



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 11:19 PM EDT

PDB ID : 9DX1 / pdb_00009dx1
EMDB ID : EMD-47277
Title : Human GATOR2 complex - Sestrin2 bound state
Authors : Wranik, M.; Rogala, K.B.
Deposited on : 2024-10-10
Resolution : 3.36 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

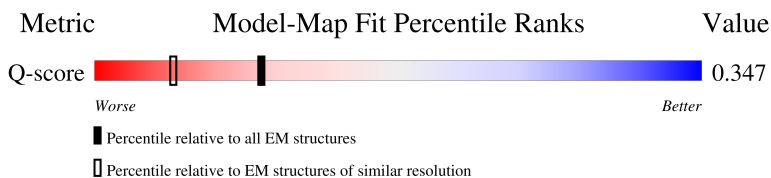
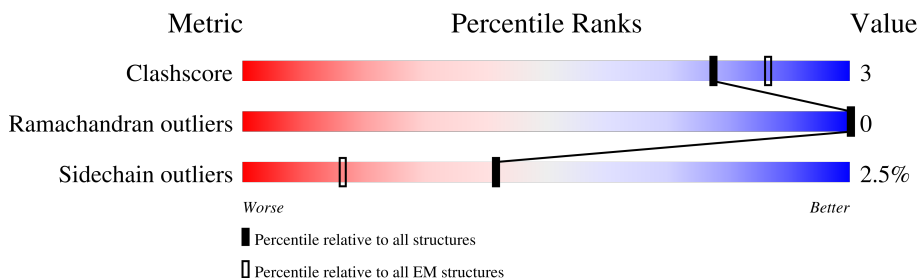
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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	1116	 9% 66% 5% 29%
1	B	1116	 9% 88% 9% ..
2	C	595	 92% 7%
3	D	564	 91% 9%

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Mol	Chain	Length	Quality of chain
4	E	335	<div><div></div><div>5%</div><div>96%</div><div></div><div></div></div>
5	F	729	<div><div></div><div>9%</div><div>89%</div><div>10%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30499 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 GATOR2 complex protein MIOS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	791	Total	C	N	O	S	0	0
			6027	3795	1072	1111	49		
1	B	1089	Total	C	N	O	S	0	0
			7467	4656	1361	1405	45		

- Molecule 2 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	595	Total	C	N	O	S	0	0
			4577	2879	814	844	40		

- Molecule 3 is a protein called Protein SEC13 homolog.

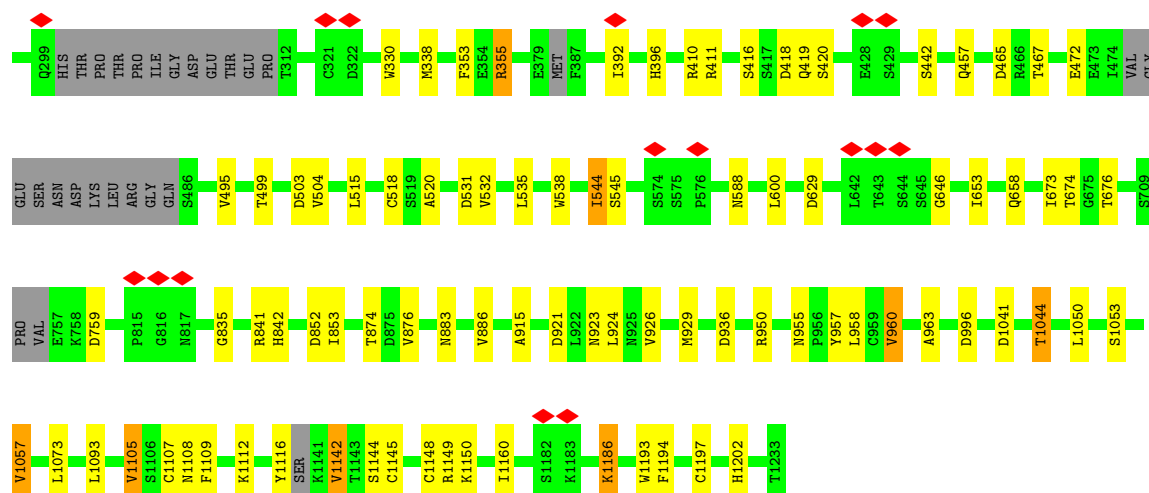
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	564	Total	C	N	O	S	0	0
			4244	2670	757	795	22		

- Molecule 4 is a protein called Sestrin2.

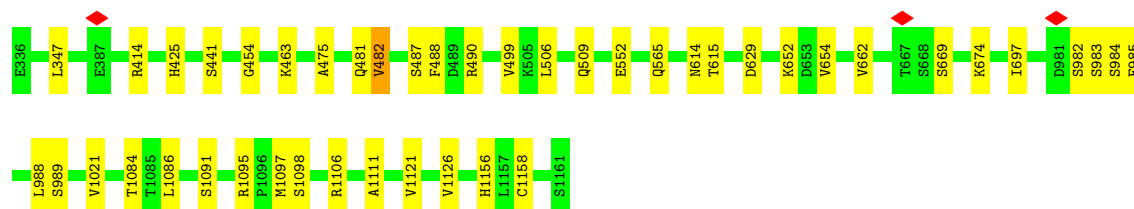
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	335	Total	C	N	O	S	0	0
			2682	1736	466	467	13		

- Molecule 5 is a protein called GATOR2 complex protein WDR24.

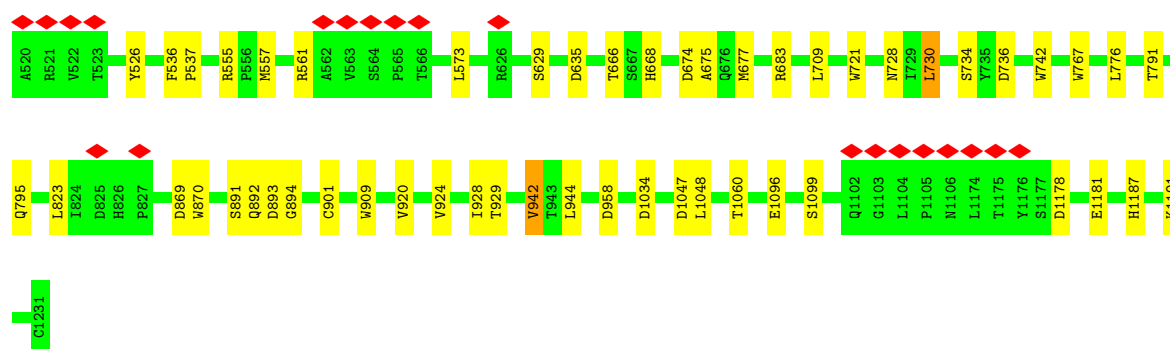
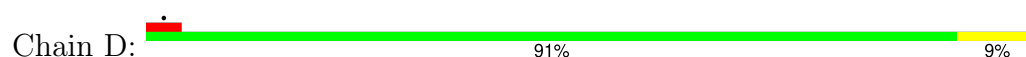
Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	729	Total	C	N	O	S	0	0
			5502	3474	984	995	49		

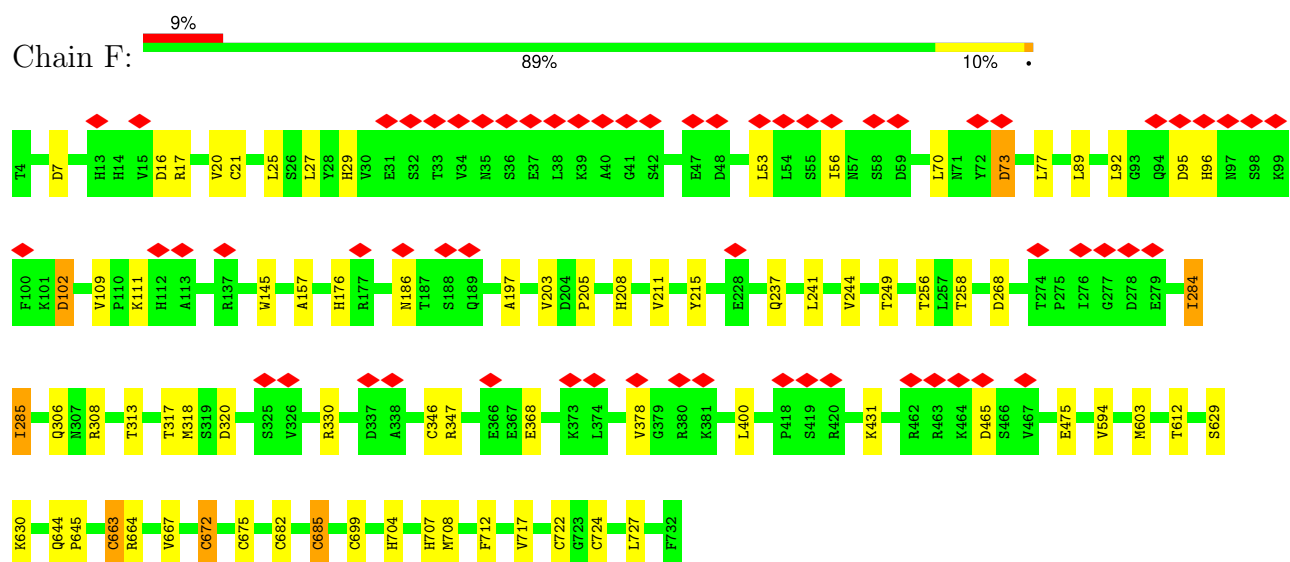


• Molecule 2: Nucleoporin SEH1



• Molecule 3: Protein SEC13 homolog





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	605308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69.44	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.520	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	417.456, 417.456, 417.456	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8697, 0.8697, 0.8697	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.11	0/6167	0.24	0/8381
1	B	0.12	0/7602	0.24	0/10392
2	C	0.10	0/4692	0.24	0/6374
3	D	0.14	0/4348	0.28	0/5927
4	E	0.10	0/2761	0.21	0/3757
5	F	0.11	0/5650	0.28	0/7718
All	All	0.11	0/31220	0.25	0/42549

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

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	6027	0	5709	29	0
1	B	7467	0	6266	55	0
2	C	4577	0	4349	24	0
3	D	4244	0	3983	26	0
4	E	2682	0	2582	7	0
5	F	5502	0	5067	37	0
All	All	30499	0	27956	169	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 (169) 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)
5:F:157:ALA:HB3	5:F:176:HIS:HB2	1.70	0.73
1:A:790:ASP:HB3	1:A:793:LEU:HB2	1.72	0.71
5:F:722:CYS:SG	5:F:724:CYS:N	2.58	0.70
1:A:978:GLU:O	1:A:986:ARG:NH1	2.28	0.66
5:F:685:CYS:SG	5:F:707:HIS:ND1	2.67	0.66
5:F:249:THR:HG21	5:F:306:GLN:HA	1.77	0.65
5:F:73:ASP:N	5:F:73:ASP:OD1	2.28	0.65
1:B:1112:LYS:NZ	1:B:1145:CYS:SG	2.69	0.65
5:F:53:LEU:HD11	5:F:56:ILE:HD11	1.78	0.65
2:C:490:ARG:HB2	4:E:354:ARG:HH22	1.61	0.65
4:E:340:GLN:HE22	4:E:406:ASP:H	1.44	0.65
1:B:1193:TRP:HD1	1:B:1194:PHE:H	1.46	0.64
5:F:682:CYS:SG	5:F:685:CYS:N	2.67	0.63
1:B:1193:TRP:CD1	1:B:1194:PHE:H	2.17	0.62
3:D:734:SER:OG	3:D:736:ASP:OD1	2.17	0.62
1:A:995:SER:OG	1:A:998:GLN:OE1	2.18	0.61
5:F:197:ALA:HA	5:F:215:TYR:HB2	1.83	0.60
5:F:330:ARG:NH2	5:F:368:GLU:OE1	2.35	0.60
1:A:419:GLN:NE2	1:A:443:GLY:O	2.34	0.59
4:E:135:GLU:OE1	4:E:138:GLN:NE2	2.36	0.59
5:F:308:ARG:NH1	5:F:320:ASP:OD2	2.35	0.59
2:C:614:ASN:ND2	2:C:669:SER:O	2.36	0.58
1:B:243:PHE:HA	1:B:248:VAL:HA	1.86	0.58
1:B:1107:CYS:SG	1:B:1108:ASN:N	2.77	0.57
1:B:835:GLY:N	1:B:996:ASP:OD2	2.36	0.57
5:F:16:ASP:OD1	5:F:16:ASP:N	2.38	0.57
5:F:268:ASP:HB3	5:F:285:ILE:HG13	1.87	0.56
2:C:414:ARG:NH1	2:C:454:GLY:O	2.39	0.56
1:B:1112:LYS:HB2	1:B:1112:LYS:HZ2	1.71	0.56
2:C:552:GLU:OE1	2:C:565:GLN:NE2	2.39	0.56
2:C:629:ASP:OD2	2:C:652:LYS:NZ	2.35	0.56
5:F:102:ASP:OD1	5:F:102:ASP:N	2.27	0.56
1:A:923:ASN:N	1:A:923:ASN:OD1	2.39	0.56
5:F:346:CYS:SG	5:F:347:ARG:N	2.80	0.55
1:B:465:ASP:OD1	1:B:467:THR:OG1	2.19	0.54
1:B:467:THR:HG22	1:B:495:VAL:HG12	1.88	0.54
1:A:924:LEU:HA	1:A:927:VAL:HG12	1.89	0.54
1:A:1196:TRP:HB3	2:C:1086:LEU:HD12	1.90	0.54
1:A:990:ALA:HA	1:A:994:LEU:HD23	1.90	0.54
2:C:1097:MET:HE1	2:C:1111:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:244:VAL:HG22	5:F:256:THR:HG22	1.89	0.54
1:A:508:PRO:HD2	1:A:511:MET:HE2	1.90	0.53
1:B:419:GLN:NE2	1:B:442:SER:O	2.39	0.53
5:F:313:THR:HG1	5:F:317:THR:HG1	1.48	0.53
3:D:869:ASP:OD1	3:D:870:TRP:N	2.31	0.53
2:C:1095:ARG:HH11	2:C:1106:ARG:HB2	1.73	0.52
1:B:144:ILE:O	1:B:178:LEU:N	2.42	0.52
4:E:352:ILE:HD11	4:E:472:LEU:HD11	1.91	0.52
3:D:891:SER:OG	3:D:893:ASP:OD1	2.27	0.52
3:D:555:ARG:HH11	3:D:635:ASP:HB3	1.75	0.52
1:A:1187:LEU:HD11	2:C:499:VAL:HG11	1.91	0.52
1:B:416:SER:OG	1:B:418:ASP:OD1	2.27	0.52
2:C:988:LEU:HD13	3:D:944:LEU:HD11	1.91	0.51
3:D:674:ASP:OD1	3:D:675:ALA:N	2.43	0.51
1:B:531:ASP:OD1	1:B:532:VAL:N	2.44	0.51
1:B:1144:SER:HB2	1:B:1149:ARG:HA	1.91	0.51
1:B:1116:TYR:HE1	1:B:1142:VAL:HG22	1.76	0.51
1:B:853:ILE:HD11	1:B:876:VAL:HA	1.93	0.50
2:C:347:LEU:HD12	2:C:697:ILE:HD13	1.94	0.50
3:D:928:ILE:HG23	3:D:929:THR:HG23	1.94	0.50
1:A:799:THR:HG22	1:A:803:MET:HE2	1.94	0.49
3:D:683:ARG:NH1	3:D:728:ASN:OD1	2.42	0.49
1:A:764:MET:HE3	1:A:1043:GLN:HB2	1.94	0.49
5:F:685:CYS:SG	5:F:704:HIS:ND1	2.85	0.49
2:C:982:SER:H	2:C:985:PHE:HB3	1.77	0.49
3:D:1047:ASP:OD1	3:D:1048:LEU:N	2.45	0.49
4:E:195:ILE:HG13	4:E:355:LEU:HD23	1.94	0.49
1:B:1197:CYS:HB3	1:B:1202:HIS:H	1.77	0.49
5:F:672:CYS:SG	5:F:675:CYS:N	2.86	0.49
1:B:503:ASP:OD1	1:B:504:VAL:N	2.46	0.49
1:A:1157:LEU:HD12	1:A:1208:HIS:HB3	1.95	0.48
1:B:67:ALA:HB3	1:B:79:ALA:HB3	1.95	0.48
1:B:411:ARG:NH1	1:B:457:GLN:OE1	2.46	0.48
1:B:915:ALA:HA	1:B:924:LEU:HD12	1.95	0.48
1:B:955:ASN:HB3	1:B:958:LEU:HD13	1.96	0.48
5:F:284:ILE:HD13	5:F:285:ILE:H	1.78	0.48
1:A:1032:MET:HE2	1:A:1045:ALA:HA	1.96	0.48
1:B:140:PHE:HA	1:B:183:GLN:HA	1.96	0.47
1:B:188:LEU:N	1:B:203:GLY:O	2.46	0.47
3:D:1096:GLU:O	3:D:1099:SER:OG	2.28	0.47
5:F:16:ASP:OD2	5:F:29:HIS:NE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:TRP:HA	1:B:178:LEU:H	1.79	0.47
2:C:506:LEU:HD23	2:C:509:GLN:HE21	1.79	0.47
1:B:1186:LYS:NZ	5:F:712:PHE:O	2.47	0.47
1:A:1102:GLN:O	2:C:1091:SER:OG	2.28	0.47
1:B:852:ASP:N	1:B:852:ASP:OD1	2.47	0.47
3:D:1187:HIS:CD2	3:D:1191:LYS:HE3	2.50	0.47
5:F:237:GLN:HG3	5:F:241:LEU:HD21	1.97	0.47
1:A:1201:ARG:NH2	2:C:1098:SER:O	2.47	0.47
4:E:46:ALA:HB2	4:E:217:LEU:HD21	1.97	0.47
1:B:926:VAL:HA	1:B:929:MET:HE2	1.97	0.46
3:D:666:THR:HB	3:D:668:HIS:HD2	1.79	0.46
1:A:583:GLN:HG2	1:A:599:THR:HG23	1.97	0.46
1:B:535:LEU:O	1:B:538:TRP:NE1	2.49	0.46
3:D:526:TYR:HD2	3:D:629:SER:HB2	1.81	0.46
1:A:905:ARG:O	1:A:905:ARG:NH1	2.49	0.46
5:F:17:ARG:HG2	5:F:27:LEU:HD11	1.96	0.46
3:D:1178:ASP:OD2	3:D:1181:GLU:N	2.47	0.45
3:D:892:GLN:HA	3:D:920:VAL:HG23	1.98	0.45
3:D:1034:ASP:N	3:D:1034:ASP:OD1	2.50	0.45
1:A:915:ALA:HB2	1:A:924:LEU:HB2	1.98	0.45
1:B:353:PHE:O	1:B:355:ARG:NH2	2.37	0.45
1:B:115:GLN:O	1:B:134:ASP:N	2.49	0.45
1:B:629:ASP:OD2	1:B:658:GLN:NE2	2.40	0.45
1:B:1053:SER:HB3	1:B:1057:VAL:HG11	2.00	0.44
3:D:536:PHE:CG	3:D:537:PRO:HD2	2.53	0.44
1:B:1148:CYS:SG	1:B:1150:LYS:HD3	2.58	0.44
1:B:1160:ILE:HD13	1:B:1160:ILE:HA	1.91	0.44
1:A:779:VAL:HG11	1:A:1051:GLN:HE22	1.83	0.44
1:B:116:CYS:HA	1:B:133:LEU:HA	1.99	0.44
5:F:603:MET:HE3	5:F:645:PRO:HG3	2.00	0.44
1:A:693:ASN:HD21	1:A:697:ASN:HB2	1.82	0.44
1:B:330:TRP:HA	1:B:338:MET:HA	1.99	0.44
1:B:588:ASN:ND2	1:B:646:GLY:O	2.49	0.43
1:B:676:THR:OG1	1:B:759:ASP:OD1	2.34	0.43
1:B:1105:VAL:HG11	1:B:1116:TYR:CE2	2.53	0.43
3:D:677:MET:HG3	3:D:683:ARG:O	2.18	0.43
3:D:557:MET:HE2	3:D:557:MET:HB2	1.86	0.43
2:C:988:LEU:HD21	3:D:942:VAL:HG23	1.99	0.43
1:A:705:LYS:HG3	1:A:711:VAL:HG22	2.01	0.43
1:B:600:LEU:HD23	1:B:653:ILE:HD13	2.00	0.43
3:D:901:CYS:HB2	3:D:909:TRP:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:203:VAL:HG22	5:F:211:VAL:HG12	2.00	0.43
1:A:1035:TYR:O	1:A:1039:THR:HG22	2.19	0.43
2:C:983:SER:OG	2:C:984:SER:N	2.52	0.43
2:C:989:SER:OG	3:D:958:ASP:O	2.34	0.43
1:B:883:ASN:O	1:B:886:VAL:HG12	2.18	0.43
1:A:893:ARG:NH1	1:A:985:ASP:OD2	2.51	0.43
1:B:1041:ASP:OD2	1:B:1044:THR:OG1	2.26	0.43
5:F:663:CYS:HB3	5:F:675:CYS:HB3	1.84	0.43
1:A:899:LEU:HD13	1:A:961:MET:HG3	2.01	0.42
1:B:242:SER:O	1:B:249:ALA:N	2.43	0.42
1:B:921:ASP:OD2	1:B:923:ASN:ND2	2.52	0.42
2:C:425:HIS:NE2	2:C:441:SER:OG	2.45	0.42
1:B:544:ILE:HG22	1:B:545:SER:H	1.84	0.42
5:F:667:VAL:HG21	5:F:672:CYS:HA	2.01	0.42
2:C:487:SER:OG	2:C:488:PHE:N	2.53	0.42
3:D:893:ASP:OD1	3:D:894:GLY:N	2.52	0.42
1:A:1056:ASP:OD1	1:A:1056:ASP:N	2.43	0.42
3:D:767:TRP:CZ3	3:D:776:LEU:HB2	2.54	0.42
1:B:499:THR:HB	1:B:520:ALA:HB3	2.01	0.42
5:F:77:LEU:HD11	5:F:89:LEU:HB3	2.02	0.41
1:A:693:ASN:HD22	1:A:699:LYS:HE3	1.85	0.41
5:F:465:ASP:OD1	5:F:465:ASP:N	2.52	0.41
1:B:1050:LEU:O	1:B:1093:LEU:HD13	2.21	0.41
2:C:475:ALA:HB3	2:C:482:VAL:HG22	2.03	0.41
5:F:53:LEU:HD21	5:F:56:ILE:HG12	2.02	0.41
1:B:841:ARG:O	1:B:842:HIS:ND1	2.50	0.41
5:F:157:ALA:O	5:F:176:HIS:N	2.53	0.41
5:F:644:GLN:HA	5:F:645:PRO:HD3	1.95	0.41
5:F:664:ARG:HD2	5:F:664:ARG:HA	1.81	0.41
1:A:1060:ASP:OD1	1:A:1061:GLU:N	2.54	0.41
1:B:629:ASP:OD1	1:B:629:ASP:N	2.52	0.41
1:B:1109:PHE:CD2	1:B:1150:LYS:HE3	2.56	0.41
5:F:205:PRO:O	5:F:208:HIS:NE2	2.53	0.41
5:F:629:SER:OG	5:F:630:LYS:N	2.54	0.41
2:C:1156:HIS:CE1	2:C:1158:CYS:HA	2.56	0.41
1:B:673:ILE:HG23	1:B:674:THR:HG23	2.03	0.40
1:B:950:ARG:HH21	1:B:963:ALA:HB2	1.85	0.40
5:F:21:CYS:HA	5:F:25:LEU:HD23	2.04	0.40
5:F:708:MET:HE3	5:F:712:PHE:HE2	1.87	0.40
1:B:416:SER:OG	1:B:420:SER:OG	2.26	0.40
1:B:957:TYR:O	1:B:960:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:721:TRP:CE2	3:D:730:LEU:HD11	2.56	0.40
4:E:338:ARG:HD3	4:E:338:ARG:HA	1.89	0.40
2:C:662:VAL:HG11	2:C:674:LYS:HB2	2.03	0.40
3:D:709:LEU:HD13	3:D:742:TRP:CD2	2.56	0.40
1:A:392:ILE:HG22	1:A:393:ALA:H	1.86	0.40
2:C:463:LYS:HE3	2:C:463:LYS:HB2	1.83	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	781/1116 (70%)	745 (95%)	36 (5%)	0	100	100
1	B	1073/1116 (96%)	1027 (96%)	46 (4%)	0	100	100
2	C	583/595 (98%)	566 (97%)	17 (3%)	0	100	100
3	D	556/564 (99%)	525 (94%)	31 (6%)	0	100	100
4	E	329/335 (98%)	319 (97%)	10 (3%)	0	100	100
5	F	721/729 (99%)	682 (95%)	39 (5%)	0	100	100
All	All	4043/4455 (91%)	3864 (96%)	179 (4%)	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	626/980 (64%)	616 (98%)	10 (2%)	55	67
1	B	612/980 (62%)	595 (97%)	17 (3%)	38	60
2	C	490/511 (96%)	482 (98%)	8 (2%)	55	67
3	D	431/479 (90%)	422 (98%)	9 (2%)	47	64
4	E	273/289 (94%)	269 (98%)	4 (2%)	57	68
5	F	564/644 (88%)	536 (95%)	28 (5%)	22	49
All	All	2996/3883 (77%)	2920 (98%)	76 (2%)	42	61

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	CYS
1	A	599	THR
1	A	603	VAL
1	A	649	THR
1	A	878	VAL
1	A	923	ASN
1	A	931	LEU
1	A	1056	ASP
1	A	1108	ASN
1	A	1187	LEU
1	B	355	ARG
1	B	392	ILE
1	B	396	HIS
1	B	410	ARG
1	B	472	GLU
1	B	515	LEU
1	B	518	CYS
1	B	544	ILE
1	B	874	THR
1	B	936	ASP
1	B	960	VAL
1	B	1044	THR
1	B	1057	VAL
1	B	1073	LEU
1	B	1105	VAL
1	B	1142	VAL
1	B	1186	LYS
2	C	481	GLN
2	C	482	VAL
2	C	615	THR

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Mol	Chain	Res	Type
2	C	654	VAL
2	C	1021	VAL
2	C	1084	THR
2	C	1121	VAL
2	C	1126	VAL
3	D	561	ARG
3	D	573	LEU
3	D	730	LEU
3	D	791	THR
3	D	795	GLN
3	D	823	LEU
3	D	924	VAL
3	D	942	VAL
3	D	1060	THR
4	E	138	GLN
4	E	159	LEU
4	E	371	TYR
4	E	442	LEU
5	F	7	ASP
5	F	20	VAL
5	F	70	LEU
5	F	73	ASP
5	F	92	LEU
5	F	95	ASP
5	F	96	HIS
5	F	102	ASP
5	F	109	VAL
5	F	111	LYS
5	F	145	TRP
5	F	186	ASN
5	F	258	THR
5	F	284	ILE
5	F	285	ILE
5	F	318	MET
5	F	378	VAL
5	F	400	LEU
5	F	431	LYS
5	F	475	GLU
5	F	594	VAL
5	F	612	THR
5	F	663	CYS
5	F	672	CYS

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Mol	Chain	Res	Type
5	F	685	CYS
5	F	699	CYS
5	F	717	VAL
5	F	727	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	HIS
1	A	608	HIS
1	A	661	ASN
1	A	662	HIS
1	A	901	ASN
1	A	909	GLN
1	A	1008	ASN
1	A	1043	GLN
1	A	1069	ASN
1	A	1089	HIS
1	A	1230	GLN
1	B	373	HIS
1	B	654	HIS
1	B	697	ASN
1	B	923	ASN
1	B	1208	HIS
2	C	481	GLN
2	C	509	GLN
2	C	561	GLN
2	C	632	HIS
2	C	685	ASN
2	C	686	HIS
2	C	1022	GLN
2	C	1149	HIS
3	D	638	ASN
3	D	673	HIS
4	E	465	GLN
5	F	13	HIS
5	F	430	HIS
5	F	607	HIS
5	F	671	GLN
5	F	701	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	5
1	A	4
5	F	3
3	D	3
4	E	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	324:PHE	C	325:SER	N	143.98
1	F	646:VAL	C	647:PRO	N	74.17
1	C	830:PRO	C	981:ASP	N	40.92
1	D	1106:ASN	C	1174:LEU	N	27.78
1	C	731:ASN	C	778:GLY	N	24.73
1	A	711:VAL	C	757:GLU	N	22.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1166:VAL	C	1182:SER	N	21.56
1	E	55:ARG	C	77:ASP	N	19.86
1	B	1166:VAL	C	1182:SER	N	18.54
1	C	361:ALA	C	387:GLU	N	17.74
1	E	219:GLU	C	309:HIS	N	13.84
1	A	1116:TYR	C	1140:SER	N	13.61
1	D	581:THR	C	626:ARG	N	13.27
1	D	958:ASP	C	996:ALA	N	12.95
1	C	499:VAL	C	505:LYS	N	11.42
1	F	147:ILE	C	148:PRO	N	10.71
1	B	148:CYS	C	174:VAL	N	9.29
1	C	404:PRO	C	410:MET	N	5.22
1	A	379:GLU	C	386:MET	N	3.23

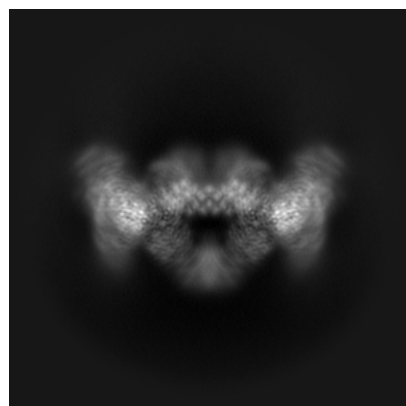
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47277. These allow visual inspection of the internal detail of the map and identification of artifacts.

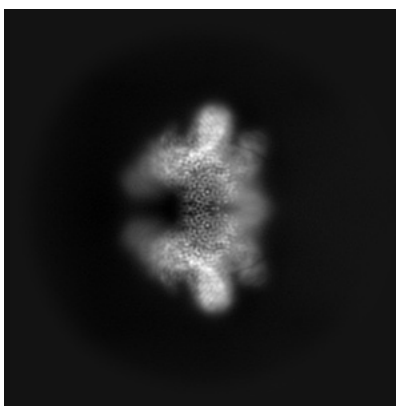
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

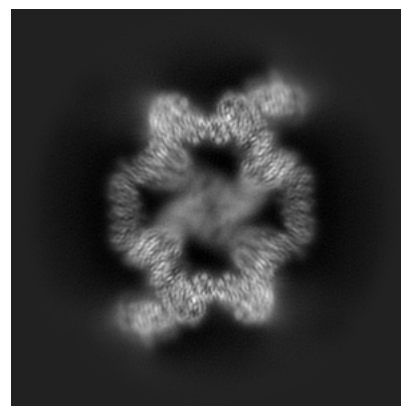
6.1.1 Primary map



X

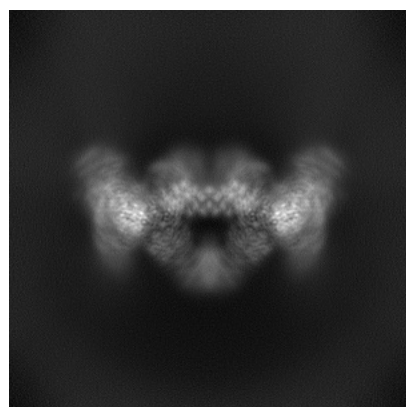


Y

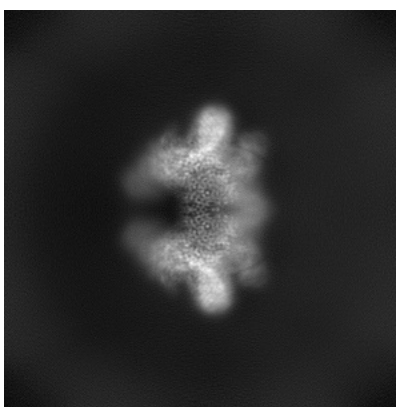


Z

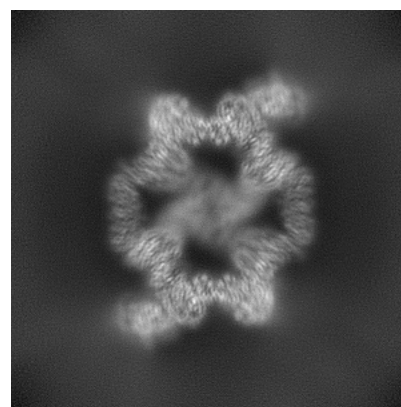
6.1.2 Raw map



X



Y

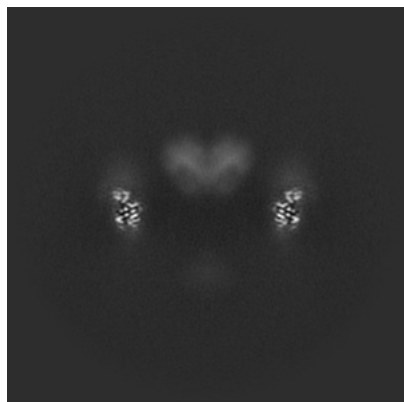


Z

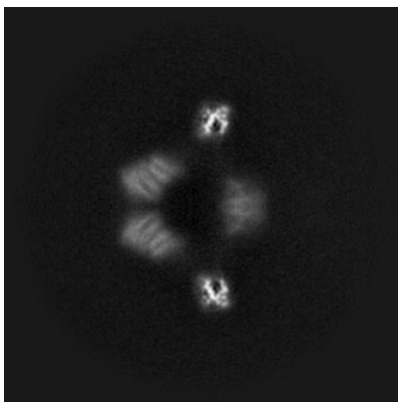
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

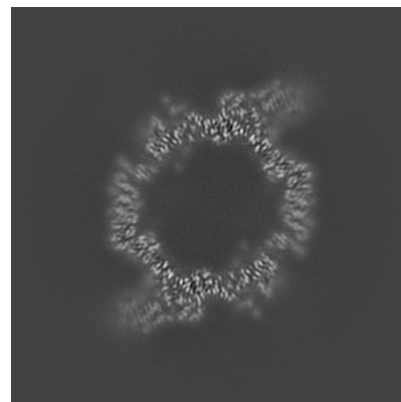
6.2.1 Primary map



X Index: 240

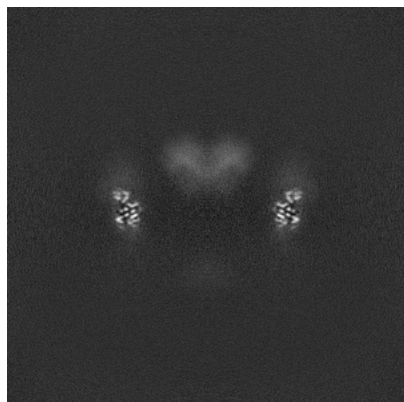


Y Index: 240

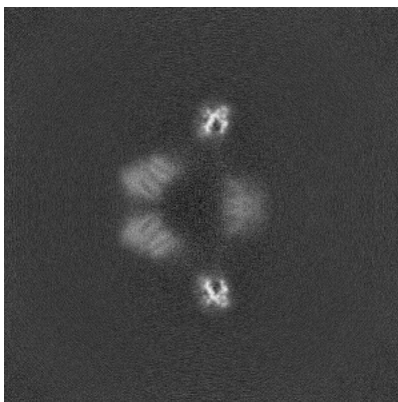


Z Index: 240

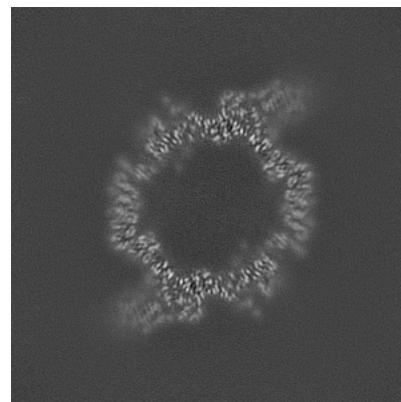
6.2.2 Raw map



X Index: 240



Y Index: 240

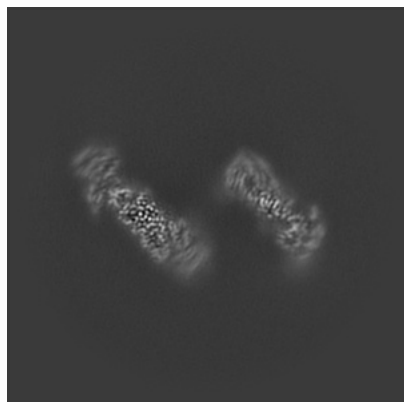


Z Index: 240

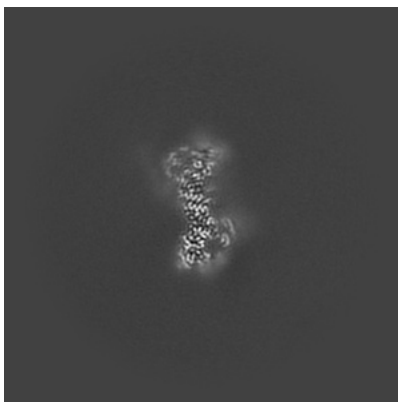
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

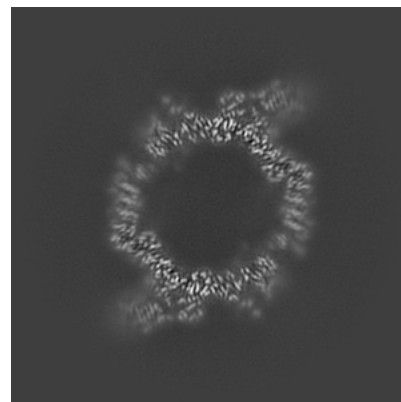
6.3.1 Primary map



X Index: 184

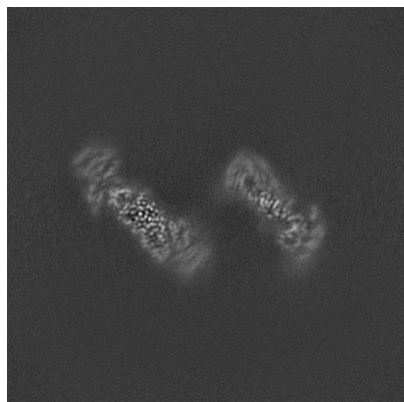


Y Index: 151

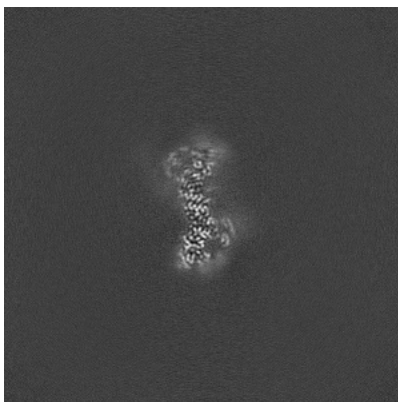


Z Index: 238

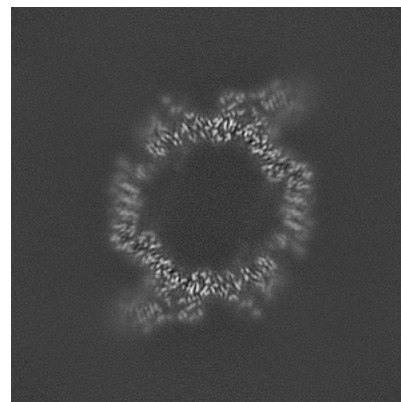
6.3.2 Raw map



X Index: 184



Y Index: 151

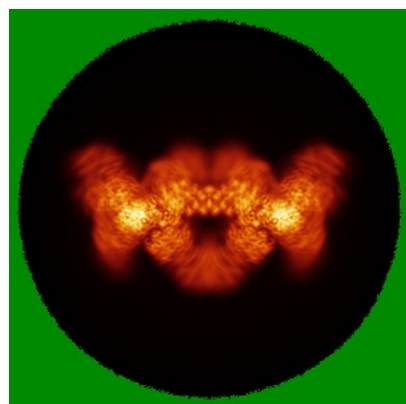


Z Index: 238

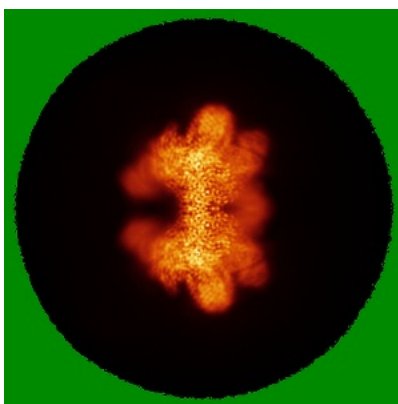
The images above show the largest variance slices of the map in three orthogonal directions.

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

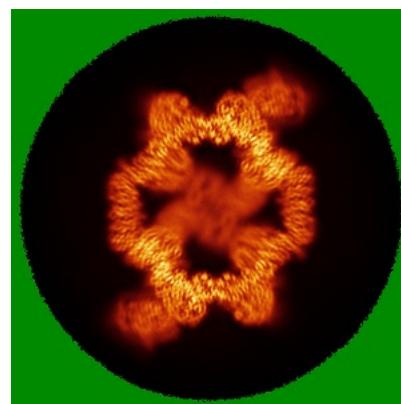
6.4.1 Primary map



X

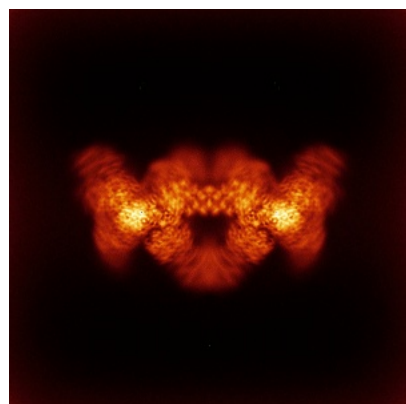


Y

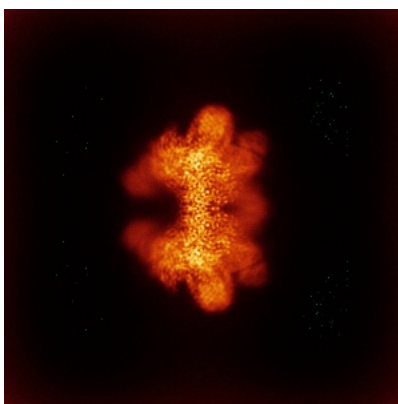


Z

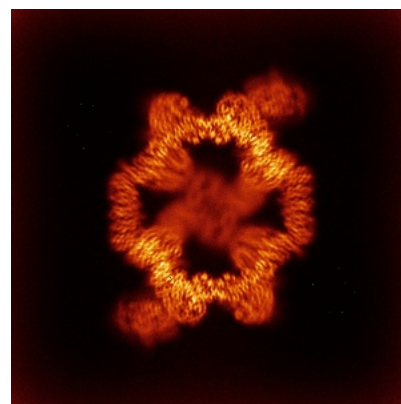
6.4.2 Raw map



X



Y

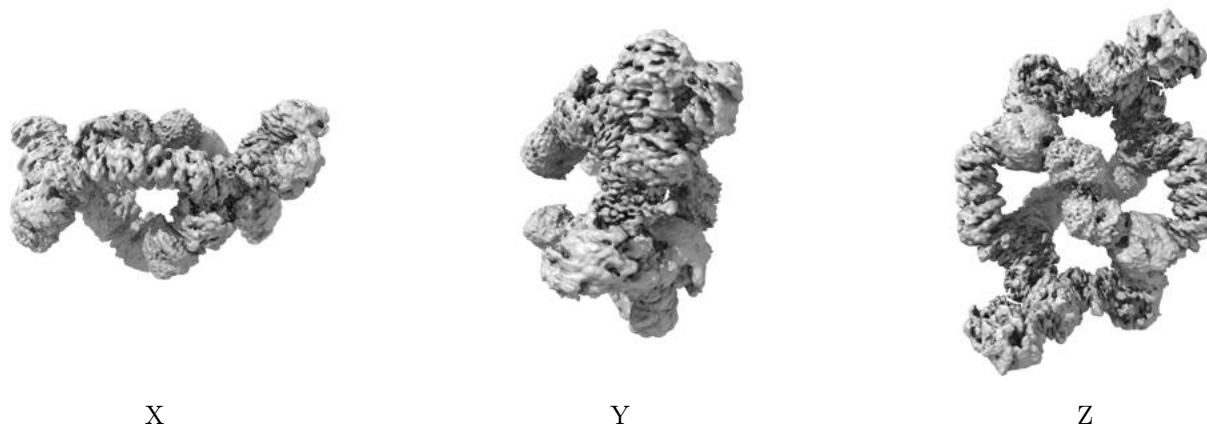


Z

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.

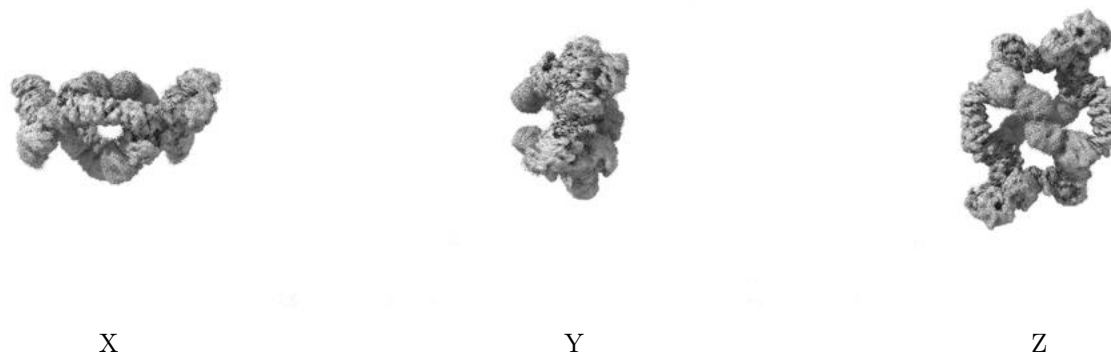
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

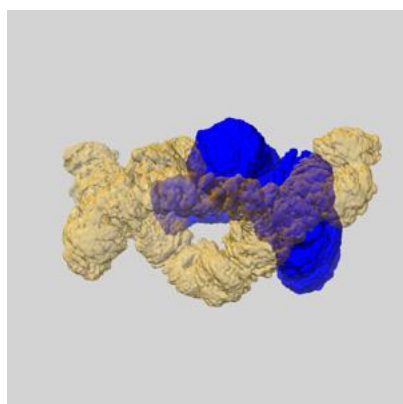
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

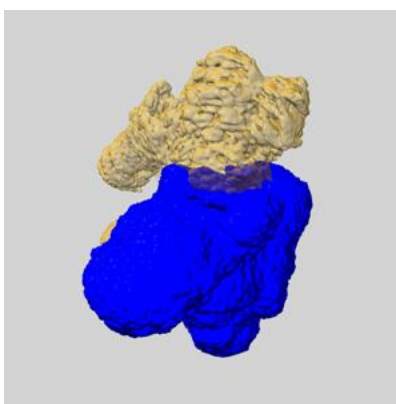
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

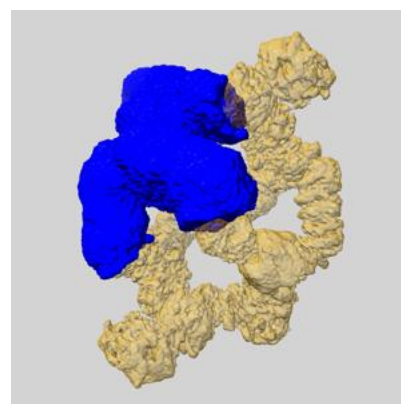
6.6.1 emd_47277_msk_4.map [i](#)



X

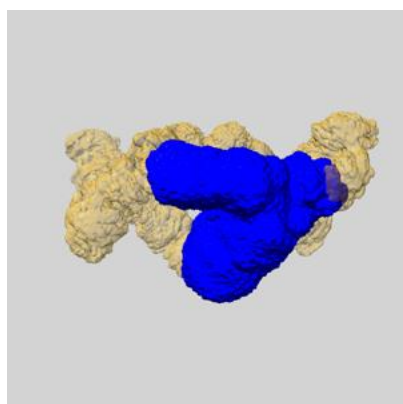


Y

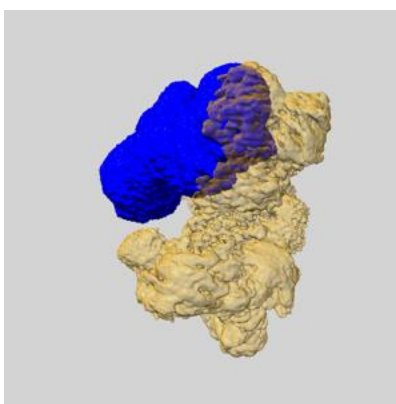


Z

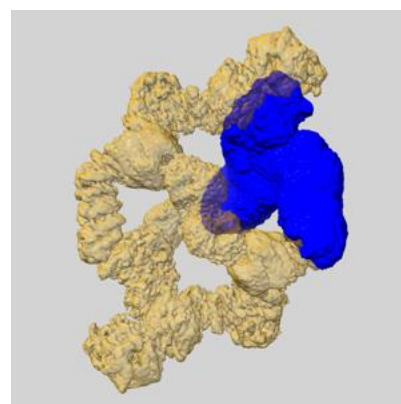
6.6.2 emd_47277_msk_3.map [i](#)



X

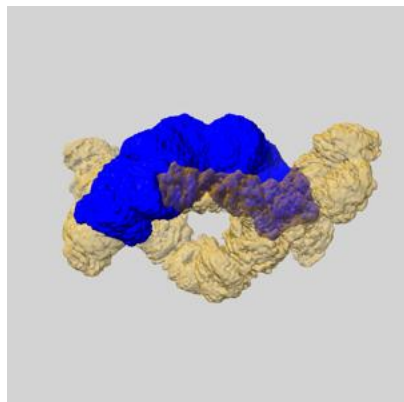


Y

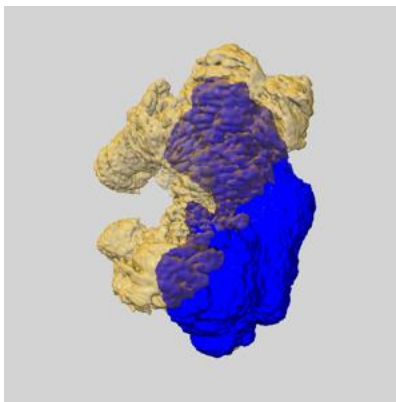


Z

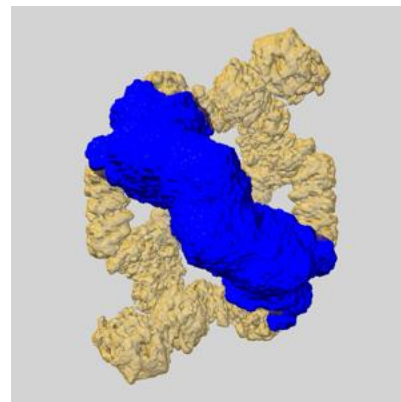
6.6.3 emd_47277_msk_2.map [i](#)



X

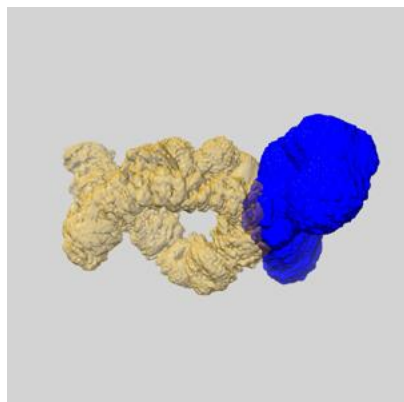


Y

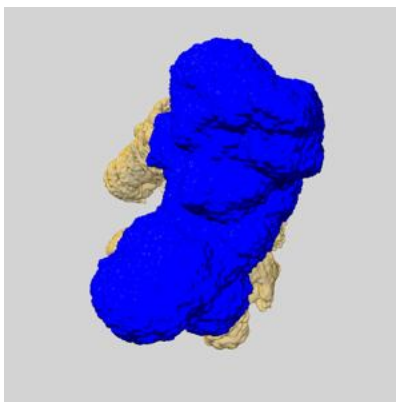


Z

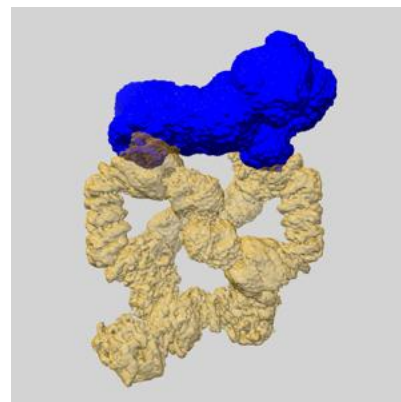
6.6.4 emd_47277_msk_1.map [i](#)



X



Y

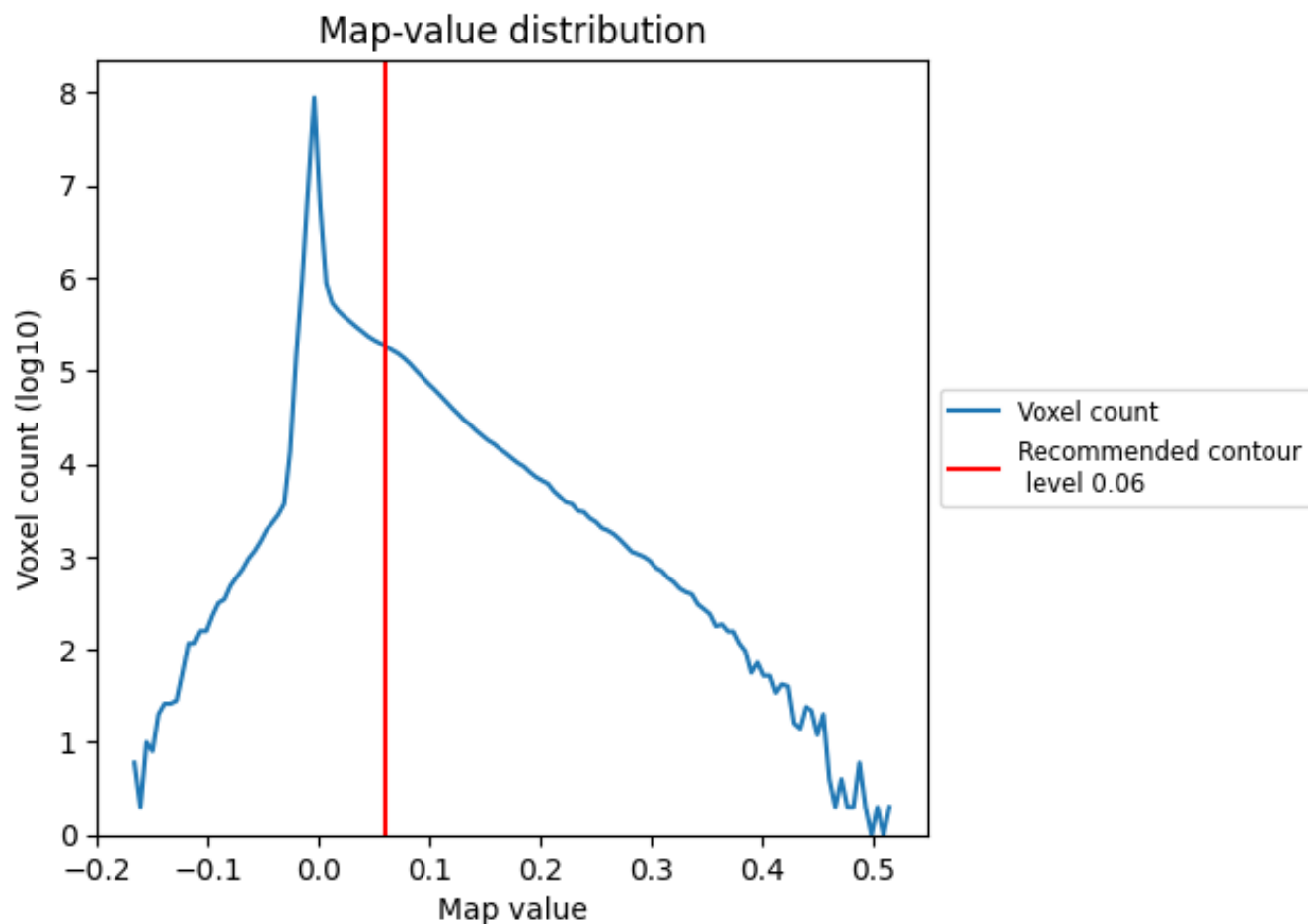


Z

7 Map analysis [i](#)

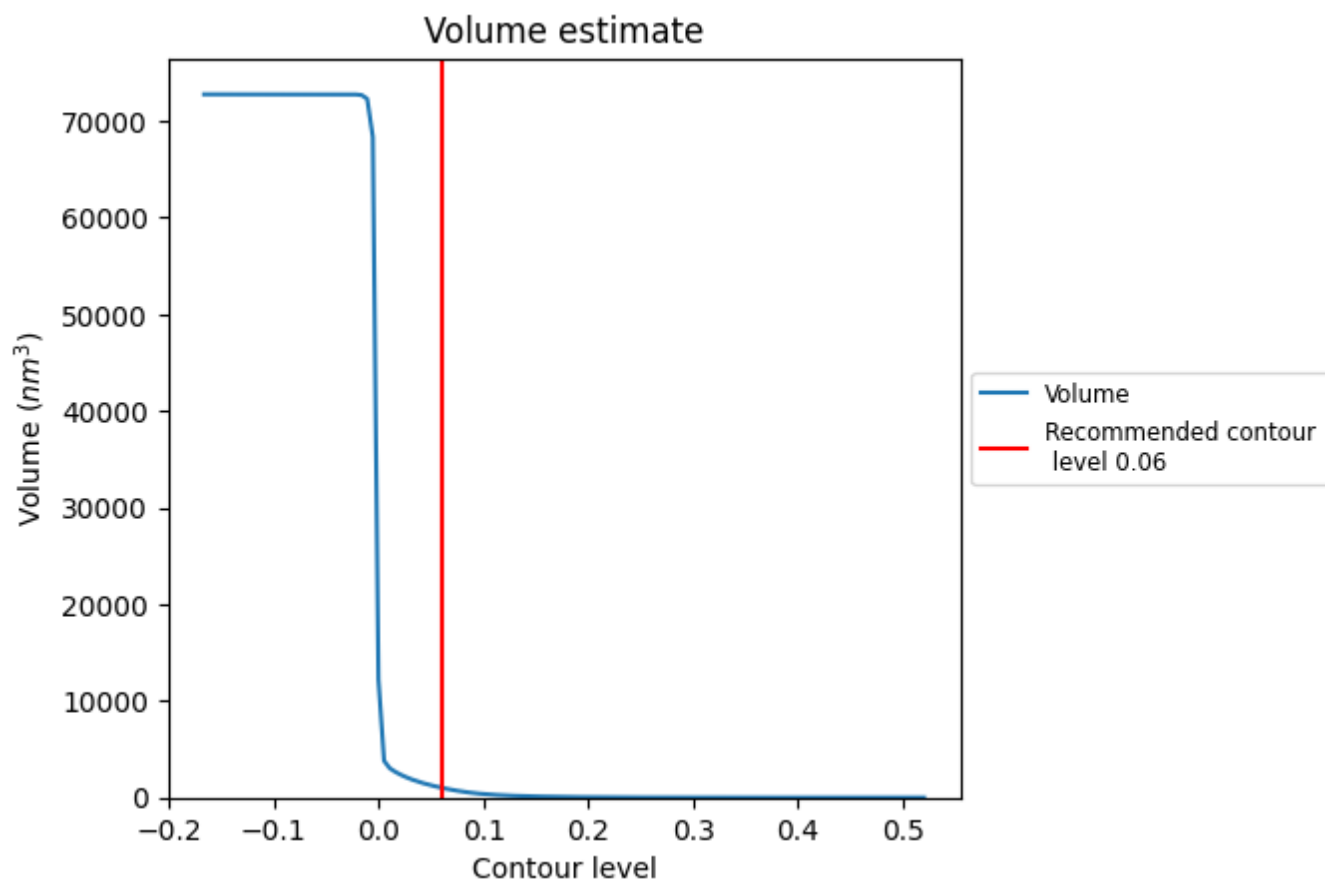
This section contains the results of statistical analysis of the map.

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.

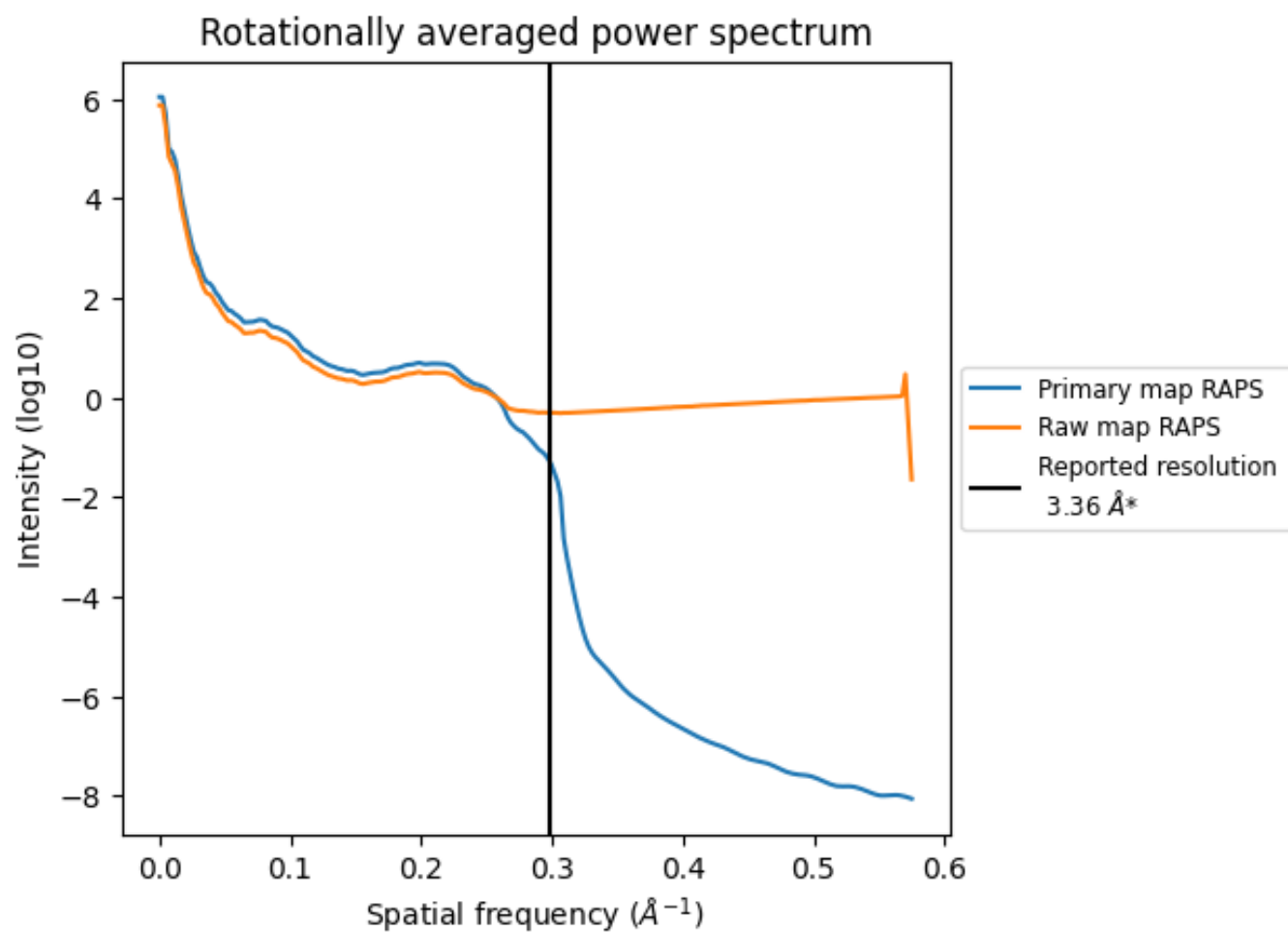
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1023 nm^3 ; this corresponds to an approximate mass of 924 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 ⓘ

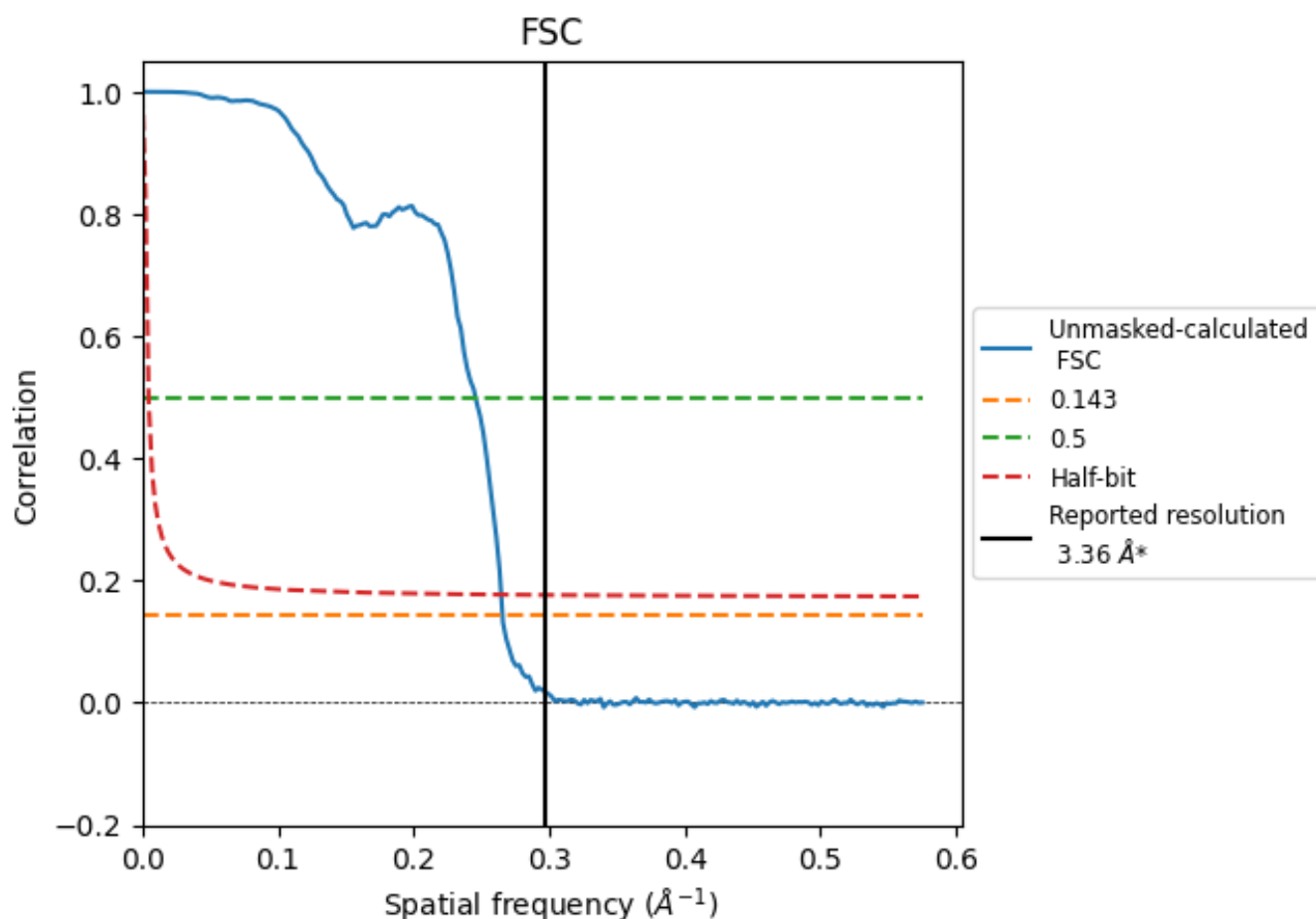


*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

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 0.298 \AA^{-1}

8.2 Resolution estimates [i](#)

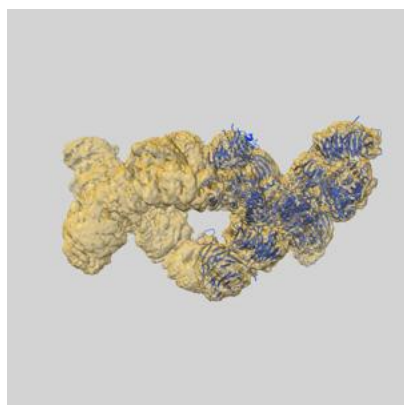
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.77	4.07	3.78

*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 3.77 differs from the reported value 3.36 by more than 10 %

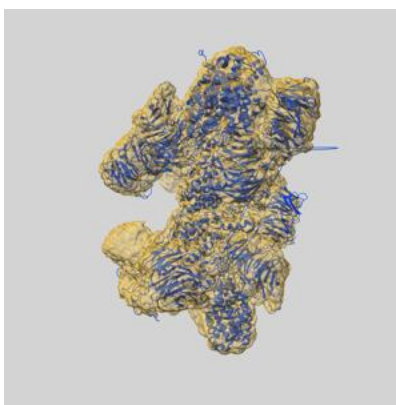
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47277 and PDB model 9DX1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

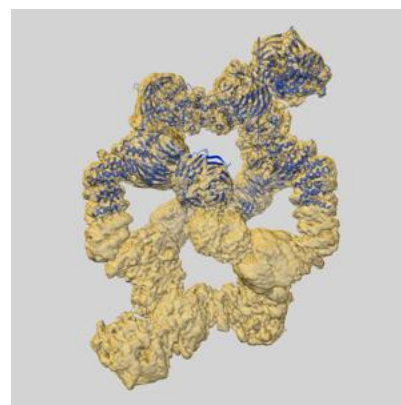
9.1 Map-model overlay [i](#)



X



Y



Z

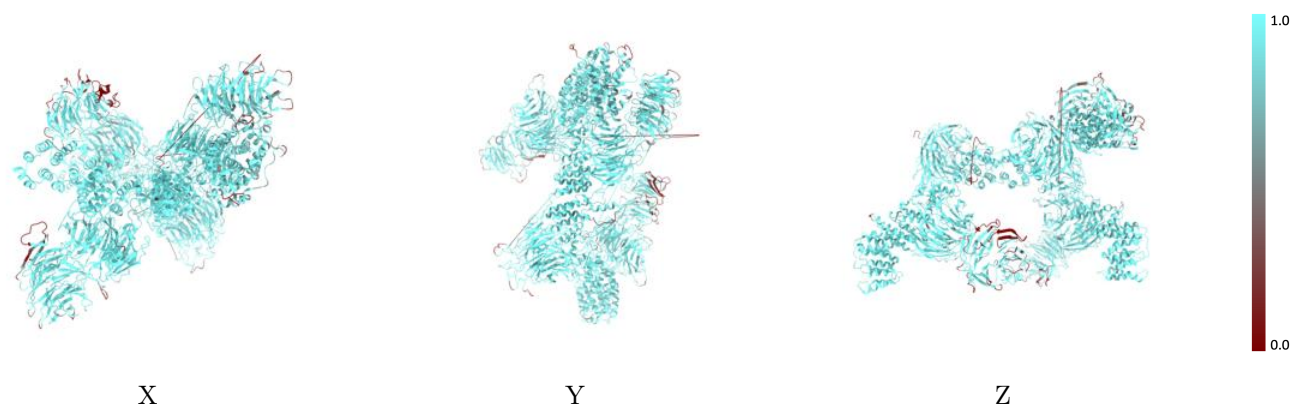
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



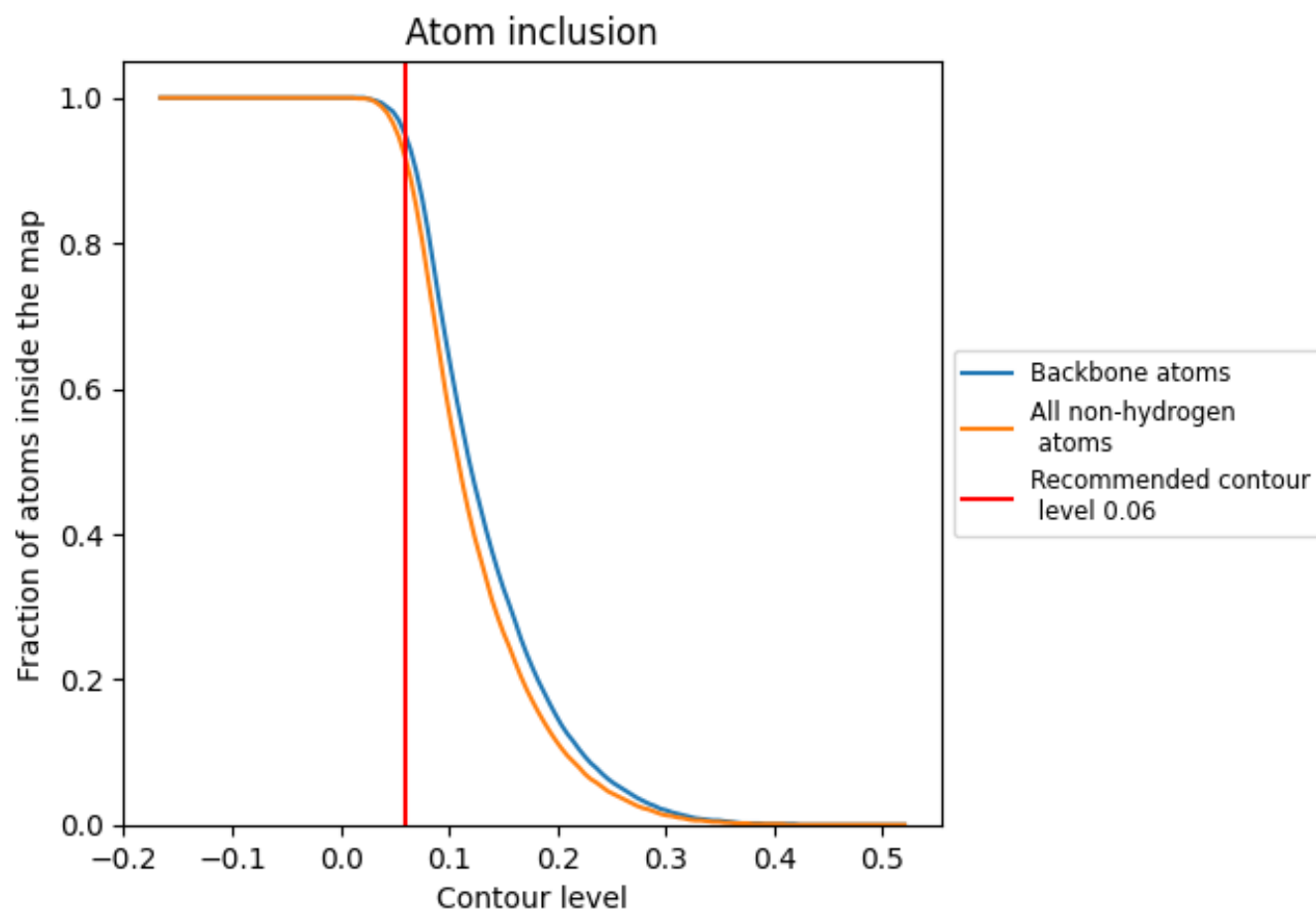
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9160	<div></div> 0.3470
A	<div></div> 0.9610	<div></div> 0.4210
B	<div></div> 0.8970	<div></div> 0.2590
C	<div></div> 0.9730	<div></div> 0.4770
D	<div></div> 0.9370	<div></div> 0.3960
E	<div></div> 0.8490	<div></div> 0.3260
F	<div></div> 0.8630	<div></div> 0.2510

