



## wwPDB EM Validation Summary Report ⓘ

Oct 8, 2024 – 02:29 pm BST

PDB ID : 8R0F  
EMDB ID : EMD-18791  
Title : Capsid structure of Giardavirus (GLV) HP strain  
Authors : Wang, H.; Gianluca, M.; Munke, A.; Hassan, M.M.; Lalle, M.; Okamoto, K.  
Deposited on : 2023-10-31  
Resolution : 2.14 Å (reported)  
Based on initial model : 6S2C

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

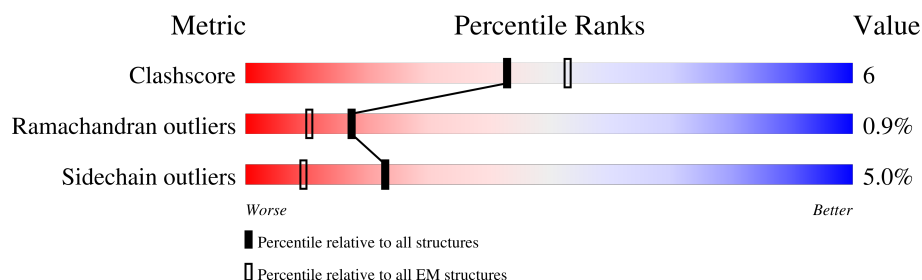
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.14 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  $\geq 3$ , 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	929	
1	B	929	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12852 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	858	Total	C	N	O	S	0	0
			6753	4332	1130	1264	27		
1	A	775	Total	C	N	O	S	0	0
			6099	3921	1020	1133	25		

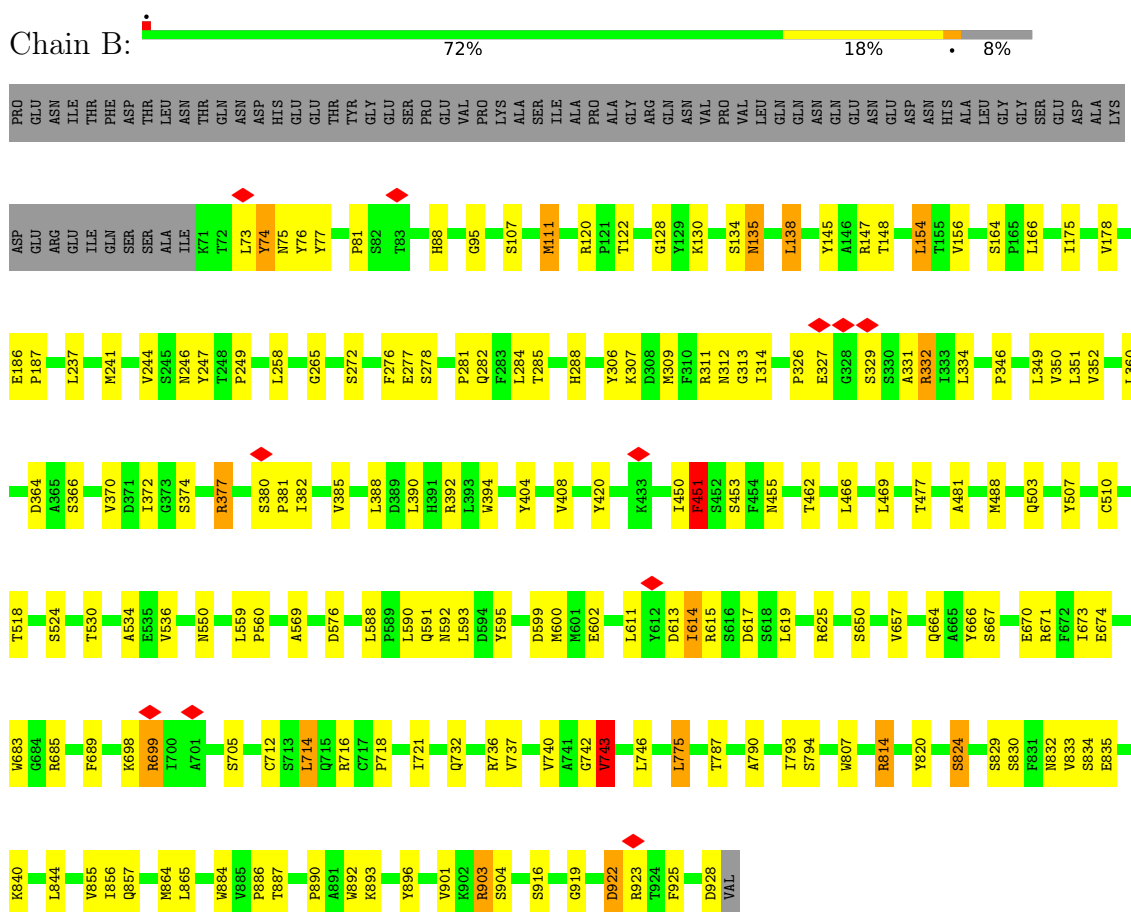
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	178	VAL	UNK	conflict	UNP A0A8F6AHR5
B	516	ASN	UNK	conflict	UNP A0A8F6AHR5
B	684	GLY	UNK	conflict	UNP A0A8F6AHR5
B	793	ILE	LEU	conflict	UNP A0A8F6AHR5
A	178	VAL	UNK	conflict	UNP A0A8F6AHR5
A	516	ASN	UNK	conflict	UNP A0A8F6AHR5
A	684	GLY	UNK	conflict	UNP A0A8F6AHR5
A	793	ILE	LEU	conflict	UNP A0A8F6AHR5

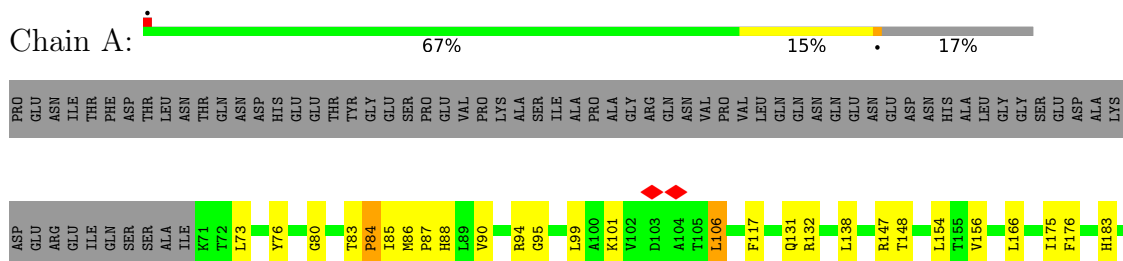
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Capsid protein



#### • Molecule 1: Capsid protein



LEU	SER	R739	A569	P187
	ASP	ASP	T369	H188
ASP	PRO	VAL	A578	M189
VAL	TYR	ALA	L596	E198
	TYR	GLY	M601	S380
	GLU	R743		
	GLU	L746	T608	P382
	SER	Q747		
	THR	Q747	T608	D384
	THR	Q747		
	THR	D754	L619	V385
	VAL	L763		
	VAL	L763	S621	T220
	SER	G764		
	ALA	T765	L643	P419
	ASP	T765		
	ASN	R770	V646	D227
	GLU	T770		
	TRP	T787	V657	T231
	VAL	T788		
	PRO	C789	S659	G434
	THR	T789		
	SER	T800	S667	L284
	GLY	T800		
	PRO	T806	V659	E439
	ALA	T806		
	TRP	A815	R671	L258
	LYS	A815		
	VAL	Y820	E674	F451
	PRO	T821		
	TYR	S824	R685	T462
	LEU	S824		
	GLU	S830	C686	Y307
	ASN	S830		
	VAL	E835	R699	M309
	LYS	E835		
	ARG	F838	A701	R311
	SER	N839		
	GLY	T840	G702	I314
	ARG	T841		
	ARG	T842	A794	S318
	LEU	T842		
	LEU	D849	S519	E327
	ALA	ASP		
	GLU	THR	L714	G328
	LEU	SER		
	ARG	GLN	Q715	S329
	ILE	THR		
	ALA	THR	C717	S330
	SER	ILE		
	ASN	ASN	P718	M344
	ASN	ASN		
	GLY	LEU	L719	T330
	SER	SER		
	ASP	MET	W721	T531
	PRO	GLN		
	THR	PHE	M723	T533
	PHE	PHE		
			G727	S362
			R736	A365

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28342	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.547	Depositor
Minimum map value	-3.394	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.227	Depositor
Recommended contour level	0.68	Depositor
Map size (Å)	678.39996, 678.39996, 678.39996	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.71	2/6269 (0.0%)	0.80	5/8561 (0.1%)
1	B	0.29	0/6940	0.52	0/9479
All	All	0.53	2/13209 (0.0%)	0.67	5/18040 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	SER	C-N	-42.53	0.36	1.34
1	A	209	LYS	C-N	-28.57	0.68	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LYS	O-C-N	-32.68	70.42	122.70
1	A	208	SER	CA-C-N	-31.71	47.45	117.20
1	A	208	SER	C-N-CA	-28.88	49.51	121.70
1	A	209	LYS	CA-C-N	13.38	146.63	117.20
1	A	208	SER	O-C-N	-9.85	106.94	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	SER	Mainchain
1	A	209	LYS	Mainchain
1	A	83	THR	Peptide
1	B	450	ILE	Peptide

## 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	6099	0	5984	68	0
1	B	6753	0	6611	99	0
All	All	12852	0	12595	162	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 6.

The worst 5 of 162 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:B:73:LEU:HD23	1:B:74:TYR:H	1.39	0.87
1:B:503:GLN:NE2	1:B:714:LEU:O	2.08	0.86
1:B:122:THR:HG23	1:B:145:TYR:HB3	1.70	0.72
1:B:380:SER:HB2	1:B:840:LYS:HD2	1.72	0.71
1:B:312:ASN:HB3	1:A:314:ILE:HD12	1.74	0.69

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	771/929 (83%)	725 (94%)	39 (5%)	7 (1%)	14	8
1	B	856/929 (92%)	800 (94%)	49 (6%)	7 (1%)	16	10
All	All	1627/1858 (88%)	1525 (94%)	88 (5%)	14 (1%)	17	8

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	614	ILE
1	A	210	THR
1	A	824	SER
1	B	743	VAL
1	A	209	LYS

### 5.3.2 Protein sidechains ⓘ

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	677/811 (84%)	639 (94%)	38 (6%)	17	13
1	B	750/811 (92%)	716 (96%)	34 (4%)	23	19
All	All	1427/1622 (88%)	1355 (95%)	72 (5%)	23	16

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	658	THR
1	A	849	ASP
1	A	667	SER
1	A	716	ARG
1	B	743	VAL

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	209:LYS	C	210:THR	N	0.68
1	A	208:SER	C	209:LYS	N	0.36

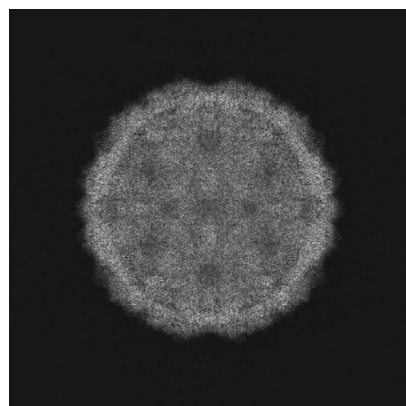
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18791. These allow visual inspection of the internal detail of the map and identification of artifacts.

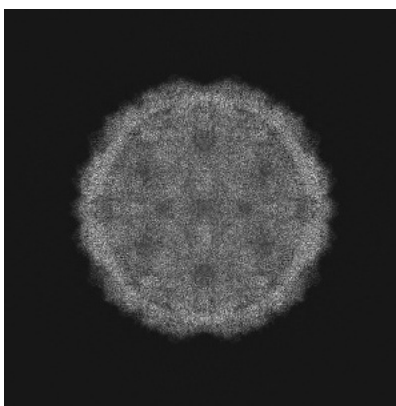
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

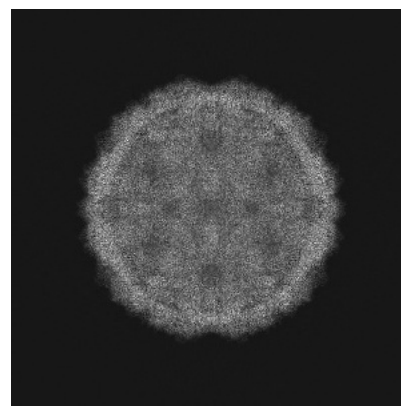
#### 6.1.1 Primary map



X

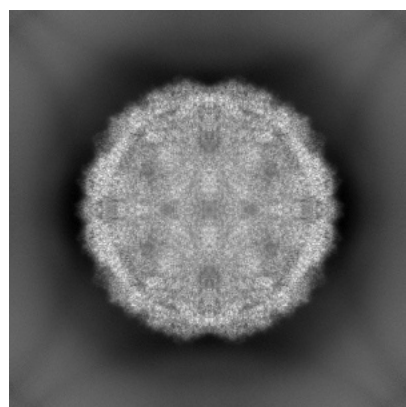


Y

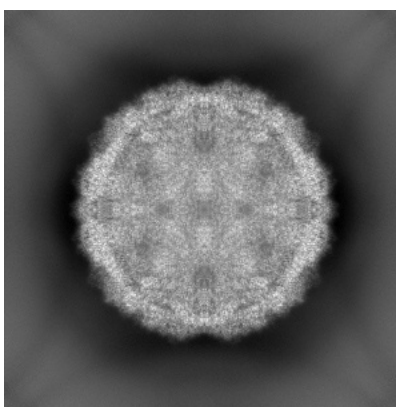


Z

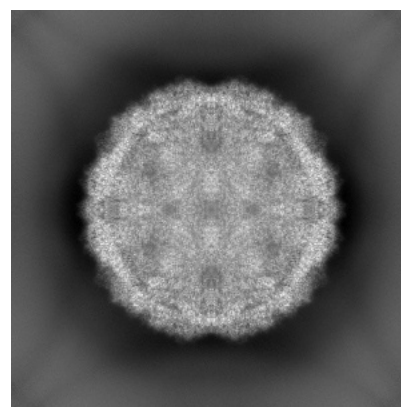
#### 6.1.2 Raw map



X



Y

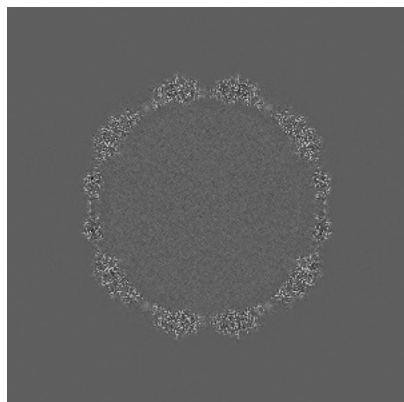


Z

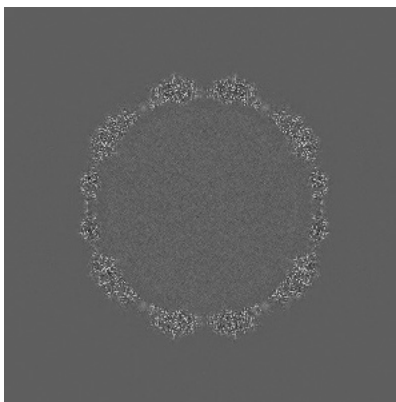
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

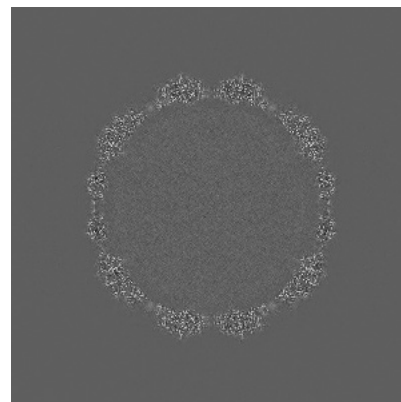
### 6.2.1 Primary map



X Index: 320

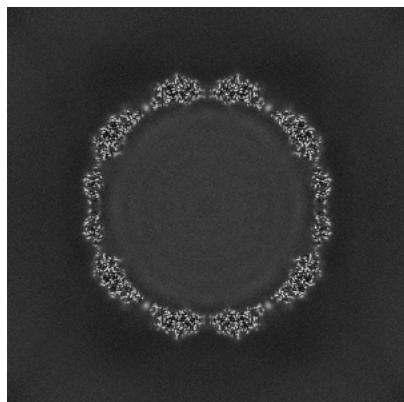


Y Index: 320

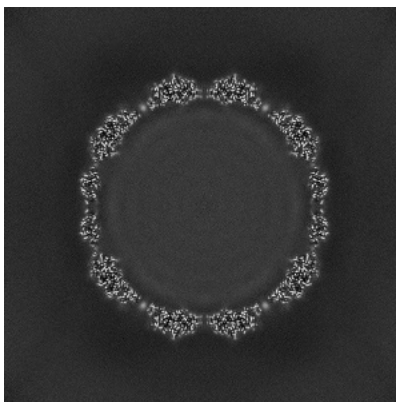


Z Index: 320

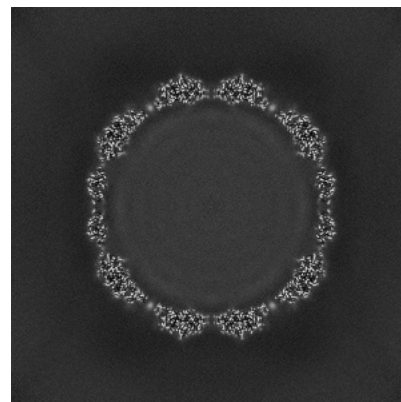
### 6.2.2 Raw map



X Index: 320



Y Index: 320

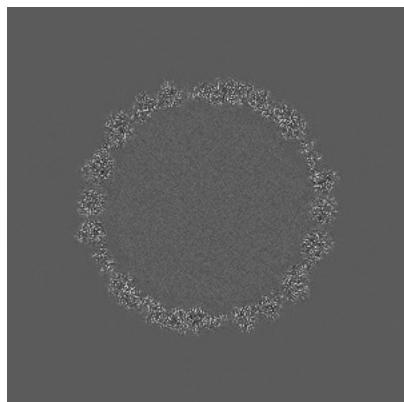


Z Index: 320

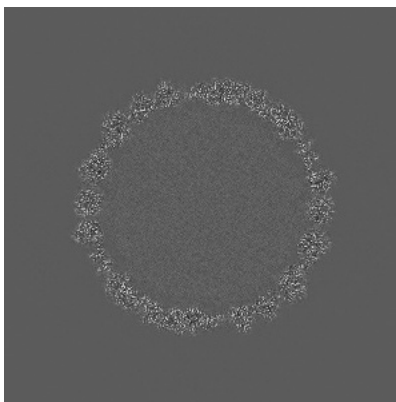
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

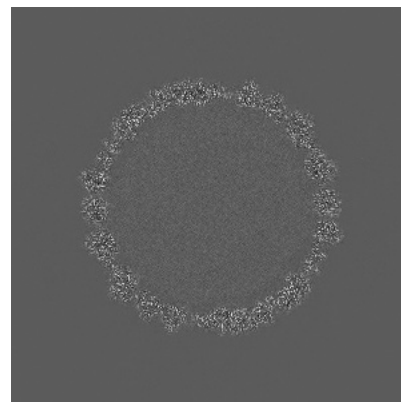
### 6.3.1 Primary map



X Index: 287

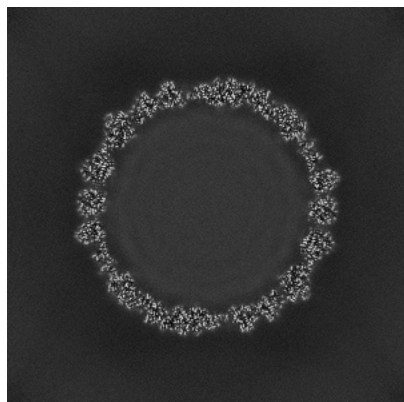


Y Index: 287

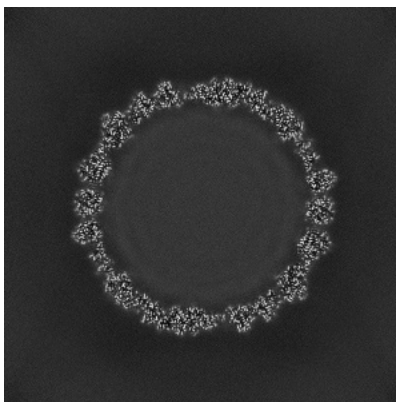


Z Index: 353

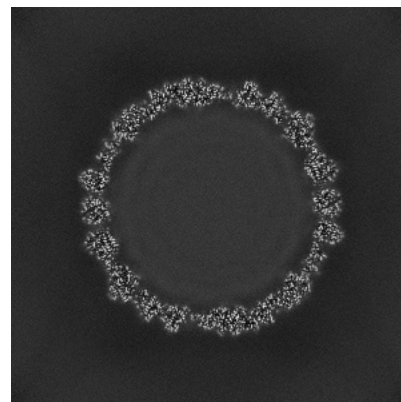
### 6.3.2 Raw map



X Index: 286



Y Index: 286

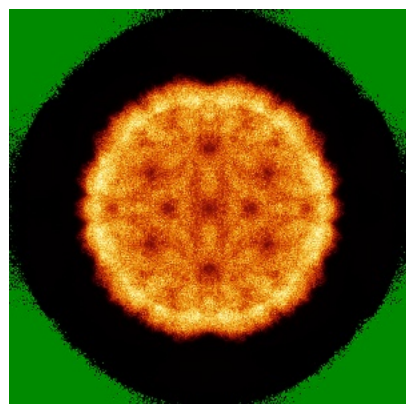


Z Index: 354

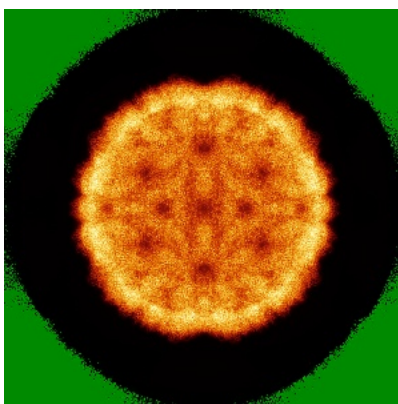
The images above show the largest variance slices of the map in three orthogonal directions.

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

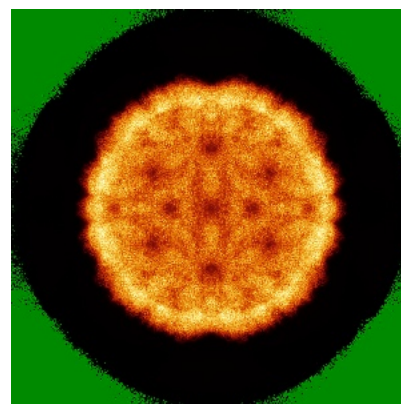
### 6.4.1 Primary map



X

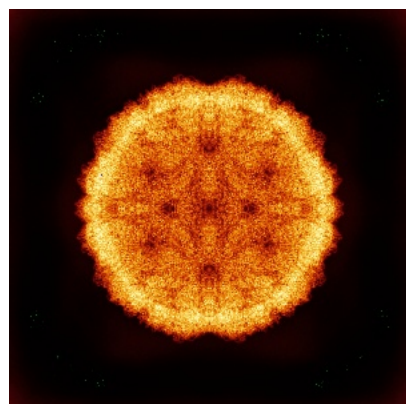


Y

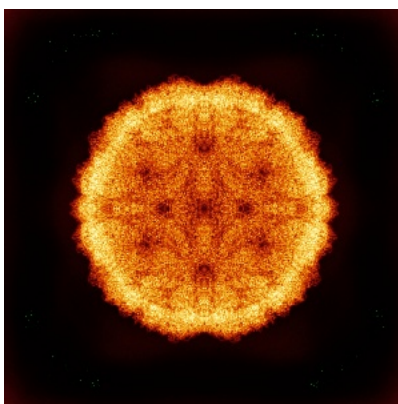


Z

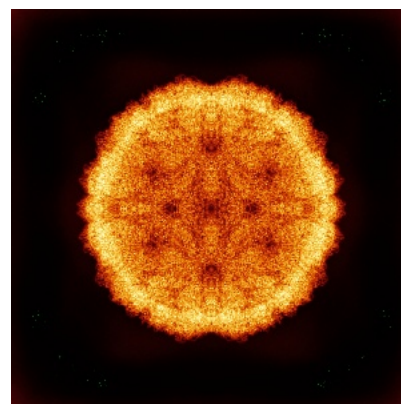
### 6.4.2 Raw map



X



Y



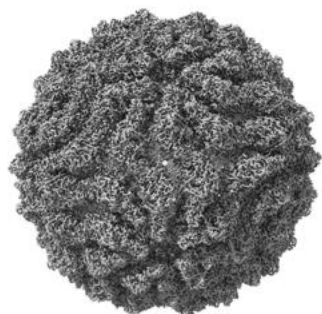
Z

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.

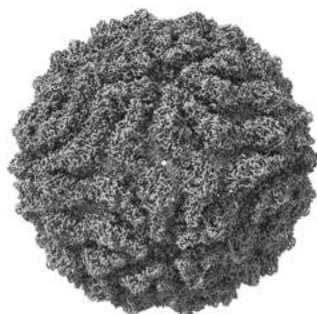


## 6.5 Orthogonal surface views [i](#)

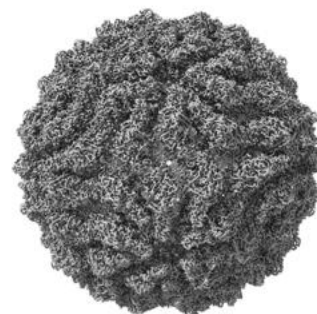
### 6.5.1 Primary map



X



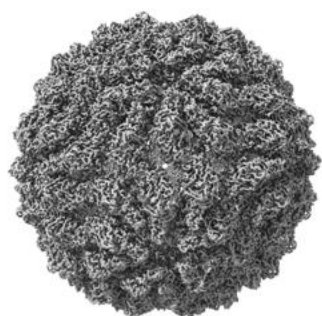
Y



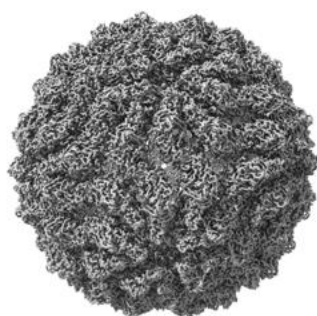
Z

The images above show the 3D surface view of the map at the recommended contour level 0.68. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

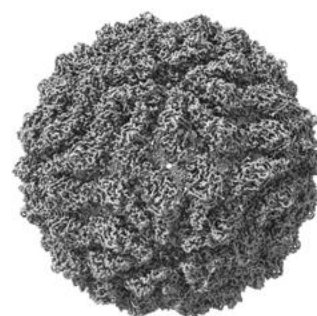
### 6.5.2 Raw map



X



Y



Z

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.

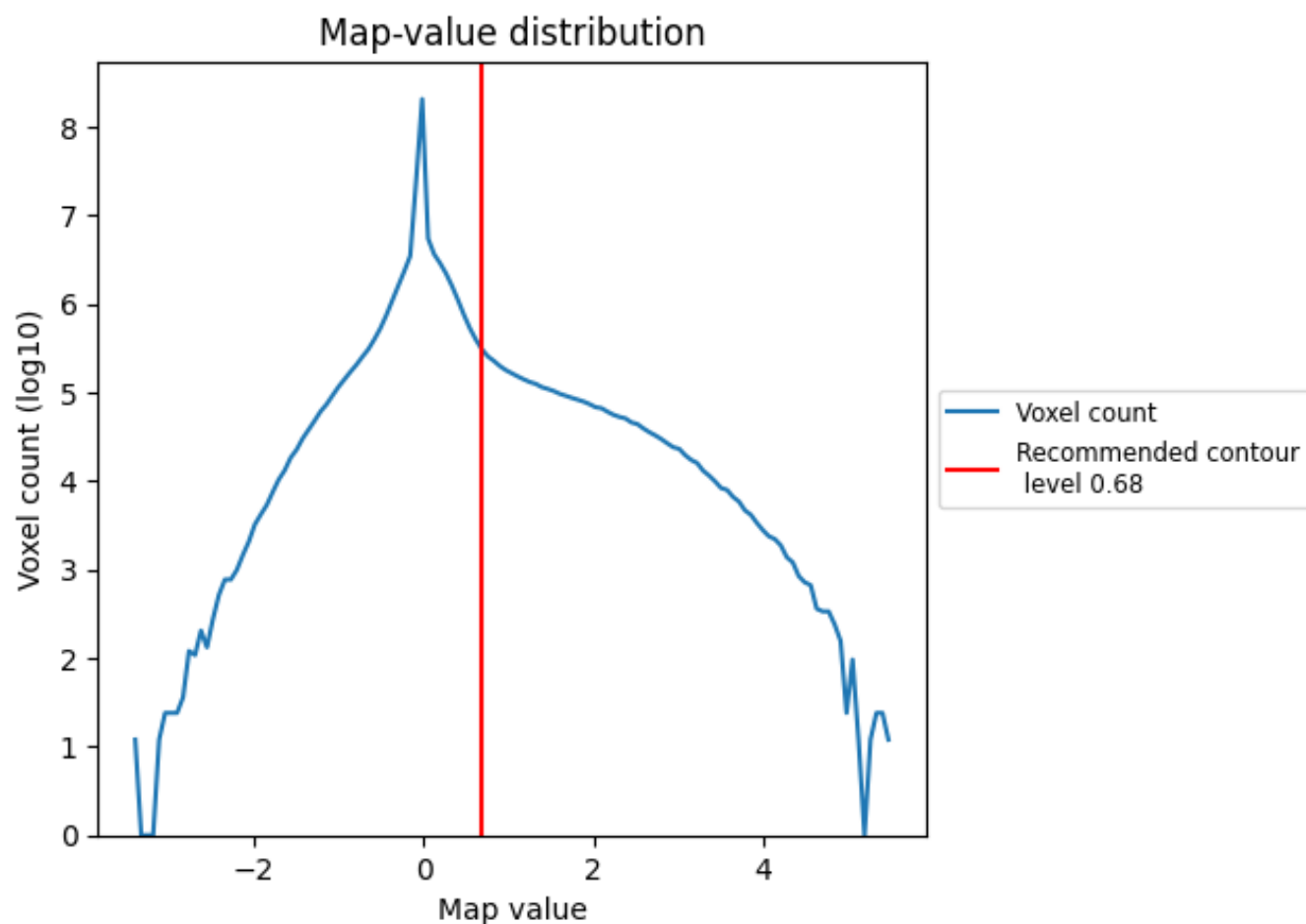
## 6.6 Mask visualisation [i](#)

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.

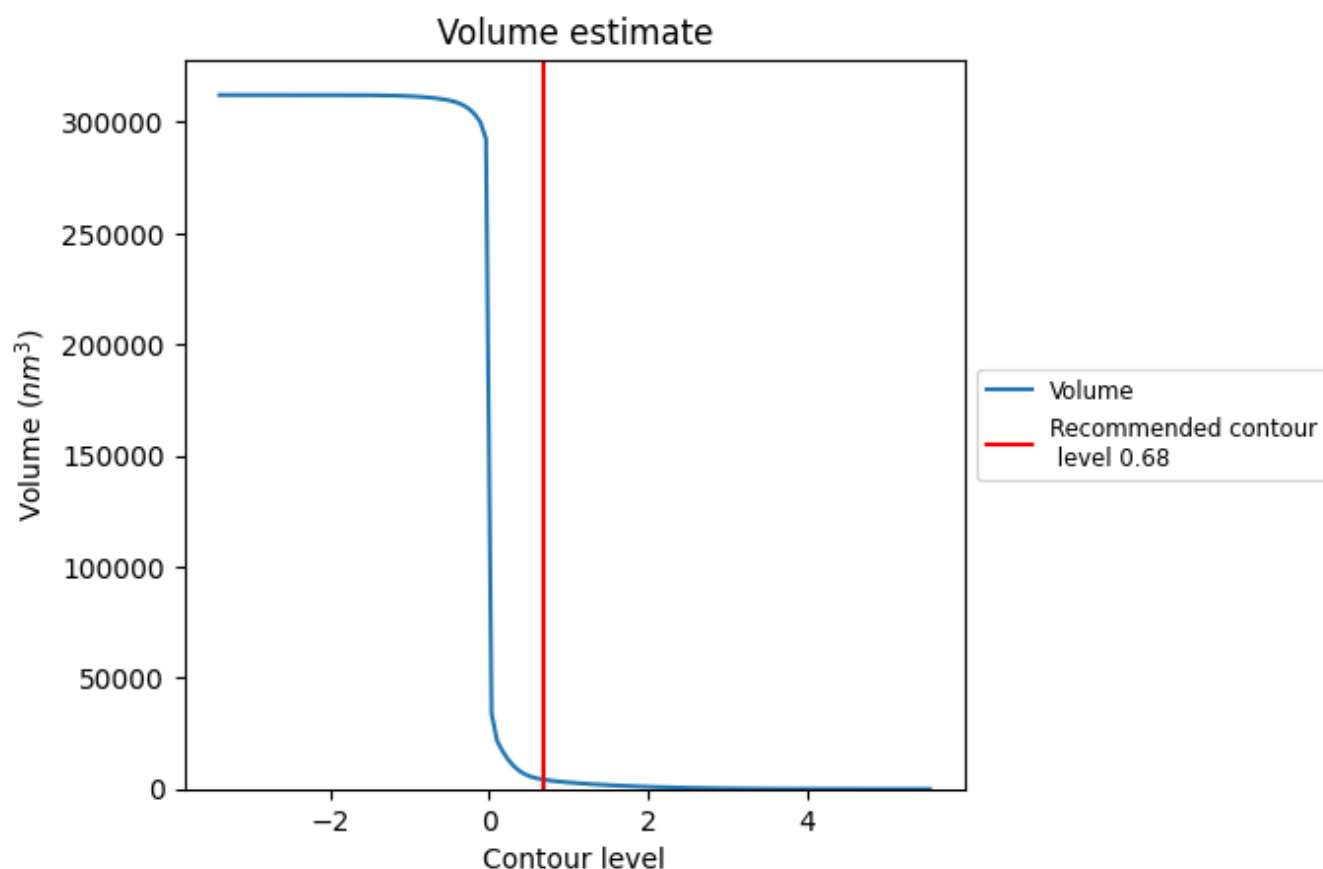
### 7.1 Map-value distribution [i](#)



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.



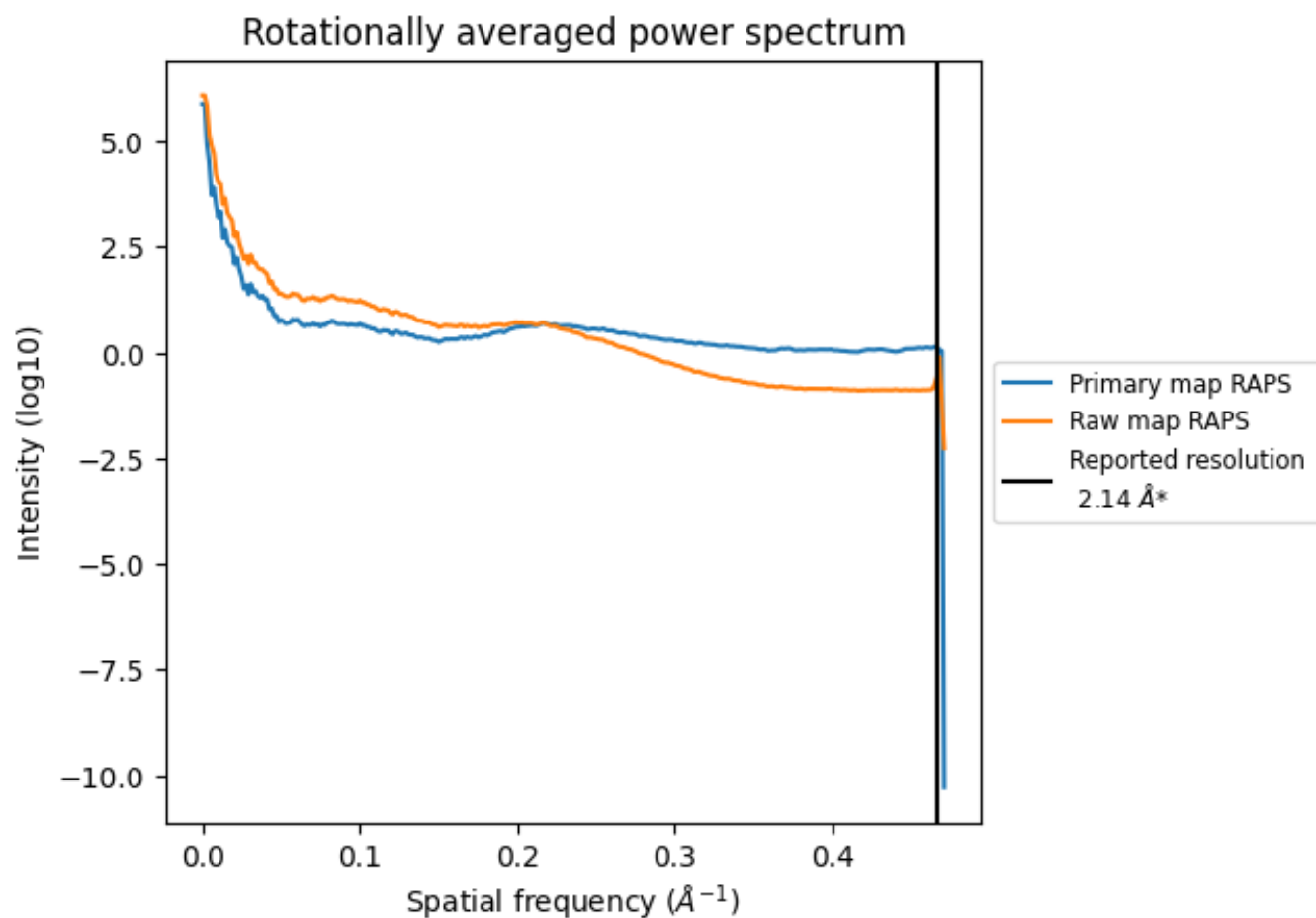
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4229 nm<sup>3</sup>; this corresponds to an approximate mass of 3820 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 ⓘ

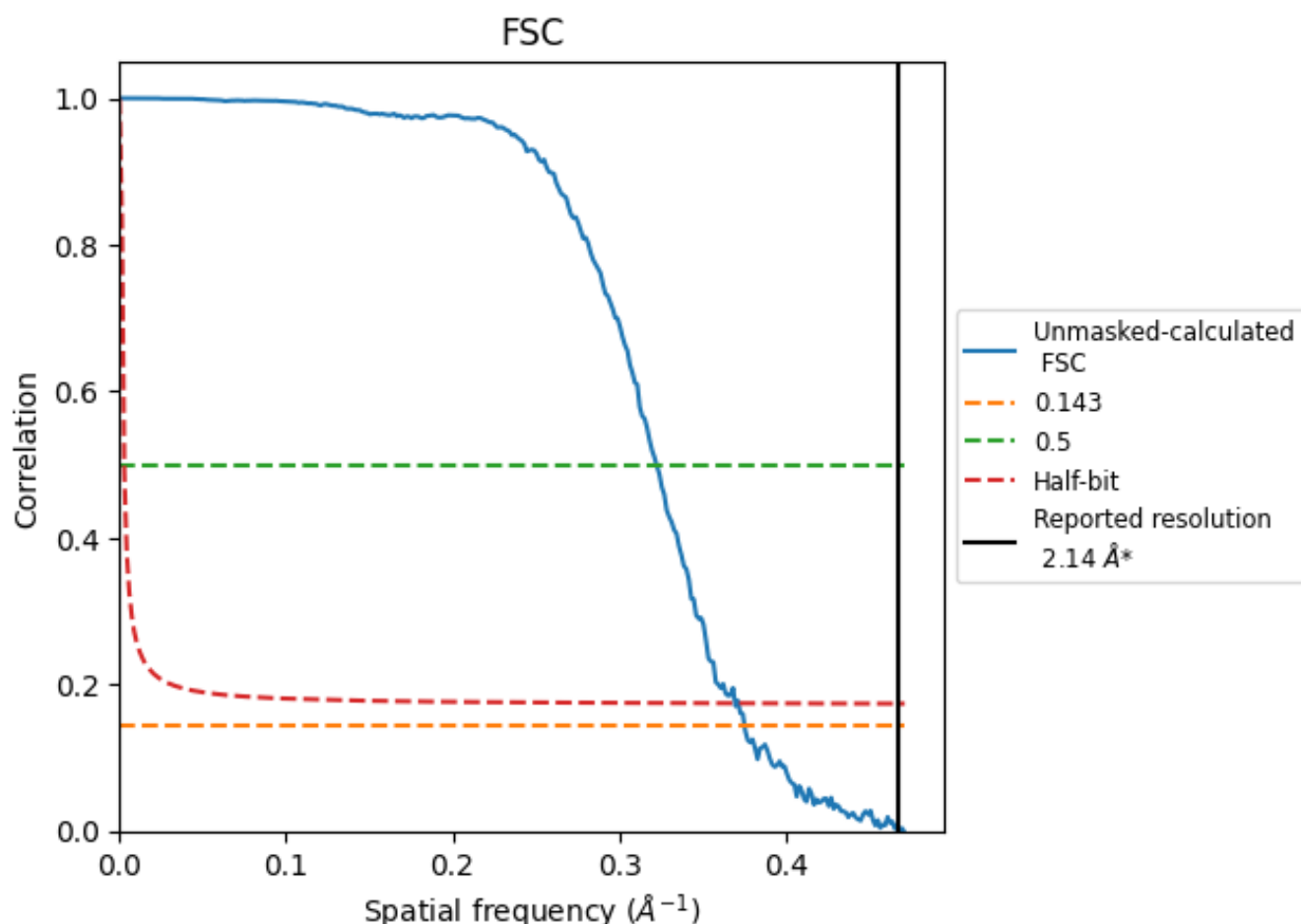


\*Reported resolution corresponds to spatial frequency of  $0.467 \text{ \AA}^{-1}$

## 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 0.467 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.66	3.10	2.70

\*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 2.66 differs from the reported value 2.14 by more than 10 %

## 9 Map-model fit [i](#)

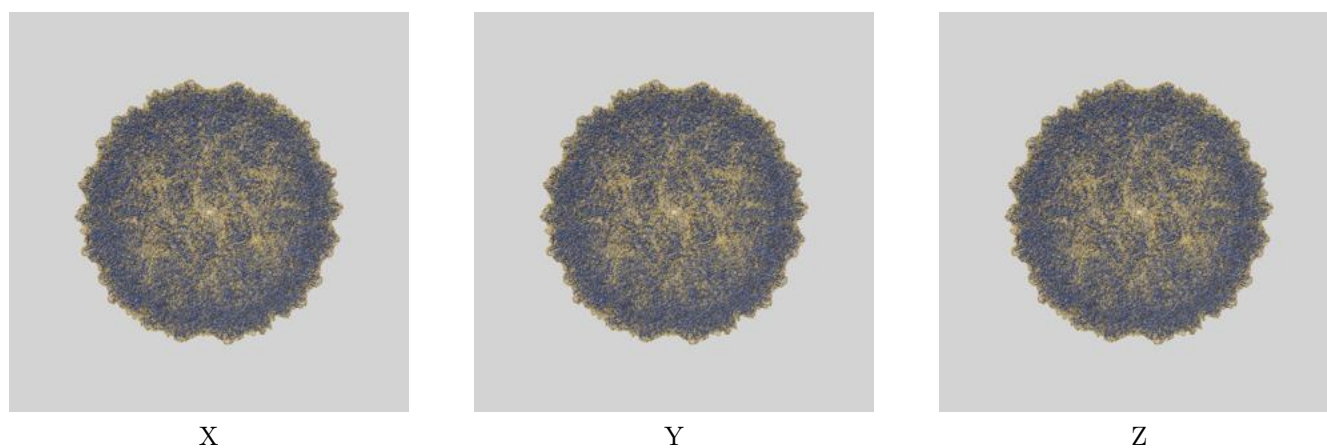
This section contains information regarding the fit between EMDB map EMD-18791 and PDB model 8R0F. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

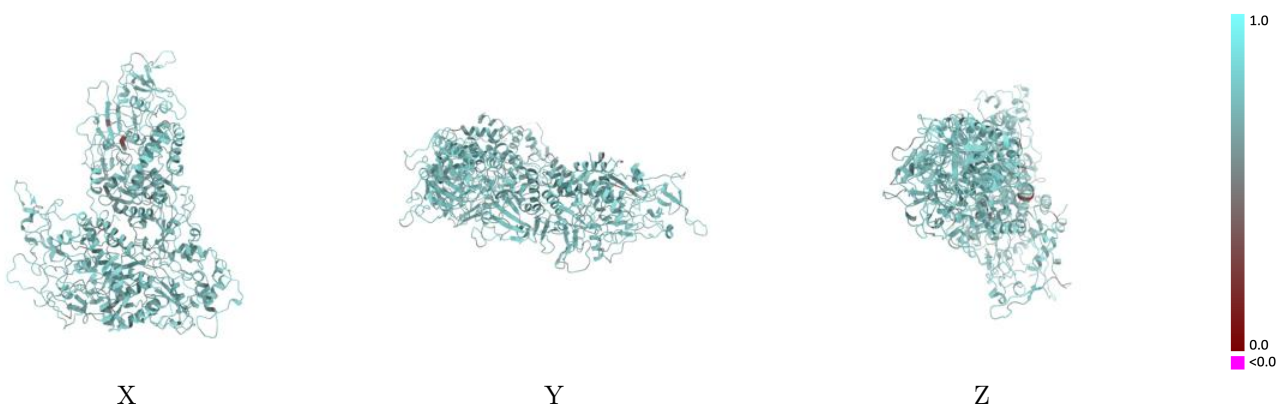


#### 9.1.2 Map-model assembly overlay [i](#)



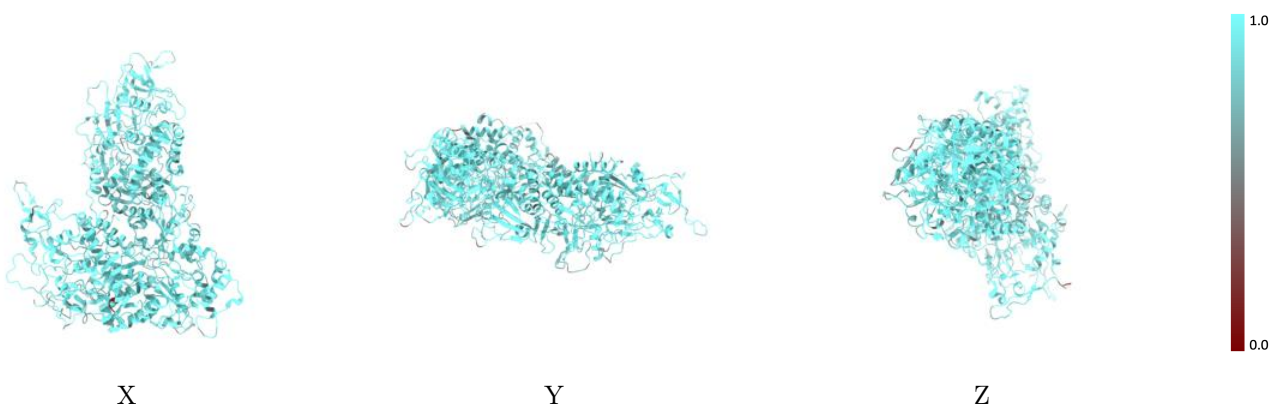
The images above show the 3D surface view of the map at the recommended contour level 0.68 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



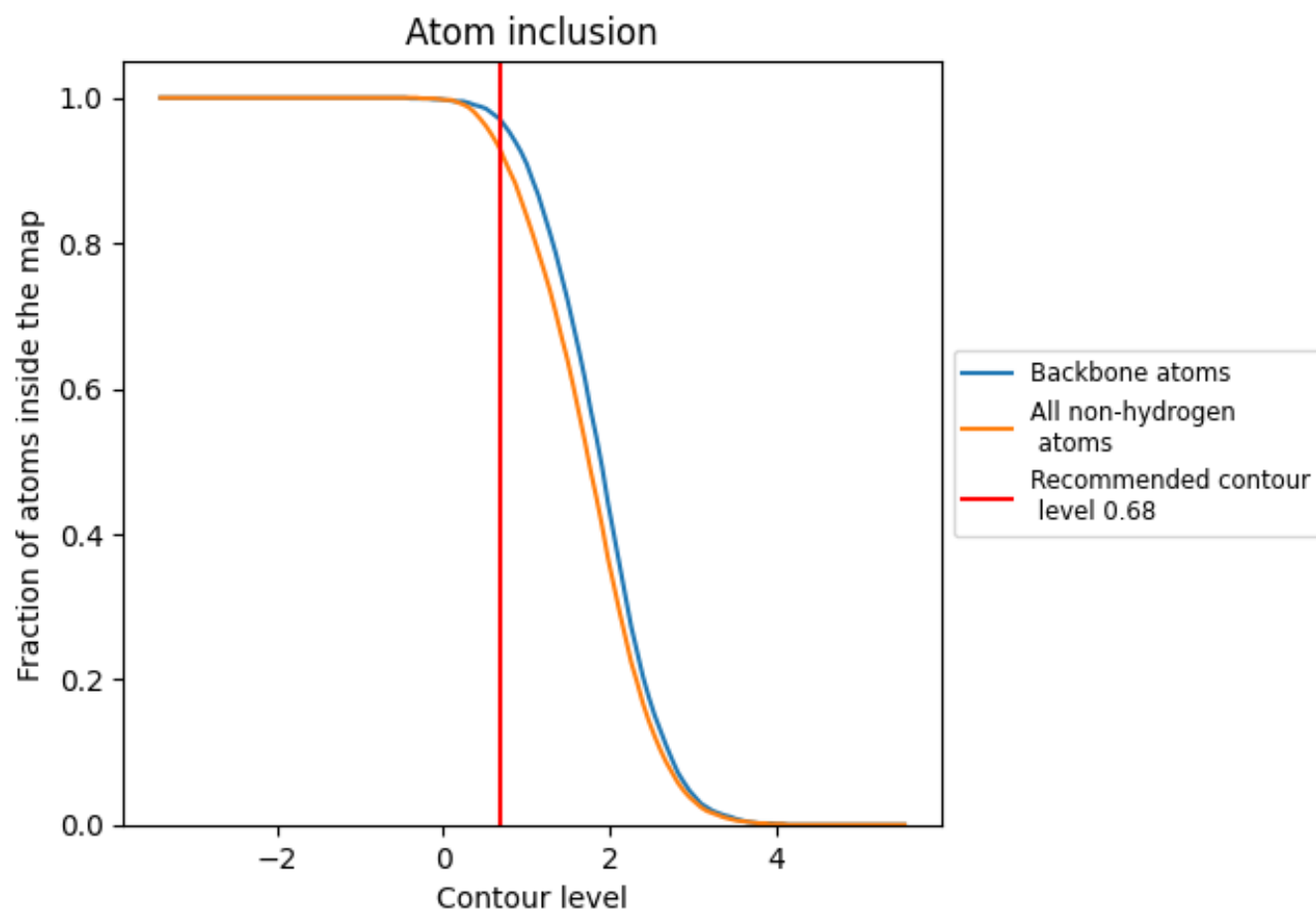
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.68).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.68) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9310	<div></div> 0.6990
A	<div></div> 0.9280	<div></div> 0.6960
B	<div></div> 0.9340	<div></div> 0.7020

