10	1.58	1 (12%)	7,12,14	1.29	1 (14%)
8	SEP	S	232	8	8,9,10	1.61	1 (12%)	7,12,14	1.13	1 (14%)

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
8	SEP	S	228	8	-	3/6/8/10	-
8	SEP	S	232	8	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	232	SEP	P-O1P	3.51	1.61	1.50
8	S	228	SEP	P-O1P	3.44	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	228	SEP	OG-CB-CA	2.65	110.72	108.14
8	S	232	SEP	OG-CB-CA	2.26	110.34	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	228	SEP	CB-OG-P-O1P
8	S	228	SEP	CB-OG-P-O3P
8	S	232	SEP	CA-CB-OG-P
8	S	228	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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.

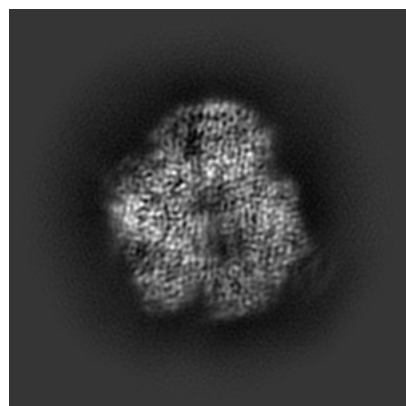
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50033. These allow visual inspection of the internal detail of the map and identification of artifacts.

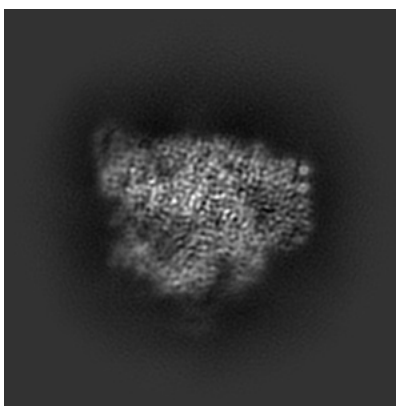
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

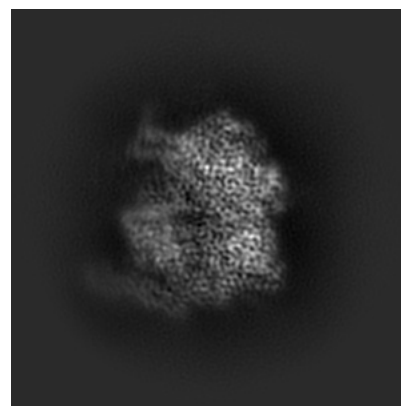
6.1.1 Primary map



X

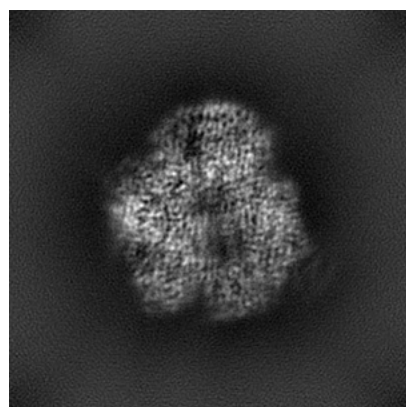


Y

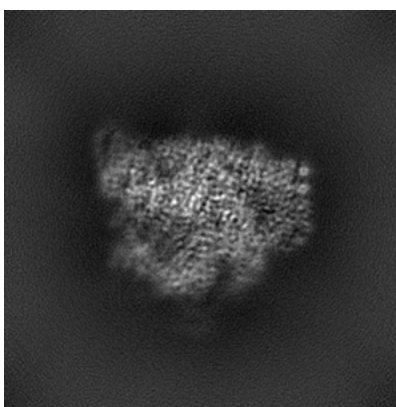


Z

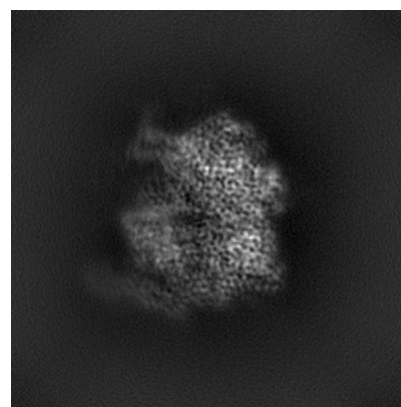
6.1.2 Raw map



X



Y

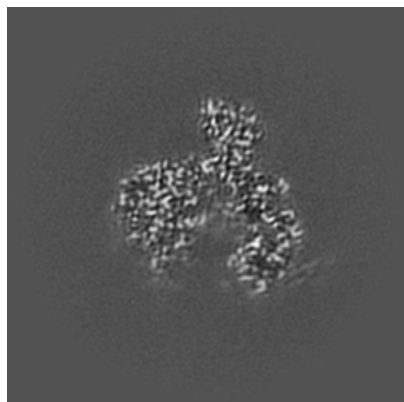


Z

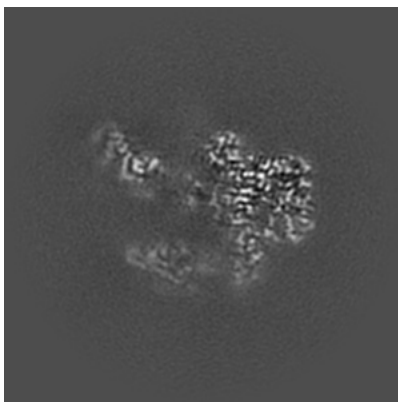
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

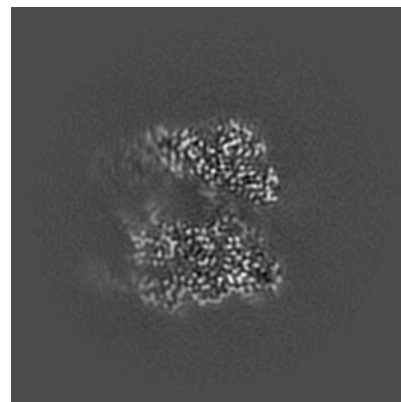
6.2.1 Primary map



X Index: 128

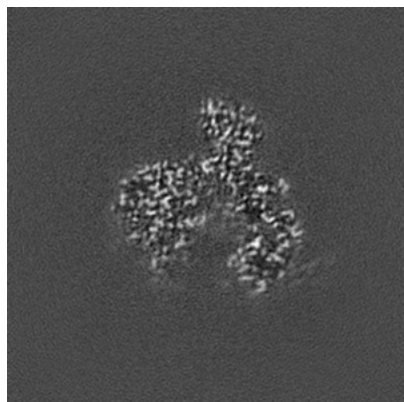


Y Index: 128

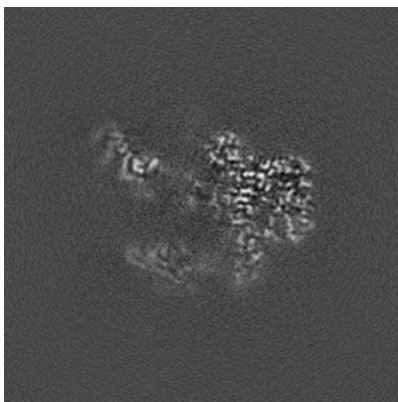


Z Index: 128

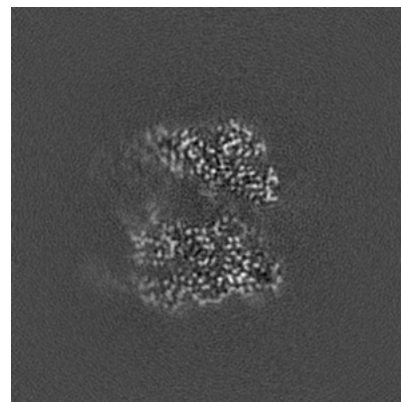
6.2.2 Raw map



X Index: 128



Y Index: 128

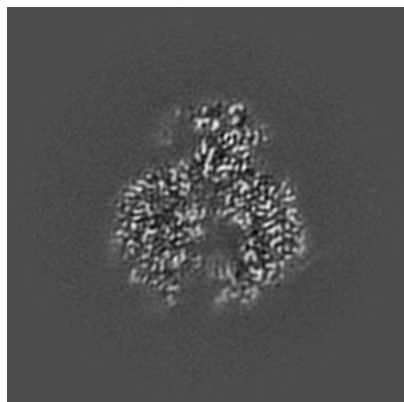


Z Index: 128

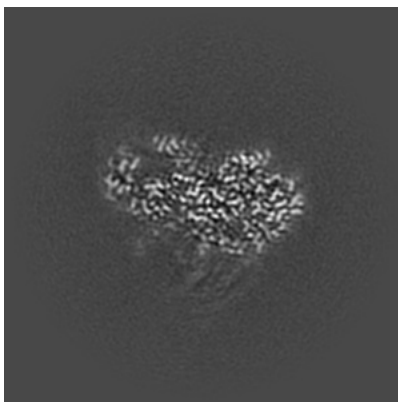
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

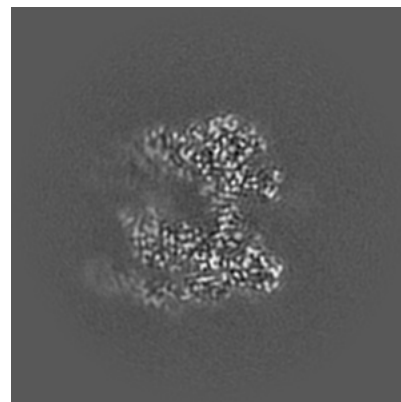
6.3.1 Primary map



X Index: 137

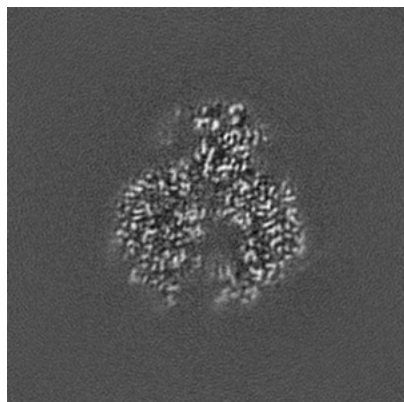


Y Index: 154

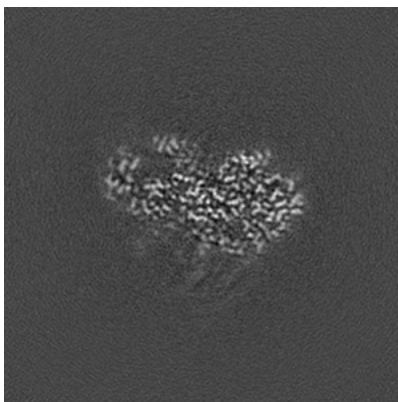


Z Index: 124

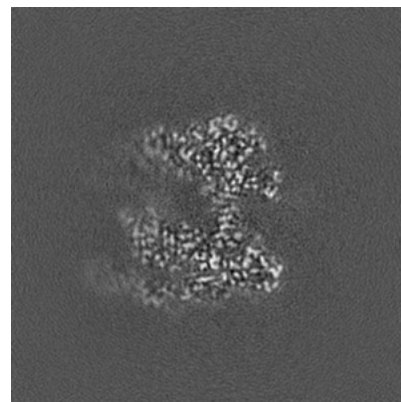
6.3.2 Raw map



X Index: 137



Y Index: 154

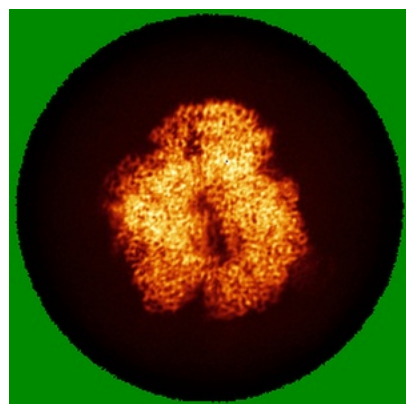


Z Index: 124

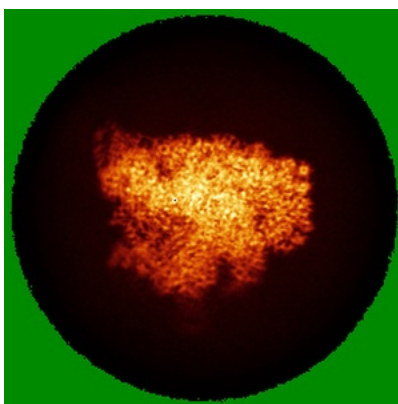
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

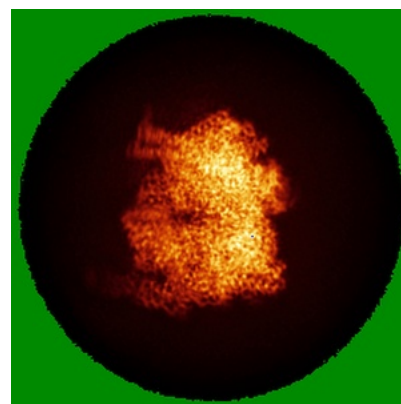
6.4.1 Primary map



X

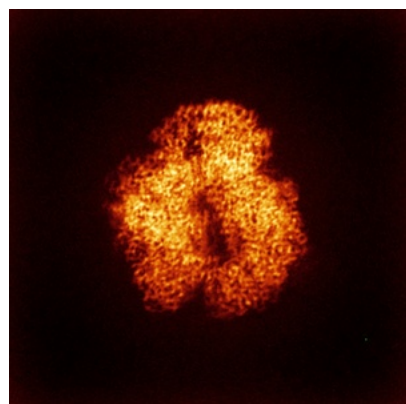


Y

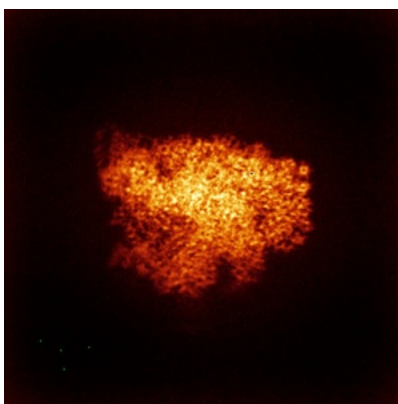


Z

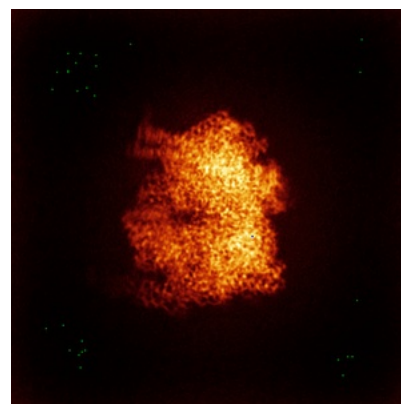
6.4.2 Raw map



X



Y

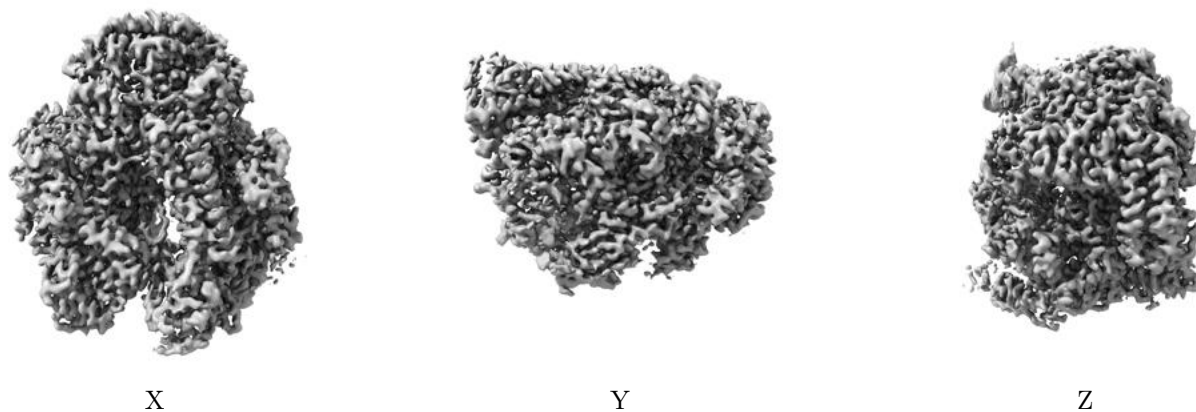


Z

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.

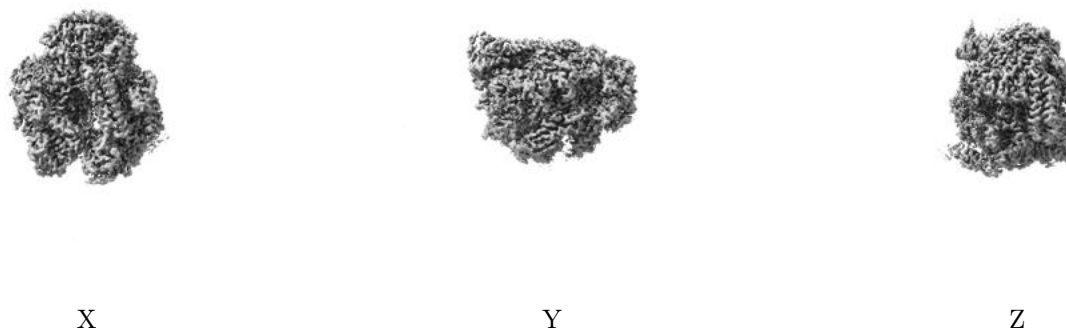
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

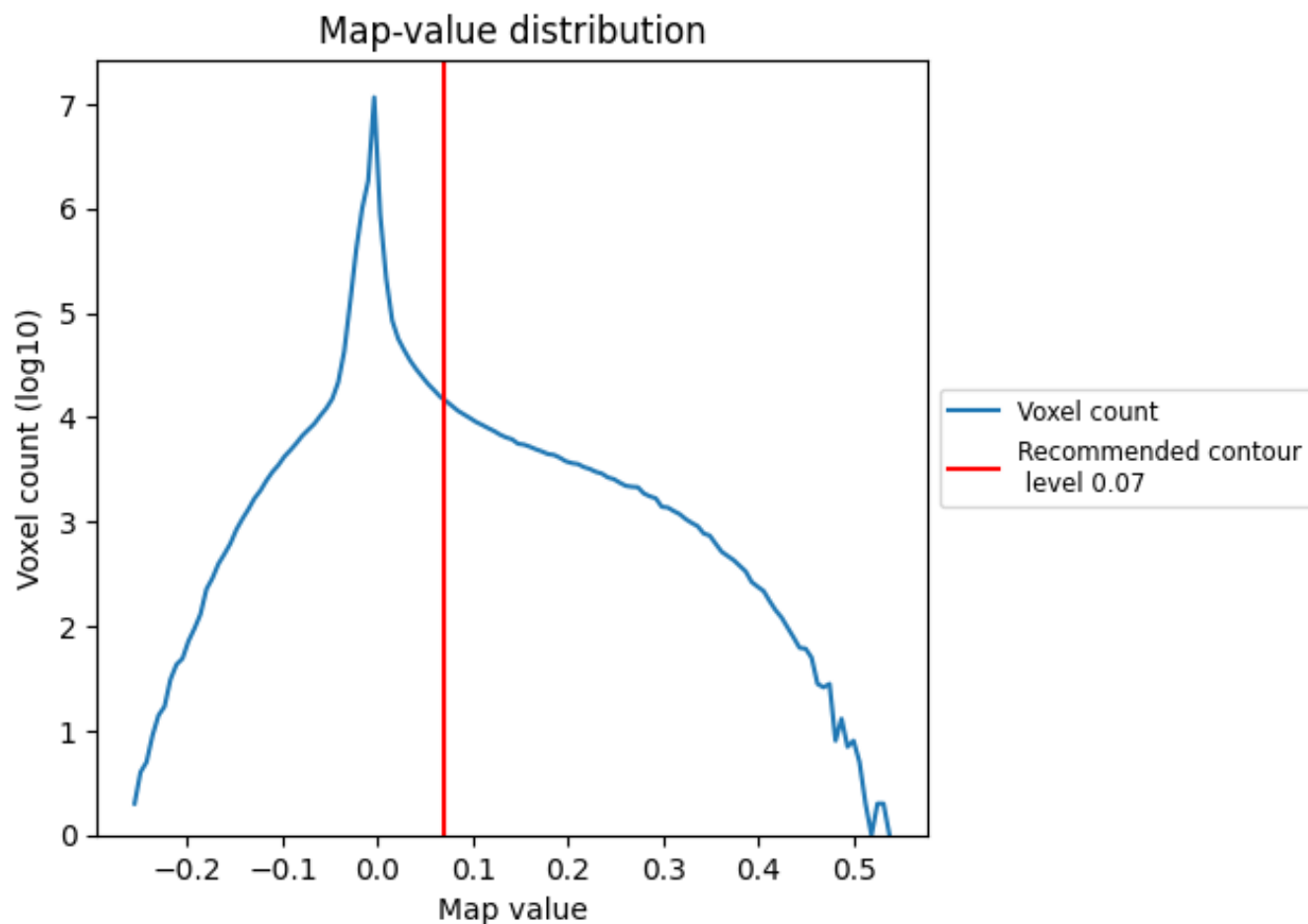
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

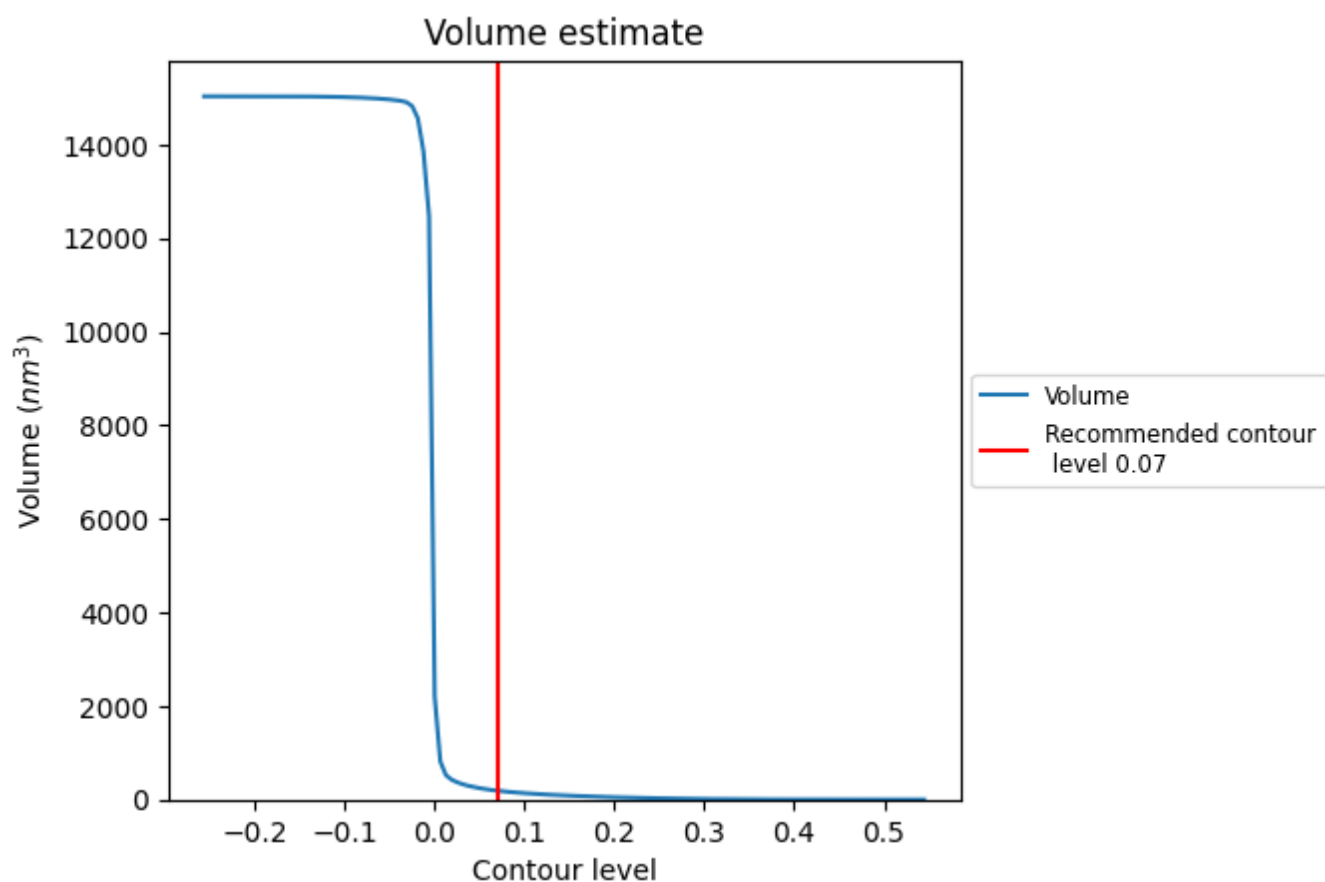
This section contains the results of statistical analysis of the map.

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.

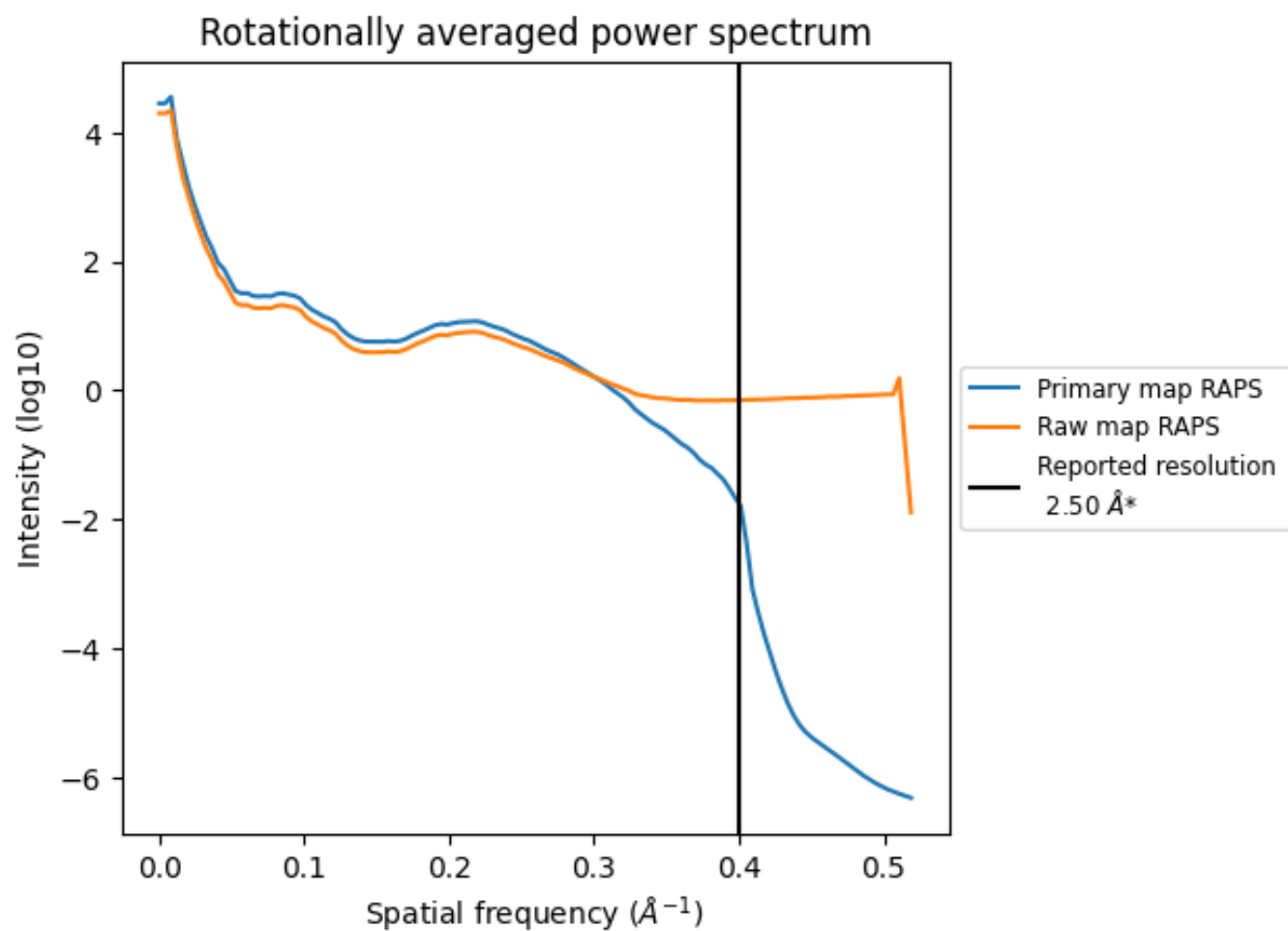
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 190 nm³; this corresponds to an approximate mass of 171 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 ⓘ

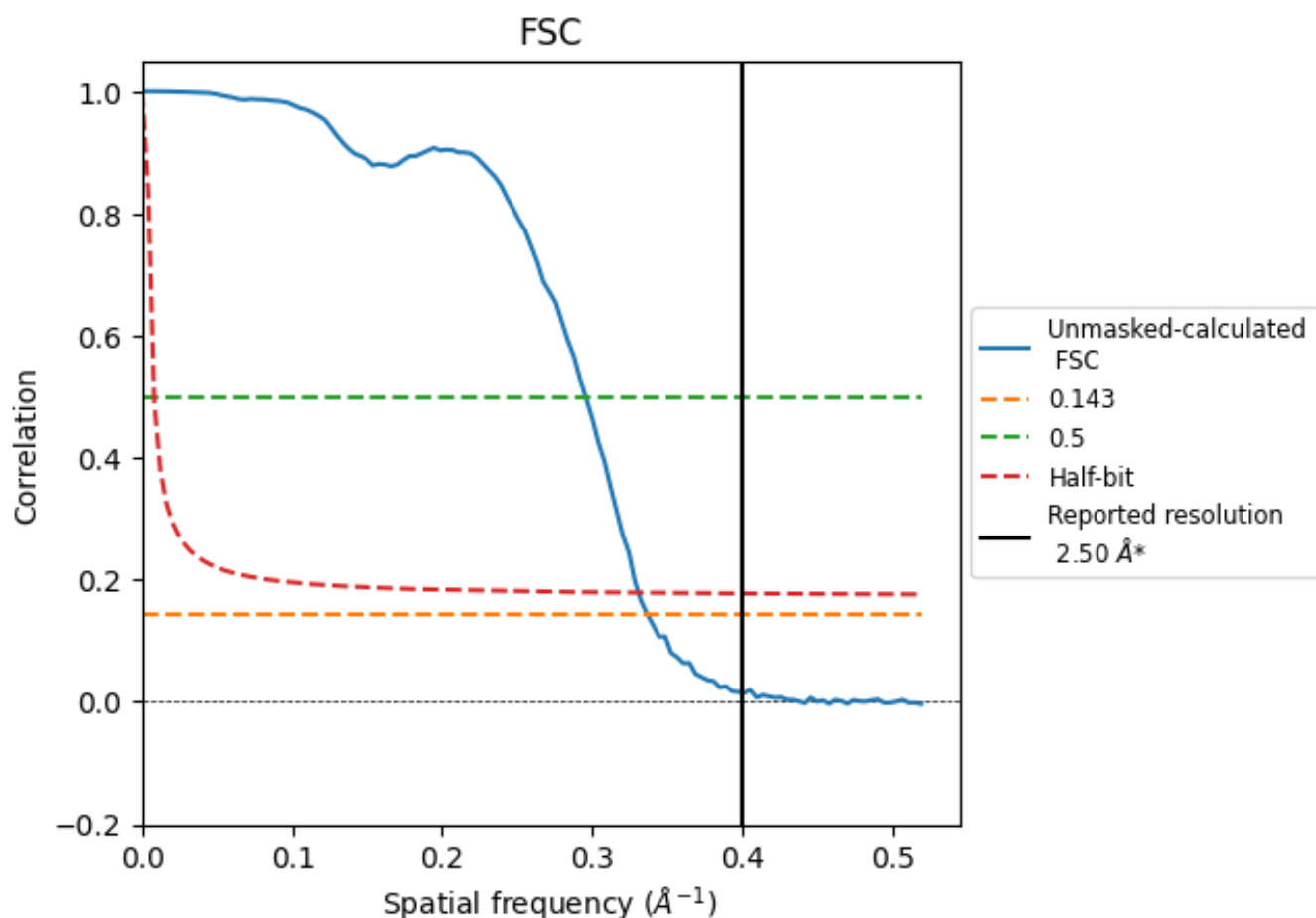


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

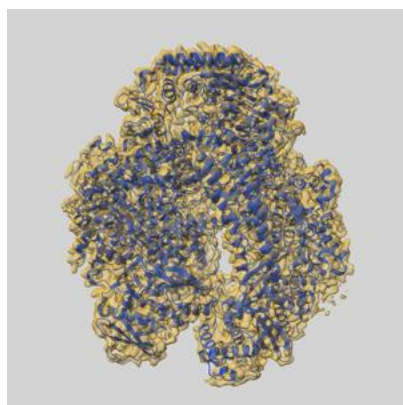
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.97	3.39	3.02

*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 2.97 differs from the reported value 2.5 by more than 10 %

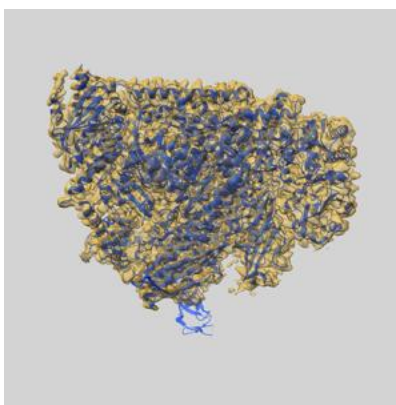
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50033 and PDB model 9EX9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

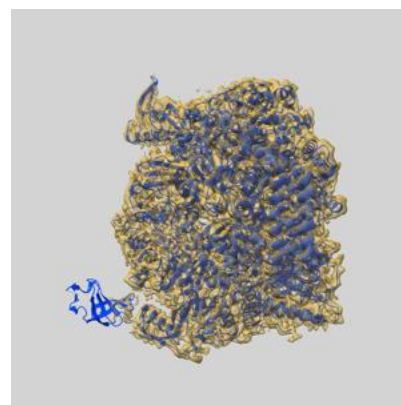
9.1 Map-model overlay [i](#)



X



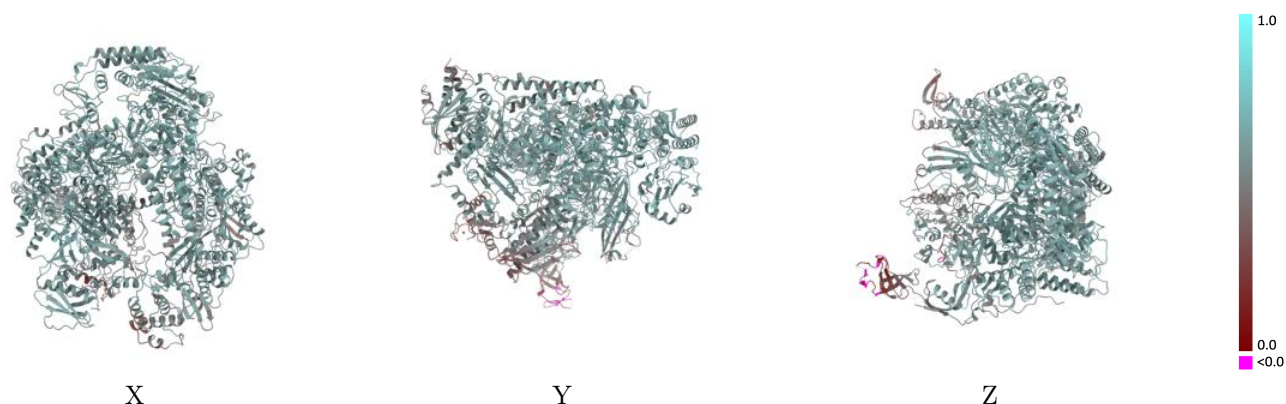
Y



Z

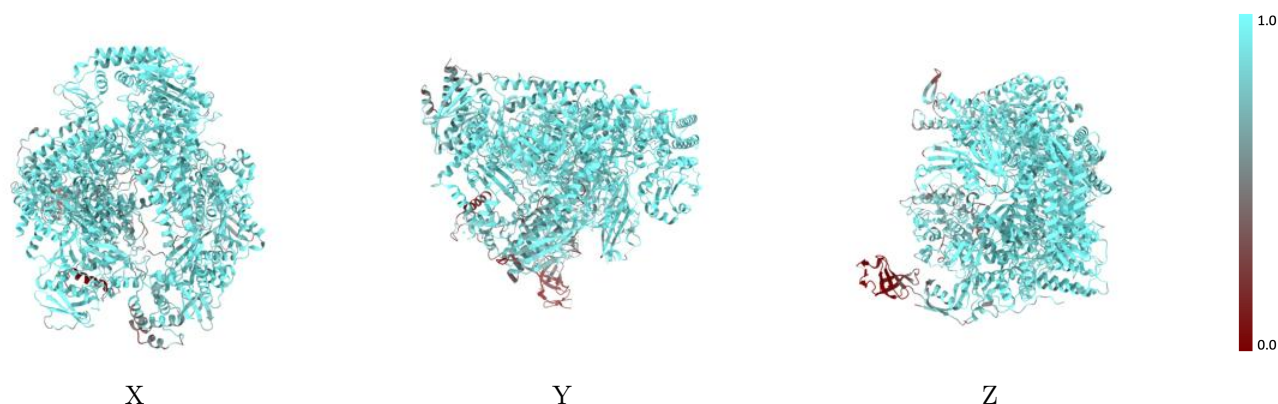
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



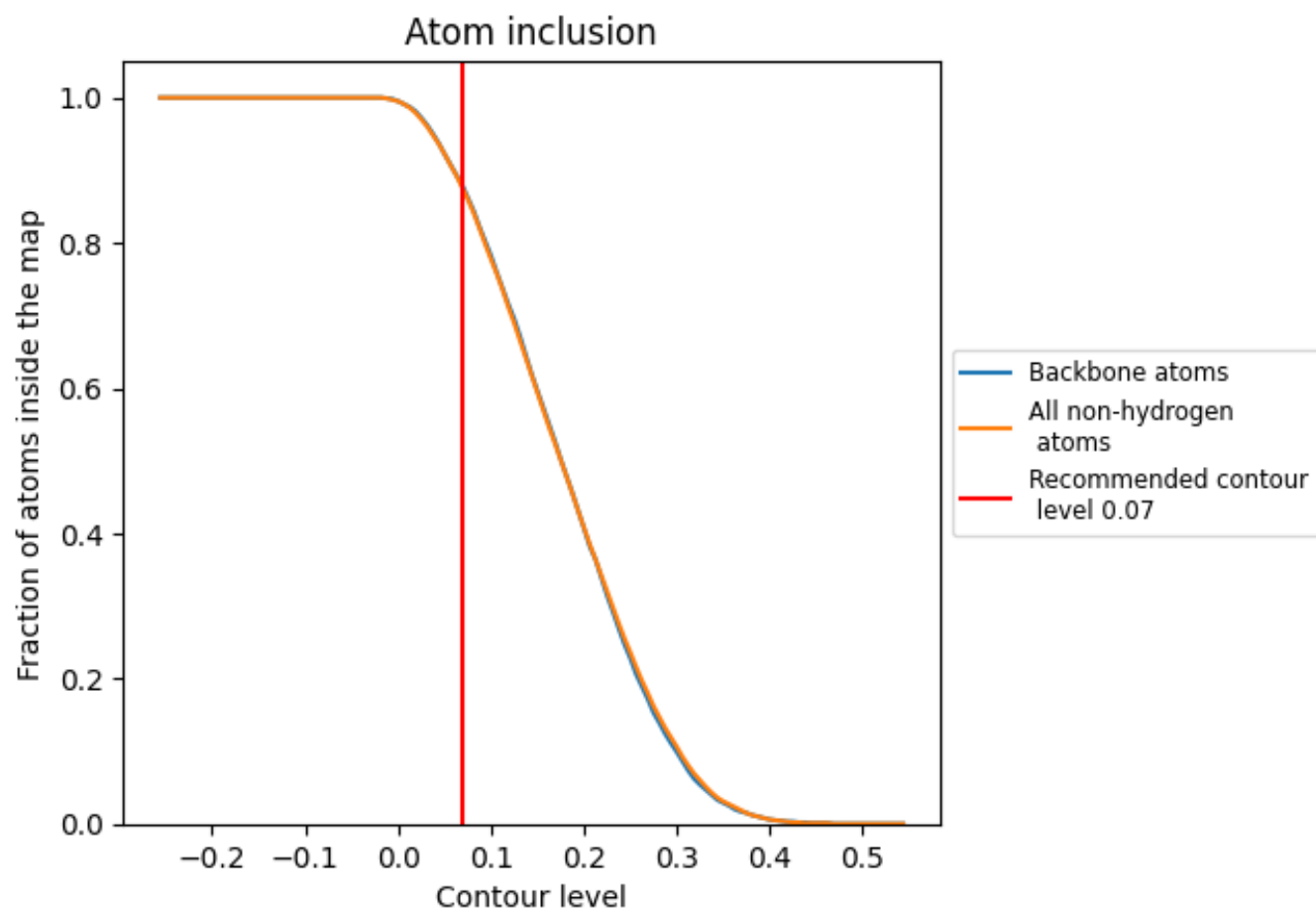
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.5690
A	0.8890	0.5650
B	0.9130	0.5850
C	0.9570	0.6000
E	0.9460	0.5950
F	0.9410	0.6040
G	0.4320	0.3970
J	0.9630	0.6110
S	0.6570	0.5150

