wwPDB EM Validation Summary Report

Nov 9, 2026 – 02:38 PM JST

PDB ID	:	9XMU / pdb_00009xmu
EMDB ID	:	EMD-67033
Title	:	The tail structure of AbP20
Authors	:	Xue, H.; Rao, G.; Cao, S.; Yang, H.
Deposited on	:	2025-11-11
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Validation Summary 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:

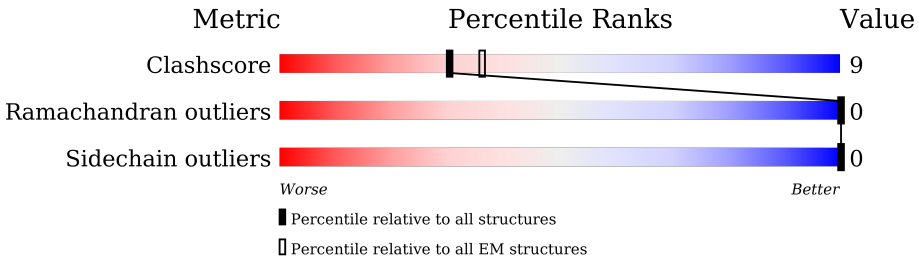
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

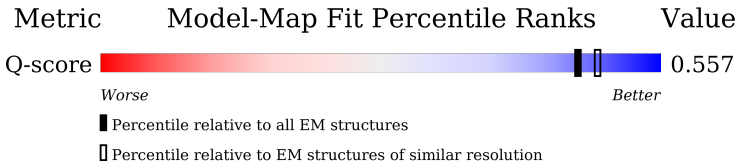
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 <=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	208	73% 17% 11%
1	B	208	75% 13% 12%
2	D	518	10% 63% 21% 16%
2	E	518	8% 65% 17% 18%

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Mol	Chain	Length	Quality of chain
3	F	763	
4	I	808	
4	J	808	
4	K	808	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18749 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 Tail tubular protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	186	Total	C	N	O	S	0	0
			1523	966	273	280	4		
1	B	183	Total	C	N	O	S	0	0
			1495	951	267	274	3		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ALA	VAL	conflict	UNP A0AAF0RU91
A	101	ILE	VAL	conflict	UNP A0AAF0RU91
A	117	ASP	ASN	conflict	UNP A0AAF0RU91
A	135	PRO	THR	conflict	UNP A0AAF0RU91
B	91	ALA	VAL	conflict	UNP A0AAF0RU91
B	101	ILE	VAL	conflict	UNP A0AAF0RU91
B	117	ASP	ASN	conflict	UNP A0AAF0RU91
B	135	PRO	THR	conflict	UNP A0AAF0RU91

- Molecule 2 is a protein called Head-to-tail joining protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	437	Total	C	N	O	S	0	0
			3524	2228	607	681	8		
2	E	424	Total	C	N	O	S	0	0
			3419	2166	588	657	8		

- Molecule 3 is a protein called nozzle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	763	Total	C	N	O	S	0	0
			5954	3763	981	1191	19		

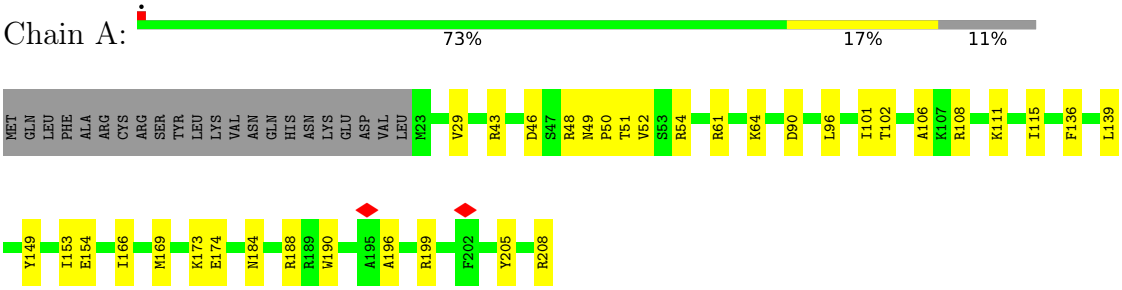
- Molecule 4 is a protein called fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	126	Total	C	N	O	S	0	0
			1005	641	162	199	3		
4	J	118	Total	C	N	O	S	0	0
			943	603	150	187	3		
4	K	110	Total	C	N	O	S	0	0
			886	568	144	172	2		

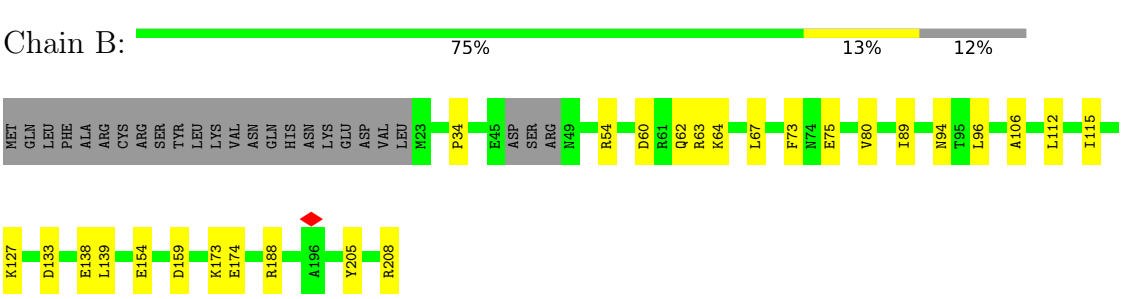
3 Residue-property plots (i)

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.

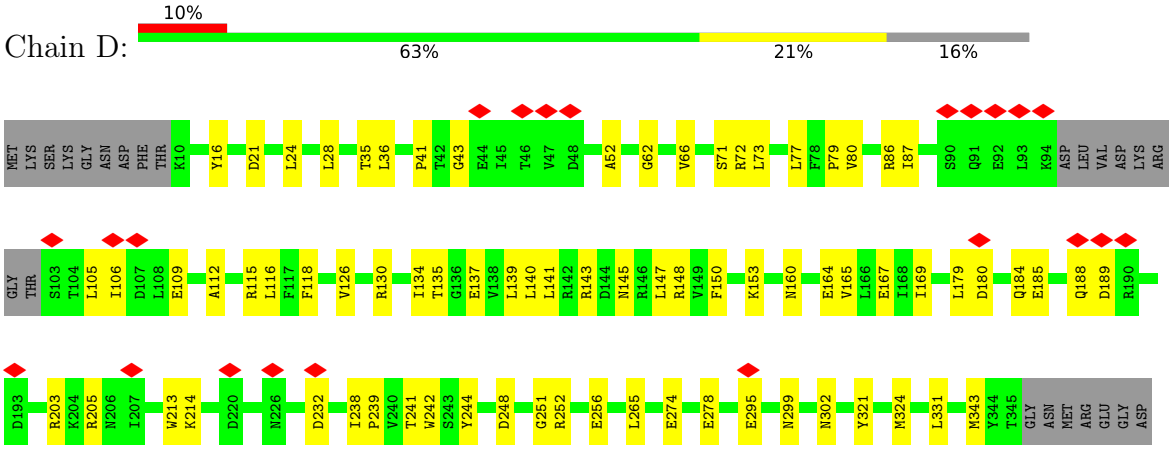
• Molecule 1: Tail tubular protein A

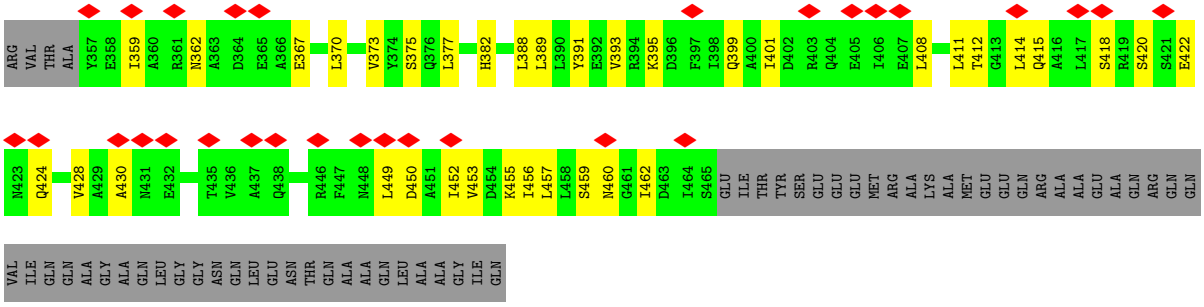


• Molecule 1: Tail tubular protein A



• Molecule 2: Head-to-tail joining protein

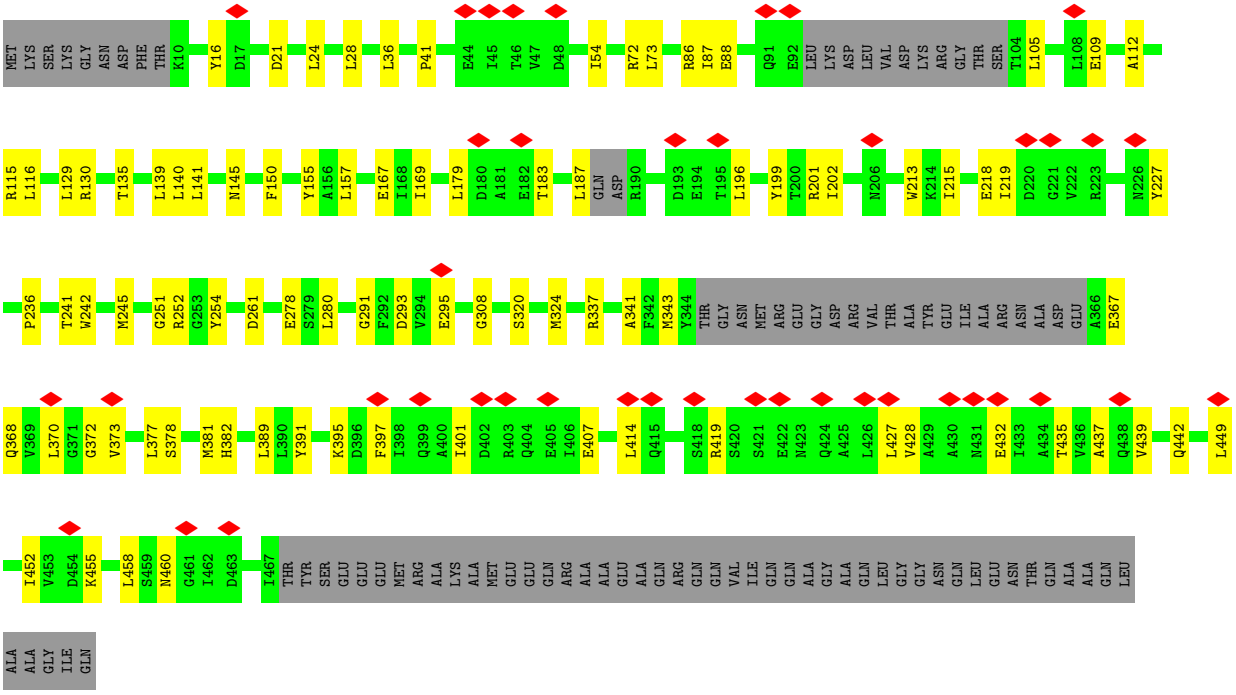




• Molecule 2: Head-to-tail joining protein

Chain E:

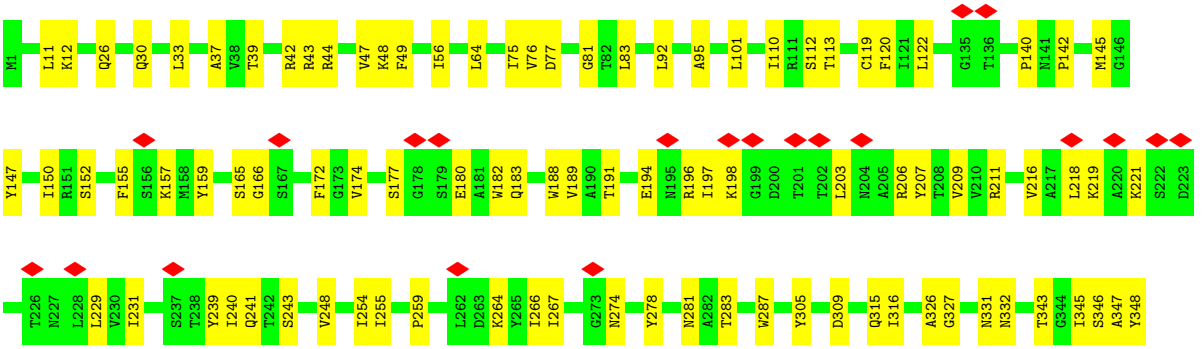


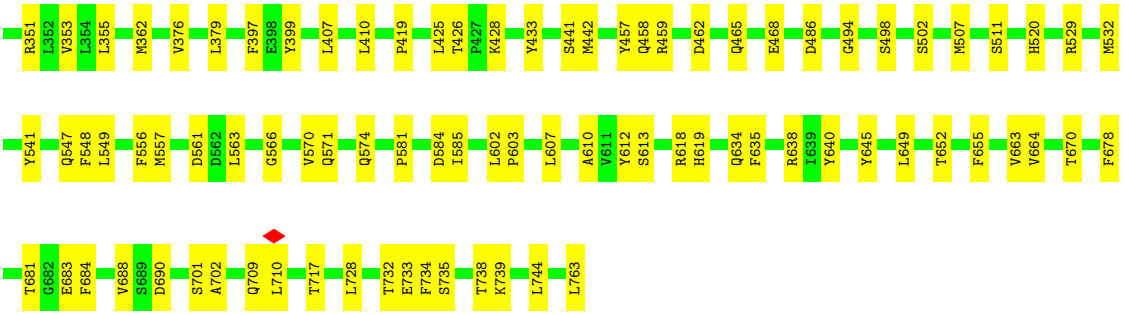


• Molecule 3: nozzle protein

Chain F:



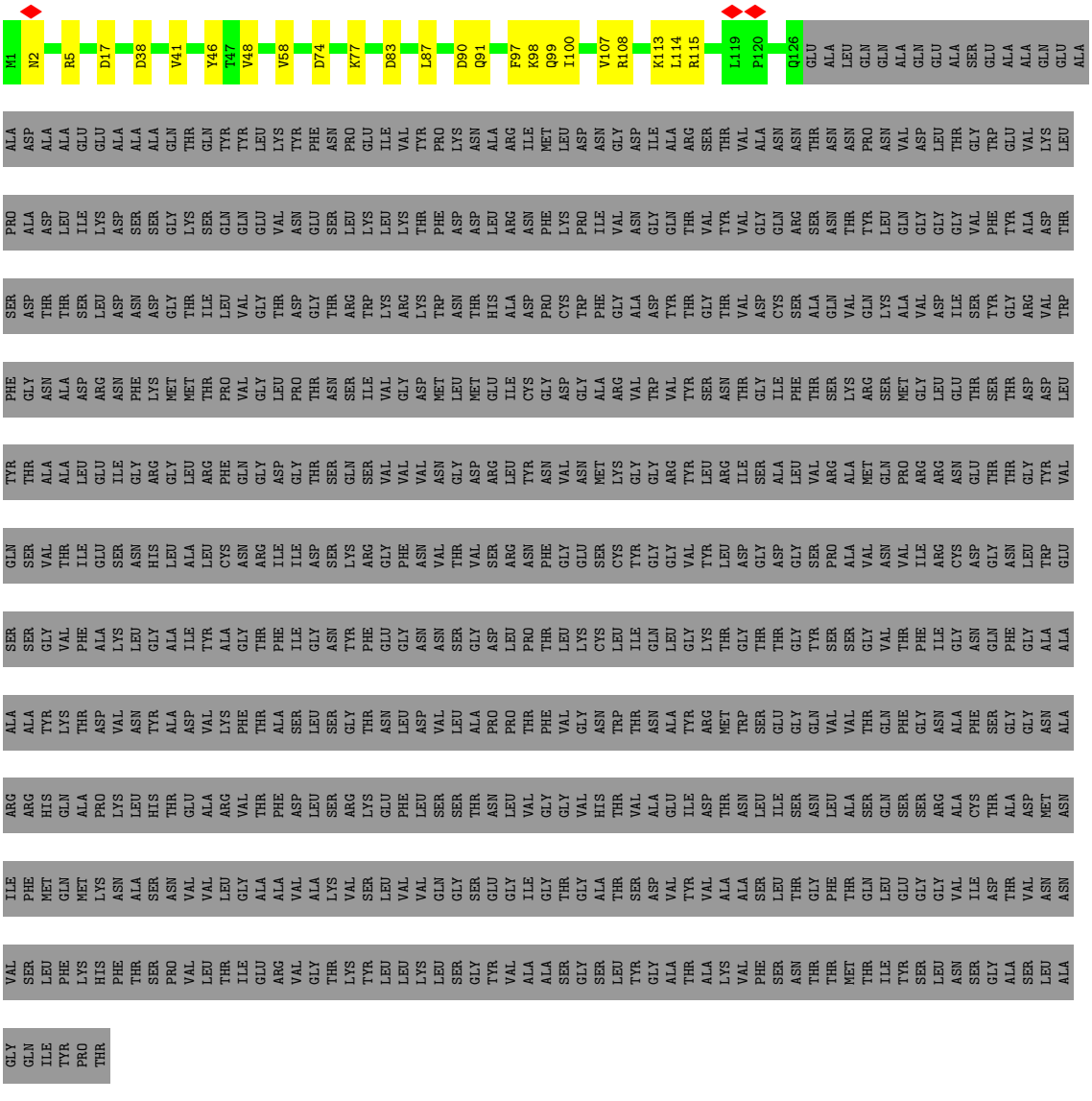




• Molecule 4: fiber protein

Chain I:

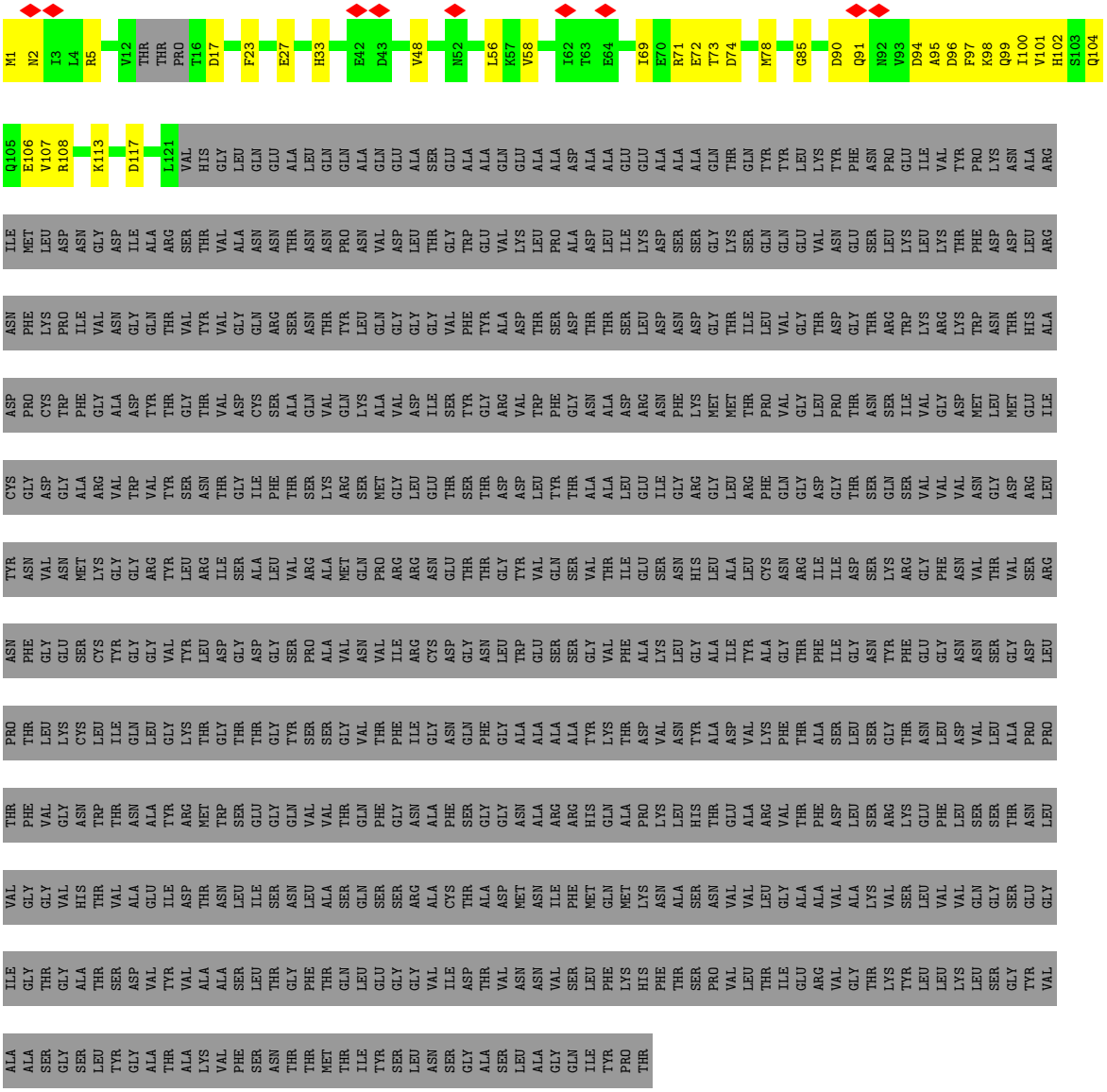




• Molecule 4: fiber protein

Chain J:

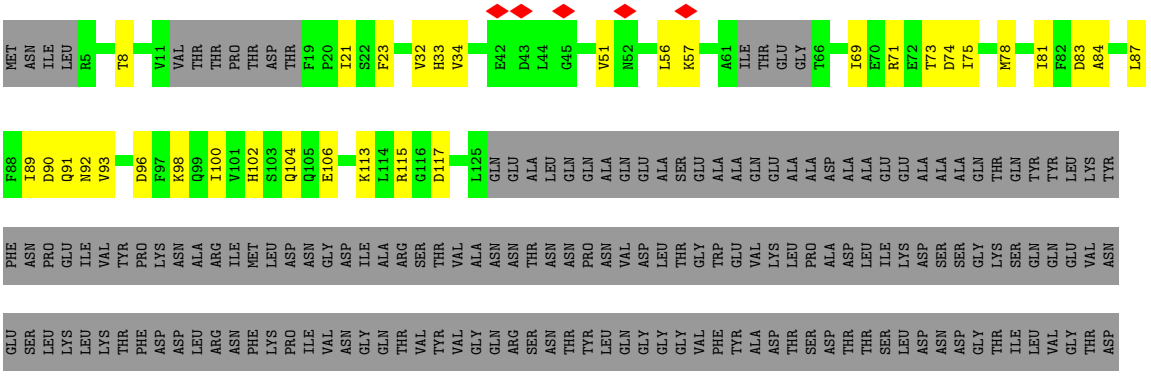


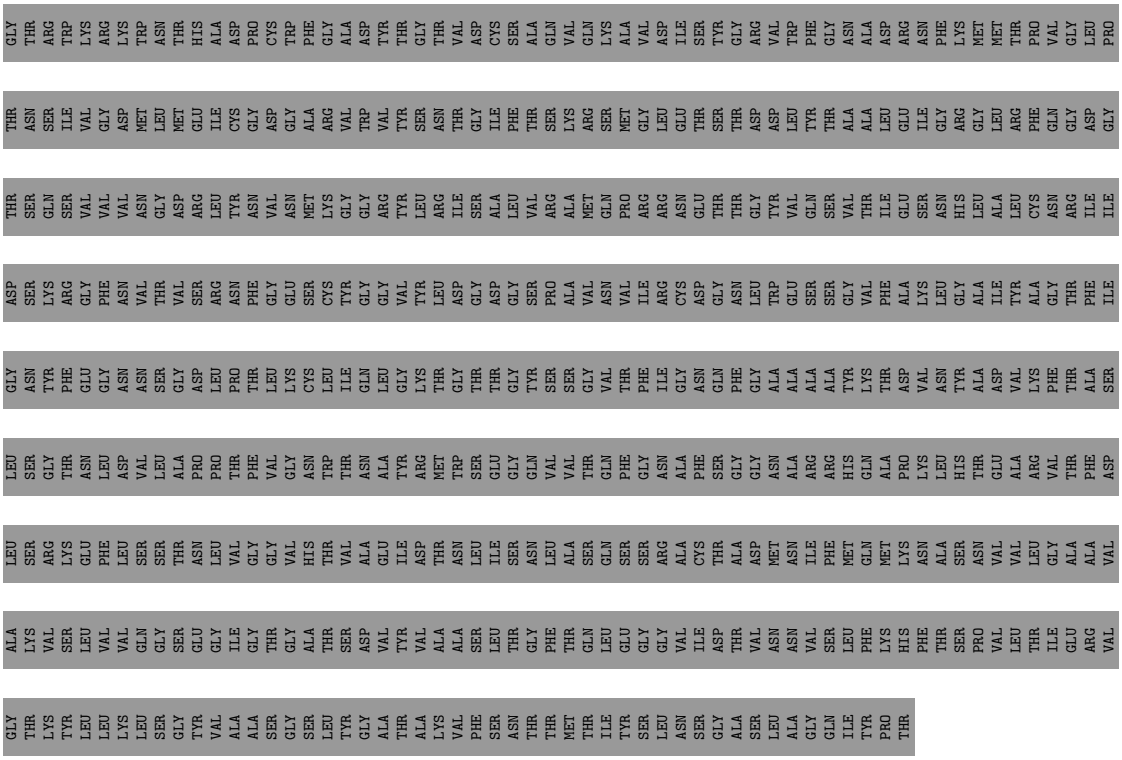


- Molecule 4: fiber protein

Chain K:






GLY THR ARG TRP LYS ARG LYS TRP ASN THR HIS ALA ASP PRO CYS TRP PHE GLY ALA ASP TYR THR GLY THR VAL ASP CYS SER ALA GLN VAL GLN LYS ALA VAL ASP ILE SER TYR GLY ARG VAL TRP PHE GLY ASN ALA ASP ARG ASN PHE LYS MET MET THR PRO VAL GLY LEU PRO
THR ASN SER ILE VAL GLY ASP MET LEU MET GLU ILE CYS GLY ASP GLY ALA ARG VAL TRP VAL TYR SER ASN THR GLY ILE PHE THR SER LYS ARG SER MET GLY LEU GLU THR SER THR ASP ASP LEU TYR THR ALA ALA LEU GLU GLU ILE GLY ARG GLY LEU ARG PHE GLN GLY ASP
THR SER GLN SER VAL VAL VAL ASN GLY ASP ARG LEU TYR ASN VAL ASN MET LYS GLY GLY ARG TYR LEU ARG ILE SER ALA LEU VAL ARG ALA MET GLN PRO ARG ARG ASN GLU THR THR GLY TYR VAL GLN SER VAL THR ILE GLU SER ASN HIS LEU ALA LEU GLU SER ARG ILE
ASP SER LYS ARG GLY PHE ASN VAL THR VAL SER ARG ASN PHE GLY GLU SER CYS TYR GLY GLY VAL TYR LEU ASP GLY ASP GLY SER PRO ALA VAL ASN VAL ILE ARG CYS ASP GLY ASN LEU TRP GLU SER SER VAL GLY VAL PHE ALA LYS LEU GLY ALA ILE TYR ALA GLY THR PHE ILE
GLY ASN TYR PHE GLU GLY ASN ASN SER GLY ASP LEU PRO THR LEU LYS CYS LEU ILE GLN LEU GLY LYS THR GLY THR THR GLY TYR SER SER GLY VAL GLY PHE ILE GLY ASN GLN PHE GLY ALA ALA ALA ALA TYR LYS THR ASP VAL LYS PHE THR ALA SER
LEU SER GLY THR ASN LEU ASP VAL LEU ALA PRO PRO THR PHE VAL GLY ASN TRP THR ASN ALA TYR ARG MET TRP SER GLU GLY GLN VAL VAL THR GLN PHE GLY GLY ASN ALA PHE SER GLY GLY ASN ALA ARG HIS GLN ALA PRO LYS LEU HIS THR GLU ALA ARG VAL THR PHE ASP
LEU SER ARG LYS GLU PHE LEU SER SER THR ASN LEU VAL GLY GLY VAL HIS THR VAL ALA GLU ILE ASP THR ASN LEU ALA SER GLN SER SER ARG ALA CYS THR ALA ASP MET ASN ILE PHE MET GLN MET LYS ASN ALA SER ASN VAL VAL LEU GLY ALA ALA VAL
ALA LYS VAL SER LEU VAL VAL GLN GLY SER GLU GLY ILE GLY THR GLY ALA THR SER ASP VAL TYR VAL ALA ALA SER LEU THR GLY PHE THR GLN LEU GLU GLY GLY VAL ILE ASP THR VAL ASN ASN VAL SER LEU PHE LYS HIS PHE THR SER PRO VAL LEU THR ILE GLU ARG VAL
GLY THR LYS TYR LEU LEU LYS LEU SER GLY TYR VAL ALA ALA SER GLY SER LEU TYR GLY ALA THR ALA LYS VAL PHE SER ASN THR THR MET THR ILE TYR SER LEU ASN SER GLY ALA SER LEU ALA GLY GLN ILE TYR PRO THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.044	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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	0.37	0/1552	0.48	0/2104
1	B	0.35	0/1523	0.47	0/2065
2	D	0.29	0/3579	0.44	0/4847
2	E	0.28	0/3472	0.45	0/4701
3	F	0.34	0/6079	0.48	0/8277
4	I	0.30	0/1023	0.46	0/1391
4	J	0.32	0/958	0.54	0/1299
4	K	0.31	0/901	0.54	0/1219
All	All	0.32	0/19087	0.47	0/25903

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	1523	0	1535	25	0
1	B	1495	0	1505	18	0
2	D	3524	0	3497	78	0
2	E	3419	0	3400	60	0
3	F	5954	0	5820	118	0
4	I	1005	0	986	17	0
4	J	943	0	922	26	0
4	K	886	0	861	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18749	0	18526	335	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 9.

The worst 5 of 335 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:F:709:GLN:HG3	3:F:710:LEU:H	1.36	0.90
2:D:428:VAL:HG23	2:D:460:ASN:HD22	1.43	0.83
2:E:116:LEU:HB2	2:E:389:LEU:HD21	1.64	0.79
4:K:89:ILE:HG13	4:K:92:ASN:H	1.47	0.79
3:F:634:GLN:HE22	4:K:92:ASN:HD21	1.30	0.78

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	184/208 (88%)	178 (97%)	6 (3%)	0	100	100
1	B	179/208 (86%)	170 (95%)	9 (5%)	0	100	100
2	D	431/518 (83%)	406 (94%)	25 (6%)	0	100	100
2	E	416/518 (80%)	396 (95%)	20 (5%)	0	100	100
3	F	761/763 (100%)	713 (94%)	48 (6%)	0	100	100
4	I	124/808 (15%)	118 (95%)	6 (5%)	0	100	100
4	J	114/808 (14%)	105 (92%)	9 (8%)	0	100	100
4	K	104/808 (13%)	103 (99%)	1 (1%)	0	100	100
All	All	2313/4639 (50%)	2189 (95%)	124 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	163/185 (88%)	163 (100%)	0	100	100
1	B	159/185 (86%)	159 (100%)	0	100	100
2	D	382/444 (86%)	382 (100%)	0	100	100
2	E	371/444 (84%)	371 (100%)	0	100	100
3	F	665/665 (100%)	665 (100%)	0	100	100
4	I	113/664 (17%)	113 (100%)	0	100	100
4	J	105/664 (16%)	105 (100%)	0	100	100
4	K	98/664 (15%)	98 (100%)	0	100	100
All	All	2056/3915 (52%)	2056 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	465	GLN
3	F	587	GLN
3	F	571	GLN
3	F	634	GLN
2	D	362	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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.

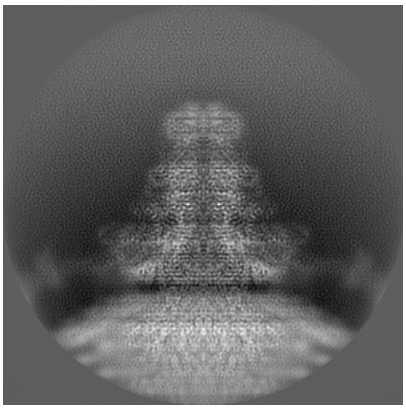
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67033. These allow visual inspection of the internal detail of the map and identification of artifacts.

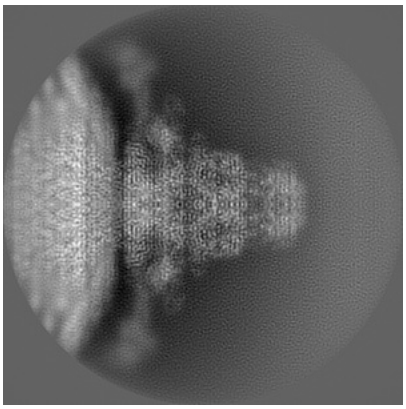
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

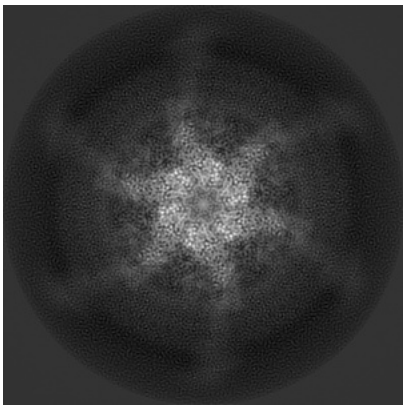
6.1.1 Primary map



X

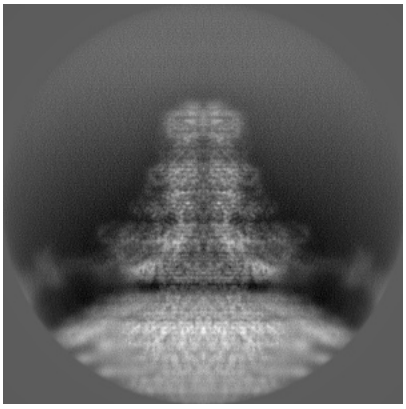


Y

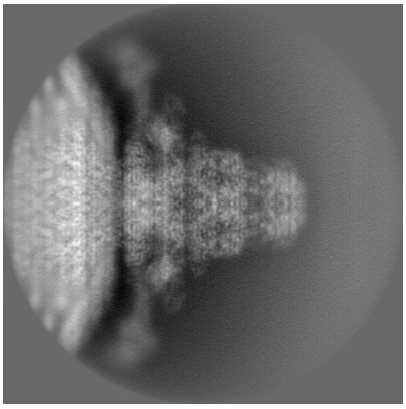


Z

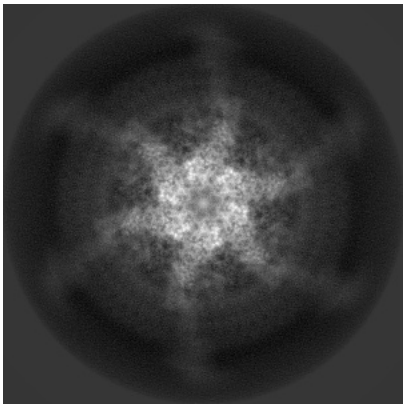
6.1.2 Raw map



X



Y

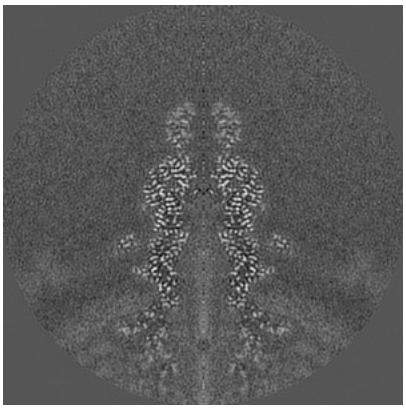


Z

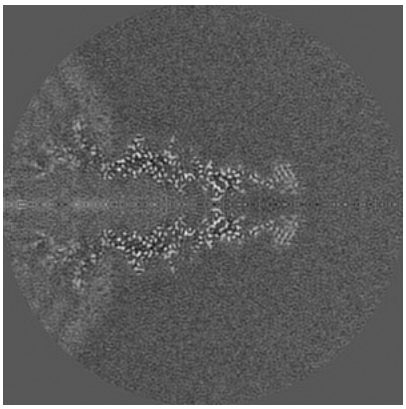
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

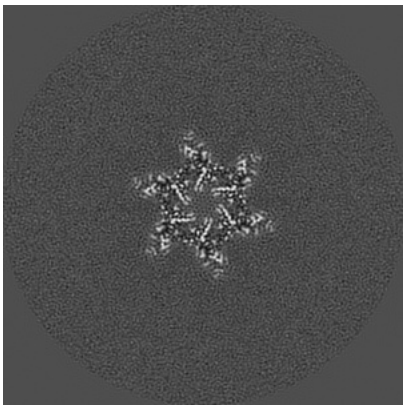
6.2.1 Primary map



X Index: 200

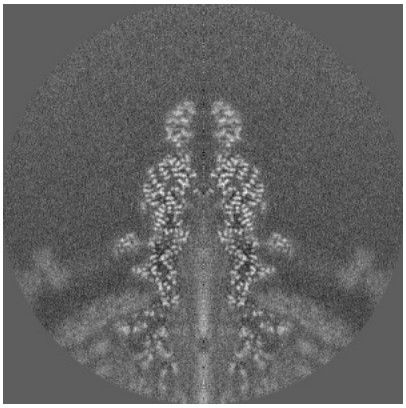


Y Index: 200

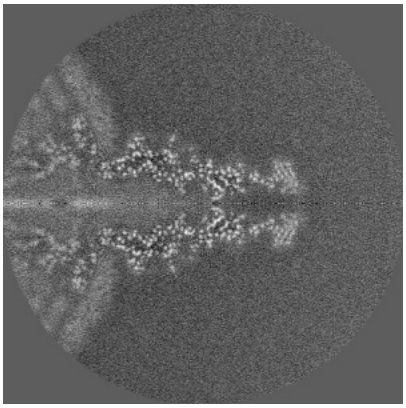


Z Index: 200

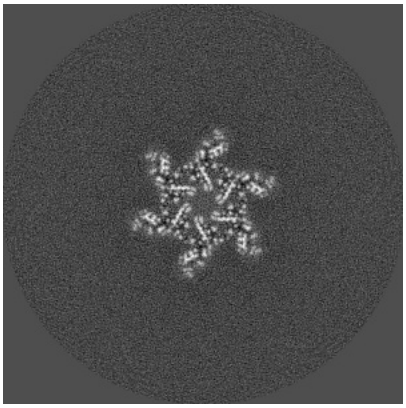
6.2.2 Raw map



X Index: 200



Y Index: 200

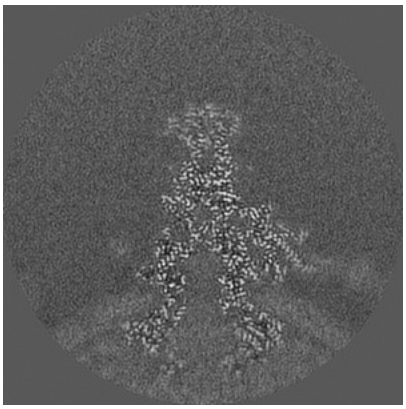


Z Index: 200

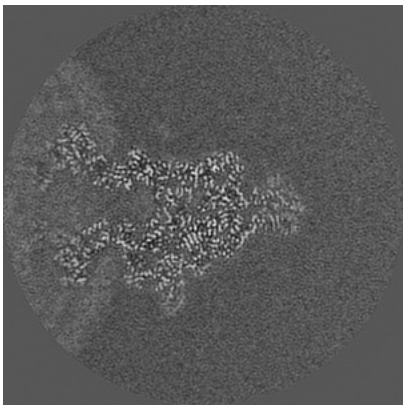
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

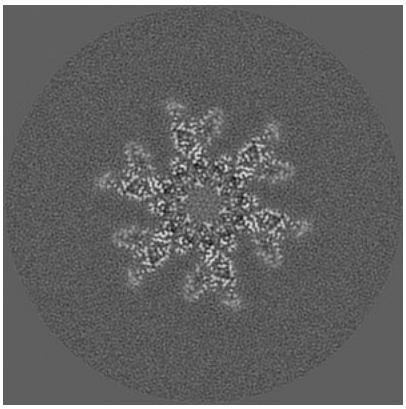
6.3.1 Primary map



X Index: 180

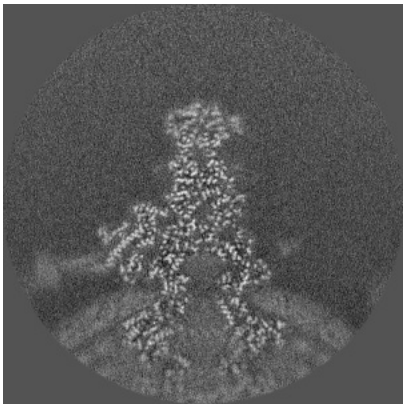


Y Index: 221

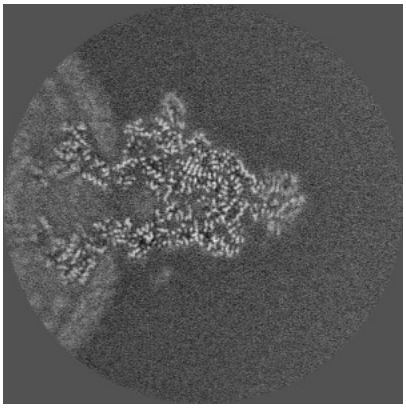


Z Index: 162

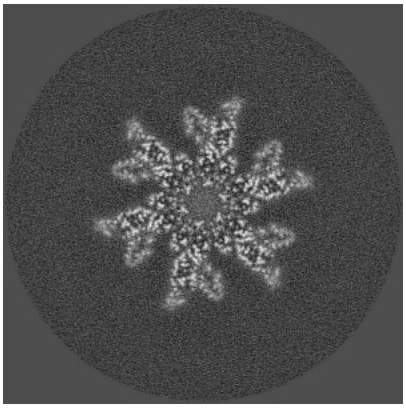
6.3.2 Raw map



X Index: 179



Y Index: 221

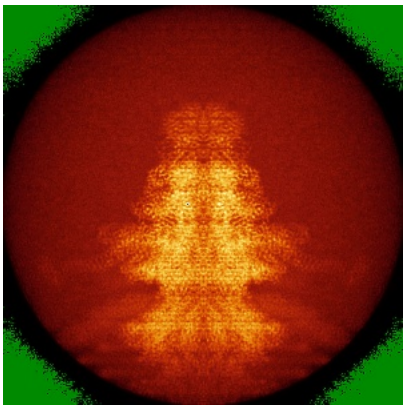


Z Index: 162

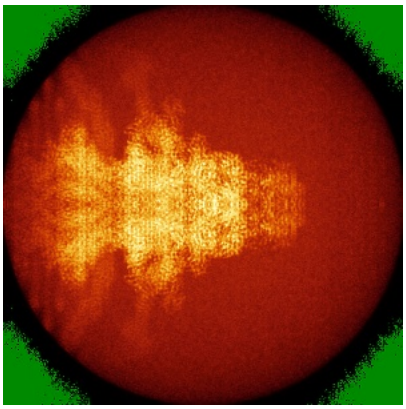
The images above show the largest variance slices of the map in three orthogonal directions.

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

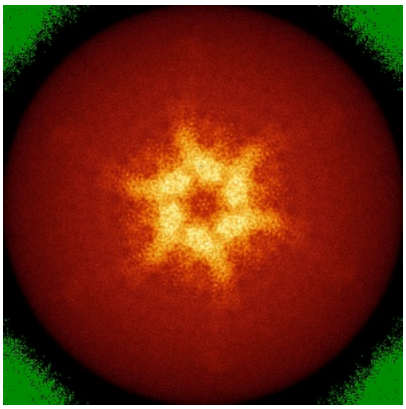
6.4.1 Primary map



X

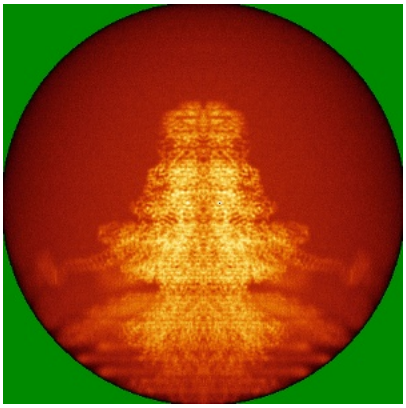


Y

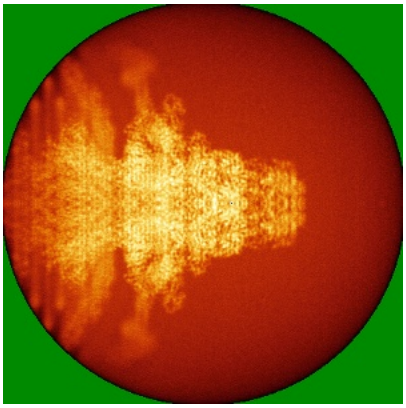


Z

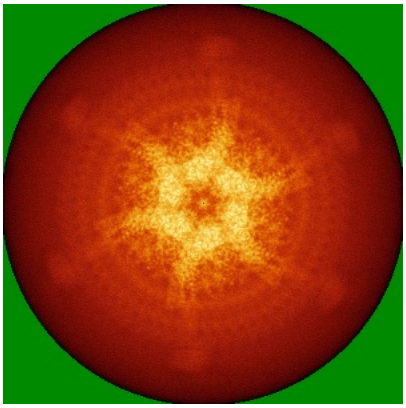
6.4.2 Raw map



X



Y

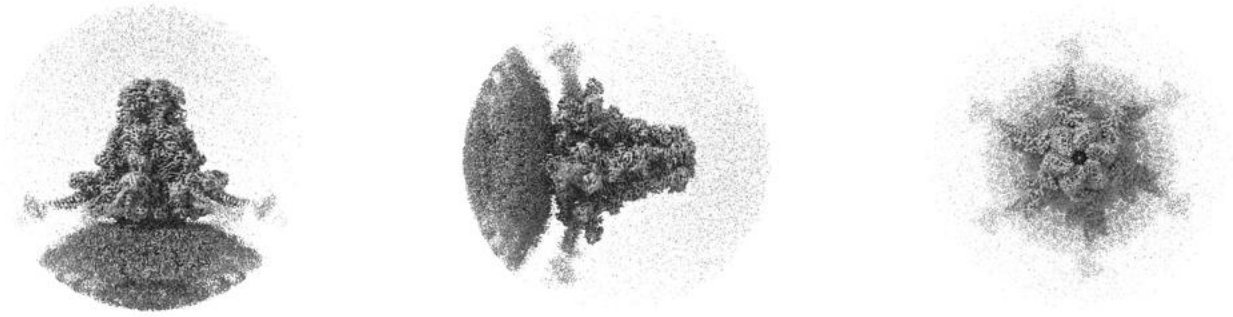


Z

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)

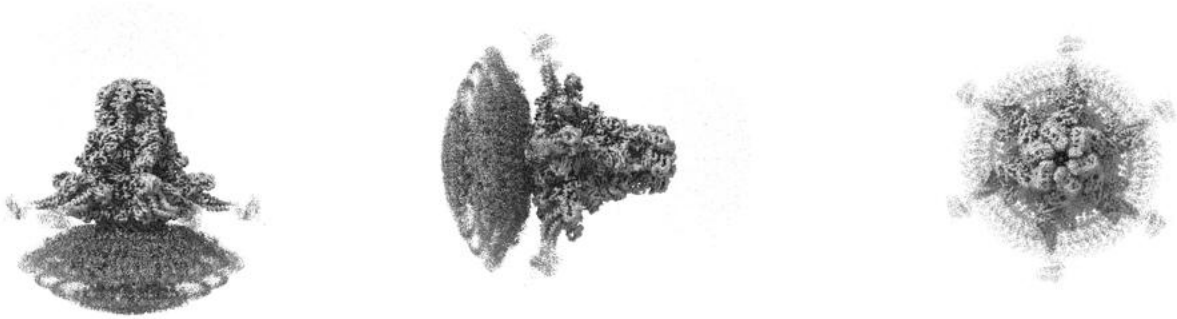
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

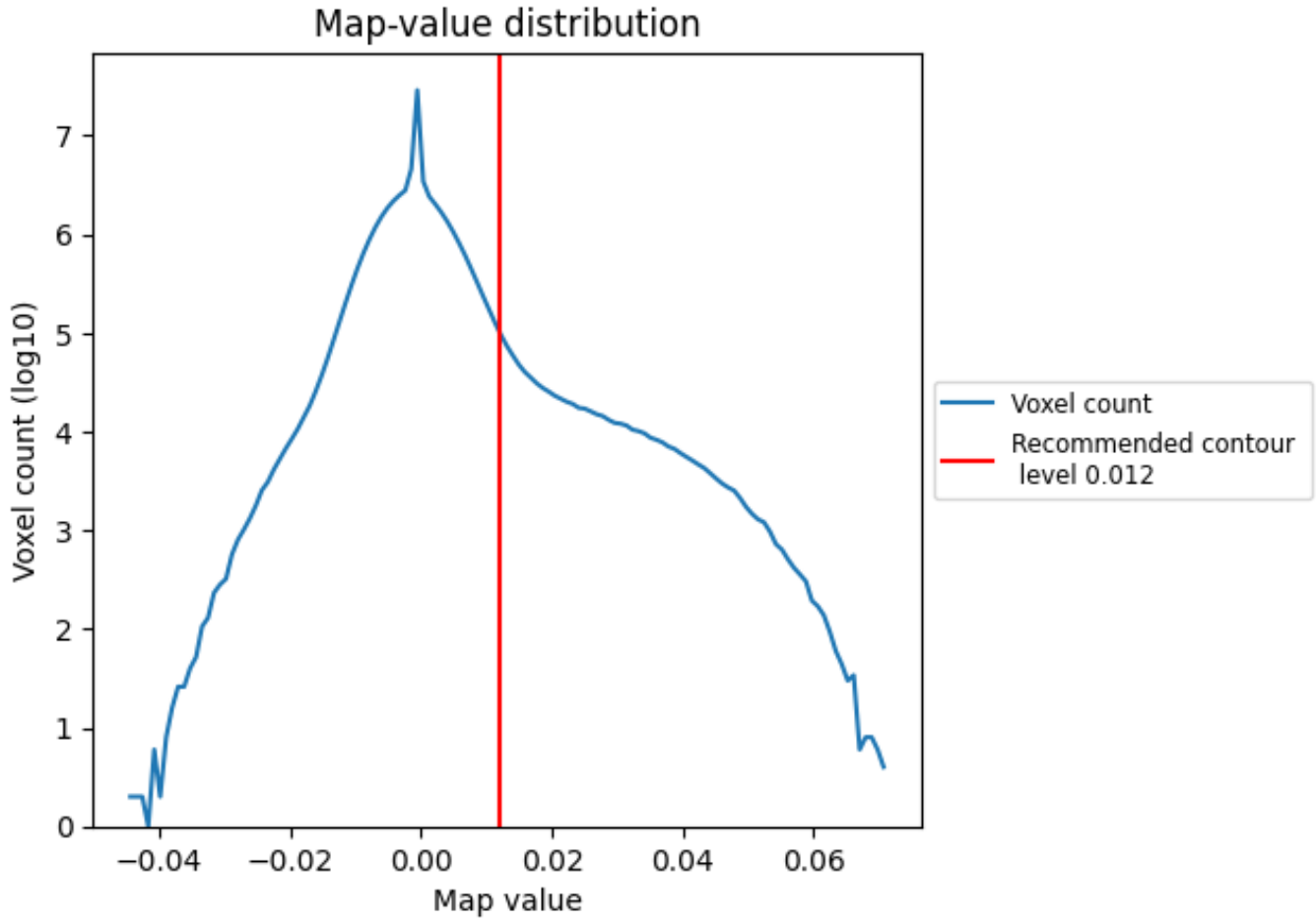
6.6 Mask visualisation (i)

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

7 Map analysis

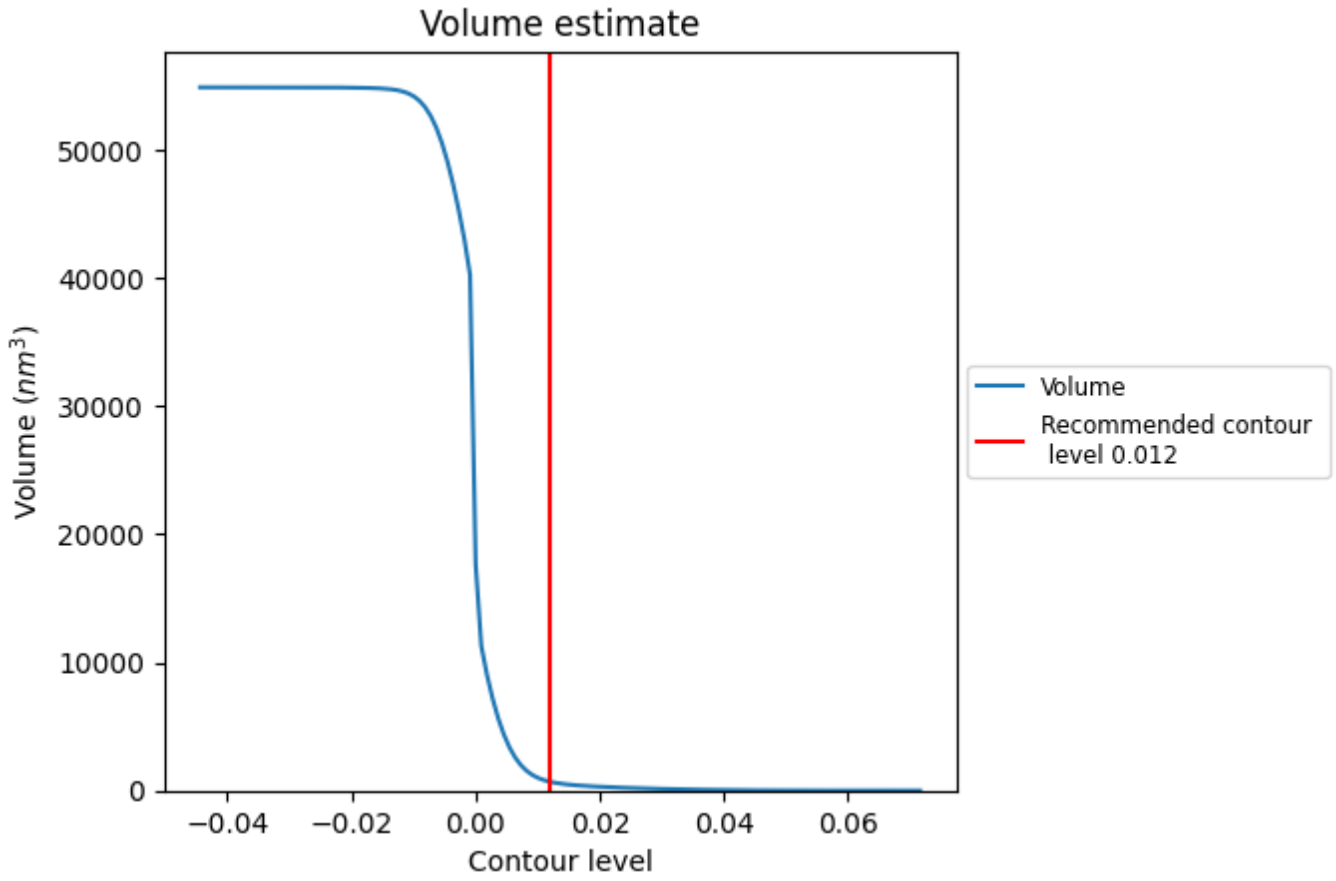
This section contains the results of statistical analysis of the map.

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.

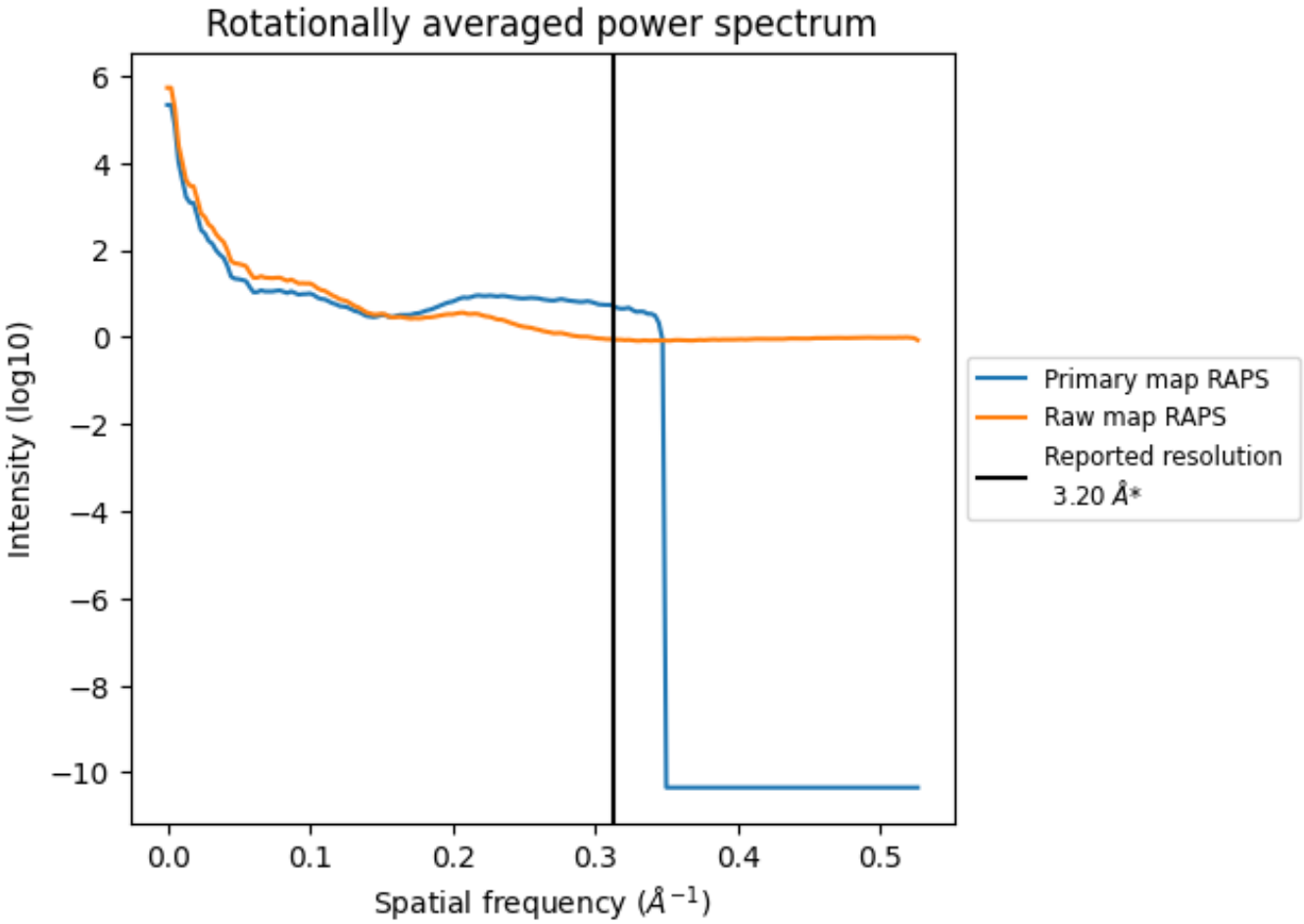
7.2 Volume estimate (i)



The volume at the recommended contour level is 691 nm^3; this corresponds to an approximate mass of 624 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)

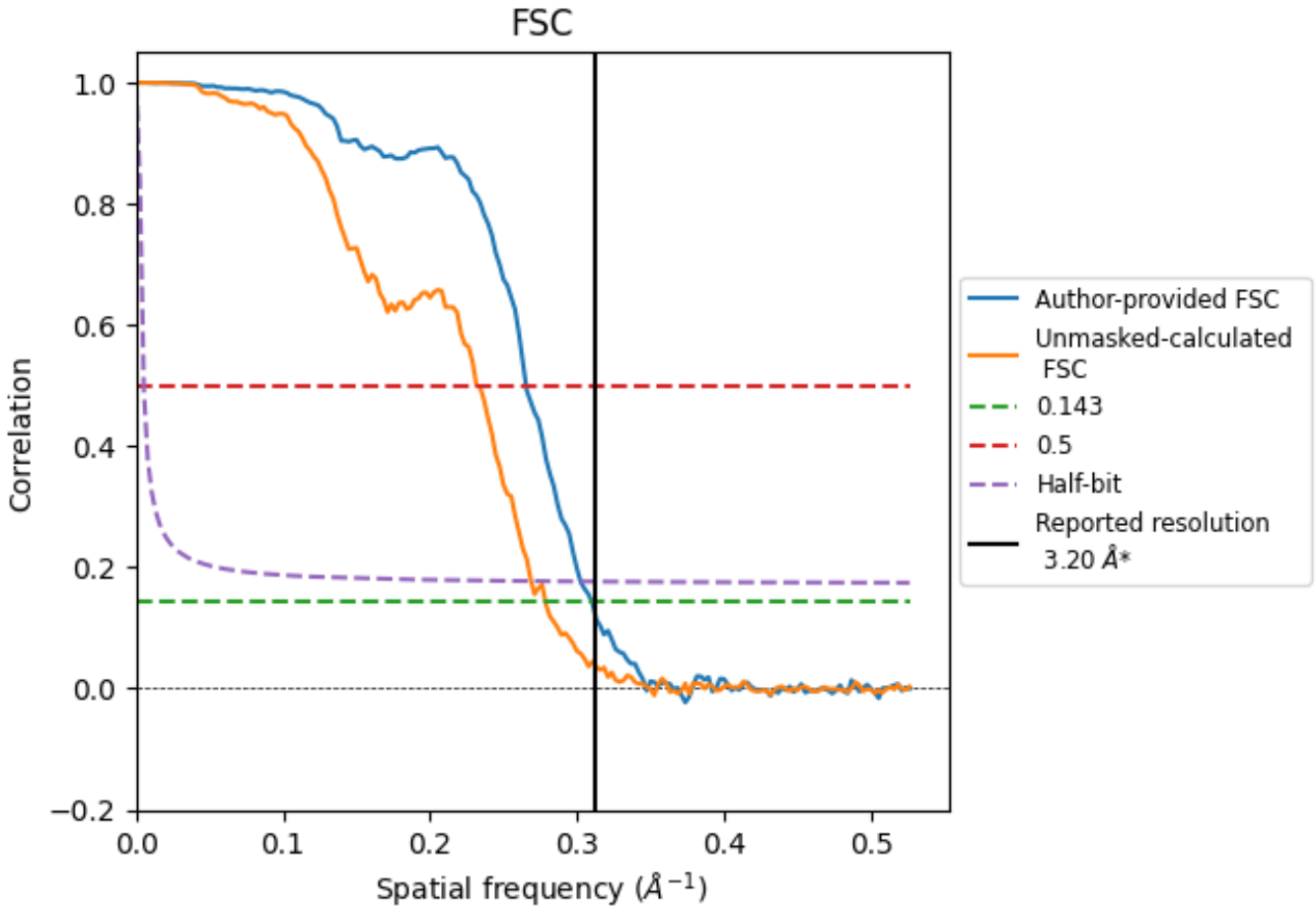


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.77	3.31
Unmasked-calculated*	3.59	4.31	3.72

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67033 and PDB model 9XMU. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

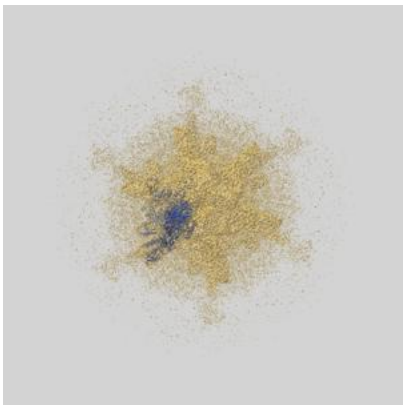
9.1.1 Map-model overlay



X

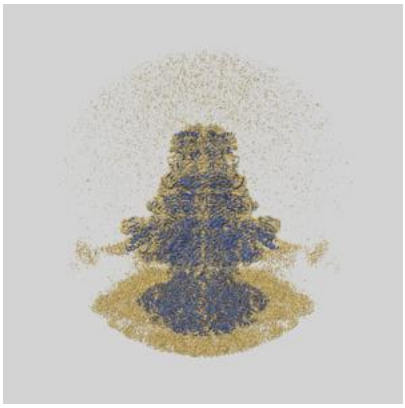


Y

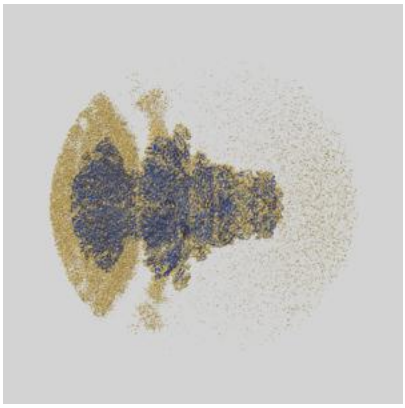


Z

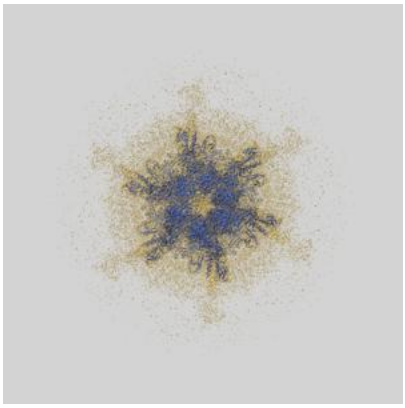
9.1.2 Map-model assembly overlay



X



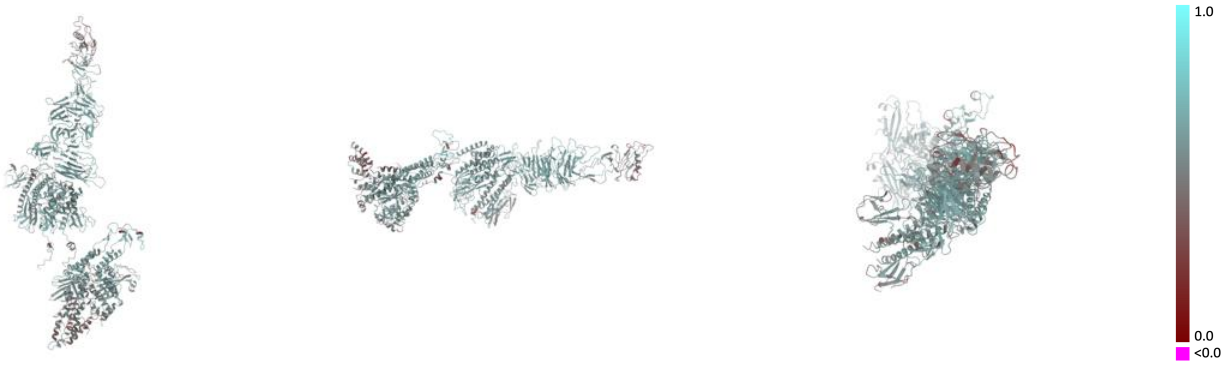
Y



Z

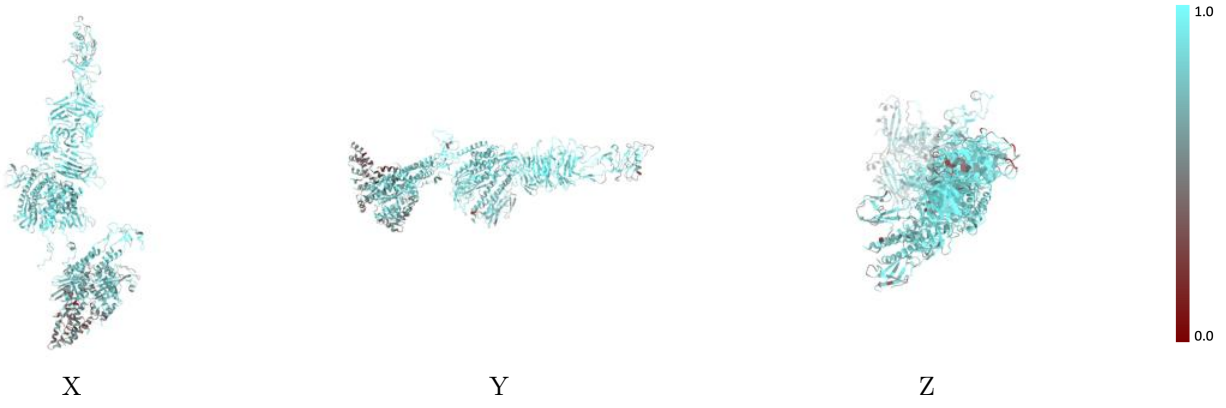
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



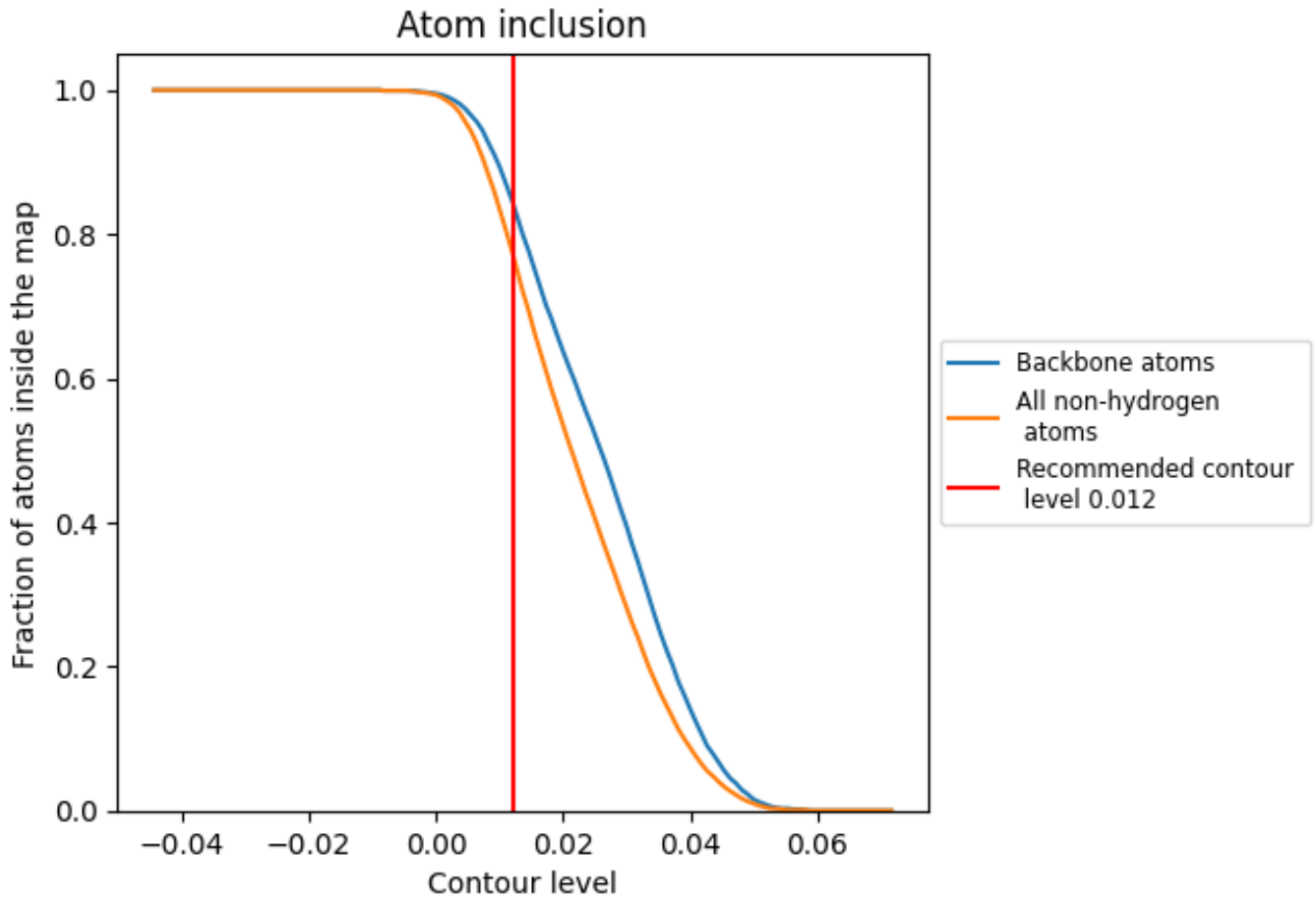
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.5570
A	0.8430	0.5800
B	0.8560	0.5860
D	0.6880	0.5370
E	0.7040	0.5470
F	0.8340	0.5690
I	0.7890	0.5650
J	0.7430	0.5310
K	0.7490	0.5240

