



Full wwPDB EM Validation Report ⓘ

Jun 6, 2024 – 04:12 pm BST

PDB ID : 8QPF
EMDB ID : EMD-18549
Title : Ammonium Transporter Amt1 from *Shewanella denitrificans*
Authors : Gschell, M.; Zhang, L.; Einsle, O.; Andrade, S.
Deposited on : 2023-10-01
Resolution : 2.53 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.dev92
MolProbity : **FAILED**
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 2.53 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 9085 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 Ammonium transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	389	2961	1950	478	514	19	0	0
1	B	389	2961	1950	478	514	19	0	0
1	C	389	2961	1950	478	514	19	0	0

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	LEU	-	expression tag	UNP Q12R70
A	646	ASP	-	expression tag	UNP Q12R70
A	647	GLU	-	expression tag	UNP Q12R70
A	648	ASN	-	expression tag	UNP Q12R70
A	649	LEU	-	expression tag	UNP Q12R70
A	650	TYR	-	expression tag	UNP Q12R70
A	651	PHE	-	expression tag	UNP Q12R70
A	652	GLN	-	expression tag	UNP Q12R70
A	653	GLY	-	expression tag	UNP Q12R70
A	654	PHE	-	expression tag	UNP Q12R70
A	655	GLU	-	expression tag	UNP Q12R70
A	656	HIS	-	expression tag	UNP Q12R70
A	657	HIS	-	expression tag	UNP Q12R70
A	658	HIS	-	expression tag	UNP Q12R70
A	659	HIS	-	expression tag	UNP Q12R70
A	660	HIS	-	expression tag	UNP Q12R70
A	661	HIS	-	expression tag	UNP Q12R70
B	645	LEU	-	expression tag	UNP Q12R70
B	646	ASP	-	expression tag	UNP Q12R70
B	647	GLU	-	expression tag	UNP Q12R70
B	648	ASN	-	expression tag	UNP Q12R70
B	649	LEU	-	expression tag	UNP Q12R70
B	650	TYR	-	expression tag	UNP Q12R70
B	651	PHE	-	expression tag	UNP Q12R70

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Chain	Residue	Modelled	Actual	Comment	Reference
B	652	GLN	-	expression tag	UNP Q12R70
B	653	GLY	-	expression tag	UNP Q12R70
B	654	PHE	-	expression tag	UNP Q12R70
B	655	GLU	-	expression tag	UNP Q12R70
B	656	HIS	-	expression tag	UNP Q12R70
B	657	HIS	-	expression tag	UNP Q12R70
B	658	HIS	-	expression tag	UNP Q12R70
B	659	HIS	-	expression tag	UNP Q12R70
B	660	HIS	-	expression tag	UNP Q12R70
B	661	HIS	-	expression tag	UNP Q12R70
C	645	LEU	-	expression tag	UNP Q12R70
C	646	ASP	-	expression tag	UNP Q12R70
C	647	GLU	-	expression tag	UNP Q12R70
C	648	ASN	-	expression tag	UNP Q12R70
C	649	LEU	-	expression tag	UNP Q12R70
C	650	TYR	-	expression tag	UNP Q12R70
C	651	PHE	-	expression tag	UNP Q12R70
C	652	GLN	-	expression tag	UNP Q12R70
C	653	GLY	-	expression tag	UNP Q12R70
C	654	PHE	-	expression tag	UNP Q12R70
C	655	GLU	-	expression tag	UNP Q12R70
C	656	HIS	-	expression tag	UNP Q12R70
C	657	HIS	-	expression tag	UNP Q12R70
C	658	HIS	-	expression tag	UNP Q12R70
C	659	HIS	-	expression tag	UNP Q12R70
C	660	HIS	-	expression tag	UNP Q12R70
C	661	HIS	-	expression tag	UNP Q12R70

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	AltConf
2	A	66	Total O 66 66	0
2	B	70	Total O 70 70	0
2	C	66	Total O 66 66	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	477507	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.466	Depositor
Minimum map value	-0.275	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	168.0, 168.0, 168.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84, 0.84, 0.84	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

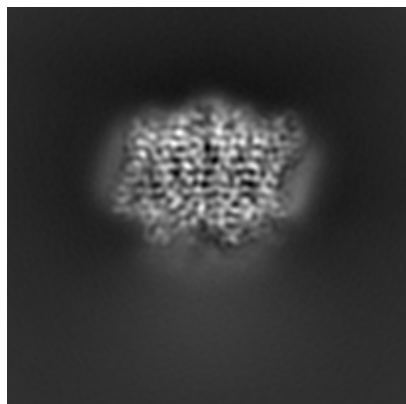
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18549. These allow visual inspection of the internal detail of the map and identification of artifacts.

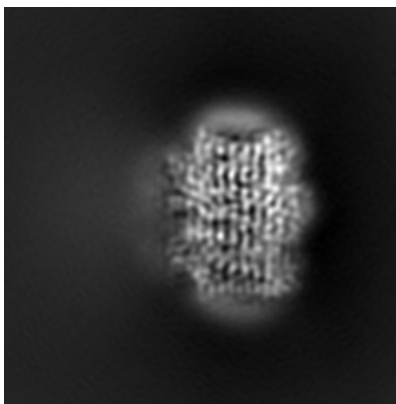
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

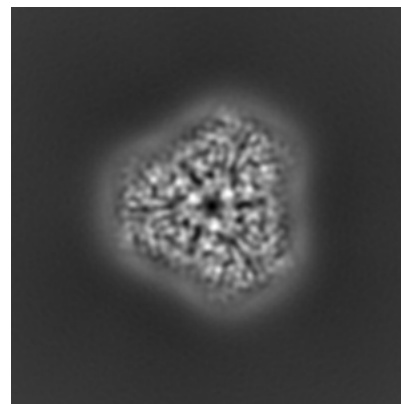
5.1.1 Primary map



X

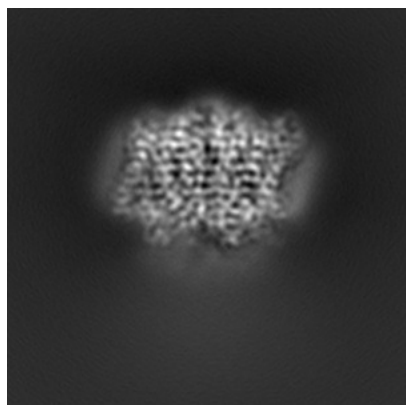


Y

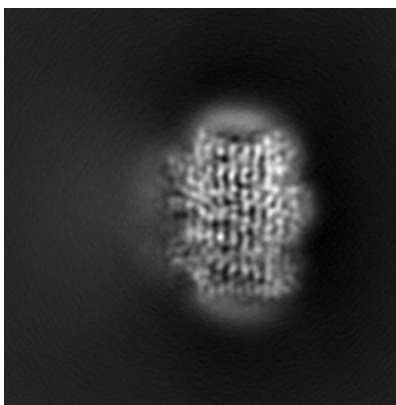


Z

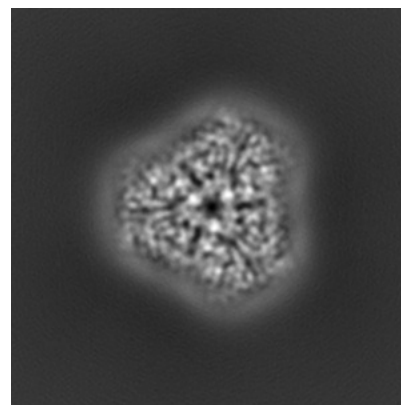
5.1.2 Raw map



X



Y

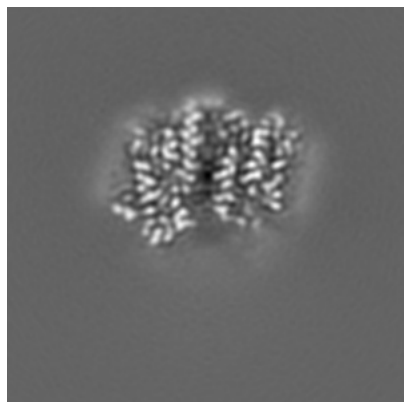


Z

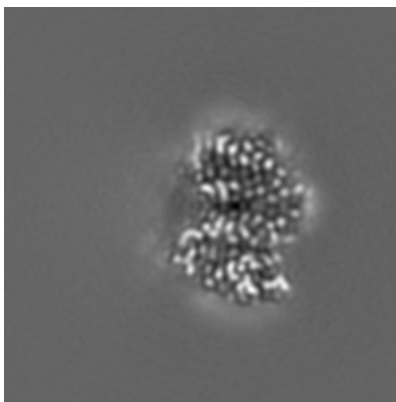
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

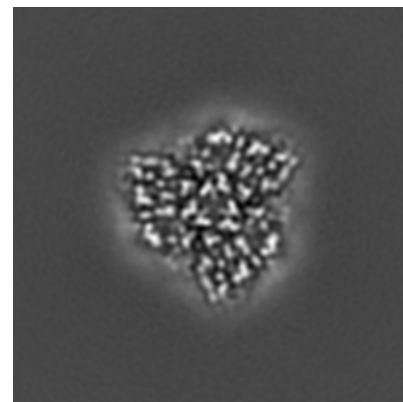
5.2.1 Primary map



X Index: 100

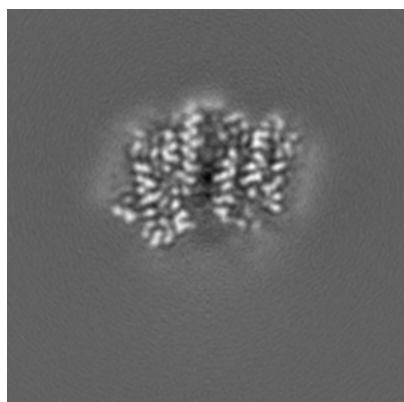


Y Index: 100

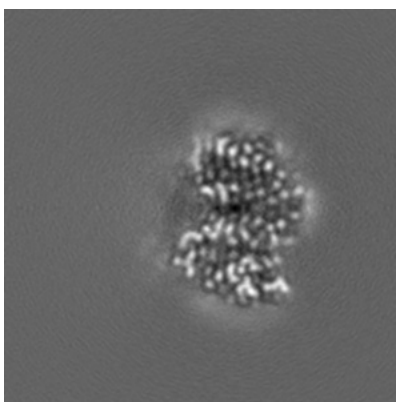


Z Index: 100

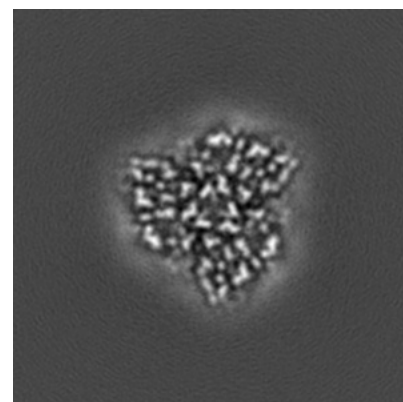
5.2.2 Raw map



X Index: 100



Y Index: 100

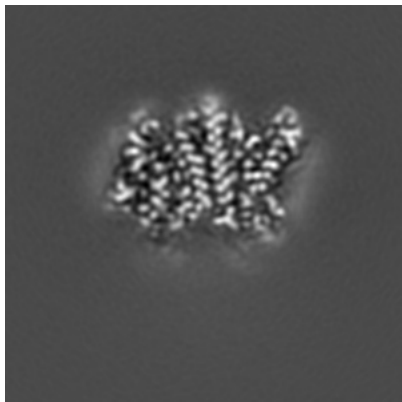


Z Index: 100

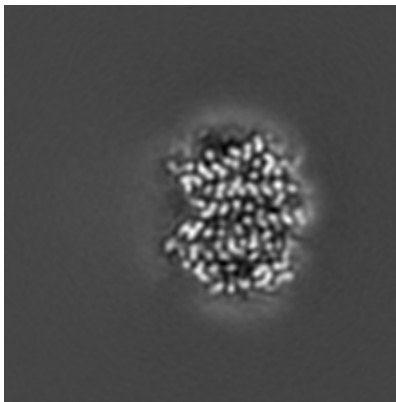
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

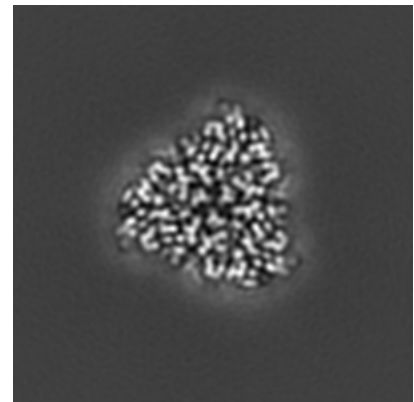
5.3.1 Primary map



X Index: 108

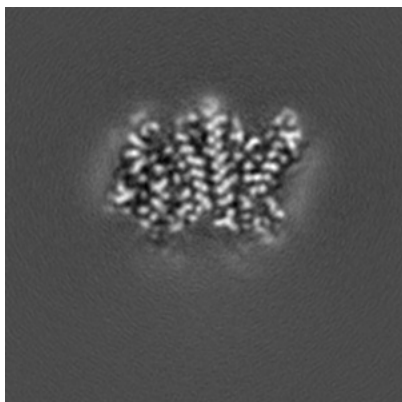


Y Index: 107

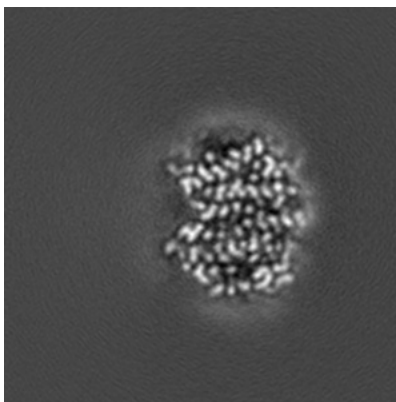


Z Index: 132

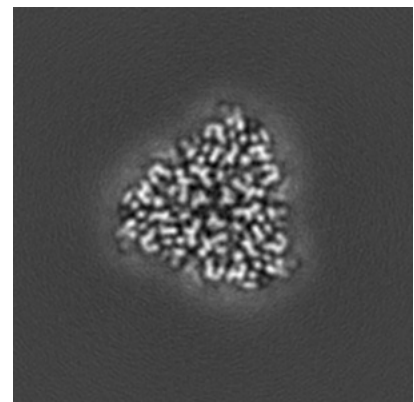
5.3.2 Raw map



X Index: 108



Y Index: 107

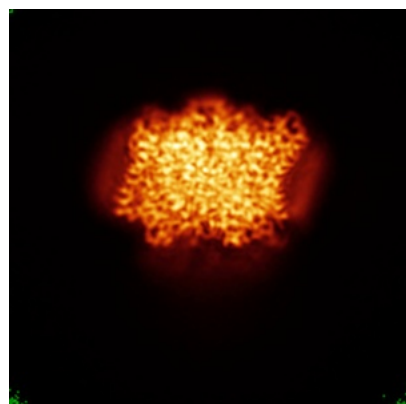


Z Index: 132

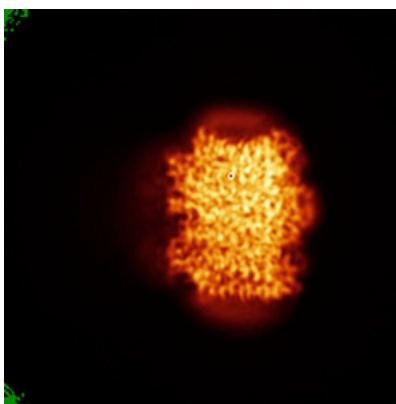
The images above show the largest variance slices of the map in three orthogonal directions.

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

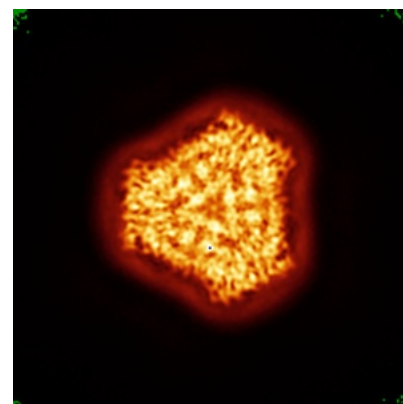
5.4.1 Primary map



X

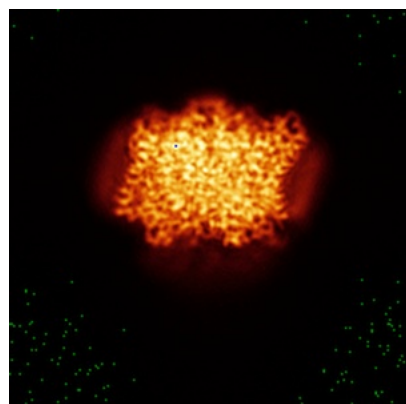


Y

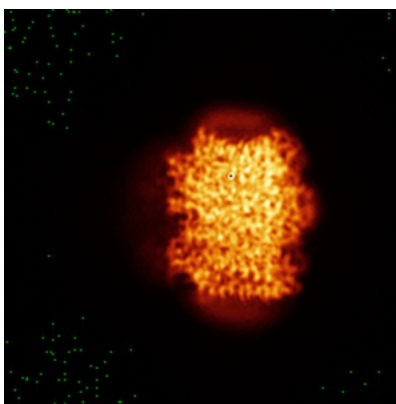


Z

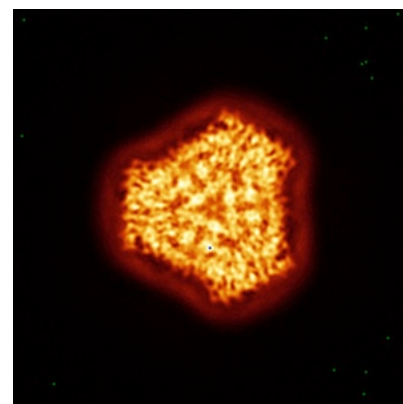
5.4.2 Raw map



X



Y

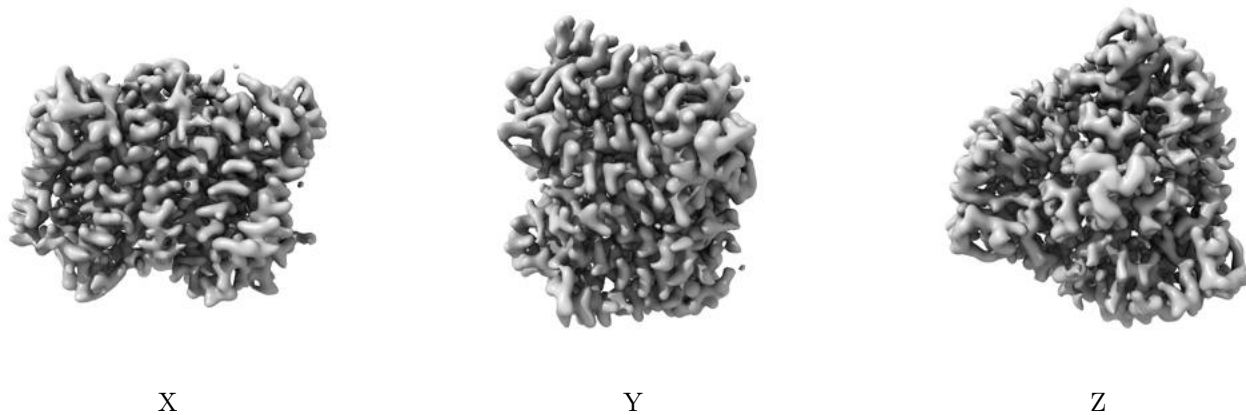


Z

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.

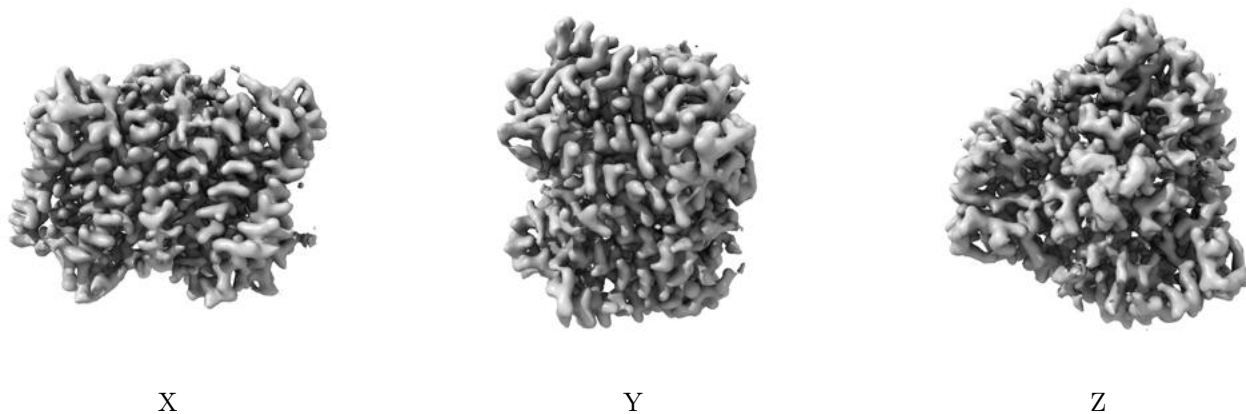
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

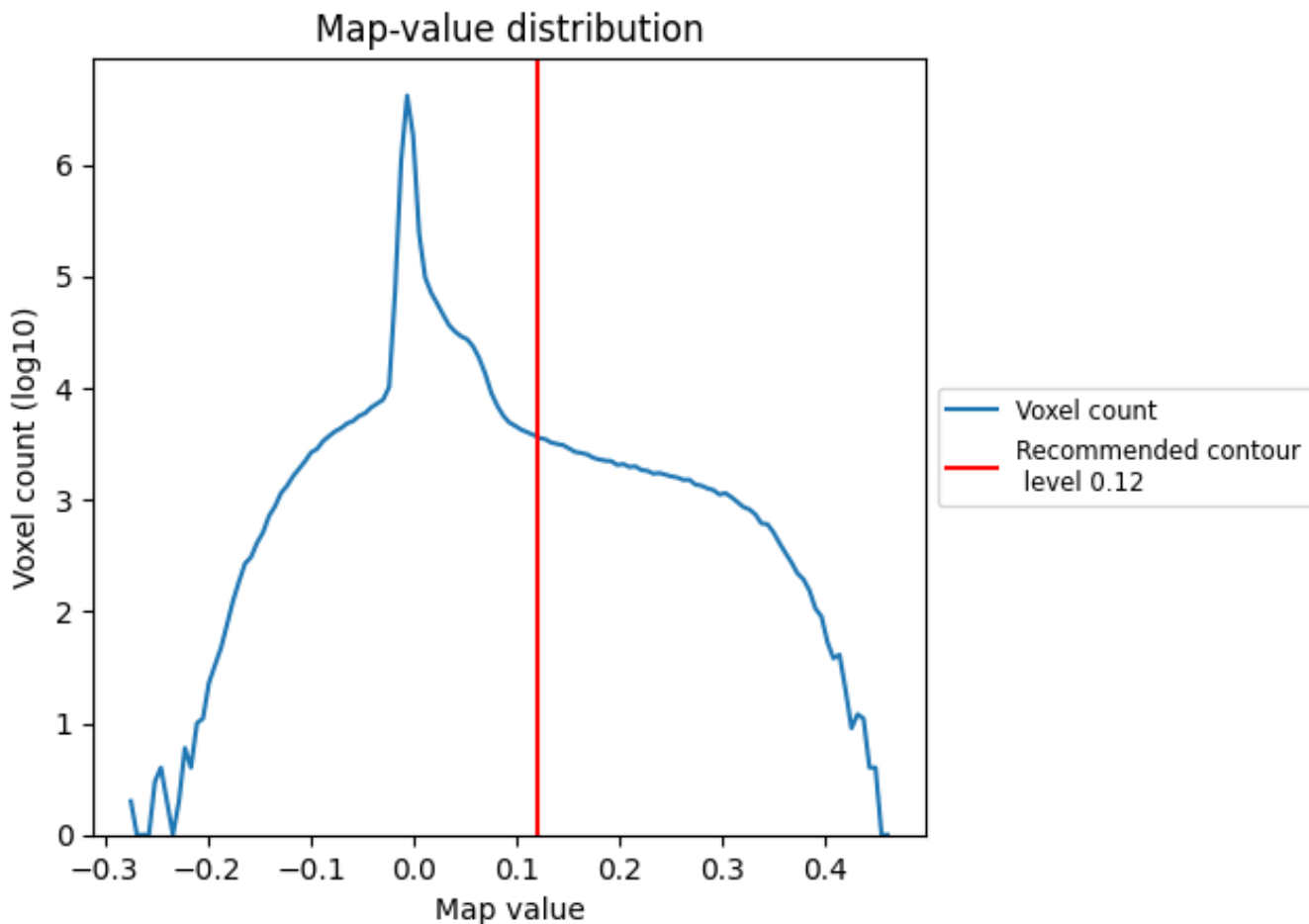
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

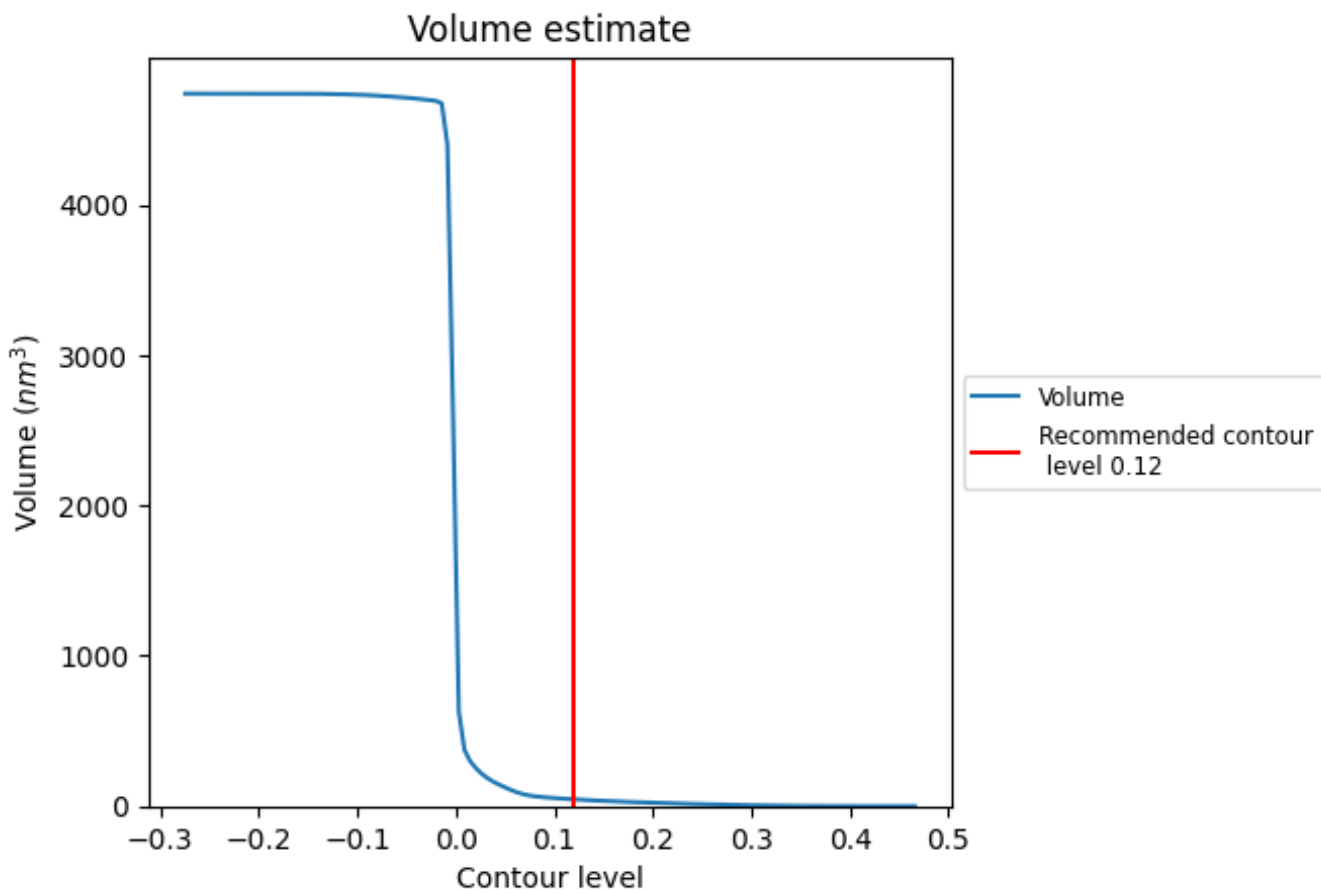
This section contains the results of statistical analysis of the map.

6.1 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.

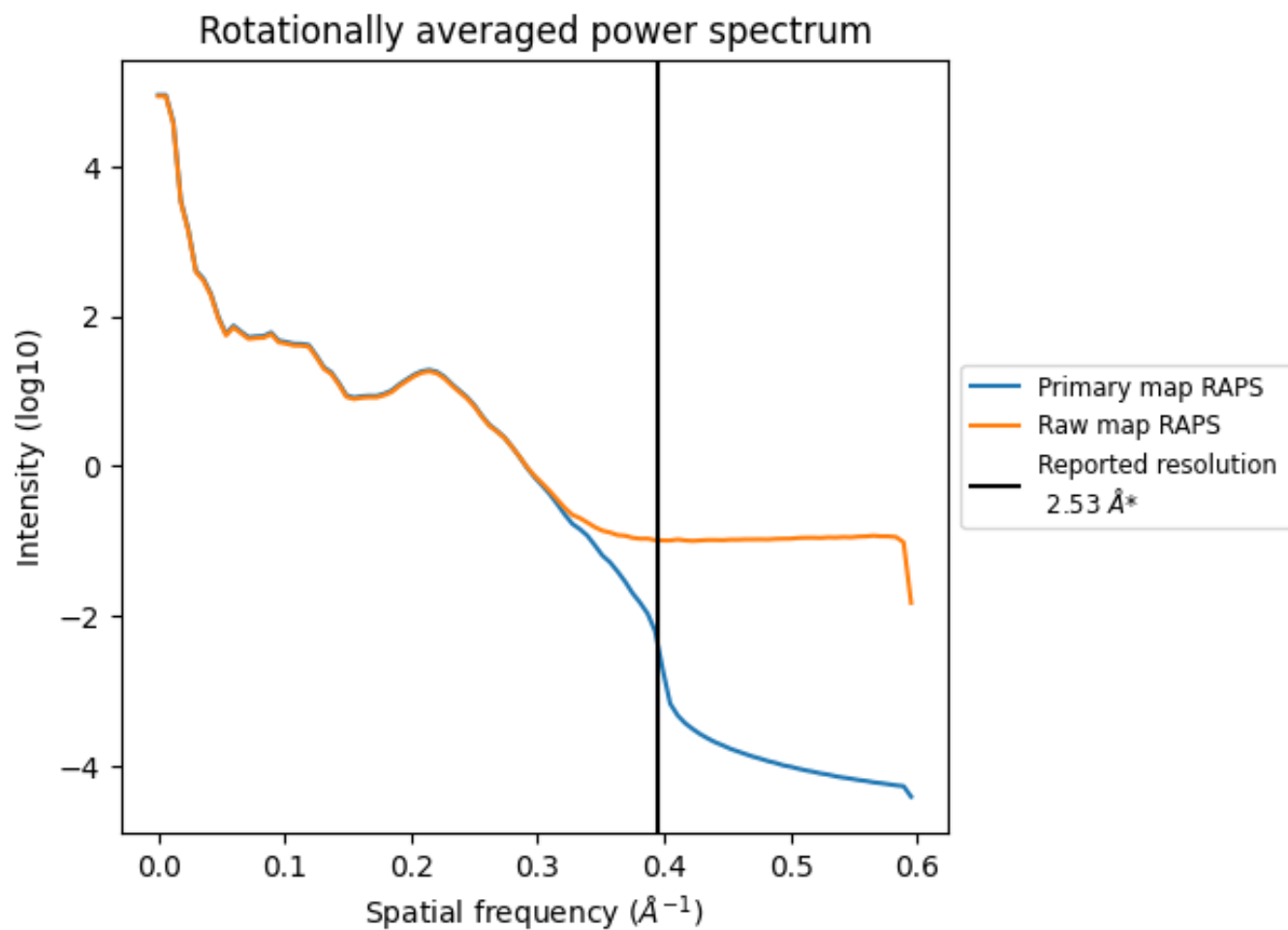
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 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.

6.3 Rotationally averaged power spectrum i

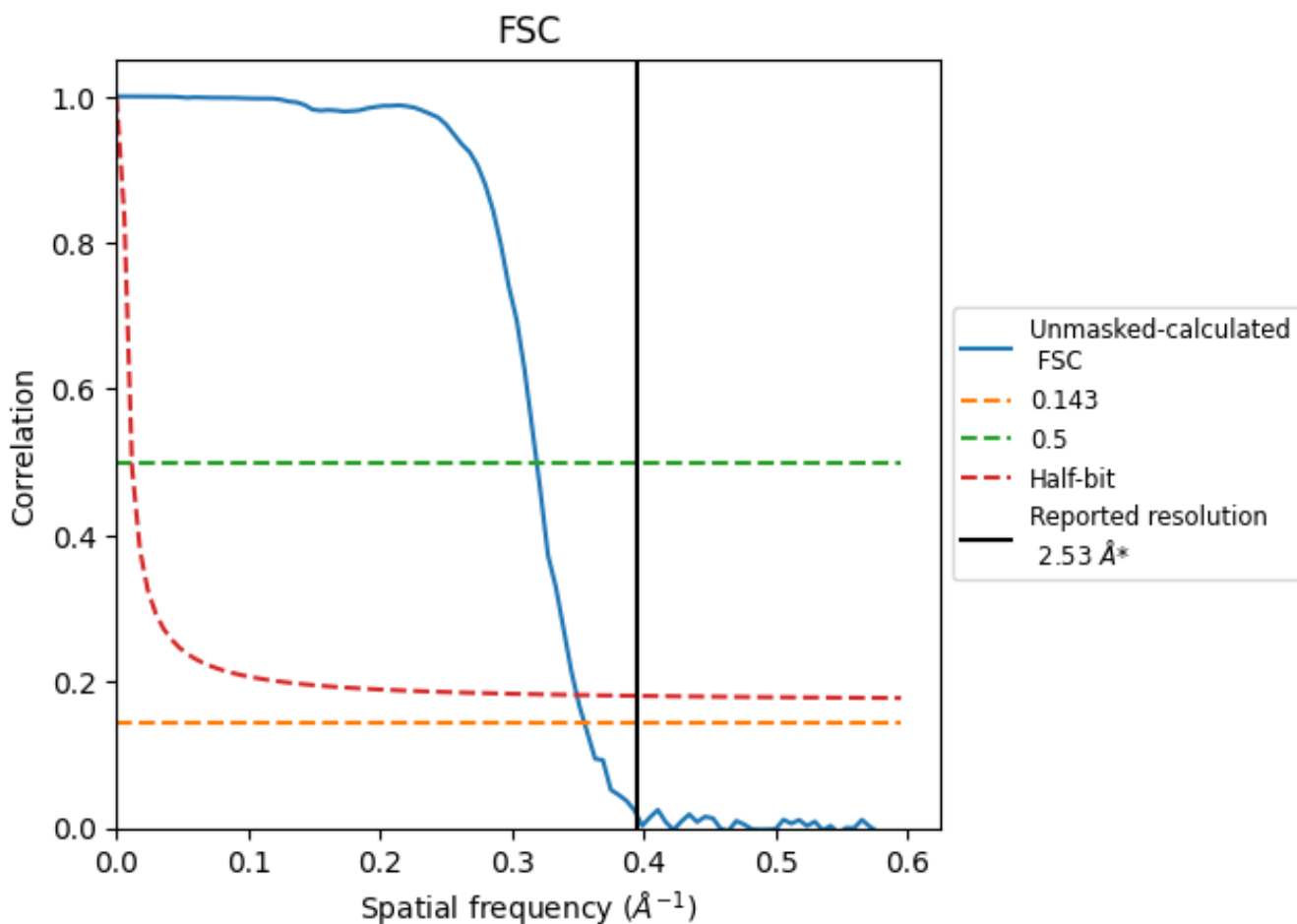


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

7.2 Resolution estimates [i](#)

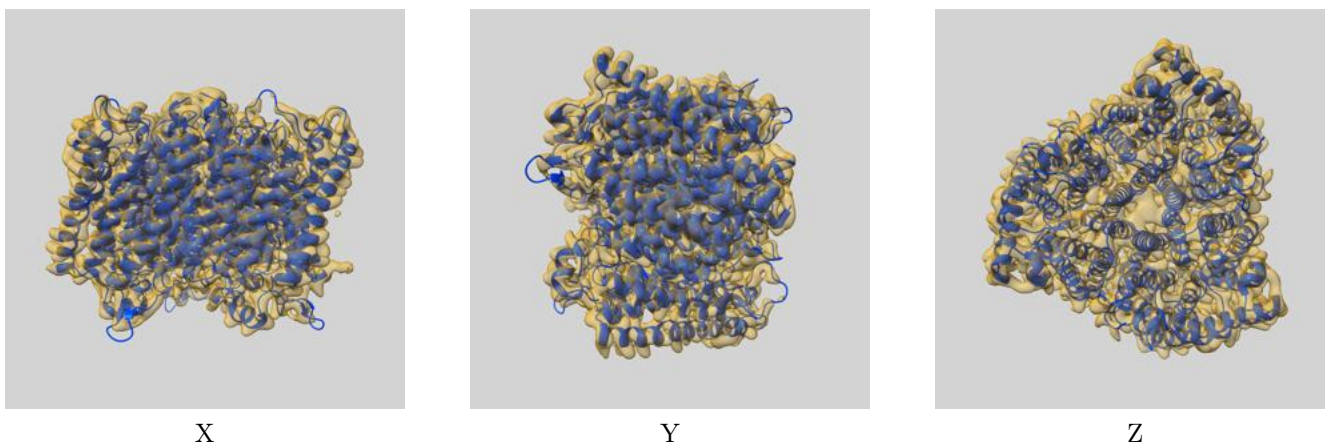
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.82	3.14	2.86

*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 2.82 differs from the reported value 2.53 by more than 10 %

8 Map-model fit [i](#)

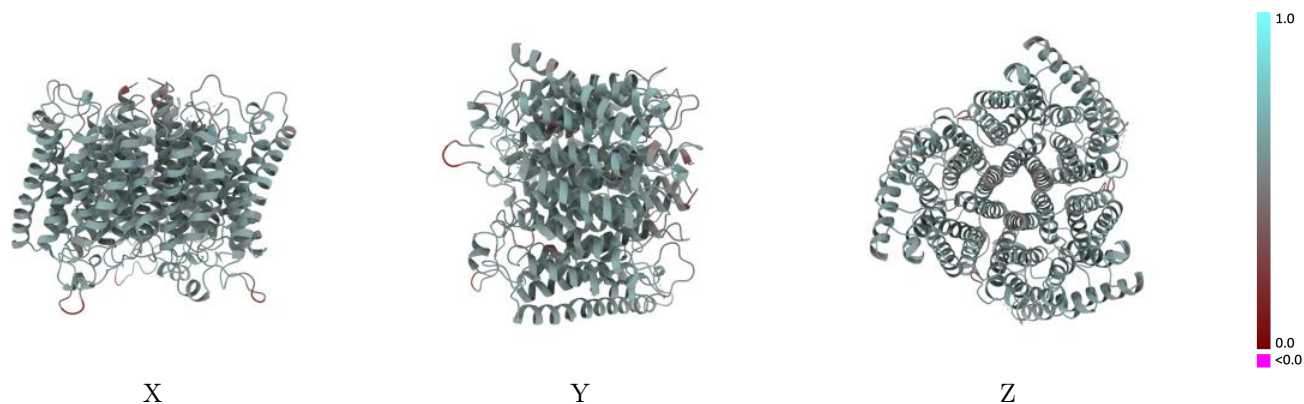
This section contains information regarding the fit between EMDB map EMD-18549 and PDB model 8QPF. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



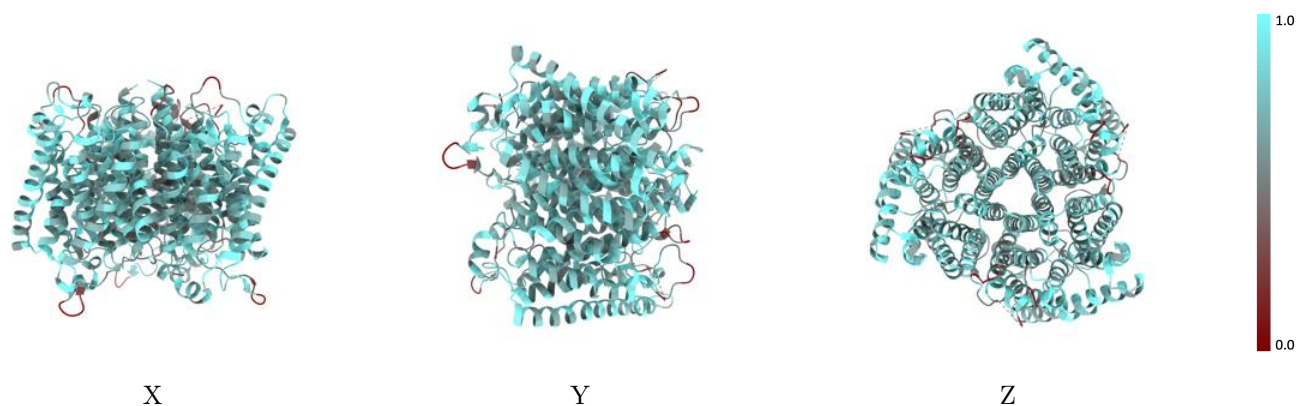
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



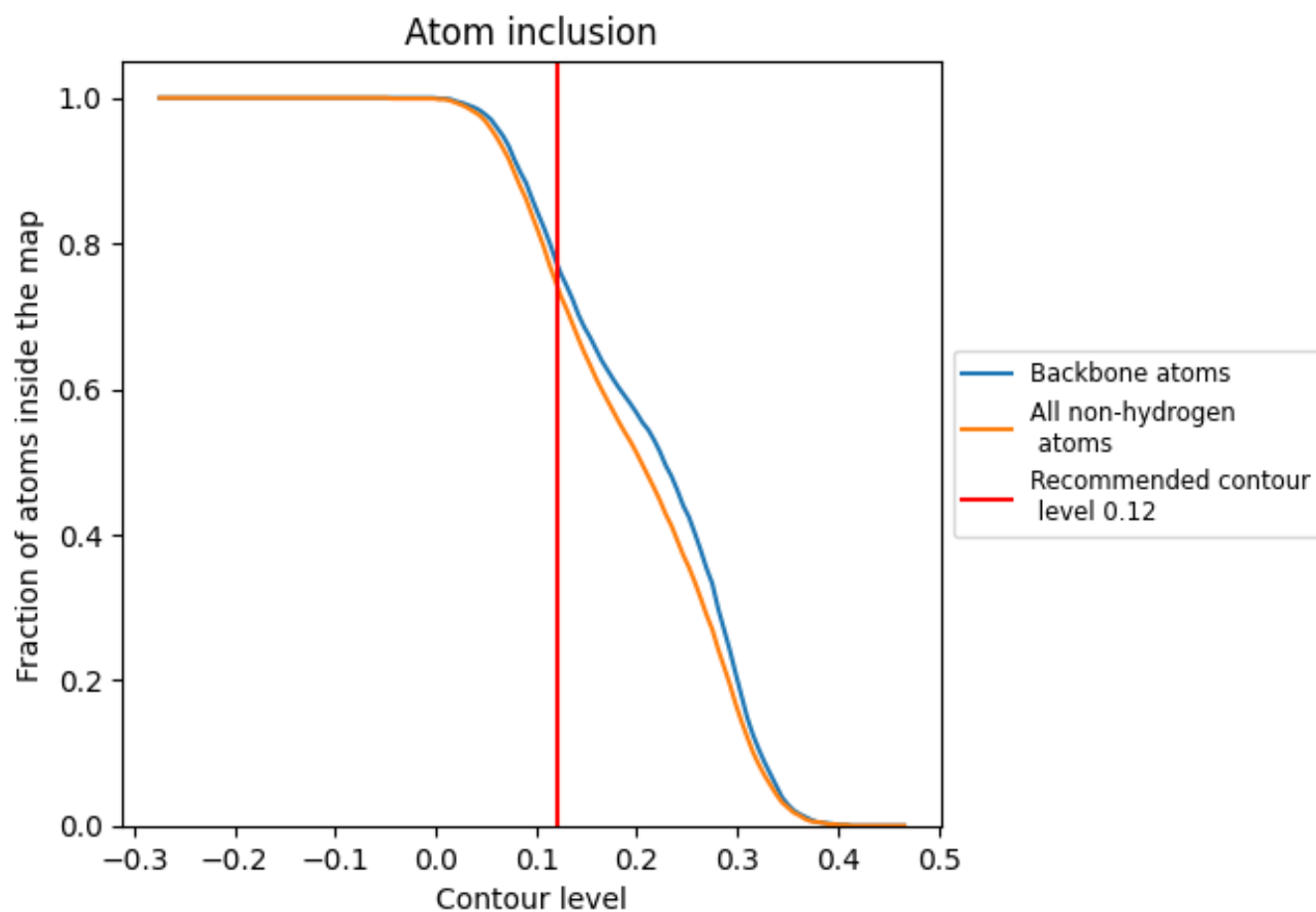
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.12).









8.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.5520
A	 0.7490	 0.5500
B	 0.7450	 0.5520
C	 0.7480	 0.5520

