Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 05:00 pm BST

PDB ID	:	9HG6 / pdb_00009hg6
EMDB ID	:	EMD-52127
Title	:	BAM-SurA complex in the swing-in state
Authors	:	Lehner, P.A.; Jakob, R.P.; Hiller, S.
Deposited on	:	2024-11-19
Resolution	:	2.73 Å(reported)
Based on initial models	:	., 5LJO

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:

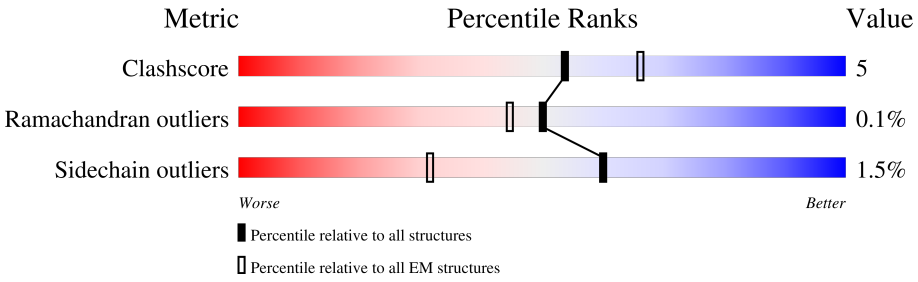
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.73 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	790	90% 10%
2	B	381	89% 8%
3	C	320	81% 78% 21%
4	D	226	87% 9%
5	E	102	82% 14%
6	F	412	41% 62% 10% 27%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31980 atoms, of which 15755 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	790	12200	3940	5953	1052	1239	16	0	0

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	371	5534	1754	2739	478	557	6	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	393	TRP	-	expression tag	UNP P77774
B	394	SER	-	expression tag	UNP P77774
B	395	HIS	-	expression tag	UNP P77774
B	396	PRO	-	expression tag	UNP P77774
B	397	GLN	-	expression tag	UNP P77774
B	398	PHE	-	expression tag	UNP P77774
B	399	GLU	-	expression tag	UNP P77774
B	400	LYS	-	expression tag	UNP P77774

- Molecule 3 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	318	4747	1485	2348	422	483	9	0	0

- Molecule 4 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	218	3461	1109	1700	309	336	7	0	0

- Molecule 5 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	88	Total	C	H	N	O	S	0	0
			1363	435	672	120	134	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	LYS	-	expression tag	UNP P0A937
E	115	LEU	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937
E	120	HIS	-	expression tag	UNP P0A937
E	121	HIS	-	expression tag	UNP P0A937

- Molecule 6 is a protein called Chaperone SurA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	300	Total	C	H	N	O	S	0	0
			4675	1430	2343	435	455	12		

There are 4 discrepancies between the modelled and reference sequences:

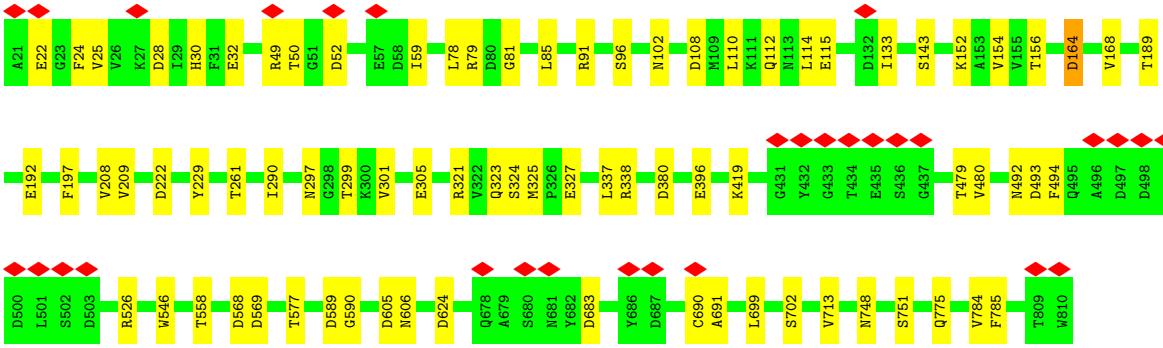
Chain	Residue	Modelled	Actual	Comment	Reference
F	17	GLY	-	expression tag	UNP P0ABZ6
F	18	SER	-	expression tag	UNP P0ABZ6
F	19	HIS	-	expression tag	UNP P0ABZ6
F	20	MET	-	expression tag	UNP P0ABZ6

3 Residue-property plots (i)

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.

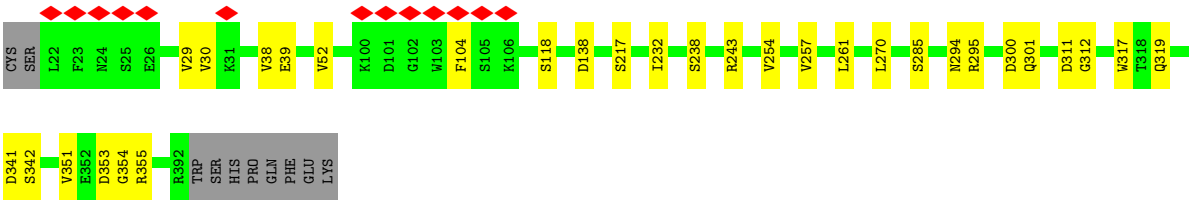
• Molecule 1: Outer membrane protein assembly factor BamA

Chain A:



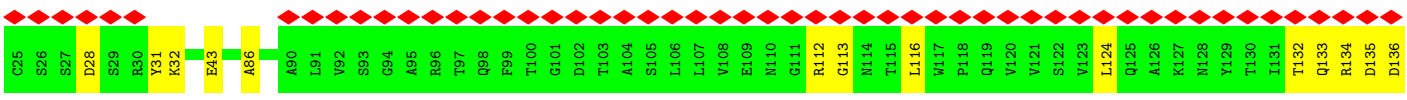
• Molecule 2: Outer membrane protein assembly factor BamB

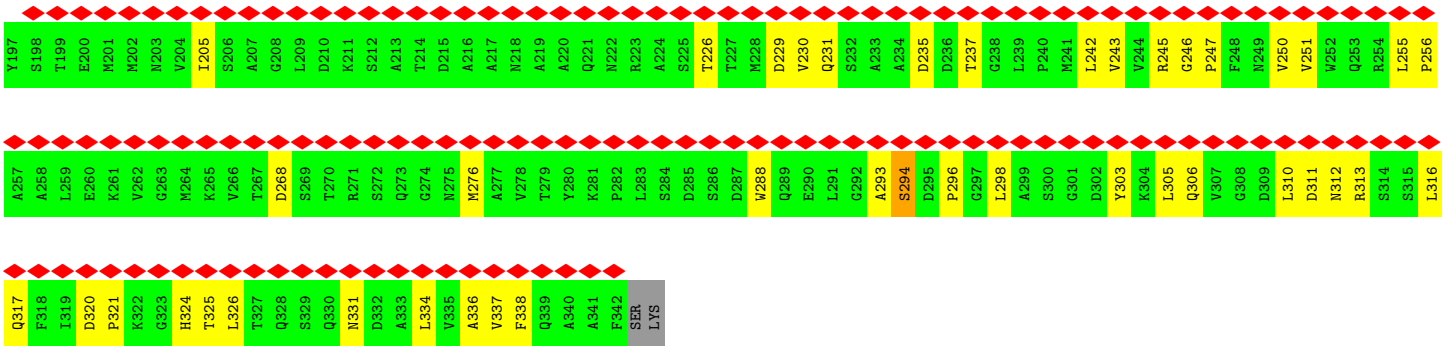
Chain B:



• Molecule 3: Outer membrane protein assembly factor BamC

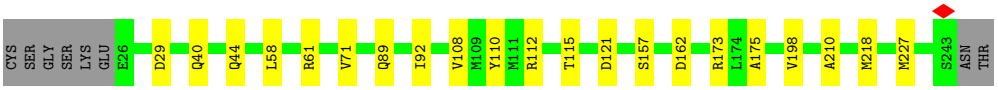
Chain C:





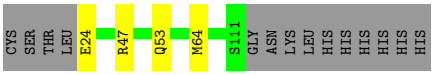
• Molecule 4: Outer membrane protein assembly factor BamD

Chain D:



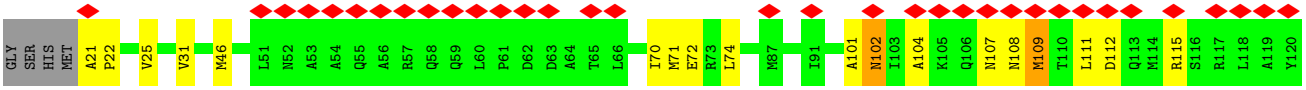
• Molecule 5: Outer membrane protein assembly factor BamE

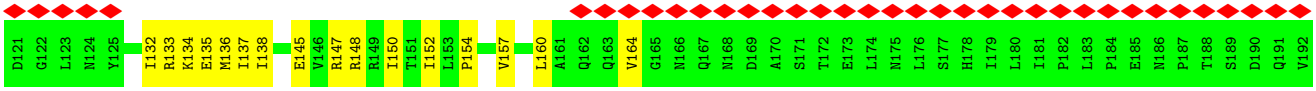
Chain E:

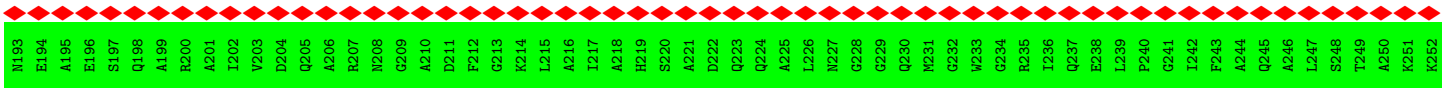


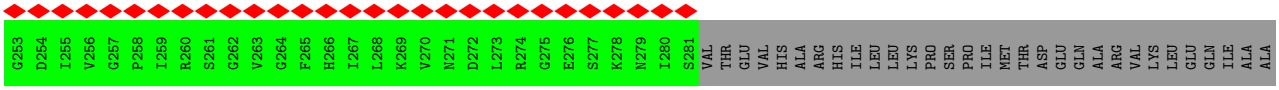
• Molecule 6: Chaperone SurA

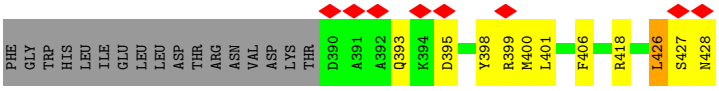
Chain F:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1088801	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.317	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	280.32, 280.32, 280.32	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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	0.28	0/6392	0.49	0/8671
2	B	0.27	0/2846	0.51	0/3881
3	C	0.26	0/2441	0.56	1/3324 (0.0%)
4	D	0.30	0/1801	0.48	0/2447
5	E	0.29	0/706	0.52	0/963
6	F	0.28	0/2355	0.55	0/3171
All	All	0.28	0/16541	0.52	1/22457 (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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	294	SER	C-N-CA	5.66	135.86	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	61	ARG	Sidechain

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	6247	5953	5952	52	0
2	B	2795	2739	2738	18	0
3	C	2399	2348	2347	49	0
4	D	1761	1700	1699	13	0
5	E	691	672	671	3	0
6	F	2332	2343	2341	35	0
All	All	16225	15755	15748	161	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 5.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:THR:OG1	3:C:133:GLN:OE1	1.98	0.80
2:B:300:ASP:OD1	2:B:301:GLN:N	2.15	0.79
6:F:145:GLU:OE2	6:F:148:ARG:NH2	2.15	0.79
5:E:53:GLN:N	5:E:53:GLN:OE1	2.17	0.78
1:A:156:THR:OG1	3:C:306:GLN:NE2	2.18	0.77
5:E:24:GLU:OE1	5:E:24:GLU:N	2.20	0.76
6:F:107:ASN:ND2	6:F:112:ASP:OD1	2.21	0.73
6:F:108:ASN:OD1	6:F:111:LEU:HD21	1.89	0.72
2:B:319:GLN:NE2	2:B:354:GLY:O	2.24	0.71
3:C:310:LEU:O	3:C:312:ASN:N	2.22	0.70
1:A:301:VAL:HG22	1:A:337:LEU:HD11	1.72	0.70
1:A:290:ILE:HD12	1:A:290:ILE:O	1.96	0.65
1:A:25:VAL:HG13	1:A:52:ASP:OD1	1.98	0.63
3:C:293:ALA:HB1	3:C:336:ALA:HB3	1.82	0.62
1:A:305:GLU:OE2	1:A:324:SER:OG	2.05	0.61
1:A:96:SER:OG	1:A:164:ASP:OD1	2.16	0.61
3:C:229:ASP:OD2	3:C:245:ARG:NH2	2.33	0.61
1:A:208:VAL:HG12	1:A:208:VAL:O	2.00	0.60
2:B:238:SER:O	2:B:243:ARG:NH1	2.36	0.59
2:B:353:ASP:OD2	2:B:355:ARG:NH1	2.36	0.59
1:A:28:ASP:OD2	1:A:30:HIS:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:ASP:OD1	2:B:312:GLY:N	2.36	0.58
3:C:151:LEU:H	3:C:151:LEU:HD12	1.67	0.58
1:A:59:ILE:CD1	6:F:25:VAL:HG11	2.34	0.58
6:F:133:ARG:O	6:F:137:ILE:HG13	2.04	0.56
1:A:32:GLU:OE2	1:A:85:LEU:HD11	2.03	0.56
1:A:154:VAL:HG11	3:C:317:GLN:OE1	2.06	0.56
3:C:32:LYS:NZ	4:D:44:GLN:O	2.30	0.56
6:F:21:ALA:HB3	6:F:22:PRO:CD	2.36	0.56
1:A:690:CYS:SG	1:A:691:ALA:N	2.79	0.56
3:C:242:LEU:HD23	3:C:338:PHE:CE2	2.40	0.56
3:C:288:TRP:HB3	3:C:294:SER:HA	1.87	0.56
4:D:89:GLN:HG2	4:D:115:THR:HG21	1.88	0.56
2:B:52:VAL:HG12	2:B:52:VAL:O	2.07	0.55
1:A:25:VAL:HG13	1:A:52:ASP:CG	2.27	0.55
1:A:59:ILE:HD13	6:F:25:VAL:HG11	1.89	0.55
4:D:40:GLN:OE1	4:D:44:GLN:NE2	2.40	0.55
1:A:25:VAL:HG22	1:A:52:ASP:OD1	2.06	0.55
2:B:294:ASN:OD1	2:B:294:ASN:N	2.40	0.54
6:F:150:ILE:HD11	6:F:406:PHE:HA	1.89	0.54
3:C:296:PRO:HD3	3:C:334:LEU:HD21	1.90	0.54
4:D:198:VAL:HG11	4:D:218:MET:HB2	1.90	0.54
3:C:231:GLN:HG3	3:C:243:VAL:HB	1.89	0.54
6:F:134:LYS:O	6:F:138:ILE:HG23	2.07	0.54
4:D:92:ILE:HG23	4:D:108:VAL:HG12	1.91	0.53
6:F:104:ALA:HB3	6:F:107:ASN:HB3	1.91	0.53
3:C:230:VAL:HG21	3:C:338:PHE:HB3	1.91	0.53
2:B:261:LEU:HD21	2:B:285:SER:OG	2.09	0.52
1:A:209:VAL:HG22	1:A:209:VAL:O	2.10	0.52
3:C:310:LEU:C	3:C:312:ASN:H	2.12	0.52
3:C:255:LEU:N	3:C:256:PRO:HD2	2.25	0.52
6:F:21:ALA:HB3	6:F:22:PRO:HD3	1.92	0.52
1:A:192:GLU:OE2	1:A:229:TYR:OH	2.27	0.51
3:C:190:ASP:OD2	3:C:192:ALA:HB3	2.09	0.51
6:F:31:VAL:HG23	6:F:426:LEU:HD11	1.93	0.51
3:C:134:ARG:NE	3:C:136:ASP:OD1	2.44	0.51
1:A:189:THR:HG21	2:B:104:PHE:CD1	2.46	0.51
6:F:427:SER:O	6:F:428:ASN:C	2.49	0.51
2:B:355:ARG:NH1	2:B:355:ARG:HB3	2.26	0.50
3:C:43:GLU:HA	3:C:43:GLU:OE1	2.12	0.50
3:C:231:GLN:OE1	3:C:313:ARG:NH1	2.44	0.50
6:F:72:GLU:OE2	6:F:418:ARG:NE	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:160:LEU:HD21	6:F:400:MET:SD	2.52	0.50
6:F:111:LEU:H	6:F:111:LEU:HD23	1.76	0.50
1:A:108:ASP:O	1:A:112:GLN:OE1	2.30	0.49
4:D:92:ILE:HG21	4:D:112:ARG:HB2	1.94	0.49
3:C:294:SER:O	3:C:334:LEU:HD23	2.12	0.49
3:C:205:ILE:N	3:C:205:ILE:HD13	2.27	0.49
6:F:102:ASN:O	6:F:102:ASN:ND2	2.46	0.49
2:B:295:ARG:NH2	2:B:351:VAL:O	2.46	0.48
3:C:235:ASP:OD1	3:C:237:THR:HG22	2.13	0.48
3:C:298:LEU:HD23	3:C:303:TYR:CE2	2.48	0.48
1:A:110:LEU:O	1:A:114:LEU:HD23	2.14	0.48
6:F:46:MET:HA	6:F:46:MET:HE2	1.95	0.48
3:C:242:LEU:HD11	3:C:331:ASN:HB2	1.95	0.48
1:A:301:VAL:CG2	1:A:337:LEU:HD11	2.39	0.48
1:A:699:LEU:HD12	1:A:699:LEU:N	2.29	0.48
6:F:71:MET:HA	6:F:71:MET:CE	2.44	0.47
4:D:58:LEU:HD23	4:D:71:VAL:HG21	1.96	0.47
2:B:232:ILE:HD11	2:B:270:LEU:HD21	1.95	0.47
4:D:58:LEU:HD23	4:D:71:VAL:CG2	2.45	0.47
1:A:526:ARG:NH1	1:A:577:THR:OG1	2.38	0.47
3:C:298:LEU:HD23	3:C:303:TYR:CD2	2.49	0.47
6:F:108:ASN:O	6:F:112:ASP:HB3	2.14	0.47
3:C:116:LEU:HD23	3:C:165:VAL:CG1	2.45	0.46
1:A:197:PHE:CD2	1:A:222:ASP:OD2	2.69	0.46
6:F:132:ILE:O	6:F:136:MET:HE2	2.15	0.46
1:A:79:ARG:HG2	1:A:81:GLY:H	1.81	0.45
3:C:247:PRO:O	3:C:251:VAL:HG13	2.17	0.45
1:A:52:ASP:OD1	1:A:52:ASP:O	2.34	0.45
2:B:341:ASP:OD1	2:B:342:SER:N	2.50	0.45
3:C:255:LEU:HD21	3:C:305:LEU:HD22	1.99	0.45
6:F:135:GLU:O	6:F:138:ILE:HG12	2.17	0.45
6:F:111:LEU:HD23	6:F:111:LEU:N	2.32	0.45
1:A:589:ASP:OD1	1:A:590:GLY:N	2.50	0.44
1:A:775:GLN:HG2	1:A:784:VAL:HG13	1.99	0.44
1:A:78:LEU:HD13	1:A:85:LEU:HD23	1.99	0.44
1:A:396:GLU:N	1:A:419:LYS:O	2.48	0.44
6:F:395:ASP:O	6:F:399:ARG:HG2	2.18	0.44
2:B:38:VAL:HG22	2:B:39:GLU:N	2.32	0.44
1:A:156:THR:HG21	3:C:306:GLN:CD	2.38	0.44
6:F:46:MET:CE	6:F:70:ILE:HD12	2.48	0.43
1:A:114:LEU:HD13	1:A:133:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:THR:HG22	1:A:480:VAL:N	2.33	0.43
2:B:254:VAL:O	2:B:257:VAL:HG12	2.18	0.43
2:B:317:TRP:NE1	2:B:351:VAL:O	2.49	0.43
3:C:298:LEU:HD21	3:C:326:LEU:CD1	2.47	0.43
3:C:310:LEU:HB2	3:C:313:ARG:O	2.18	0.43
4:D:29:ASP:O	4:D:29:ASP:CG	2.56	0.43
3:C:116:LEU:HD23	3:C:165:VAL:HG13	2.00	0.43
2:B:29:VAL:HG22	2:B:30:VAL:H	1.83	0.43
4:D:110:TYR:OH	4:D:162:ASP:OD2	2.34	0.43
1:A:380:ASP:OD1	1:A:380:ASP:N	2.52	0.43
1:A:112:GLN:O	1:A:115:GLU:HG3	2.19	0.43
3:C:86:ALA:HB3	3:C:196:ARG:HA	2.01	0.43
1:A:197:PHE:CG	1:A:222:ASP:OD1	2.71	0.43
1:A:321:ARG:NH1	1:A:323:GLN:OE1	2.52	0.43
6:F:101:ALA:HA	6:F:109:MET:SD	2.59	0.43
1:A:325:MET:SD	1:A:325:MET:N	2.92	0.42
4:D:92:ILE:HG23	4:D:108:VAL:CG1	2.49	0.42
3:C:113:GLY:O	3:C:172:GLN:OE1	2.37	0.42
3:C:145:TRP:NE1	3:C:160:ARG:NH1	2.67	0.42
3:C:293:ALA:HB2	3:C:337:VAL:HB	2.01	0.42
1:A:327:GLU:OE1	1:A:338:ARG:NH2	2.53	0.42
1:A:114:LEU:HD13	1:A:133:ILE:HD12	2.02	0.42
3:C:135:ASP:O	3:C:139:GLN:N	2.52	0.42
1:A:492:ASN:OD1	1:A:493:ASP:N	2.53	0.42
3:C:242:LEU:O	3:C:316:LEU:HD13	2.20	0.42
3:C:28:ASP:O	3:C:31:TYR:HD1	2.03	0.42
3:C:298:LEU:HD21	3:C:326:LEU:HD11	2.02	0.42
1:A:108:ASP:OD1	1:A:108:ASP:C	2.58	0.42
3:C:226:THR:HG21	3:C:246:GLY:HA2	2.02	0.42
3:C:247:PRO:HG2	3:C:250:VAL:HG22	2.02	0.42
1:A:558:THR:HG22	1:A:558:THR:O	2.20	0.42
6:F:112:ASP:HA	6:F:115:ARG:HH11	1.85	0.42
6:F:147:ARG:HA	6:F:150:ILE:HD12	2.02	0.42
1:A:152:LYS:HB2	1:A:152:LYS:NZ	2.36	0.41
3:C:268:ASP:O	3:C:276:MET:HG3	2.20	0.41
4:D:227:MET:HE2	5:E:64:MET:HE1	2.02	0.41
6:F:152:ILE:HD11	6:F:401:LEU:HD23	2.03	0.41
3:C:124:LEU:HD13	3:C:124:LEU:C	2.41	0.41
6:F:70:ILE:O	6:F:74:LEU:HD23	2.21	0.41
3:C:334:LEU:O	3:C:338:PHE:HB2	2.21	0.41
2:B:29:VAL:HG22	2:B:30:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:154:PRO:HA	6:F:157:VAL:HG12	2.03	0.41
1:A:102:ASN:OD1	1:A:102:ASN:N	2.51	0.41
1:A:49:ARG:O	1:A:50:THR:C	2.59	0.41
1:A:261:THR:O	1:A:261:THR:HG23	2.21	0.41
1:A:493:ASP:OD1	1:A:494:PHE:N	2.54	0.41
1:A:624:ASP:OD1	1:A:624:ASP:O	2.39	0.41
6:F:104:ALA:HB3	6:F:107:ASN:CB	2.51	0.41
3:C:320:ASP:N	3:C:324:HIS:O	2.47	0.41
6:F:46:MET:HE2	6:F:46:MET:CA	2.50	0.41
6:F:152:ILE:HD11	6:F:401:LEU:CD2	2.51	0.41
6:F:164:VAL:HG11	6:F:393:GLN:NE2	2.37	0.40
3:C:112:ARG:HD3	3:C:116:LEU:HD13	2.02	0.40
1:A:168:VAL:HG11	3:C:325:THR:HG23	2.03	0.40
1:A:297:ASN:OD1	1:A:299:THR:HG22	2.21	0.40
1:A:569:ASP:OD2	1:A:606:ASN:ND2	2.54	0.40
3:C:303:TYR:CE2	3:C:321:PRO:HD3	2.57	0.40
4:D:175:ALA:HB1	4:D:210:ALA:HB3	2.02	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	788/790 (100%)	772 (98%)	15 (2%)	1 (0%)	48 70
2	B	369/381 (97%)	355 (96%)	14 (4%)	0	100 100
3	C	316/320 (99%)	301 (95%)	14 (4%)	1 (0%)	37 55
4	D	216/226 (96%)	212 (98%)	4 (2%)	0	100 100
5	E	86/102 (84%)	83 (96%)	3 (4%)	0	100 100
6	F	296/412 (72%)	284 (96%)	12 (4%)	0	100 100
All	All	2071/2231 (93%)	2007 (97%)	62 (3%)	2 (0%)	50 70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	311	ASP
1	A	22	GLU

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	672/672 (100%)	659 (98%)	13 (2%)	52	71
2	B	302/312 (97%)	299 (99%)	3 (1%)	73	84
3	C	256/258 (99%)	254 (99%)	2 (1%)	79	88
4	D	183/190 (96%)	180 (98%)	3 (2%)	58	75
5	E	77/90 (86%)	76 (99%)	1 (1%)	65	80
6	F	250/341 (73%)	246 (98%)	4 (2%)	58	75
All	All	1740/1863 (93%)	1714 (98%)	26 (2%)	60	76

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

Mol	Chain	Res	Type
1	A	24	PHE
1	A	91	ARG
1	A	143	SER
1	A	164	ASP
1	A	546	TRP
1	A	568	ASP
1	A	605	ASP
1	A	683	ASP
1	A	702	SER
1	A	713	VAL
1	A	748	ASN
1	A	751	SER
1	A	785	PHE
2	B	118	SER
2	B	138	ASP

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Mol	Chain	Res	Type
2	B	217	SER
3	C	152	ASP
3	C	195	GLN
4	D	121	ASP
4	D	157	SER
4	D	173	ARG
5	E	47	ARG
6	F	102	ASN
6	F	109	MET
6	F	398	TYR
6	F	426	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	172	GLN
3	C	306	GLN

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)

There are no chain breaks in this entry.

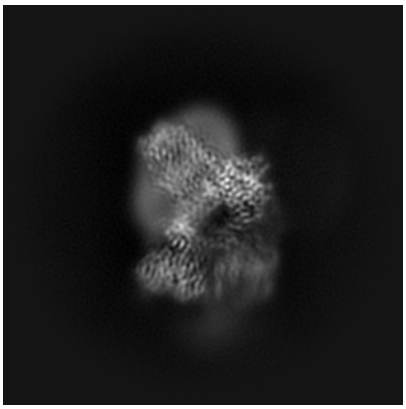
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52127. These allow visual inspection of the internal detail of the map and identification of artifacts.

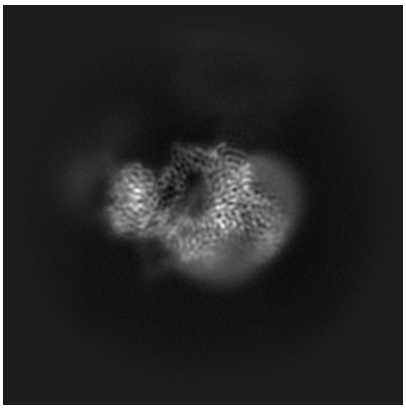
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

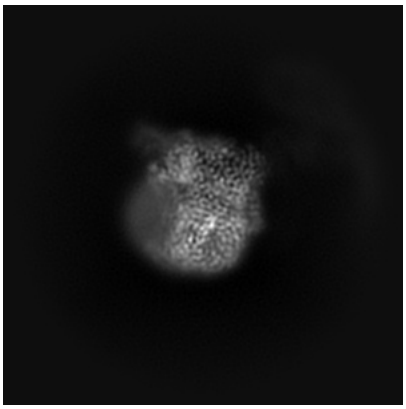
6.1.1 Primary map



X

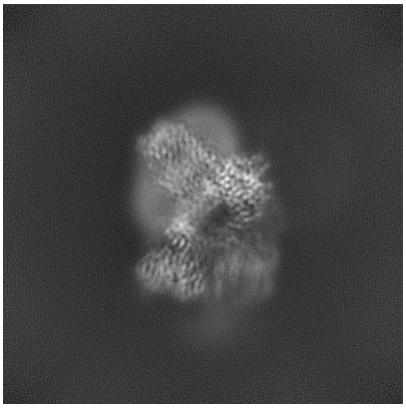


Y

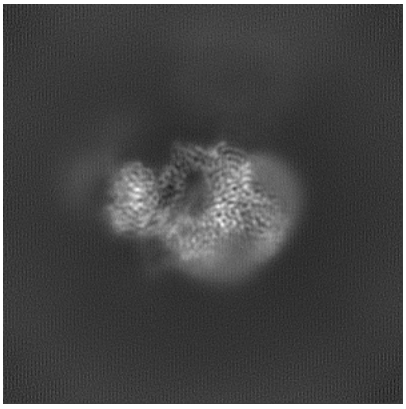


Z

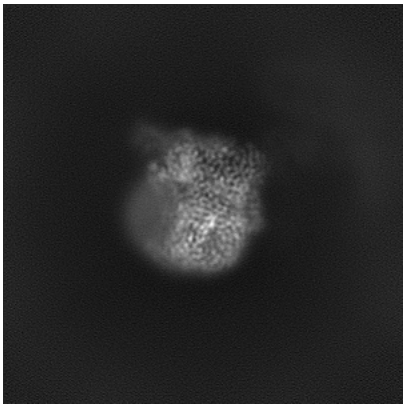
6.1.2 Raw map



X



Y

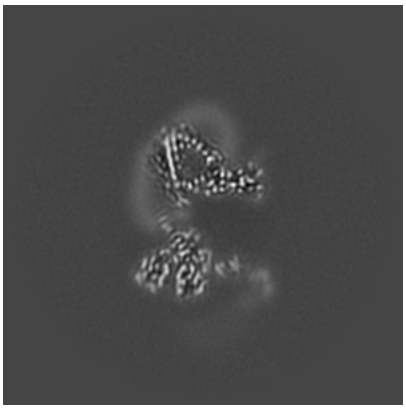


Z

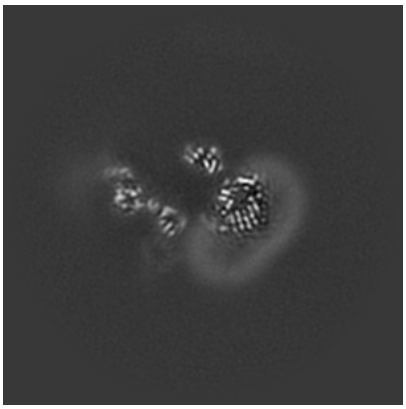
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

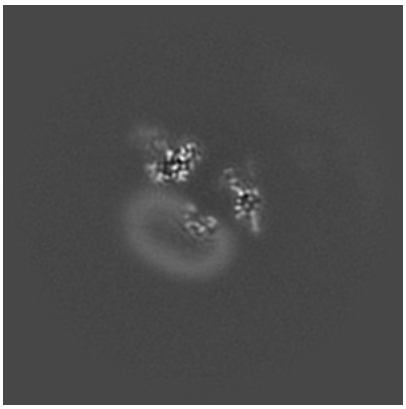
6.2.1 Primary map



X Index: 192

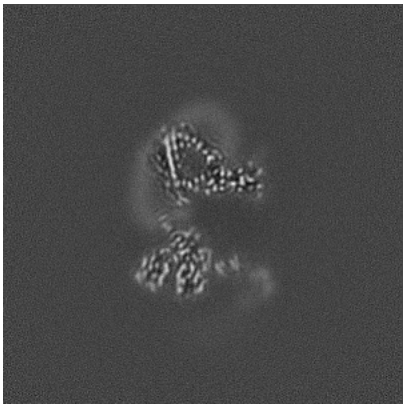


Y Index: 192

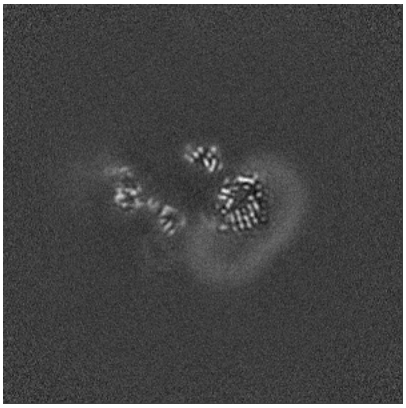


Z Index: 192

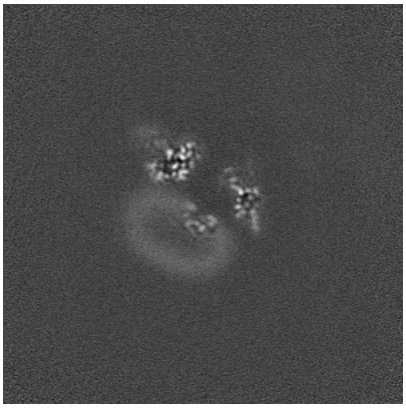
6.2.2 Raw map



X Index: 192



Y Index: 192

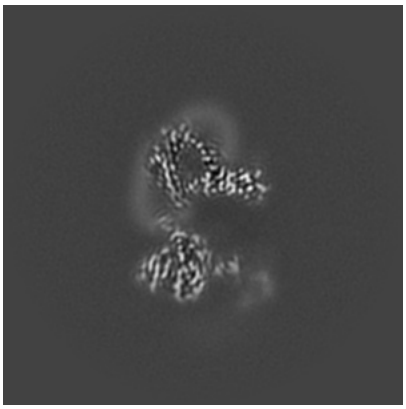


Z Index: 192

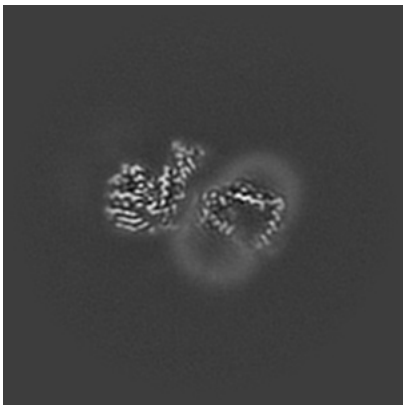
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

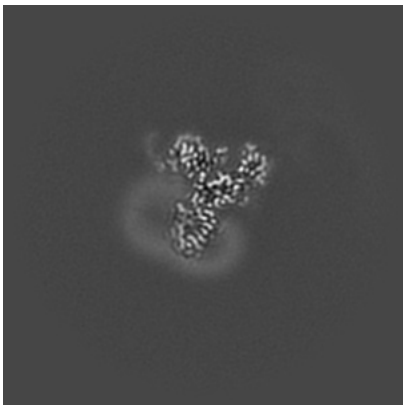
6.3.1 Primary map



X Index: 190

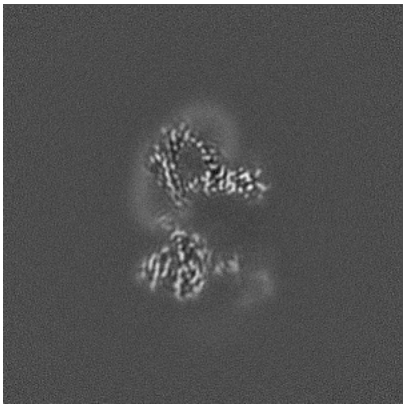


Y Index: 172

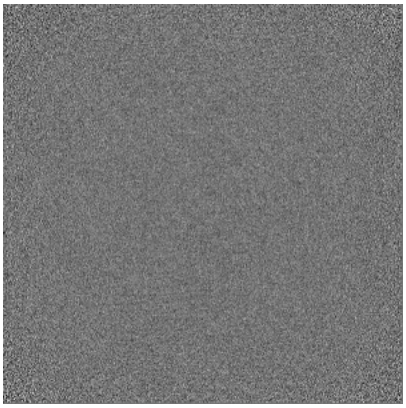


Z Index: 210

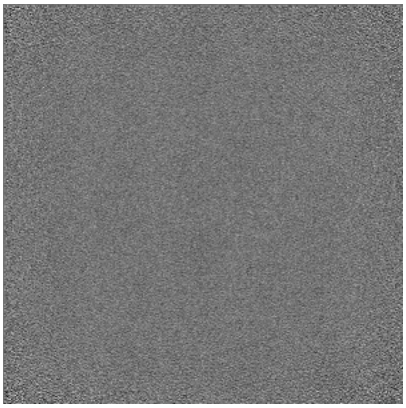
6.3.2 Raw map



X Index: 190



Y Index: 0

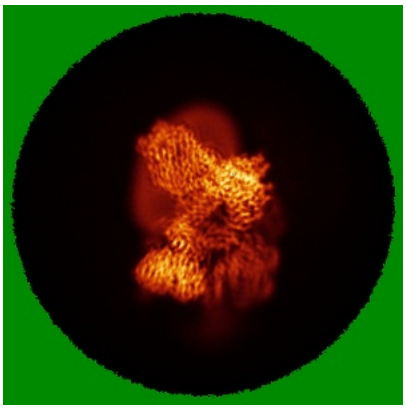


Z Index: 0

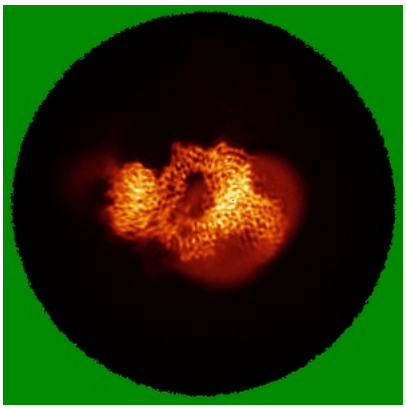
The images above show the largest variance slices of the map in three orthogonal directions.

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

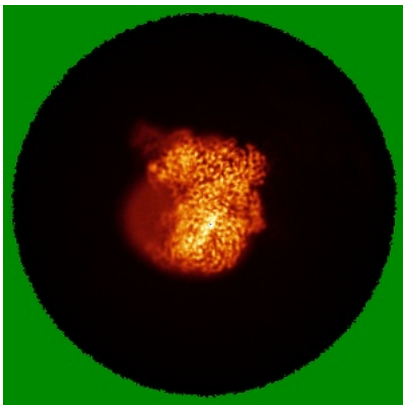
6.4.1 Primary map



X

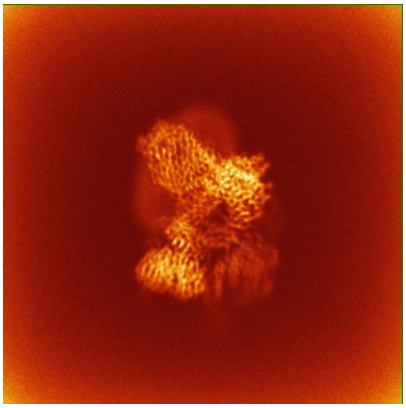


Y

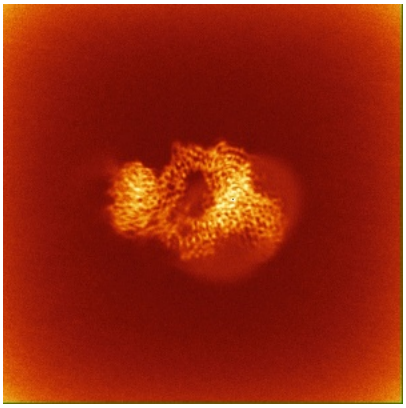


Z

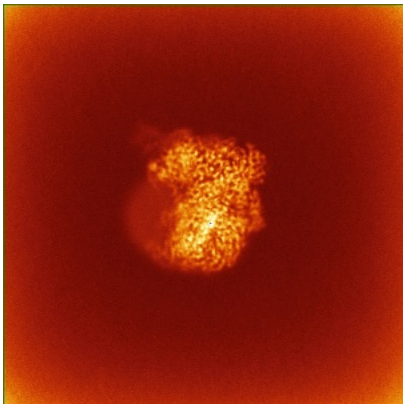
6.4.2 Raw map



X



Y

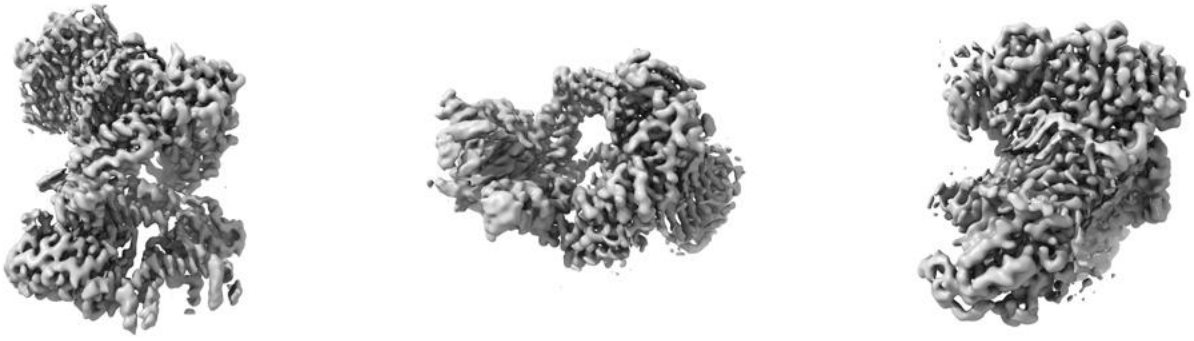


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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

X Y Z

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.

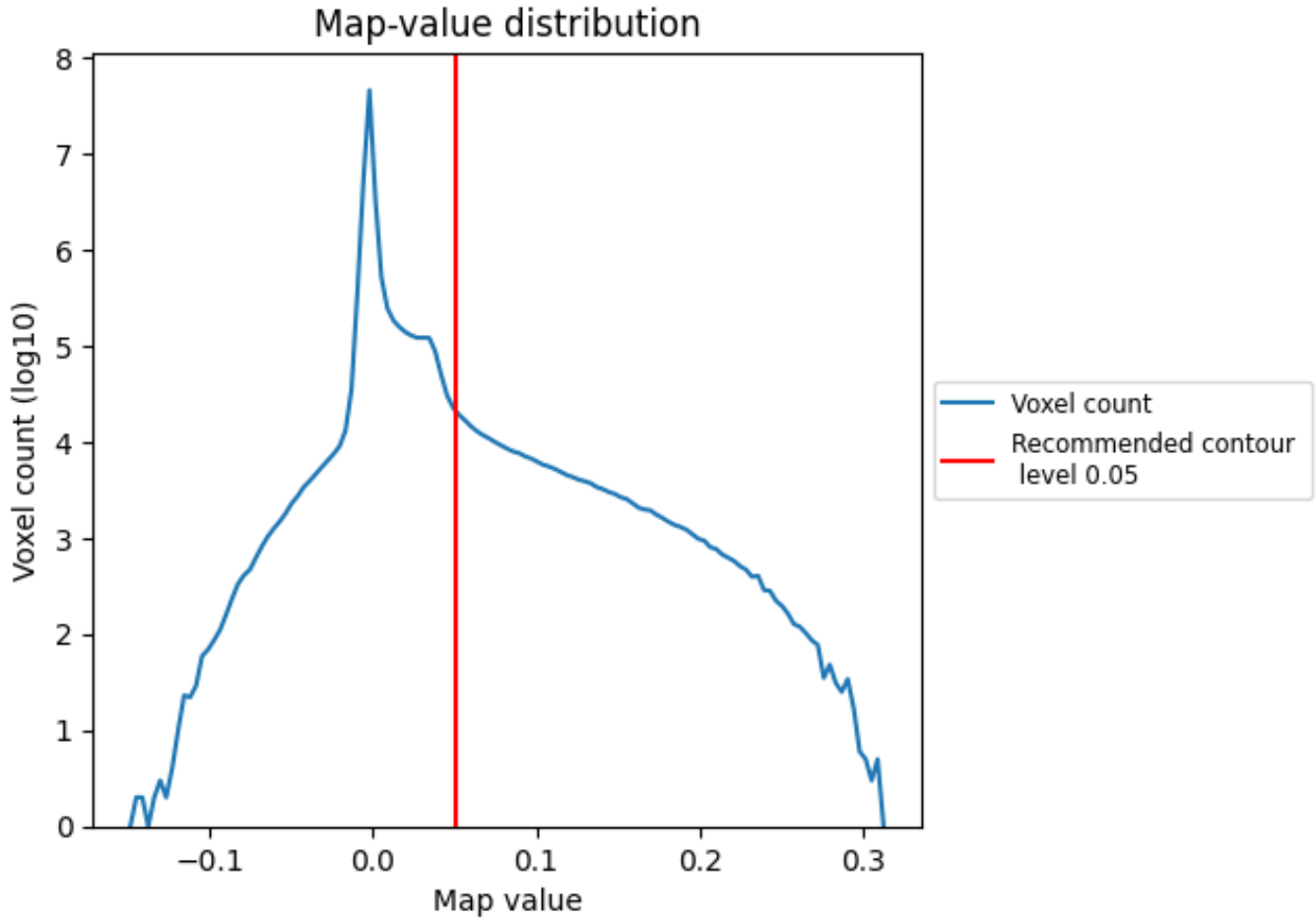
6.6 Mask visualisation (i)

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

7 Map analysis

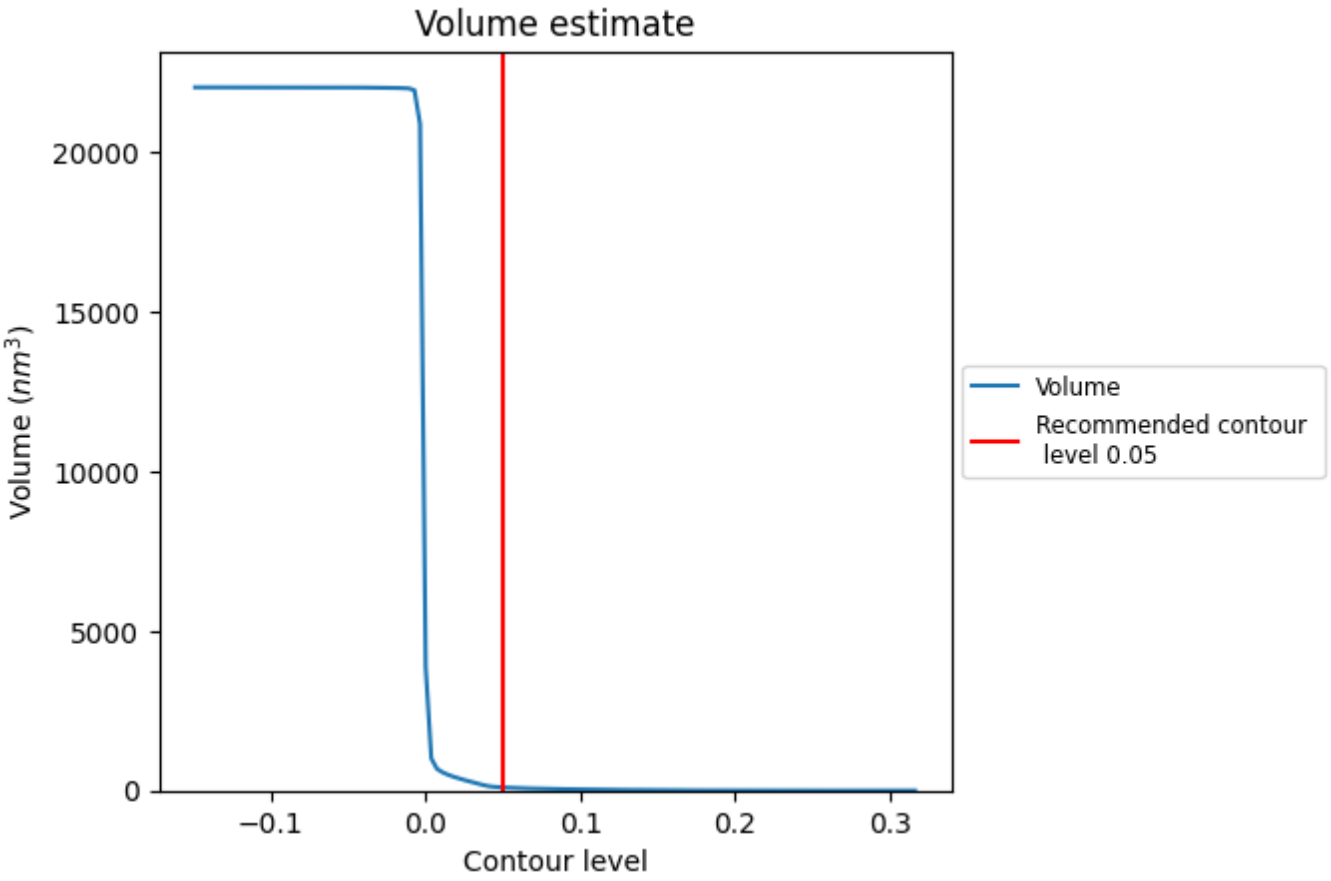
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

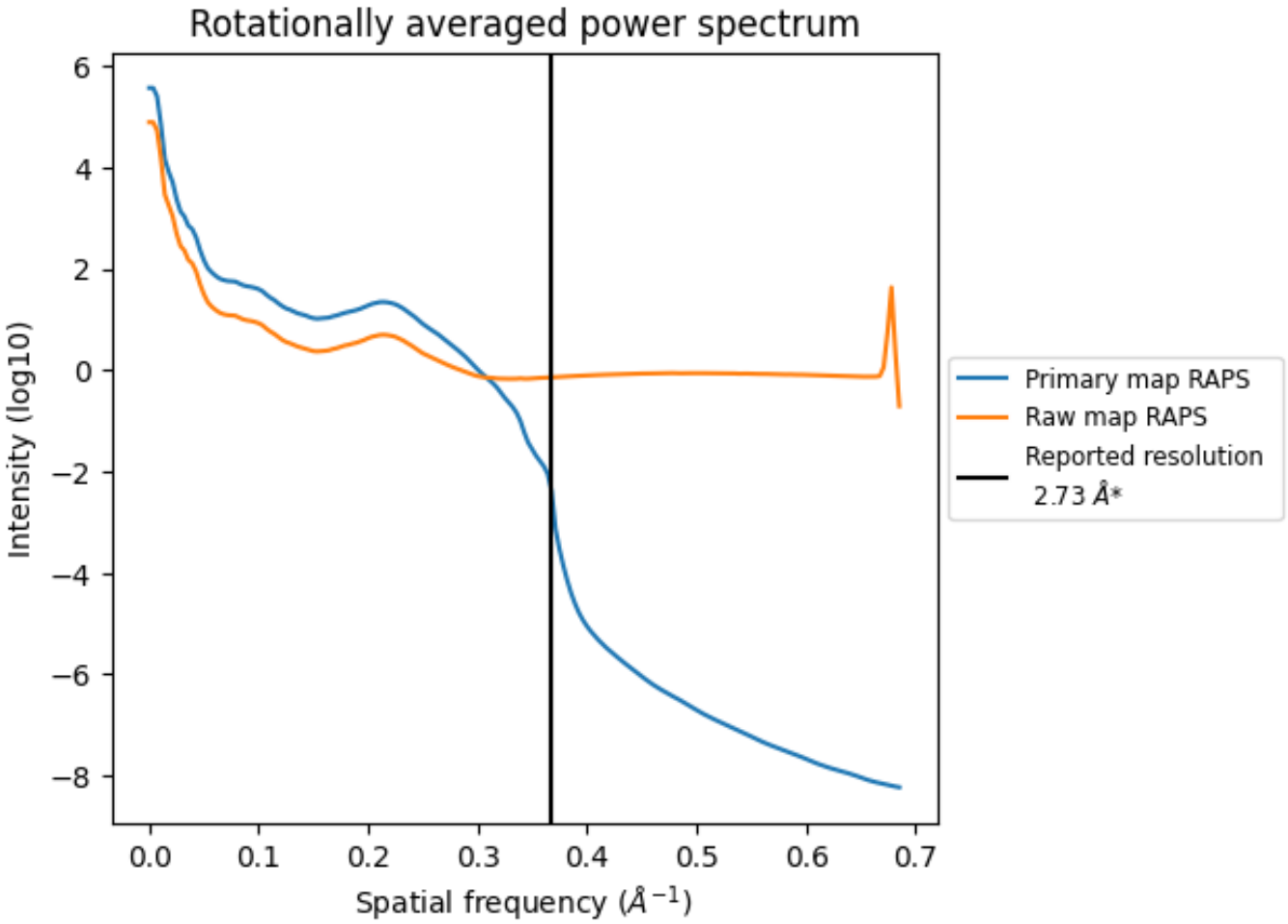
7.2 Volume estimate (i)



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 89 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 (i)

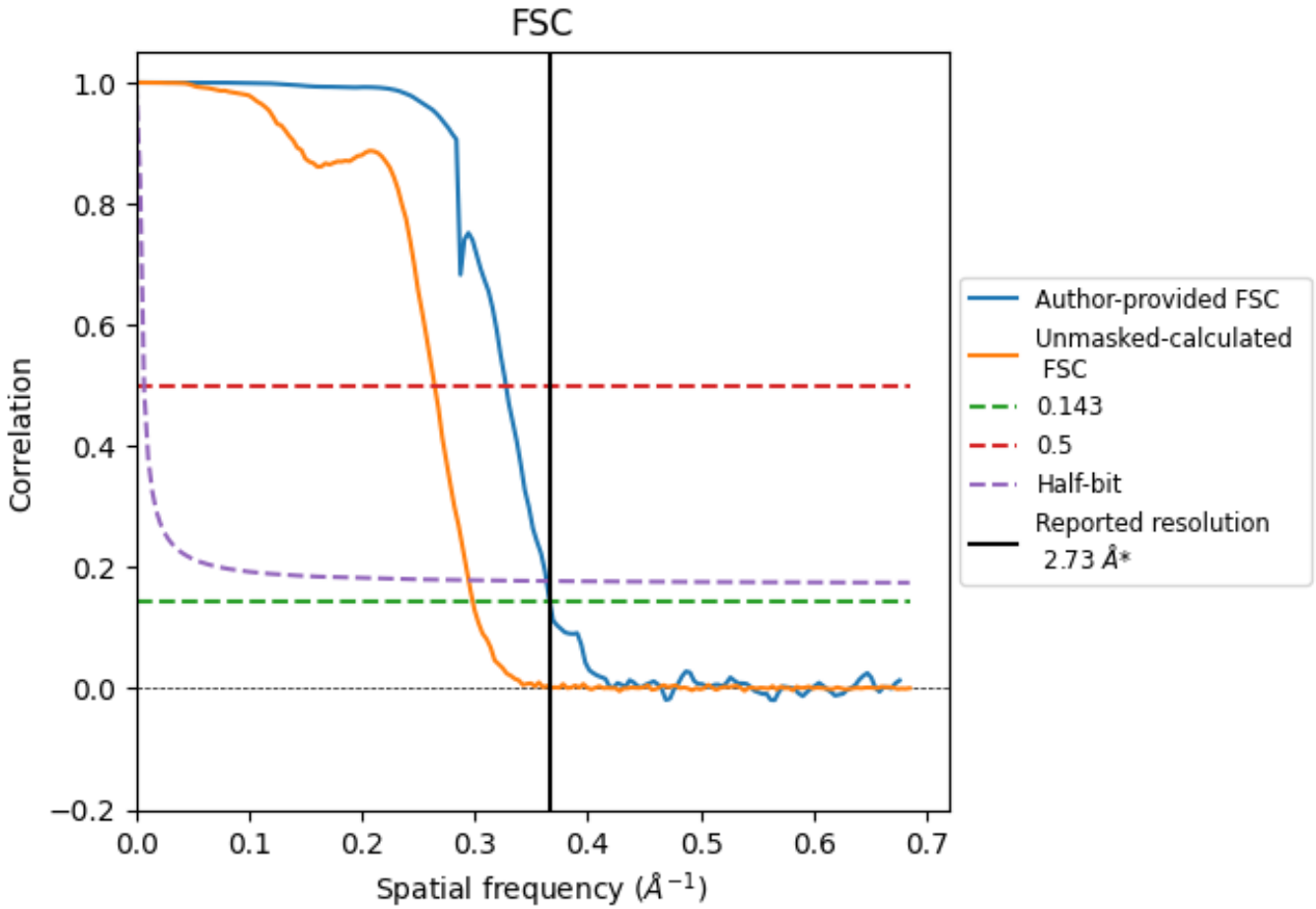


*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8.2 Resolution estimates (i)

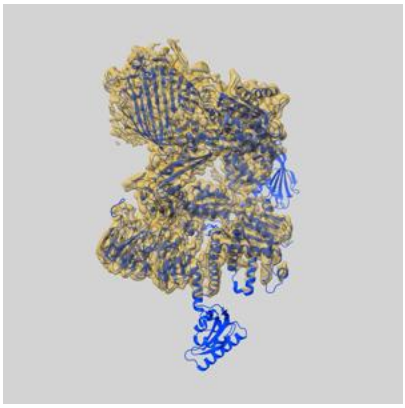
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.05	2.75
Unmasked-calculated*	3.35	3.78	3.40

*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 3.35 differs from the reported value 2.73 by more than 10 %

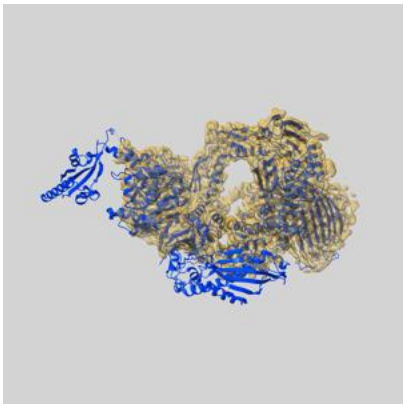
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52127 and PDB model 9HG6. Per-residue inclusion information can be found in section 3 on page 5.

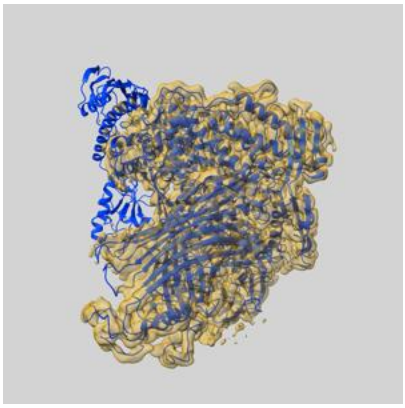
9.1 Map-model overlay



X



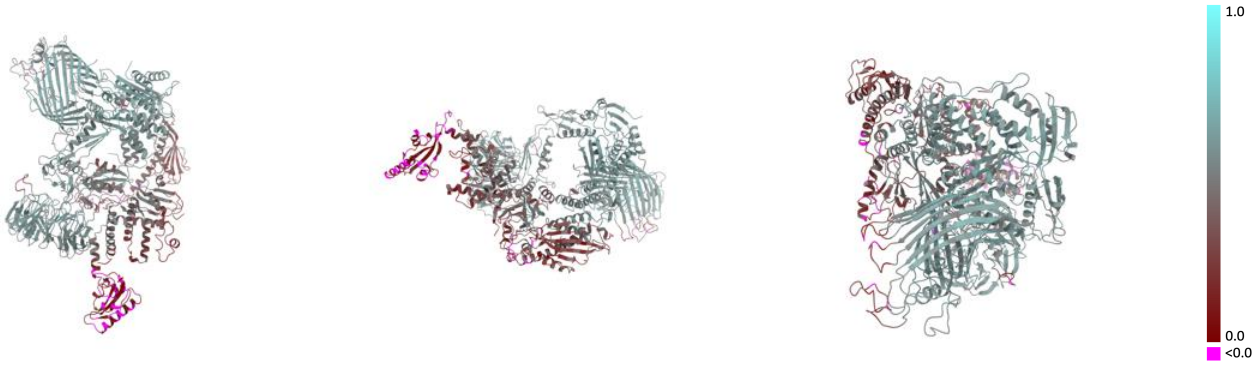
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

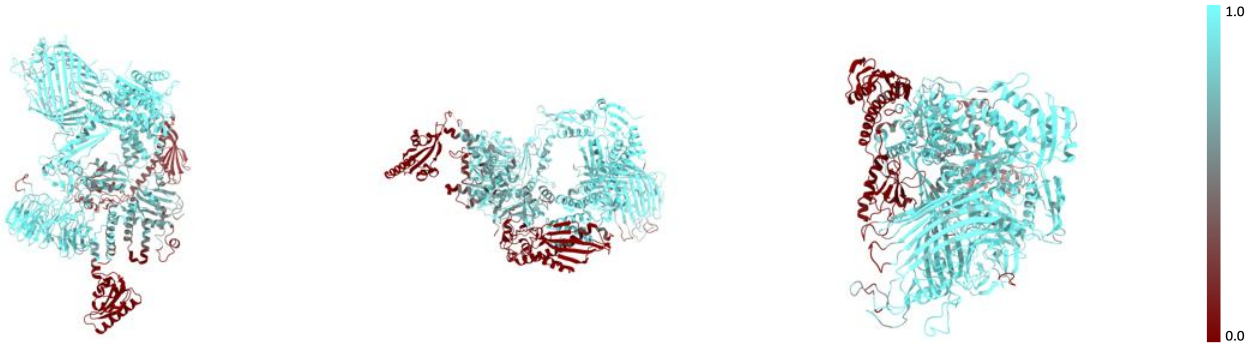
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

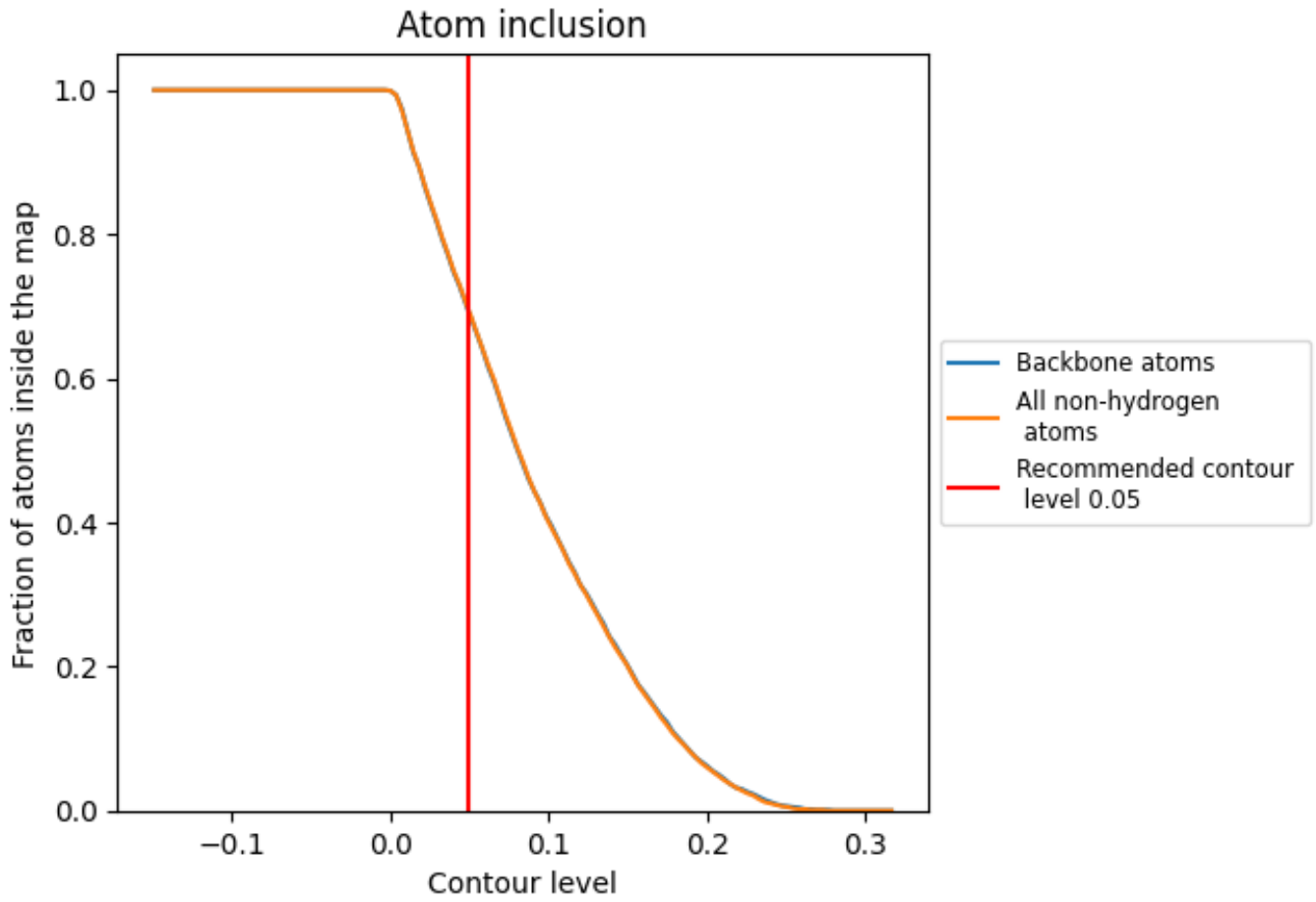
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.4550
A	0.8530	0.5220
B	0.8880	0.5270
C	0.1670	0.3080
D	0.9330	0.5540
E	0.9530	0.5670
F	0.3470	0.2340