



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:14 AM UTC

PDB ID : 6RDF / pdb_00006rdf
EMDB ID : EMD-4816
Title : CryoEM structure of Polytomella F-ATP synthase, Primary rotary state 3, monomer-masked refinement
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 3.20 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:

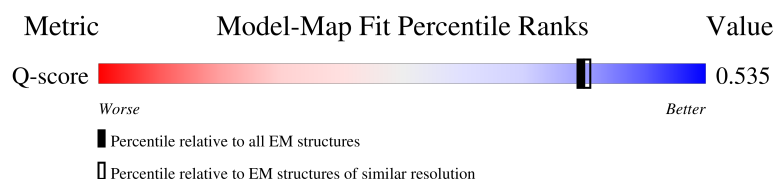
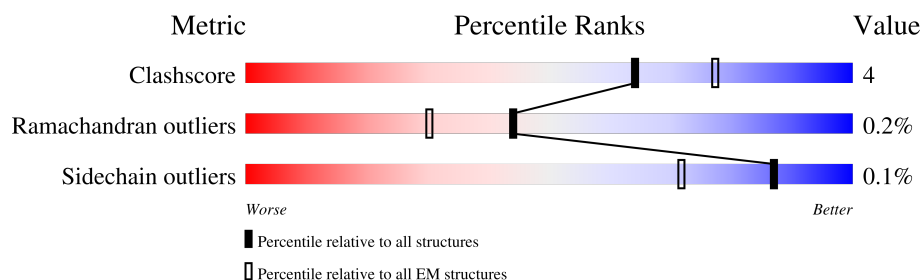
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.20 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	15020 (2.70 - 3.70)

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	0	82	7% 93% 6%
2	1	618	10% 86% 10%
3	2	441	15% 85% 14%
4	3	325	16% 67% 8% 25%

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Mol	Chain	Length	Quality of chain
5	4	294	
6	5	123	
7	6	151	
8	7	190	
9	8	89	
10	9	97	
11	M	327	
12	P	229	
13	T	562	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 19855 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	81	Total	C	N	O	S	0	0
			607	388	107	110	2		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	441	Total	C	N	O	0	0
			3163	2020	532	611		

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	245	Total	C	N	O	S	0	0
			1874	1204	299	370	1		

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	290	Total	C	N	O	S	0	0
			2177	1385	356	434	2		

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	97	Total	C	N	O	S	0	0
			776	514	124	132	6		

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	80	Total	C	N	O	S	0	0
			646	418	105	120	3		

- Molecule 13 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	T	40	Total	C	N	O	0	0
			330	215	56	59		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40

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

Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total Zn 1 1	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	AltConf
15	1	2	Total O 2 2	0
15	5	3	Total O 3 3	0
15	6	2	Total O 2 2	0
15	M	22	Total O 22 22	0

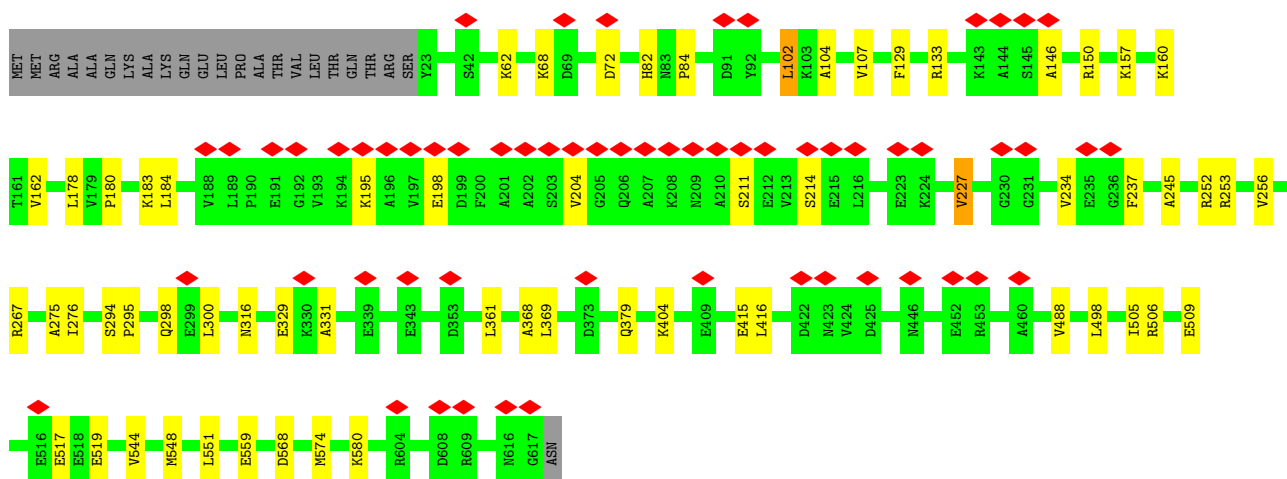
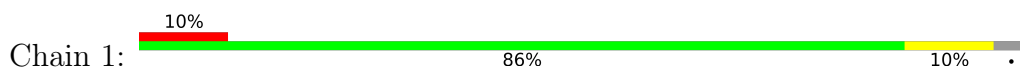
3 Residue-property plots [i](#)

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.

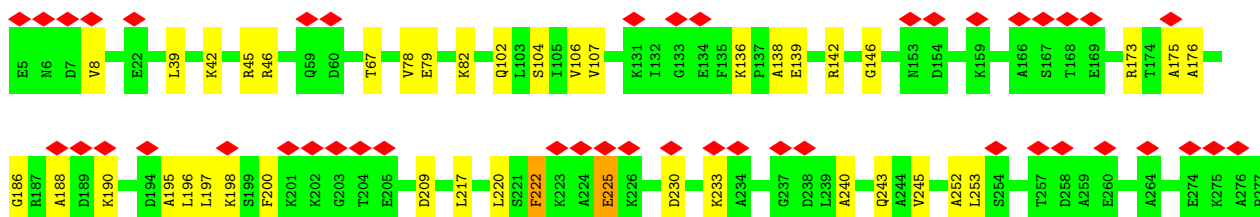
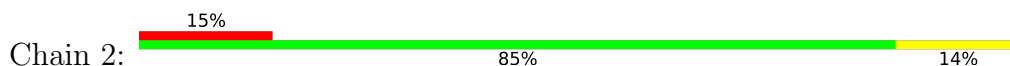
- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

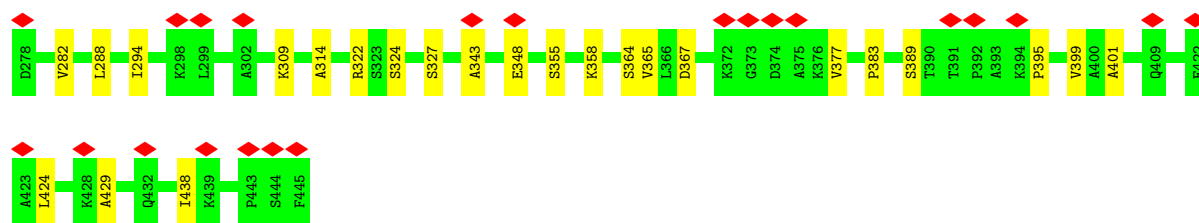


- Molecule 2: ATP synthase associated protein ASA1

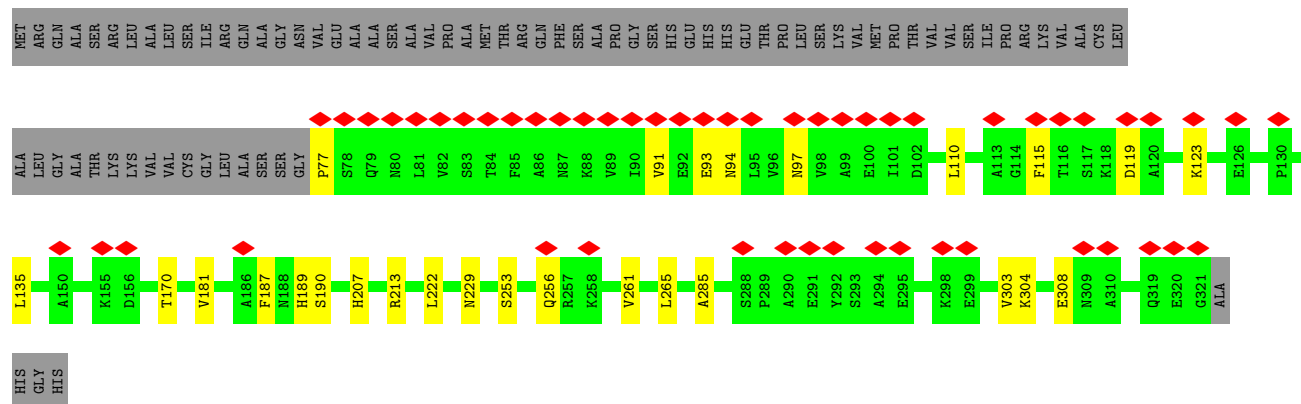


- Molecule 3: ASA-2: *Polytomella* F-ATP synthase associated subunit 2

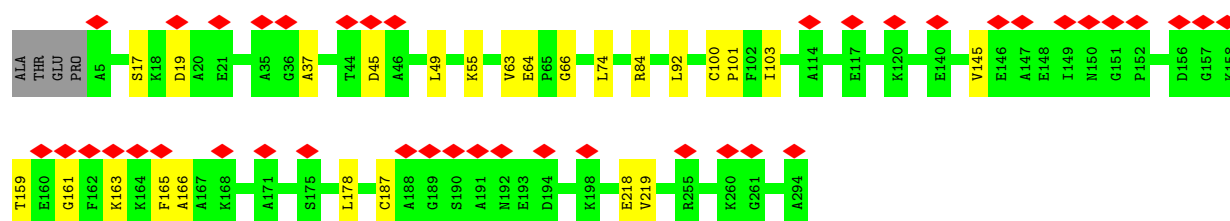




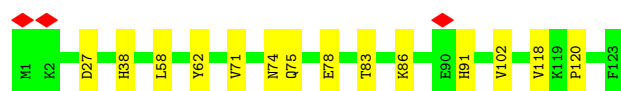
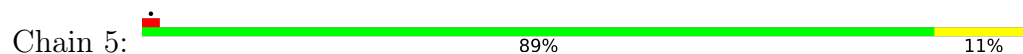
- Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein



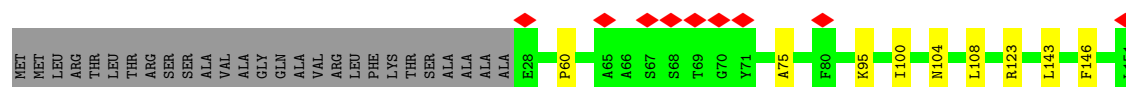
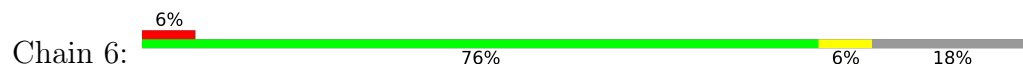
- Molecule 5: Mitochondrial ATP synthase associated protein ASA4



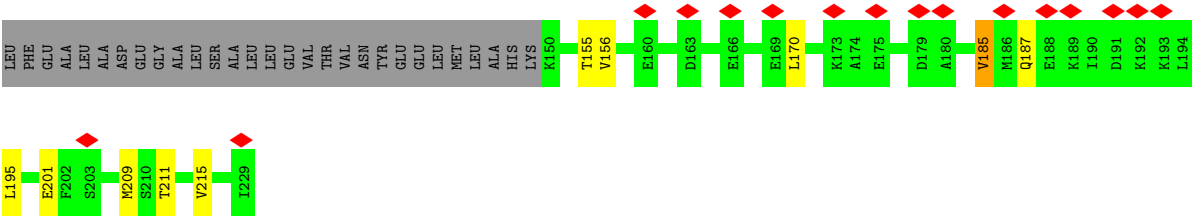
- Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein



- Molecule 7: Mitochondrial ATP synthase subunit ASA6



- | |
|-----|
| ALA | ALA | LYS | GLU | ASN | GLN | LEU | ASP | GLU | LEU | TYR | GLN | PHE | ILE | GLU | LEU | PHE | LYS | GLN | HIS | SER | LEU | ARG | ARG | LEU | ALA | THR | ASP | PRO | PHE | VAL | PRO | THR | LEU | VAL | ARG | THR | LYS | ILE | ILE | SER | SER | VAL | LEU | LYS | ASP | SER | GLY | ALA | SER | GLU | ILE | THR | LYS |
|-----|



• Molecule 13: ATP synthase subunit alpha



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163259	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.233	Depositor
Minimum map value	-0.147	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0	0.32	0/628	0.49	0/856
2	1	0.34	0/4750	0.48	0/6434
3	2	0.28	0/3212	0.54	4/4371 (0.1%)
4	3	0.31	0/1911	0.51	1/2601 (0.0%)
5	4	0.31	0/2216	0.48	0/3000
6	5	0.44	0/1011	0.56	0/1376
7	6	0.37	0/946	0.58	0/1287
8	7	0.37	0/1374	0.52	2/1865 (0.1%)
9	8	0.37	0/715	0.54	0/974
10	9	0.27	0/802	0.55	0/1084
11	M	0.42	0/1683	0.59	0/2295
12	P	0.26	0/653	0.60	0/872
13	T	0.35	0/338	0.68	0/454
All	All	0.34	0/20239	0.53	7/27469 (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
12	P	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	157	VAL	CA-C-N	7.21	126.10	120.33
8	7	157	VAL	C-N-CA	7.21	126.10	120.33
4	3	77	PRO	N-CA-CB	6.67	110.34	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	222	PHE	CA-C-N	5.84	132.70	121.54
3	2	222	PHE	C-N-CA	5.84	132.70	121.54
3	2	225	GLU	CA-C-N	5.73	132.48	121.54
3	2	225	GLU	C-N-CA	5.73	132.48	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	P	185	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	607	0	584	4	0
2	1	4661	0	4695	39	0
3	2	3163	0	3262	40	0
4	3	1874	0	1826	16	0
5	4	2177	0	2169	18	0
6	5	986	0	1021	13	0
7	6	926	0	941	9	0
8	7	1347	0	1345	25	0
9	8	692	0	694	6	0
10	9	776	0	757	4	0
11	M	1640	0	1665	19	0
12	P	646	0	681	6	0
13	T	330	0	342	6	0
14	M	1	0	0	0	0
15	1	2	0	0	0	0
15	5	3	0	0	0	0
15	6	2	0	0	0	0
15	M	22	0	0	6	0
All	All	19855	0	19982	164	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 4.

All (164) 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)
11:M:224:LEU:HG	15:M:709:HOH:O	1.66	0.93
11:M:224:LEU:CD2	15:M:709:HOH:O	2.21	0.87
11:M:224:LEU:CG	15:M:709:HOH:O	2.22	0.86
11:M:199:LYS:HE3	11:M:313:ASP:OD2	1.78	0.84
11:M:224:LEU:HD23	15:M:709:HOH:O	1.77	0.81
2:1:316:ASN:HD21	2:1:331:ALA:H	1.43	0.66
8:7:123:HIS:HD2	8:7:125:GLU:H	1.43	0.66
8:7:170:HIS:HD2	8:7:172:ALA:H	1.44	0.65
3:2:136:LYS:HE3	3:2:138:ALA:HB3	1.79	0.64
7:6:100:ILE:O	7:6:104:ASN:ND2	2.32	0.62
12:P:209:MET:HG2	13:T:79:PRO:HG2	1.81	0.62
2:1:180:PRO:HG2	2:1:183:LYS:HB3	1.82	0.62
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.83	0.60
2:1:267:ARG:NH1	2:1:519:GLU:OE1	2.34	0.59
2:1:544:VAL:HG12	2:1:548:MET:HE2	1.83	0.59
3:2:67:THR:HG21	3:2:102:GLN:HB3	1.86	0.58
3:2:245:VAL:HG22	3:2:288:LEU:HD13	1.85	0.58
7:6:108:LEU:HD11	11:M:281:LEU:HD13	1.84	0.58
2:1:245:ALA:HB1	2:1:498:LEU:HD13	1.86	0.57
3:2:253:LEU:HD11	3:2:401:ALA:HB2	1.85	0.56
2:1:368:ALA:O	2:1:379:GLN:NE2	2.34	0.56
3:2:188:ALA:HB2	3:2:220:LEU:HD22	1.87	0.55
2:1:295:PRO:HA	2:1:298:GLN:HG2	1.89	0.55
4:3:190:SER:OG	4:3:229:ASN:ND2	2.40	0.55
3:2:8:VAL:HG13	3:2:39:LEU:HD23	1.89	0.55
6:5:83:THR:O	8:7:119:TYR:OH	2.24	0.55
2:1:84:PRO:HG2	6:5:71:VAL:HG11	1.89	0.55
2:1:404:LYS:NZ	6:5:74:ASN:OD1	2.39	0.55
11:M:163:ASN:ND2	11:M:175:THR:OG1	2.40	0.54
3:2:197:LEU:HD22	3:2:225:GLU:HG3	1.88	0.54
3:2:209:ASP:OD1	3:2:209:ASP:N	2.38	0.54
5:4:45:ASP:OD2	5:4:45:ASP:N	2.39	0.54
2:1:195:LYS:HA	2:1:198:GLU:HG2	1.89	0.54
3:2:107:VAL:HG12	3:2:146:GLY:HA3	1.90	0.53
4:3:119:ASP:O	4:3:123:LYS:NZ	2.34	0.53
4:3:181:VAL:HG21	4:3:222:LEU:HD13	1.89	0.53
8:7:170:HIS:CD2	8:7:172:ALA:H	2.25	0.53
5:4:74:LEU:HD23	5:4:219:VAL:HG13	1.90	0.52
11:M:223:PRO:O	11:M:227:ILE:HG12	2.08	0.52
2:1:253:ARG:HD3	2:1:369:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:506:ARG:NH1	2:1:509:GLU:OE1	2.43	0.52
1:0:51:PRO:HD2	1:0:54:TYR:HB2	1.92	0.51
10:9:70:PRO:HA	11:M:264:SER:HA	1.92	0.51
12:P:156:VAL:HG11	12:P:170:LEU:HD21	1.92	0.51
3:2:195:ALA:HA	3:2:198:LYS:HE3	1.93	0.51
2:1:329:GLU:OE2	7:6:123:ARG:NH1	2.44	0.51
5:4:17:SER:OG	5:4:19:ASP:OD1	2.28	0.51
1:0:12:PHE:HB3	7:6:75:ALA:HB2	1.92	0.51
4:3:261:VAL:HG11	4:3:285:ALA:HB2	1.91	0.51
3:2:309:LYS:NZ	5:4:37:ALA:O	2.38	0.50
5:4:63:VAL:HA	5:4:92:LEU:HD11	1.94	0.50
12:P:155:THR:HG23	12:P:201:GLU:HB2	1.93	0.50
3:2:230:ASP:HA	3:2:233:LYS:HG3	1.93	0.50
6:5:86:LYS:NZ	8:7:135:ASP:OD1	2.44	0.50
12:P:155:THR:HA	12:P:187:GLN:HB3	1.93	0.50
2:1:104:ALA:HB1	2:1:294:SER:HB2	1.94	0.50
3:2:136:LYS:HB3	3:2:139:GLU:HG2	1.94	0.50
8:7:16:THR:O	8:7:73:LYS:NZ	2.42	0.50
3:2:355:SER:O	3:2:358:LYS:NZ	2.36	0.50
6:5:75:GLN:HA	6:5:78:GLU:HG2	1.95	0.49
3:2:240:ALA:H	3:2:243:GLN:HE21	1.60	0.49
2:1:102:LEU:HD23	2:1:107:VAL:HG22	1.94	0.48
2:1:568:ASP:HB2	2:1:580:LYS:HE3	1.94	0.48
11:M:101:LYS:NZ	15:M:706:HOH:O	2.38	0.48
2:1:68:LYS:NZ	8:7:117:ASP:OD1	2.39	0.48
2:1:568:ASP:OD2	6:5:38:HIS:NE2	2.43	0.48
3:2:377:VAL:HG11	3:2:438:ILE:HG23	1.95	0.48
4:3:91:VAL:HG23	4:3:93:GLU:H	1.79	0.48
3:2:322:ARG:NH1	3:2:367:ASP:OD2	2.41	0.48
3:2:78:VAL:HA	8:7:74:ILE:HB	1.96	0.47
5:4:64:GLU:OE2	8:7:166:ARG:NH2	2.42	0.47
2:1:559:GLU:OE2	4:3:207:HIS:NE2	2.41	0.47
3:2:104:SER:HB2	3:2:142:ARG:HB2	1.96	0.47
11:M:199:LYS:NZ	15:M:708:HOH:O	2.47	0.47
3:2:197:LEU:HD21	3:2:217:LEU:HD11	1.96	0.47
3:2:424:LEU:HD12	3:2:429:ALA:HB1	1.97	0.47
3:2:42:LYS:NZ	8:7:69:LEU:O	2.43	0.47
3:2:175:ALA:HB1	3:2:196:LEU:HB3	1.97	0.47
2:1:129:PHE:HZ	2:1:133:ARG:HH21	1.63	0.47
5:4:218:GLU:OE2	8:7:165:ARG:NH1	2.48	0.47
3:2:82:LYS:HA	5:4:84:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:49:LEU:HD11	12:P:215:VAL:HG12	1.97	0.46
3:2:173:ARG:HG3	8:7:67:ARG:HH12	1.80	0.46
4:3:213:ARG:NH1	11:M:143:ASP:OD1	2.49	0.46
2:1:72:ASP:OD1	8:7:121:ARG:NH2	2.45	0.46
2:1:157:LYS:HB2	2:1:160:LYS:HB2	1.98	0.46
11:M:155:PHE:HA	11:M:158:THR:HG22	1.97	0.46
5:4:163:LYS:HA	5:4:166:ALA:HB3	1.98	0.46
3:2:395:PRO:HB2	3:2:399:VAL:HG21	1.98	0.45
10:9:26:LEU:HA	10:9:29:PHE:HD2	1.81	0.45
5:4:101:PRO:HG3	8:7:170:HIS:CD2	2.51	0.45
4:3:265:LEU:HD22	4:3:303:VAL:HG11	1.98	0.45
2:1:551:LEU:HD21	4:3:170:THR:HB	1.98	0.45
5:4:100:CYS:HB3	5:4:103:ILE:HG13	1.99	0.45
3:2:67:THR:HG22	3:2:106:VAL:HG23	1.99	0.45
7:6:60:PRO:HB3	9:8:15:PRO:HB2	1.98	0.45
2:1:415:GLU:HG3	2:1:416:LEU:HD12	1.97	0.45
5:4:178:LEU:HD11	8:7:183:THR:HG21	1.98	0.45
5:4:159:THR:HG22	5:4:161:GLY:H	1.81	0.45
3:2:282:VAL:HG12	3:2:314:ALA:HB2	1.98	0.45
9:8:26:HIS:CD2	9:8:28:PHE:H	2.35	0.45
6:5:27:ASP:OD2	9:8:44:HIS:NE2	2.50	0.44
13:T:44:ALA:HB3	13:T:47:GLU:HG3	1.98	0.44
13:T:62:VAL:O	13:T:66:LEU:N	2.49	0.44
4:3:253:SER:H	4:3:256:GLN:HE21	1.65	0.44
8:7:40:ALA:HB3	8:7:47:GLU:HB2	1.99	0.44
4:3:110:LEU:HB3	4:3:115:PHE:HB3	1.98	0.44
4:3:304:LYS:NZ	4:3:308:GLU:OE2	2.48	0.44
3:2:186:GLY:O	3:2:389:SER:OG	2.33	0.44
6:5:62:TYR:OH	7:6:146:PHE:O	2.23	0.44
6:5:91:HIS:CG	8:7:111:THR:HG21	2.53	0.44
11:M:251:LEU:HD21	11:M:285:VAL:HG22	1.99	0.43
3:2:79:GLU:HB3	8:7:15:LEU:HD23	2.00	0.43
3:2:324:SER:HA	3:2:327:SER:HB2	2.00	0.43
2:1:184:LEU:HG	2:1:488:VAL:HG21	2.01	0.43
1:0:64:ALA:HA	7:6:95:LYS:HE2	2.00	0.43
2:1:517:GLU:HA	9:8:2:VAL:HG12	2.00	0.43
6:5:91:HIS:ND1	8:7:138:TYR:OH	2.34	0.42
7:6:143:LEU:HD12	7:6:143:LEU:HA	1.86	0.42
2:1:150:ARG:HA	2:1:150:ARG:HD3	1.89	0.42
3:2:343:ALA:HB1	3:2:348:GLU:HG3	2.01	0.42
5:4:66:GLY:HA3	5:4:92:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:36:ALA:HA	9:8:40:LEU:HB3	2.00	0.42
3:2:176:ALA:HB2	3:2:200:PHE:HZ	1.84	0.42
11:M:200:THR:OG1	11:M:201:GLY:N	2.52	0.42
11:M:314:LYS:HE3	11:M:314:LYS:HB3	1.89	0.42
3:2:46:ARG:HA	3:2:46:ARG:HD2	1.91	0.42
2:1:252:ARG:HG3	2:1:505:ILE:HG21	2.01	0.42
3:2:190:LYS:HG3	3:2:222:PHE:HE1	1.84	0.42
5:4:187:CYS:HB2	8:7:184:ASN:HD21	1.83	0.42
13:T:55:SER:O	13:T:57:TYR:N	2.52	0.42
3:2:45:ARG:NH2	8:7:74:ILE:O	2.48	0.42
3:2:364:SER:OG	3:2:365:VAL:N	2.53	0.42
4:3:187:PHE:O	4:3:189:HIS:N	2.53	0.42
5:4:145:VAL:HG21	5:4:165:PHE:HA	2.02	0.42
2:1:276:ILE:HD12	2:1:300:LEU:HG	2.02	0.41
3:2:78:VAL:HG22	8:7:74:ILE:HG13	2.02	0.41
5:4:55:LYS:HE3	5:4:55:LYS:HB3	1.88	0.41
6:5:118:VAL:HG21	8:7:94:LEU:HD22	2.03	0.41
1:0:69:PRO:HD3	10:9:60:ASN:HB3	2.01	0.41
2:1:211:SER:O	2:1:214:SER:OG	2.34	0.41
2:1:227:VAL:HG13	2:1:234:VAL:HG23	2.02	0.41
2:1:256:VAL:HG11	2:1:505:ILE:HG23	2.01	0.41
10:9:66:ILE:HG13	10:9:68:MET:HG2	2.03	0.41
13:T:55:SER:C	13:T:57:TYR:H	2.29	0.41
3:2:252:ALA:HB1	3:2:294:ILE:HB	2.02	0.41
6:5:58:LEU:HD23	6:5:58:LEU:HA	1.93	0.41
11:M:301:ILE:O	11:M:304:THR:OG1	2.37	0.41
2:1:227:VAL:HG11	2:1:237:PHE:CD2	2.56	0.41
4:3:213:ARG:NH2	11:M:143:ASP:OD2	2.54	0.41
3:2:197:LEU:HD23	3:2:197:LEU:HA	1.94	0.41
9:8:26:HIS:H	9:8:29:GLN:HE21	1.68	0.41
12:P:195:LEU:O	12:P:211:THR:OG1	2.37	0.41
2:1:275:ALA:HA	2:1:361:LEU:HD13	2.03	0.40
7:6:146:PHE:HD1	7:6:146:PHE:HA	1.74	0.40
11:M:163:ASN:HB3	11:M:292:ALA:HB1	2.02	0.40
2:1:178:LEU:HD23	2:1:178:LEU:HA	1.92	0.40
2:1:574:MET:HE2	2:1:574:MET:HB3	1.89	0.40
4:3:94:ASN:HA	4:3:97:ASN:HB2	2.03	0.40
8:7:39:VAL:HG12	8:7:48:VAL:HG23	2.03	0.40
2:1:82:HIS:NE2	8:7:120:TYR:O	2.49	0.40
2:1:162:VAL:HG11	6:5:102:VAL:HG12	2.04	0.40
4:3:135:LEU:HD23	4:3:135:LEU:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:72:GLU:HA	13:T:75:LYS:HG2	2.04	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	0	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
2	1	593/618 (96%)	574 (97%)	19 (3%)	0	100	100
3	2	439/441 (100%)	417 (95%)	21 (5%)	1 (0%)	43	73
4	3	243/325 (75%)	234 (96%)	9 (4%)	0	100	100
5	4	288/294 (98%)	277 (96%)	11 (4%)	0	100	100
6	5	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	16	50
7	6	122/151 (81%)	111 (91%)	11 (9%)	0	100	100
8	7	174/190 (92%)	171 (98%)	3 (2%)	0	100	100
9	8	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
10	9	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
11	M	213/327 (65%)	206 (97%)	7 (3%)	0	100	100
12	P	78/229 (34%)	71 (91%)	6 (8%)	1 (1%)	9	40
13	T	38/562 (7%)	31 (82%)	6 (16%)	1 (3%)	4	26
All	All	2569/3528 (73%)	2445 (95%)	120 (5%)	4 (0%)	44	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	383	PRO
13	T	56	LYS

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Mol	Chain	Res	Type
6	5	120	PRO
12	P	185	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	490 (99%)	3 (1%)	78	84
3	2	312/312 (100%)	312 (100%)	0	100	100
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
6	5	107/107 (100%)	107 (100%)	0	100	100
7	6	96/115 (84%)	96 (100%)	0	100	100
8	7	140/150 (93%)	140 (100%)	0	100	100
9	8	71/72 (99%)	71 (100%)	0	100	100
10	9	79/79 (100%)	79 (100%)	0	100	100
11	M	178/272 (65%)	178 (100%)	0	100	100
12	P	73/196 (37%)	73 (100%)	0	100	100
13	T	36/448 (8%)	36 (100%)	0	100	100
All	All	2063/2808 (74%)	2060 (100%)	3 (0%)	87	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	102	LEU
2	1	204	VAL
2	1	227	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	48	ASN
1	0	60	GLN
1	0	61	HIS
1	0	79	HIS
2	1	100	GLN
2	1	209	ASN
2	1	316	ASN
2	1	428	HIS
2	1	438	GLN
2	1	482	ASN
2	1	542	HIS
2	1	547	HIS
2	1	587	ASN
2	1	590	HIS
3	2	68	ASN
3	2	122	ASN
3	2	153	ASN
3	2	243	GLN
3	2	380	GLN
3	2	427	GLN
4	3	179	GLN
4	3	189	HIS
4	3	206	ASN
4	3	229	ASN
4	3	256	GLN
5	4	240	GLN
6	5	29	GLN
6	5	107	ASN
6	5	117	GLN
7	6	74	GLN
8	7	86	HIS
8	7	91	ASN
8	7	123	HIS
8	7	170	HIS
8	7	184	ASN
9	8	26	HIS
9	8	29	GLN
10	9	80	GLN
10	9	97	ASN
11	M	108	ASN
11	M	121	ASN
11	M	163	ASN
12	P	220	ASN

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Mol	Chain	Res	Type
12	P	223	ASN
13	T	61	HIS
13	T	64	GLN
13	T	78	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

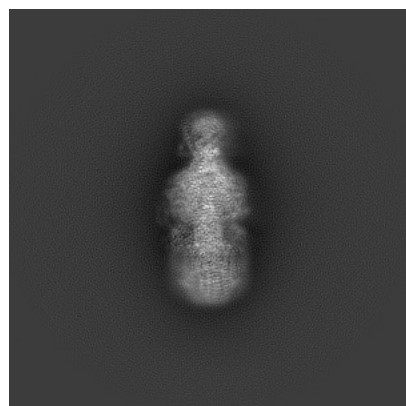
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4816. These allow visual inspection of the internal detail of the map and identification of artifacts.

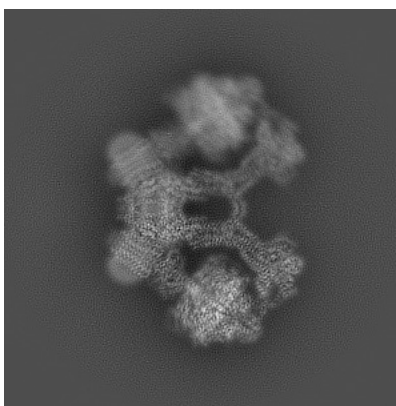
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

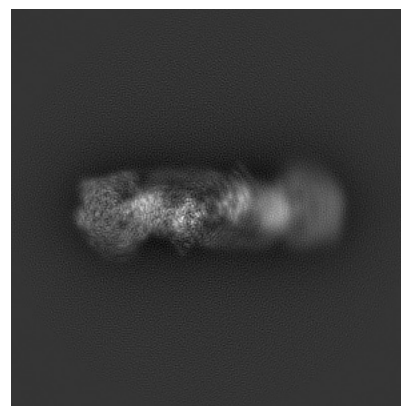
6.1.1 Primary map



X

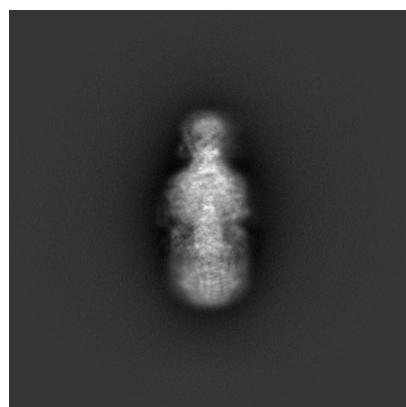


Y

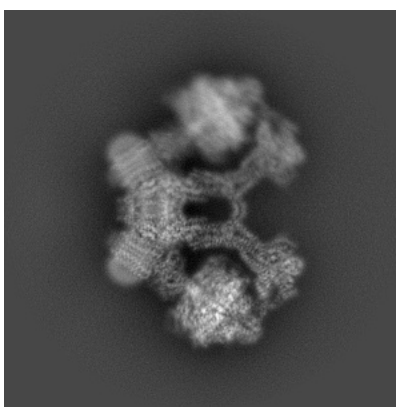


Z

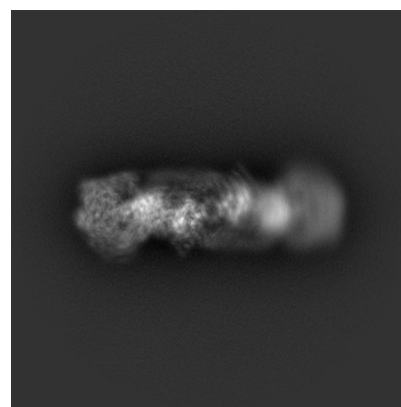
6.1.2 Raw map



X



Y



Z

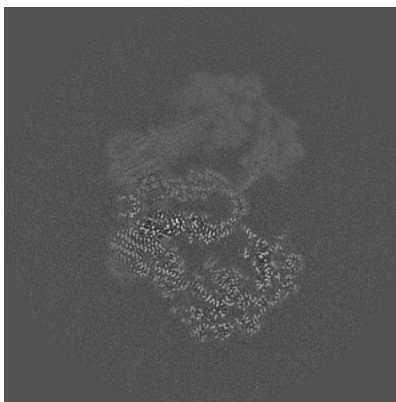
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

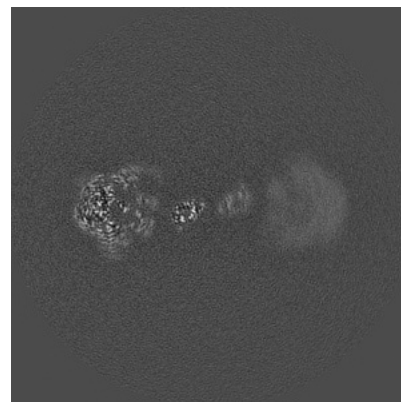
6.2.1 Primary map



X Index: 240

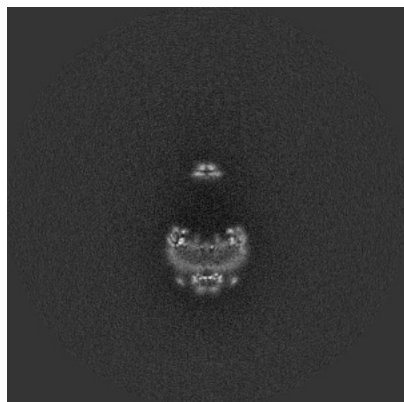


Y Index: 240

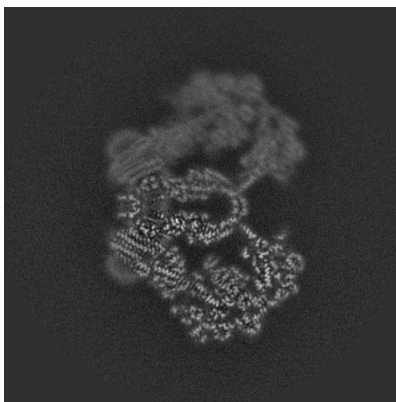


Z Index: 240

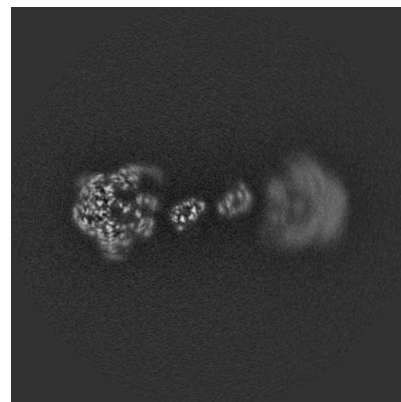
6.2.2 Raw map



X Index: 240



Y Index: 240

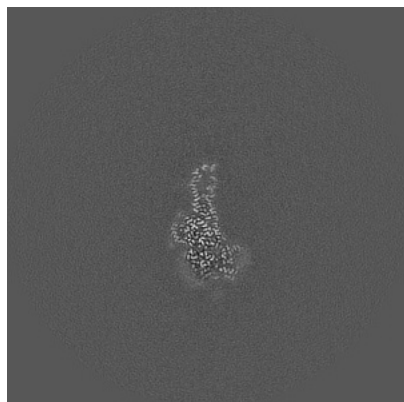


Z Index: 240

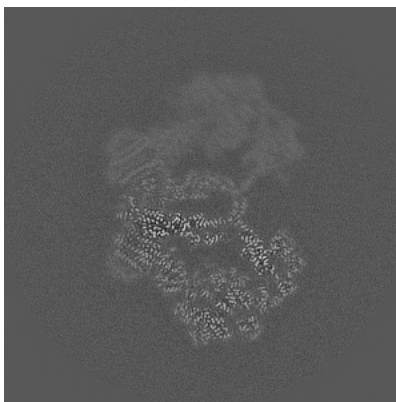
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 216

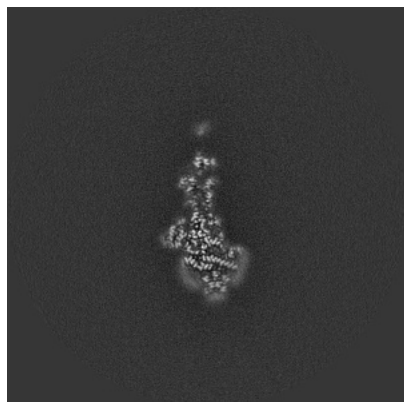


Y Index: 235

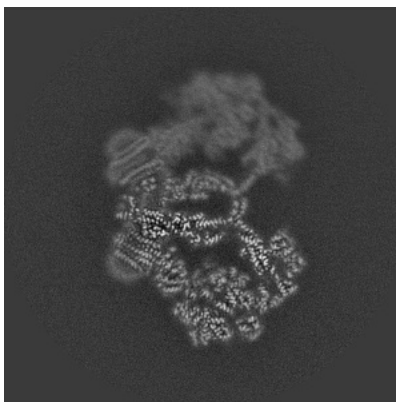


Z Index: 255

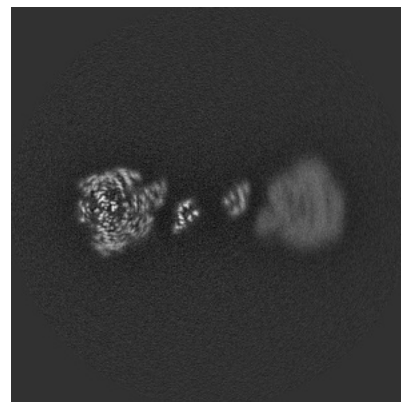
6.3.2 Raw map



X Index: 209



Y Index: 235

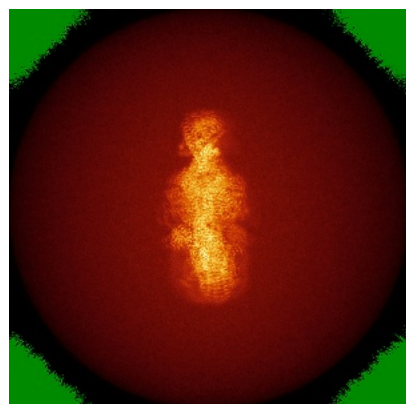


Z Index: 256

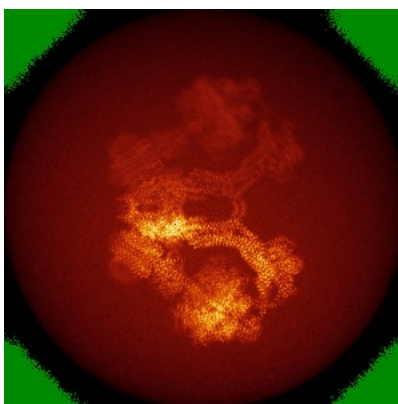
The images above show the largest variance slices of the map in three orthogonal directions.

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

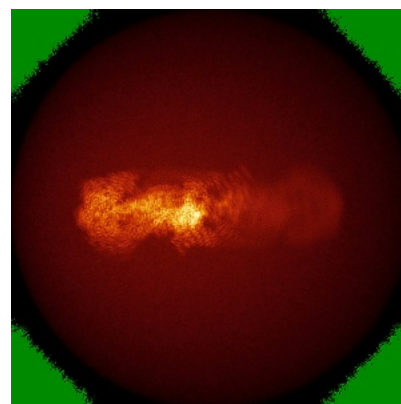
6.4.1 Primary map



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



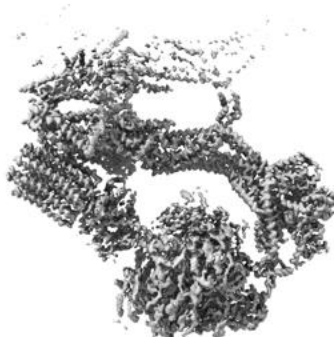
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

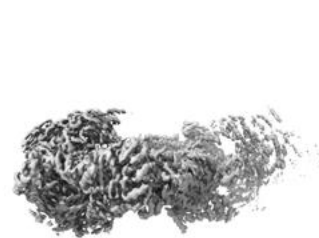
6.5.2 Raw map



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.

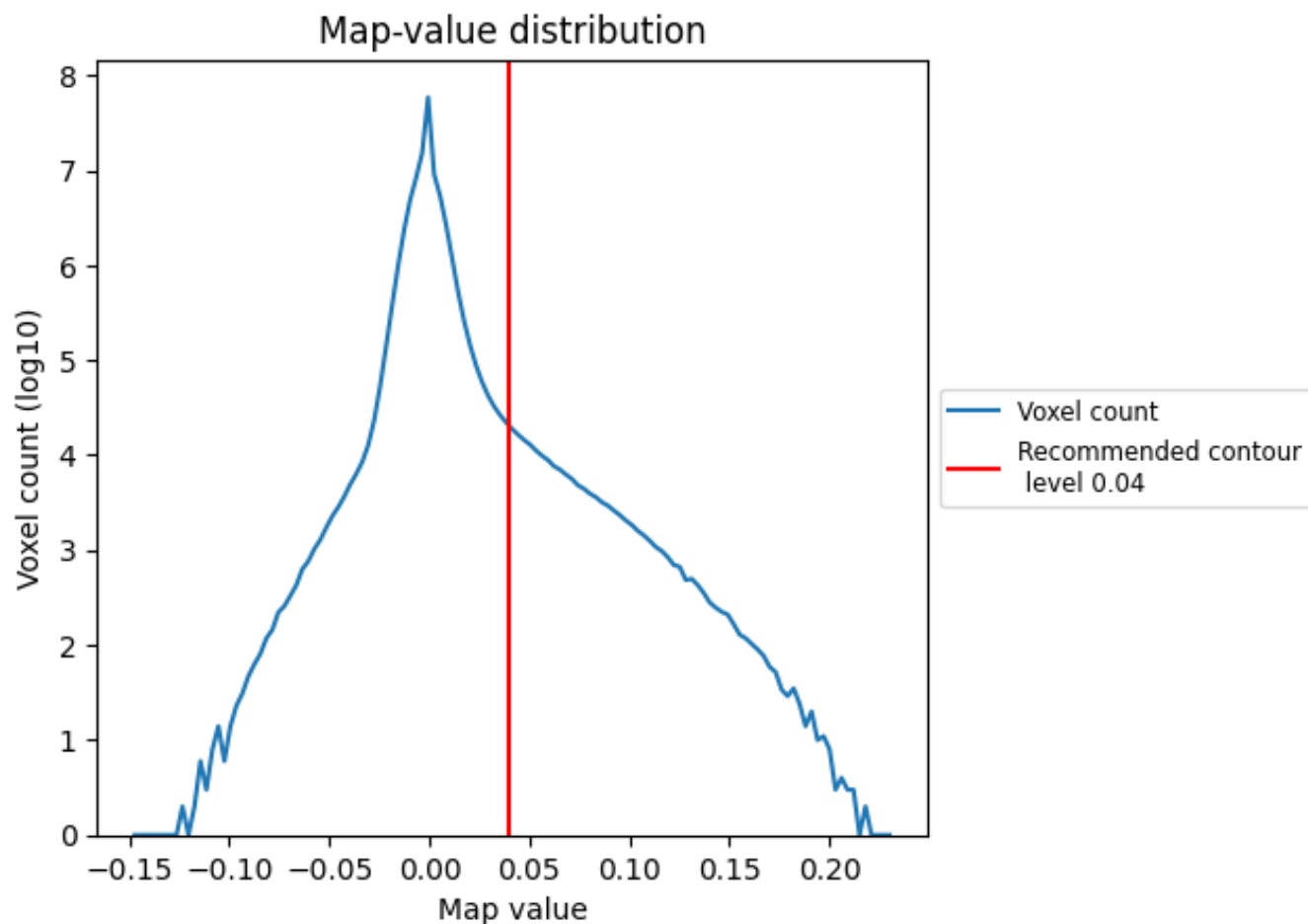
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

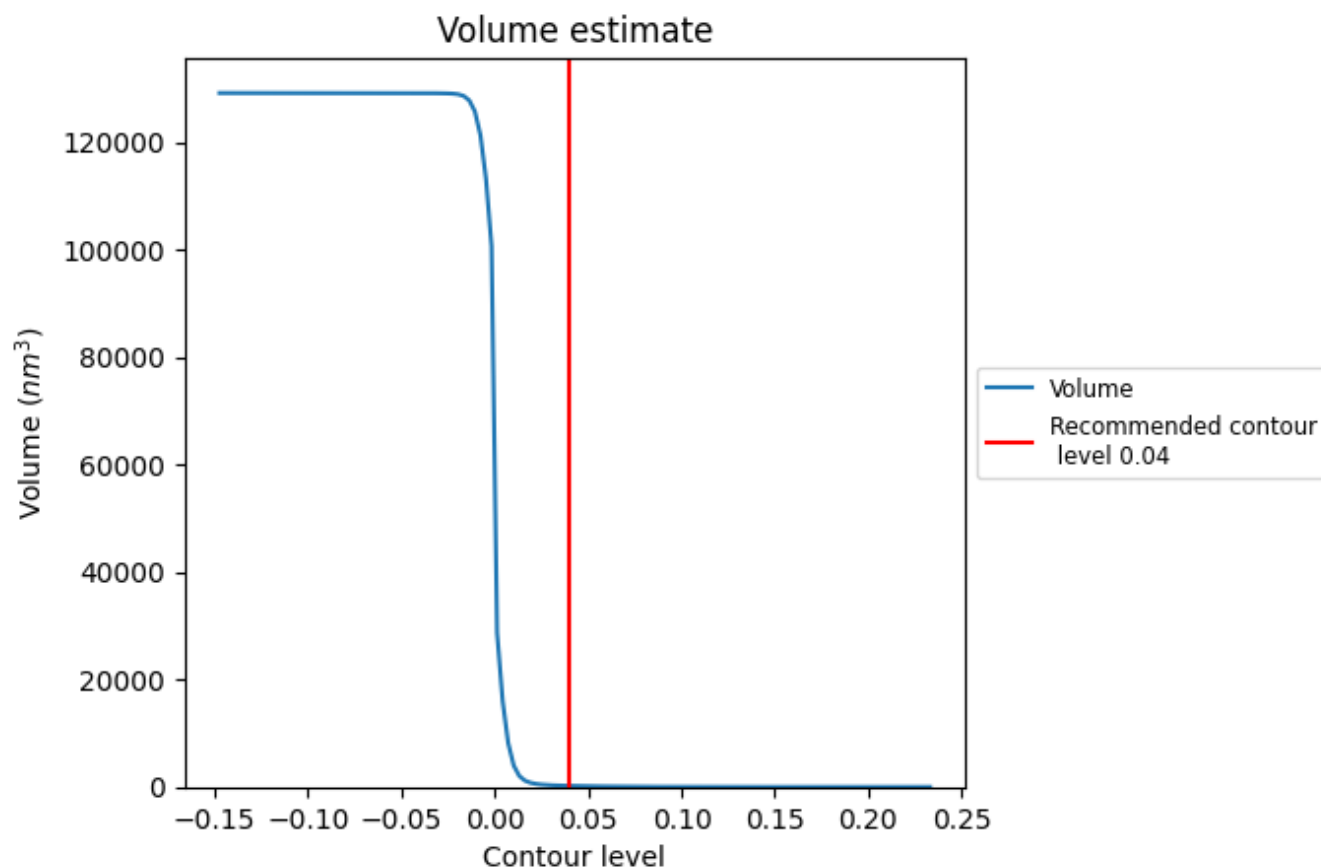
This section contains the results of statistical analysis of the map.

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.

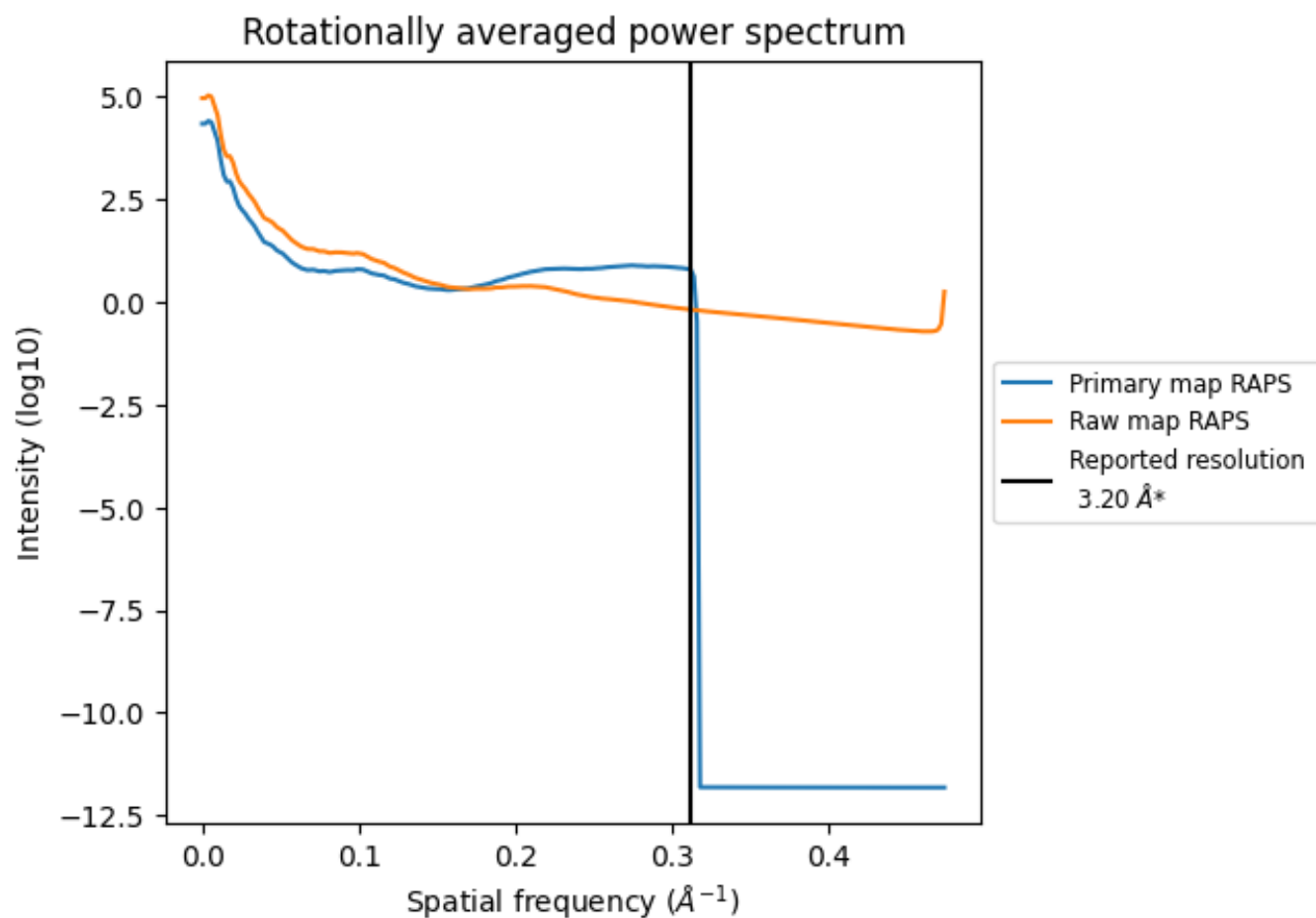
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm³; this corresponds to an approximate mass of 183 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 ⓘ

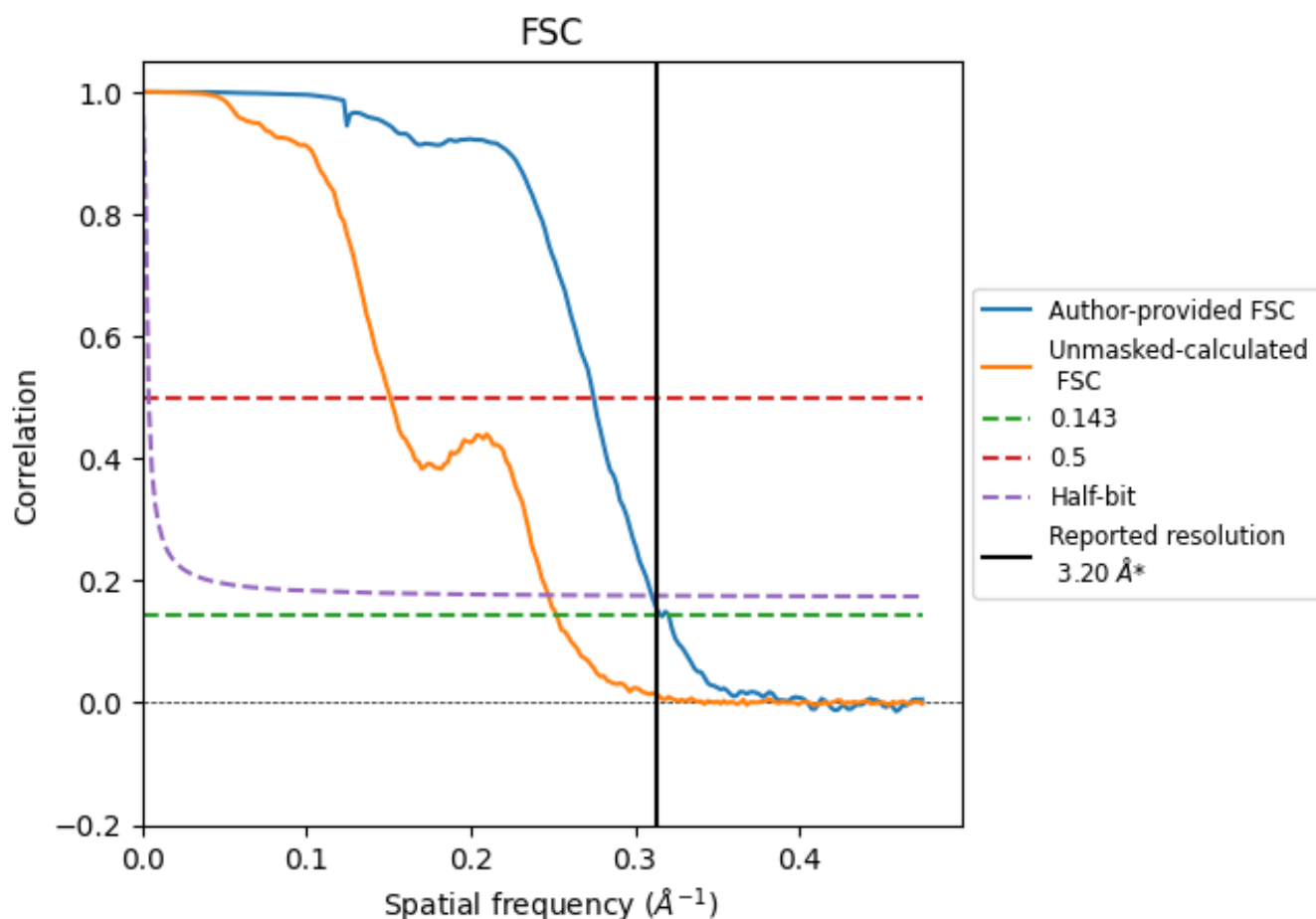


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates

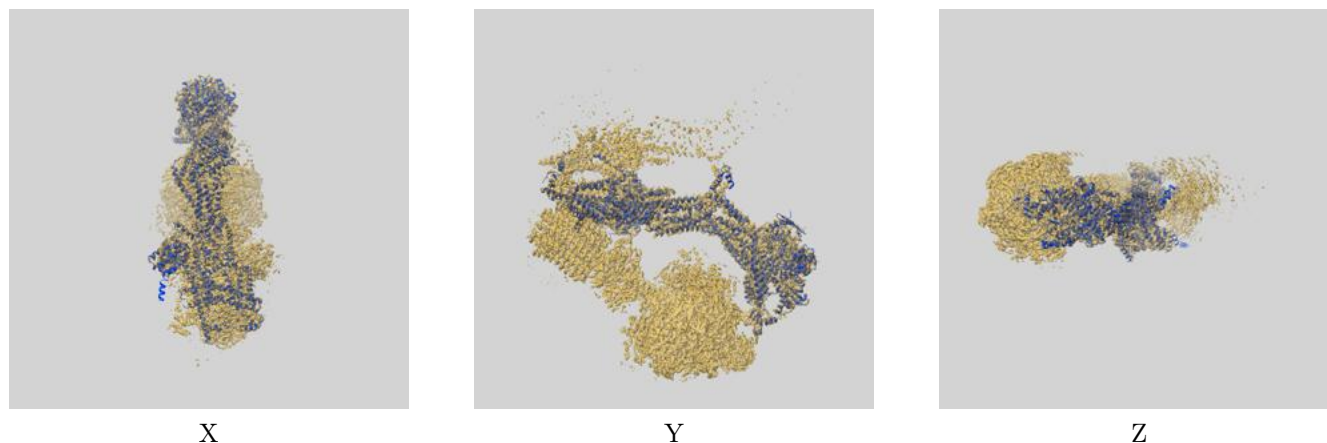
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.64	3.22
Unmasked-calculated*	3.97	6.62	4.05

*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 3.97 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

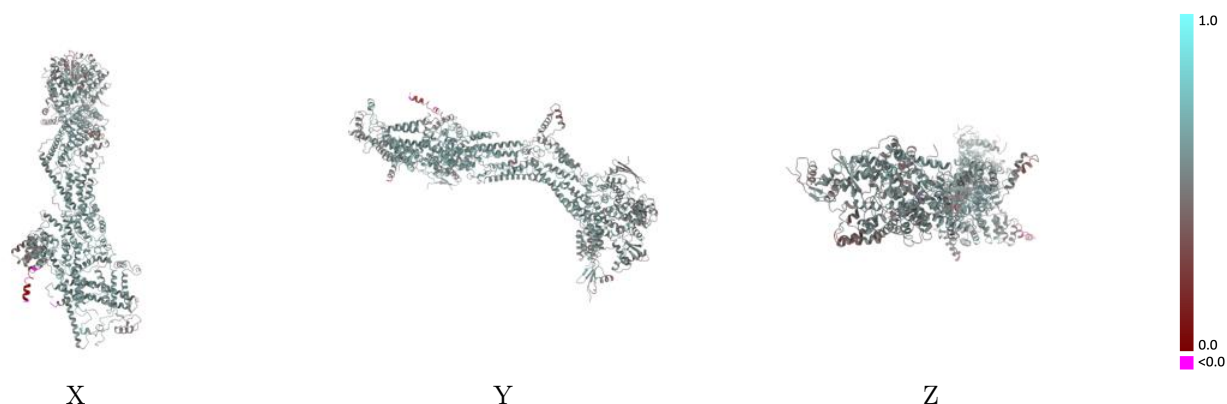
This section contains information regarding the fit between EMDB map EMD-4816 and PDB model 6RDF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



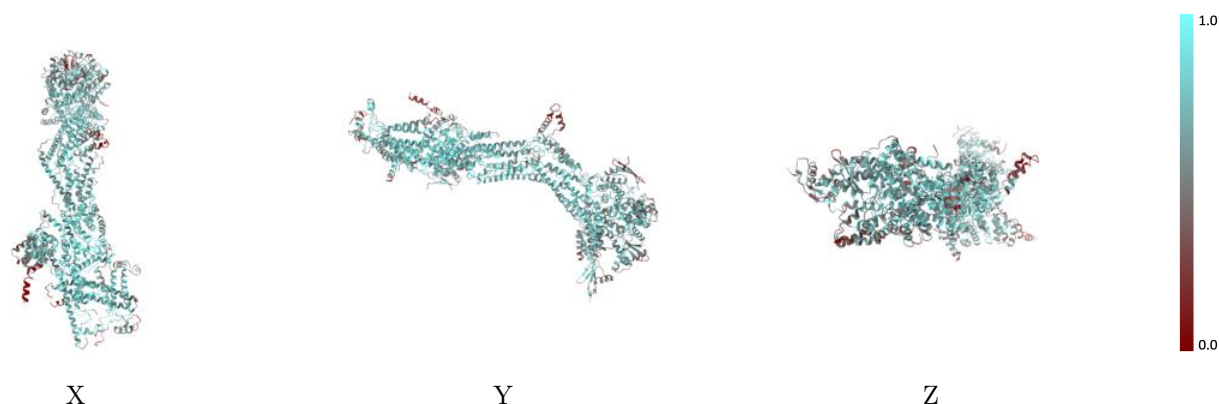
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



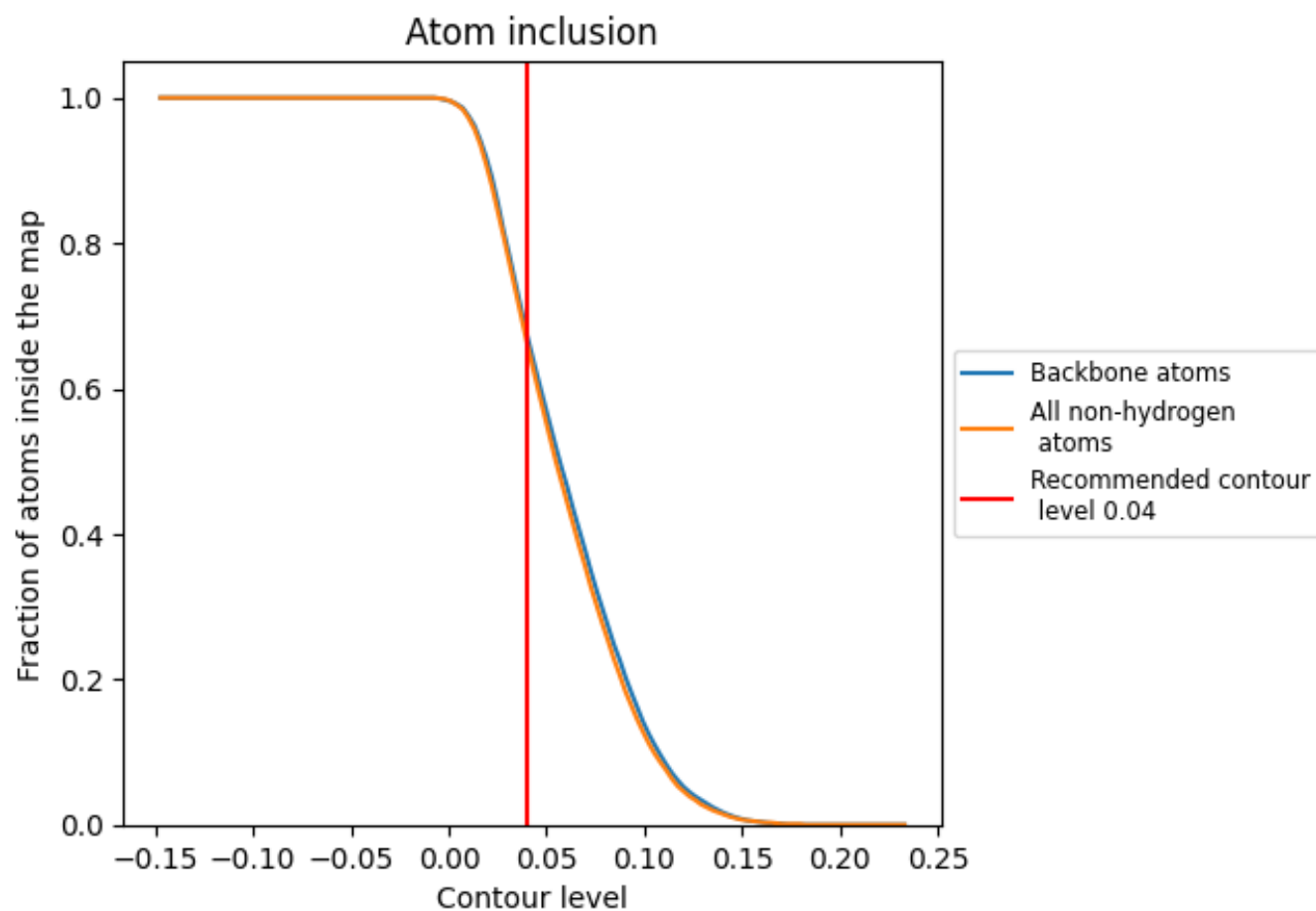
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 66% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6630	0.5350
0	0.6890	0.5440
1	0.6930	0.5510
2	0.6170	0.5150
3	0.5990	0.4830
4	0.6400	0.5230
5	0.7890	0.5770
6	0.7120	0.5530
7	0.7170	0.5520
8	0.7460	0.5700
9	0.5600	0.4910
M	0.7100	0.5590
P	0.5630	0.4990
T	0.6860	0.5510

1.0

0.0

<0.0