



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:55 PM UTC

PDB ID : 8R0G / pdb_00008r0g
EMDB ID : EMD-18792
Title : Capsid structure of Giardavirus (GLV) CAT strain
Authors : Wang, H.; Gianluca, M.; Munke, A.; Hassan, M.M.; Lalle, M.; Okamoto, K.
Deposited on : 2023-10-31
Resolution : 2.60 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

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

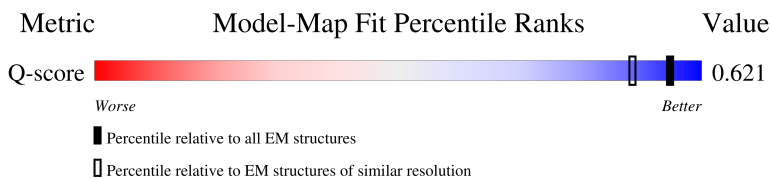
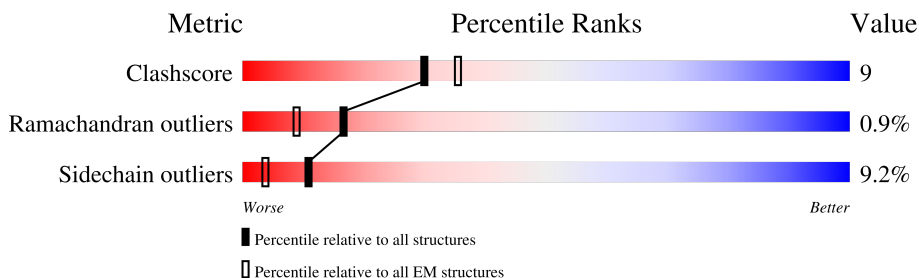
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	929	 67% 23% • 8%
1	B	929	 67% 21% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13445 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	A	855	Total	C	N	O	S	0	0
			6732	4320	1124	1260	28		
1	B	853	Total	C	N	O	S	0	0
			6713	4305	1124	1256	28		

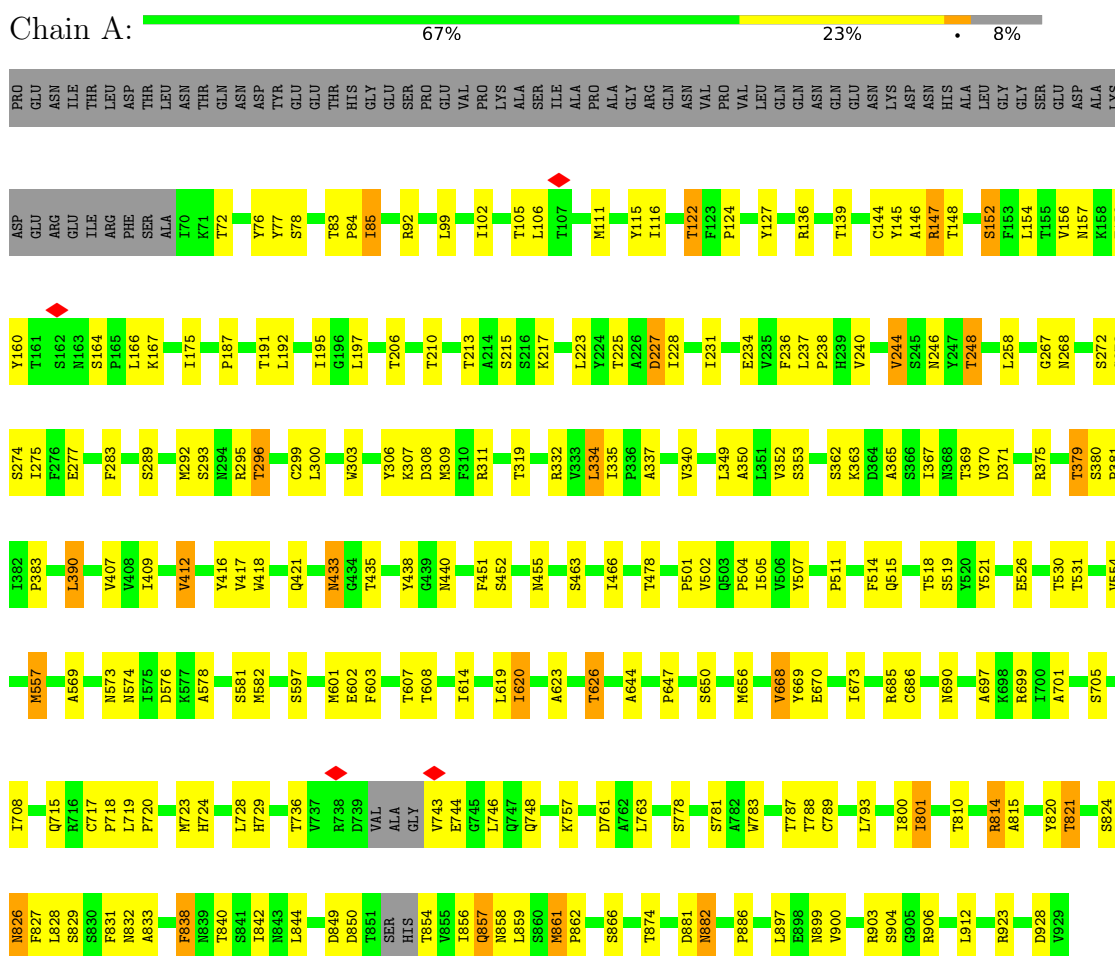
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	SER	ASN	conflict	UNP A0A8F6AGH5
A	202	GLN	LEU	conflict	UNP A0A8F6AGH5
A	203	ASN	ALA	conflict	UNP A0A8F6AGH5
A	204	LEU	THR	conflict	UNP A0A8F6AGH5
A	205	ALA	SER	conflict	UNP A0A8F6AGH5
A	206	THR	GLN	conflict	UNP A0A8F6AGH5
B	201	SER	ASN	conflict	UNP A0A8F6AGH5
B	202	GLN	LEU	conflict	UNP A0A8F6AGH5
B	203	ASN	ALA	conflict	UNP A0A8F6AGH5
B	204	LEU	THR	conflict	UNP A0A8F6AGH5
B	205	ALA	SER	conflict	UNP A0A8F6AGH5
B	206	THR	GLN	conflict	UNP A0A8F6AGH5

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



P836	I837	F838	N839	T840	S841	I842	N843	L844		S852	H853	T854	V855	Q856	N857	N858	L859	S860		S873	T874	V877	V878		D881	T887	P890	A891	W892	V900	R906		N917		S920	G921	F925		V929																			
Q715	D576	V585	L719	F720	I721	I722	M723		Y612	T726	G727	L728	H729		N618	L619	I620	L621	S622		Q748	V759	V760	D761		T765	L780	S781	A782	W783	T787	T788	C789	L793	S794		I801	T810	R813		Y820	T821	S824	F825	N826	F827	L828	S829	S830	F831	N832	A833	S834	E835				
Y404	V407	V408	I409	W410	G411	V412		T435		I450	F451		V458	N459	V460		L470		W473	N474	H475	I476	T477	T478	T479	E483	E484	E485	V486	T487		I490	K491		P501	V502	C510	P511		H517		E535		V554	L555	Q556	M557	T558	L559		Q563	P564	T565		A569			
W303	S304	A305	Y306	F310	F311	N312	G313	I314		P321	THR	LEU	ALA	PRO		G328	S329	S330		L334	I335	P336		L339	V340	T341		L349	A350	V352	S353	S354		Q357		S362		N368		R375		T379	S380	P381	I382	P383	D384	V385		L390		L393	R398		G401			
R190	Q202	S208	K209	T210	T213	A214	S215	S216	K217	V218	F219	T220		L229	S230	I231		V235	F236	L237		M241	Q242	P243	V244		N246	Y247	T248	R253	A254	L255	L256		I259		N268		S273	S274	I275		I280		T290	N291	M292		R295	T296	C299	L300	H301	T302				
ASP	GLU	ARG	GLU	ILE	ARG	PHE	SER	ALA	ALA	ILE	K71	T72	Y76		T83	P84	I85		G95		A104	T105	L106	T107	K108		Y115		T122	S134	N135	R136		T140		Y145	A146	R147	T148	S152	F153	L154	T155	V156		T159		L166		I175	F176	N177		V184		P187		G

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5804	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	2.947	Depositor
Minimum map value	-1.352	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.45	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 [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	0.12	0/6918	0.33	0/9453
1	B	0.29	3/6899 (0.0%)	0.42	5/9426 (0.1%)
All	All	0.22	3/13817 (0.0%)	0.38	5/18879 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	660	PRO	CG-CD	-11.53	1.11	1.50
1	B	208	SER	CA-C	-7.62	1.43	1.52
1	B	660	PRO	N-CD	6.02	1.56	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	660	PRO	N-CD-CG	-13.39	83.11	103.20
1	B	660	PRO	CA-N-CD	-12.45	94.58	112.00
1	B	208	SER	N-CA-C	-7.65	95.79	108.34
1	B	660	PRO	CA-CB-CG	-7.28	90.66	104.50
1	B	660	PRO	N-CA-CB	-5.60	97.37	103.25

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	6732	0	6584	124	0
1	B	6713	0	6560	119	0
All	All	13445	0	13144	241	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 9.

The worst 5 of 241 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:A:83:THR:HG23	1:A:84:PRO:HD3	1.58	0.85
1:B:296:THR:HG21	1:B:353:SER:HB3	1.66	0.76
1:A:85:ILE:HD11	1:B:925:PHE:HB3	1.68	0.76
1:A:296:THR:HG21	1:A:353:SER:HB3	1.66	0.75
1:A:76:TYR:O	1:A:92:ARG:NH2	2.26	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	849/929 (91%)	797 (94%)	44 (5%)	8 (1%)	14	30
1	B	849/929 (91%)	805 (95%)	37 (4%)	7 (1%)	16	34
All	All	1698/1858 (91%)	1602 (94%)	81 (5%)	15 (1%)	16	30

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	A	701	ALA
1	B	619	LEU

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Mol	Chain	Res	Type
1	A	882	ASN
1	B	209	LYS

5.3.2 Protein sidechains [i](#)

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	748/810 (92%)	684 (91%)	64 (9%)	10	22
1	B	745/810 (92%)	672 (90%)	73 (10%)	7	17
All	All	1493/1620 (92%)	1356 (91%)	137 (9%)	11	19

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	737	VAL
1	B	810	THR
1	B	860	SER
1	A	736	THR
1	A	728	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	618	ASN
1	B	732	GLN
1	B	863	GLN
1	B	711	HIS
1	B	203	ASN

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.

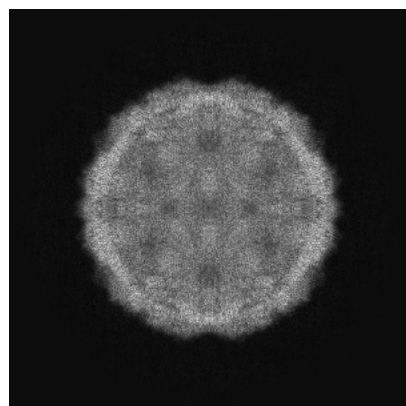
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18792. These allow visual inspection of the internal detail of the map and identification of artifacts.

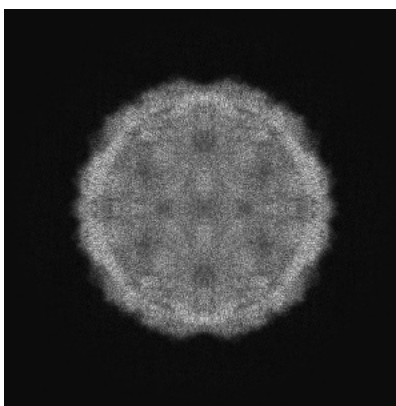
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

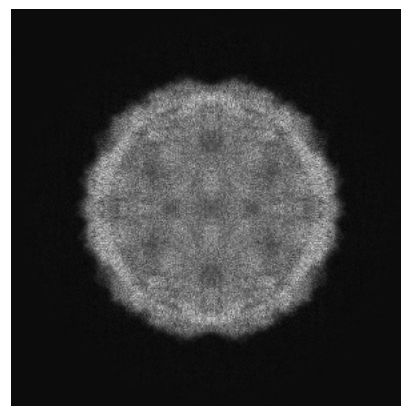
6.1.1 Primary map



X

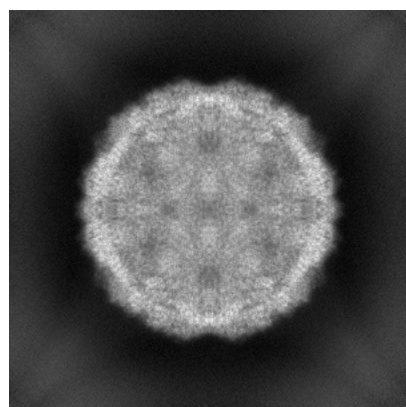


Y

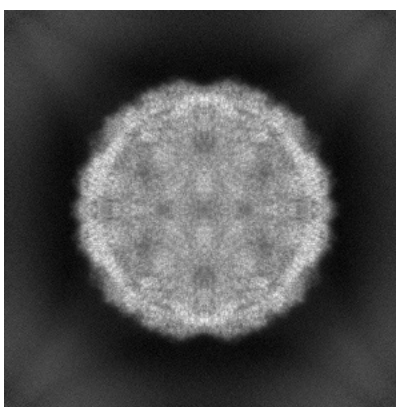


Z

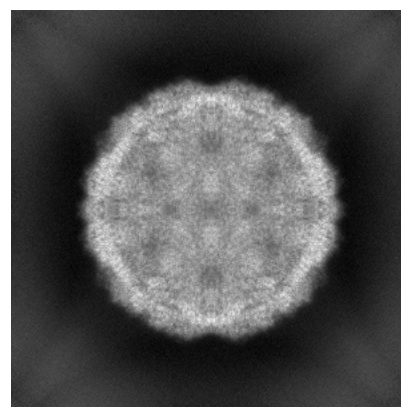
6.1.2 Raw map



X



Y

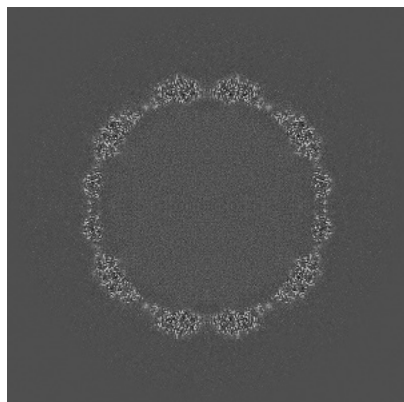


Z

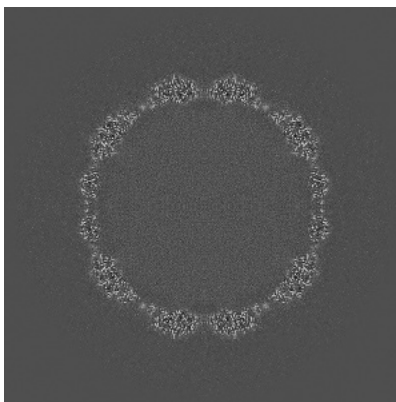
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

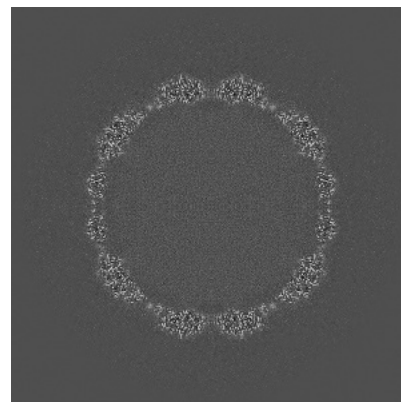
6.2.1 Primary map



X Index: 320

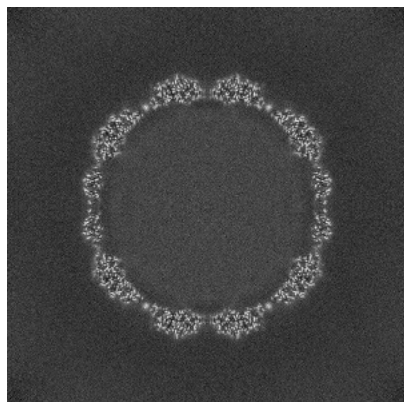


Y Index: 320

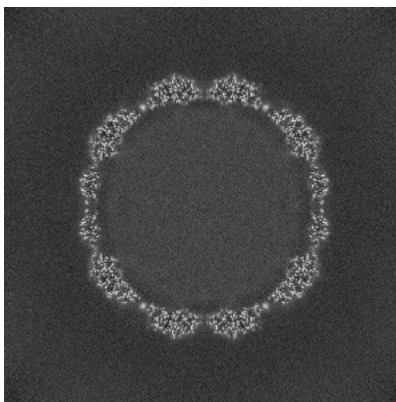


Z Index: 320

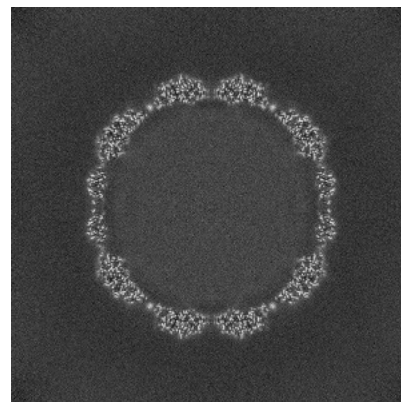
6.2.2 Raw map



X Index: 320



Y Index: 320

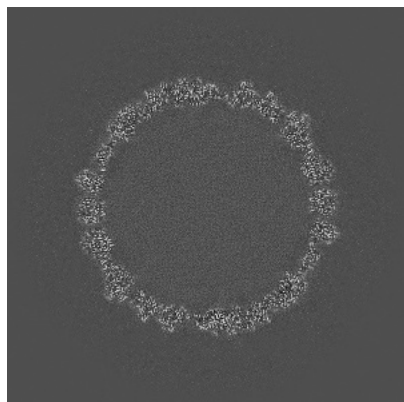


Z Index: 320

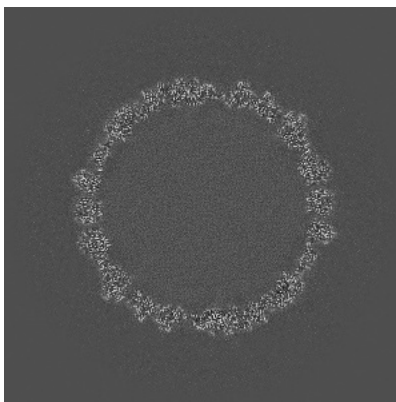
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

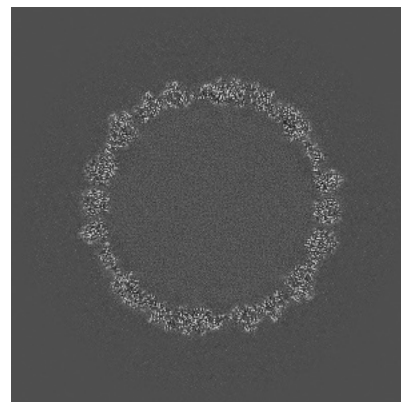
6.3.1 Primary map



X Index: 355

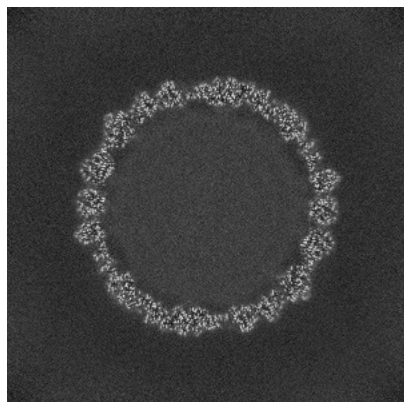


Y Index: 355

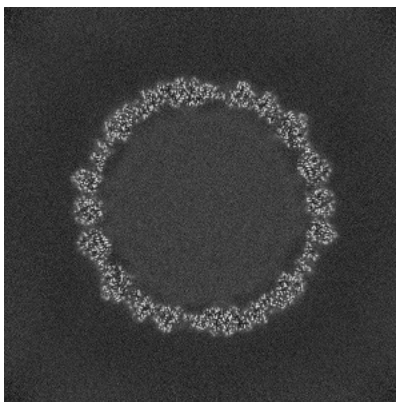


Z Index: 285

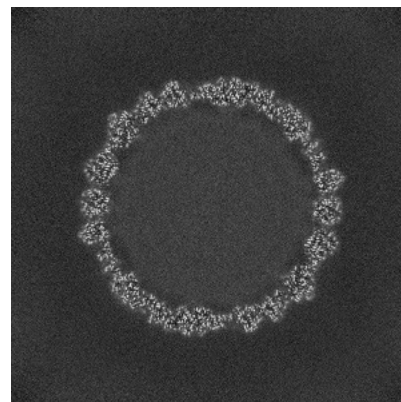
6.3.2 Raw map



X Index: 286



Y Index: 354

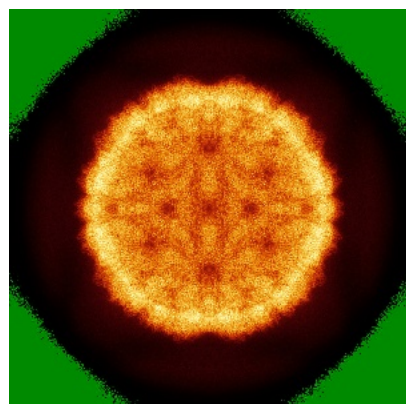


Z Index: 286

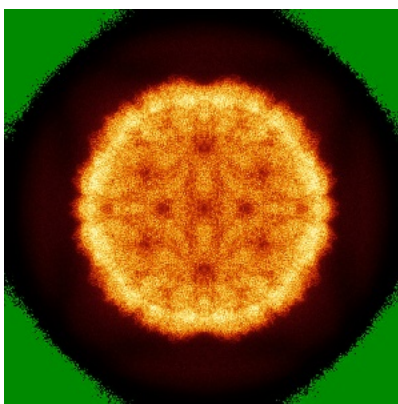
The images above show the largest variance slices of the map in three orthogonal directions.

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

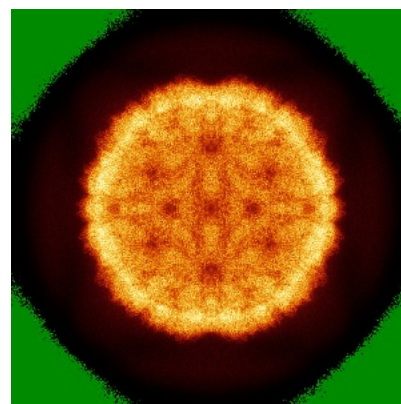
6.4.1 Primary map



X

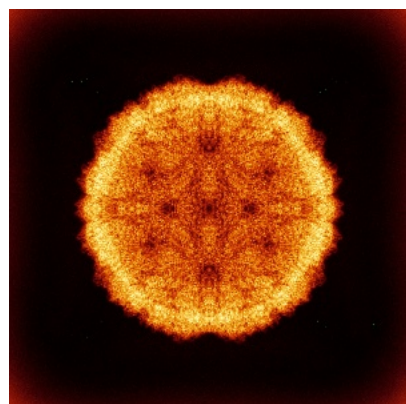


Y

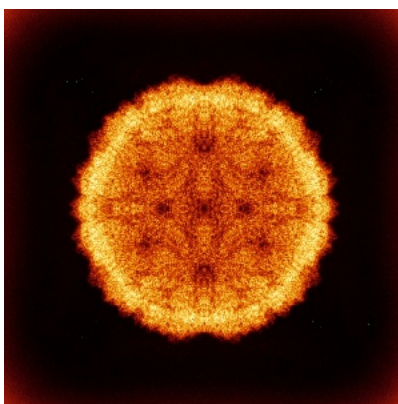


Z

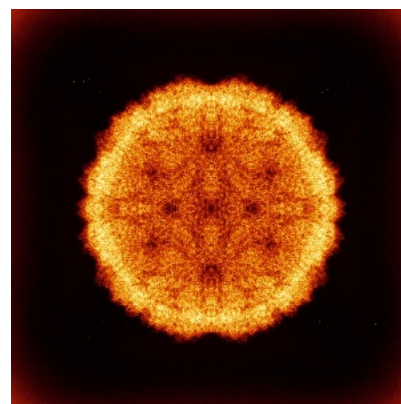
6.4.2 Raw map



X



Y

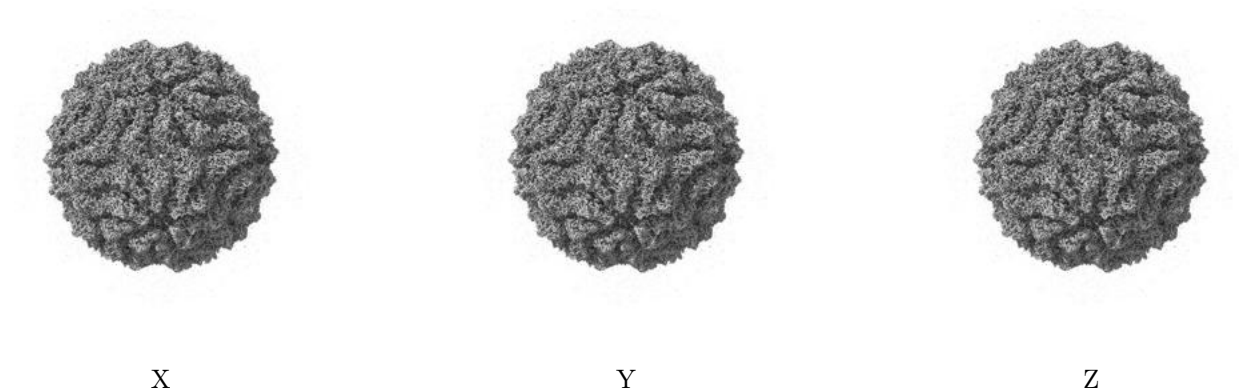


Z

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

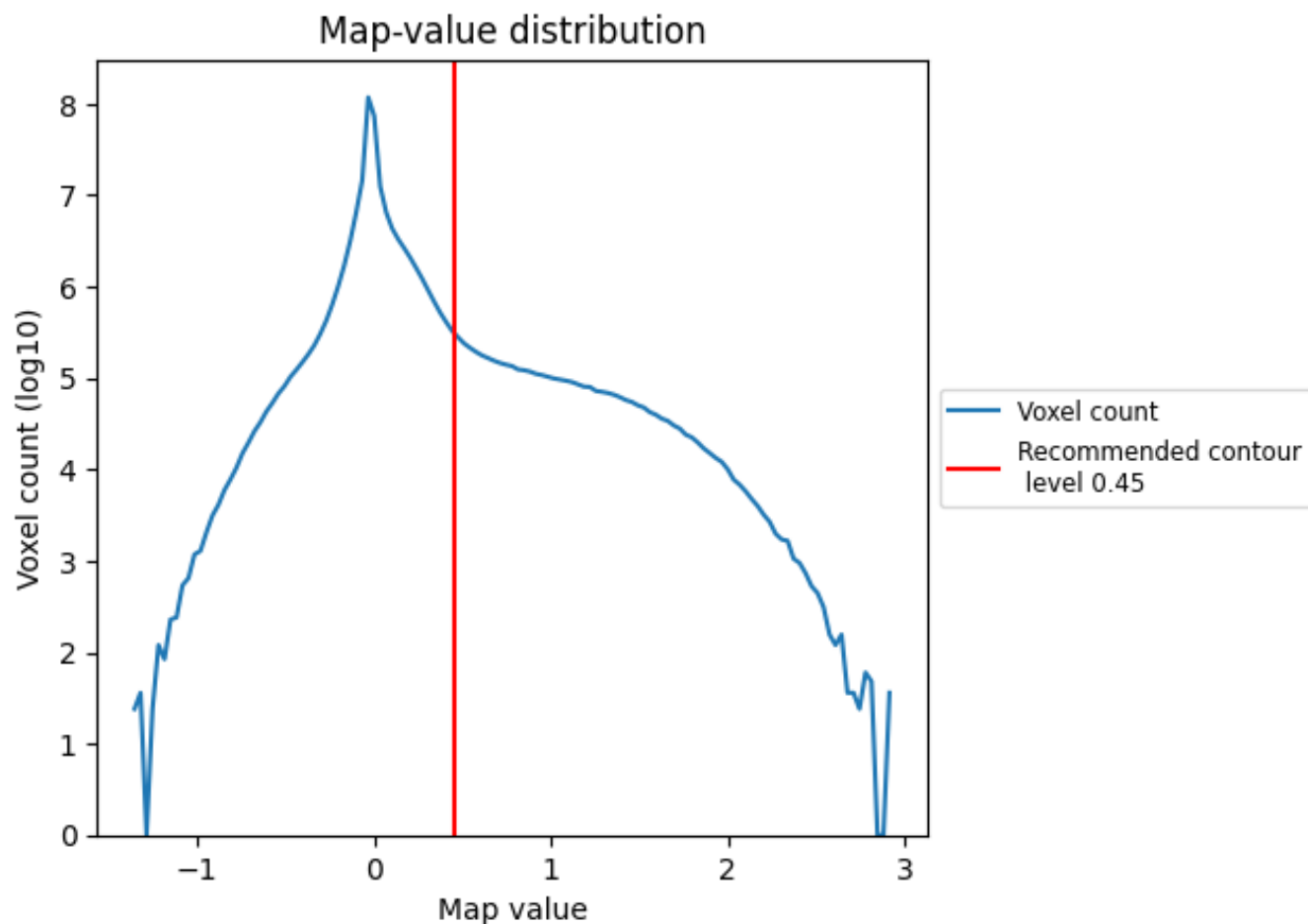
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

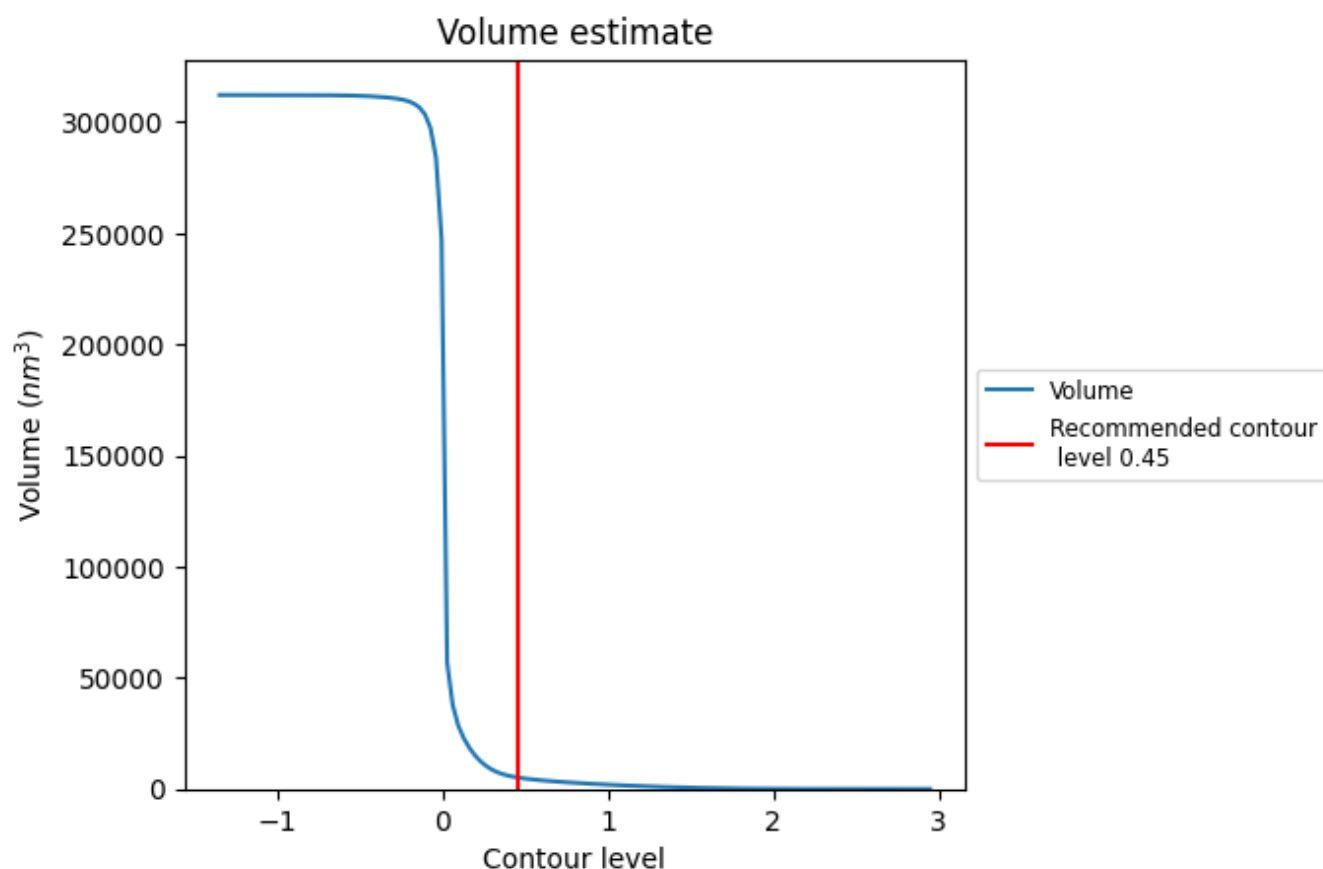
This section contains the results of statistical analysis of the map.

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.

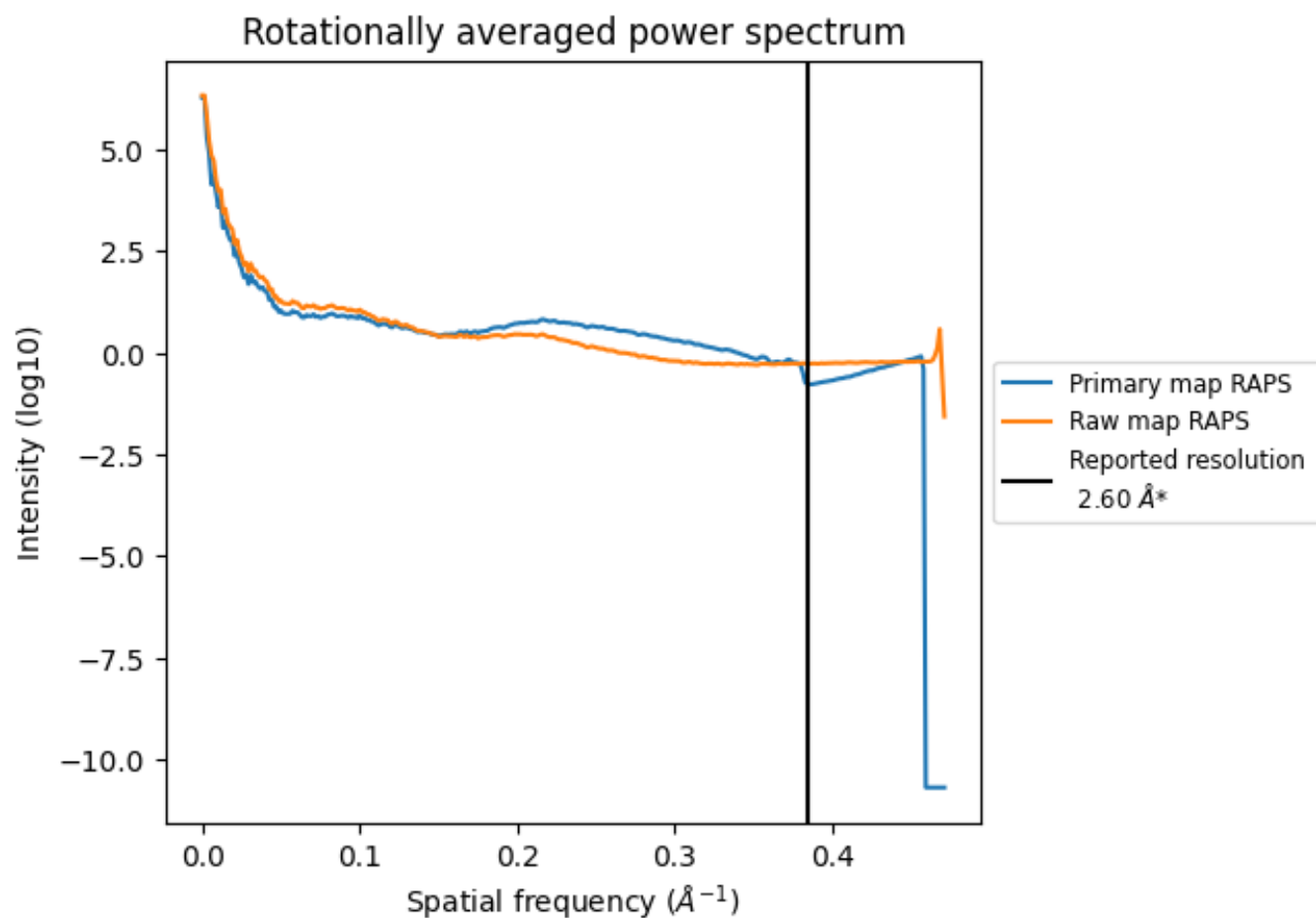
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5174 nm³; this corresponds to an approximate mass of 4674 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 ⓘ

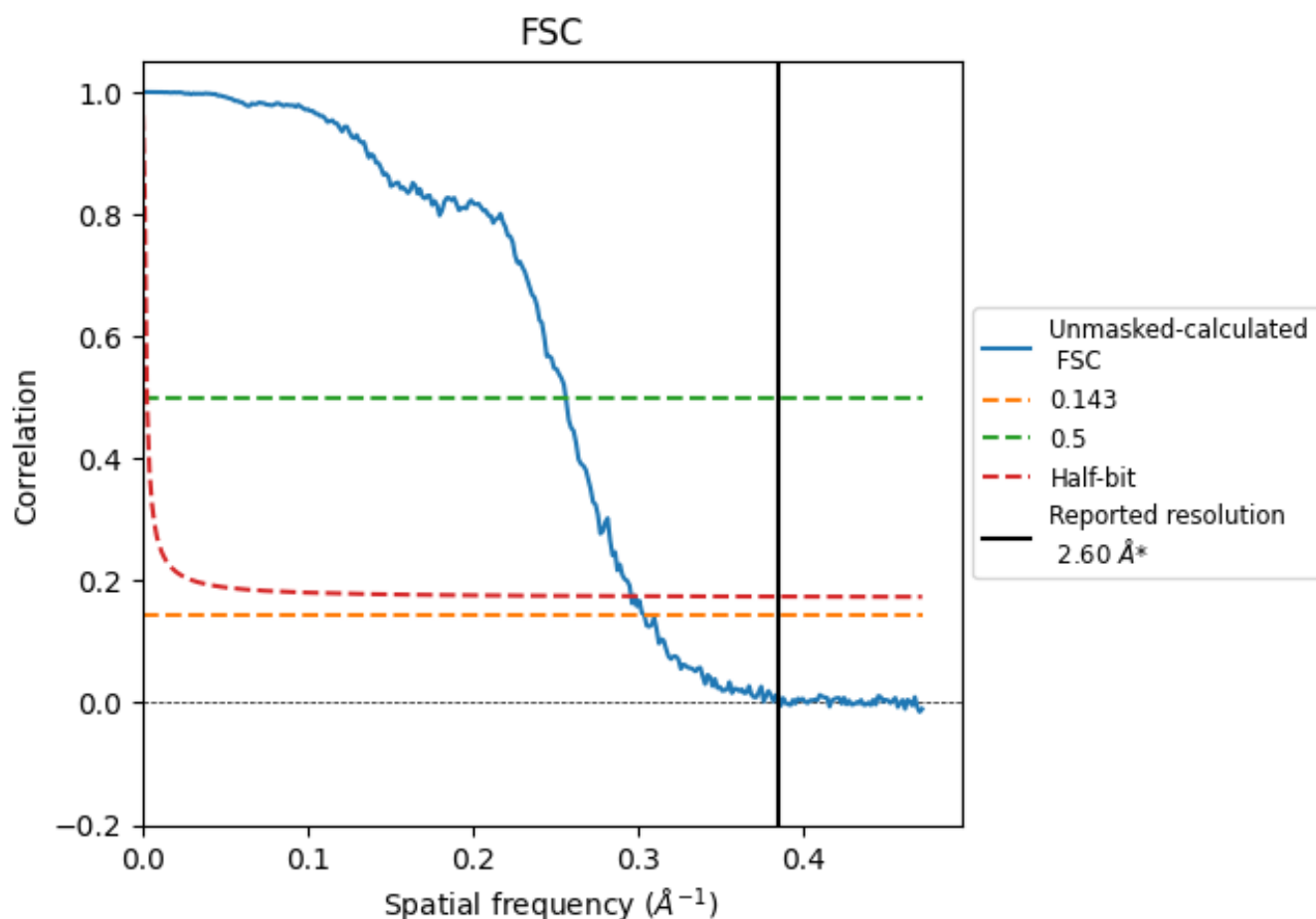


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	3.90	3.38

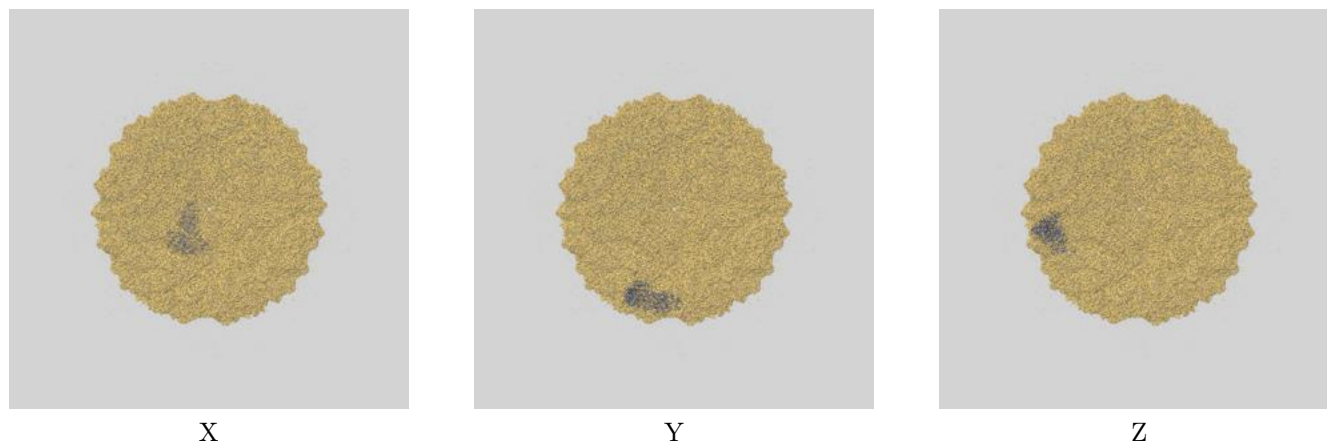
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18792 and PDB model 8R0G. Per-residue inclusion information can be found in section [3](#) on page [4](#).

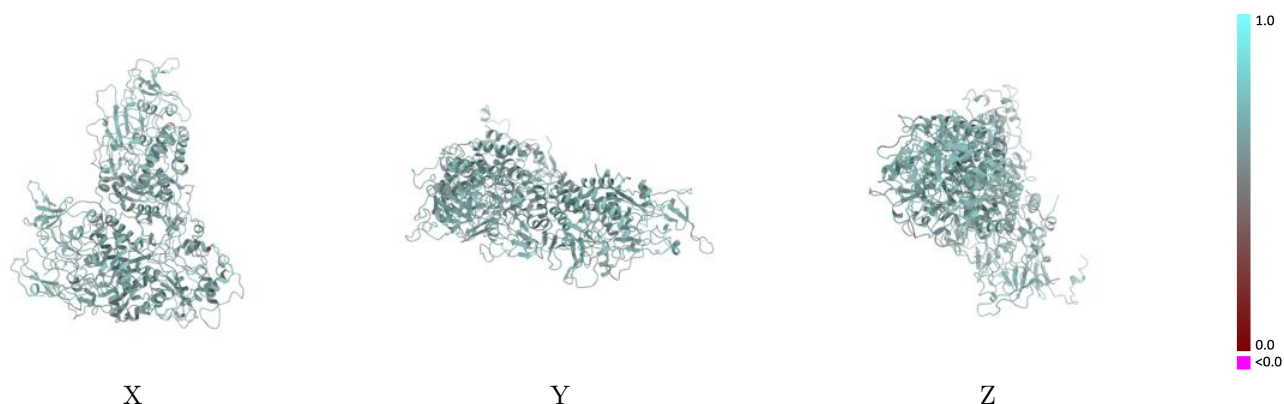
9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



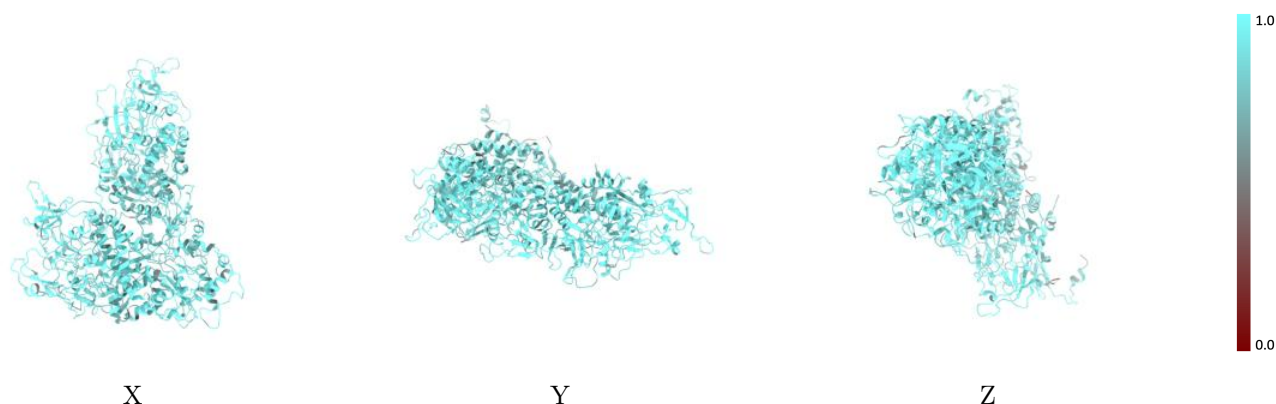
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



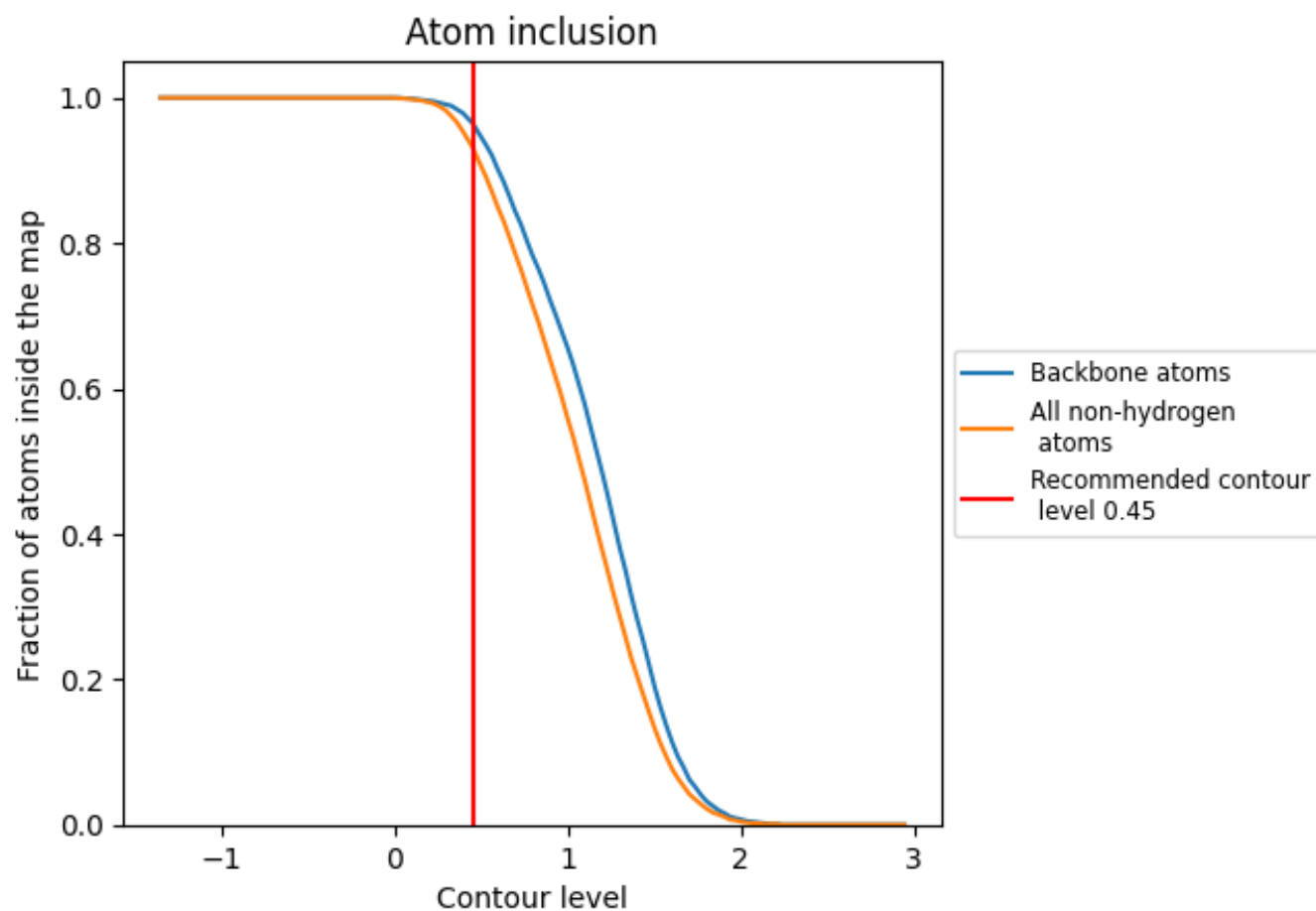
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.6210
A	0.9220	0.6170
B	0.9410	0.6250

