



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 07:17 PM EDT

PDB ID : 8W22
EMDB ID : EMD-43737
Title : Umb1 umbrella toxin particle (local refinement of UmbB1 bound ALF of UmbC1 and UmbA1)
Authors : Park, Y.J.; Zhao, Q.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); DiMaio, F.; Mougous, J.D.; Veesler, D.
Deposited on : 2024-02-19
Resolution : 4.00 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

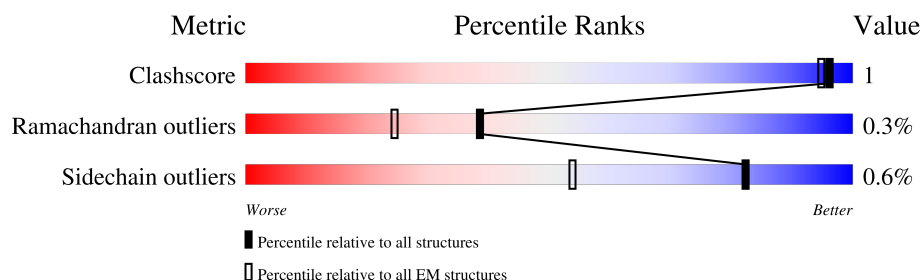
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1368	<div> <div>7%</div> <div>93%</div> </div>
2	B	166	<div> <div>74%</div> <div>25%</div> </div>
3	C	515	<div> <div>8%</div> <div>78%</div> <div>21%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3750 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 Intein C-terminal splicing domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	99	Total	C	N	O	S	0	0
			685	426	134	123	2		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9ACV2
A	2	ARG	-	expression tag	UNP Q9ACV2
A	3	ARG	-	expression tag	UNP Q9ACV2
A	4	ARG	-	expression tag	UNP Q9ACV2
A	5	ILE	-	expression tag	UNP Q9ACV2
A	6	PRO	-	expression tag	UNP Q9ACV2
A	7	SER	-	expression tag	UNP Q9ACV2
A	8	ARG	-	expression tag	UNP Q9ACV2
A	9	THR	-	expression tag	UNP Q9ACV2
A	10	PRO	-	expression tag	UNP Q9ACV2
A	11	GLY	-	expression tag	UNP Q9ACV2
A	12	SER	-	expression tag	UNP Q9ACV2
A	13	GLY	-	expression tag	UNP Q9ACV2
A	14	ALA	-	expression tag	UNP Q9ACV2
A	15	LYS	-	expression tag	UNP Q9ACV2
A	16	GLN	-	expression tag	UNP Q9ACV2
A	17	LYS	-	expression tag	UNP Q9ACV2
A	18	SER	-	expression tag	UNP Q9ACV2
A	19	TRP	-	expression tag	UNP Q9ACV2
A	20	PHE	-	expression tag	UNP Q9ACV2
A	21	PRO	-	expression tag	UNP Q9ACV2
A	22	ARG	-	expression tag	UNP Q9ACV2
A	23	ARG	-	expression tag	UNP Q9ACV2
A	24	SER	-	expression tag	UNP Q9ACV2
A	25	LEU	-	expression tag	UNP Q9ACV2
A	26	GLN	-	expression tag	UNP Q9ACV2
A	27	VAL	-	expression tag	UNP Q9ACV2
A	28	LEU	-	expression tag	UNP Q9ACV2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LEU	-	expression tag	UNP Q9ACV2
A	30	SER	-	expression tag	UNP Q9ACV2
A	31	ALA	-	expression tag	UNP Q9ACV2
A	32	GLY	-	expression tag	UNP Q9ACV2

- Molecule 2 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	125	Total	C	N	O	S	0	0
			805	517	143	139	6		

- Molecule 3 is a protein called Secreted esterase.

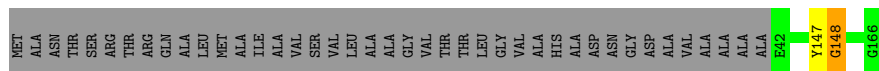
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	405	Total	C	N	O	S	0	0
			2260	1390	446	419	5		

There are 10 discrepancies between the modelled and reference sequences:

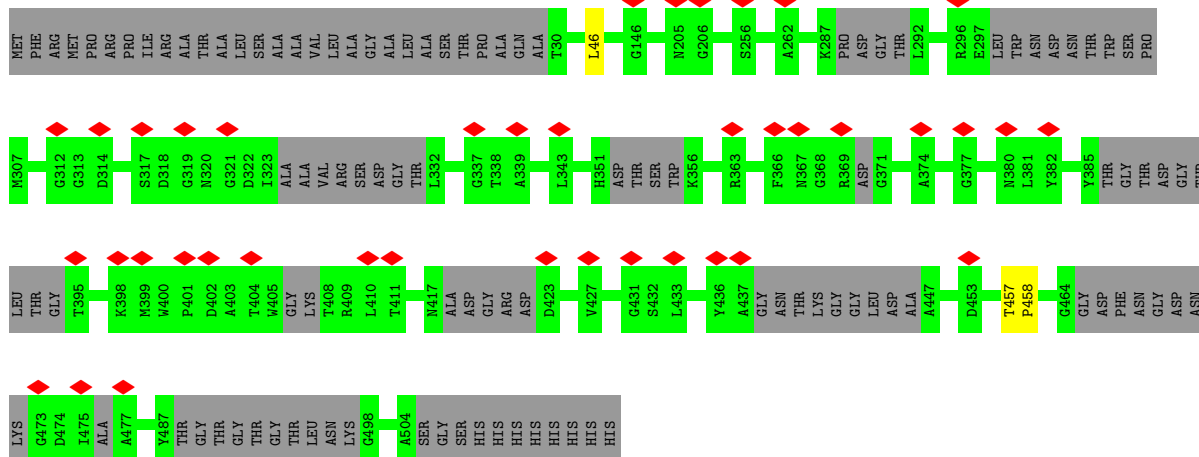
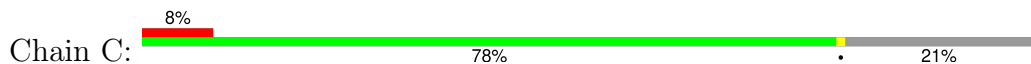
Chain	Residue	Modelled	Actual	Comment	Reference
C	506	GLY	-	expression tag	UNP Q9ACV4
C	507	SER	-	expression tag	UNP Q9ACV4
C	508	HIS	-	expression tag	UNP Q9ACV4
C	509	HIS	-	expression tag	UNP Q9ACV4
C	510	HIS	-	expression tag	UNP Q9ACV4
C	511	HIS	-	expression tag	UNP Q9ACV4
C	512	HIS	-	expression tag	UNP Q9ACV4
C	513	HIS	-	expression tag	UNP Q9ACV4
C	514	HIS	-	expression tag	UNP Q9ACV4
C	515	HIS	-	expression tag	UNP Q9ACV4

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

- Molecule 2: Secreted protein



- Molecule 3: Secreted esterase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	386275	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.149	Depositor
Minimum map value	-6.592	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.9	Depositor
Map size (\AA)	512.544, 512.544, 512.544	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.686, 1.686, 1.686	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	0.59	0/692	0.48	0/936
2	B	0.46	0/822	0.53	0/1126
3	C	0.39	0/2282	0.48	0/3133
All	All	0.45	0/3796	0.49	0/5195

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	685	0	637	2	0
2	B	805	0	678	1	0
3	C	2260	0	1487	2	0
All	All	3750	0	2802	5	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 1.

All (5) 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:A:140:GLU:N	1:A:141:PRO:CD	2.66	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:TYR:O	2:B:148:GLY:C	2.50	0.49
3:C:457:THR:N	3:C:458:PRO:CD	2.78	0.47
3:C:457:THR:N	3:C:458:PRO:HD2	2.35	0.41
1:A:140:GLU:N	1:A:141:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/1368 (7%)	94 (97%)	2 (2%)	1 (1%)	13	47
2	B	123/166 (74%)	115 (94%)	7 (6%)	1 (1%)	16	53
3	C	379/515 (74%)	371 (98%)	8 (2%)	0	100	100
All	All	599/2049 (29%)	580 (97%)	17 (3%)	2 (0%)	38	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	148	GLY
1	A	121	ASP

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	53/961 (6%)	53 (100%)	0	100	100
2	B	53/123 (43%)	53 (100%)	0	100	100
3	C	74/395 (19%)	73 (99%)	1 (1%)	62	75
All	All	180/1479 (12%)	179 (99%)	1 (1%)	82	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

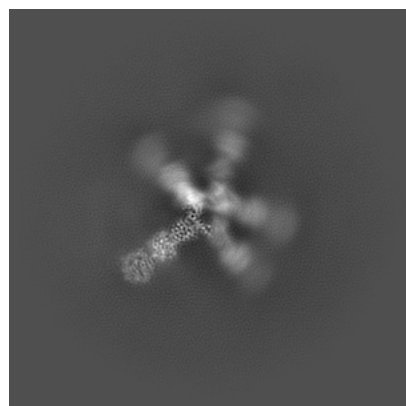
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43737. These allow visual inspection of the internal detail of the map and identification of artifacts.

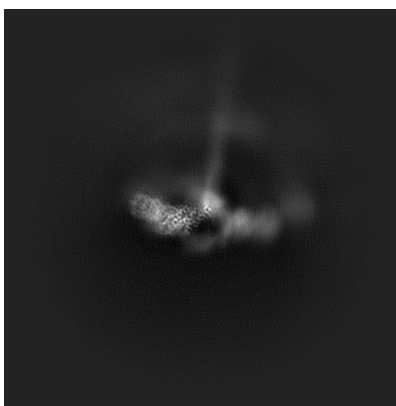
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

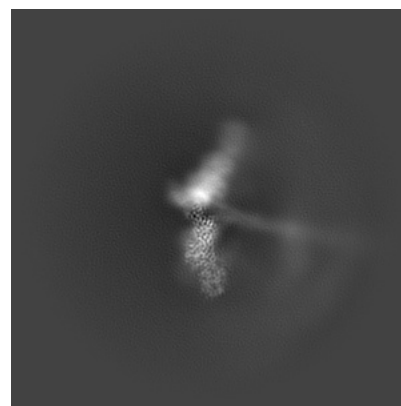
6.1.1 Primary map



X

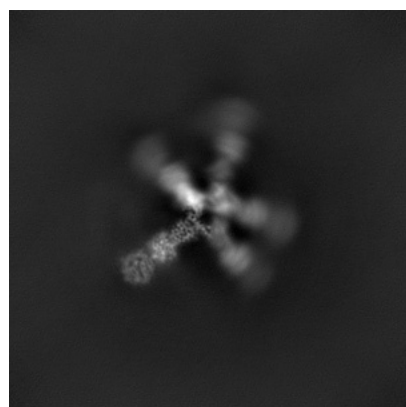


Y

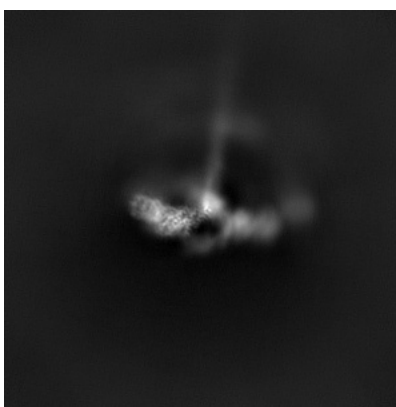


Z

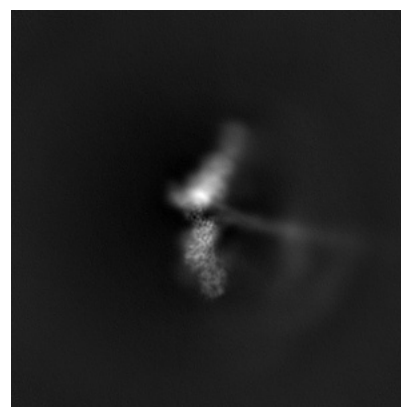
6.1.2 Raw map



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: 152

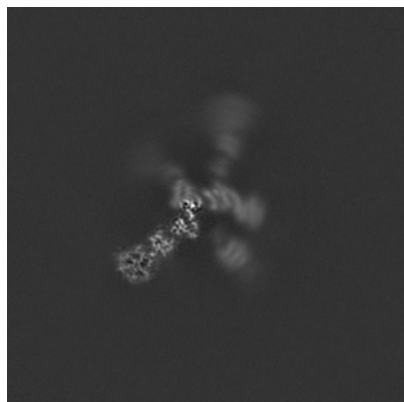


Y Index: 152

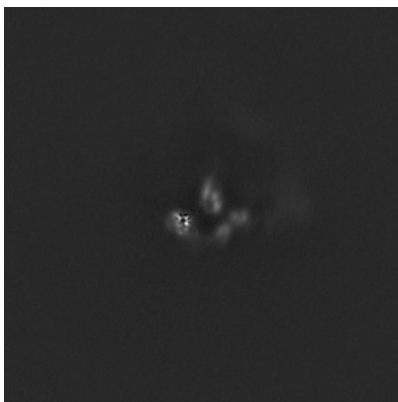


Z Index: 152

6.2.2 Raw map



X Index: 152



Y Index: 152

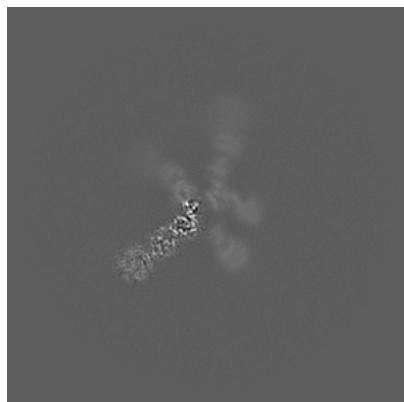


Z Index: 152

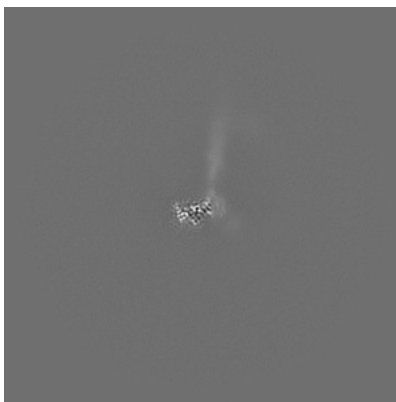
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

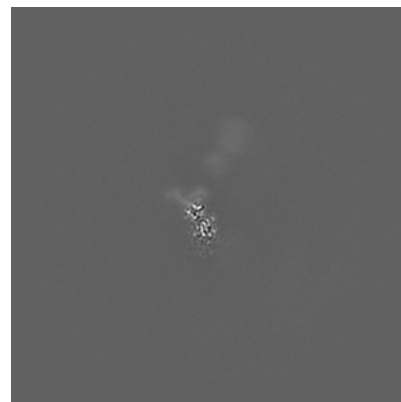
6.3.1 Primary map



X Index: 149

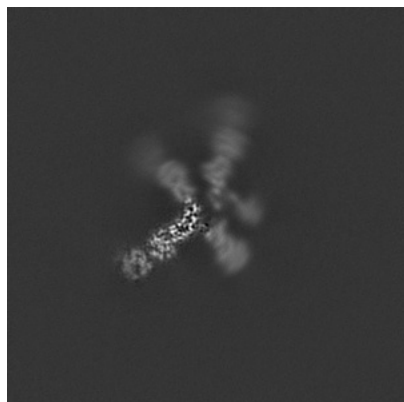


Y Index: 139

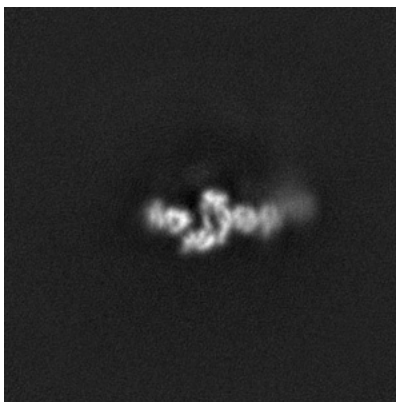


Z Index: 138

6.3.2 Raw map



X Index: 146



Y Index: 162

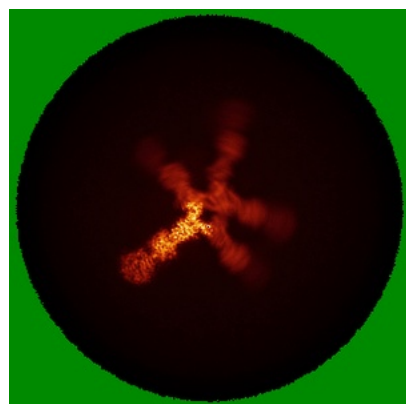


Z Index: 154

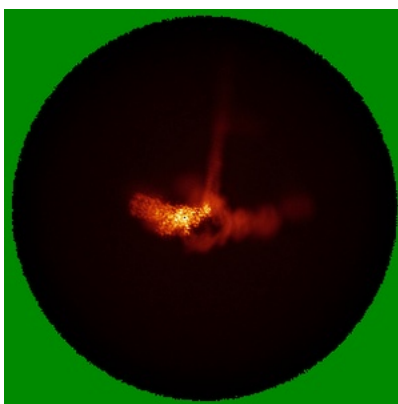
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

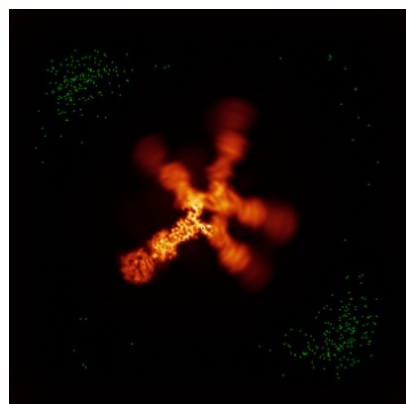


Y

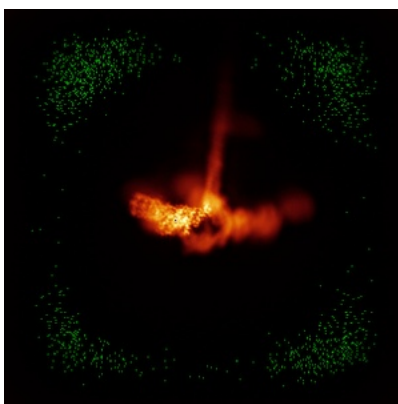


Z

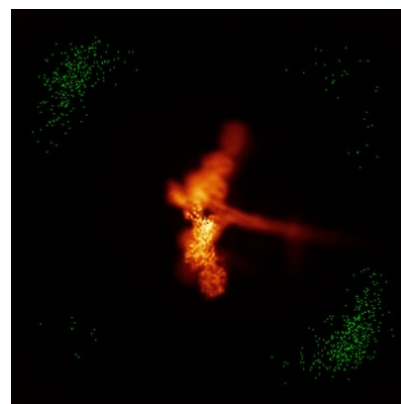
6.4.2 Raw map



X



Y

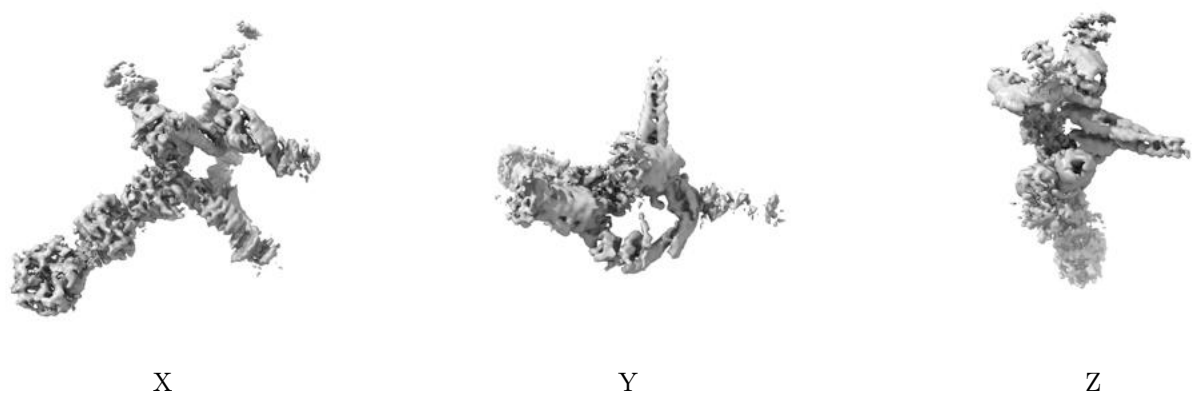


Z

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.

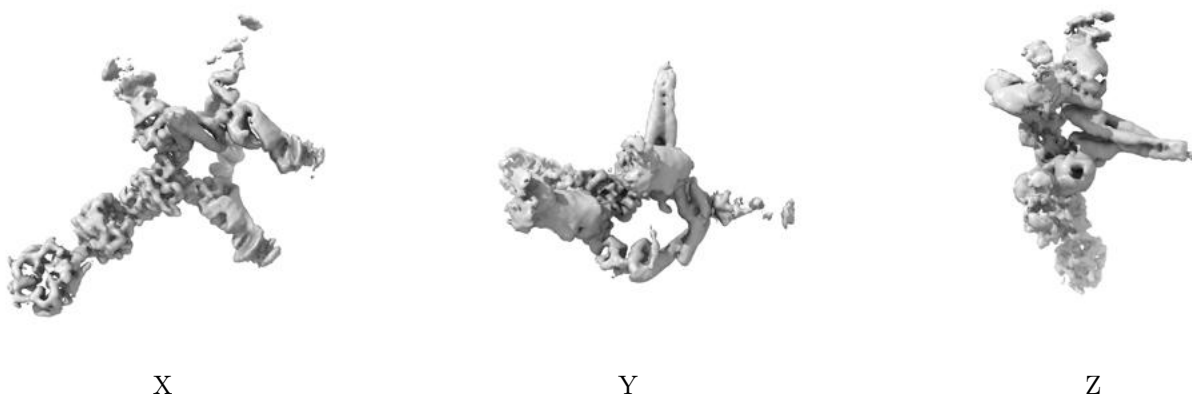
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

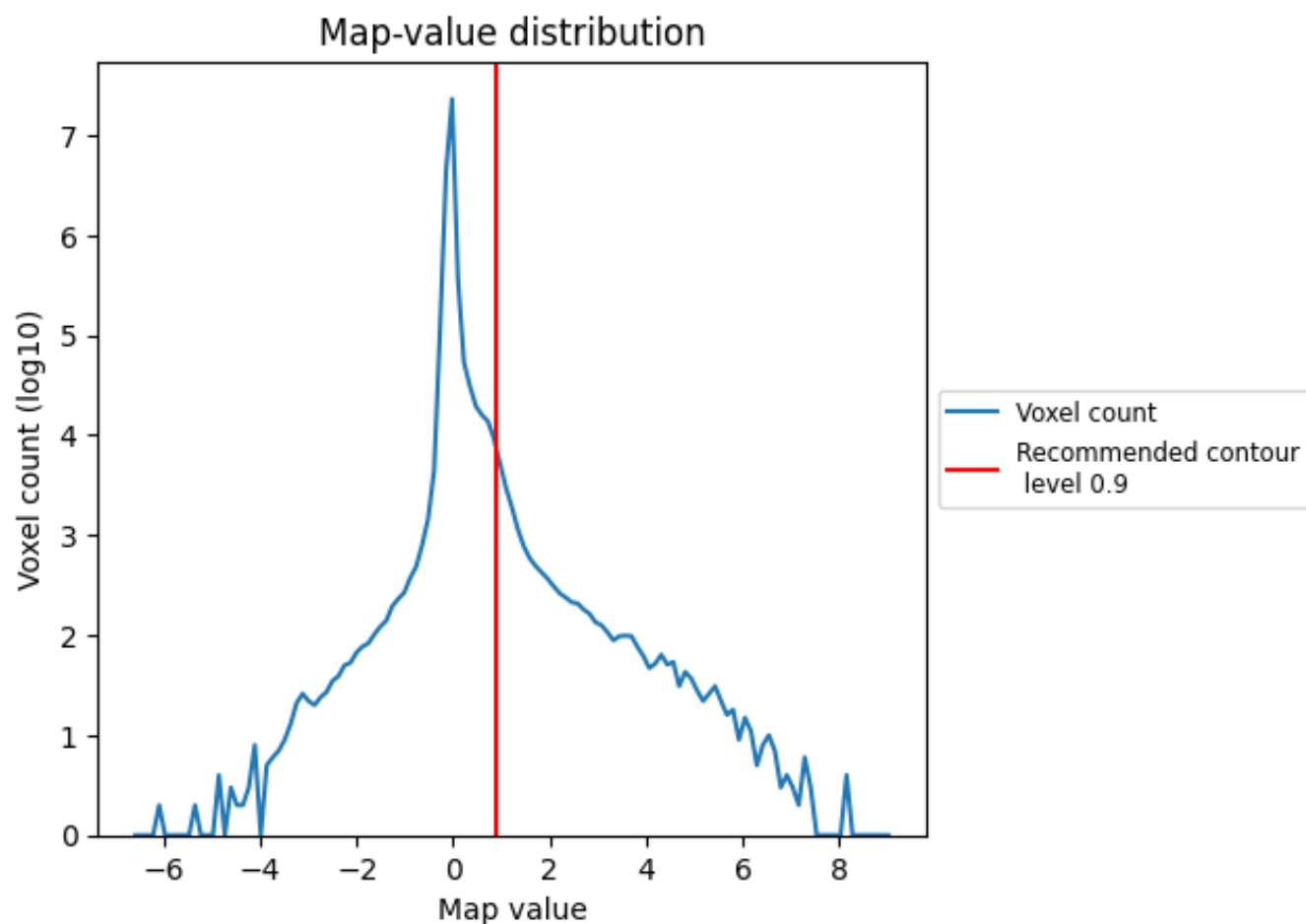
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

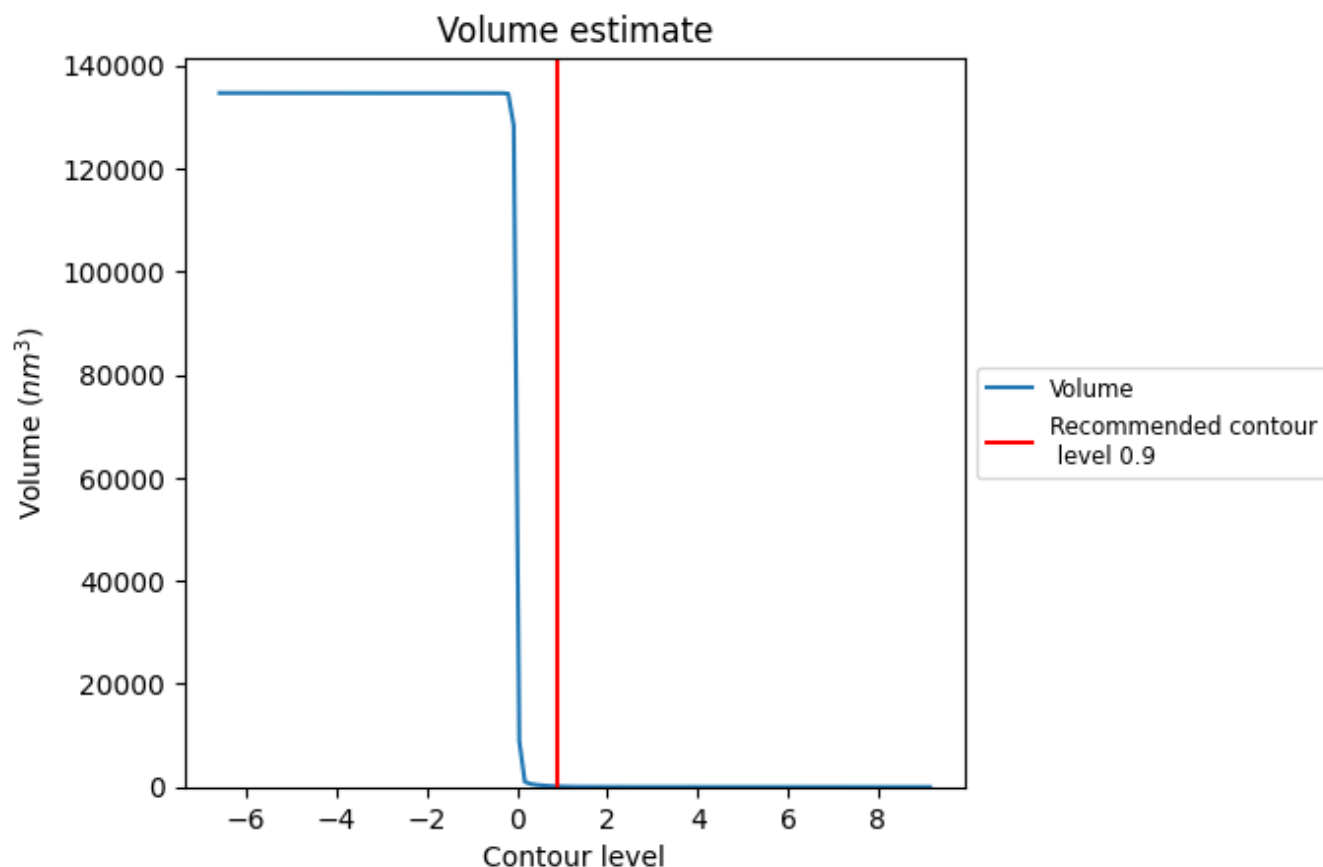
This section contains the results of statistical analysis of the map.

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.

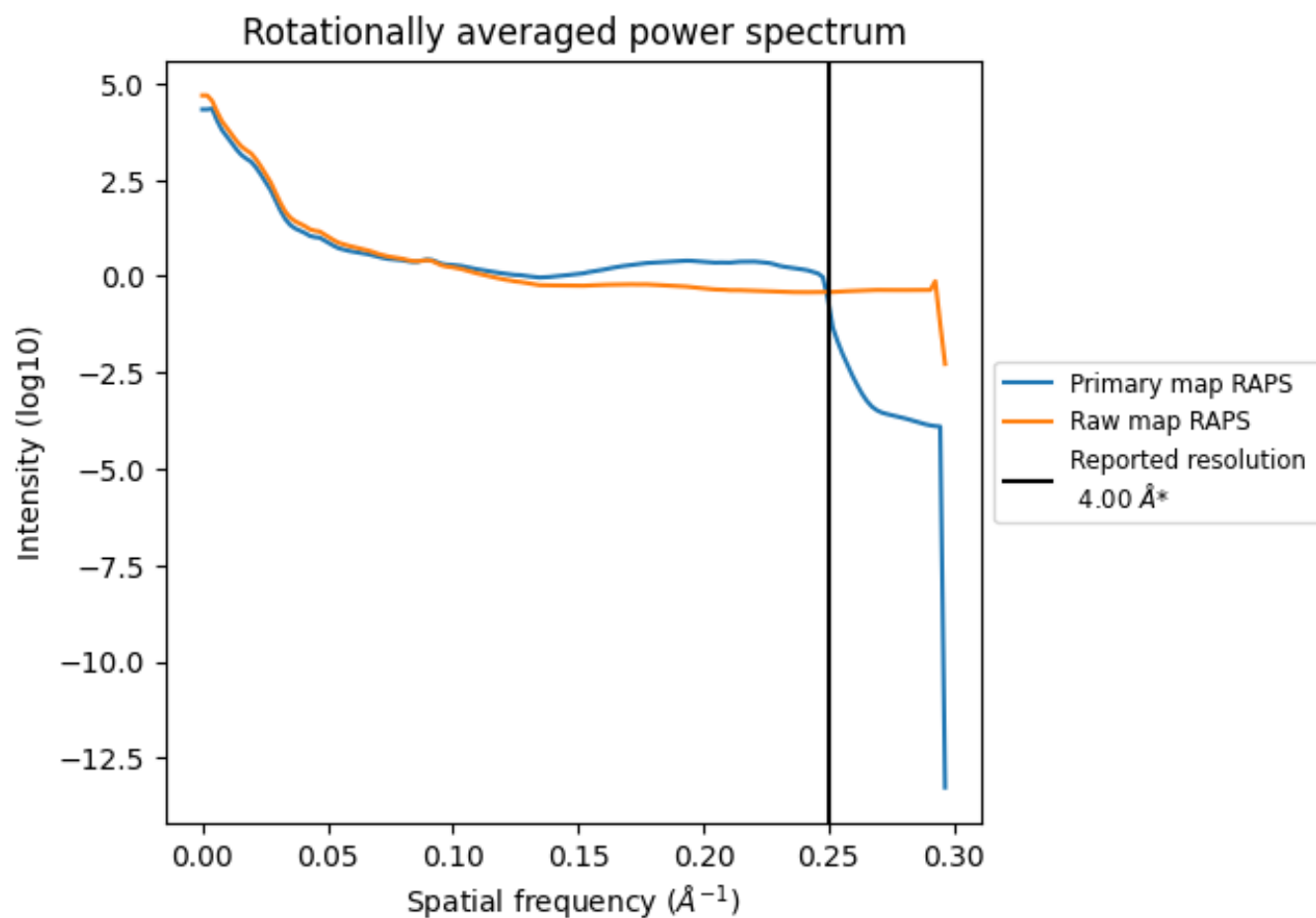
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm^3 ; this corresponds to an approximate mass of 95 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 ⓘ

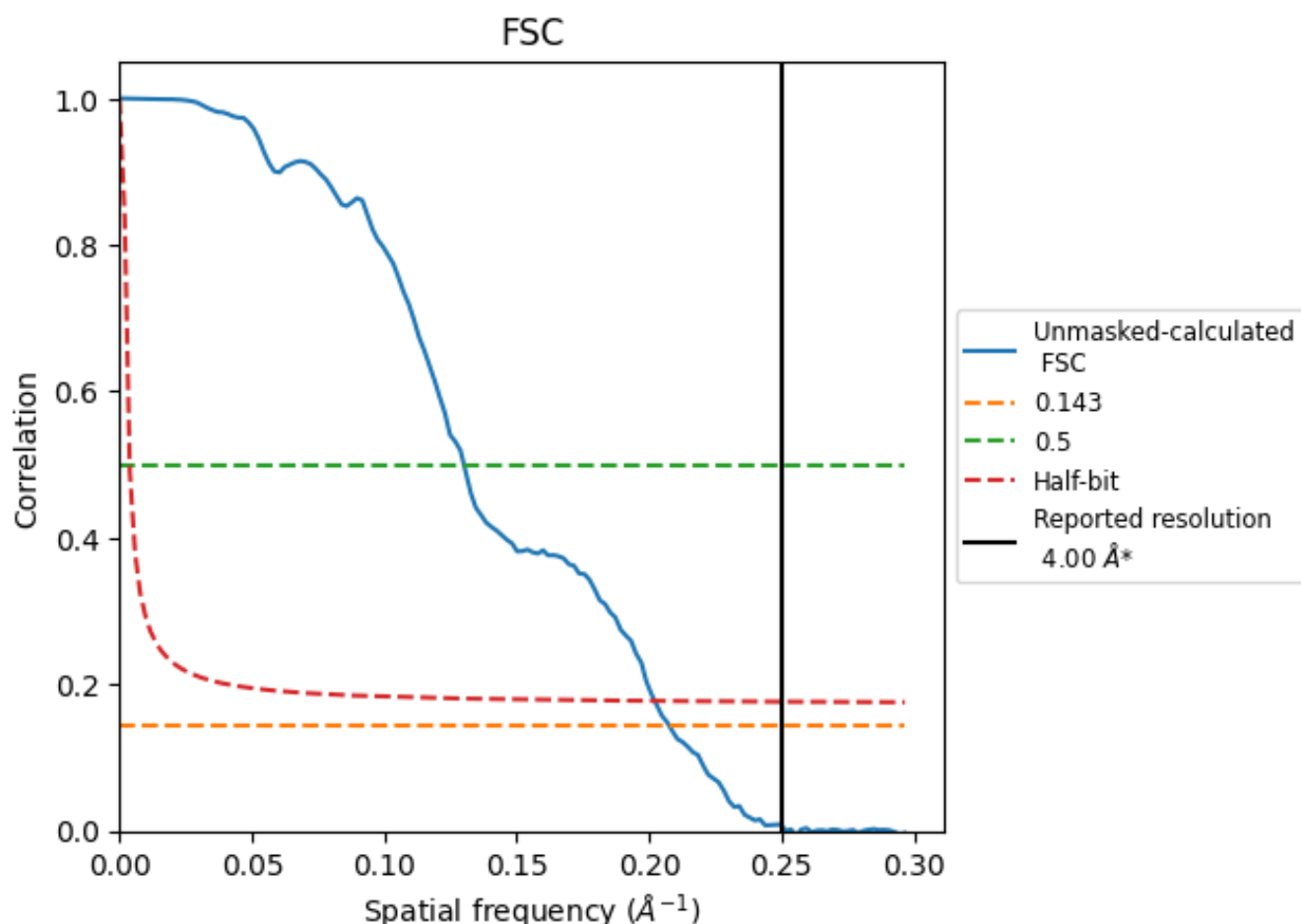


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

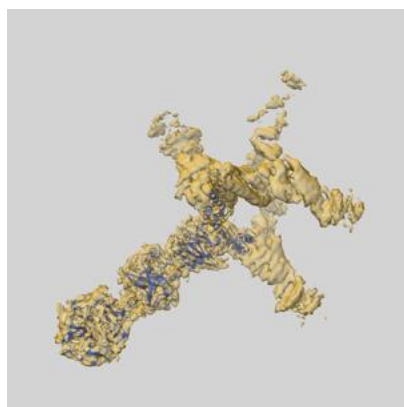
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.81	7.69	4.95

*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 4.81 differs from the reported value 4.0 by more than 10 %

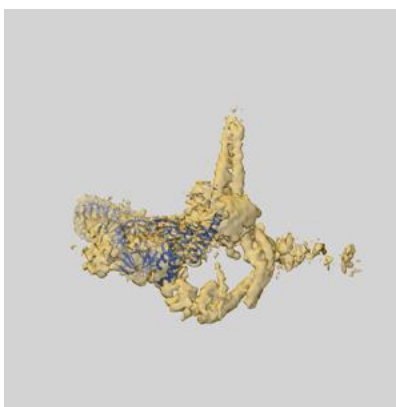
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43737 and PDB model 8W22. Per-residue inclusion information can be found in section [3](#) on page [5](#).

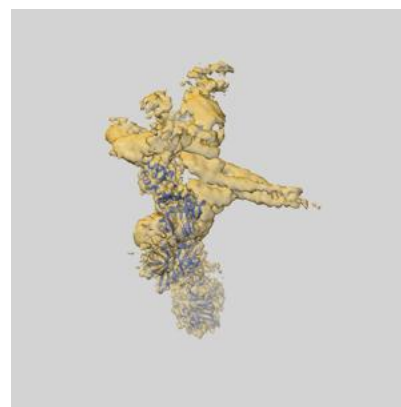
9.1 Map-model overlay [i](#)



X



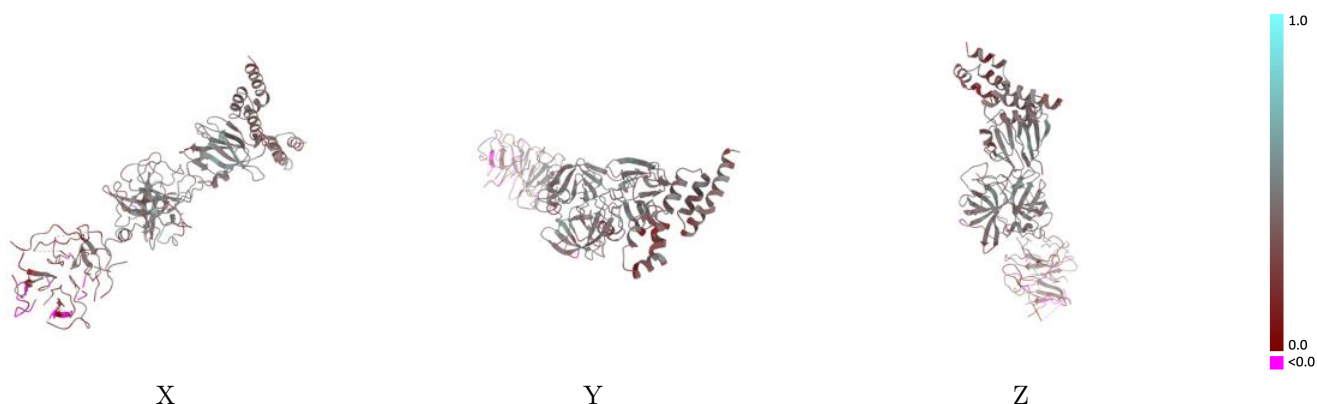
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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](#)



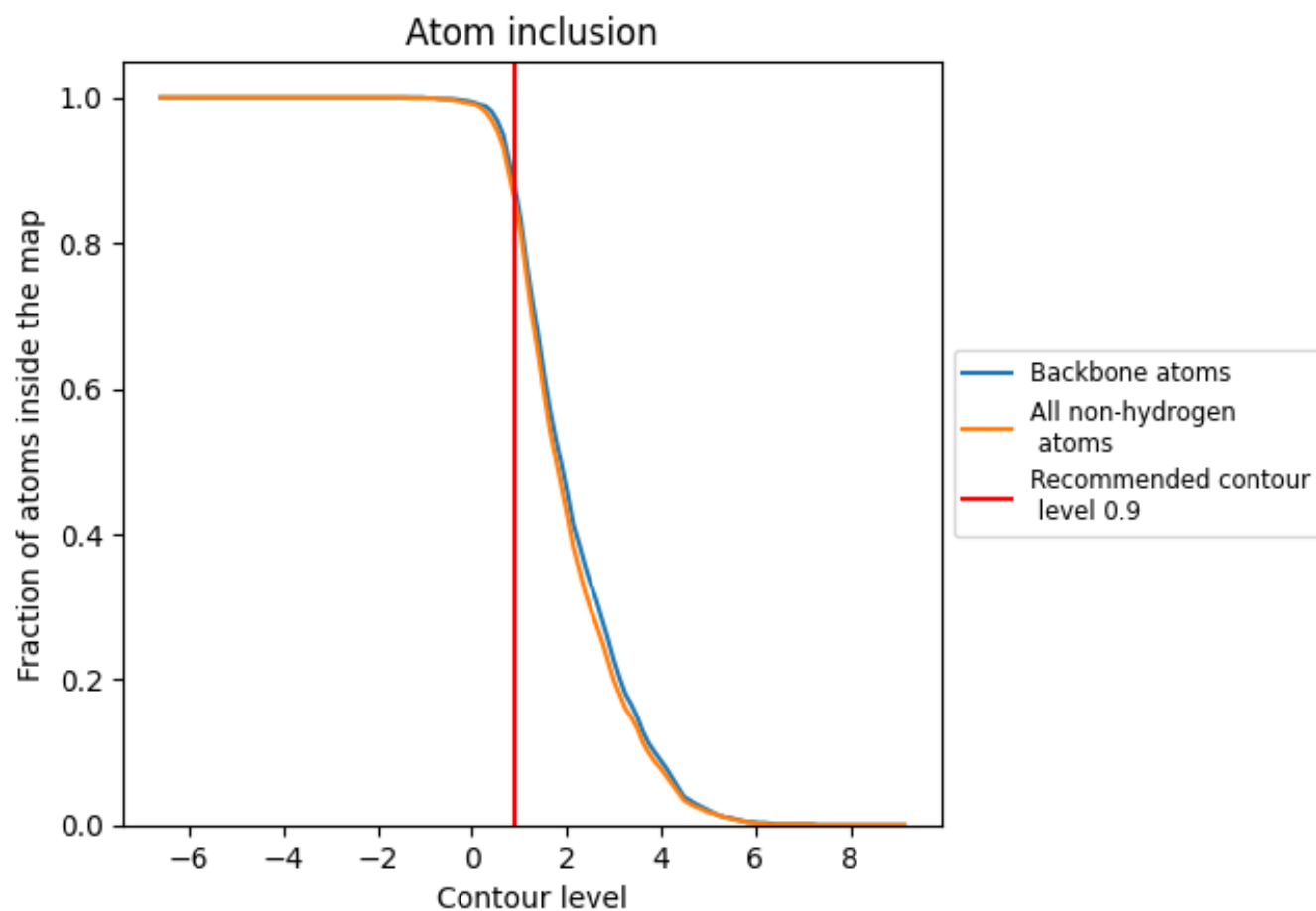
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8610	<div><div></div></div> 0.3860
A	<div><div></div></div> 0.8920	<div><div></div></div> 0.3750
B	<div><div></div></div> 0.9270	<div><div></div></div> 0.4470
C	<div><div></div></div> 0.8280	<div><div></div></div> 0.3670

