



Full wwPDB EM Validation Report ⓘ

Aug 6, 2024 – 12:32 AM JST

PDB ID : 8YF9
EMDB ID : EMD-39215
Title : Cryo-EM structure of Dragon Grouper nervous necrosis virion at pH6.5 (3.12Å)
Authors : Wang, C.H.; Chang, W.H.
Deposited on : 2024-02-24
Resolution : 3.12 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

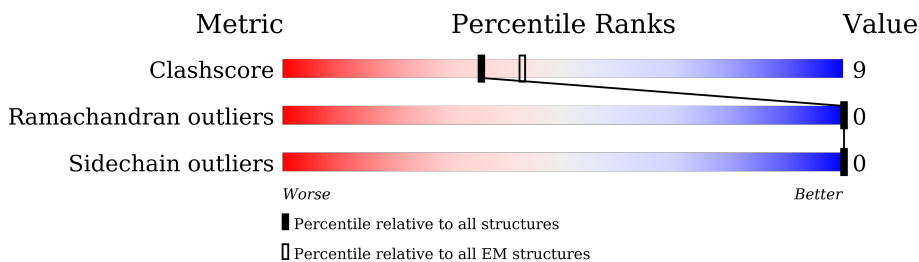
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.12 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	338	
1	B	338	
1	C	338	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3895 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	164	1259	793	224	237	5	0	0
1	B	164	1259	793	224	237	5	0	0
1	C	181	1374	863	245	261	5	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	C	2	Total	Ca	0
			2	2	

ASN	L128	ASN	GLY
ASP	H136	ASP	THR
SER	L141	PRO	ALA
LEU	T144	GLY	TRP
SER	R145	PHE	ARG
THR	V149	TRP	TRP
ASN	L150	GLY	ILE
ASP	K151	ILE	TRP
PHE	W152	ASP	ASP
LEU	W153	ASN	ASN
LEU	E154	LYS	PHE
GLY	S155	THR	THR
SER	R156	PRO	PHE
THR	Q161	LEU	THR
PRO	L166	ASP	ASP
ASP	E174	ILE	GLY
ASP	Q175	ALA	VAL
ALA	R176	PRO	VAL
ALA	R182	VAL	ALA
VAL	L183	ALA	TYR
VAL	I184	TYR	TYR
VAL	L185	SER	SER
VAL	L186	ASP	ASP
VAL	V195	GLN	GLU
VAL	R202	LEU	GLN
VAL	W203	ILE	GLN
VAL	S204	LEU	PRO
VAL	V205	LEU	VAL
VAL	R206	THR	GLY
VAL	L207	CYS	THR
VAL	S211	THR	CYS
VAL	L212	ARG	THR
VAL	P215	VAL	ARG
VAL	GLU	ASP	ASP
VAL	GLU	SER	SER
VAL	THR	GLU	GLU
VAL	THR	ALA	GLU
VAL	ALA	VAL	ASN
VAL	THR	TYR	ASN
VAL	ALA	TRP	ASN
VAL	HIS	HIS	ALA
VAL	LEU	LEU	ALA
VAL	LYS	LYS	ALA
VAL	LYS	LYS	ALA
VAL	PHE	PHE	ALA
VAL	GLN	GLN	ALA
VAL	ALA	ALA	ALA
VAL	SER	SER	ALA
VAL	GLY	GLY	ALA
VAL	ASN	ASN	ALA
VAL	ALA	ALA	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9626	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	450	Depositor
Maximum defocus (nm)	3050	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	3.907	Depositor
Minimum map value	-1.065	Depositor
Average map value	0.118	Depositor
Map value standard deviation	0.300	Depositor
Recommended contour level	0.717	Depositor
Map size (Å)	522.62396, 522.62396, 522.62396	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.361, 1.361, 1.361	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.26	0/1288	0.54	0/1764
1	B	0.26	0/1288	0.54	0/1764
1	C	0.27	0/1405	0.55	0/1923
All	All	0.27	0/3981	0.54	0/5451

There are no bond length outliers.

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	1259	0	1250	28	0
1	B	1259	0	1250	17	0
1	C	1374	0	1364	25	0
2	A	1	0	0	0	0
2	C	2	0	0	0	0
All	All	3895	0	3864	67	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.

All (67) 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:C:141:LEU:HD21	1:C:184:ILE:HB	1.60	0.82
1:B:61:SER:HB2	1:B:90:PRO:HD2	1.72	0.71
1:A:65:GLN:HE21	1:A:196:ASN:HD21	1.39	0.70
1:A:141:LEU:HD21	1:A:184:ILE:HB	1.72	0.70
1:B:60:MET:SD	1:B:202:ARG:NH2	2.68	0.67
1:B:139:ASP:HB3	1:C:212:LEU:HD13	1.80	0.64
1:B:89:LEU:HD12	1:B:92:LEU:HD23	1.79	0.63
1:C:145:ARG:HD2	1:C:161:GLN:HB2	1.80	0.63
1:B:106:THR:HB	1:B:204:SER:HB3	1.81	0.62
1:A:171:SER:O	1:C:176:ARG:NH2	2.32	0.61
1:C:78:VAL:HA	1:C:186:LEU:HD23	1.83	0.61
1:C:110:GLU:OE1	1:C:202:ARG:NH2	2.27	0.58
1:A:89:LEU:HD12	1:A:92:LEU:HD23	1.87	0.56
1:A:176:ARG:NH2	1:B:171:SER:O	2.38	0.56
1:C:103:ALA:HB2	1:C:166:LEU:HD23	1.86	0.56
1:A:67:VAL:HG22	1:A:196:ASN:HD22	1.71	0.56
1:B:89:LEU:HB2	1:B:92:LEU:HB3	1.90	0.54
1:C:68:LEU:HD21	1:C:79:VAL:HG22	1.89	0.53
1:C:81:ASP:OD1	1:C:182:ARG:NH2	2.42	0.52
1:C:102:TYR:HB3	1:C:207:LEU:HD23	1.91	0.52
1:A:89:LEU:HB2	1:A:92:LEU:HB3	1.92	0.52
1:C:79:VAL:HG12	1:C:80:VAL:HG23	1.91	0.52
1:B:104:VAL:HA	1:B:205:VAL:HG12	1.92	0.52
1:A:105:GLU:OE1	1:A:206:ARG:NH2	2.40	0.52
1:C:106:THR:HB	1:C:204:SER:HB3	1.92	0.52
1:A:68:LEU:HB3	1:A:195:VAL:HG23	1.92	0.51
1:A:173:LYS:HA	1:A:173:LYS:HE3	1.92	0.51
1:C:152:TRP:CE3	1:C:195:VAL:HG11	2.47	0.50
1:A:191:ASN:ND2	1:A:193:ASP:O	2.44	0.50
1:C:124:VAL:HG23	1:C:149:VAL:HG22	1.94	0.49
1:C:154:GLU:CD	1:C:156:ARG:HH12	2.16	0.49
1:C:54:ASP:OD1	1:C:206:ARG:NH2	2.45	0.48
1:C:174:GLU:OE2	1:C:176:ARG:HG3	2.13	0.48
1:A:89:LEU:HD13	1:A:203:TRP:CD1	2.48	0.48
1:B:164:ARG:HH11	1:B:164:ARG:HG3	1.77	0.48
1:A:70:ALA:H	1:A:194:VAL:HG12	1.79	0.48
1:C:111:ILE:HD12	1:C:185:LEU:HD12	1.96	0.47
1:A:124:VAL:HG23	1:A:149:VAL:HG22	1.97	0.47
1:A:106:THR:HB	1:A:204:SER:HB3	1.96	0.47
1:A:92:LEU:HD13	1:A:205:VAL:HG21	1.98	0.47
1:A:65:GLN:HE21	1:A:196:ASN:ND2	2.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:CZ	1:B:215:PRO:HD3	2.46	0.45
1:B:84:ILE:O	1:B:180:PRO:HD2	2.17	0.44
1:A:89:LEU:O	1:A:93:GLY:N	2.46	0.44
1:B:72:THR:O	1:B:72:THR:HG22	2.18	0.44
1:C:83:THR:HA	1:C:182:ARG:HG2	2.00	0.44
1:B:79:VAL:HG12	1:B:80:VAL:HG23	2.00	0.43
1:C:136:HIS:CE1	1:C:182:ARG:HH22	2.37	0.43
1:B:92:LEU:HD12	1:B:95:ALA:HB3	2.00	0.43
1:C:128:LEU:HD23	1:C:144:THR:HG21	1.99	0.42
1:C:151:LYS:HD2	1:C:153:TRP:CZ2	2.54	0.42
1:A:151:LYS:HZ3	1:A:153:TRP:HB3	1.84	0.42
1:A:128:LEU:HD13	1:A:184:ILE:HD12	2.02	0.42
1:C:211:SER:OG	1:C:212:LEU:N	2.52	0.42
1:A:111:ILE:HD12	1:A:185:LEU:HD12	2.01	0.42
1:C:85:VAL:HG23	1:C:88:LEU:H	1.85	0.42
1:B:63:ILE:HG13	1:B:64:SER:N	2.34	0.41
1:A:86:PRO:HB3	1:A:92:LEU:HG	2.01	0.41
1:A:130:ASP:OD1	1:A:176:ARG:NH1	2.53	0.41
1:B:139:ASP:HA	1:B:142:GLN:HG2	2.02	0.41
1:A:68:LEU:HD23	1:A:69:PRO:O	2.21	0.41
1:A:96:ALA:HB1	1:A:169:THR:HB	2.02	0.40
1:A:151:LYS:NZ	1:A:153:TRP:HB3	2.37	0.40
1:B:68:LEU:HB3	1:B:195:VAL:HB	2.02	0.40
1:A:85:VAL:HG22	1:A:88:LEU:HD23	2.04	0.40
1:A:104:VAL:HG21	1:A:180:PRO:HG3	2.04	0.40
1:C:136:HIS:HE1	1:C:182:ARG:HH22	1.68	0.40

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	162/338 (48%)	159 (98%)	3 (2%)	0	100	100
1	B	162/338 (48%)	154 (95%)	8 (5%)	0	100	100
1	C	179/338 (53%)	171 (96%)	8 (4%)	0	100	100
All	All	503/1014 (50%)	484 (96%)	19 (4%)	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	A	139/284 (49%)	139 (100%)	0	100	100
1	B	139/284 (49%)	139 (100%)	0	100	100
1	C	151/284 (53%)	151 (100%)	0	100	100
All	All	429/852 (50%)	429 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	196	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

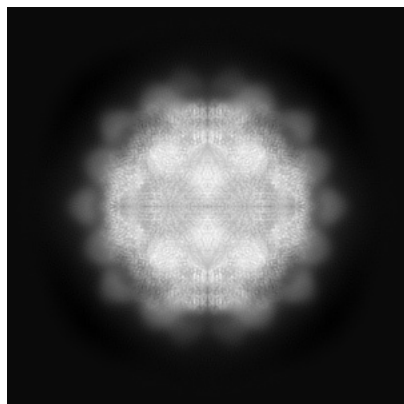
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39215. These allow visual inspection of the internal detail of the map and identification of artifacts.

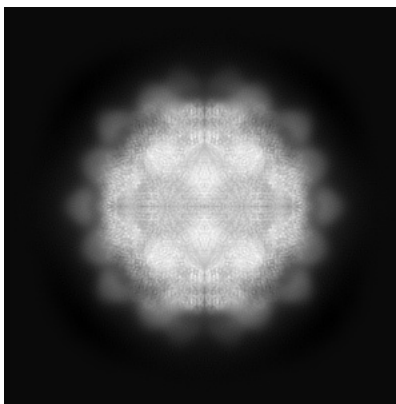
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

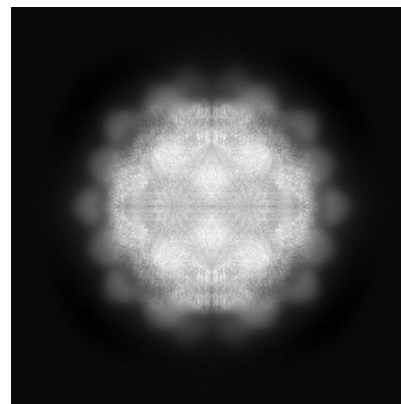
6.1.1 Primary map



X

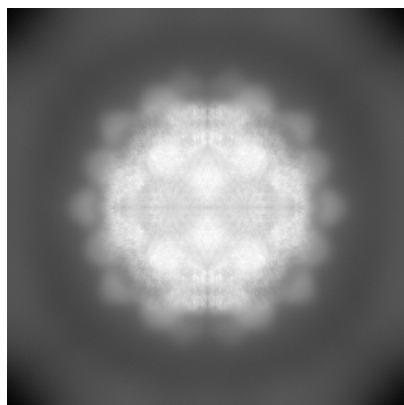


Y

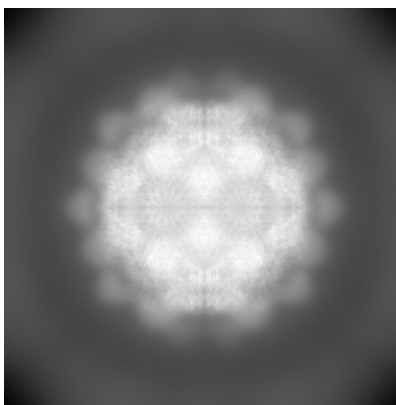


Z

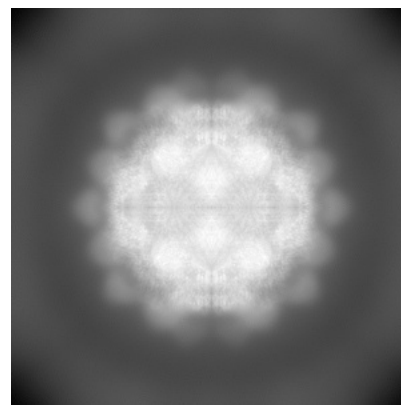
6.1.2 Raw map



X



Y

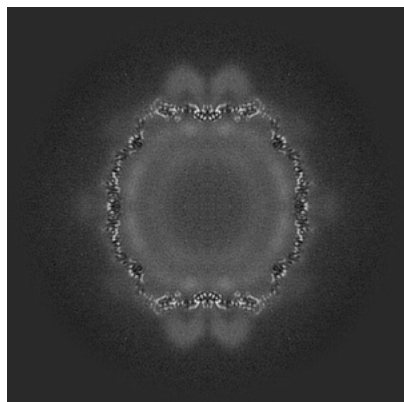


Z

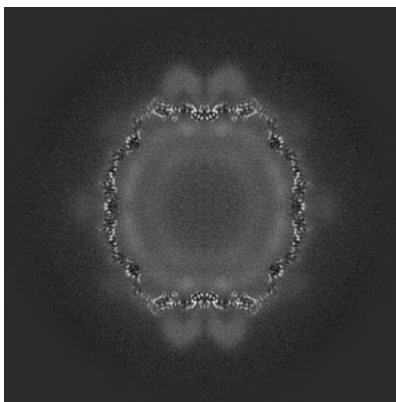
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

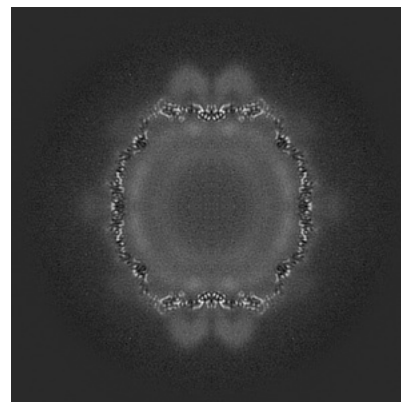
6.2.1 Primary map



X Index: 192

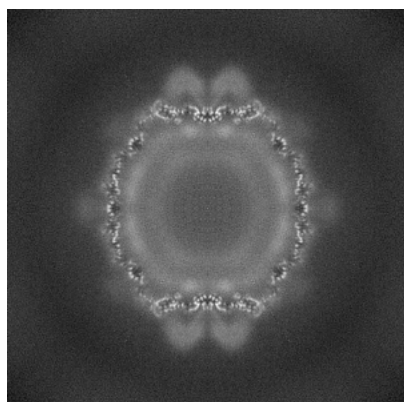


Y Index: 192

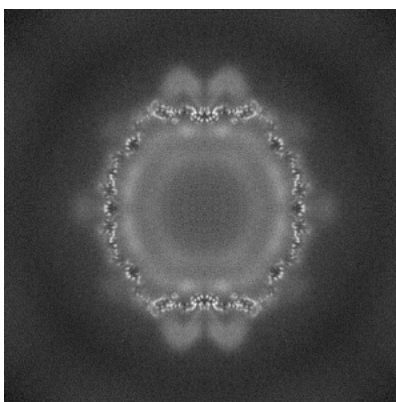


Z Index: 192

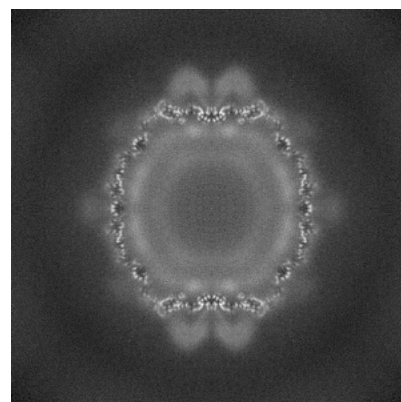
6.2.2 Raw map



X Index: 192



Y Index: 192

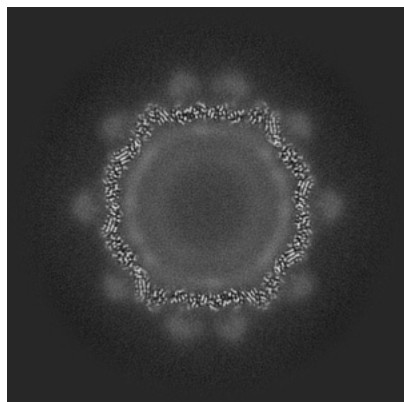


Z Index: 192

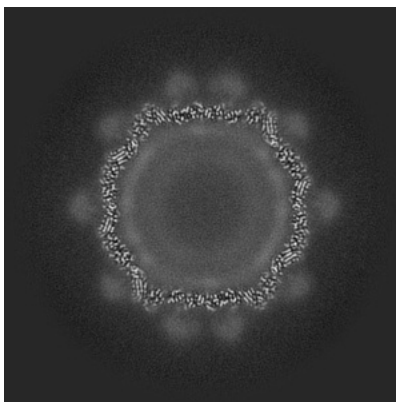
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

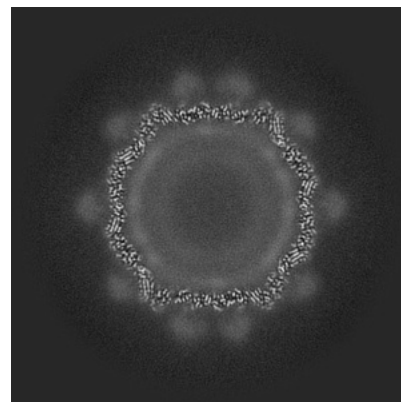
6.3.1 Primary map



X Index: 180

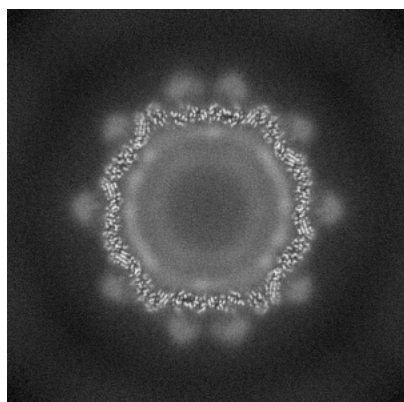


Y Index: 180

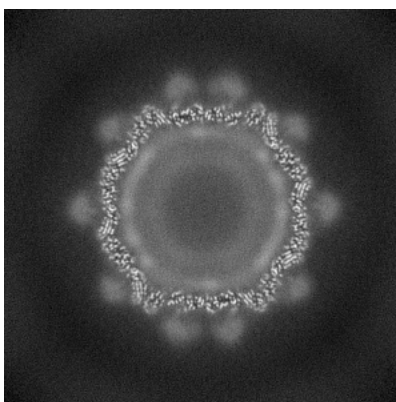


Z Index: 180

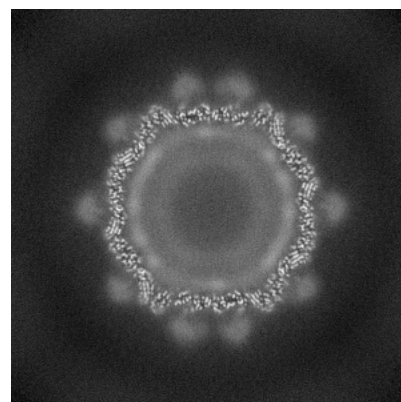
6.3.2 Raw map



X Index: 204



Y Index: 180

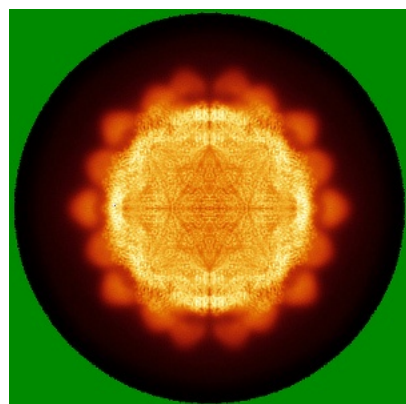


Z Index: 180

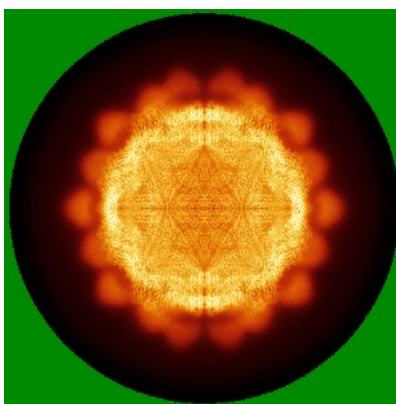
The images above show the largest variance slices of the map in three orthogonal directions.

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

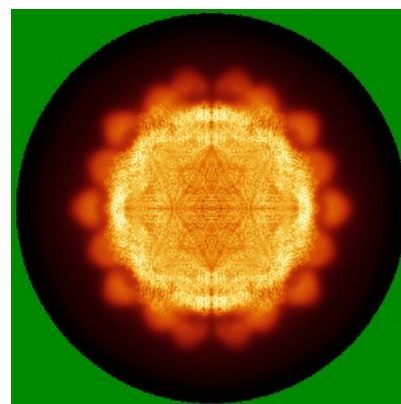
6.4.1 Primary map



X

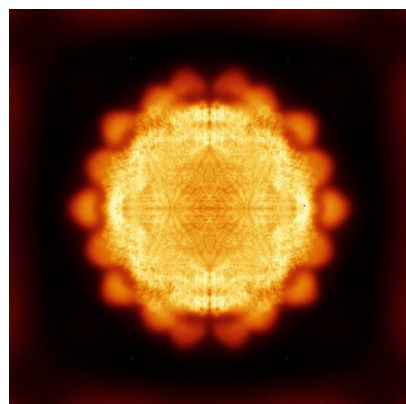


Y

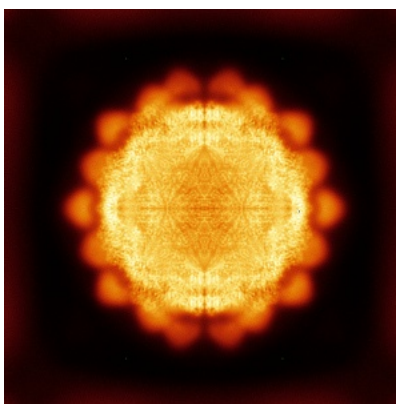


Z

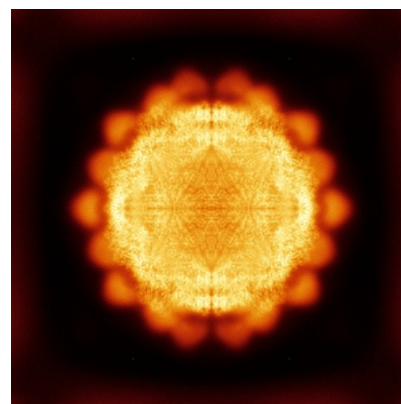
6.4.2 Raw map



X



Y

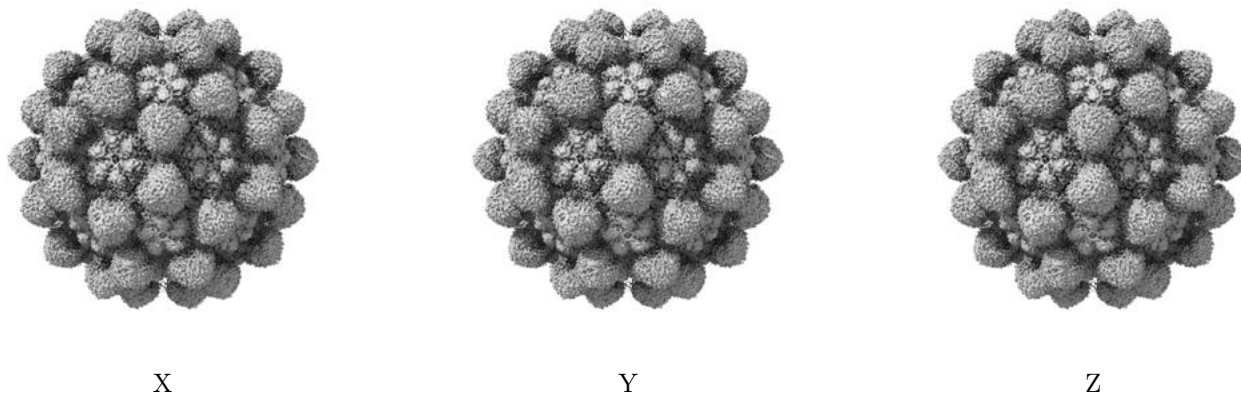


Z

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.

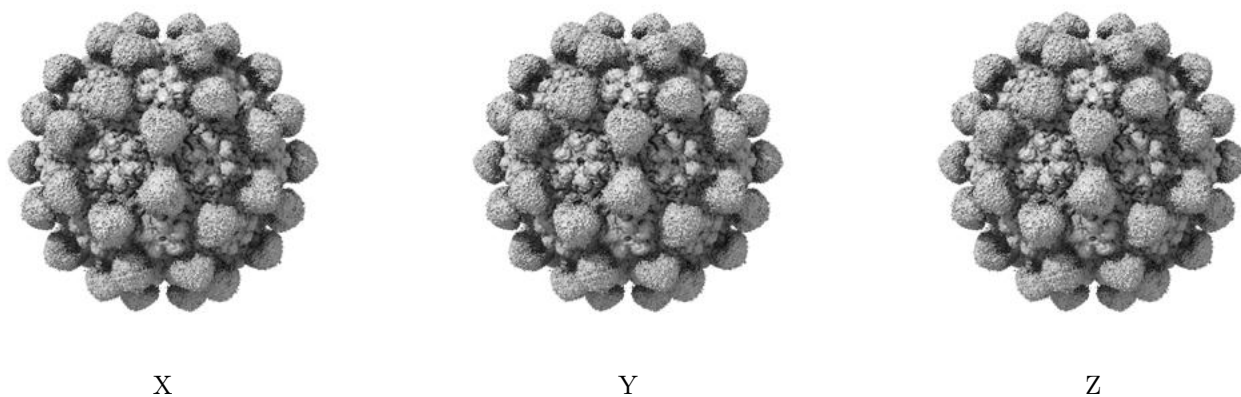
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.717. 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.

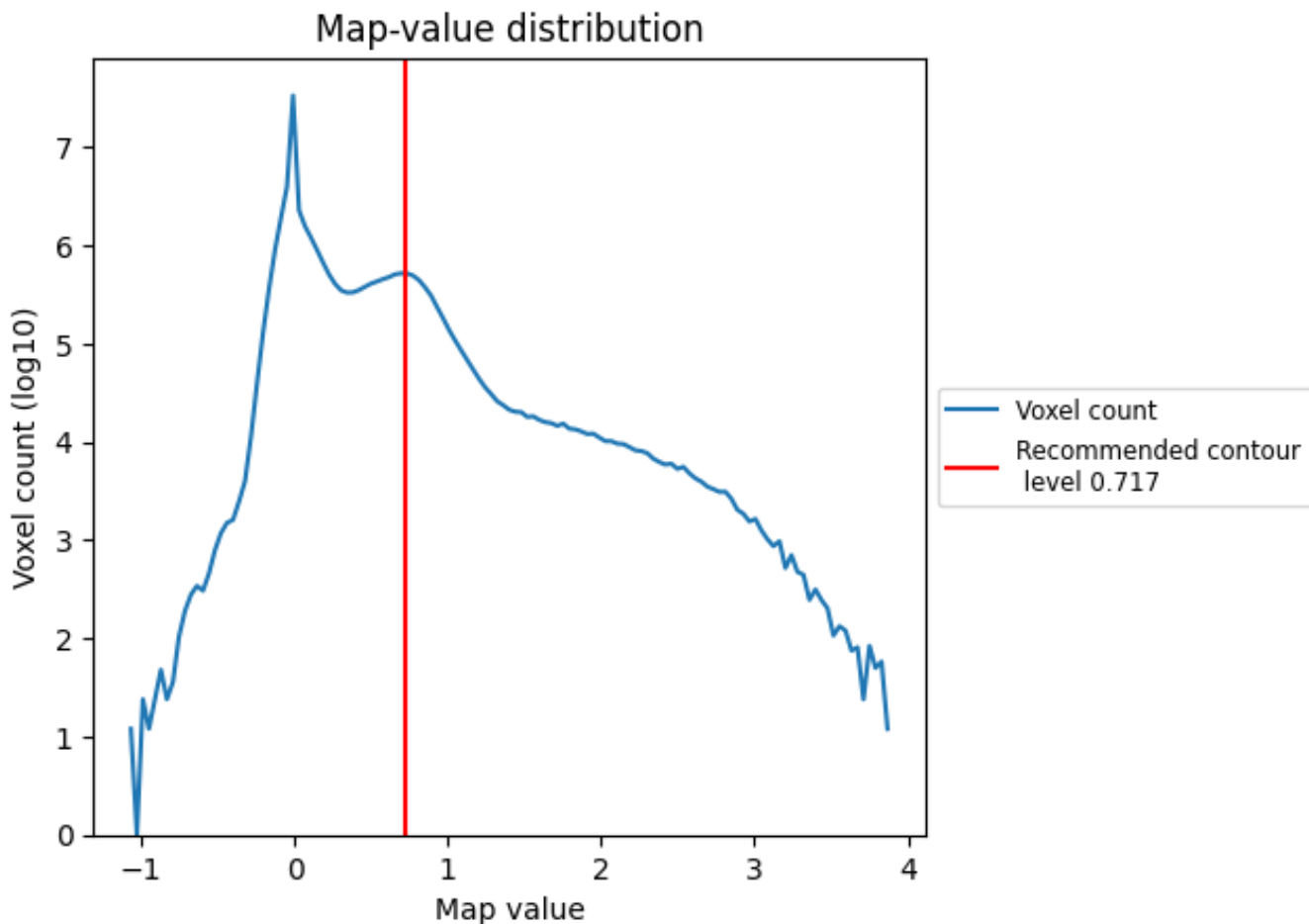
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

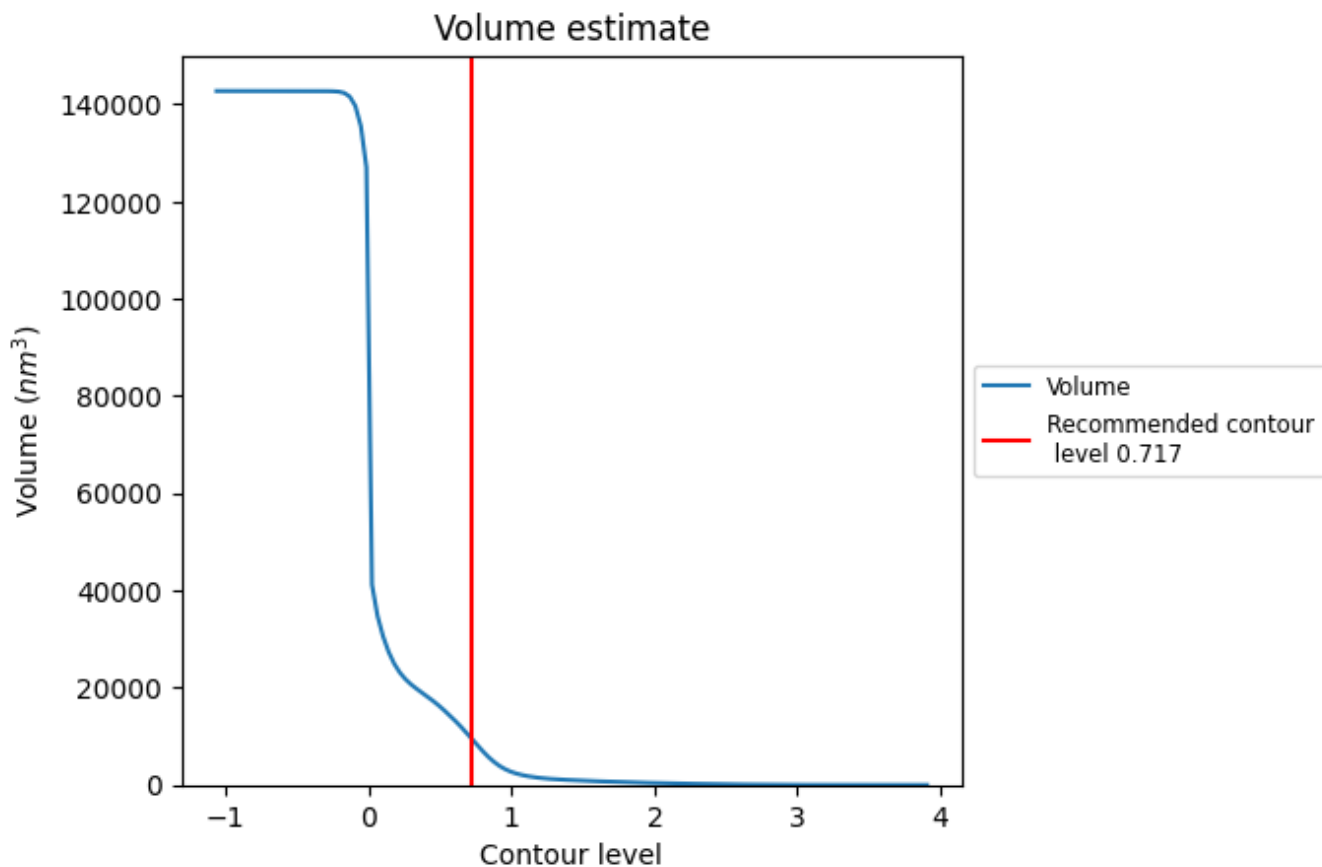
This section contains the results of statistical analysis of the map.

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.

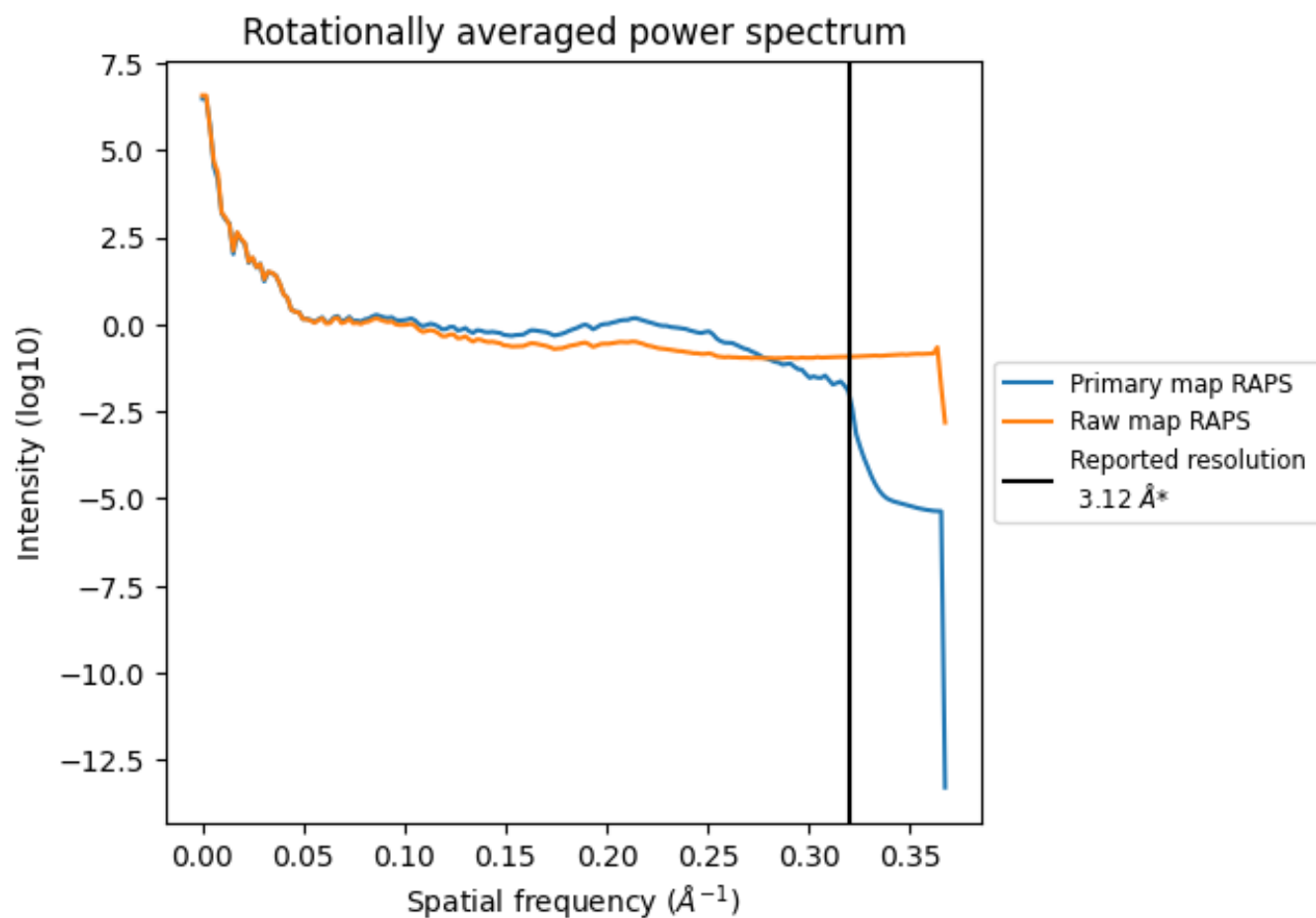
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96270 nm³; this corresponds to an approximate mass of 8697 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 [i](#)

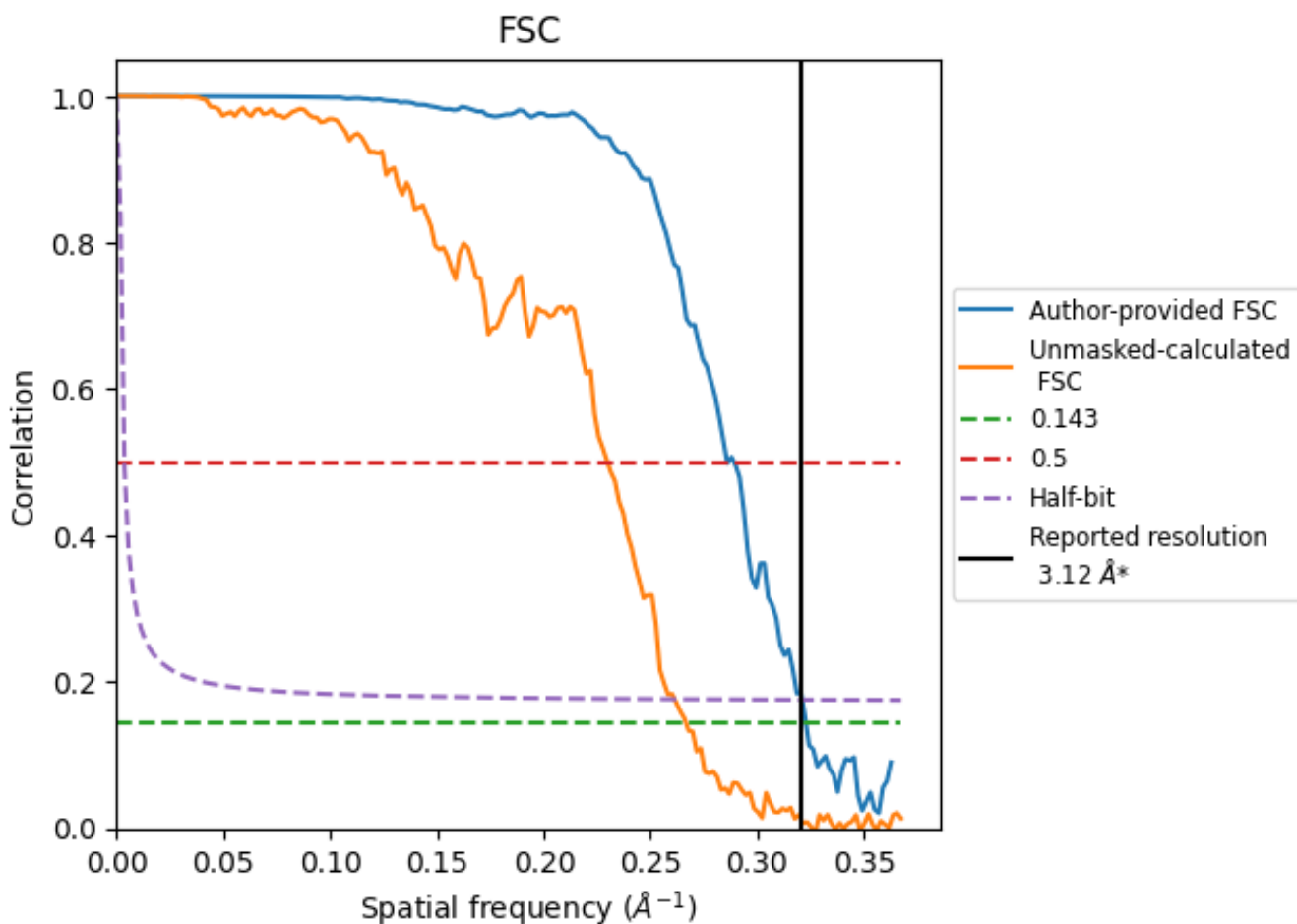


*Reported resolution corresponds to spatial frequency of 0.321 Å⁻¹

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 0.321 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	3.10	3.50	3.11
Unmasked-calculated*	3.75	4.35	3.83

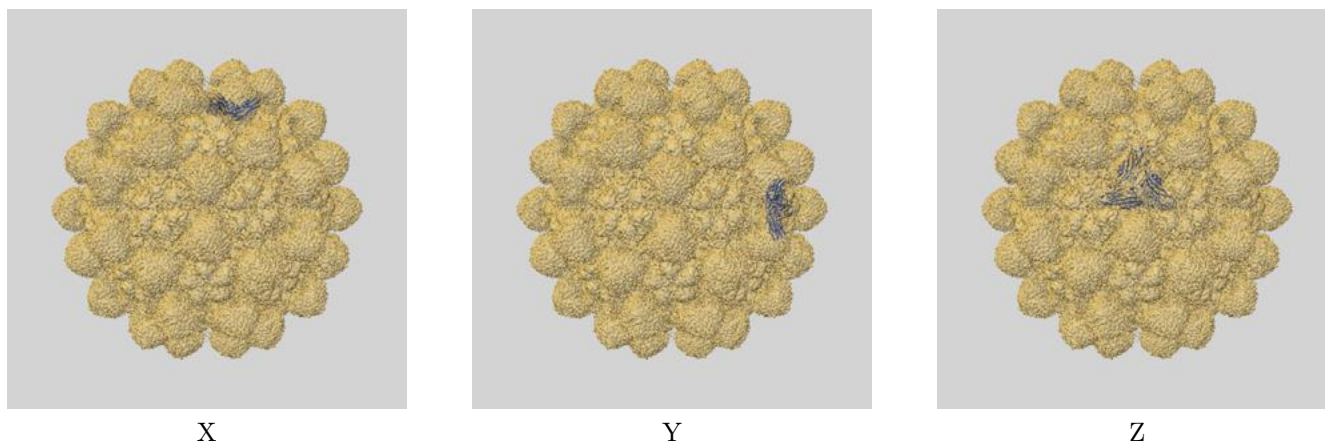
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.12 by more than 10 %

9 Map-model fit [i](#)

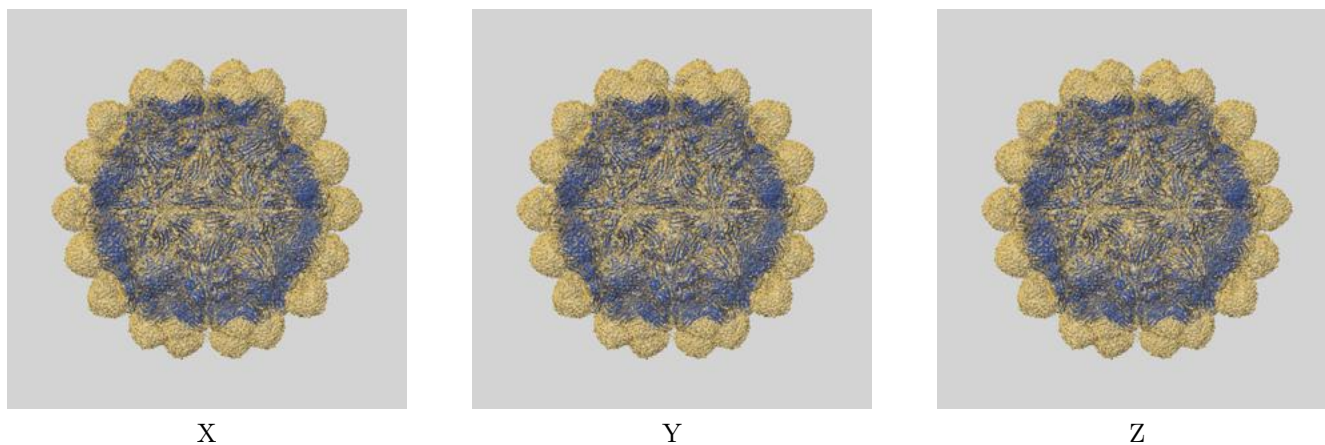
This section contains information regarding the fit between EMDB map EMD-39215 and PDB model 8YF9. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

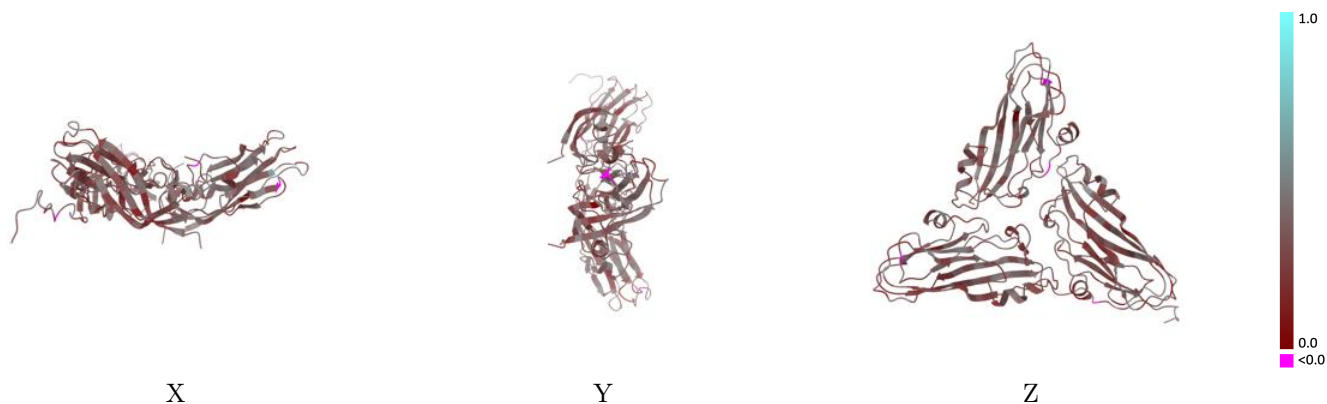


9.1.2 Map-model assembly overlay [i](#)



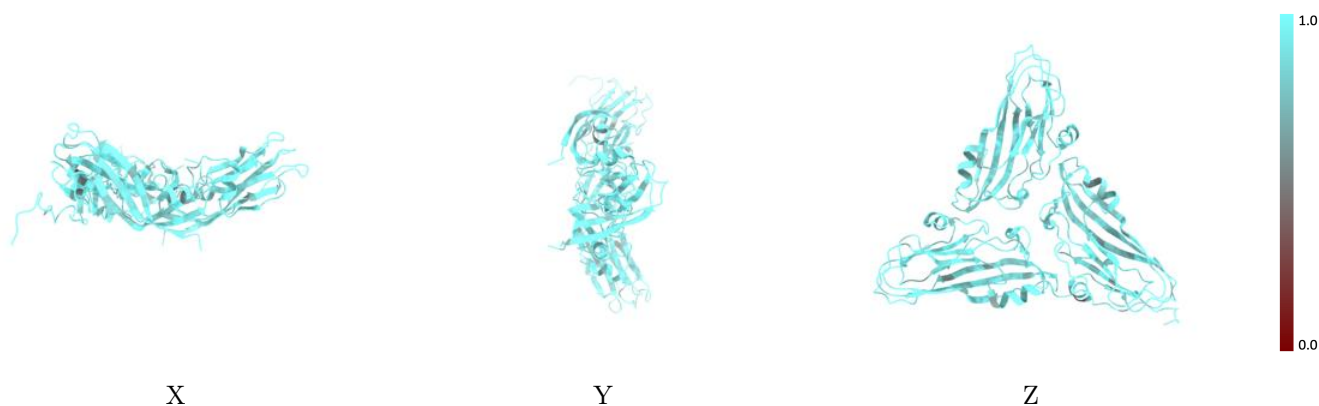
The images above show the 3D surface view of the map at the recommended contour level 0.717 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



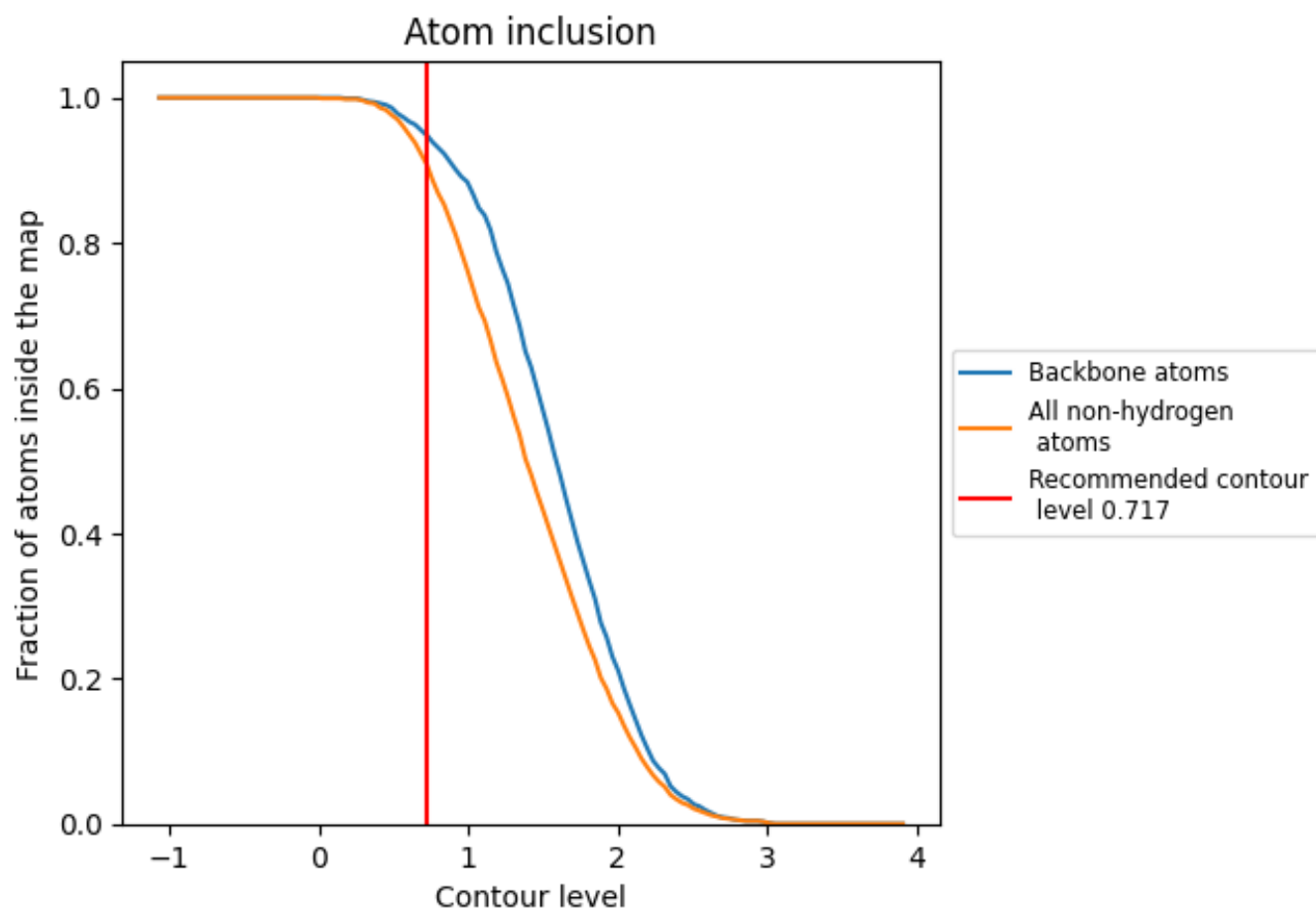
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.717).









9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.717) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.3170
A	 0.9150	 0.3220
B	 0.9050	 0.3170
C	 0.9110	 0.3120

