



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:43 PM UTC

PDB ID : 9GVJ / pdb_00009gvj
EMDB ID : EMD-51636
Title : MUC5AC mucin amino acids 28 to 1483
Authors : Haberman, M.; Kamyshinsky, R.; Fass, D.
Deposited on : 2024-09-24
Resolution : 2.91 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:

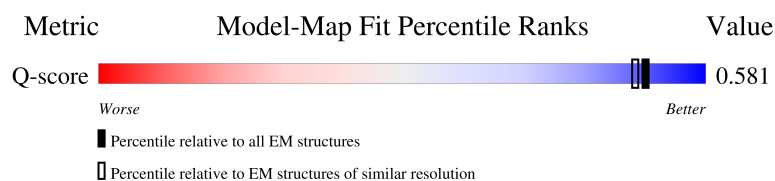
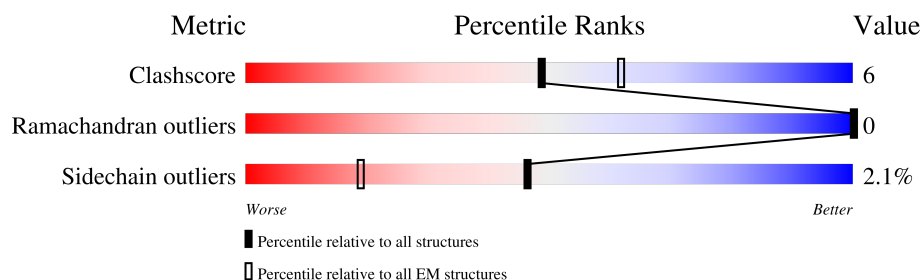
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.91 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	12972 (2.41 - 3.41)

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	1456	
1	B	1456	
1	C	1456	
1	D	1456	

2 Entry composition [i](#)

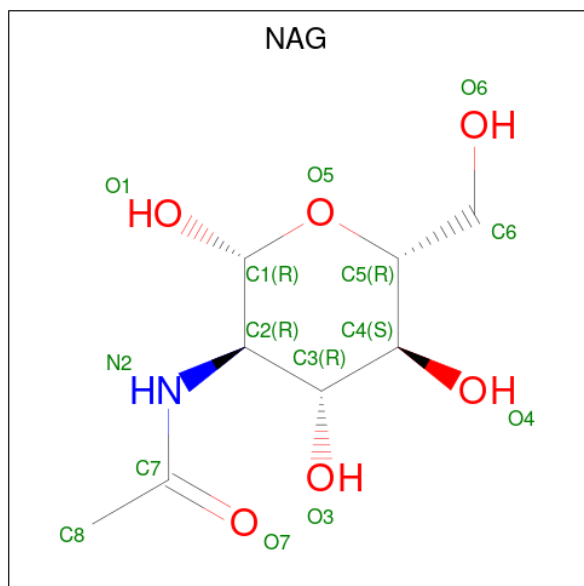
There are 5 unique types of molecules in this entry. The entry contains 17636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mucin-5AC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	690	Total	C	N	O	S	4	0
			5230	3250	903	1008	69		
1	B	688	Total	C	N	O	S	4	0
			5219	3242	903	1005	69		
1	C	463	Total	C	N	O	S	3	0
			3453	2138	596	663	56		
1	D	463	Total	C	N	O	S	4	0
			3465	2144	602	663	56		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Cu	0
			1	1	
4	B	1	Total	Cu	0
			1	1	

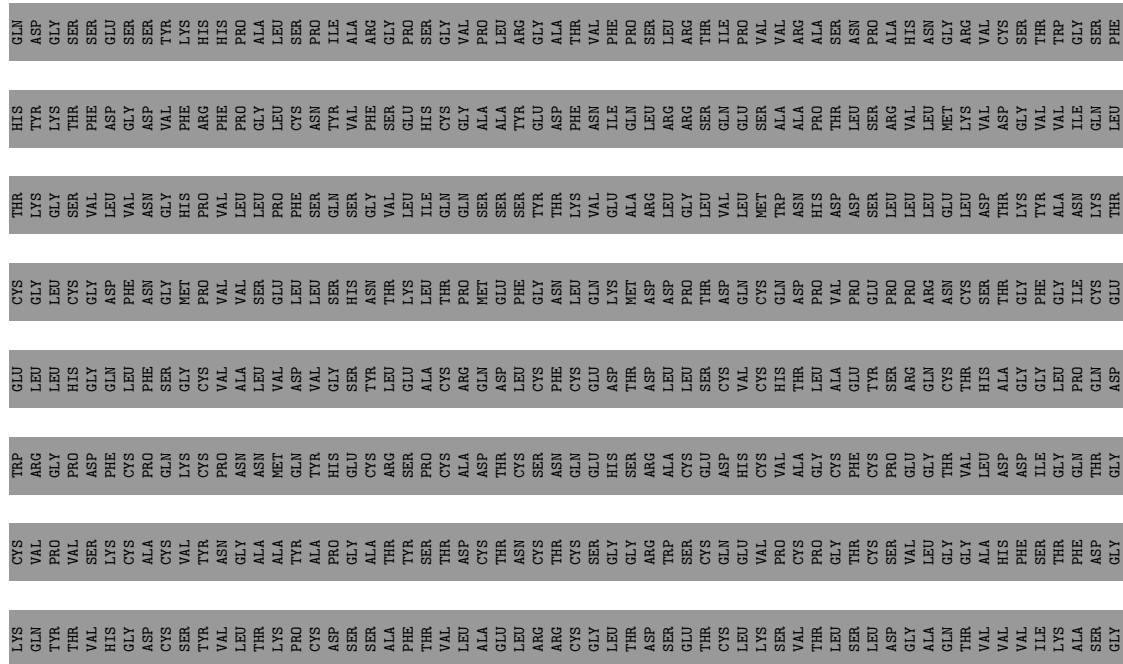
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	64	Total	O	0
			64	64	
5	B	39	Total	O	0
			39	39	
5	C	45	Total	O	0
			45	45	
5	D	29	Total	O	0
			29	29	

[illegible]

- Molecule 1: Mucin-5AC

[illegible]



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198256	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.313	Depositor
Minimum map value	-0.925	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.256	Depositor
Map size ($\text{\AA}$)	453.31, 453.31, 453.31	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8242, 0.8242, 0.8242	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: CU, NAG, CA

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	0.10	0/5356	0.26	0/7280
1	B	0.10	0/5344	0.27	0/7264
1	C	0.10	0/3548	0.28	0/4831
1	D	0.11	0/3563	0.31	0/4850
All	All	0.10	0/17811	0.28	0/24225

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5230	0	4954	51	0
1	B	5219	0	4947	61	0
1	C	3453	0	3179	43	0
1	D	3465	0	3199	48	0
2	A	42	0	39	1	0
2	B	42	0	39	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	64	0	0	0	0
5	B	39	0	0	0	0
5	C	45	0	0	0	0
5	D	29	0	0	0	0
All	All	17636	0	16357	195	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 (195) 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:C:1147:HIS:HB3	1:C:1202:GLY:HA3	1.69	0.73
1:B:548:GLN:O	1:B:553:MET:HA	1.89	0.72
1:A:660:ASP:HB3	1:A:670:CYS:HB3	1.73	0.71
1:D:1147:HIS:HB3	1:D:1202:GLY:HA3	1.74	0.70
1:C:1191:ASN:ND2	1:C:1195:ASP:O	2.25	0.70
1:C:1162:PRO:HG2	1:D:1162:PRO:HG2	1.75	0.69
1:B:183:LEU:HD11	1:B:185:LEU:HD23	1.74	0.68
1:B:430:CYS:HB3	1:B:564:ARG:HH21	1.59	0.67
1:C:1087:ARG:NH2	1:C:1131:ASP:OD2	2.20	0.67
1:A:483:SER:O	1:A:663:ASN:ND2	2.29	0.66
1:B:88:HIS:NE2	1:B:294:ASP:OD1	2.29	0.66
1:A:83:THR:OG1	1:A:124:ARG:NH2	2.29	0.65
1:D:1223:GLN:N	1:D:1223:GLN:OE1	2.30	0.65
1:B:461:THR:HG22	1:B:471:VAL:HB	1.79	0.64
1:A:548:GLN:O	1:A:553:MET:HA	1.98	0.62
1:B:454:GLY:HA2	1:B:609:ILE:HG13	1.82	0.61
1:C:968:LEU:HD23	1:C:992:PRO:HG2	1.82	0.61
1:A:354:THR:HG22	1:A:380:LEU:HB3	1.81	0.61
1:B:161:LEU:HD12	1:B:172:GLN:HB2	1.83	0.61
1:A:620:SER:HB3	1:A:623:ASN:HB2	1.83	0.61
1:C:971:PHE:HD1	1:C:984:GLY:HA2	1.66	0.60
1:A:623:ASN:HA	1:B:244:PRO:HG3	1.84	0.60
1:A:181:ALA:HB3	1:A:185:LEU:HG	1.83	0.60
1:B:170:ILE:HG23	1:B:179:VAL:HG22	1.84	0.60
1:A:382:ASP:O	1:A:385:GLN:NE2	2.35	0.59
1:B:83:THR:OG1	1:B:124:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLN:NE2	1:B:180:GLU:OE2	2.35	0.59
1:B:660:ASP:HB3	1:B:670:CYS:HB3	1.84	0.59
1:A:70:ARG:NH1	1:A:70:ARG:HB3	2.18	0.59
1:B:610:ARG:NH1	1:B:610:ARG:HB3	2.17	0.59
1:D:1080:PRO:HB3	1:D:1125:ALA:HB2	1.84	0.59
1:D:1081:CYS:HB3	1:D:1088:LYS:HG3	1.85	0.59
1:C:883:ASN:ND2	1:C:895:THR:O	2.28	0.58
1:C:1218:ASP:O	1:C:1222:MET:N	2.36	0.58
1:B:413:CYS:HA	1:B:428:VAL:HG23	1.85	0.58
1:A:183:LEU:HD11	1:A:185:LEU:HD23	1.85	0.58
1:D:926:GLU:OE2	1:D:965:LYS:NZ	2.28	0.58
1:D:930:VAL:HG12	1:D:946:VAL:HB	1.85	0.58
1:B:412:ASP:OD2	1:B:685:LYS:NZ	2.36	0.58
1:D:1049:THR:HG22	1:D:1061:PHE:HA	1.85	0.58
1:A:313:GLU:OE2	1:A:317:GLN:NE2	2.34	0.58
1:D:973:LEU:HD21	1:D:995:ILE:HD11	1.87	0.56
1:C:1049:THR:HG22	1:C:1061:PHE:HA	1.87	0.56
1:A:302:ASP:N	1:A:302:ASP:OD1	2.37	0.56
1:B:483:SER:O	1:B:663:ASN:ND2	2.38	0.55
1:A:720:THR:HG22	1:A:749:LEU:HB3	1.87	0.55
1:A:410:SER:HB2	2:A:1503:NAG:H82	1.87	0.55
1:C:900:LEU:HD22	1:C:1023:ASN:HB3	1.87	0.55
1:C:778:ASP:N	1:C:778:ASP:OD1	2.38	0.55
1:C:930:VAL:HG12	1:C:946:VAL:HB	1.89	0.54
1:B:77:ASN:HD21	1:B:321:ALA:HB2	1.73	0.54
1:A:244:PRO:HG3	1:B:623:ASN:HA	1.90	0.54
1:D:1147:HIS:CD2	1:D:1152:CYS:HA	2.44	0.53
1:B:732:SER:O	1:B:734:GLY:N	2.41	0.53
1:D:946:VAL:HG22	1:D:966:ILE:HG23	1.89	0.53
1:C:946:VAL:HG22	1:C:966:ILE:HG23	1.90	0.53
1:C:1080:PRO:HB3	1:C:1125:ALA:HB2	1.90	0.53
1:D:922[A]:ASN:HD22	1:D:1077:PRO:HG3	1.73	0.53
1:C:940:THR:HG23	1:C:941:GLN:HG2	1.90	0.52
1:B:390:PRO:HD2	1:B:393:LYS:HD3	1.90	0.52
1:B:243:ASP:HB2	1:B:246:ASP:HB2	1.92	0.52
1:D:971:PHE:HD2	1:D:984:GLY:HA3	1.74	0.52
1:B:706:LYS:H	1:B:706:LYS:CD	2.23	0.52
1:B:494:LEU:HB2	1:B:499:THR:HB	1.92	0.51
1:A:170:ILE:HG23	1:A:179:VAL:HG22	1.92	0.51
1:B:122:LEU:HD12	1:B:133:LEU:HD21	1.94	0.50
1:A:289:GLU:O	1:A:293:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1012:LEU:HD23	1:C:1020:ILE:HD11	1.93	0.50
1:D:1152:CYS:HB3	1:D:1180:PRO:HB2	1.93	0.49
1:C:849:LEU:HB3	1:C:857:CYS:HB3	1.94	0.49
1:D:889:SER:O	1:D:889:SER:OG	2.24	0.49
1:A:454:GLY:HA2	1:A:609:ILE:HG13	1.94	0.49
1:A:707:SER:HB2	1:A:755:CYS:HB2	1.94	0.49
1:D:1191:ASN:ND2	1:D:1195:ASP:O	2.46	0.49
1:B:265:ILE:HD12	1:B:265:ILE:H	1.78	0.49
1:C:905:VAL:HB	1:C:1020:ILE:HG22	1.95	0.49
1:D:928:THR:HA	1:D:947:VAL:HG22	1.95	0.49
1:B:192:ASP:N	1:B:192:ASP:OD1	2.46	0.48
1:B:750:ASP:OD2	1:B:754:LYS:NZ	2.37	0.48
1:B:87:PHE:CG	1:B:100:PRO:HA	2.48	0.48
1:D:973:LEU:HD13	1:D:993:TYR:CZ	2.48	0.48
1:A:90:LYS:HG3	1:A:96:VAL:HG22	1.96	0.48
1:B:411:THR:OG1	1:B:414:THR:HG22	2.13	0.48
1:A:610:ARG:HB2	1:A:610:ARG:NH1	2.28	0.48
1:A:732:SER:O	1:A:734:GLY:N	2.45	0.48
1:B:610:ARG:HB3	1:B:610:ARG:HH11	1.78	0.48
1:C:934:CYS:O	1:C:1052:ARG:NH2	2.47	0.48
1:A:460:LEU:HD11	1:A:473:ALA:HB2	1.95	0.48
1:C:1079:ASP:HB3	1:C:1082:THR:HB	1.96	0.48
1:B:74:PRO:O	1:B:76:HIS:ND1	2.46	0.47
1:D:1147:HIS:HD2	1:D:1152:CYS:HA	1.77	0.47
1:C:765:HIS:O	1:C:768:SER:OG	2.32	0.47
1:A:466:SER:OG	1:A:467:SER:N	2.47	0.46
1:A:529:ARG:HG3	1:A:535:ILE:HG12	1.97	0.46
1:C:973:LEU:HD11	1:C:995:ILE:HD11	1.96	0.46
1:A:87:PHE:CZ	1:A:131:PRO:HB3	2.50	0.46
1:B:273:GLN:HA	1:B:276:SER:HB3	1.96	0.46
1:D:1222:MET:HE3	1:D:1222:MET:HB3	1.81	0.46
1:D:1148:GLU:OE2	1:D:1201[A]:ARG:NH2	2.48	0.46
1:A:456:CYS:HB2	1:A:606:CYS:HB3	1.80	0.46
1:B:583[A]:ARG:HB2	1:B:589:VAL:HG22	1.98	0.46
1:B:84:TRP:CD2	1:B:313:GLU:HG2	2.51	0.46
1:A:408:THR:HG22	1:A:417:THR:HB	1.98	0.45
1:B:634:LEU:O	1:B:645:HIS:NE2	2.48	0.45
1:D:1012:LEU:HD23	1:D:1020:ILE:HD11	1.98	0.45
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.49	0.45
1:A:511:LEU:HD22	1:A:520:ILE:HG21	1.99	0.45
1:B:460:LEU:HD23	1:B:570:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:SER:OG	1:B:467:SER:N	2.47	0.45
1:C:1132:CYS:SG	1:D:1132:CYS:HB2	2.56	0.45
1:D:800:PRO:HB2	1:D:808:PHE:HE2	1.80	0.45
1:A:313:GLU:O	1:A:317:GLN:HG2	2.16	0.45
1:C:1084:ASN:HB3	1:C:1087:ARG:HD3	1.98	0.45
1:A:205:ASN:N	1:A:214:PHE:O	2.39	0.45
1:B:302:ASP:OD1	1:B:302:ASP:N	2.49	0.45
1:C:922[A]:ASN:HD22	1:C:1077:PRO:HG3	1.81	0.45
1:D:975:LEU:HD23	1:D:980:VAL:HG13	1.99	0.45
1:D:832:MET:SD	1:D:890:ARG:NH1	2.87	0.45
1:D:919:TYR:OH	1:D:1035:LEU:O	2.33	0.45
1:A:348:ARG:HB2	1:A:373:PHE:CE2	2.53	0.44
1:A:494:LEU:HB2	1:A:499:THR:HB	1.99	0.44
1:C:1185:CYS:HB3	1:C:1195:ASP:C	2.43	0.44
1:D:1024:LEU:HD11	1:D:1032:VAL:HG11	2.00	0.44
1:D:1149:VAL:HG23	1:D:1151:LEU:HD12	1.99	0.44
1:D:832:MET:HE3	1:D:832:MET:HA	1.99	0.44
1:B:456:CYS:SG	1:B:457:SER:N	2.91	0.44
1:D:1188:THR:HG23	1:D:1191:ASN:H	1.81	0.44
1:B:704:CYS:HB2	1:B:705:PRO:HD2	2.00	0.44
1:A:161:LEU:HD12	1:A:172:GLN:HB2	1.99	0.44
1:A:359:GLU:OE2	1:A:359:GLU:HA	2.17	0.44
1:A:382:ASP:OD1	1:A:382:ASP:N	2.47	0.44
1:B:448:LYS:HD2	1:B:581:ASP:HB2	2.00	0.44
1:C:877:THR:HG23	1:C:884:THR:HG23	2.00	0.44
1:A:87:PHE:CG	1:A:100:PRO:HA	2.53	0.43
1:B:138:MET:SD	1:B:187:LEU:HD22	2.59	0.43
1:B:235:PHE:O	1:B:239:GLN:HG2	2.18	0.43
1:D:922[A]:ASN:ND2	1:D:1077:PRO:HG3	2.32	0.43
1:A:437:LEU:HD13	1:A:677:SER:HB2	2.01	0.43
1:D:991:VAL:HG13	1:D:993:TYR:HD2	1.83	0.43
1:C:1090:TRP:CE2	1:C:1094:GLN:HG3	2.54	0.43
1:D:1218:ASP:O	1:D:1222:MET:N	2.52	0.43
1:C:971:PHE:CD1	1:C:984:GLY:HA2	2.51	0.43
1:A:192:ASP:OD1	1:A:192:ASP:N	2.42	0.43
1:A:84:TRP:CD2	1:A:313:GLU:HG2	2.54	0.42
1:C:1185:CYS:CA	1:C:1196:CYS:HB3	2.43	0.42
1:A:456:CYS:SG	1:A:457:SER:N	2.92	0.42
1:C:1195:ASP:C	1:C:1195:ASP:OD1	2.62	0.42
1:D:1185:CYS:HB3	1:D:1196:CYS:N	2.34	0.42
1:B:205:ASN:N	1:B:214:PHE:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:CYS:HA	1:D:775:SER:O	2.18	0.42
1:A:110:HIS:HB2	1:A:118:PHE:CE1	2.55	0.42
1:B:706:LYS:H	1:B:706:LYS:HD3	1.84	0.42
1:C:945:ARG:HG2	1:C:947:VAL:HG23	2.01	0.42
1:A:77:ASN:ND2	1:A:321:ALA:HB2	2.34	0.42
1:B:470:THR:HB	1:B:493:SER:HB3	2.02	0.42
1:D:933:HIS:HB3	1:D:937:LYS:HA	2.01	0.42
1:B:583[B]:ARG:HB2	1:B:589:VAL:HG22	2.02	0.42
1:D:1185:CYS:HB3	1:D:1196:CYS:CA	2.40	0.42
1:B:710:TYR:HA	1:B:741:CYS:HA	2.02	0.42
1:C:922[A]:ASN:ND2	1:C:1077:PRO:HG3	2.35	0.42
1:D:971:PHE:HB3	1:D:993:TYR:HE2	1.84	0.42
1:B:341:ASN:OD1	1:B:341:ASN:N	2.52	0.41
1:D:998:MET:HE3	1:D:1203:LEU:HD12	2.02	0.41
1:B:638:ASP:OD2	1:B:638:ASP:C	2.63	0.41
1:C:928:THR:HA	1:C:947:VAL:HG22	2.02	0.41
1:A:148:THR:OG1	1:A:151:SER:HB3	2.20	0.41
1:C:1210:CYS:HA	1:C:1211:PRO:HD3	1.95	0.41
1:D:877:THR:HG23	1:D:884:THR:HG23	2.02	0.41
1:B:503:ILE:HG21	1:B:547:LEU:HD13	2.03	0.41
1:B:430:CYS:HB3	1:B:564:ARG:NH2	2.30	0.41
1:B:437:LEU:HD13	1:B:677:SER:HB2	2.02	0.41
1:C:800:PRO:HG2	1:C:808:PHE:CE2	2.56	0.41
1:B:100:PRO:HD2	1:B:233:MET:HE2	2.02	0.41
1:C:973:LEU:HG	1:C:993:TYR:CE2	2.56	0.41
1:A:176:TYR:CD1	1:A:176:TYR:C	2.99	0.41
1:B:538:GLN:NE2	1:B:539:THR:O	2.53	0.41
1:A:118:PHE:HA	1:A:139:LYS:O	2.21	0.41
1:C:975:LEU:HD23	1:C:980:VAL:HG13	2.02	0.41
1:C:1215:PRO:HD2	1:C:1226:ALA:HA	2.01	0.41
1:D:1198:ARG:C	1:D:1200:VAL:H	2.29	0.41
1:A:114:ALA:HB3	1:D:1096:SER:HB2	2.03	0.41
1:A:699:LYS:HB3	1:A:699:LYS:HE3	1.76	0.41
1:B:456:CYS:HB2	1:B:606:CYS:HB3	1.81	0.41
1:A:480:LEU:HD13	1:C:782:ILE:HG21	2.03	0.41
1:B:415:ASN:OD1	2:B:1503:NAG:N2	2.53	0.41
1:B:603:GLN:HG2	1:D:822:GLY:O	2.21	0.41
1:A:289:GLU:OE1	1:A:293:GLN:NE2	2.54	0.40
1:C:783:CYS:HA	1:C:792:CYS:HA	2.03	0.40
1:B:84:TRP:CE2	1:B:313:GLU:HG2	2.56	0.40
1:C:1181:CYS:HA	1:C:1202:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1126:CYS:SG	1:D:1131:ASP:HA	2.61	0.40
1:D:852:ASP:HB3	1:D:854:GLU:HG3	2.03	0.40
1:B:200:ASP:OD1	1:B:201:THR:N	2.55	0.40
1:C:1191:ASN:ND2	1:C:1195:ASP:OD1	2.54	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	688/1456 (47%)	671 (98%)	17 (2%)	0	100	100
1	B	686/1456 (47%)	665 (97%)	21 (3%)	0	100	100
1	C	462/1456 (32%)	446 (96%)	16 (4%)	0	100	100
1	D	463/1456 (32%)	443 (96%)	20 (4%)	0	100	100
All	All	2299/5824 (40%)	2225 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	591/1233 (48%)	576 (98%)	15 (2%)	42	73
1	B	590/1233 (48%)	575 (98%)	15 (2%)	42	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	378/1233 (31%)	372 (98%)	6 (2%)	55 81
1	D	380/1233 (31%)	373 (98%)	7 (2%)	51 79
All	All	1939/4932 (39%)	1896 (98%)	43 (2%)	46 75

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	108	SER
1	A	140	VAL
1	A	173	SER
1	A	276	SER
1	A	284	VAL
1	A	302	ASP
1	A	417	THR
1	A	424	SER
1	A	480	LEU
1	A	517	GLN
1	A	541	LEU
1	A	704	CYS
1	A	731	CYS
1	A	732	SER
1	B	133	LEU
1	B	140	VAL
1	B	165	GLN
1	B	185	LEU
1	B	186	VAL
1	B	192	ASP
1	B	284	VAL
1	B	306	CYS
1	B	349	SER
1	B	526	THR
1	B	671	LEU
1	B	717	CYS
1	B	747	THR
1	B	751	ASP
1	B	759	SER
1	C	943	SER
1	C	1114[A]	ARG
1	C	1114[B]	ARG
1	C	1157	THR

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Mol	Chain	Res	Type
1	C	1185	CYS
1	C	1186	LEU
1	D	769	MET
1	D	877	THR
1	D	947	VAL
1	D	1114[A]	ARG
1	D	1114[B]	ARG
1	D	1196	CYS
1	D	1219	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	A	340	ASN
1	A	385	GLN
1	A	546	ASN
1	B	293	GLN
1	B	426	GLN
1	B	498	GLN
1	B	680	HIS
1	C	824	GLN
1	C	828	HIS
1	C	941	GLN
1	C	997	GLN
1	C	1109	HIS
1	D	824	GLN
1	D	828	HIS
1	D	838	GLN
1	D	917	GLN
1	D	1147	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
2	NAG	B	1501	1	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	A	1502	1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	A	1503	1	14,14,15	0.37	0	17,19,21	0.53	0
2	NAG	B	1503	1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	A	1501	1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	B	1502	1	14,14,15	0.29	0	17,19,21	0.48	0

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
2	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1502	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1503	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1502	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1501	NAG	C4-C5-C6-O6
2	B	1501	NAG	O5-C5-C6-O6
2	A	1501	NAG	C4-C5-C6-O6
2	B	1502	NAG	O5-C5-C6-O6
2	A	1501	NAG	O5-C5-C6-O6
2	A	1502	NAG	C4-C5-C6-O6
2	A	1502	NAG	O5-C5-C6-O6
2	B	1502	NAG	C4-C5-C6-O6
2	A	1503	NAG	C4-C5-C6-O6
2	A	1503	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1503	NAG	1	0
2	B	1503	NAG	1	0

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.

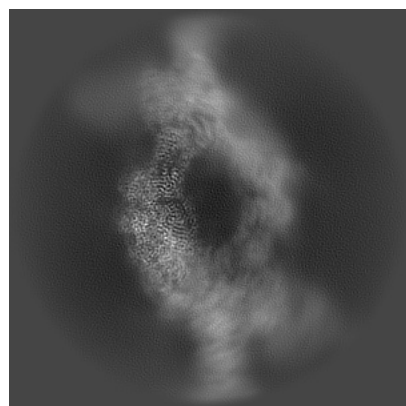
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51636. These allow visual inspection of the internal detail of the map and identification of artifacts.

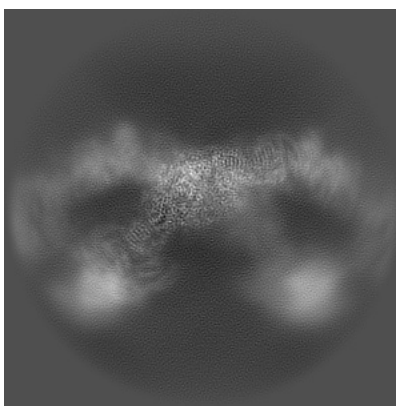
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

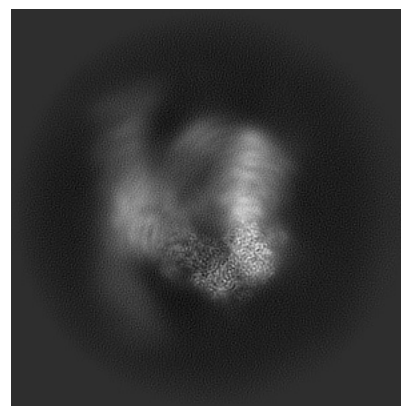
6.1.1 Primary map



X

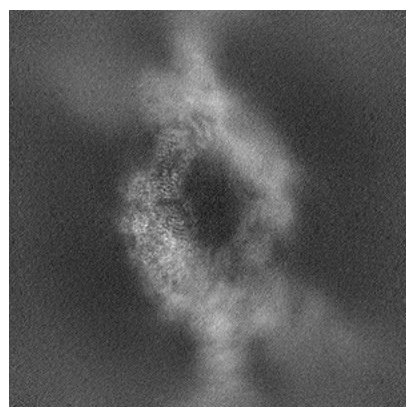


Y

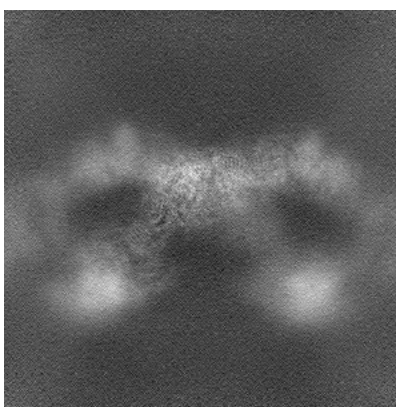


Z

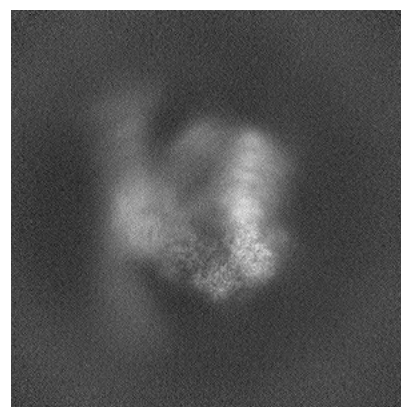
6.1.2 Raw map



X



Y

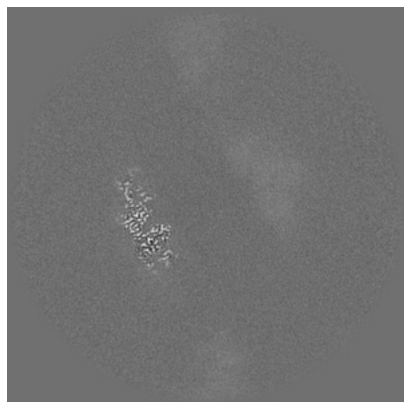


Z

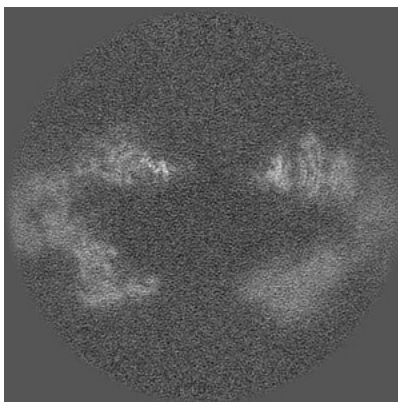
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

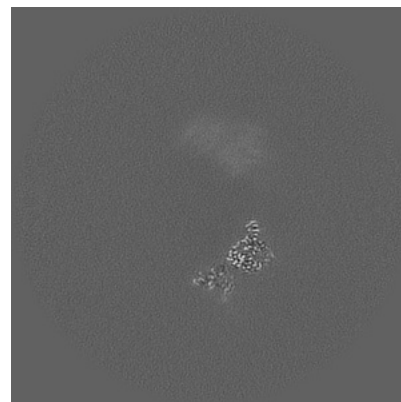
6.2.1 Primary map



X Index: 275

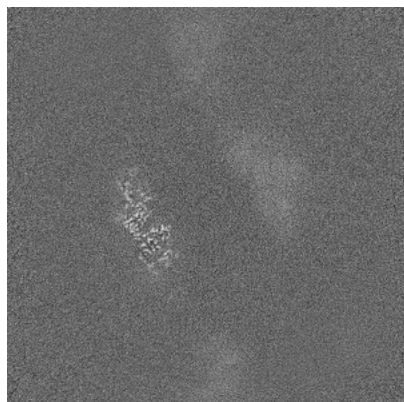


Y Index: 275

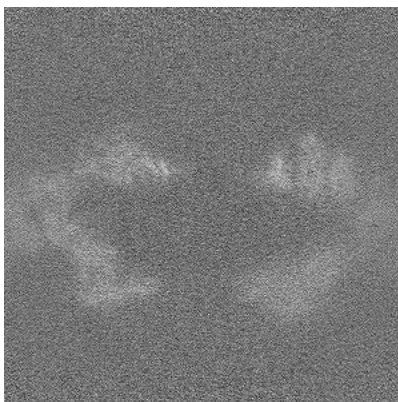


Z Index: 275

6.2.2 Raw map



X Index: 275



Y Index: 275

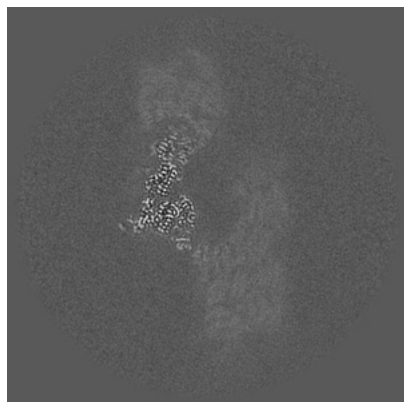


Z Index: 275

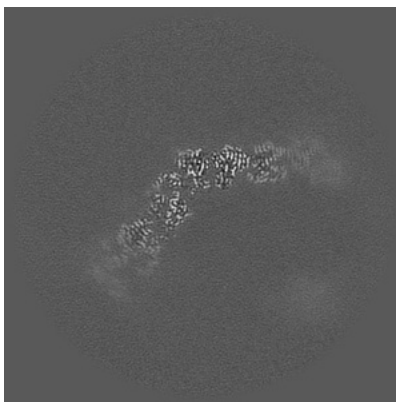
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

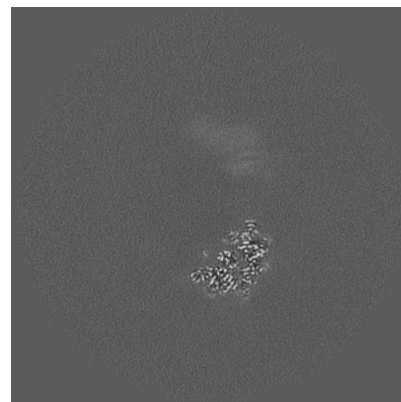
6.3.1 Primary map



X Index: 333

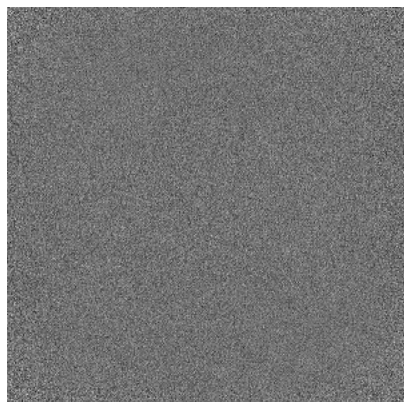


Y Index: 214

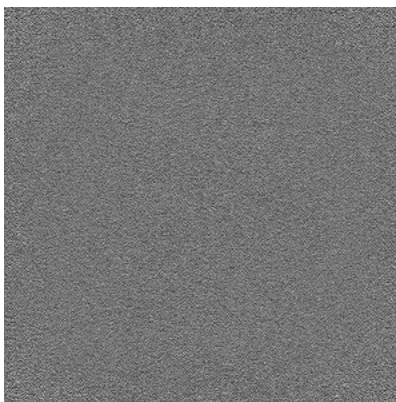


Z Index: 258

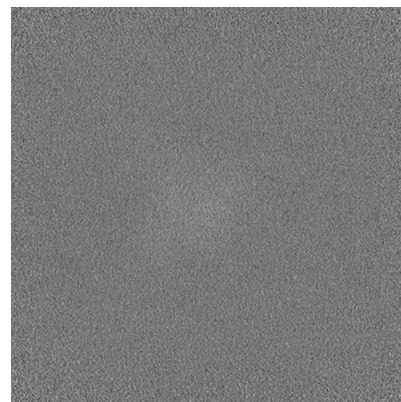
6.3.2 Raw map



X Index: 0



Y Index: 0

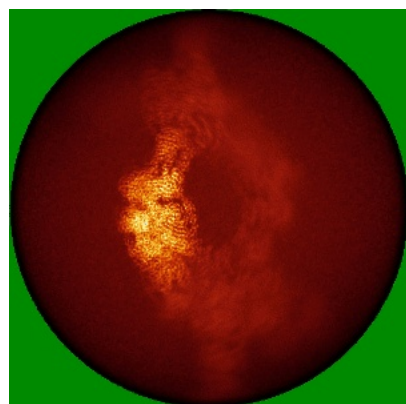


Z Index: 0

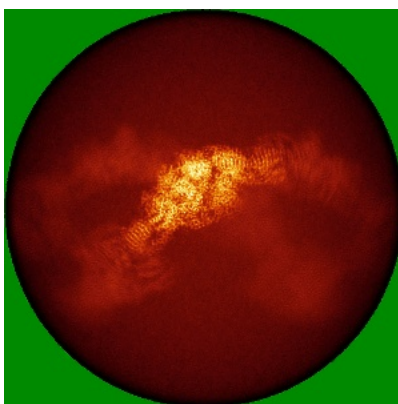
The images above show the largest variance slices of the map in three orthogonal directions.

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

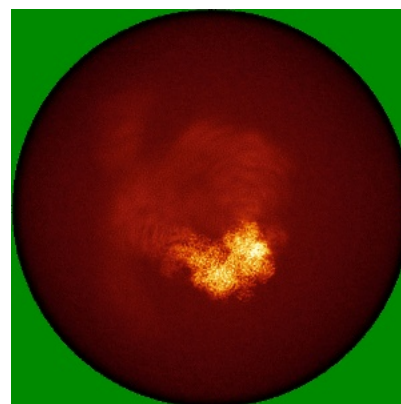
6.4.1 Primary map



X

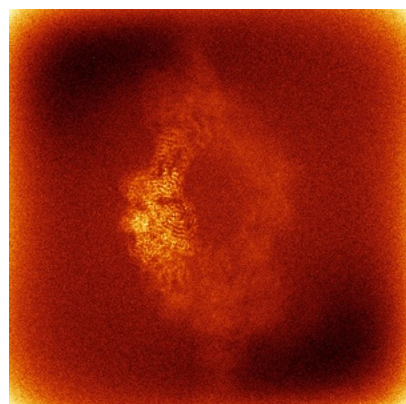


Y

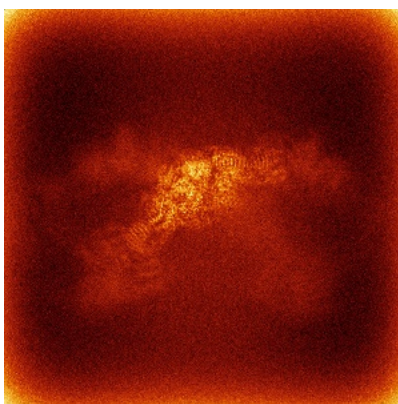


Z

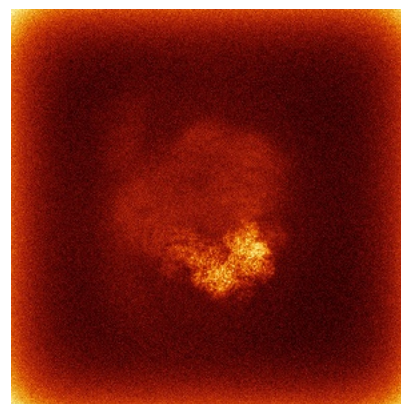
6.4.2 Raw map



X



Y

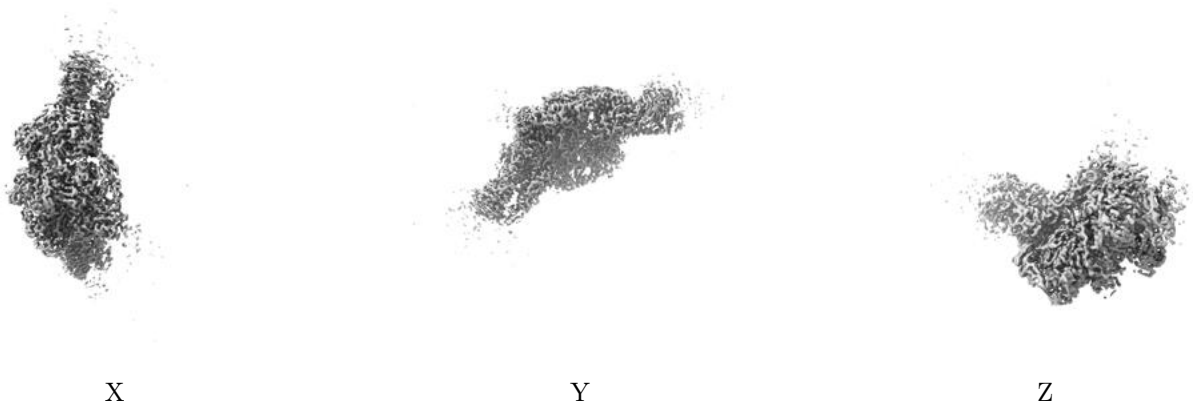


Z

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.

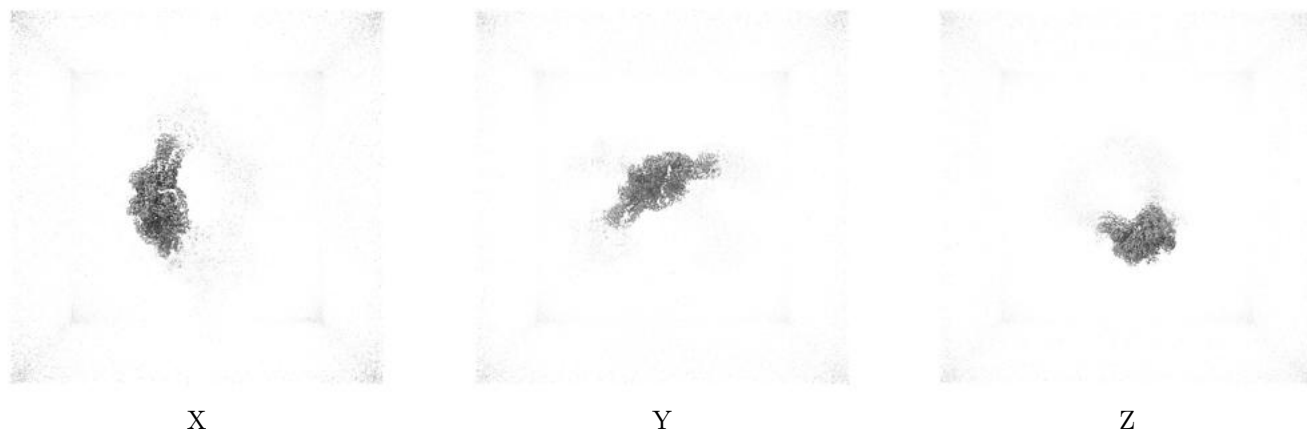
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.256. 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.

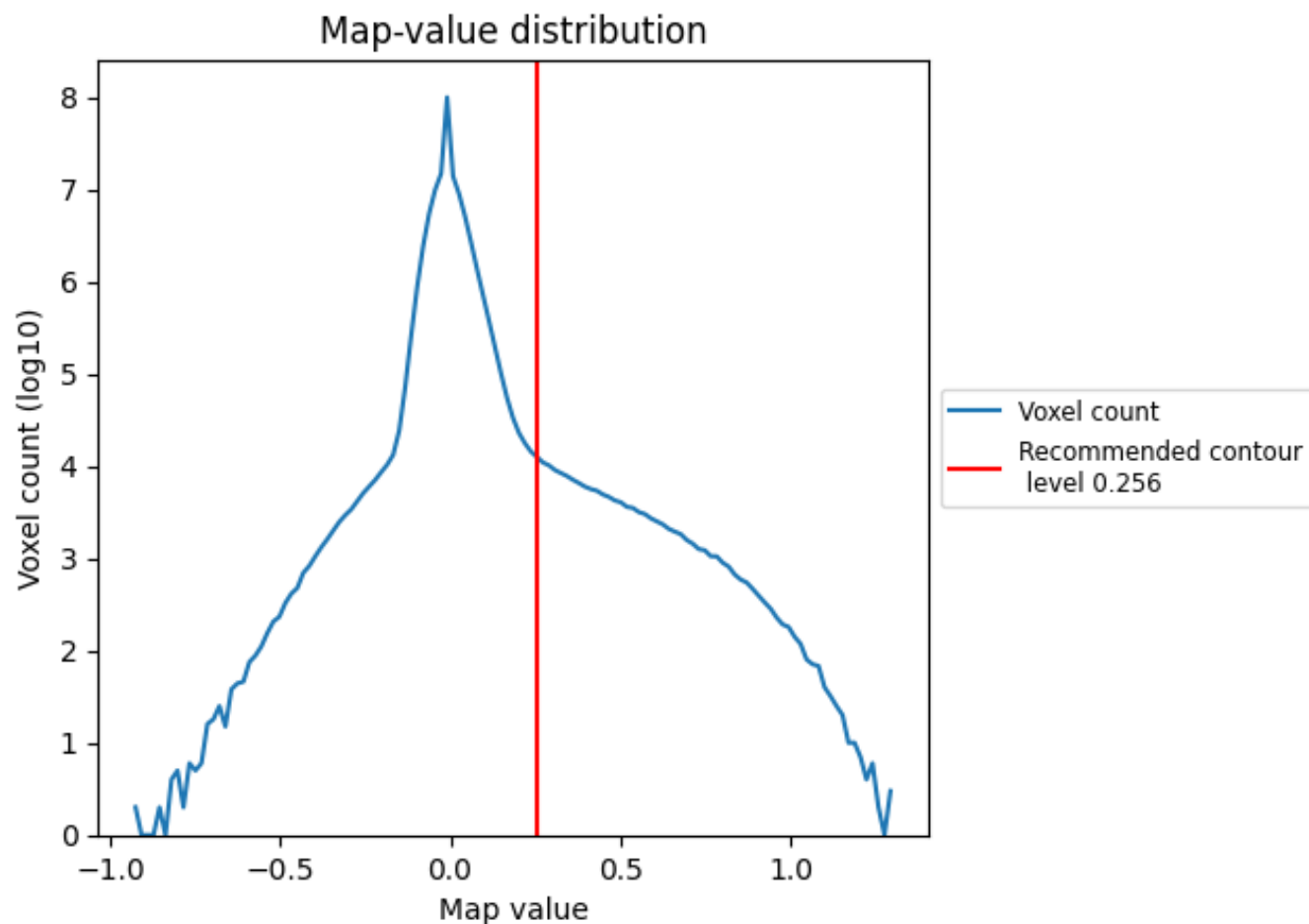
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

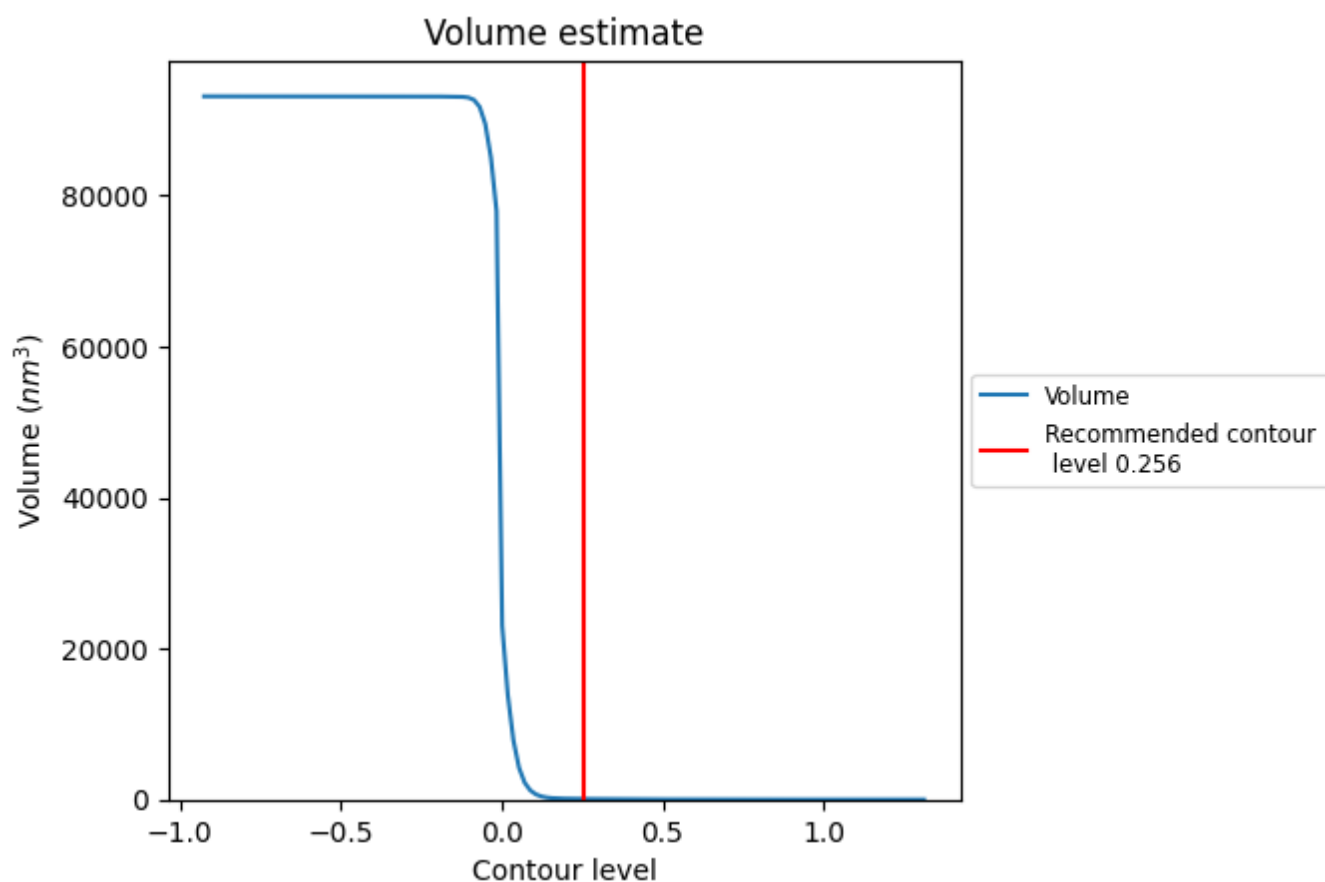
This section contains the results of statistical analysis of the map.

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.

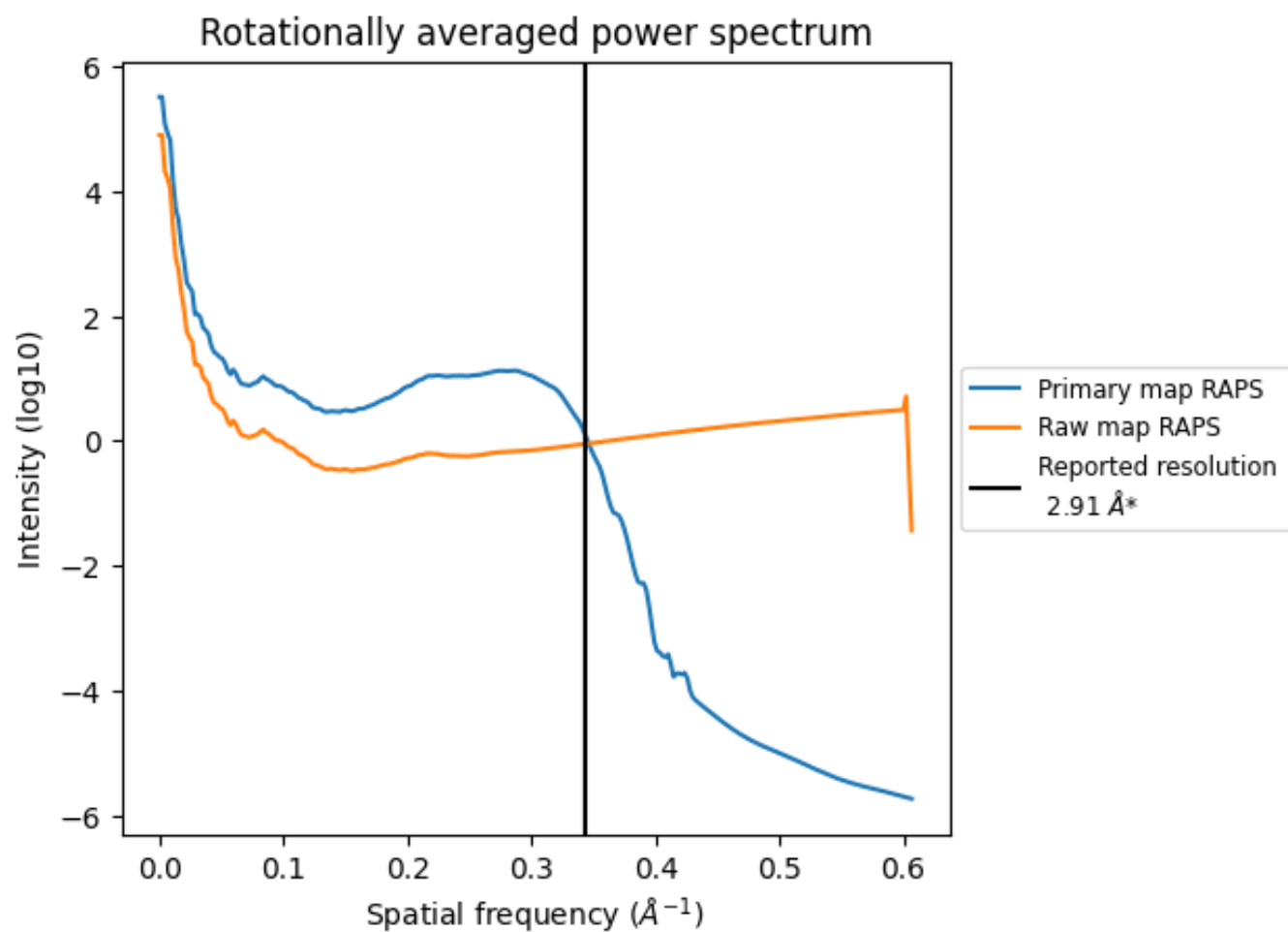
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 83 nm^3 ; this corresponds to an approximate mass of 75 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 ⓘ

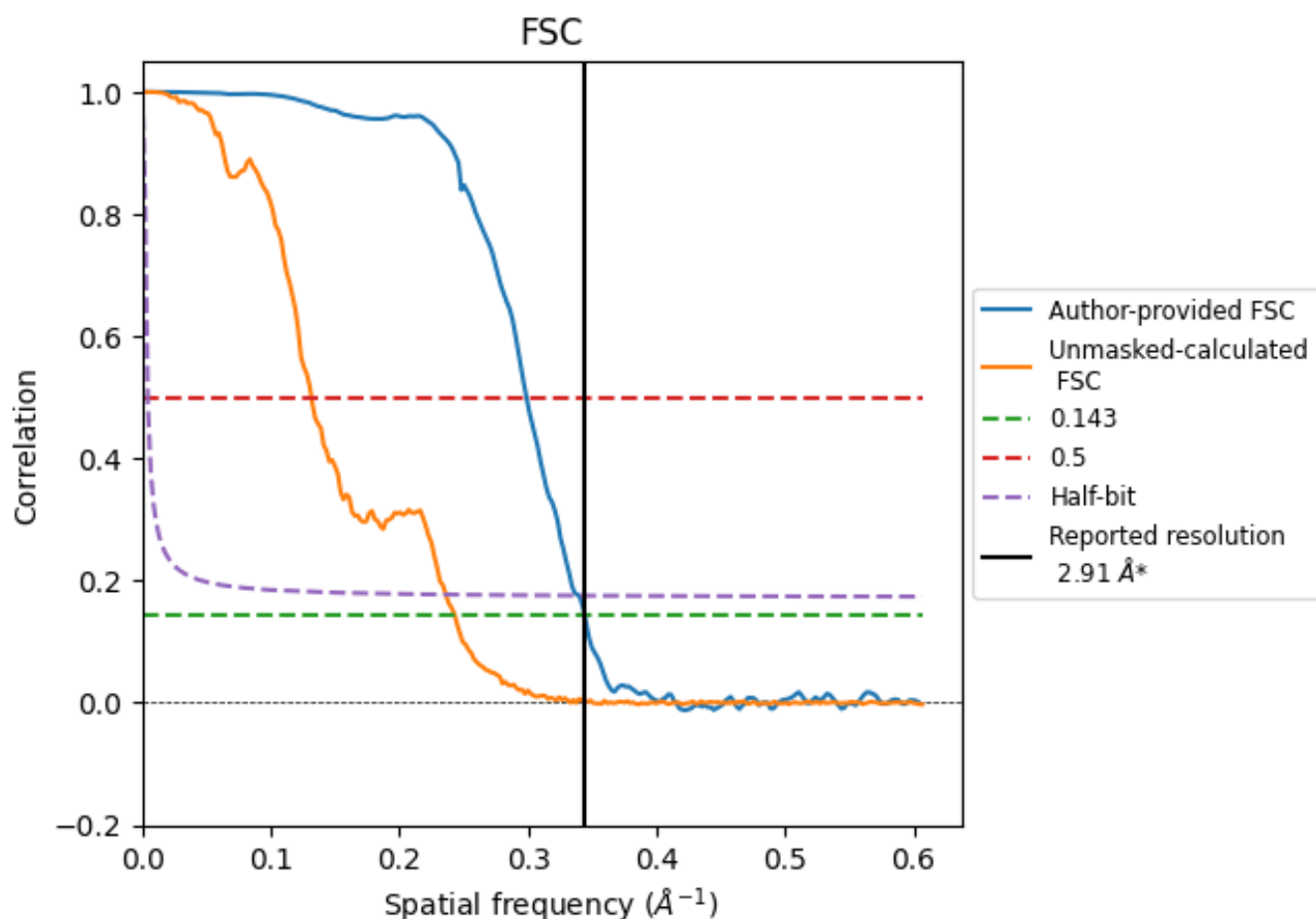


*Reported resolution corresponds to spatial frequency of 0.344 $\text{\AA}^{-1}$

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 0.344 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

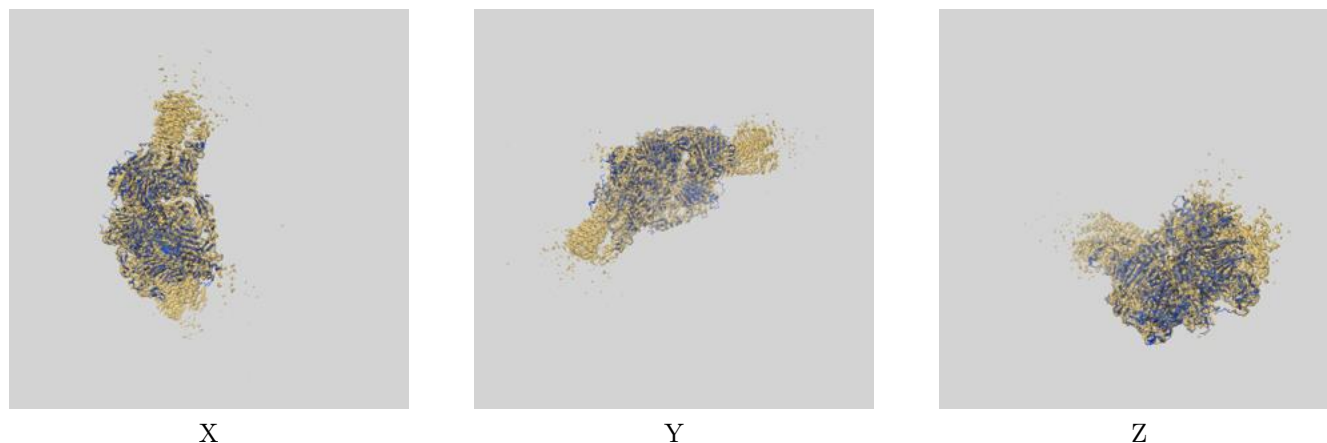
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.34	2.95
Unmasked-calculated*	4.12	7.60	4.23

*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 4.12 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

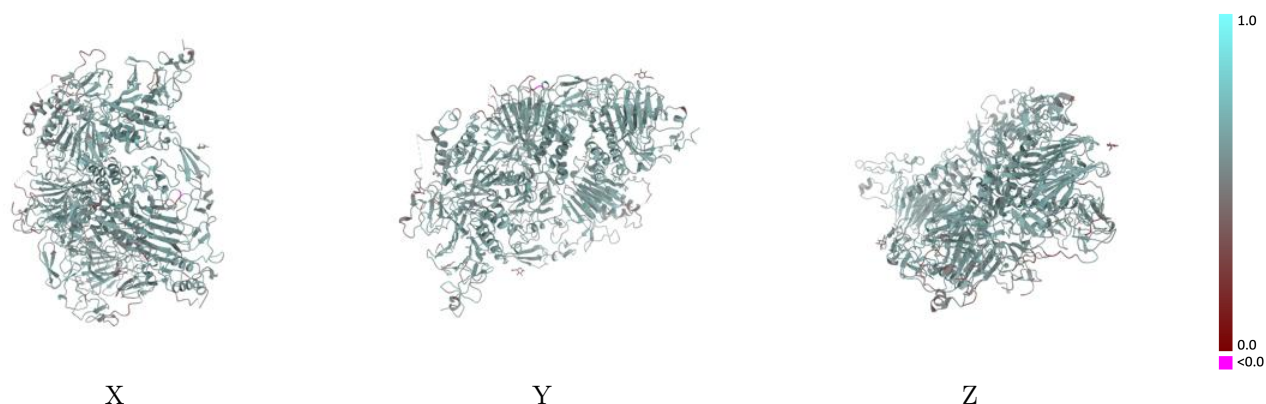
This section contains information regarding the fit between EMDB map EMD-51636 and PDB model 9GVJ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



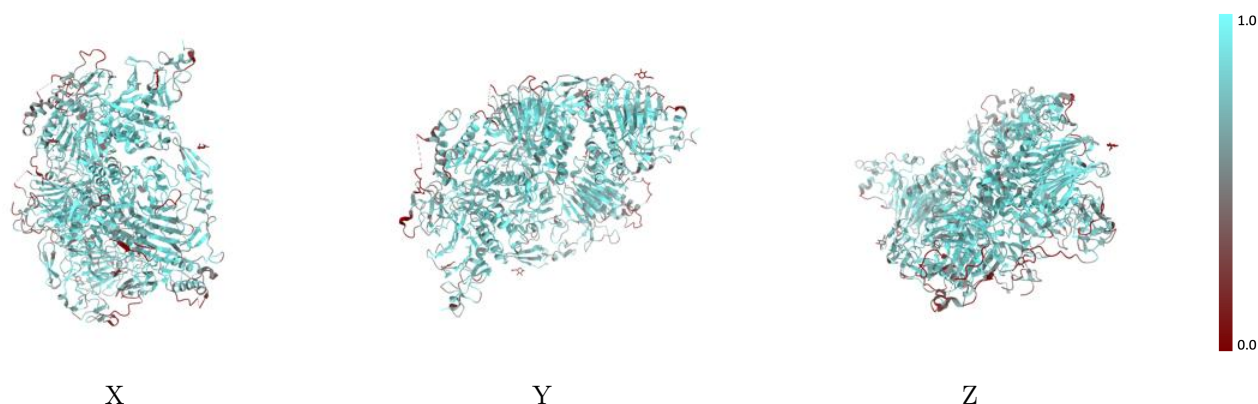
The images above show the 3D surface view of the map at the recommended contour level 0.256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



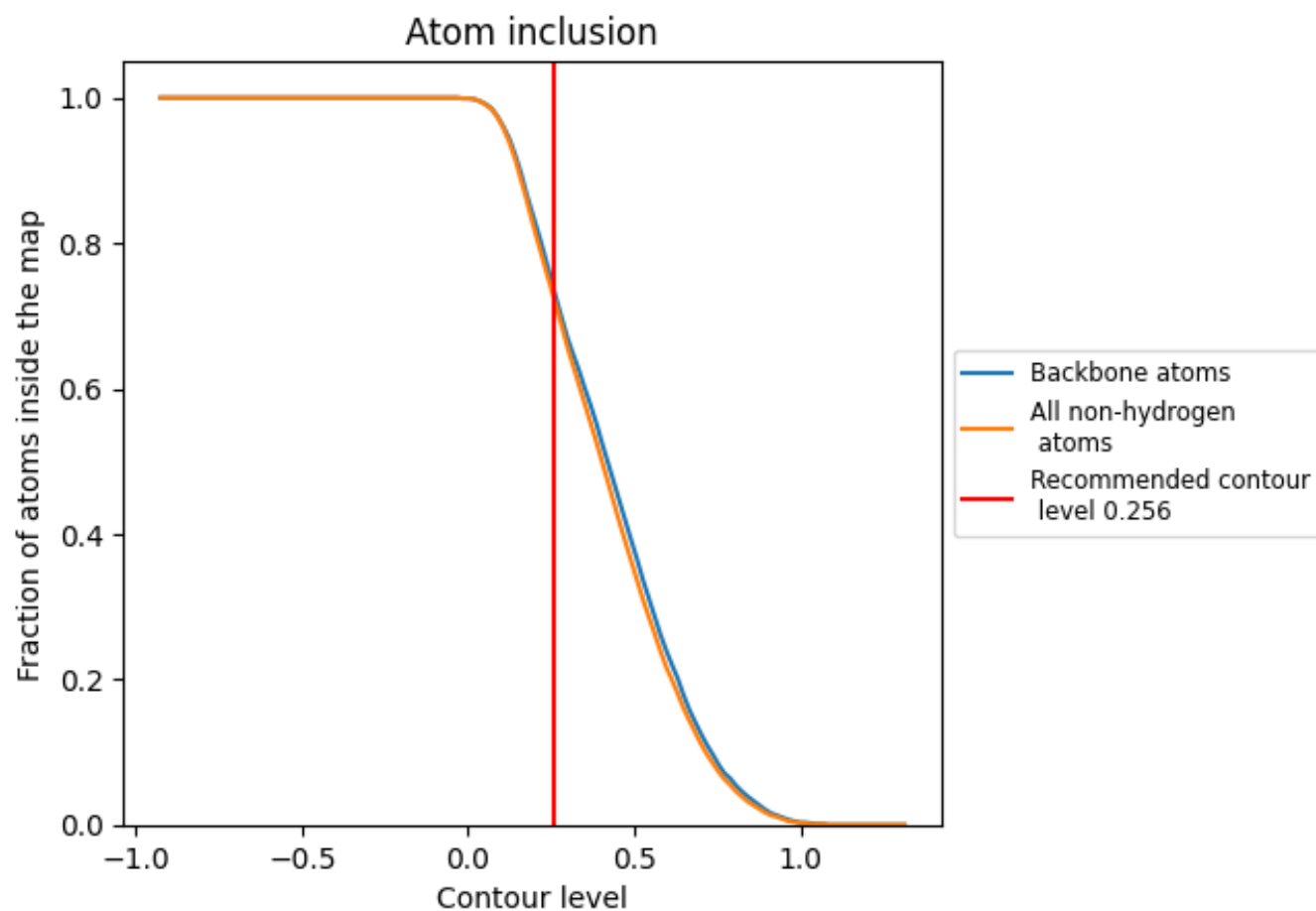
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.256).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.5810
A	0.7400	0.5890
B	0.7220	0.5810
C	0.7310	0.5750
D	0.7270	0.5720

