



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:14 PM UTC

PDB ID : 8GSC / pdb_00008gsc
EMDB ID : EMD-34231
Title : Echovirus3 A-particle in complex with 6D10 Fab
Authors : Wang, X.; Fu, W.
Deposited on : 2022-09-06
Resolution : 3.40 Å(reported)

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:

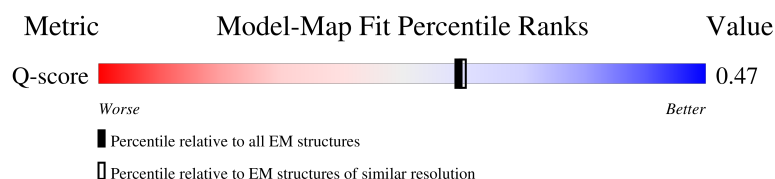
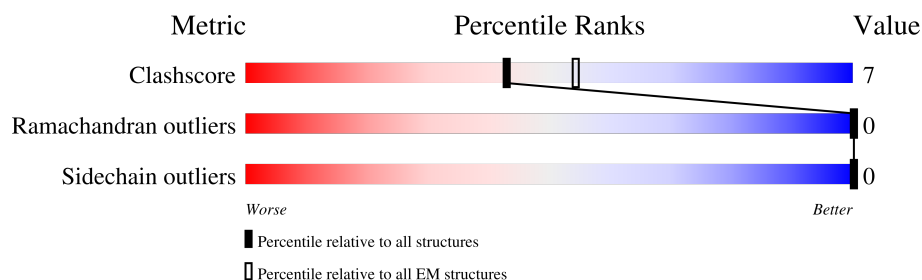
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.40 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	14717 (2.90 - 3.90)

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	1	237	7% 89% 11%
2	2	247	9% 84% 16%
3	3	234	10% 89% 11%
4	H	117	100% 74% 26%

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Mol	Chain	Length	Quality of chain	
			68%	32%
5	L	114		

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7453 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	237	Total	C	N	O	S	0	0
			1900	1210	333	348	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	80	ALA	LYS	conflict	UNP A0A060BFD5

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	247	Total	C	N	O	S	0	0
			1943	1227	328	372	16		

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	234	Total	C	N	O	S	0	0
			1816	1159	300	342	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	224	ASN	MET	conflict	UNP A0A0K0LDT3

- Molecule 4 is a protein called Heavy chain of 6D10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	117	Total	C	N	O	S	0	0
			907	577	143	183	4		

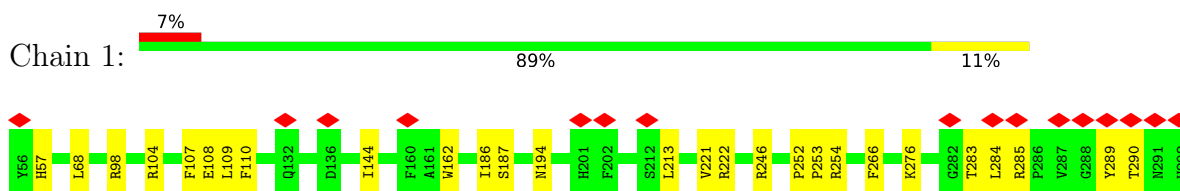
- Molecule 5 is a protein called Light chain of 6D10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	114	Total	C	N	O	S	0	0
			887	566	143	175	3		

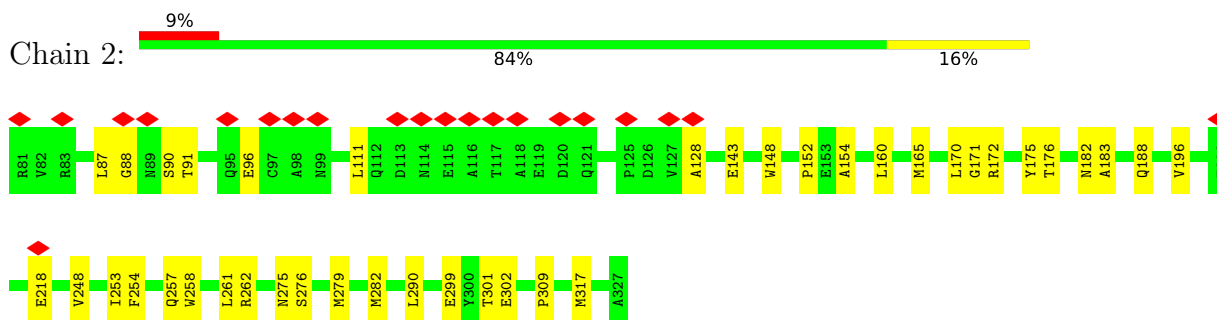
3 Residue-property plots

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.

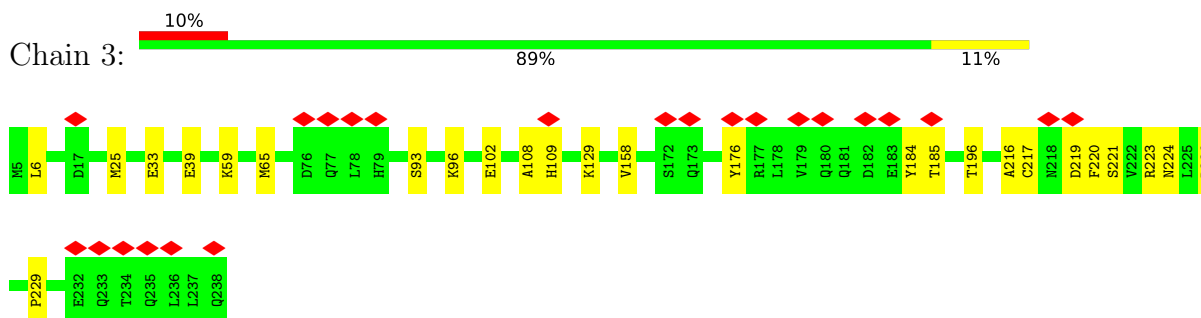
- Molecule 1: VP1



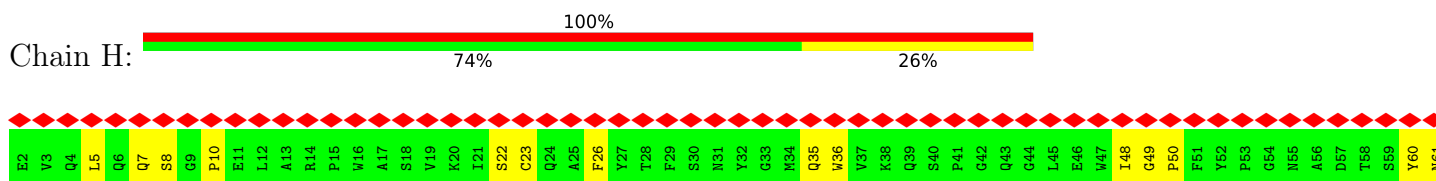
- Molecule 2: VP2



- Molecule 3: VP3



- Molecule 4: Heavy chain of 6D10



Q62	K63	F64	K65	G66	K67	A68	T69	L70	T71	A72	D73	K74	S75	S76	S77	T78	A79	Y80	M81	Q82	F83	S84	S85	L86	T87	S88	E89	D90	S91	A92	V93	Y94	Y95	C96	A97	R98	V99	V100	A101	T102	T103	D104	F105	D106	Y107	W108	G109	Q110	G111	T112	T113	V114	T115	V116	S117	S118
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• Molecule 5: Light chain of 6D10



Y1	I2	E3	A4	S5	Q6	S7	P8	S9	S10	L11	A12	V13	S14	V15	G16	E17	K18	V19	T20	M21	S22	C23	K24	S25	S26	Q27	S28	L29	L30	Y31	S32	S33	N34	Q35	K36	N37	Y38	L39	A40	W41	F42	Q43	Q44	K45	P46	G47	Q48	S49	P50	K51	L52	L53	I54	Y55	W56	A57	S58	T59	R60
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E61	S62	G63	V64	P65	D66	R67	F68	T69	G70	S71	G72	S73	G74	T75	D76	F77	T78	L79	T80	I81	S82	S83	V84	K85	A86	E87	D88	L89	A90	V91	Y92	Y93	C94	Q95	Q96	Y97	Y98	S99	Y100	P101	Y102	T103	F104	G105	G106	G107	T108	K109	L110	K111	I112	K113	R114
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55687	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	513.0, 513.0, 513.0	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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	1	0.18	0/1959	0.39	1/2673 (0.0%)
2	2	0.18	0/1992	0.35	0/2717
3	3	0.19	0/1866	0.38	0/2548
4	H	0.13	0/933	0.38	0/1270
5	L	0.13	0/909	0.36	0/1231
All	All	0.17	0/7659	0.37	1/10439 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	283	THR	CB-CA-C	-5.36	109.42	115.79

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	1	1900	0	1830	18	0
2	2	1943	0	1857	25	0
3	3	1816	0	1765	19	0
4	H	907	0	839	19	0
5	L	887	0	862	25	0
All	All	7453	0	7153	97	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 7.

The worst 5 of 97 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)
2:2:262:ARG:NH2	3:3:158:VAL:O	2.14	0.80
5:L:6:GLN:NE2	5:L:94:CYS:SG	2.58	0.76
4:H:10:PRO:HB3	4:H:113:THR:H	1.51	0.73
5:L:42:PHE:HA	5:L:52:LEU:HA	1.70	0.72
3:3:93:SER:HA	3:3:96:LYS:HE2	1.76	0.68

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	1	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
2	2	142/247 (58%)	136 (96%)	6 (4%)	0	100	100
3	3	202/234 (86%)	190 (94%)	12 (6%)	0	100	100
4	H	81/117 (69%)	78 (96%)	3 (4%)	0	100	100
5	L	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
All	All	772/949 (81%)	735 (95%)	37 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	1	209/209 (100%)	209 (100%)	0	100	100
2	2	214/214 (100%)	214 (100%)	0	100	100
3	3	205/205 (100%)	205 (100%)	0	100	100
4	H	97/98 (99%)	97 (100%)	0	100	100
5	L	98/99 (99%)	98 (100%)	0	100	100
All	All	823/825 (100%)	823 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
5	L	95	GLN
4	H	110	GLN
3	3	109	HIS
3	3	77	GLN
4	H	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

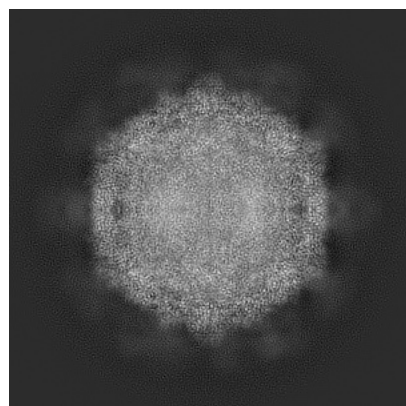
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34231. These allow visual inspection of the internal detail of the map and identification of artifacts.

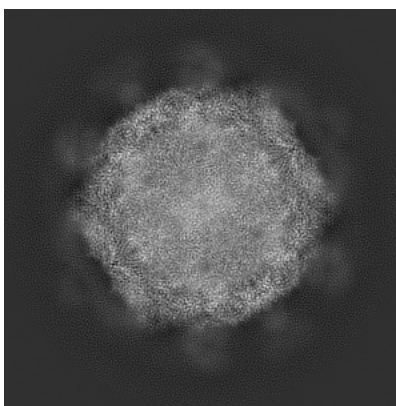
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

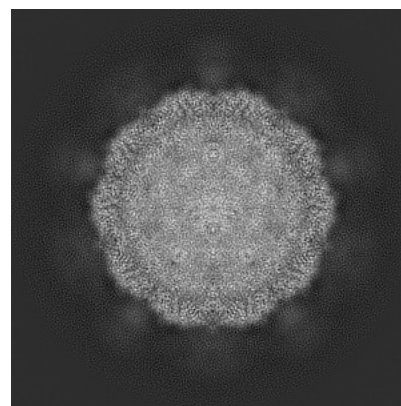
6.1.1 Primary map



X

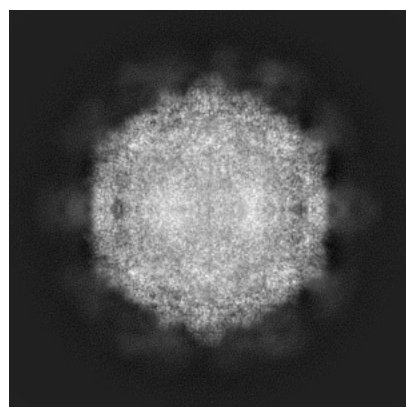


Y

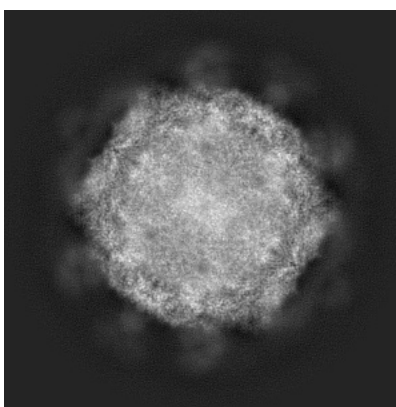


Z

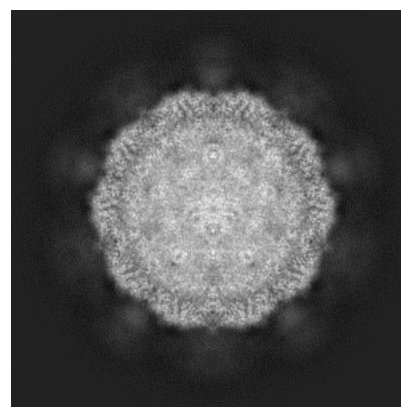
6.1.2 Raw map



X



Y

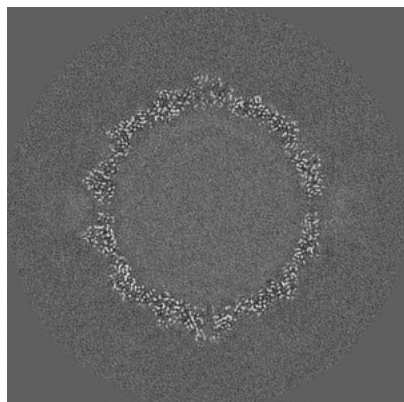


Z

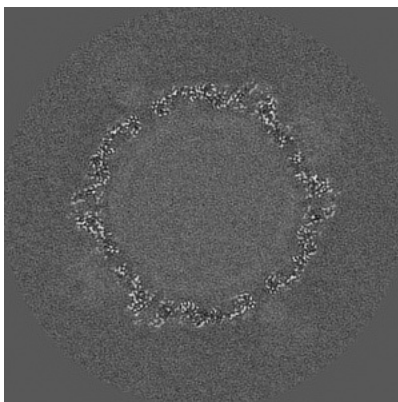
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

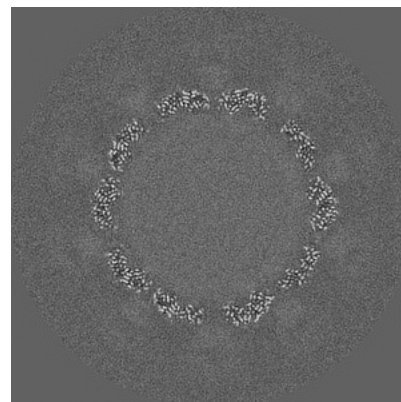
6.2.1 Primary map



X Index: 190

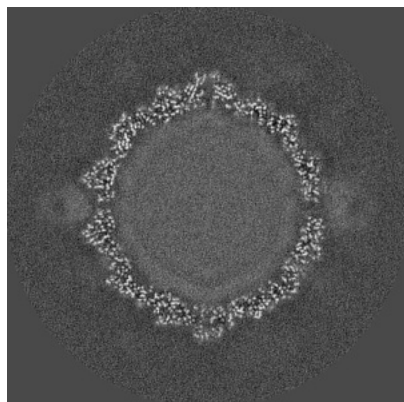


Y Index: 190

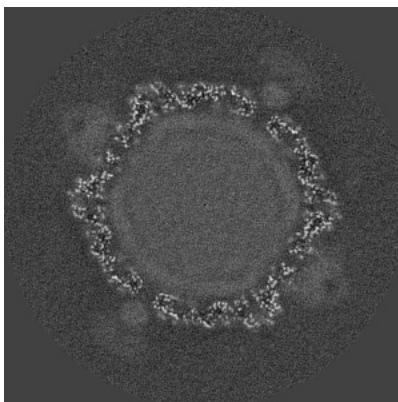


Z Index: 190

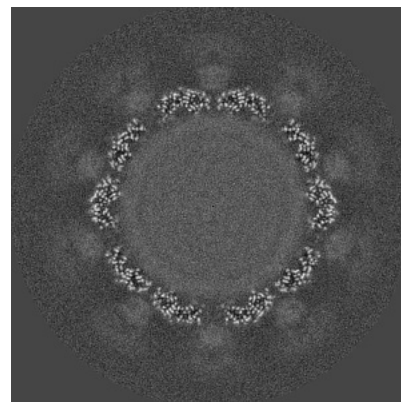
6.2.2 Raw map



X Index: 190



Y Index: 190

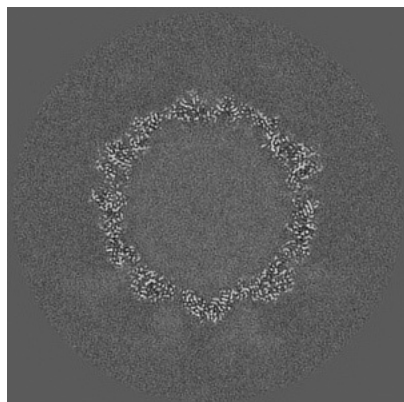


Z Index: 190

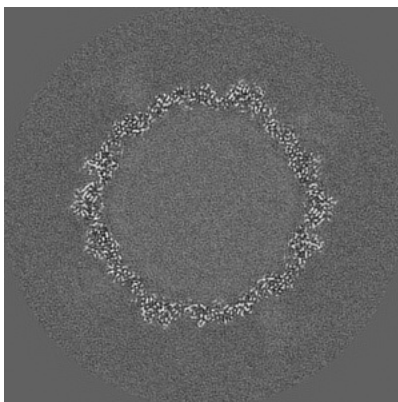
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

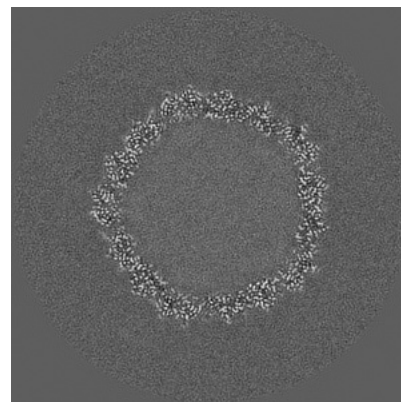
6.3.1 Primary map



X Index: 238

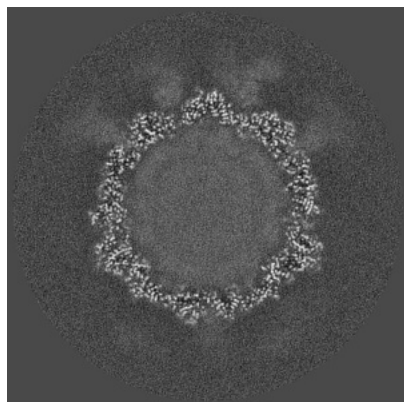


Y Index: 179

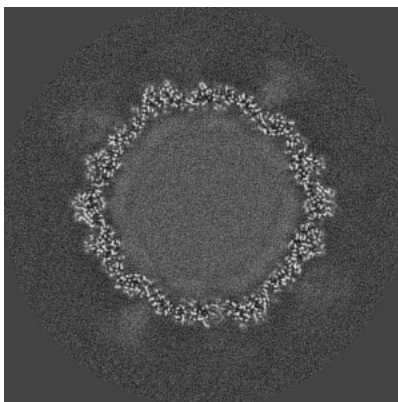


Z Index: 149

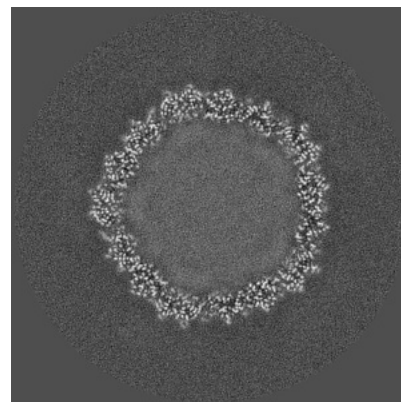
6.3.2 Raw map



X Index: 238



Y Index: 178

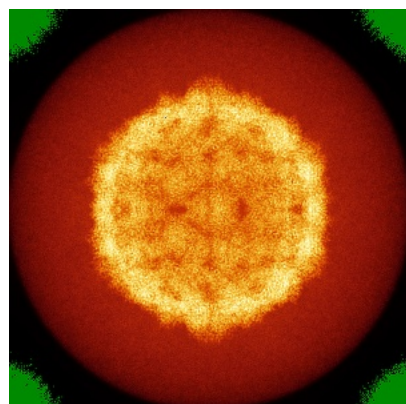


Z Index: 230

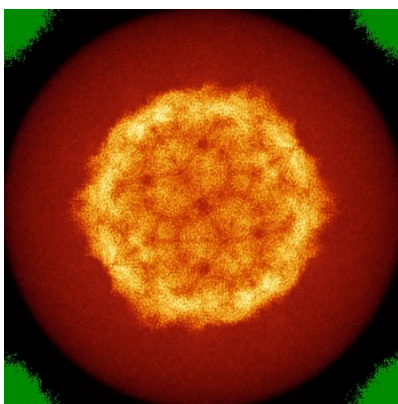
The images above show the largest variance slices of the map in three orthogonal directions.

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

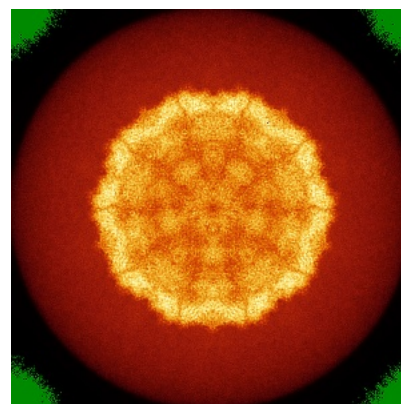
6.4.1 Primary map



X

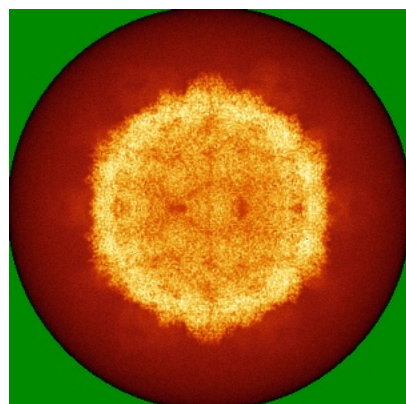


Y

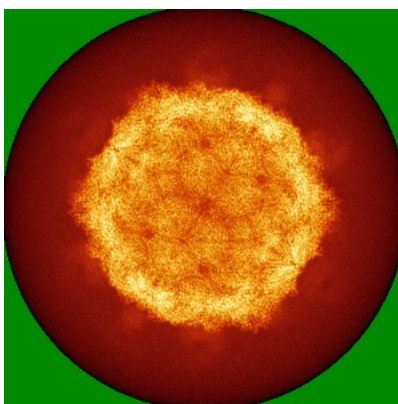


Z

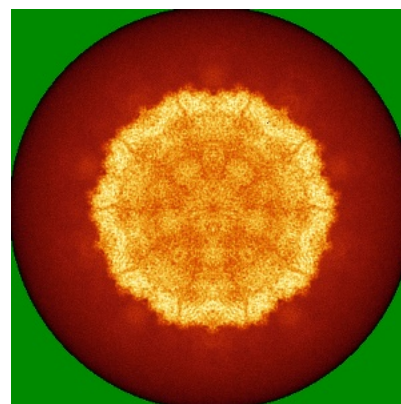
6.4.2 Raw map



X



Y

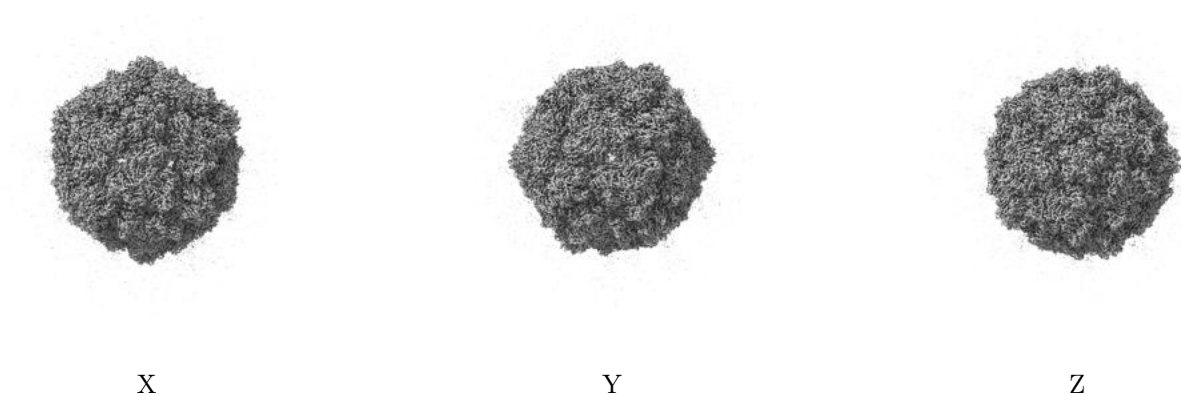


Z

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.

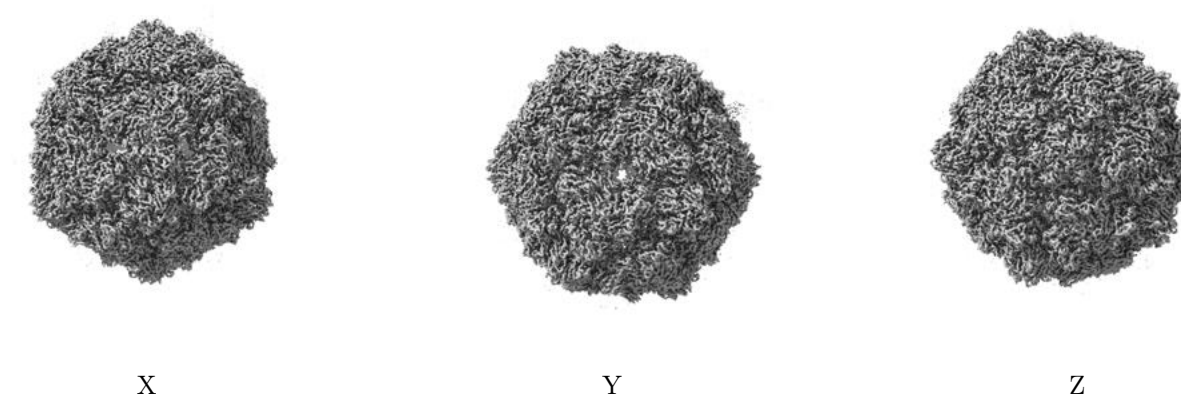
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

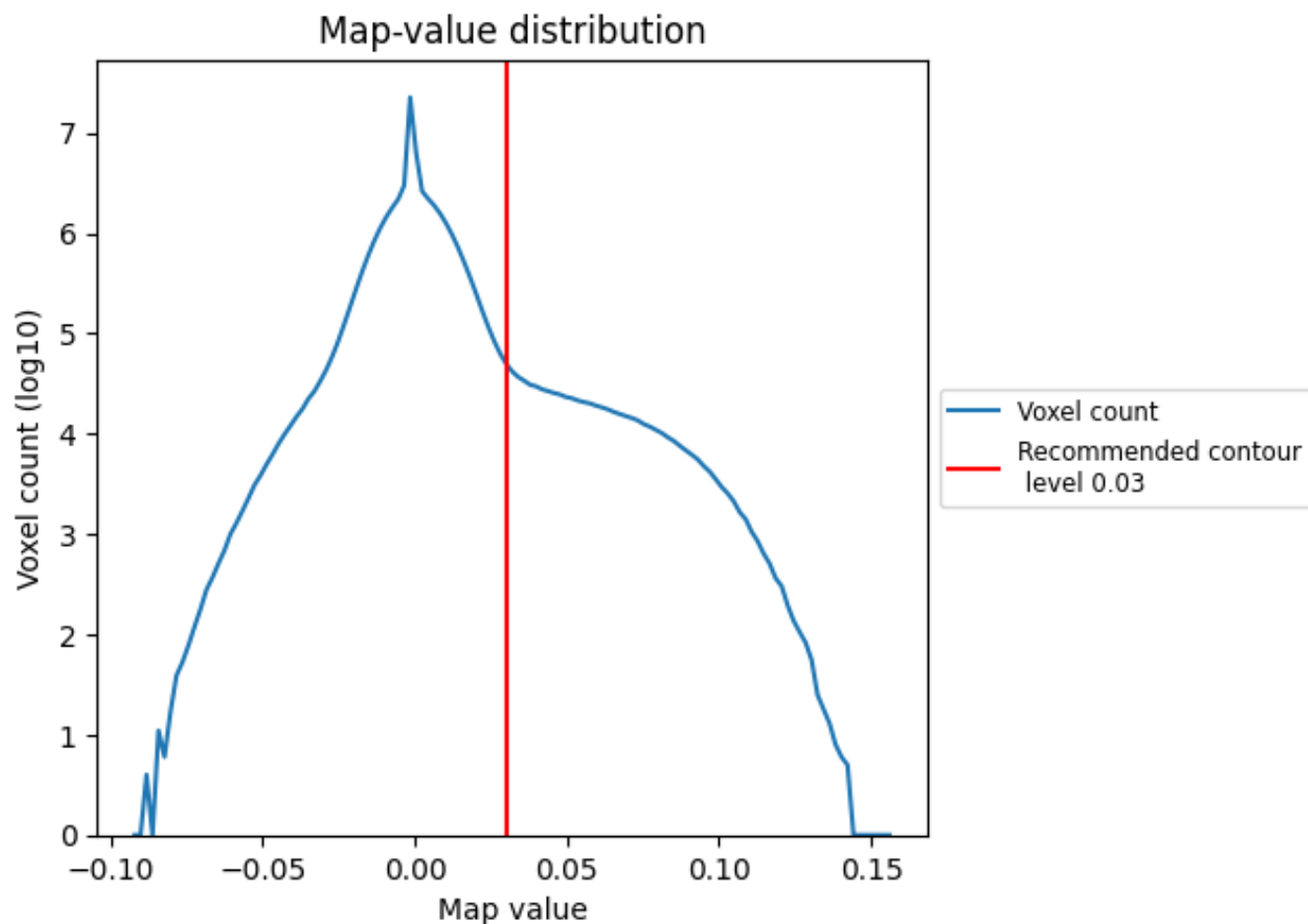
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

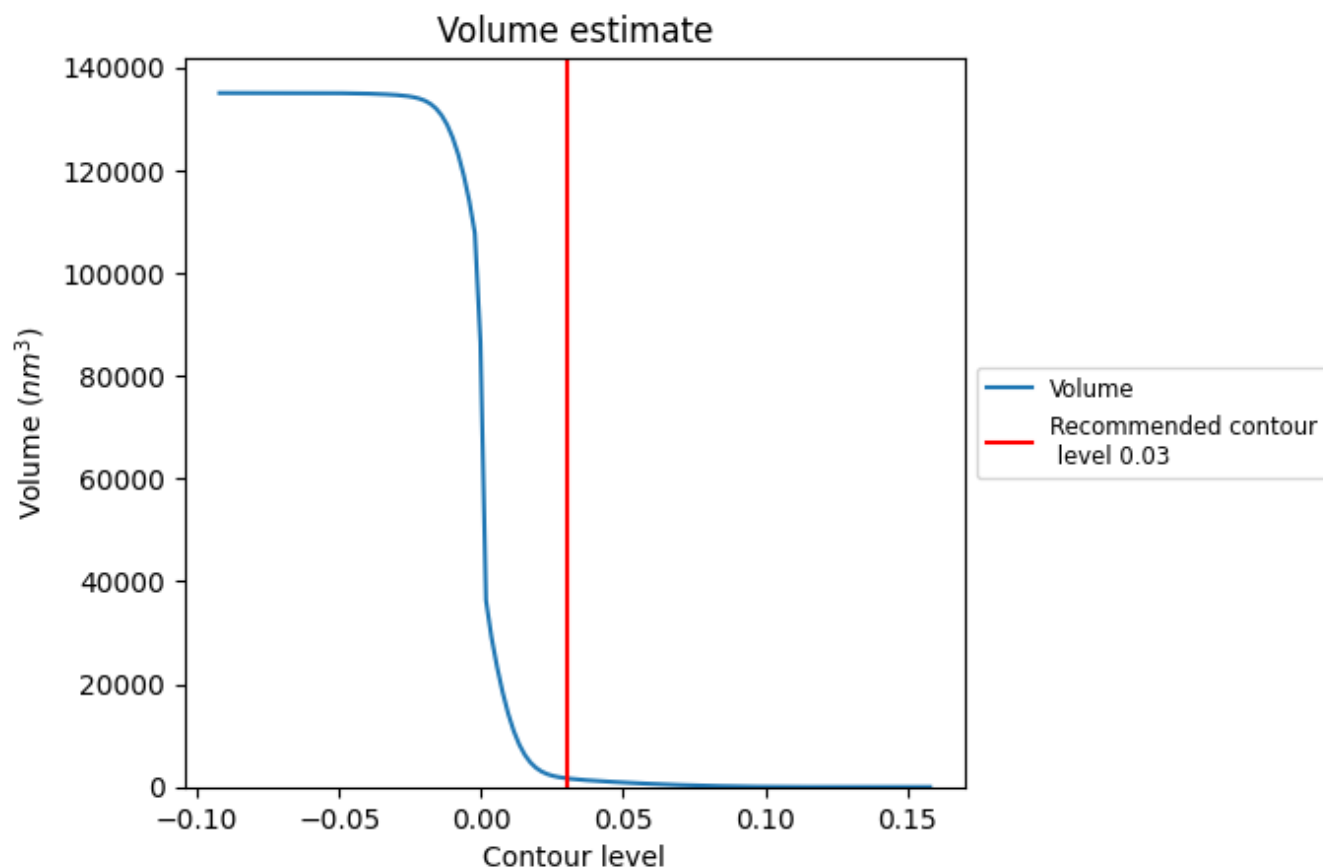
This section contains the results of statistical analysis of the map.

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.

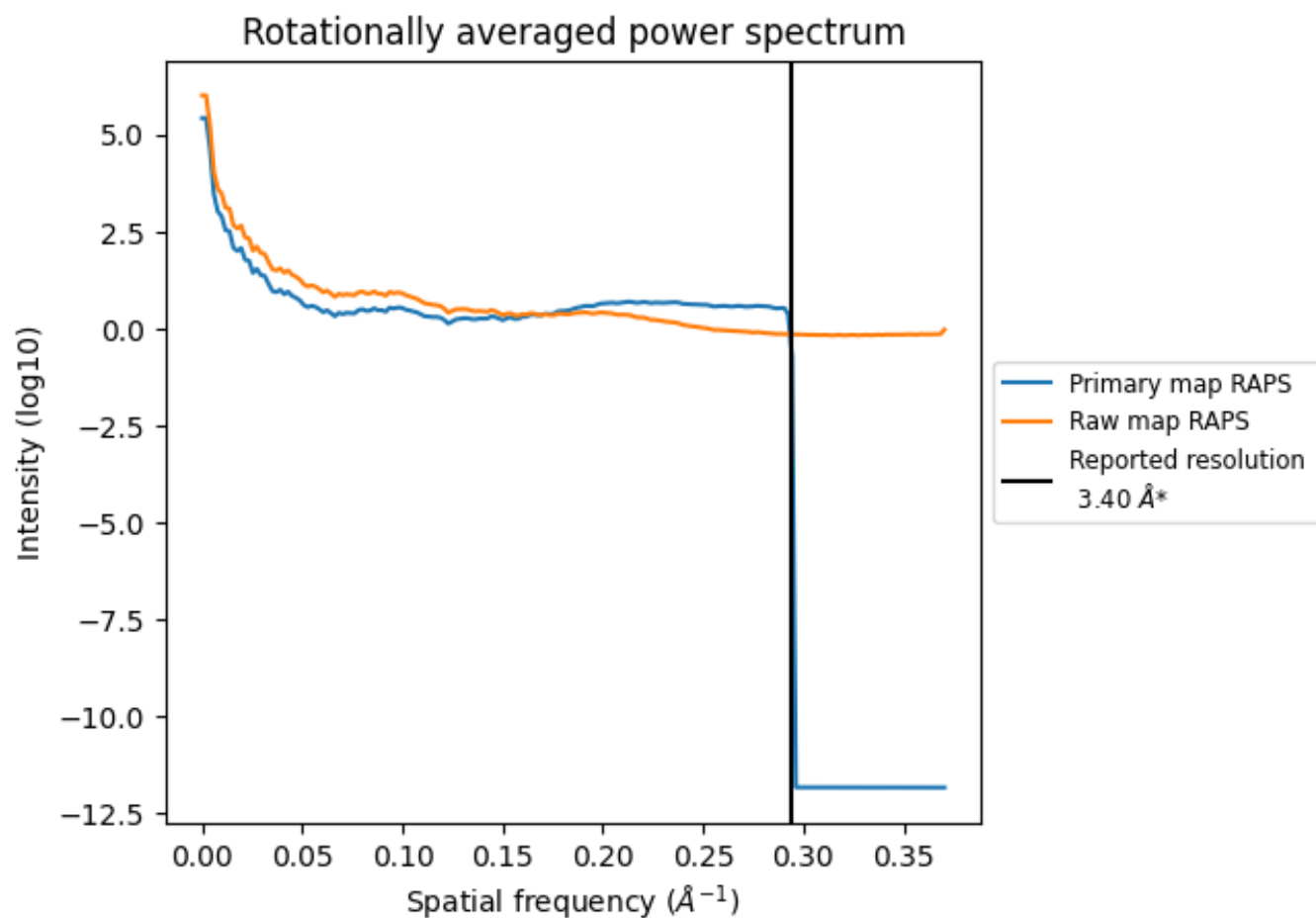
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1692 nm^3 ; this corresponds to an approximate mass of 1529 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 ⓘ

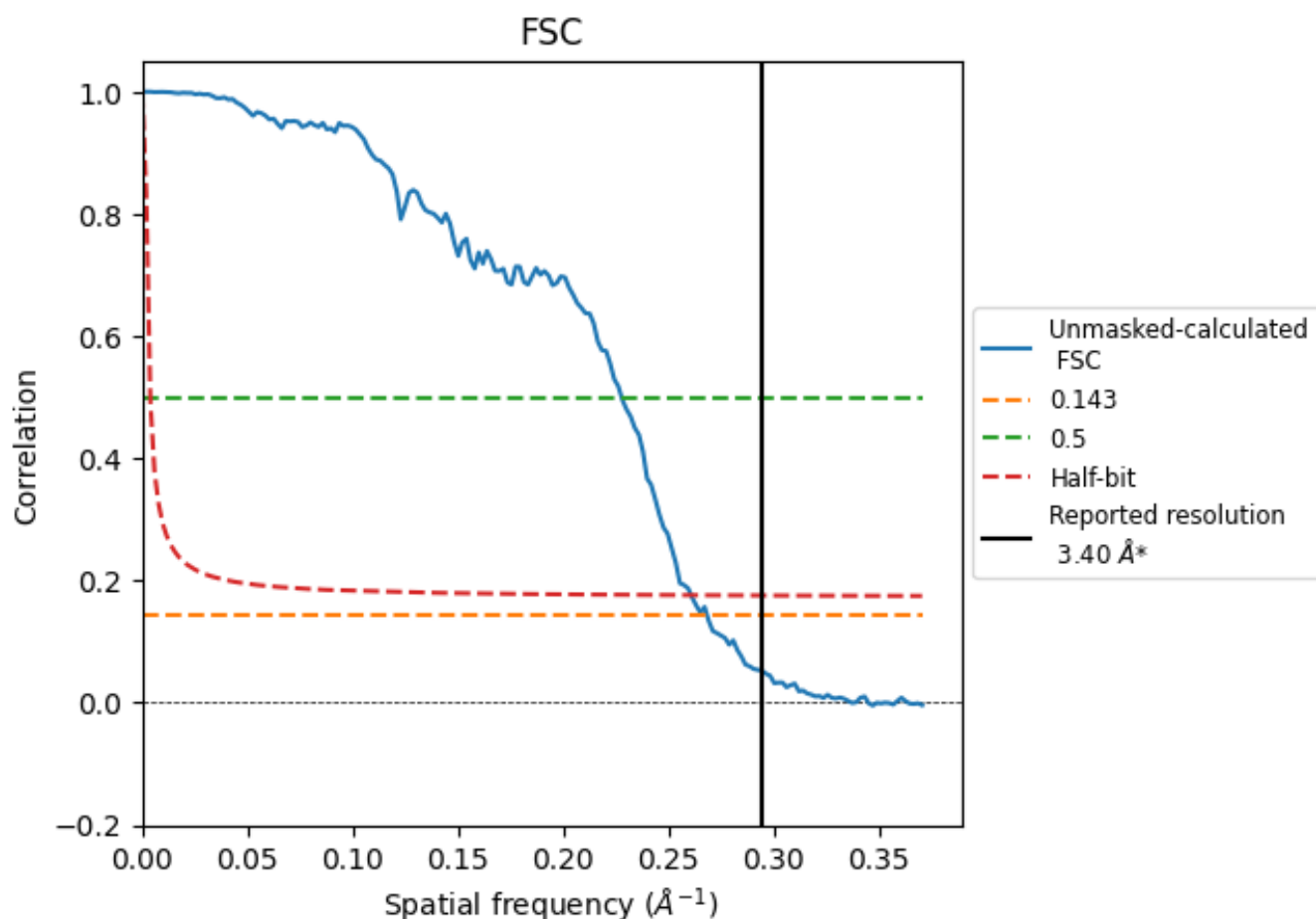


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.39	3.84

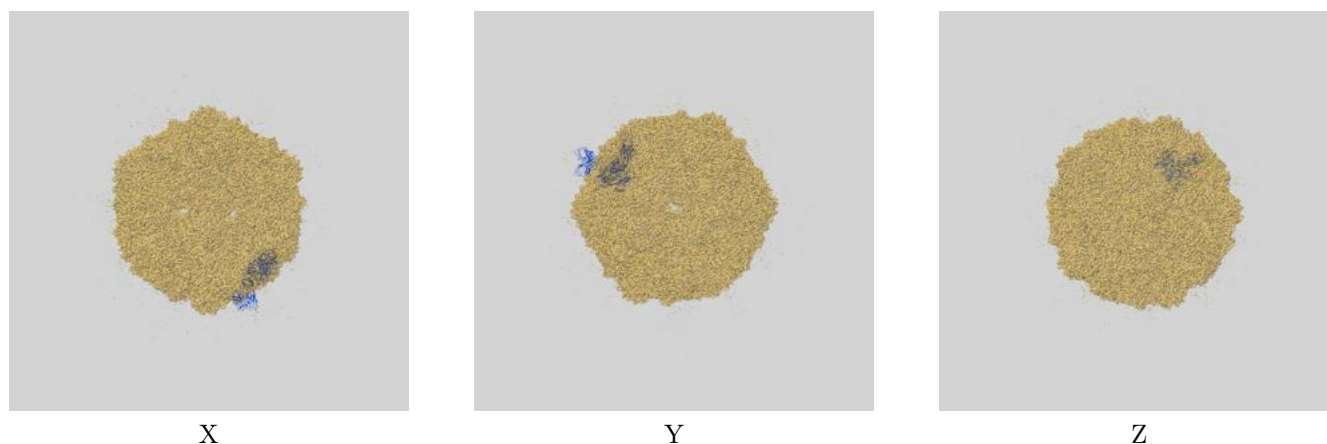
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

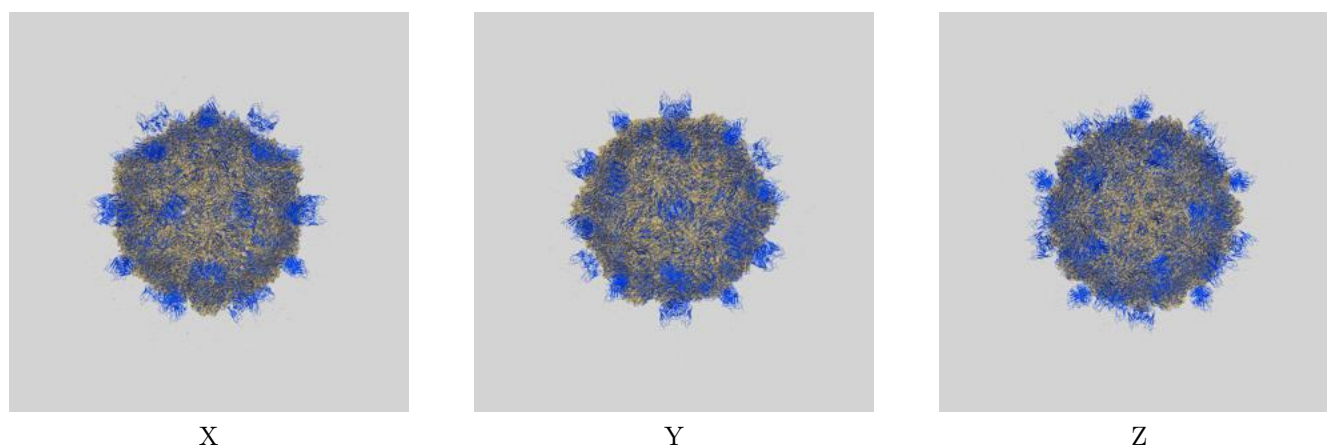
This section contains information regarding the fit between EMDB map EMD-34231 and PDB model 8GSC. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

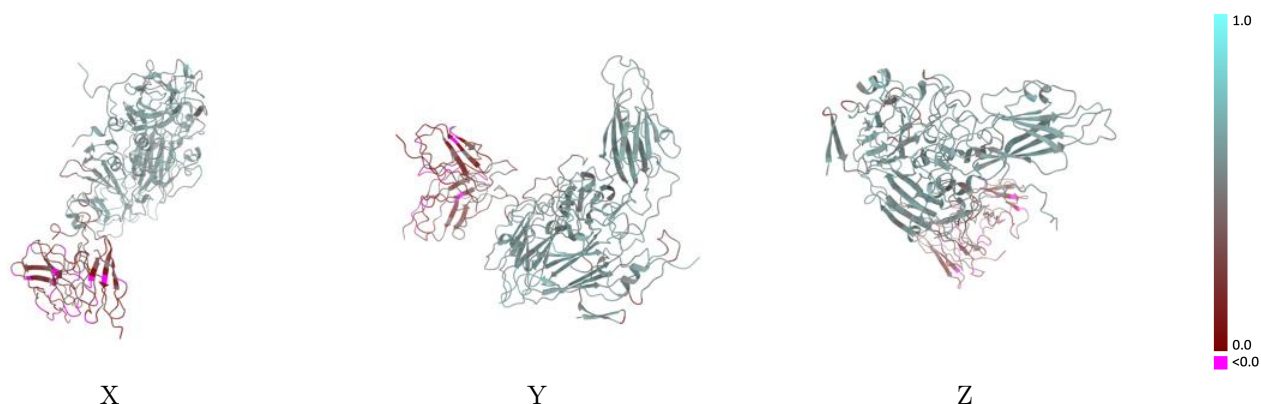


9.1.2 Map-model assembly overlay [i](#)



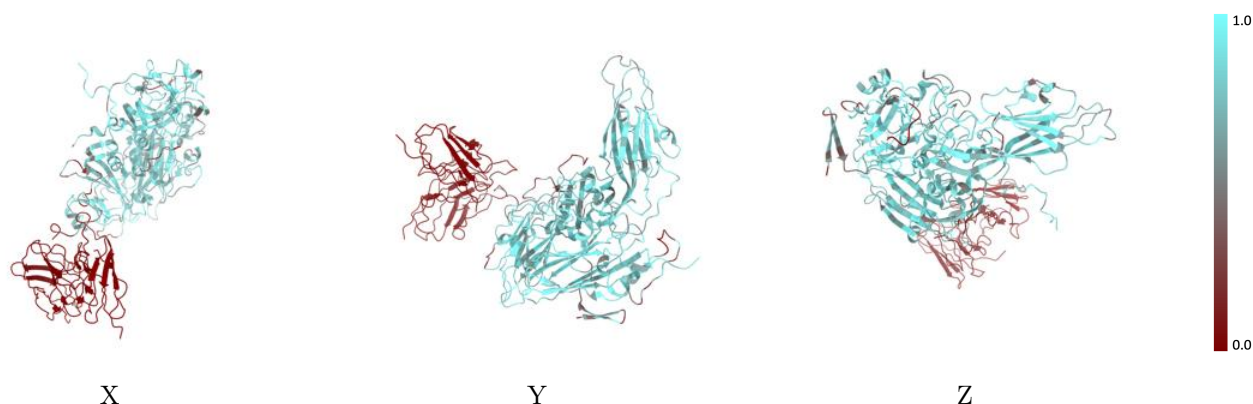
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



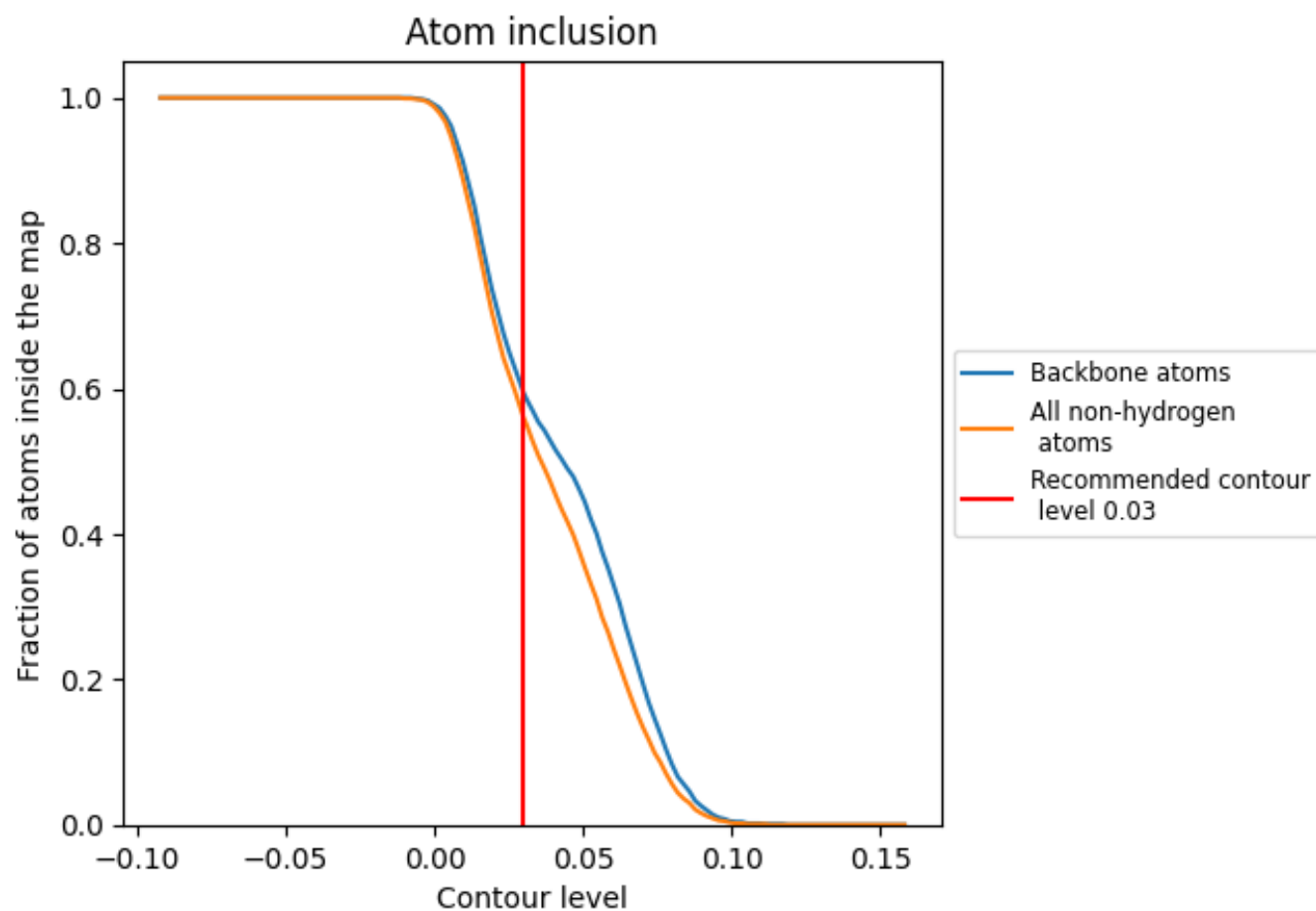
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 56% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.4700
1	0.7350	0.5490
2	0.7410	0.5560
3	0.7250	0.5420
H	0.0010	0.2040
L	0.0250	0.2340

