



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 02:45 AM UTC

PDB ID : 6HU4 / pdb_00006hu4
EMDB ID : EMD-0272
Title : F97L Hepatitis B core protein capsid
Authors : Bottcher, B.; Nassal, M.
Deposited on : 2018-10-05
Resolution : 2.64 Å (reported)
Based on initial model : 6HTX

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.dev132
MolProbity : 4-5-2 with Phenix2.0
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

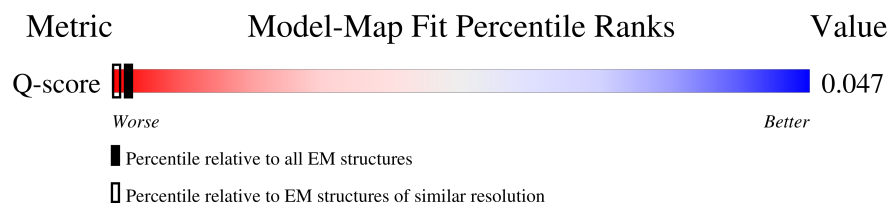
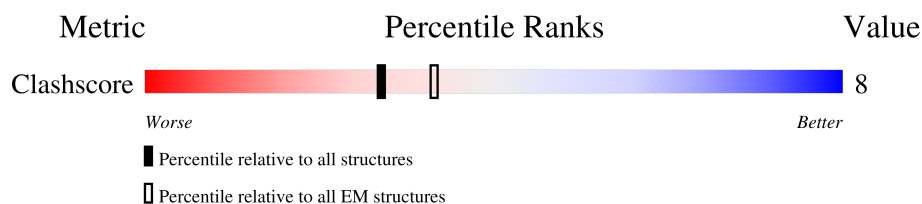
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

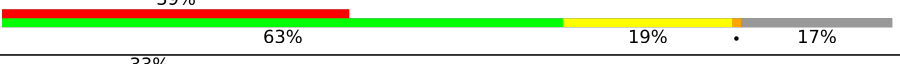
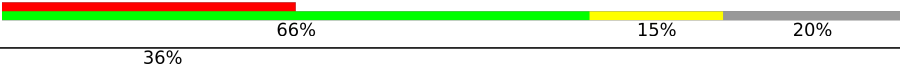
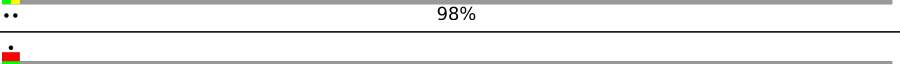
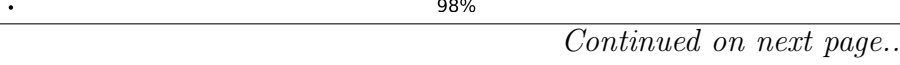
The reported resolution of this entry is 2.64 Å.

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.



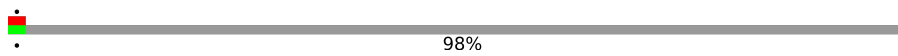
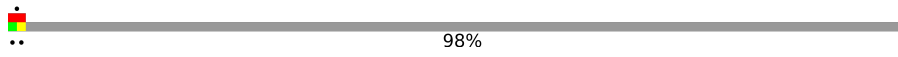
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	8968 (2.14 - 3.14)

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	183	
1	B	183	
1	C	183	
1	D	183	
1	E	183	
1	F	183	

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Mol	Chain	Length	Quality of chain
1	G	183	 98%
1	H	183	 98%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4825 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.

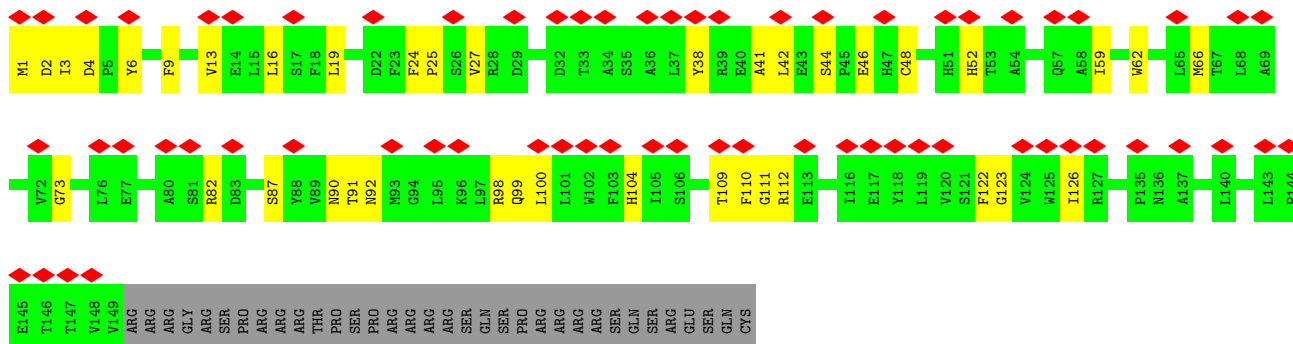
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	151	Total	C	N	O	S	0	0
			1207	781	201	219	6		
1	A	144	Total	C	N	O	S	2	0
			1167	757	195	209	6		
1	C	147	Total	C	N	O	S	0	0
			1171	759	191	215	6		
1	D	149	Total	C	N	O	S	1	0
			1196	775	197	218	6		
1	E	3	Total	C	N	O	S	0	0
			21	11	4	5	1		
1	F	3	Total	C	N	O	S	0	0
			21	11	4	5	1		
1	G	3	Total	C	N	O	S	0	0
			21	11	4	5	1		
1	H	3	Total	C	N	O	S	0	0
			21	11	4	5	1		

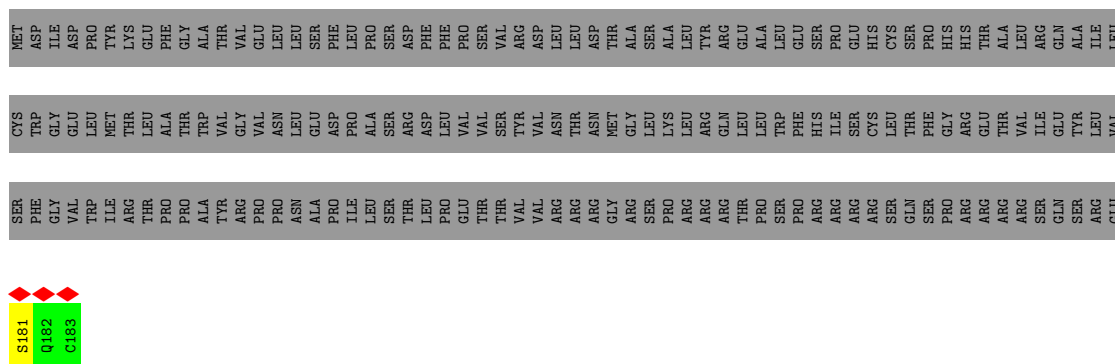
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	LEU	PHE	engineered mutation	UNP P03146
A	97	LEU	PHE	engineered mutation	UNP P03146
C	97	LEU	PHE	engineered mutation	UNP P03146
D	97	LEU	PHE	engineered mutation	UNP P03146
E	97	LEU	PHE	engineered mutation	UNP P03146
F	97	LEU	PHE	engineered mutation	UNP P03146
G	97	LEU	PHE	engineered mutation	UNP P03146
H	97	LEU	PHE	engineered mutation	UNP P03146

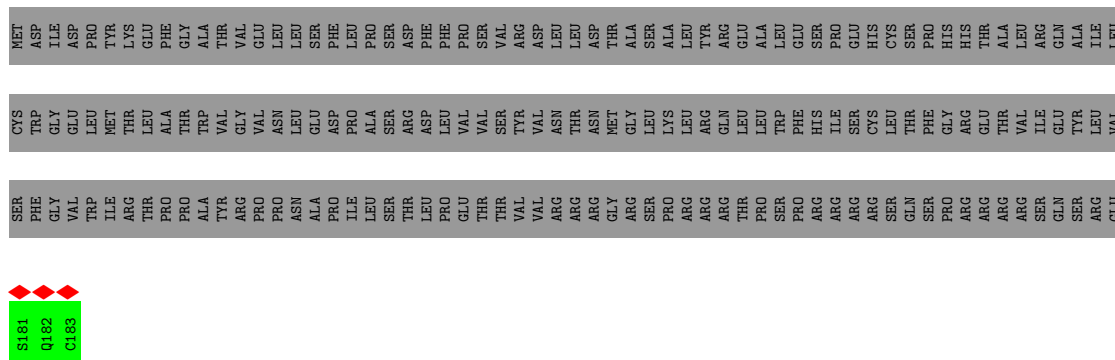
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



Chain G: 98%

S181	SER	THR	GLY	ASP	MET
Q182	PHE	TRP	GLY	ASP	ILE
C183	VAL	GLU	VAL	GLU	ASP
	THR	LEU	THR	PRO	TYR
	ILE	MET	THR	LYS	THR
	ARG	THR	LEU	GLU	GLY
	PRO	ALA	ALA	GLU	PHE
	PRO	THR	THR	THR	GLY
	ALA	TRP	VAL	ALA	THR
	TYR	GLY	VAL	VAL	THR
	ARG	GLY	VAL	GLU	VAL
	PRO	ASN	GLU	LEU	LEU
	ASN	LEU	LEU	LEU	SER
	ALA	GLU	SER	SER	PHE
	PRO	ASP	ASP	PHE	ASP
	ILE	PRO	LEU	LEU	PRO
	LEU	ALA	ALA	PRO	VAL
	SER	SER	SER	SER	VAL
	THR	ARG	THR	ARG	ARG
	LEU	ASP	LEU	ASP	THR
	PRO	LEU	VAL	LEU	THR
	GLU	VAL	GLU	LEU	THR
	THR	THR	THR	THR	THR
	VAL	VAL	VAL	VAL	THR
	ARG	ARG	ARG	LEU	ASP
	ARG	THR	THR	LEU	LEU
	ANG	ASN	ASN	ASP	ASP
	GLY	GLY	MET	THR	THR
	ARG	GLY	GLY	ALA	ALA
	SER	LEU	LEU	SER	SER
	PRO	LYS	LEU	ALA	ALA
	ARG	LEU	LEU	LEU	LEU
	ARG	ARG	GLN	ARG	THR
	THR	LEU	LEU	GLU	GLU
	PRO	LEU	THR	ALA	ALA
	SER	TRP	THR	LEU	THR
	PRO	PHE	THR	GLU	GLU
	ARG	HIS	SER	SER	SER
	ARG	ILE	ILE	PRO	PRO
	ARG	ARG	SER	GLU	GLY
	ARG	CYS	CYS	HIS	HIS
	SER	LEU	LEU	CYS	THR
	GLN	THR	THR	SER	THR
	PRO	PHE	PRO	GLY	ALA
	PRO	ARG	ARG	HIS	THR
	ARG	ARG	ARG	HIS	ALA
	ARG	THR	THR	ALA	THR
	ARG	VAL	VAL	LEU	LEU
	SER	ILE	ILE	ARG	ARG
	GLN	GLN	GLN	ALA	ALA
	SER	TYR	TYR	LEU	THR
	ARG	VAL	VAL	THR	THR

Chain H: 98%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	38292	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	370	Depositor
Maximum defocus (nm)	2560	Depositor
Magnification	75000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	539.136, 539.136, 539.136	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	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	0.25	0/1205	0.42	0/1649
1	B	0.33	1/1242 (0.1%)	0.47	0/1701
1	C	0.27	0/1206	0.44	0/1653
1	D	0.26	0/1231	0.48	0/1687
1	E	0.11	0/20	0.23	0/25
1	F	0.13	0/20	0.34	0/25
1	G	0.10	0/20	0.18	0/25
1	H	0.17	0/20	0.54	0/25
All	All	0.28	1/4964 (0.0%)	0.45	0/6790

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	LEU	C-N	7.58	1.55	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1167	0	1160	24	0
1	B	1207	0	1199	28	0
1	C	1171	0	1155	19	0
1	D	1196	0	1185	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	21	0	16	1	0
1	F	21	0	16	0	0
1	G	21	0	16	0	0
1	H	21	0	16	1	0
All	All	4825	0	4763	79	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 8.

The worst 5 of 79 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:D:2:ASP:OD1	1:D:3:ILE:N	2.12	0.83
1:B:150:ARG:NH1	1:C:143:LEU:O	2.11	0.82
1:D:44:SER:OG	1:D:46:GLU:OE1	1.98	0.80
1:B:112:ARG:HH22	1:A:47:HIS:HE1	1.31	0.78
1:B:5:PRO:HG3	1:A:60:LEU:HD13	1.73	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

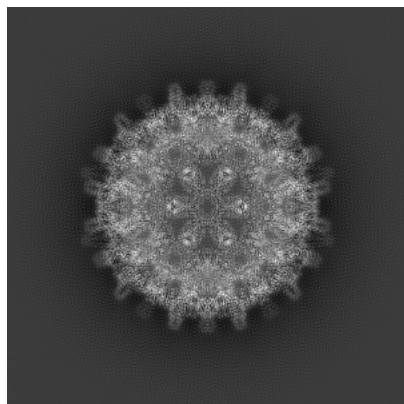
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0272. These allow visual inspection of the internal detail of the map and identification of artifacts.

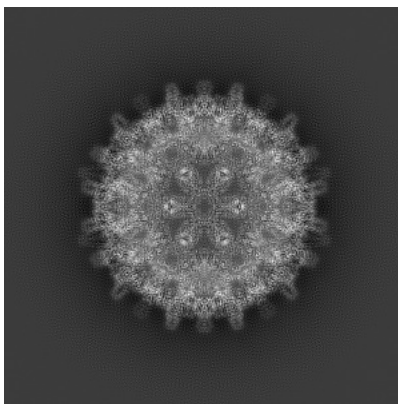
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

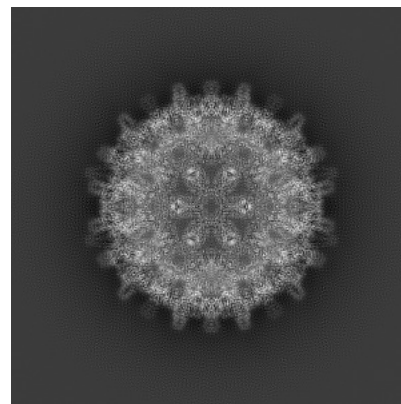
6.1.1 Primary map



X

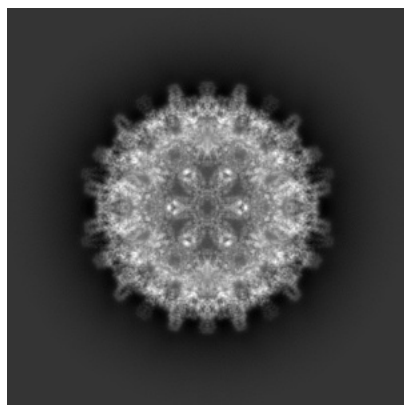


Y

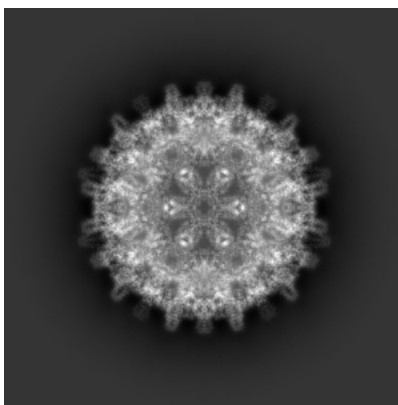


Z

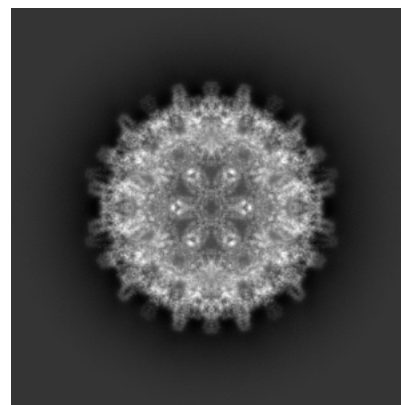
6.1.2 Raw map



X



Y

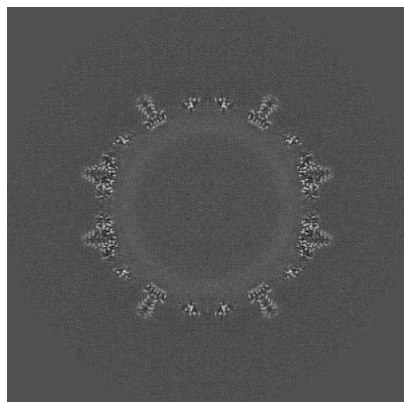


Z

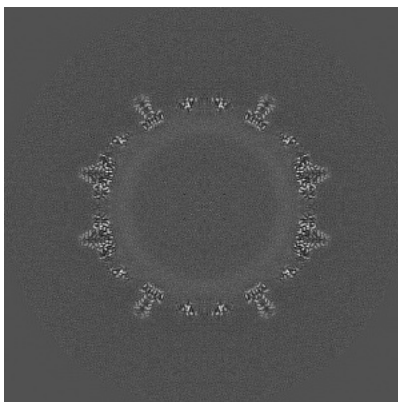
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

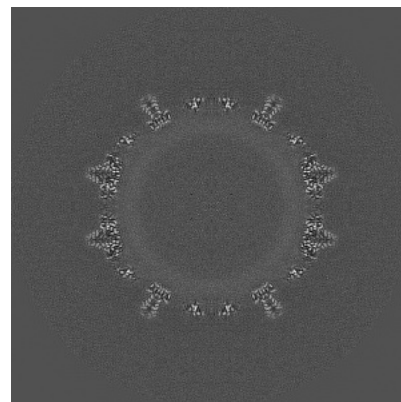
6.2.1 Primary map



X Index: 256

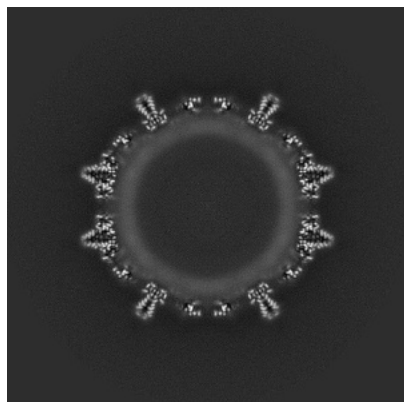


Y Index: 256

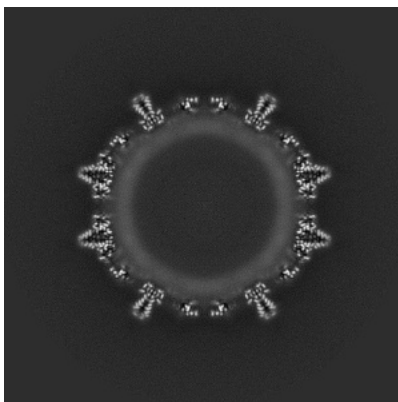


Z Index: 256

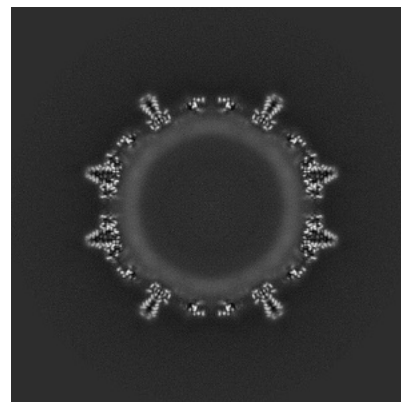
6.2.2 Raw map



X Index: 256



Y Index: 256

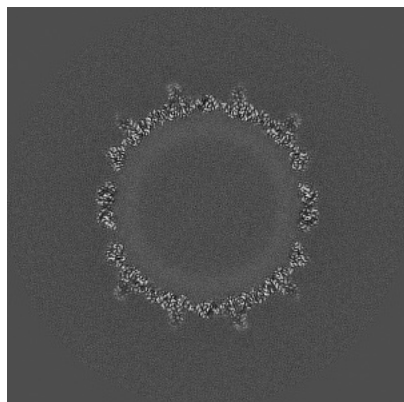


Z Index: 256

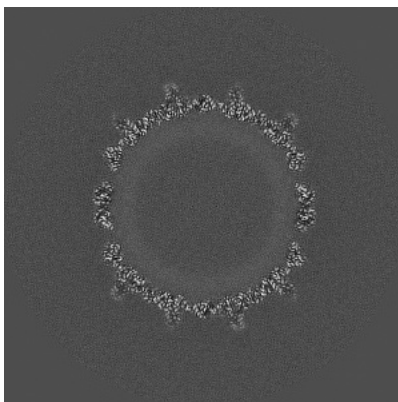
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

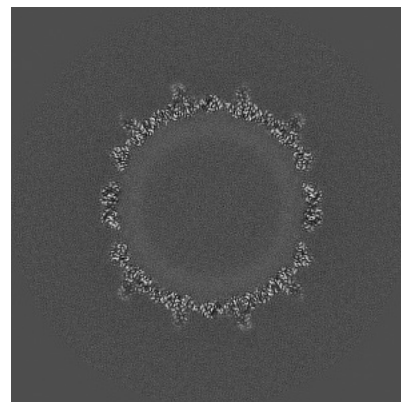
6.3.1 Primary map



X Index: 231

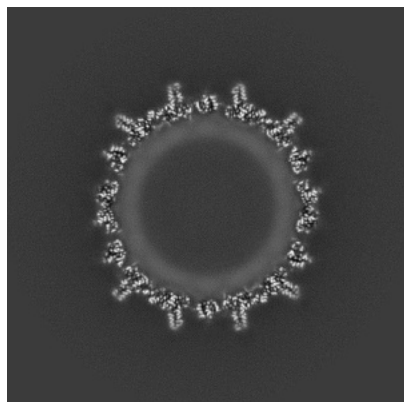


Y Index: 231

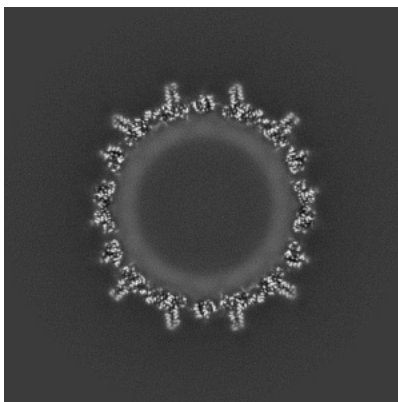


Z Index: 231

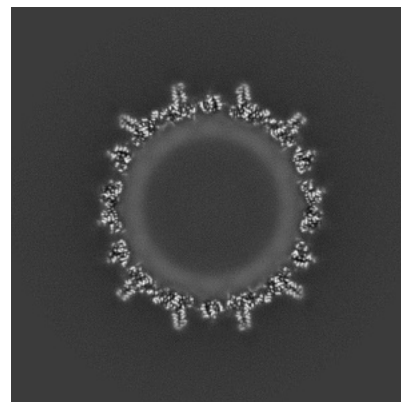
6.3.2 Raw map



X Index: 228



Y Index: 228

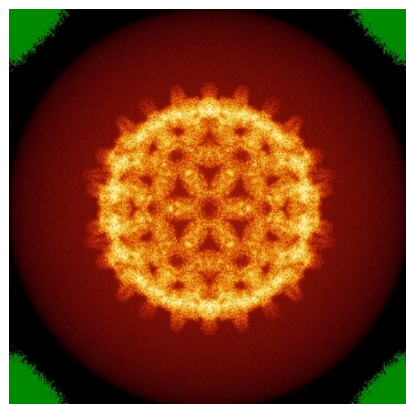


Z Index: 228

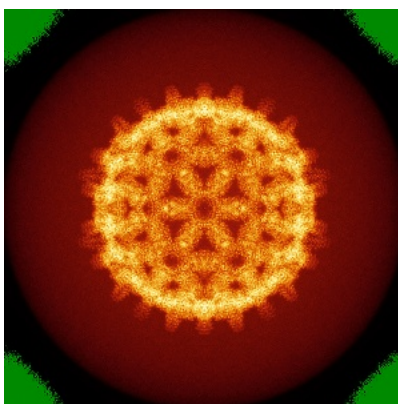
The images above show the largest variance slices of the map in three orthogonal directions.

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

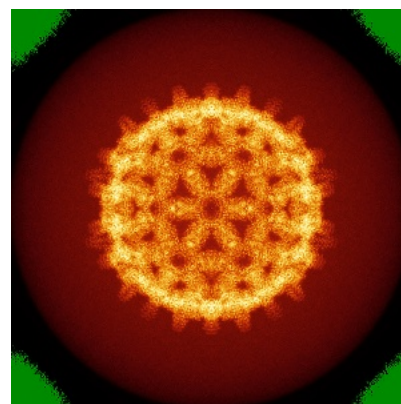
6.4.1 Primary map



X

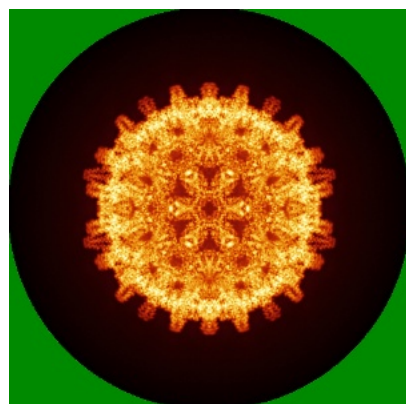


Y

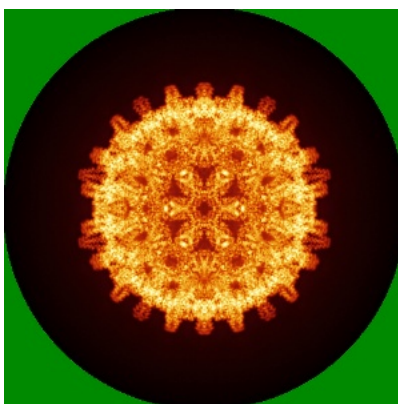


Z

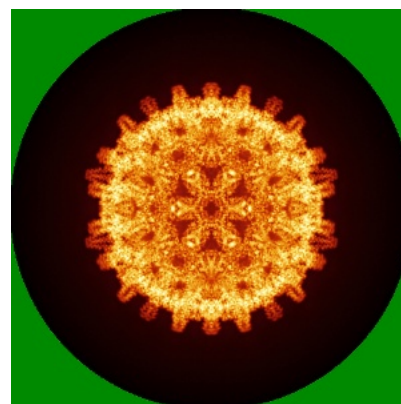
6.4.2 Raw map



X



Y

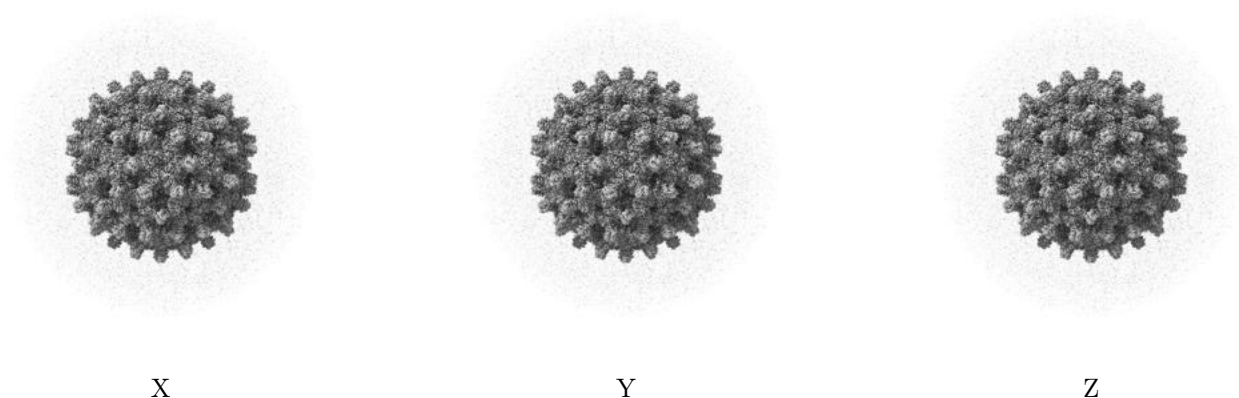


Z

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.

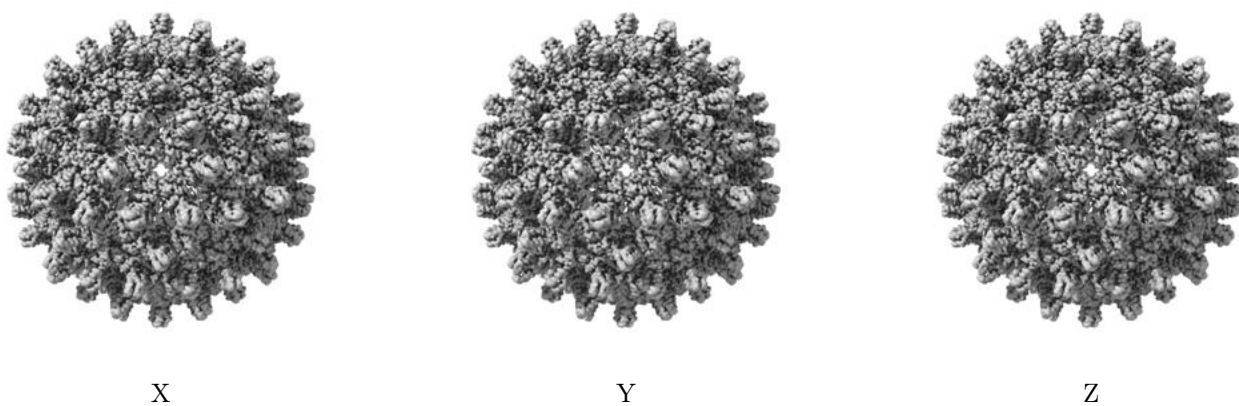
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

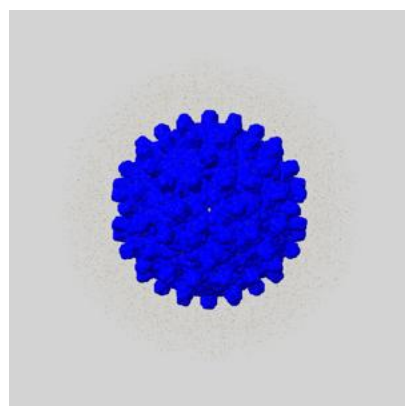
6.6 Mask visualisation [i](#)

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

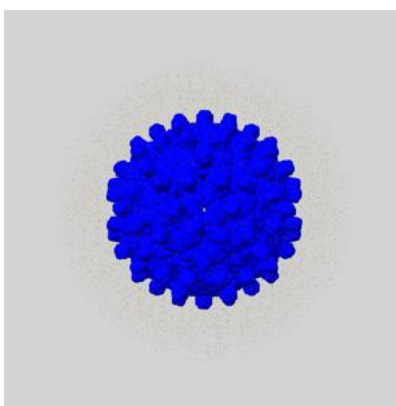
A mask typically either:

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

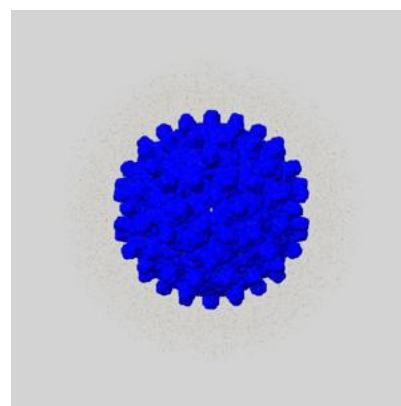
6.6.1 emd_0272_msk_1.map [i](#)



X



Y

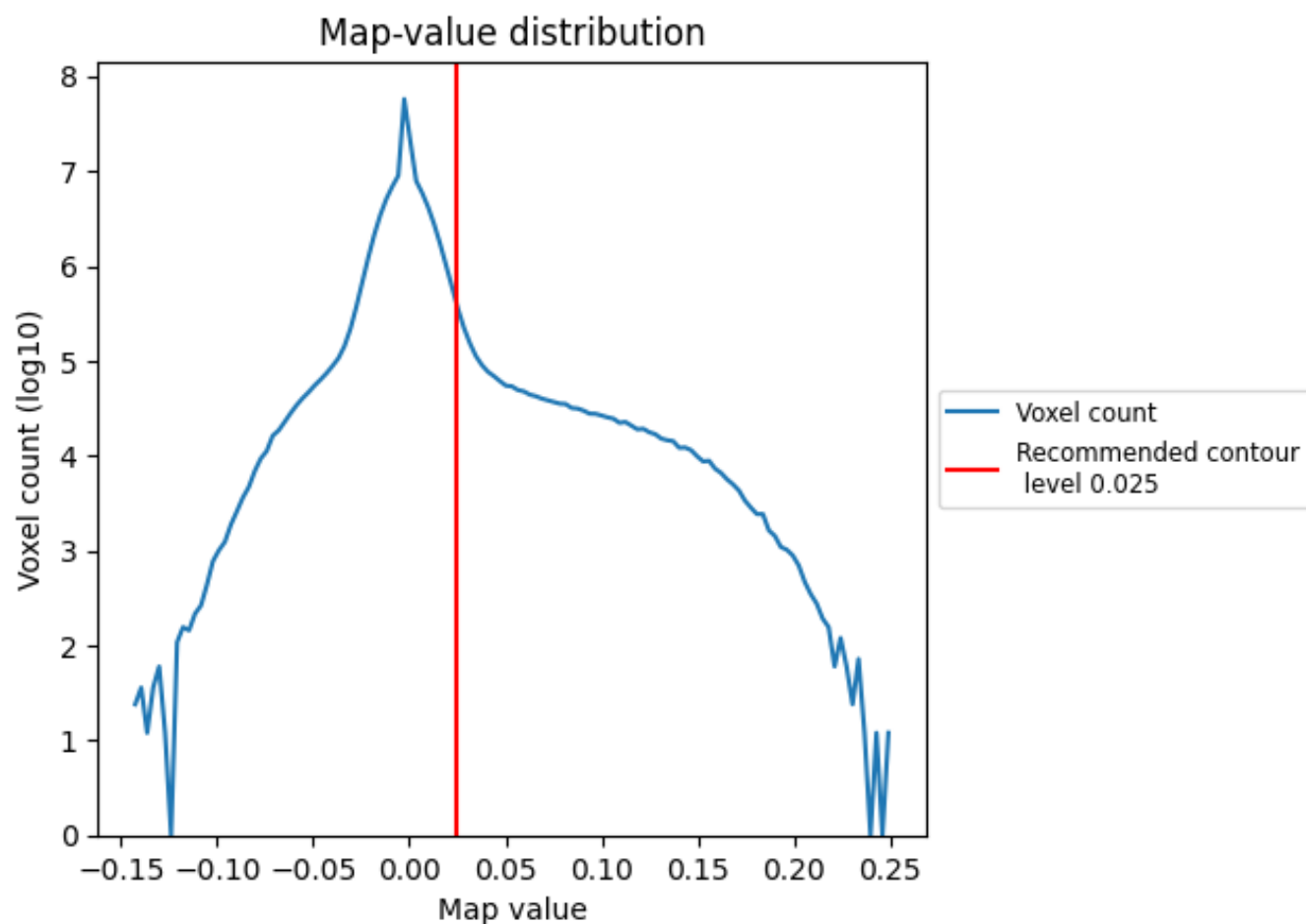


Z

7 Map analysis [i](#)

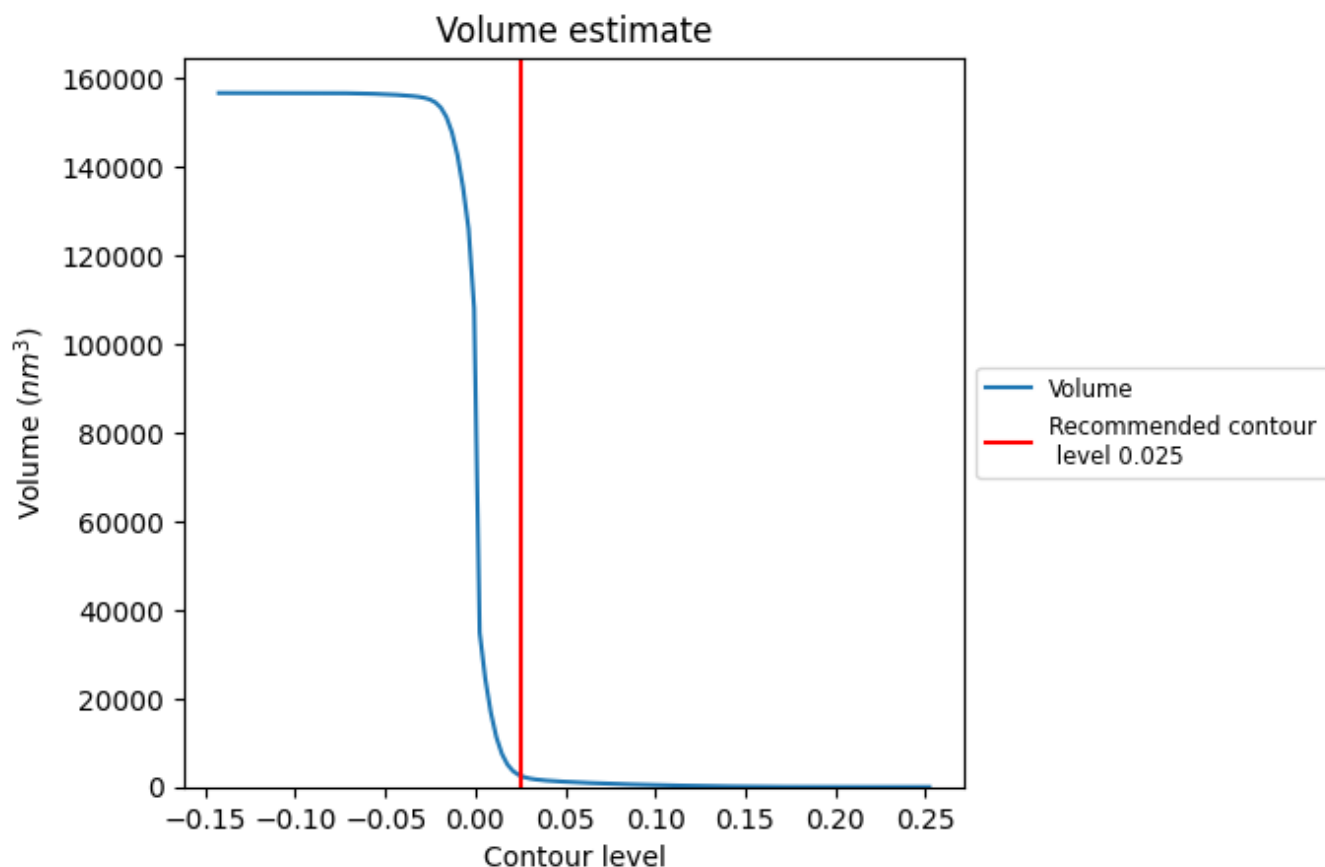
This section contains the results of statistical analysis of the map.

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.

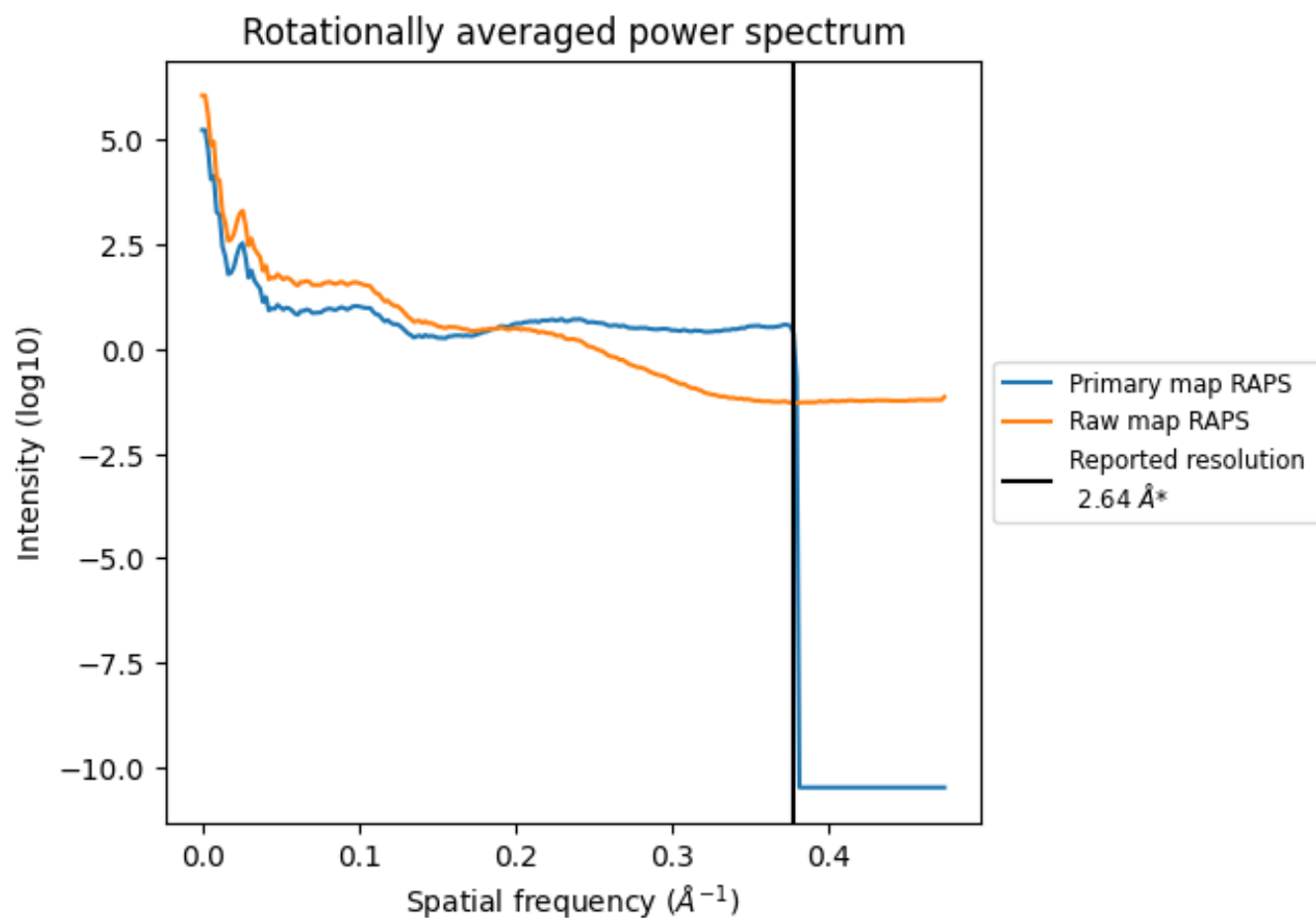
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2577 nm³; this corresponds to an approximate mass of 2328 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 ⓘ

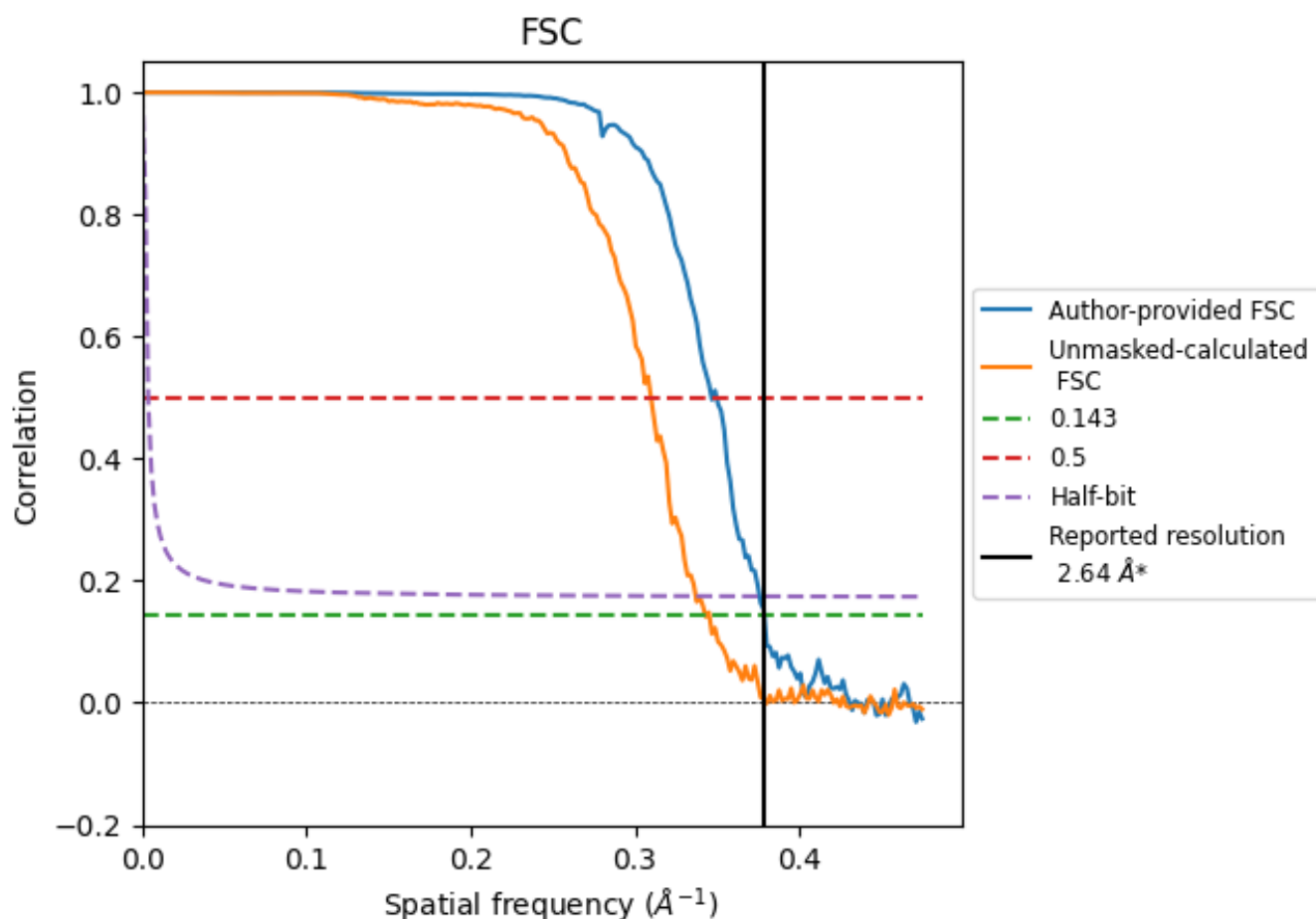


*Reported resolution corresponds to spatial frequency of $0.379 \text{ \AA}^{-1}$

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 0.379 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.64	2.89	2.66
Unmasked-calculated*	2.92	3.23	2.97

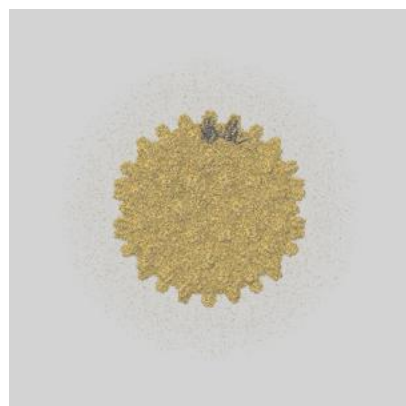
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.92 differs from the reported value 2.64 by more than 10 %

9 Map-model fit [i](#)

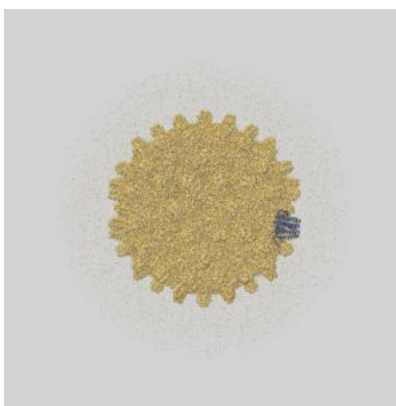
This section contains information regarding the fit between EMDB map EMD-0272 and PDB model 6HU4. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

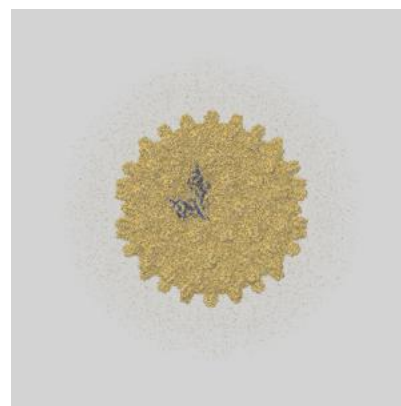
9.1.1 Map-model overlay [i](#)



X

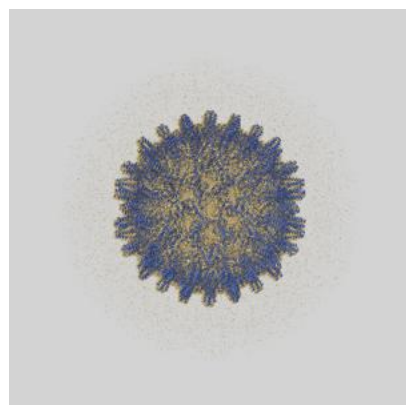


Y

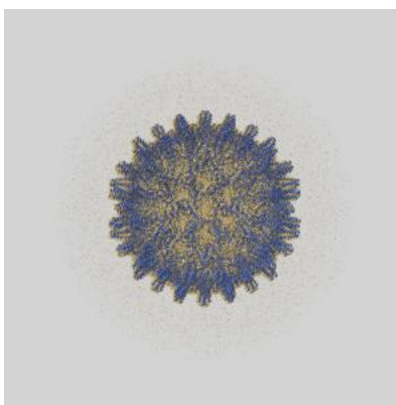


Z

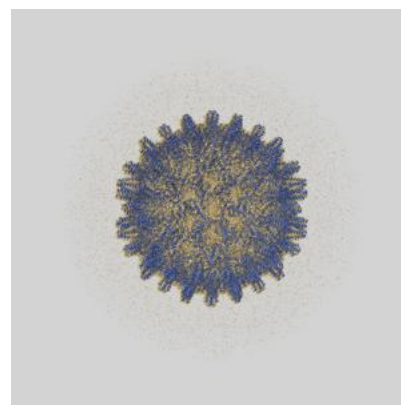
9.1.2 Map-model assembly overlay [i](#)



X



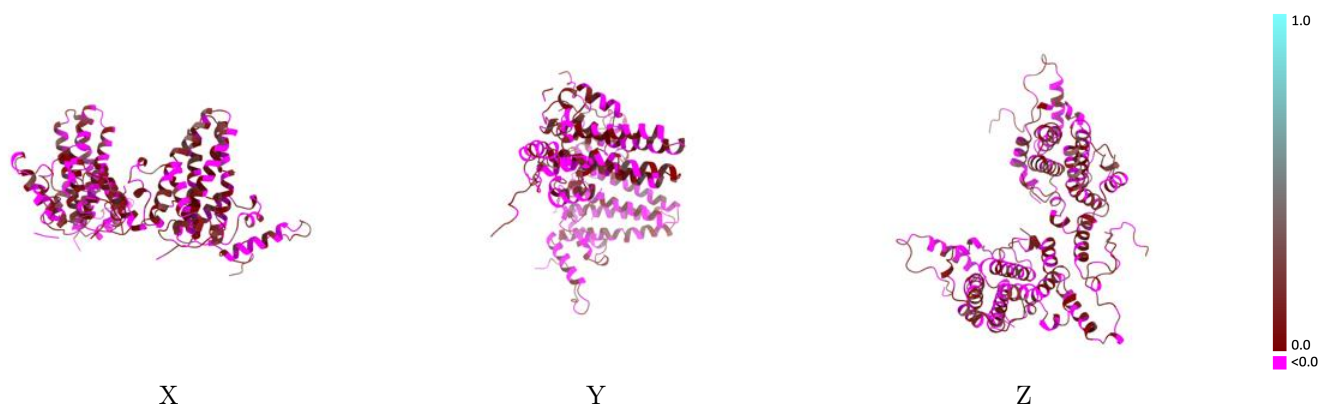
Y



Z

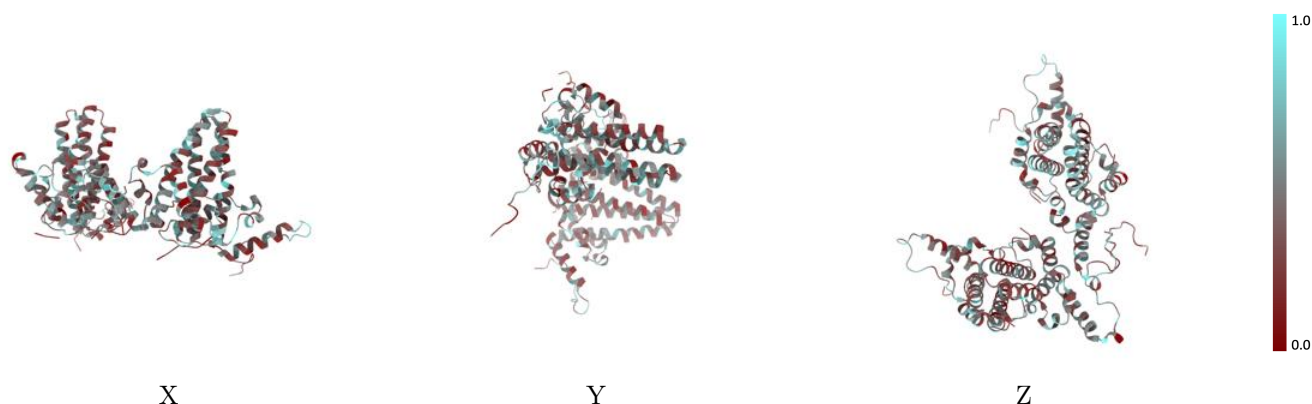
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



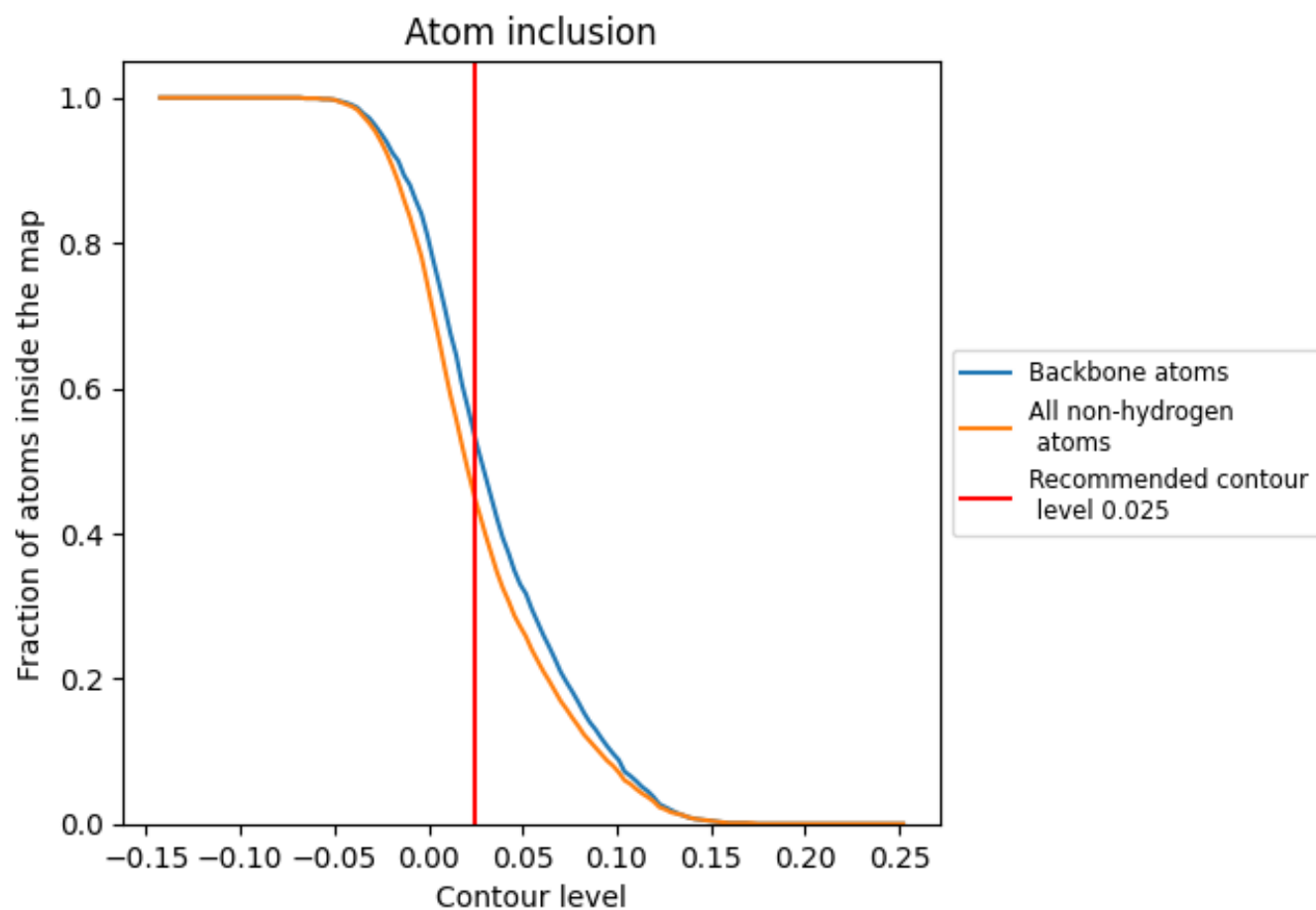
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 44% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4450	0.0470
A	0.4240	0.0270
B	0.4410	0.0400
C	0.4640	0.0560
D	0.4730	0.0650
E	0.1910	0.1070
F	0.0480	-0.1010
G	0.1910	0.0720
H	0.1910	0.1040

1.0

0.0

<0.0