



wwPDB EM Validation Summary Report ⓘ

May 11, 2024 – 04:35 pm BST

PDB ID : 6S3L
EMDB ID : EMD-10093
Title : Structure of the core of the flagellar export apparatus from *Vibrio mimicus*, the FliPQR-FlhB complex.
Authors : Kuhlen, L.; Johnson, S.; Deme, J.C.; Lea, S.M.
Deposited on : 2019-06-25
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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

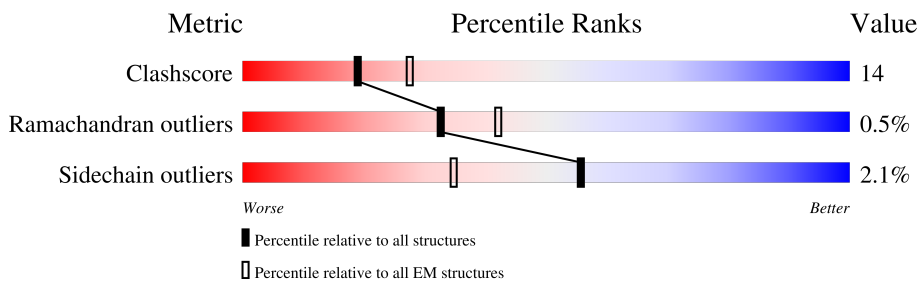
1 Overall quality at a glance

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.



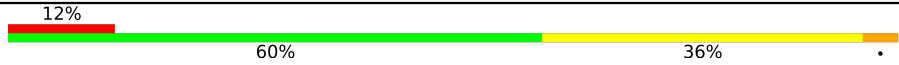


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	11% (red), 42% (green), 21% (yellow), 36% (grey)
1	B	299	15% (red), 48% (green), 17% (yellow), 35% (grey)
1	C	299	17% (red), 44% (green), 20% (yellow), 34% (grey)
1	D	299	21% (red), 43% (green), 22% (yellow), 35% (grey)
1	E	299	12% (red), 38% (green), 25% (yellow), 36% (grey)
2	F	260	5% (red), 68% (green), 28% (yellow), 1% (grey)
3	G	89	10% (red), 57% (green), 39% (yellow), 1% (grey)
3	H	89	8% (red), 60% (green), 38% (yellow), 1% (grey)

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Mol	Chain	Length	Quality of chain
3	I	89	
3	J	89	
4	K	415	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13849 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 Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	191	Total 1482	C 981	N 228	O 256	S 17	0	0
1	B	195	Total 1513	C 1003	N 232	O 260	S 18	0	0
1	C	196	Total 1520	C 1007	N 233	O 262	S 18	0	0
1	D	194	Total 1505	C 998	N 231	O 259	S 17	0	0
1	E	192	Total 1493	C 990	N 229	O 257	S 17	0	0

- Molecule 2 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	251	Total 1948	C 1294	N 304	O 331	S 19	0	0

- Molecule 3 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	89	Total 724	C 493	N 105	O 118	S 8	0	0
3	H	89	Total 724	C 493	N 105	O 118	S 8	0	0
3	I	89	Total 724	C 493	N 105	O 118	S 8	0	0
3	J	89	Total 724	C 493	N 105	O 118	S 8	0	0

- Molecule 4 is a protein called Flagellar biosynthetic protein FliB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	193	1492	993	236	255	8	0	0

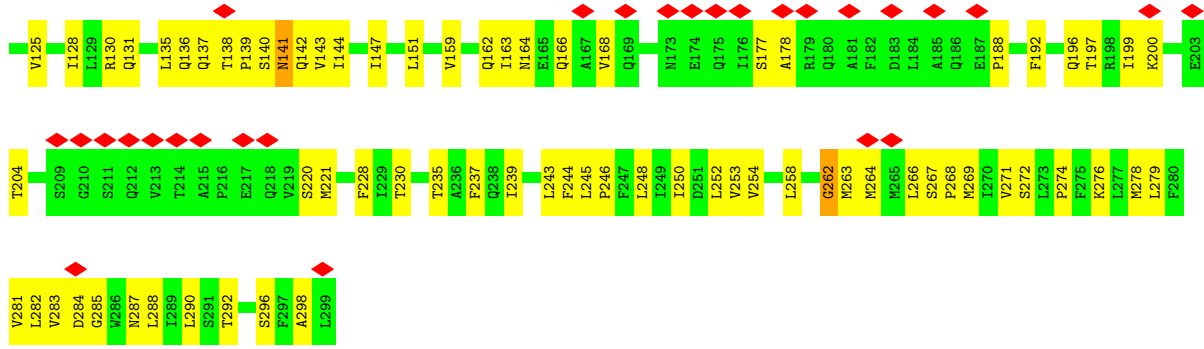
There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	377	GLU	-	expression tag	UNP A0A1D8S9F8
K	378	ASN	-	expression tag	UNP A0A1D8S9F8
K	379	LEU	-	expression tag	UNP A0A1D8S9F8
K	380	TYR	-	expression tag	UNP A0A1D8S9F8
K	381	PHE	-	expression tag	UNP A0A1D8S9F8
K	382	GLN	-	expression tag	UNP A0A1D8S9F8
K	383	GLY	-	expression tag	UNP A0A1D8S9F8
K	384	GLN	-	expression tag	UNP A0A1D8S9F8
K	385	PHE	-	expression tag	UNP A0A1D8S9F8
K	386	GLY	-	expression tag	UNP A0A1D8S9F8
K	387	SER	-	expression tag	UNP A0A1D8S9F8
K	388	TRP	-	expression tag	UNP A0A1D8S9F8
K	389	SER	-	expression tag	UNP A0A1D8S9F8
K	390	HIS	-	expression tag	UNP A0A1D8S9F8
K	391	PRO	-	expression tag	UNP A0A1D8S9F8
K	392	GLN	-	expression tag	UNP A0A1D8S9F8
K	393	PHE	-	expression tag	UNP A0A1D8S9F8
K	394	GLU	-	expression tag	UNP A0A1D8S9F8
K	395	LYS	-	expression tag	UNP A0A1D8S9F8
K	396	GLY	-	expression tag	UNP A0A1D8S9F8
K	397	GLY	-	expression tag	UNP A0A1D8S9F8
K	398	GLY	-	expression tag	UNP A0A1D8S9F8
K	399	SER	-	expression tag	UNP A0A1D8S9F8
K	400	GLY	-	expression tag	UNP A0A1D8S9F8
K	401	GLY	-	expression tag	UNP A0A1D8S9F8
K	402	GLY	-	expression tag	UNP A0A1D8S9F8
K	403	SER	-	expression tag	UNP A0A1D8S9F8
K	404	GLY	-	expression tag	UNP A0A1D8S9F8
K	405	GLY	-	expression tag	UNP A0A1D8S9F8
K	406	GLY	-	expression tag	UNP A0A1D8S9F8
K	407	SER	-	expression tag	UNP A0A1D8S9F8
K	408	TRP	-	expression tag	UNP A0A1D8S9F8
K	409	SER	-	expression tag	UNP A0A1D8S9F8
K	410	HIS	-	expression tag	UNP A0A1D8S9F8
K	411	PRO	-	expression tag	UNP A0A1D8S9F8
K	412	GLN	-	expression tag	UNP A0A1D8S9F8
K	413	PHE	-	expression tag	UNP A0A1D8S9F8

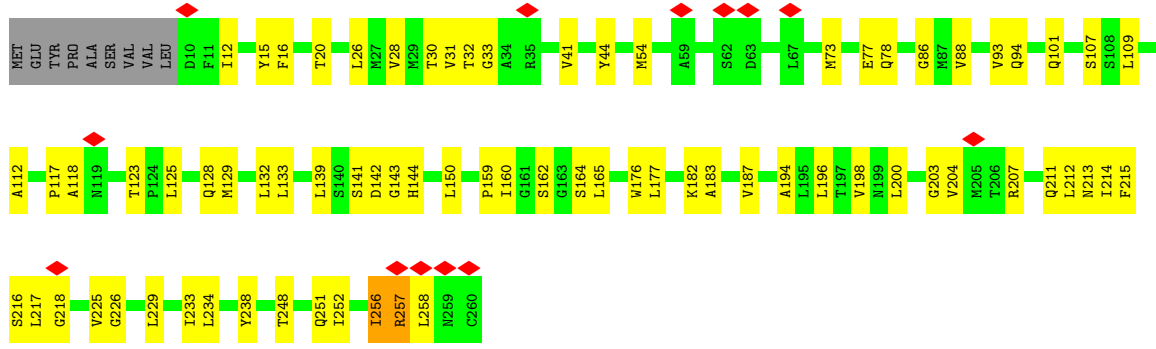
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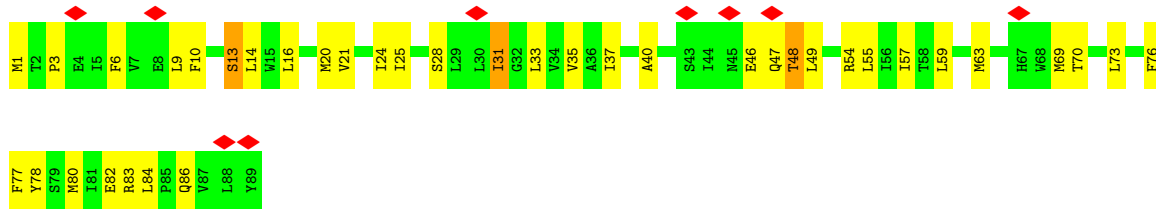
Chain	Residue	Modelled	Actual	Comment	Reference
K	414	GLU	-	expression tag	UNP A0A1D8S9F8
K	415	LYS	-	expression tag	UNP A0A1D8S9F8



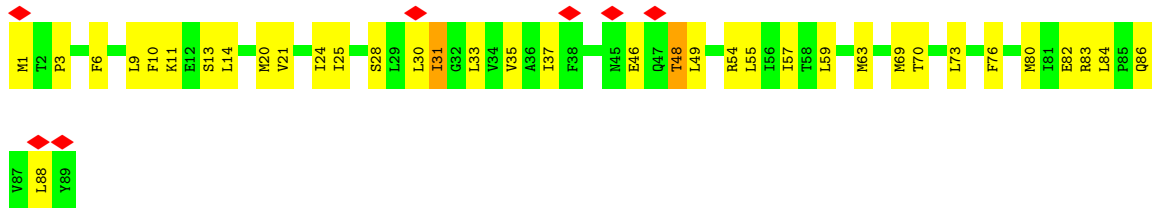
• Molecule 2: Flagellar biosynthetic protein FliR



• Molecule 3: Flagellar biosynthetic protein FliQ



• Molecule 3: Flagellar biosynthetic protein FliQ



• Molecule 3: Flagellar biosynthetic protein FliQ

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162408	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.068	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0255	Depositor
Map size (\AA)	236.73601, 236.73601, 236.73601	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.822, 0.822, 0.822	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/1510	0.52	0/2047
1	B	0.44	0/1542	0.49	0/2089
1	C	0.43	0/1549	0.56	0/2099
1	D	0.43	0/1534	0.51	0/2079
1	E	0.46	0/1522	0.56	0/2063
2	F	0.51	0/1993	0.57	0/2707
3	G	0.45	0/742	0.53	0/1009
3	H	0.46	0/742	0.53	0/1009
3	I	0.45	0/742	0.53	0/1009
3	J	0.46	0/742	0.53	0/1009
4	K	0.37	0/1520	0.48	0/2058
All	All	0.45	0/14138	0.53	0/19178

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
1	A	0	2
1	C	0	2
1	E	0	1
2	F	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	173	ASN	Peptide
1	C	136	GLN	Peptide
1	C	138	THR	Peptide
1	E	262	GLY	Peptide

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	1482	0	1569	58	0
1	B	1513	0	1601	45	0
1	C	1520	0	1608	56	0
1	D	1505	0	1592	63	0
1	E	1493	0	1578	71	0
2	F	1948	0	2021	66	0
3	G	724	0	768	33	0
3	H	724	0	768	30	0
3	I	724	0	768	34	0
3	J	724	0	768	35	0
4	K	1492	0	1582	34	0
All	All	13849	0	14623	408	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 14.

The worst 5 of 408 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLN:O	1:C:184:LEU:HB3	1.61	0.99
1:C:174:GLU:O	1:C:176:ILE:N	2.05	0.88
1:D:174:GLU:O	1:D:176:ILE:N	2.07	0.88
3:I:63:MET:O	3:J:11:LYS:NZ	2.07	0.87
2:F:133:LEU:HG	3:G:10:PHE:HE2	1.42	0.84

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	189/299 (63%)	170 (90%)	16 (8%)	3 (2%)	9	43
1	B	193/299 (64%)	179 (93%)	14 (7%)	0	100	100
1	C	194/299 (65%)	180 (93%)	11 (6%)	3 (2%)	10	44
1	D	192/299 (64%)	181 (94%)	10 (5%)	1 (0%)	29	67
1	E	190/299 (64%)	174 (92%)	15 (8%)	1 (0%)	29	67
2	F	249/260 (96%)	229 (92%)	19 (8%)	1 (0%)	34	69
3	G	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
3	H	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
3	I	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
3	J	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
4	K	191/415 (46%)	182 (95%)	9 (5%)	0	100	100
All	All	1746/2526 (69%)	1635 (94%)	102 (6%)	9 (0%)	32	67

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	138	THR
1	C	175	GLN
1	D	175	GLN
1	A	264	MET
1	E	141	ASN

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	167/252 (66%)	167 (100%)	0	100	100
1	B	170/252 (68%)	170 (100%)	0	100	100
1	C	171/252 (68%)	171 (100%)	0	100	100
1	D	169/252 (67%)	169 (100%)	0	100	100
1	E	168/252 (67%)	168 (100%)	0	100	100
2	F	211/219 (96%)	211 (100%)	0	100	100
3	G	82/82 (100%)	74 (90%)	8 (10%)	8	31
3	H	82/82 (100%)	74 (90%)	8 (10%)	8	31
3	I	82/82 (100%)	74 (90%)	8 (10%)	8	31
3	J	82/82 (100%)	74 (90%)	8 (10%)	8	31
4	K	162/344 (47%)	162 (100%)	0	100	100
All	All	1546/2151 (72%)	1514 (98%)	32 (2%)	56	79

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	48	THR
3	J	49	LEU
3	H	48	THR
3	H	35	VAL
3	J	70	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	39	GLN
3	I	47	GLN
3	I	39	GLN
3	I	86	GLN
1	D	196	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 monosaccharides 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.

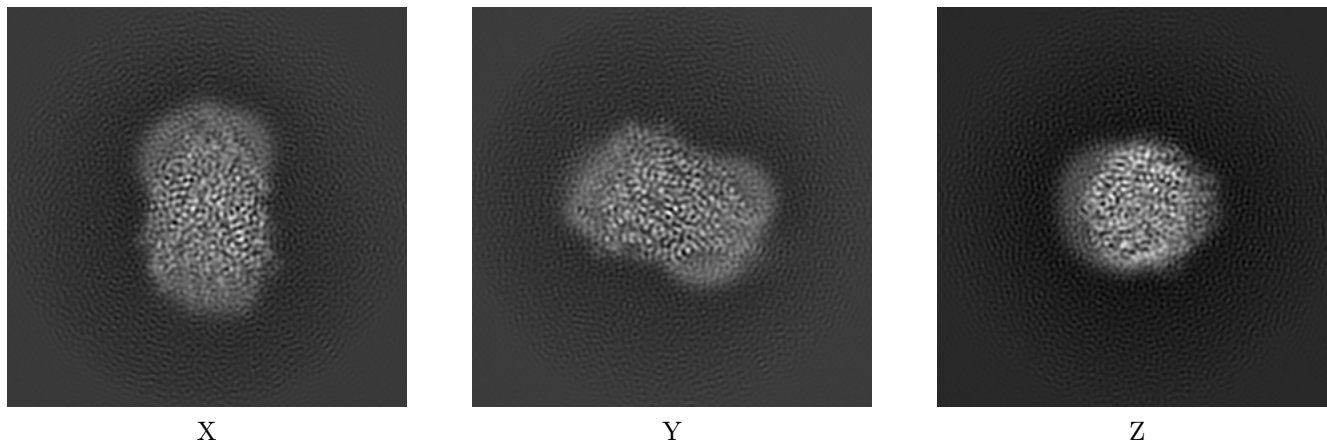
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10093. These allow visual inspection of the internal detail of the map and identification of artifacts.

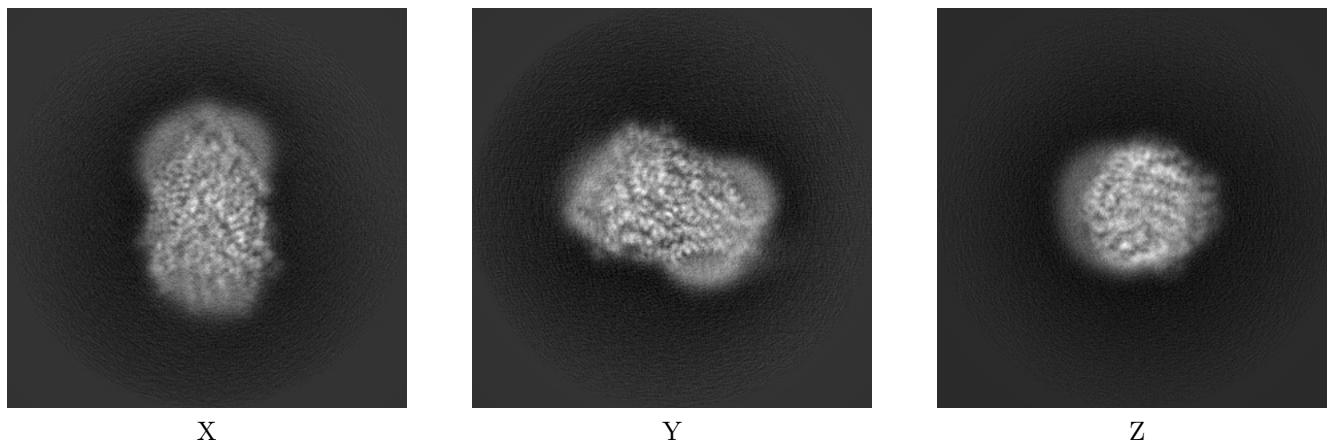
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



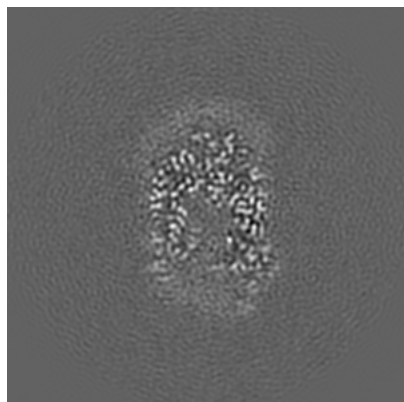
6.1.2 Raw map



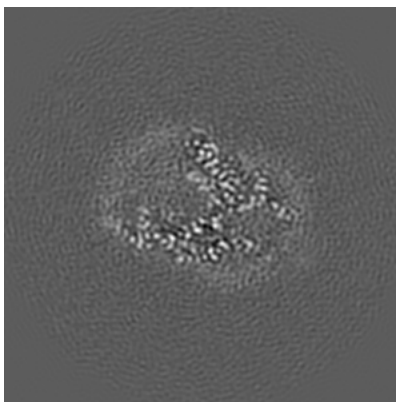
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

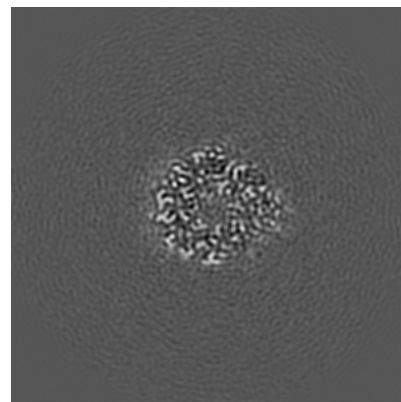
6.2.1 Primary map



X Index: 144

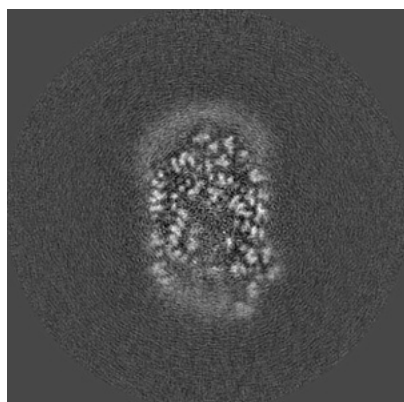


Y Index: 144

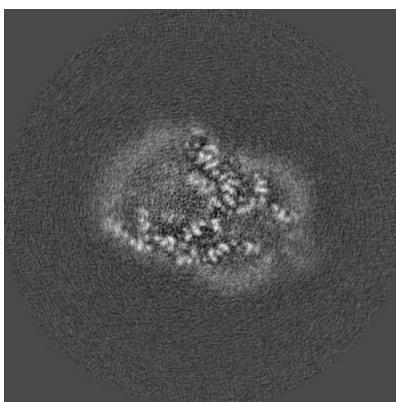


Z Index: 144

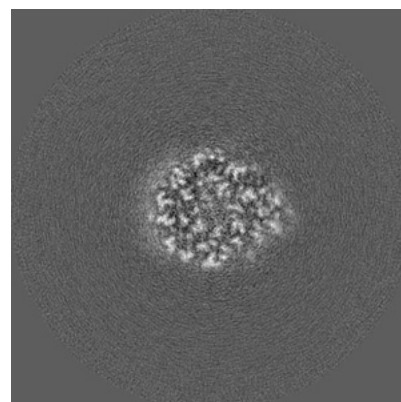
6.2.2 Raw map



X Index: 144



Y Index: 144

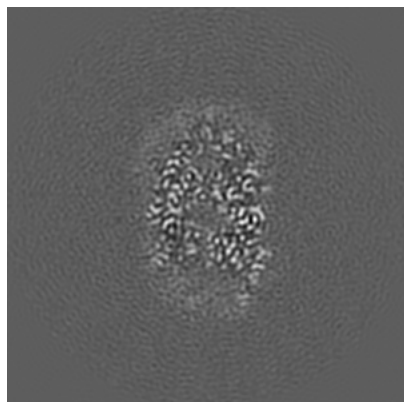


Z Index: 144

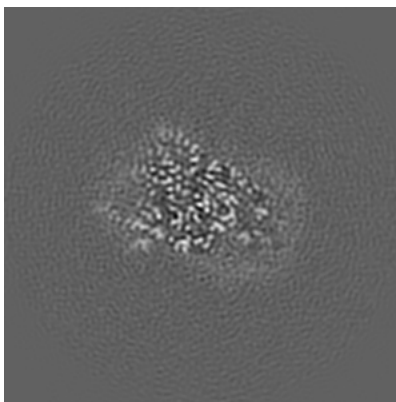
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

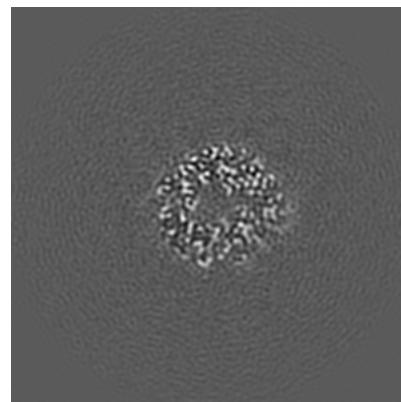
6.3.1 Primary map



X Index: 139

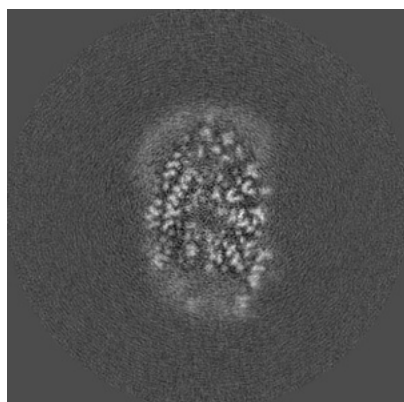


Y Index: 166

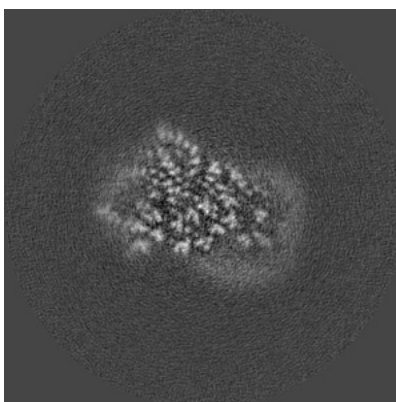


Z Index: 137

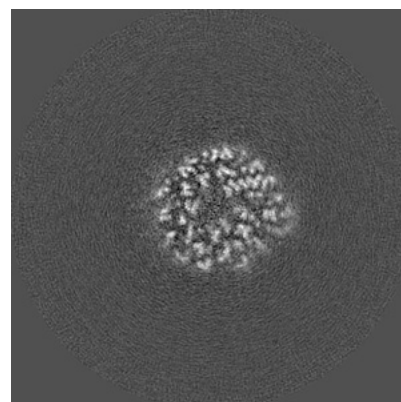
6.3.2 Raw map



X Index: 139



Y Index: 166

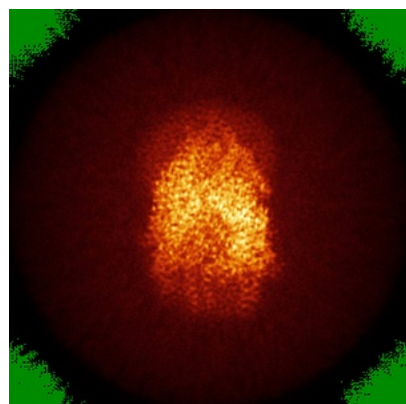


Z Index: 137

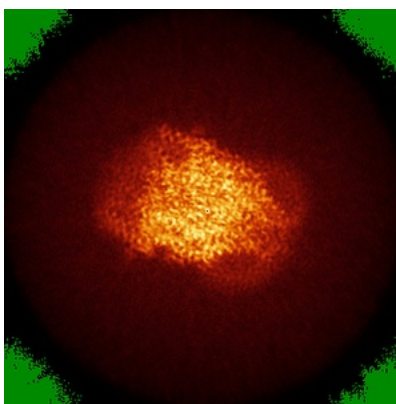
The images above show the largest variance slices of the map in three orthogonal directions.

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

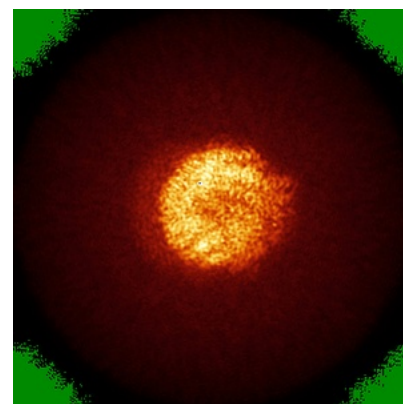
6.4.1 Primary map



X

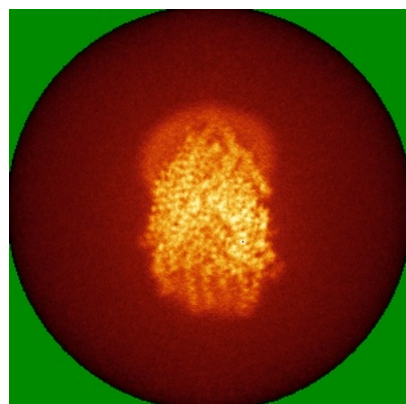


Y

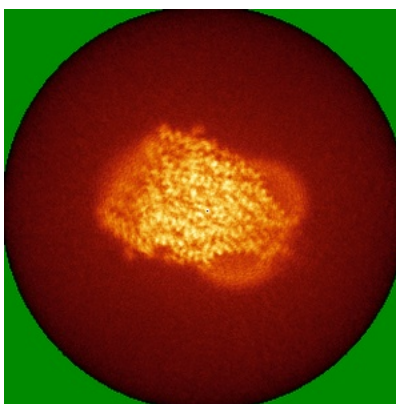


Z

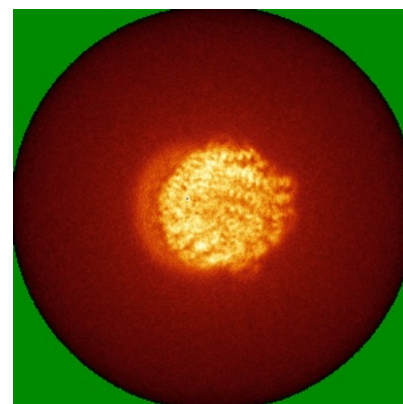
6.4.2 Raw map



X



Y

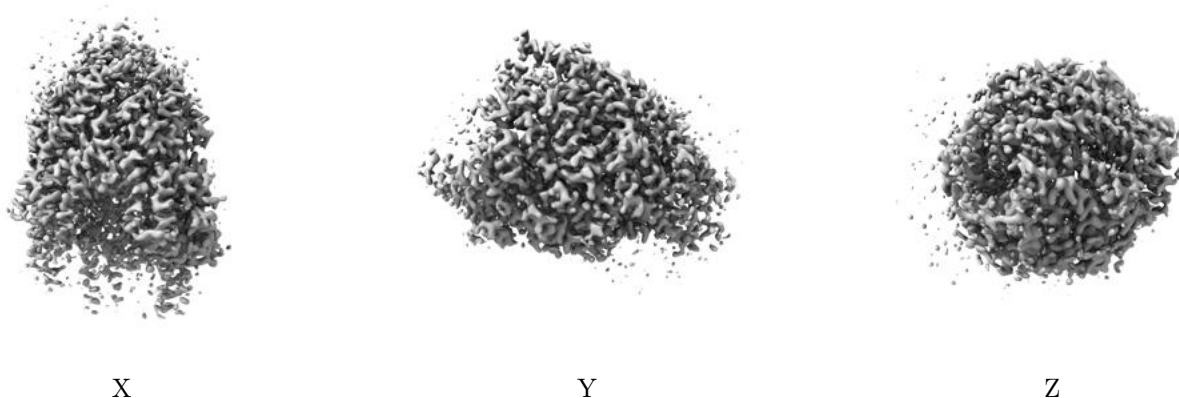


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

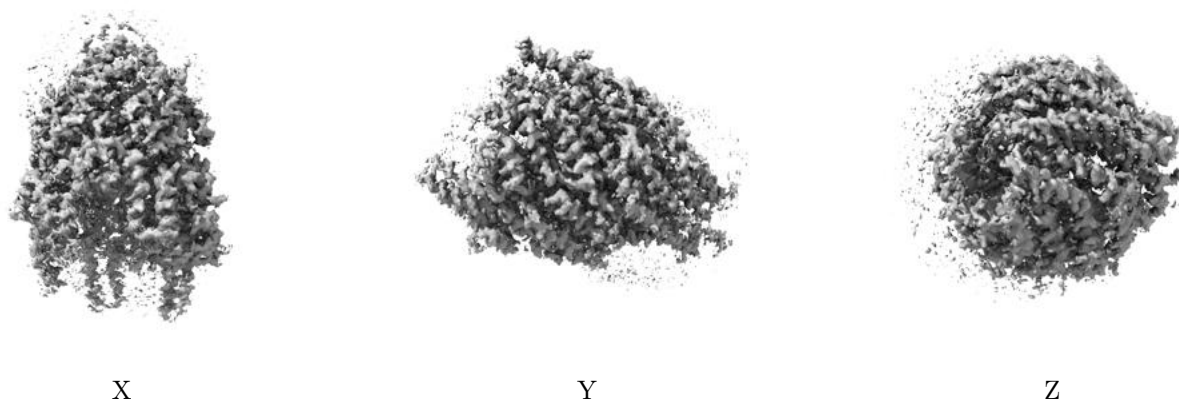
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0255. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

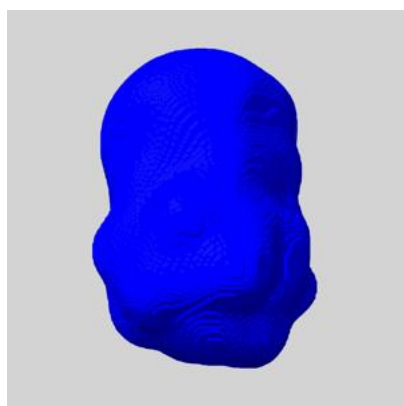
6.6 Mask visualisation [i](#)

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

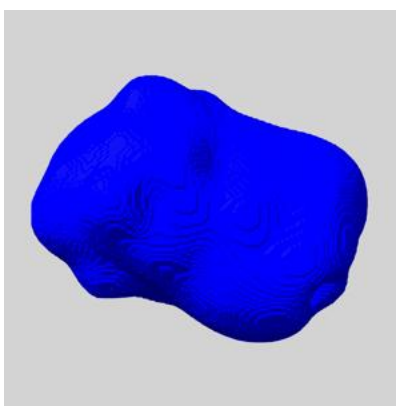
A mask typically either:

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

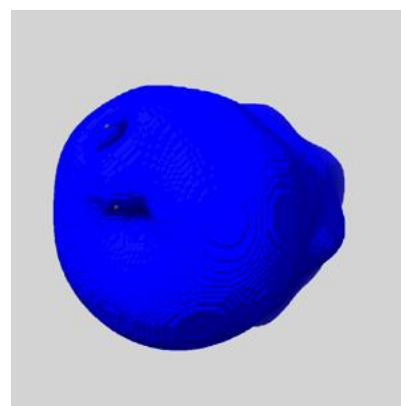
6.6.1 emd_10093_msk_1.map [i](#)



X



Y

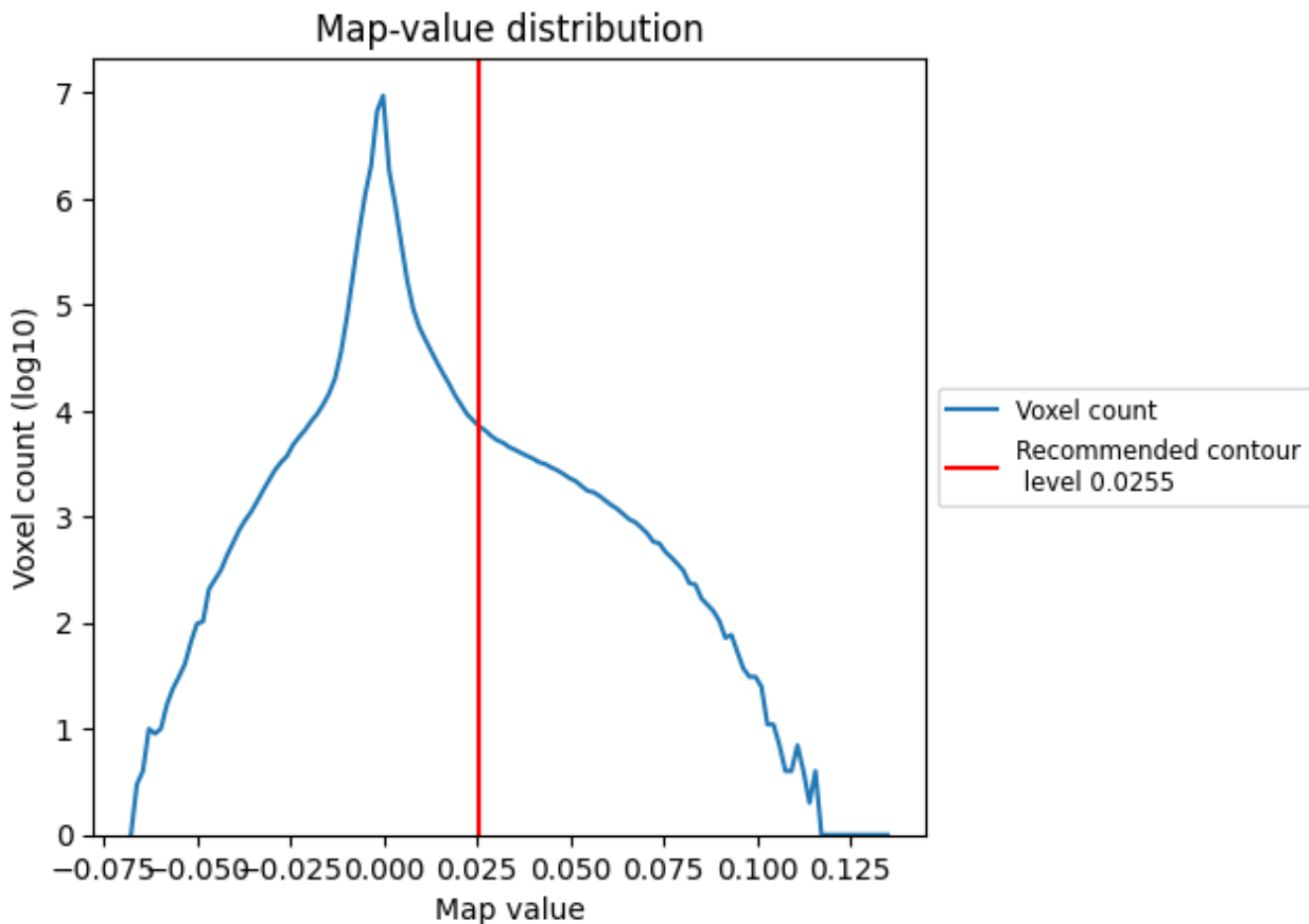


Z

7 Map analysis [i](#)

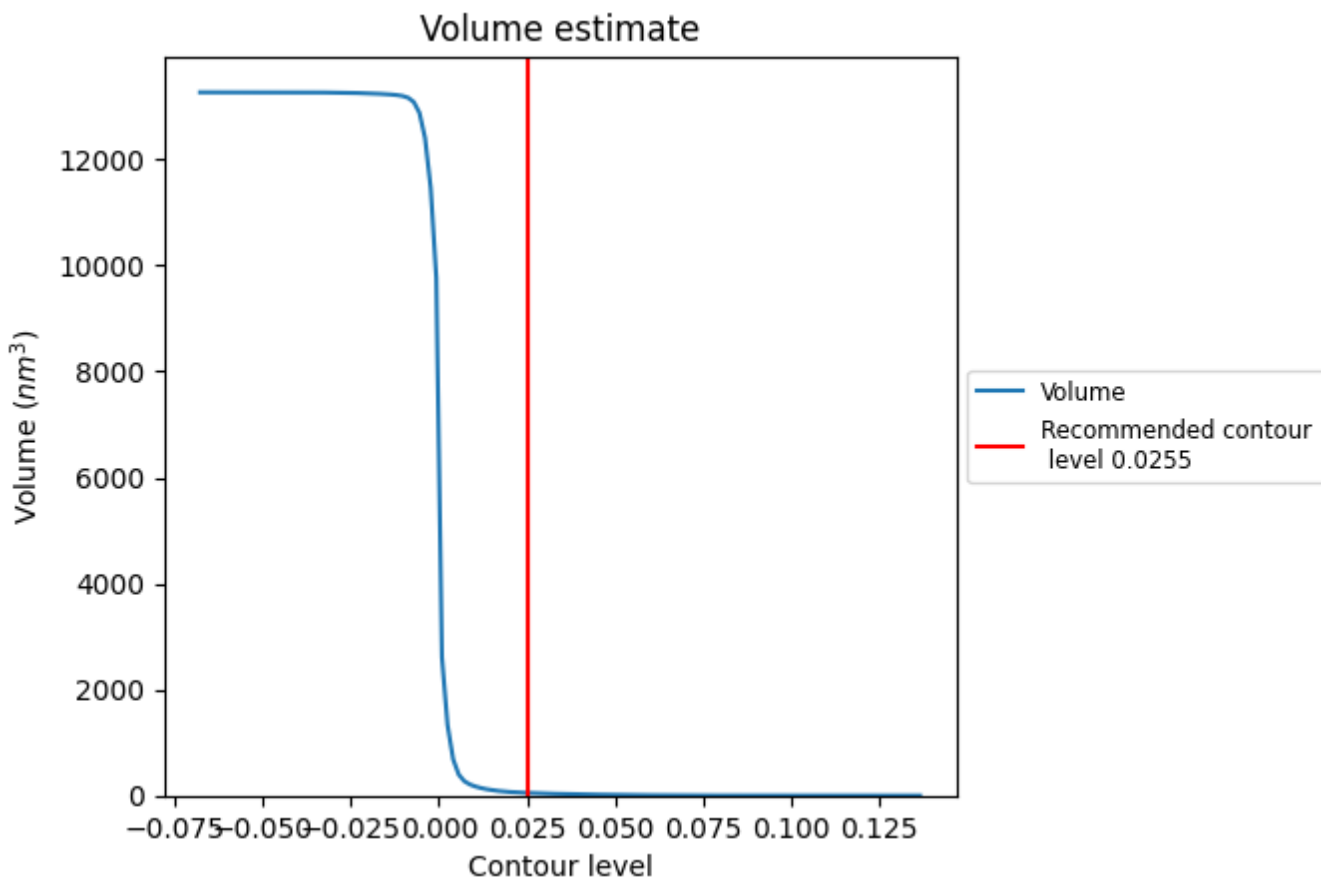
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

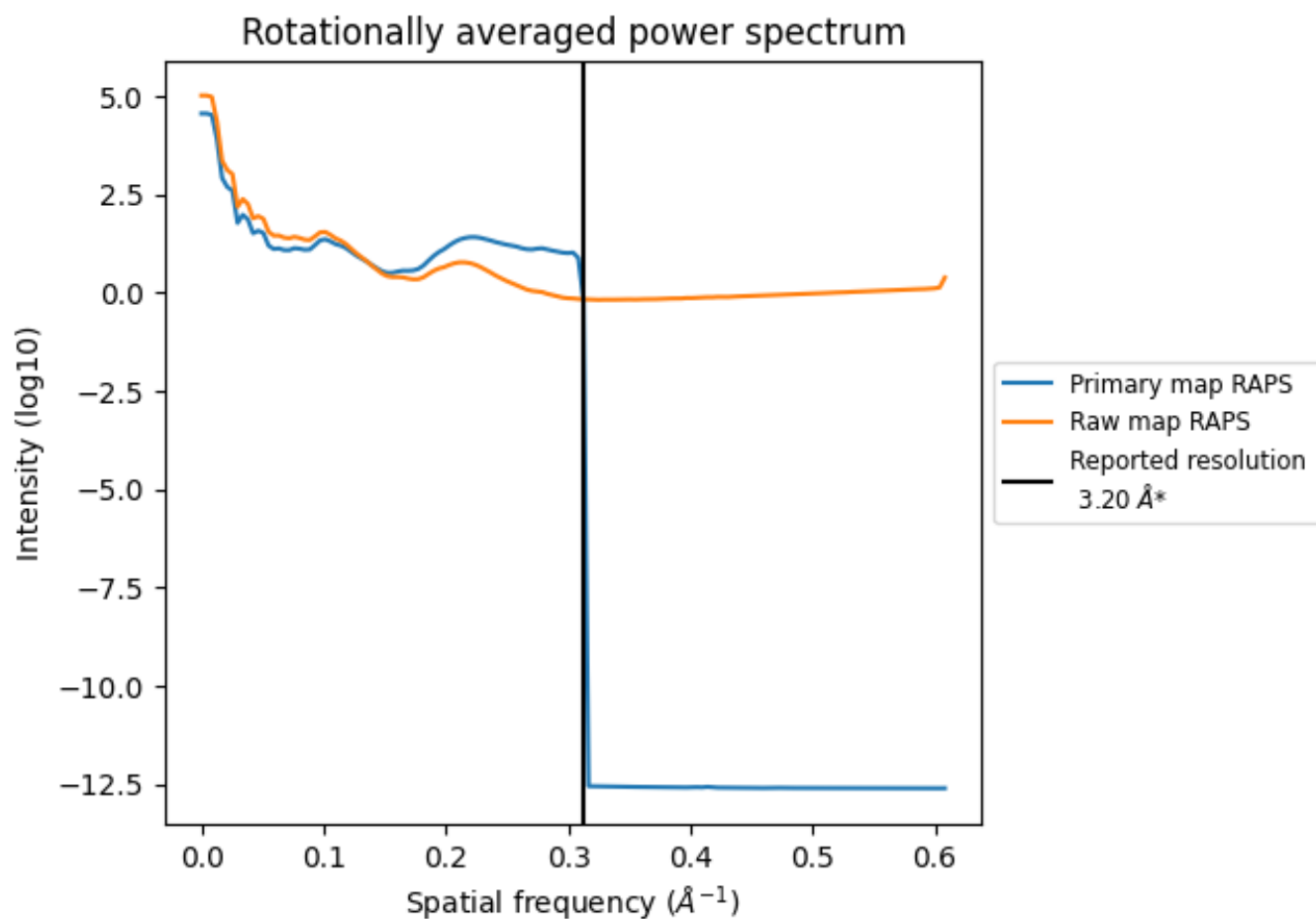
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 49 nm^3 ; this corresponds to an approximate mass of 44 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](#)

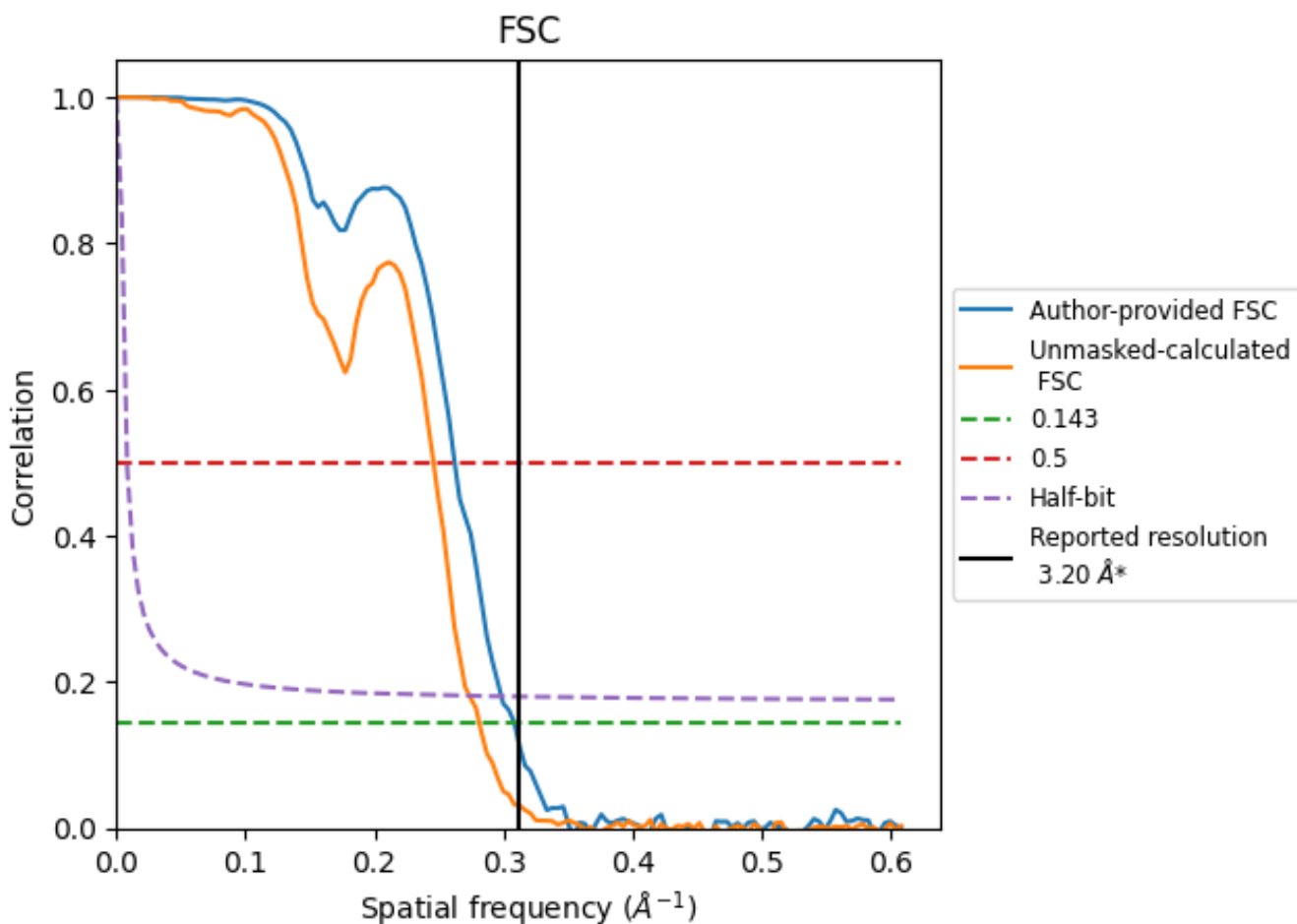


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [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 Å⁻¹

8.2 Resolution estimates [i](#)

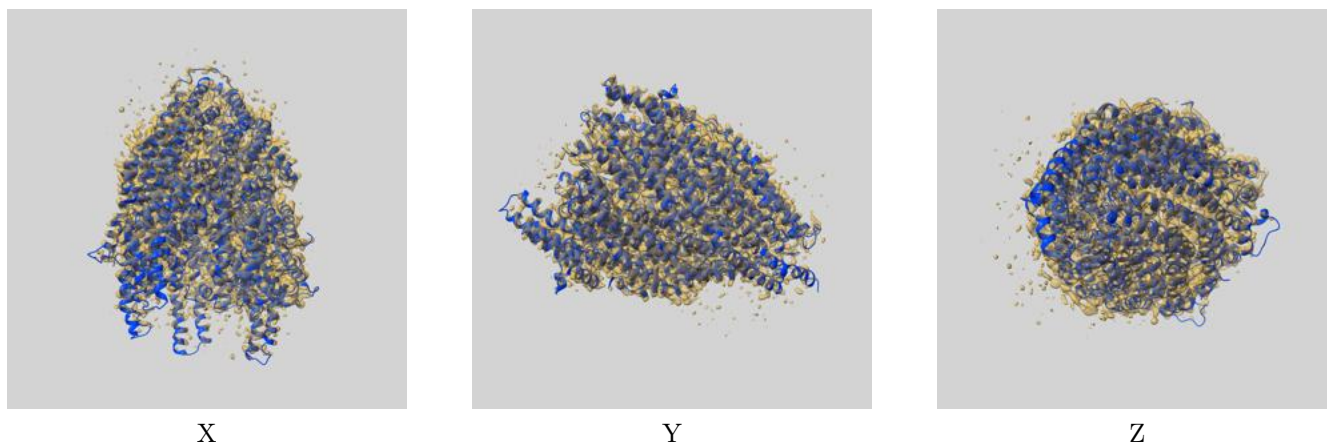
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.24	3.81	3.35
Unmasked-calculated*	3.55	4.07	3.65

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

9 Map-model fit [i](#)

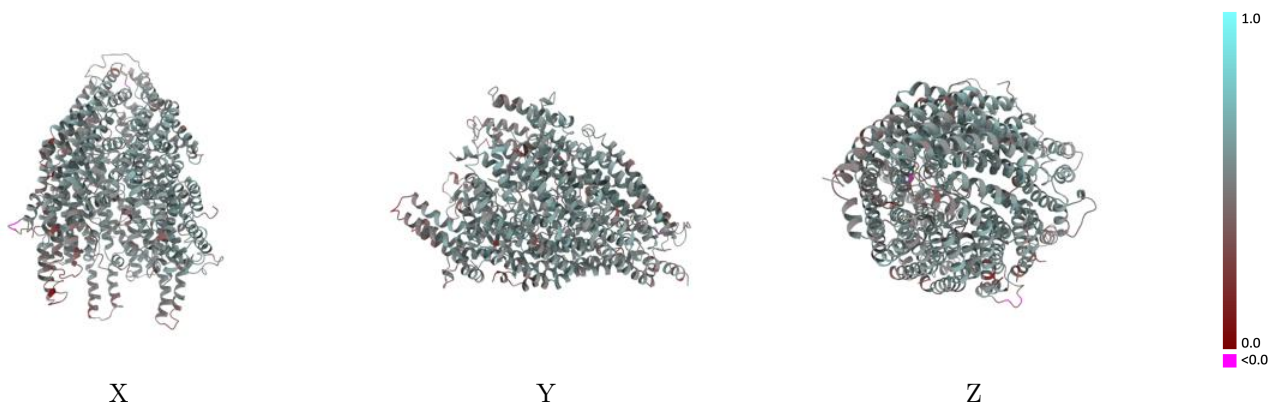
This section contains information regarding the fit between EMDB map EMD-10093 and PDB model 6S3L. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



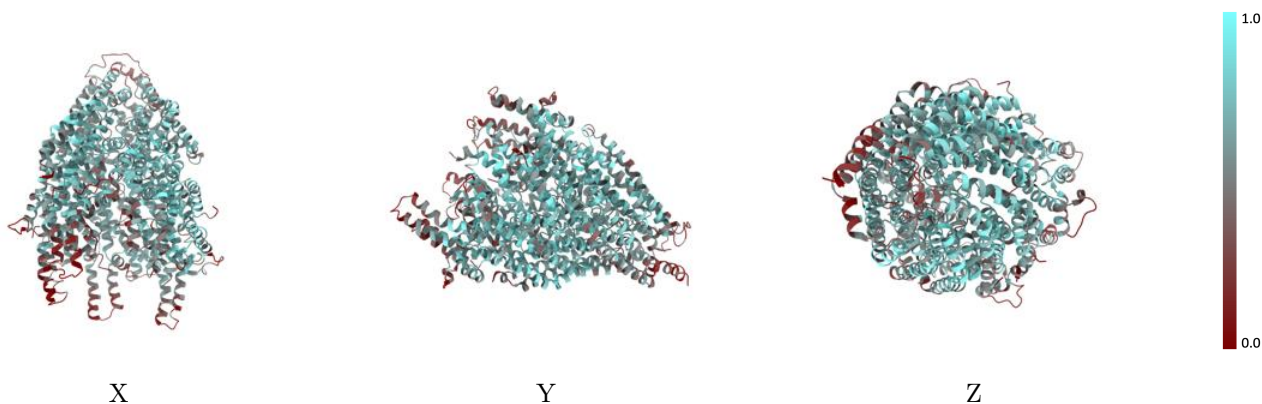
The images above show the 3D surface view of the map at the recommended contour level 0.0255 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



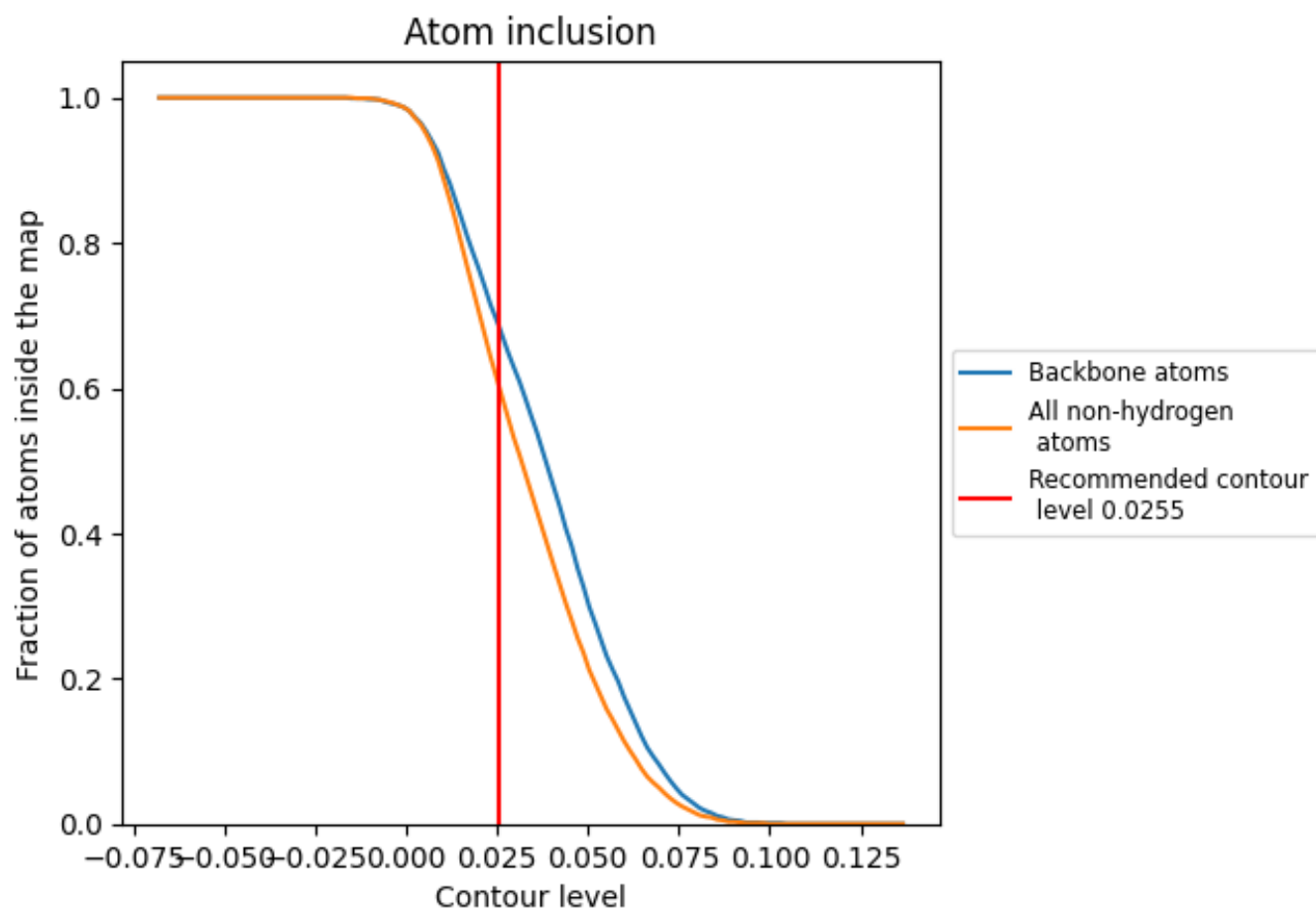
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0255).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0255) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6040	 0.5150
A	 0.6310	 0.5260
B	 0.5740	 0.5200
C	 0.5560	 0.5020
D	 0.5370	 0.4980
E	 0.6280	 0.5300
F	 0.7130	 0.5530
G	 0.6450	 0.4930
H	 0.6350	 0.5020
I	 0.6300	 0.4930
J	 0.5980	 0.4810
K	 0.5100	 0.5130

