



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:07 AM UTC

PDB ID : 9D9W / pdb_00009d9w
EMDB ID : EMD-46681
Title : Mycobacteriophage Bxb1 C1 Capsid and Portal - Composite map and model
Authors : Freeman, K.G.
Deposited on : 2024-08-21
Resolution : 3.50 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>.

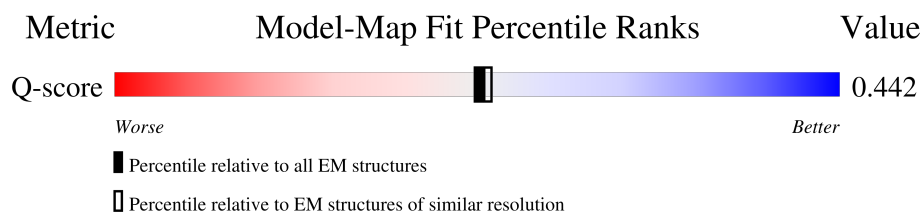
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

i

ELECTRON MICROSCOPY

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	13950 (3.00 - 4.00)

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 257618 atoms, of which 127151 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 Major capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Aa	394	Total	C	H	N	O	S	0	0
			5785	1838	2859	488	594	6		
1	Ab	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		
1	Ac	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Ad	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Ae	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Af	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Ba	394	Total	C	H	N	O	S	0	0
			5784	1838	2858	488	594	6		
1	Bb	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Bc	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Bd	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		
1	Be	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Bf	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		
1	Ca	394	Total	C	H	N	O	S	0	0
			5784	1838	2858	488	594	6		
1	Cb	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Cc	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Cd	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		
1	Ce	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Cf	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Da	394	Total	C	H	N	O	S	0	0
			5785	1838	2859	488	594	6		
1	Db	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Dc	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		
1	Dd	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		
1	De	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Df	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Ea	394	Total	C	H	N	O	S	0	0
			5784	1838	2858	488	594	6		
1	Eb	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Ec	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Ed	396	Total	C	H	N	O	S	0	0
			5811	1849	2870	490	596	6		
1	Ee	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		
1	Ef	396	Total	C	H	N	O	S	0	0
			5812	1849	2871	490	596	6		

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Fa	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fb	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fc	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fd	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fe	450	Total	C	H	N	O	S	0	0
			6952	2219	3426	603	690	14		
2	Ff	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	Fg	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fh	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fi	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fj	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fk	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		
2	Fl	450	Total	C	H	N	O	S	0	0
			6951	2219	3425	603	690	14		

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, C1	Depositor
Number of particles used	33132	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	32.850	Depositor
Minimum map value	-13.408	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.022	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	865.62006, 865.62006, 865.62006	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2366, 1.2366, 1.2366	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 ⓘ

There are no chain breaks in this entry.

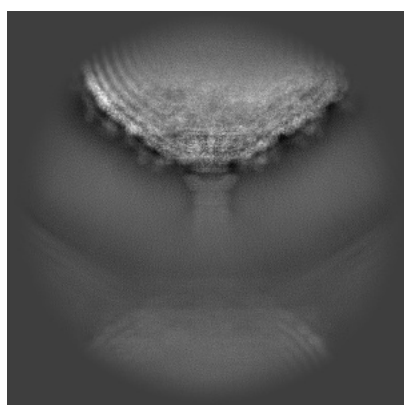
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46681. These allow visual inspection of the internal detail of the map and identification of artifacts.

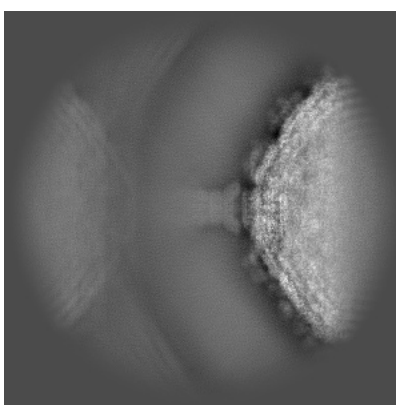
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

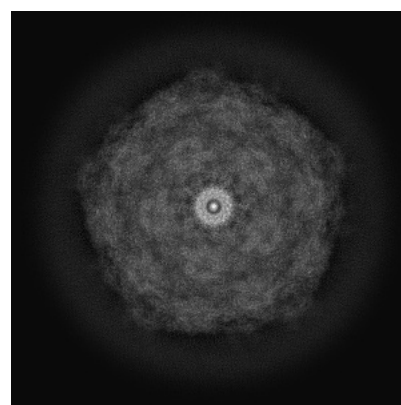
5.1.1 Primary map



X



Y

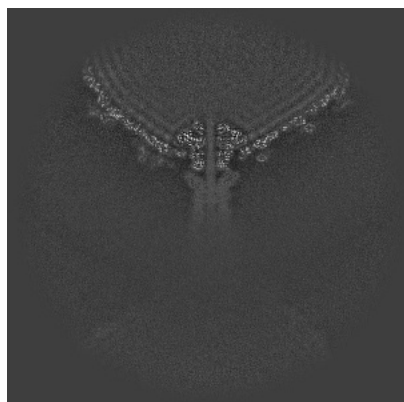


Z

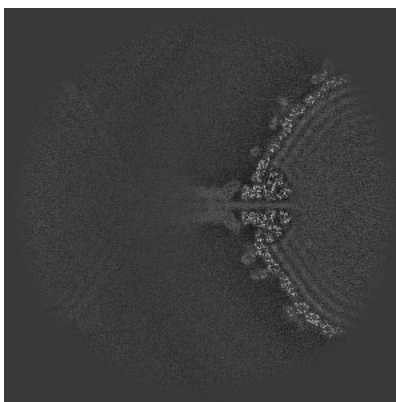
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

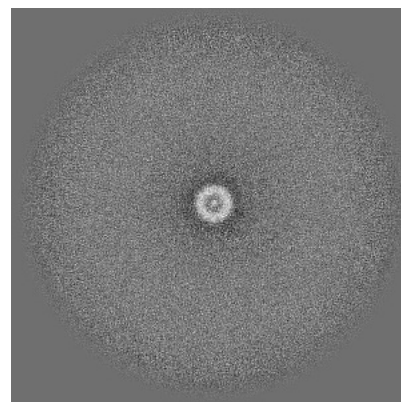
5.2.1 Primary map



X Index: 350



Y Index: 350



Z Index: 350

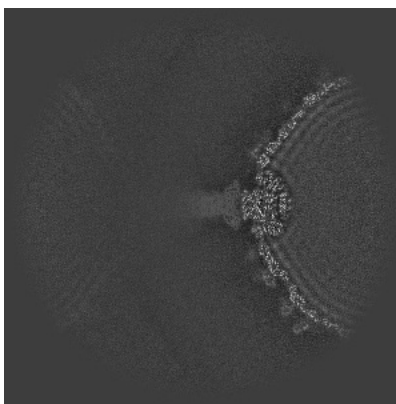
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

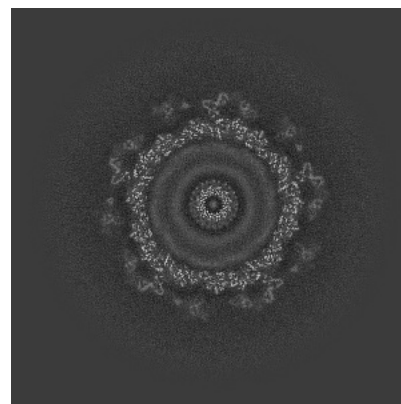
5.3.1 Primary map



X Index: 373



Y Index: 333

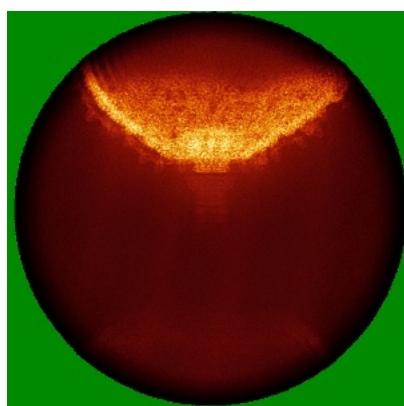


Z Index: 491

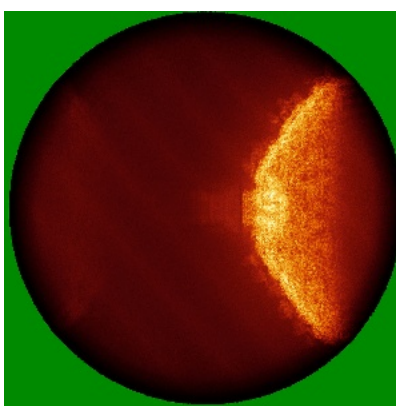
The images above show the largest variance slices of the map in three orthogonal directions.

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

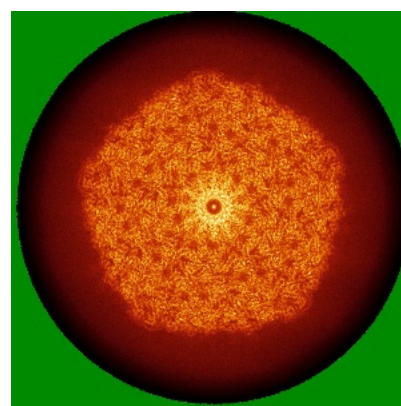
5.4.1 Primary map



X



Y

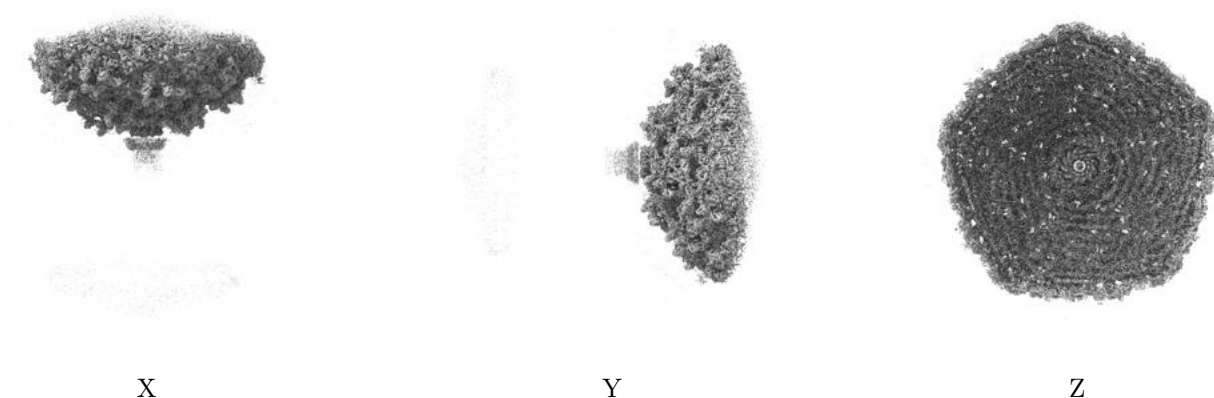


Z

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

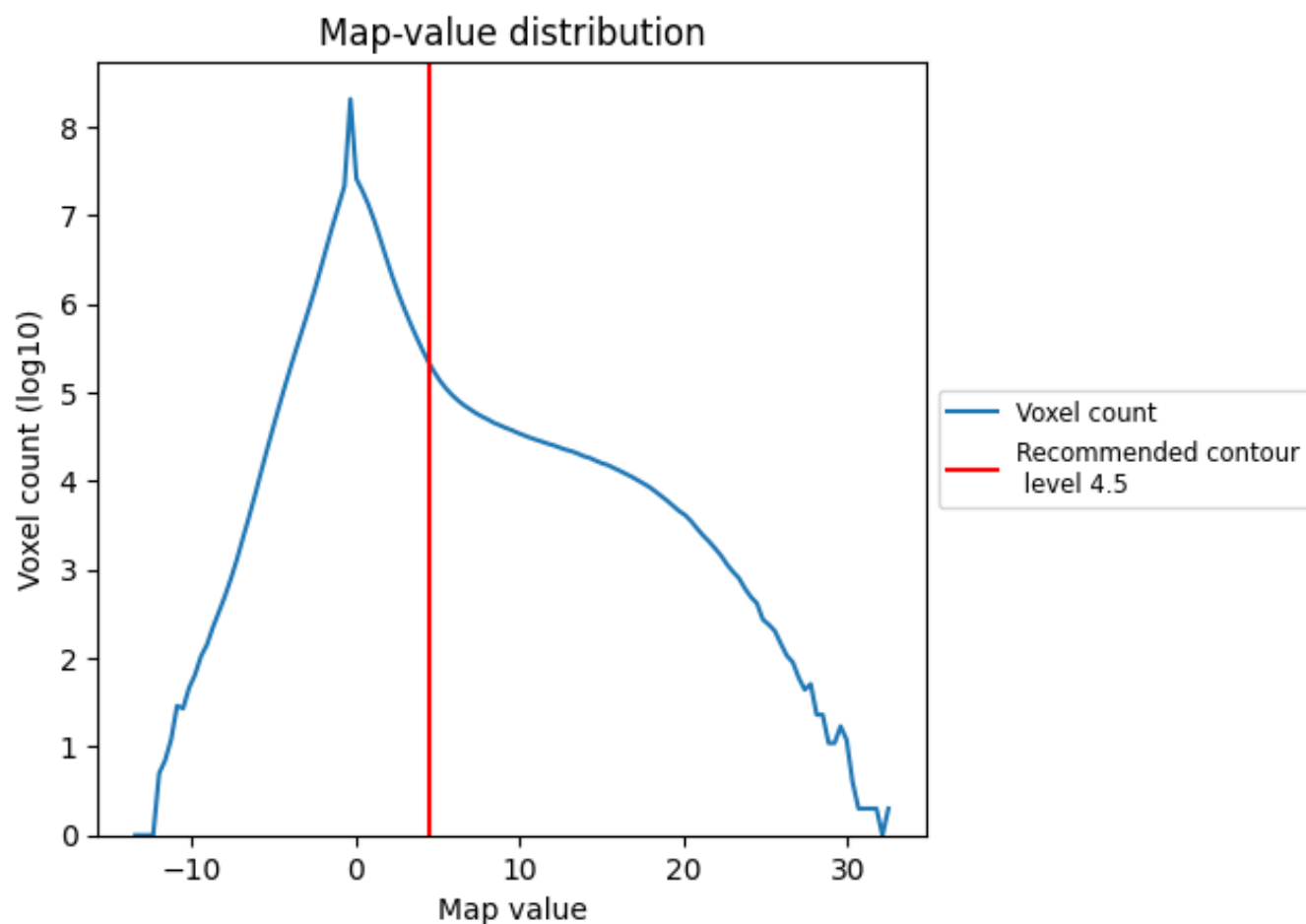
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

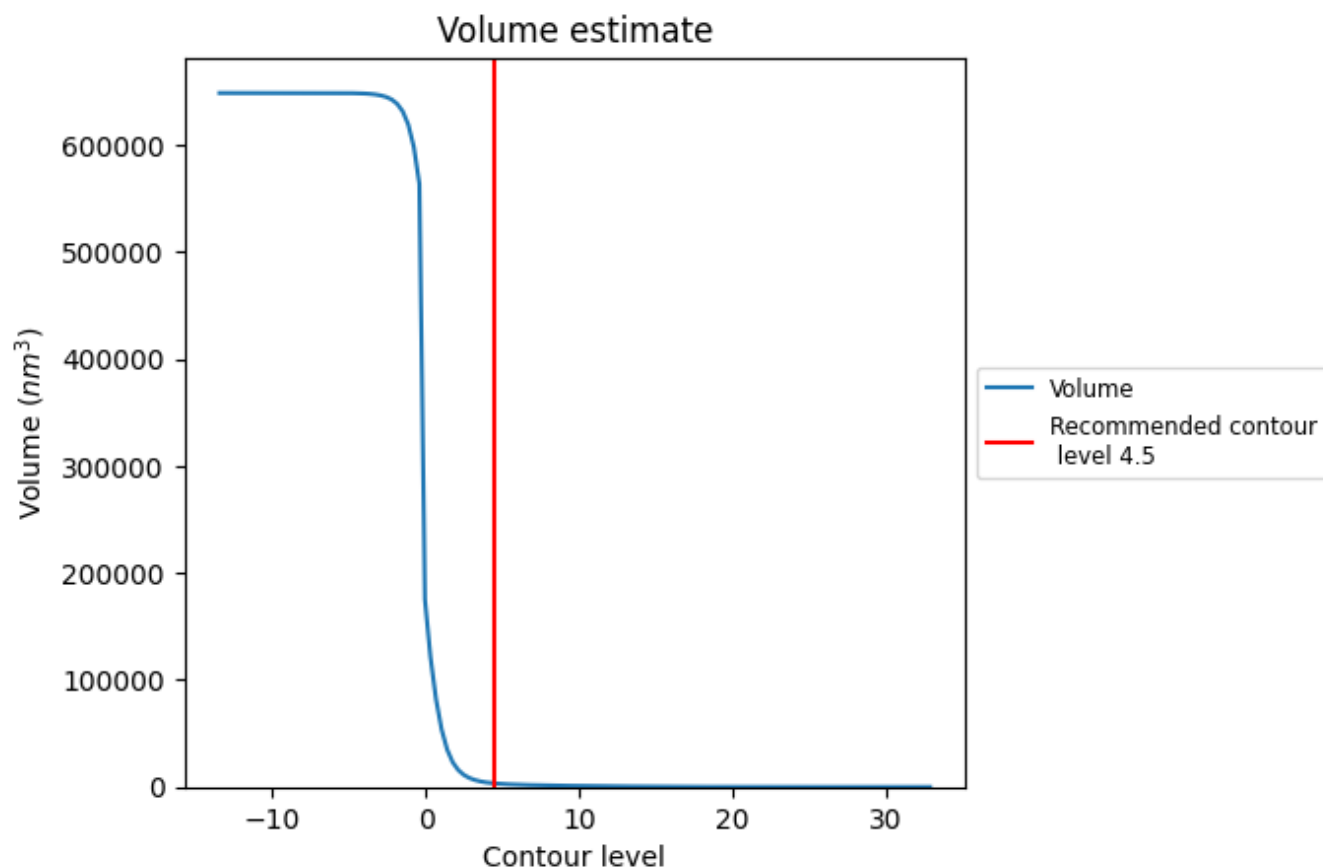
This section contains the results of statistical analysis of the map.

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.

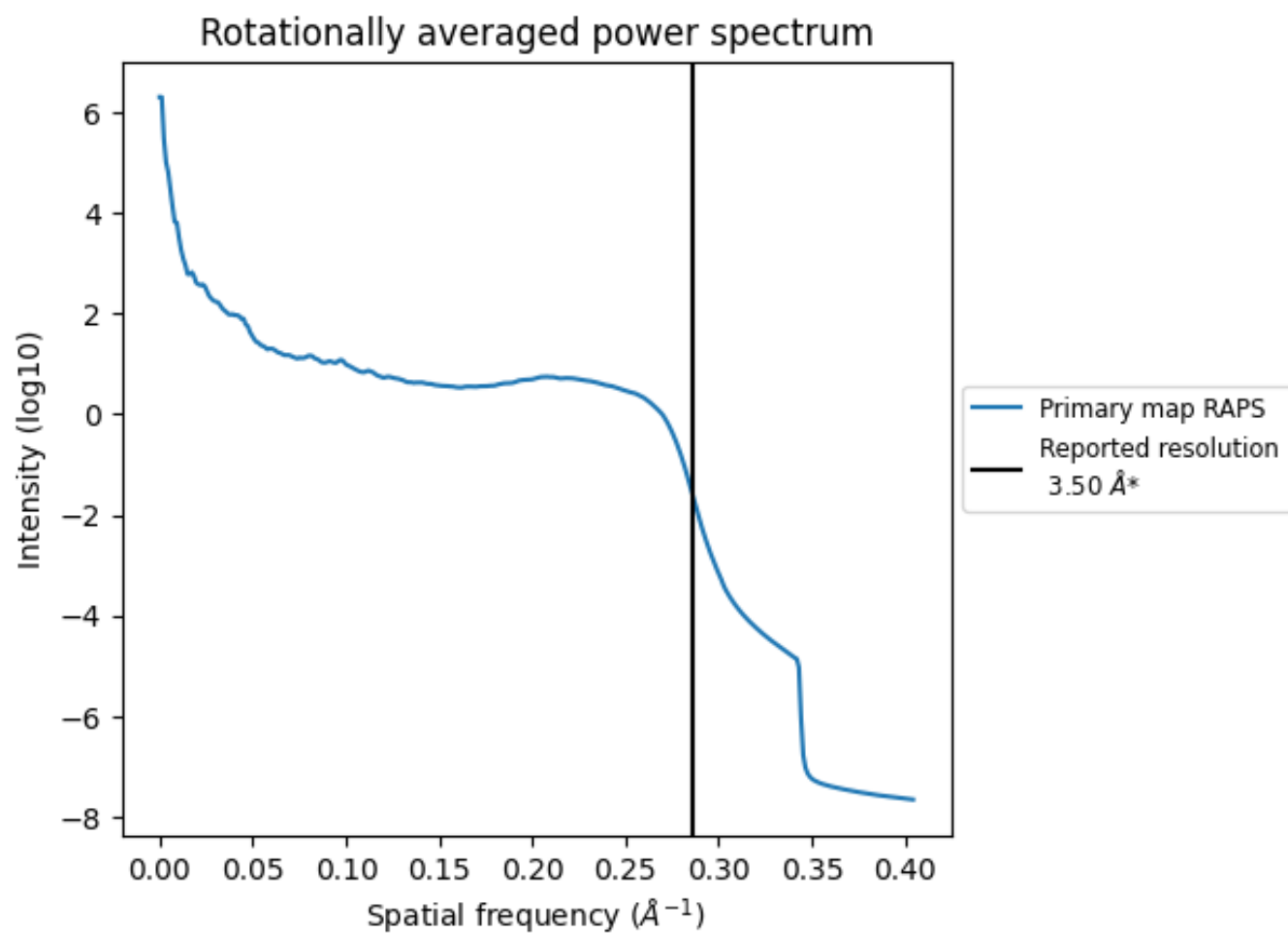
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 3345 nm^3 ; this corresponds to an approximate mass of 3022 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

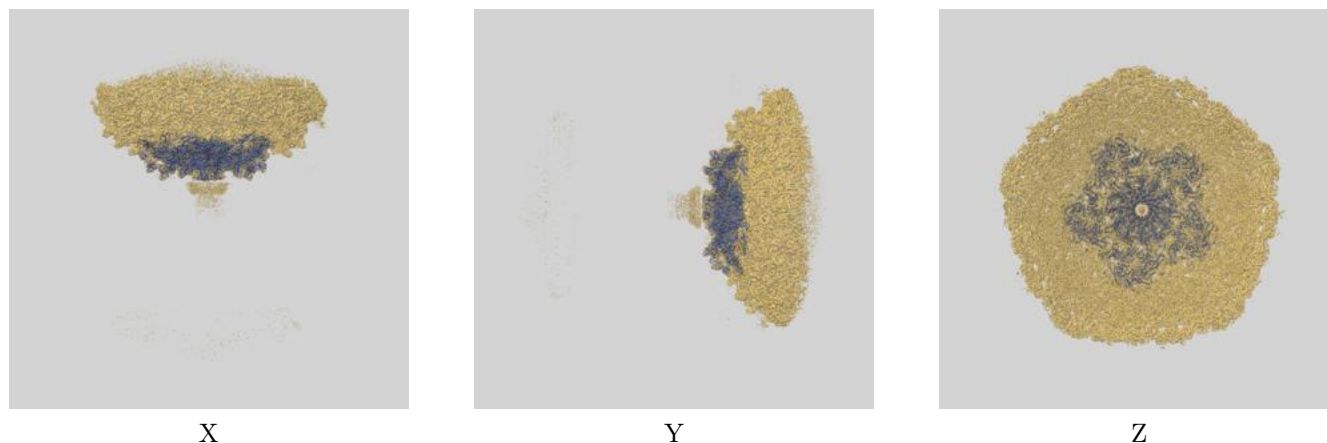
7 Fourier-Shell correlation ⓘ

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

8 Map-model fit [i](#)

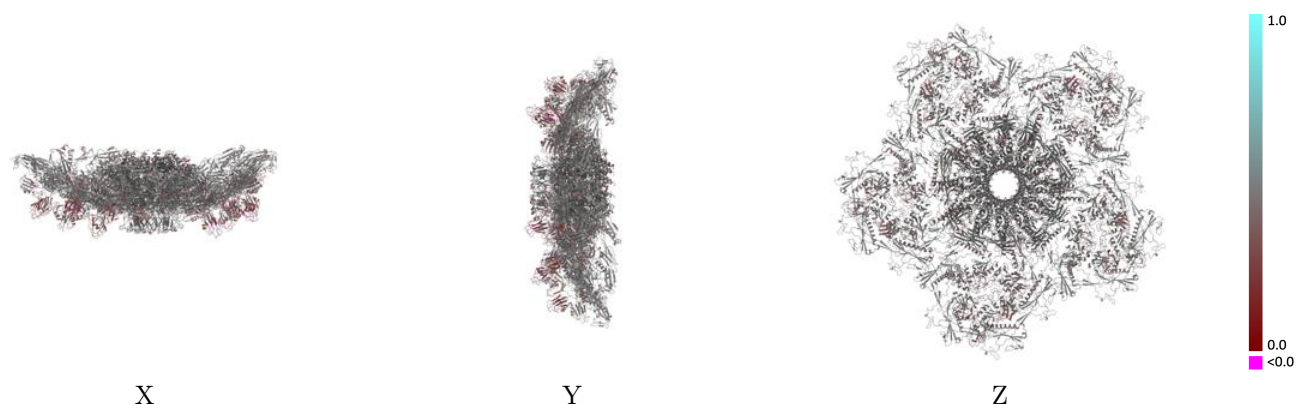
This section contains information regarding the fit between EMDB map EMD-46681 and PDB model 9D9W. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



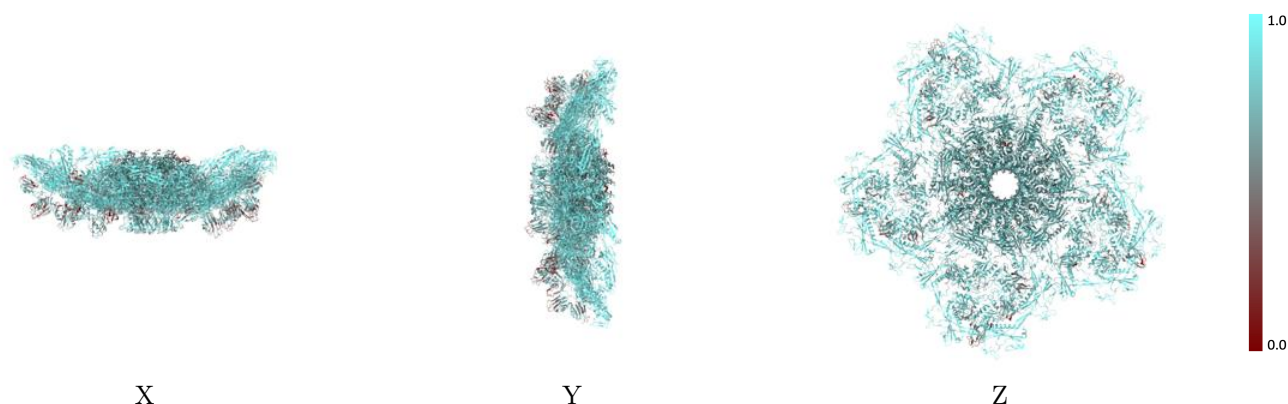
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



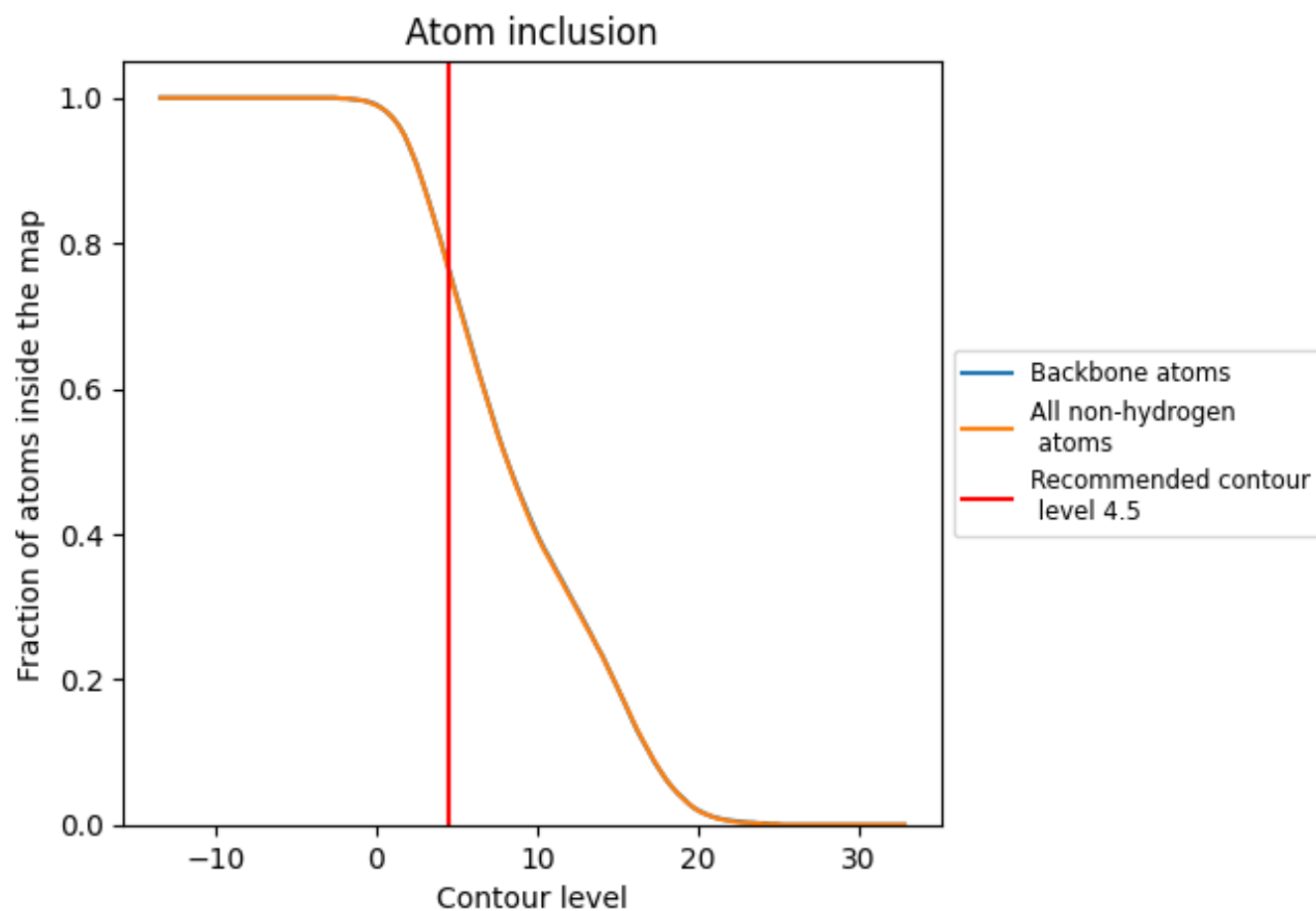
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).

8.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.4420
Aa	 0.7600	 0.4360
Ab	 0.7640	 0.4330
Ac	 0.7810	 0.4460
Ad	 0.7680	 0.4280
Ae	 0.7980	 0.4520
Af	 0.7950	 0.4370
Ba	 0.7630	 0.4360
Bb	 0.7680	 0.4270
Bc	 0.7760	 0.4460
Bd	 0.7640	 0.4260
Be	 0.7960	 0.4480
Bf	 0.7990	 0.4370
Ca	 0.7640	 0.4390
Cb	 0.7720	 0.4310
Cc	 0.7850	 0.4430
Cd	 0.7740	 0.4280
Ce	 0.7900	 0.4460
Cf	 0.7840	 0.4240
Da	 0.7720	 0.4360
Db	 0.7650	 0.4300
Dc	 0.7770	 0.4430
Dd	 0.7900	 0.4340
De	 0.7980	 0.4470
Df	 0.7820	 0.4250
Ea	 0.7720	 0.4410
Eb	 0.7670	 0.4210
Ec	 0.7680	 0.4400
Ed	 0.7790	 0.4250
Ee	 0.7950	 0.4490
Ef	 0.7830	 0.4300
Fa	 0.7550	 0.4510
Fb	 0.7590	 0.4550
Fc	 0.7750	 0.4620
Fd	 0.7620	 0.4590



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Chain	Atom inclusion	Q-score
Fe	 0.7710	 0.4620
Ff	 0.7570	 0.4480
Fg	 0.7510	 0.4500
Fh	 0.7510	 0.4520
Fi	 0.7390	 0.4470
Fj	 0.7620	 0.4540
Fk	 0.7660	 0.4590
Fl	 0.7590	 0.4530