



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:32 PM UTC

PDB ID : 3IXW / pdb_00003ixw
EMDB ID : EMD-5101
Title : Scorpion Hemocyanin activated state pseudo atomic model built based on cryo-EM density map
Authors : Cong, Y.; Zhang, Q.; Woolford, D.; Schweikardt, T.; Khant, H.; Ludtke, S.; Chiu, W.; Decker, H.
Deposited on : 2009-02-13
Resolution : 8.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

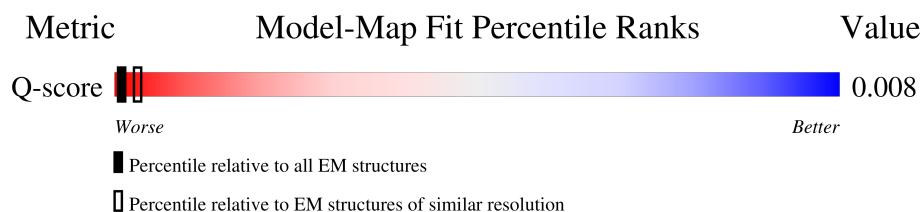
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	361 (7.50 - 8.50)

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

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 74208 atoms, of which 13476 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 Hemocyanin AA6 chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	C	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	D	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	E	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	F	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	G	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	H	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	I	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	J	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	K	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	L	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	M	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		

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, C2	Depositor
Number of particles used	13400	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1.663	Depositor
Minimum map value	-0.473	Depositor
Average map value	0.074	Depositor
Map value standard deviation	0.264	Depositor
Recommended contour level	1.16	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	1.8, 1.8, 1.8	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 oligosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	2
1	C	2
1	A	1
1	E	1
1	F	1
1	H	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	34:LYS	C	35:GLY	N	4.15
1	C	519:ALA	C	520:GLY	N	2.61
1	A	44:LEU	C	45:PHE	N	1.71
1	C	44:LEU	C	45:PHE	N	1.71
1	E	44:LEU	C	45:PHE	N	1.71
1	F	44:LEU	C	45:PHE	N	1.71
1	H	44:LEU	C	45:PHE	N	1.71
1	I	44:LEU	C	45:PHE	N	1.71
1	L	44:LEU	C	45:PHE	N	1.71

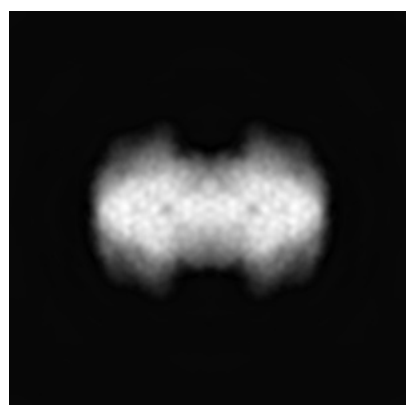
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5101. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

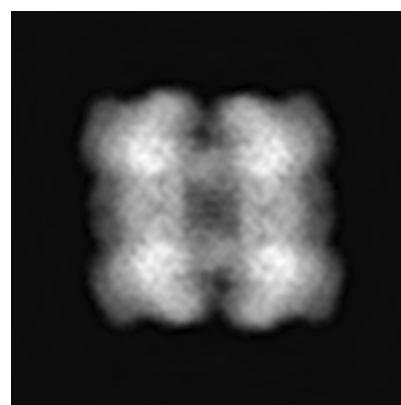
5.1.1 Primary map



X



Y



Z

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

5.2 Central slices [i](#)

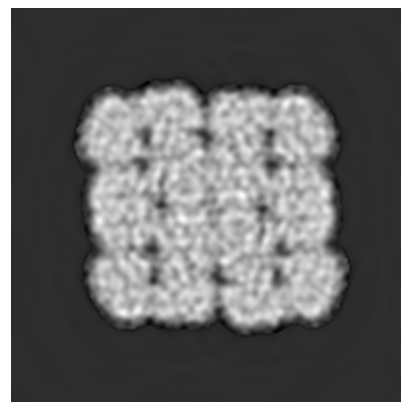
5.2.1 Primary map



X Index: 104



Y Index: 104

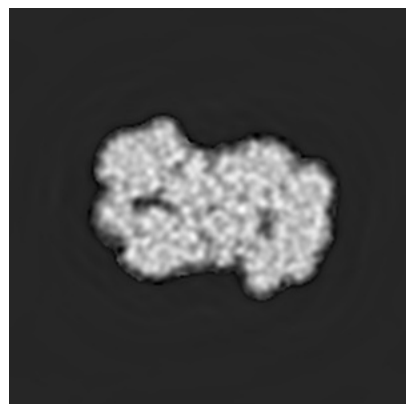


Z Index: 104

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

5.3 Largest variance slices [i](#)

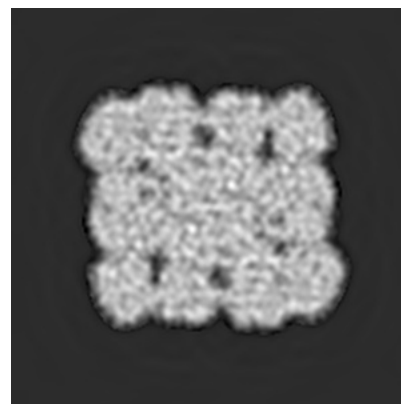
5.3.1 Primary map



X Index: 75



Y Index: 133



Z Index: 107

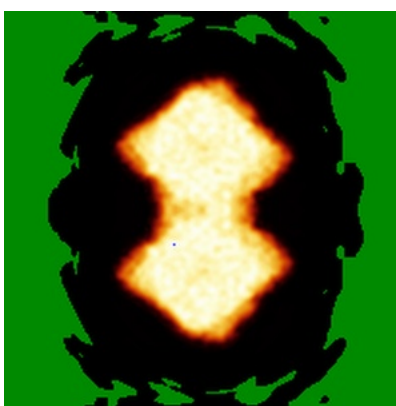
The images above show the largest variance slices of the map in three orthogonal directions.

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

5.4.1 Primary map



X



Y

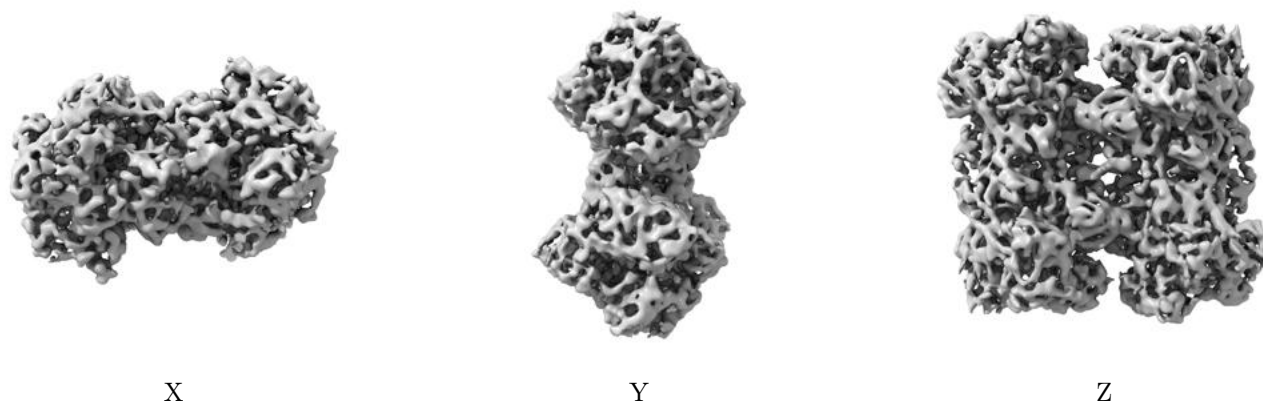


Z

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 1.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

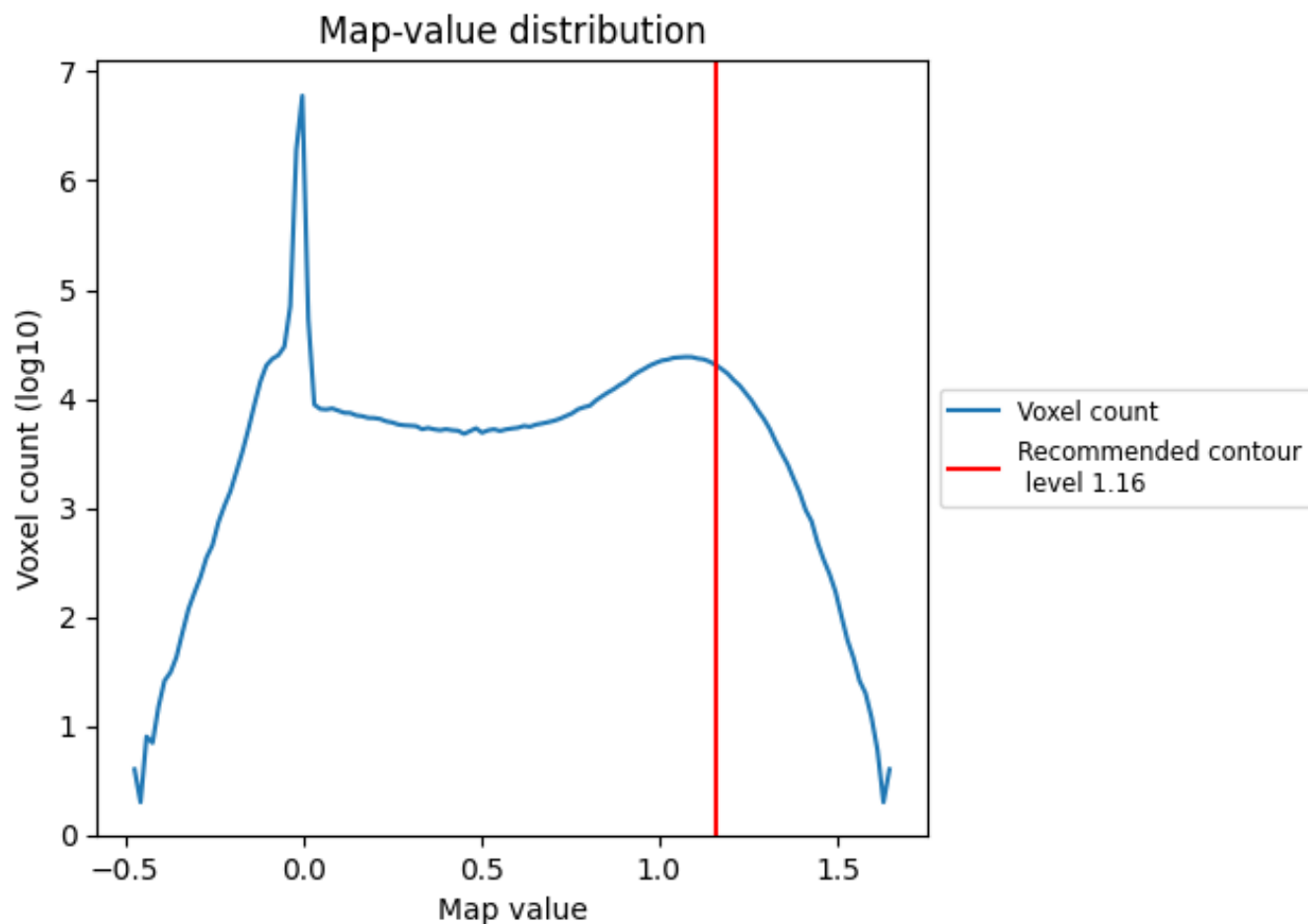
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

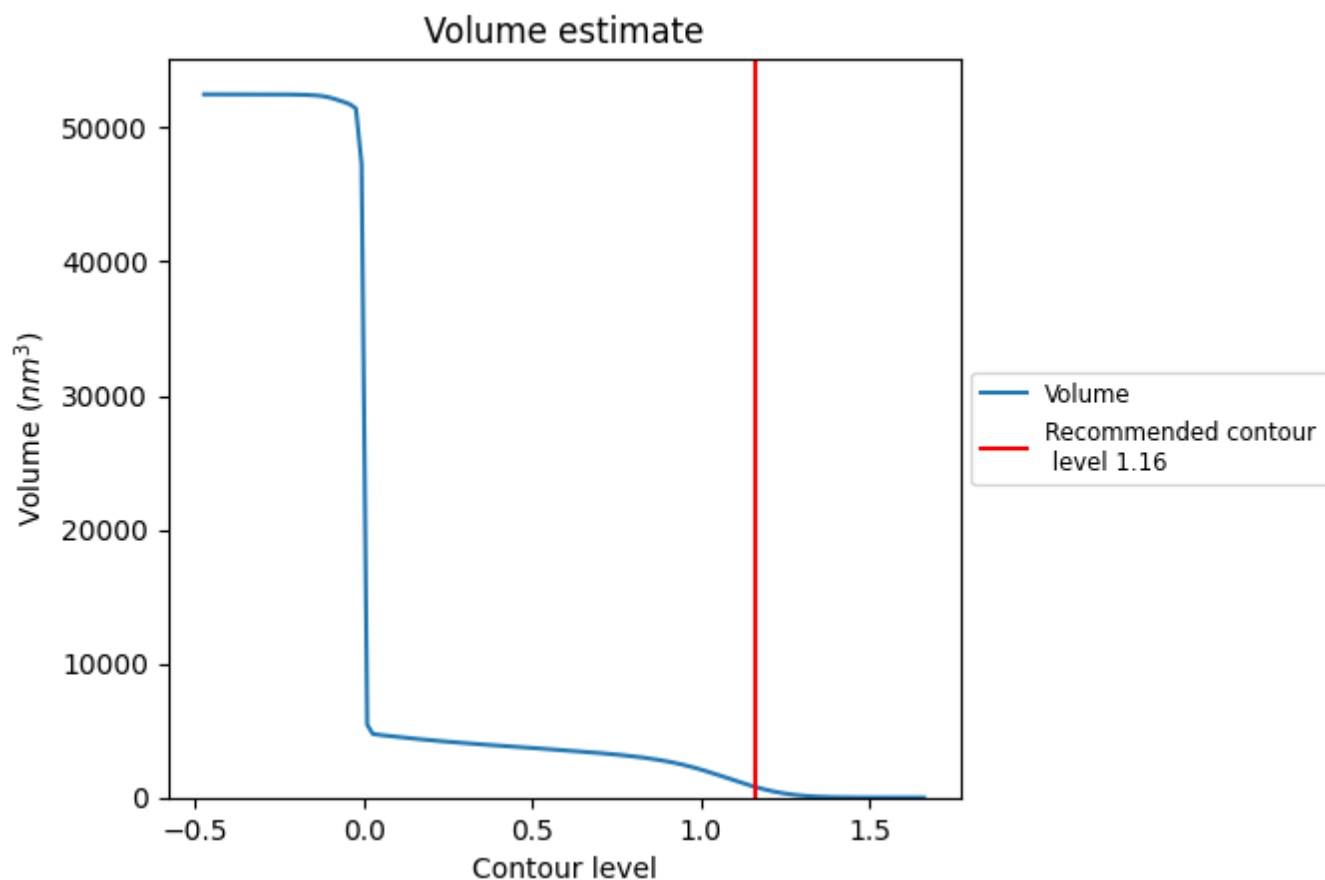
This section contains the results of statistical analysis of the map.

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.

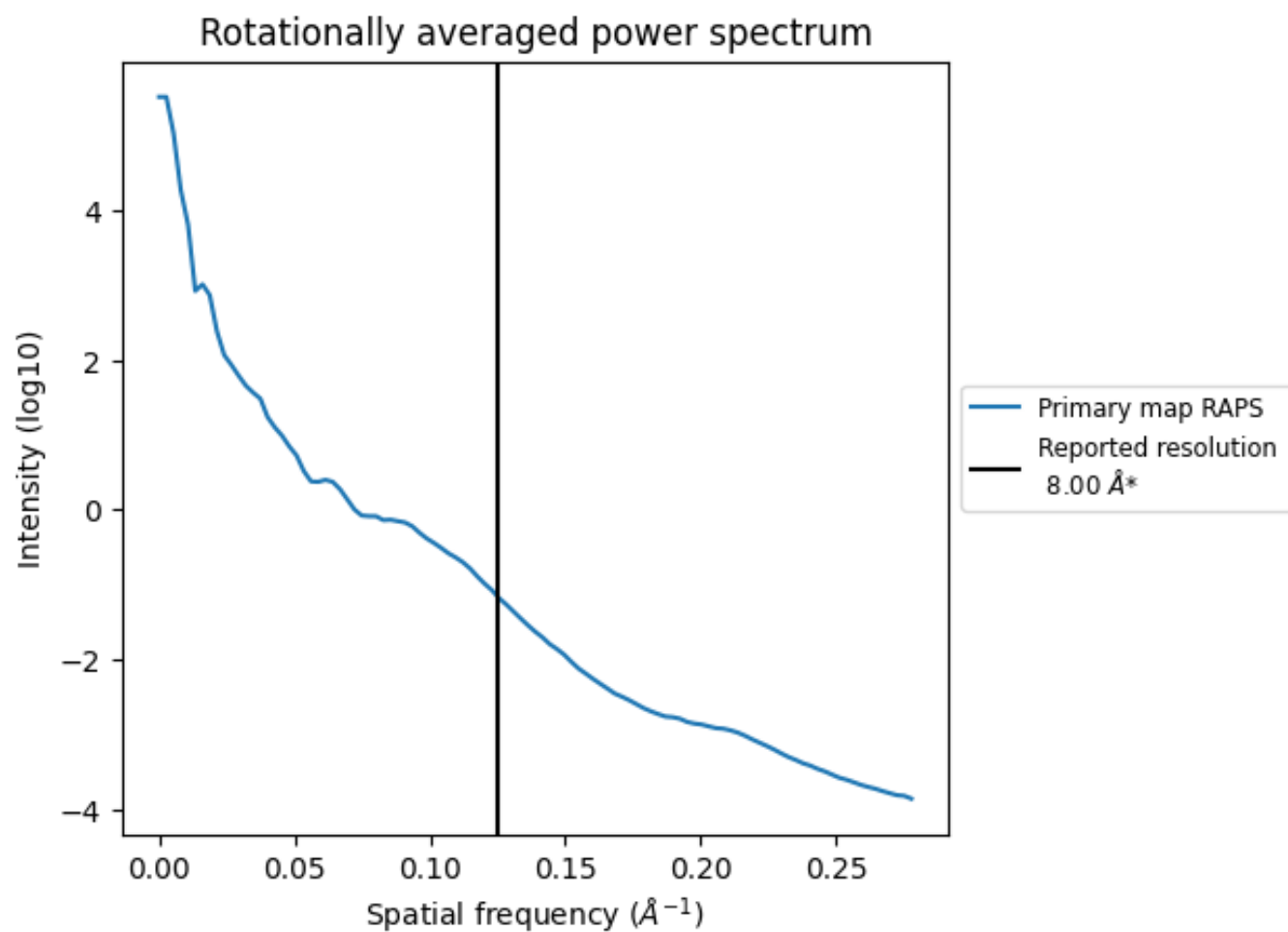
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 811 nm³; this corresponds to an approximate mass of 733 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 0.125 Å⁻¹

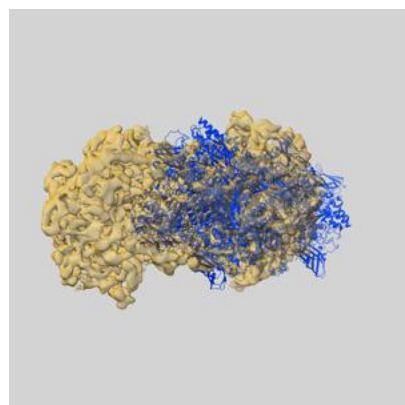
7 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

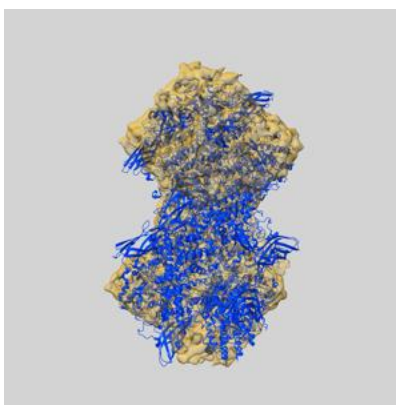
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5101 and PDB model 3IXW. Per-residue inclusion information can be found in section ?? on page ??.

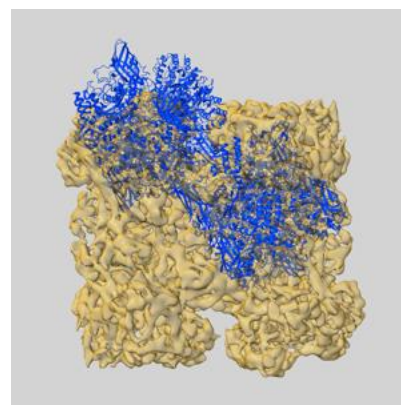
8.1 Map-model overlay [i](#)



X



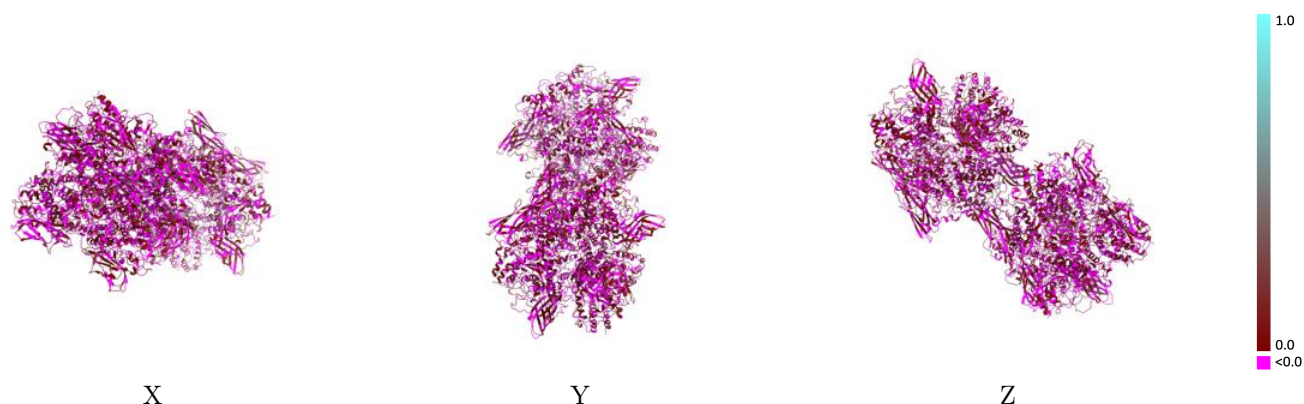
Y



Z

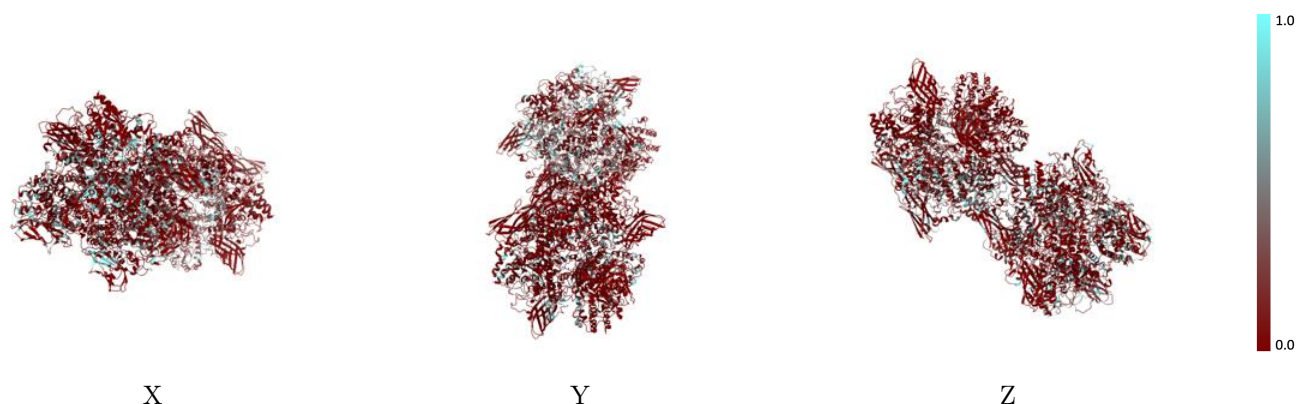
The images above show the 3D surface view of the map at the recommended contour level 1.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



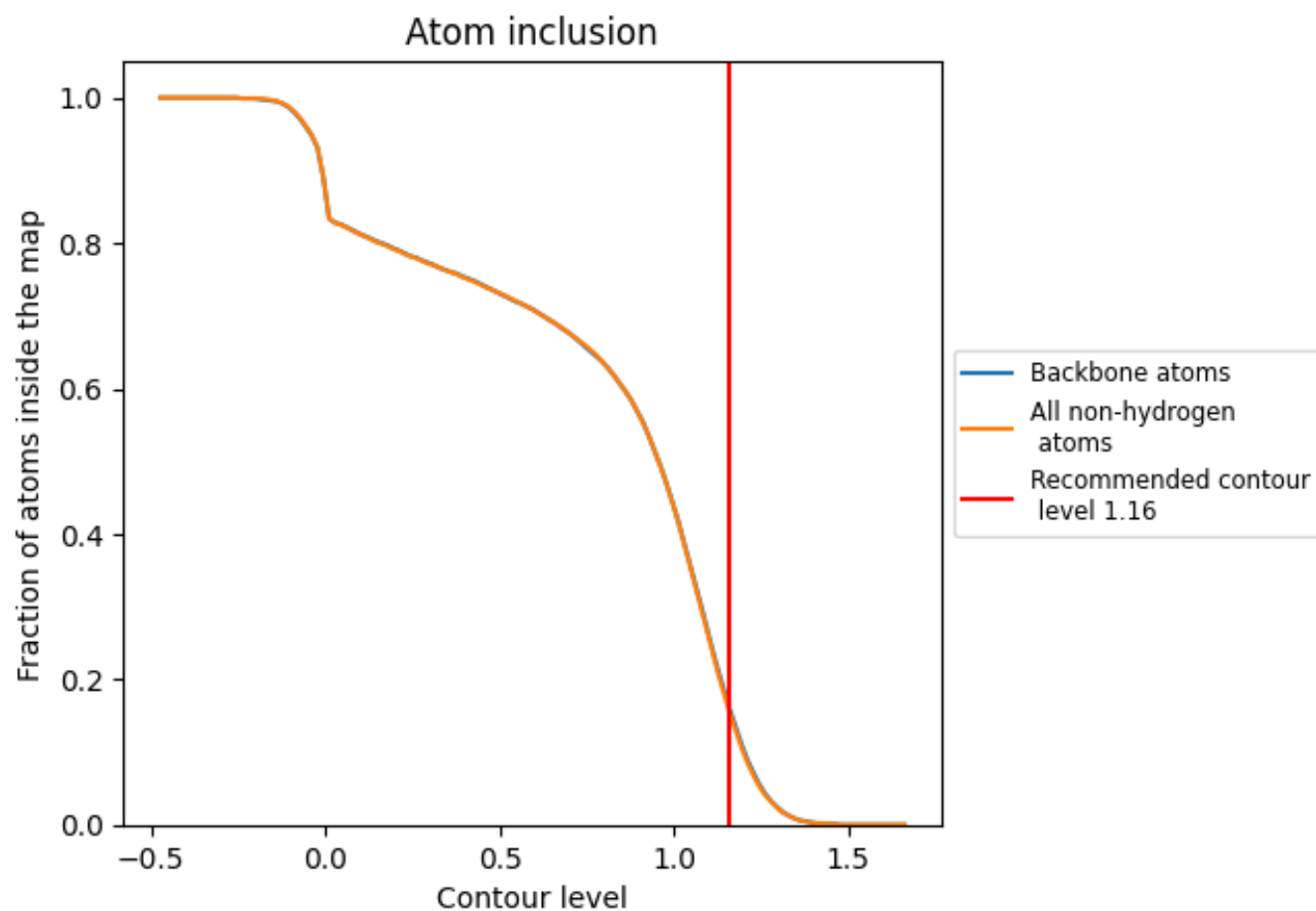
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (1.16).

8.4 Atom inclusion [i](#)



At the recommended contour level, 16% of all backbone atoms, 16% 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 (1.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1560	0.0080
A	0.2050	-0.0000
C	0.1650	0.0050
D	0.2170	0.0110
E	0.2150	0.0120
F	0.1750	0.0040
G	0.0890	0.0030
H	0.1670	0.0100
I	0.2070	0.0090
J	0.1960	0.0100
K	0.0610	0.0080
L	0.0960	0.0110
M	0.0580	0.0090

1.0

0.0

<0.0