wwPDB EM Validation Summary Report

Nov 9, 2026 – 05:04 PM JST

PDB ID	:	9XMT / pdb_00009xmt
EMDB ID	:	EMD-67032
Title	:	The self-assembled capsid protein of AbP20
Authors	:	Xue, H.; Rao, G.; Cao, S.; Yang, H.
Deposited on	:	2025-11-11
Resolution	:	3.30 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:

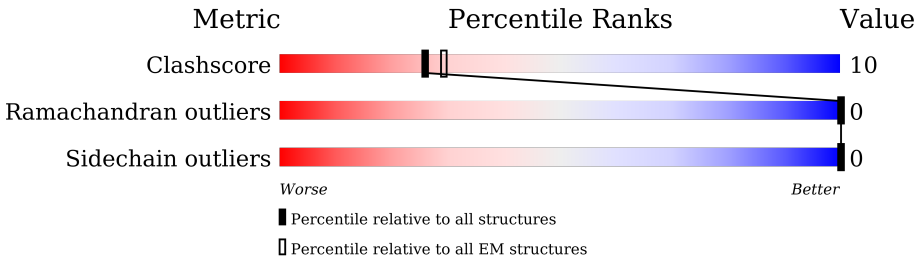
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

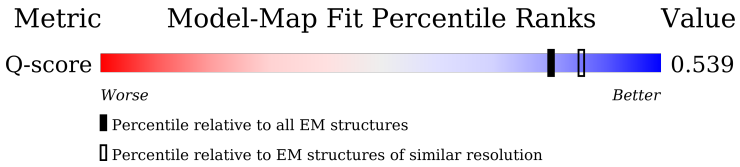
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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 <=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	286	11% 85%
1	B	286	5% 12% 85%
1	C	286	10% 9% 89%
1	D	286	11% 10% 87%

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Mol	Chain	Length	Quality of chain
1	E	286	12% 85%
1	F	286	11% 85%
1	G	286	13% 84%
2	H	343	13% 71% 21% 8%
2	I	343	7% 69% 22% 10%
2	J	343	8% 65% 25% 10%
2	K	343	9% 67% 23% 10%
2	L	343	13% 71% 22% 7%
2	M	343	10% 65% 24% 10%
2	N	343	12% 72% 20% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19594 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 Scaffolding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	43	Total 365	C 228	N 72	O 65	0	0
1	B	44	Total 369	C 230	N 73	O 66	0	0
1	C	32	Total 269	C 165	N 56	O 48	0	0
1	D	36	Total 305	C 189	N 62	O 54	0	0
1	E	43	Total 365	C 228	N 72	O 65	0	0
1	F	43	Total 365	C 228	N 72	O 65	0	0
1	G	45	Total 377	C 236	N 74	O 67	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	THR	ASN	conflict	UNP R4IPS9
A	218	THR	ALA	conflict	UNP R4IPS9
B	75	THR	ASN	conflict	UNP R4IPS9
B	218	THR	ALA	conflict	UNP R4IPS9
C	75	THR	ASN	conflict	UNP R4IPS9
C	218	THR	ALA	conflict	UNP R4IPS9
D	75	THR	ASN	conflict	UNP R4IPS9
D	218	THR	ALA	conflict	UNP R4IPS9
E	75	THR	ASN	conflict	UNP R4IPS9
E	218	THR	ALA	conflict	UNP R4IPS9
F	75	THR	ASN	conflict	UNP R4IPS9
F	218	THR	ALA	conflict	UNP R4IPS9
G	75	THR	ASN	conflict	UNP R4IPS9
G	218	THR	ALA	conflict	UNP R4IPS9

- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	314	Total	C	N	O	S	0	0
			2460	1546	433	474	7		
2	I	310	Total	C	N	O	S	0	0
			2450	1543	429	471	7		
2	J	308	Total	C	N	O	S	0	0
			2424	1526	425	466	7		
2	K	308	Total	C	N	O	S	0	0
			2428	1529	426	466	7		
2	L	319	Total	C	N	O	S	0	0
			2523	1588	443	485	7		
2	M	307	Total	C	N	O	S	0	0
			2409	1515	424	463	7		
2	N	315	Total	C	N	O	S	0	0
			2485	1565	438	475	7		

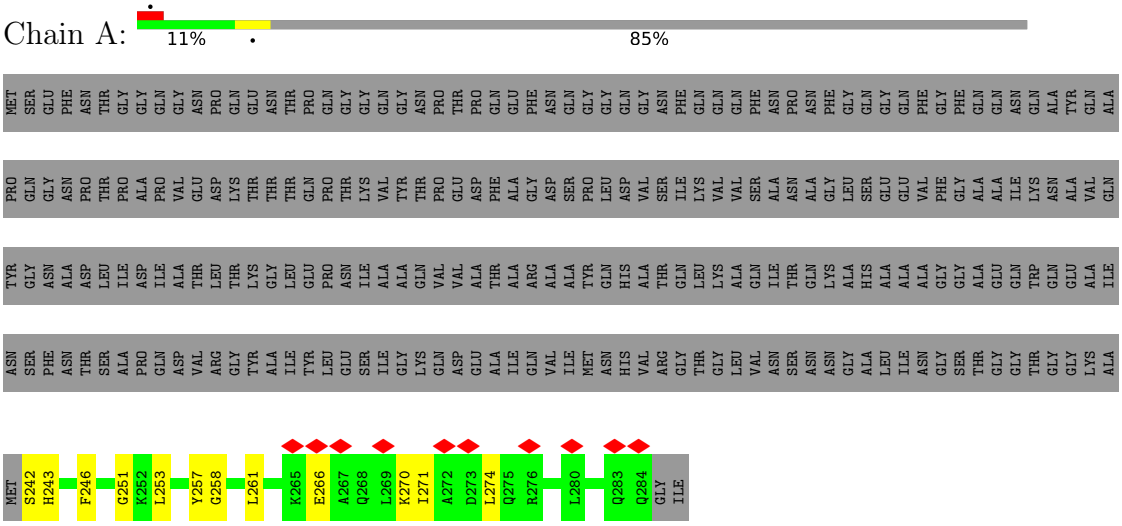
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	19	ALA	ASP	conflict	UNP A0A0P0I783
H	278	ASP	GLU	conflict	UNP A0A0P0I783
I	19	ALA	ASP	conflict	UNP A0A0P0I783
I	278	ASP	GLU	conflict	UNP A0A0P0I783
J	19	ALA	ASP	conflict	UNP A0A0P0I783
J	278	ASP	GLU	conflict	UNP A0A0P0I783
K	19	ALA	ASP	conflict	UNP A0A0P0I783
K	278	ASP	GLU	conflict	UNP A0A0P0I783
L	19	ALA	ASP	conflict	UNP A0A0P0I783
L	278	ASP	GLU	conflict	UNP A0A0P0I783
M	19	ALA	ASP	conflict	UNP A0A0P0I783
M	278	ASP	GLU	conflict	UNP A0A0P0I783
N	19	ALA	ASP	conflict	UNP A0A0P0I783
N	278	ASP	GLU	conflict	UNP A0A0P0I783

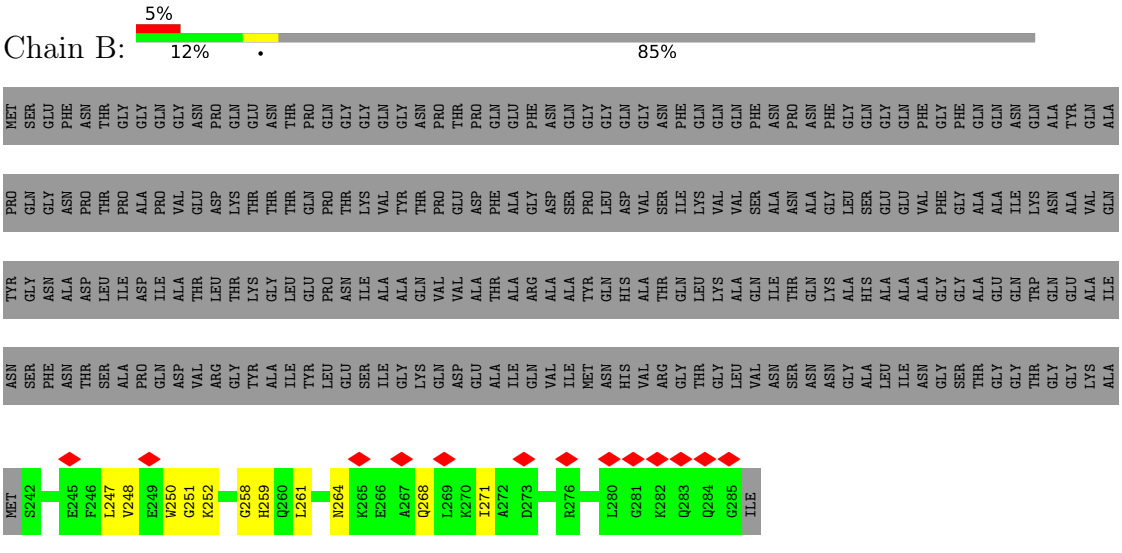
3 Residue-property plots (i)

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: Scaffolding protein

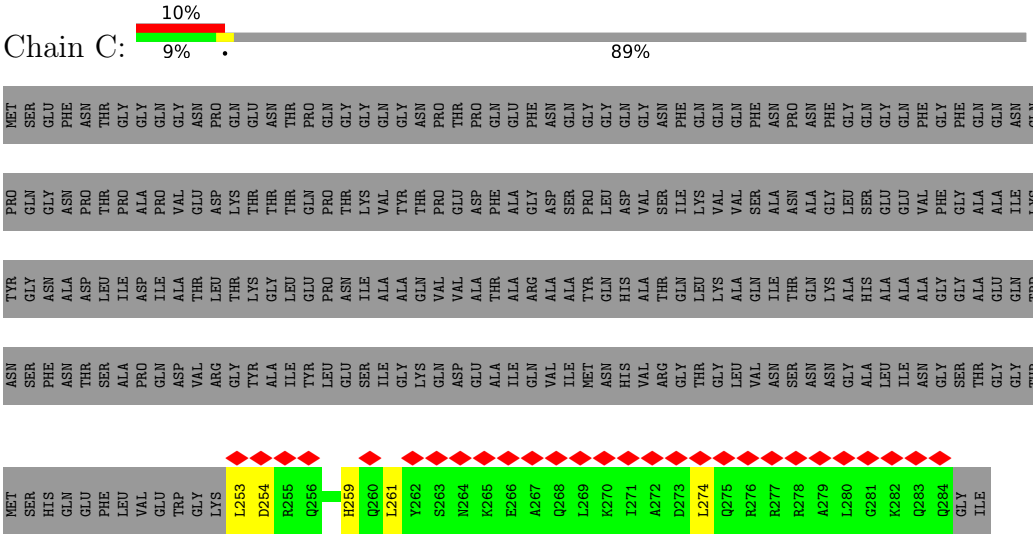


• Molecule 1: Scaffolding protein



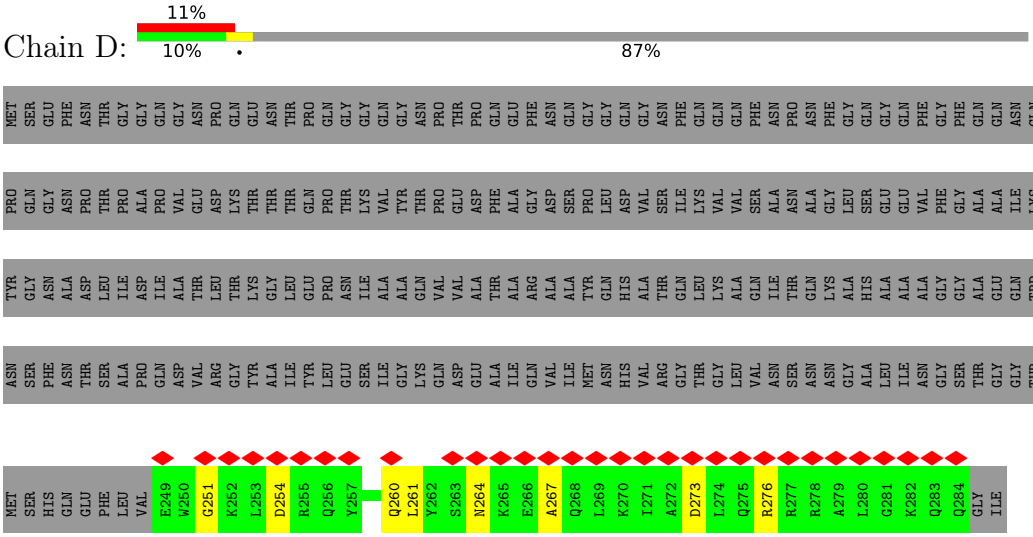
• Molecule 1: Scaffolding protein

Chain C:



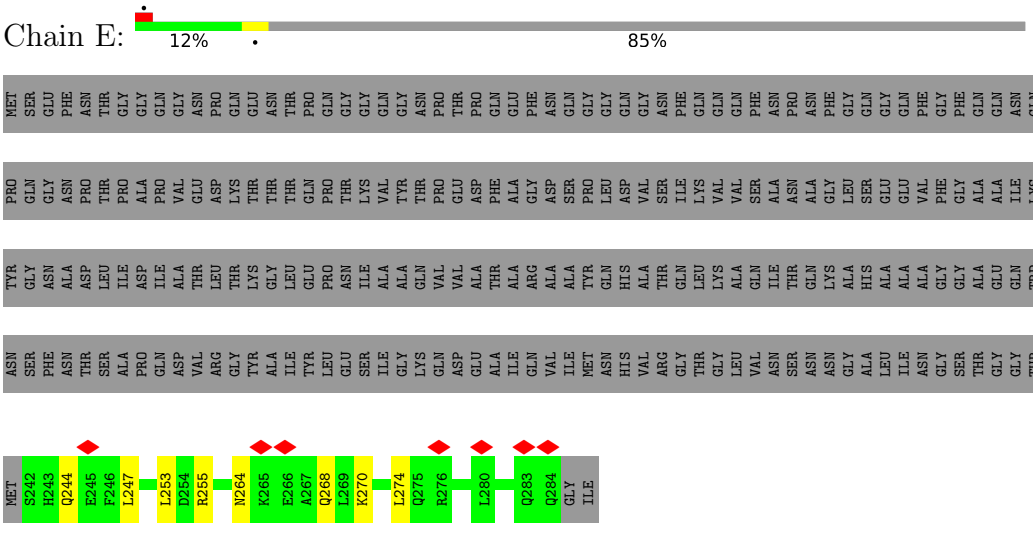
• Molecule 1: Scaffolding protein

Chain D:



• Molecule 1: Scaffolding protein

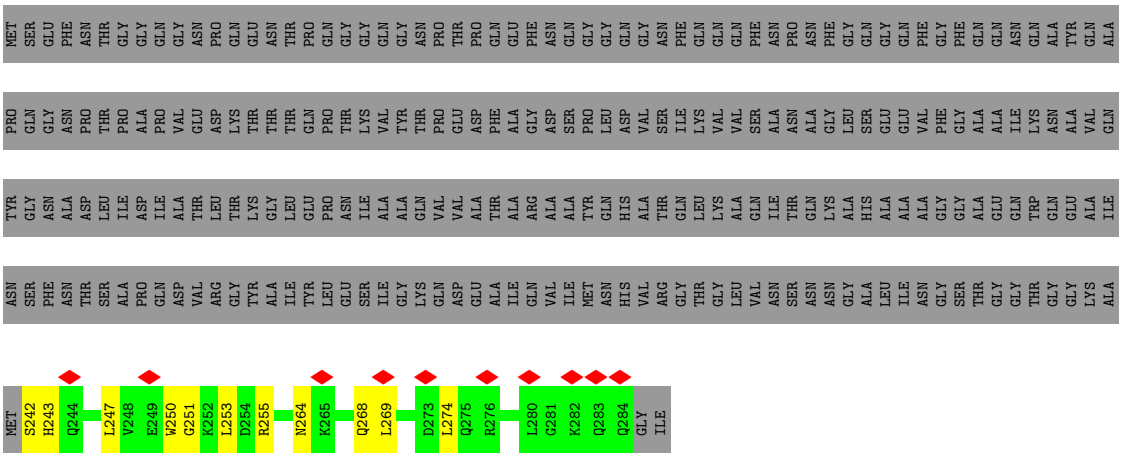
Chain E:



• Molecule 1: Scaffolding protein

Chain F:





• Molecule 1: Scaffolding protein

Chain G:

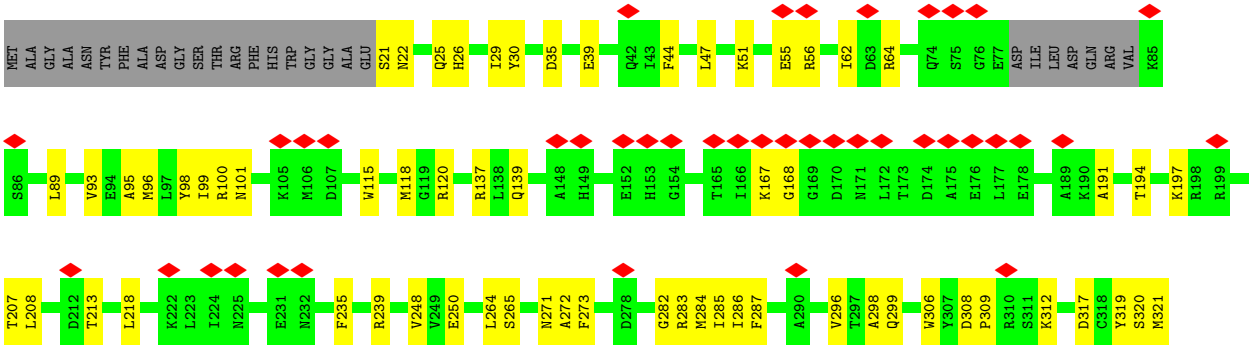


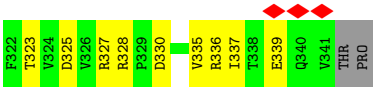


• Molecule 2: Capsid protein

Chain H:



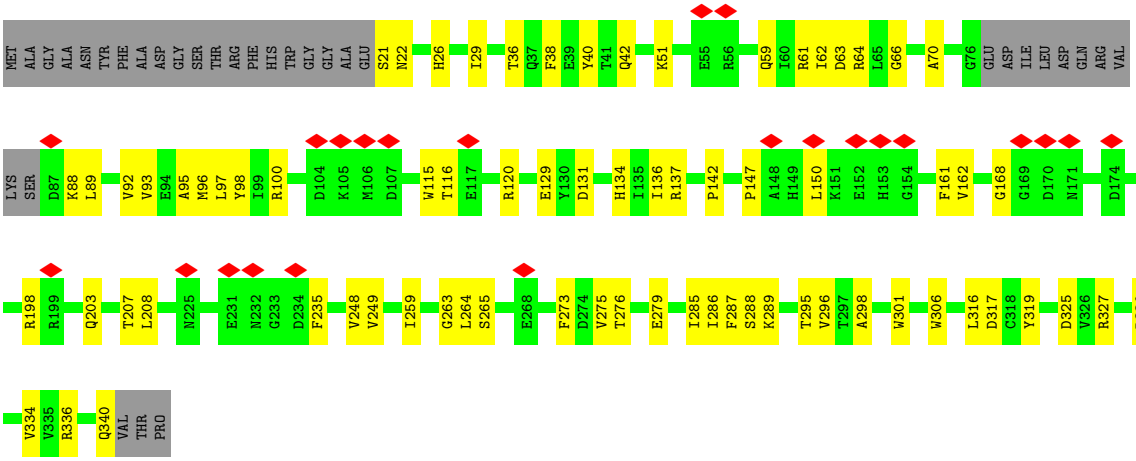




• Molecule 2: Capsid protein

Chain I:

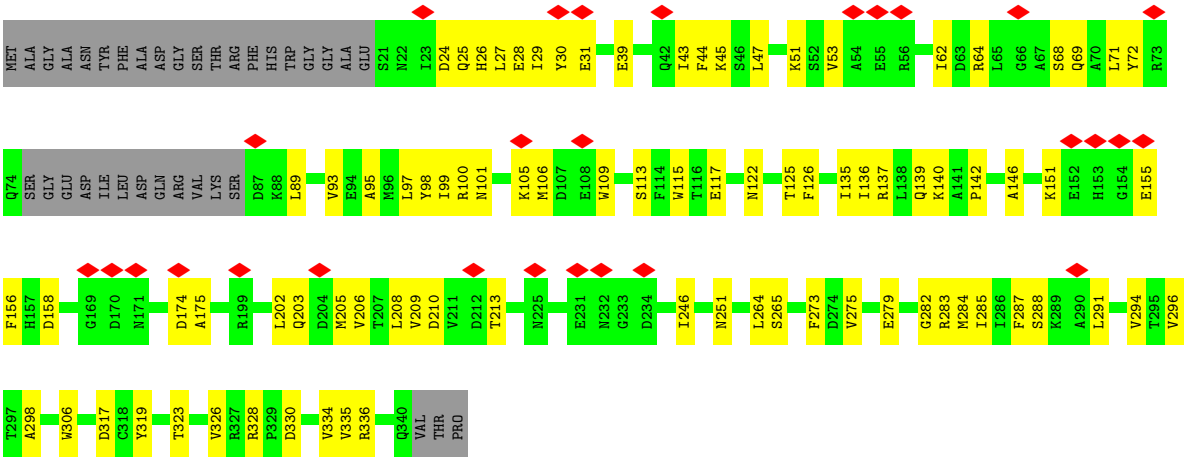




• Molecule 2: Capsid protein

Chain J:

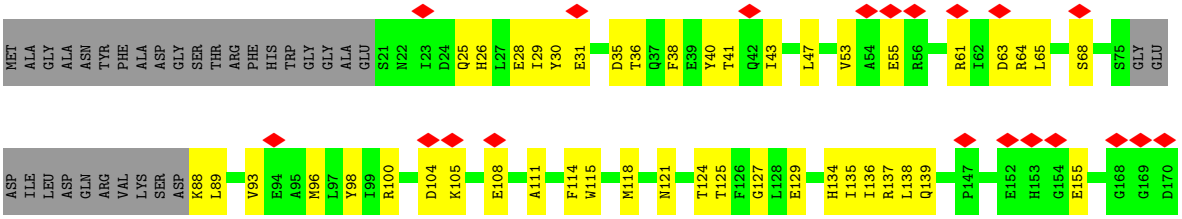


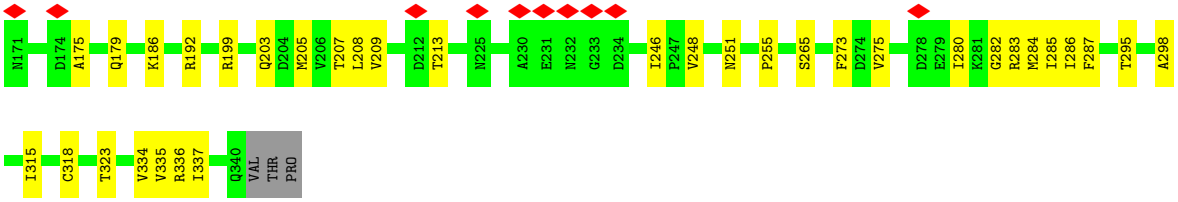


• Molecule 2: Capsid protein

Chain K:



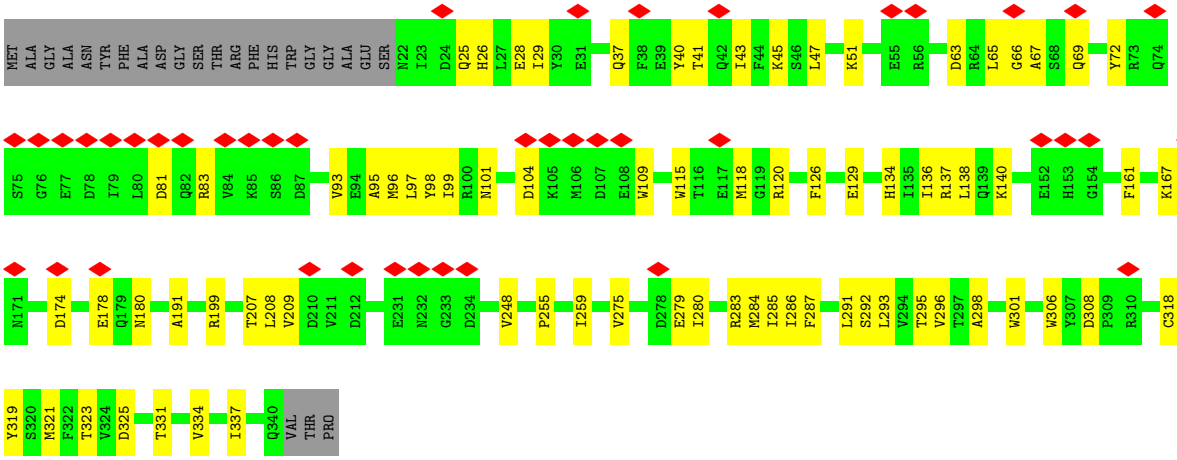




• Molecule 2: Capsid protein

Chain L:

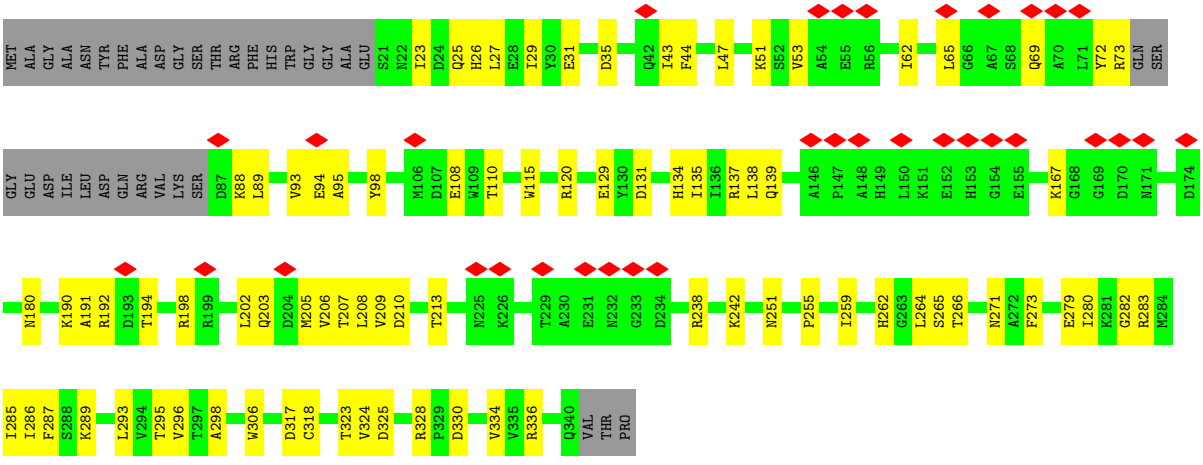




• Molecule 2: Capsid protein

Chain M:

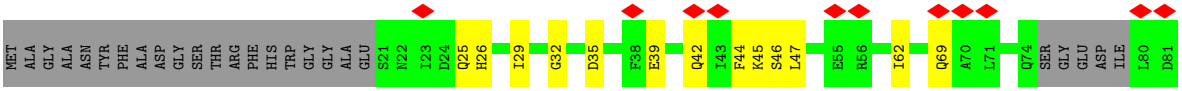


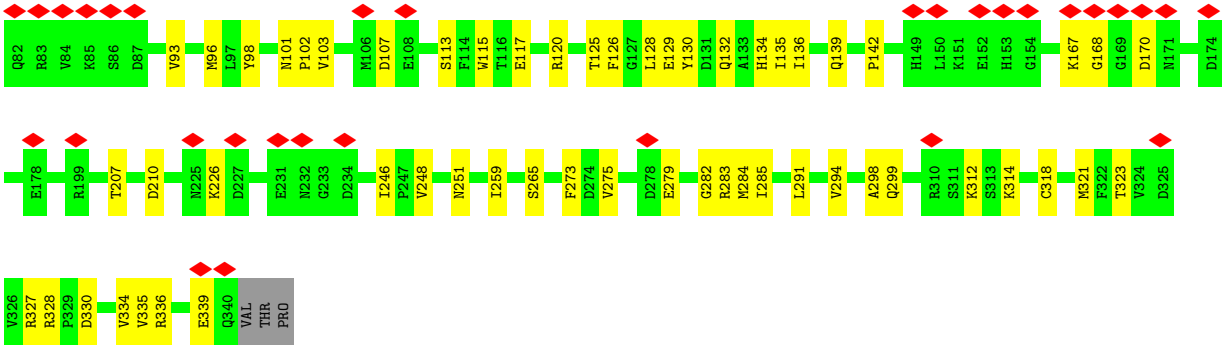


• Molecule 2: Capsid protein

Chain N:






Q82
R83
V84
K85
S86
D87
V93
M96
L97
Y98
N101
P102
V103
M106
D107
E108
S113
F114
W115
T116
E117
R120
T125
F126
G127
L128
E129
Y130
D131
Q132
A133
H134
I135
I136
Q139
P142
H149
L150
K151
E152
H153
G154
K167
G168
G169
D170
N171
D174
E178
R199
T207
D210
N225
K226
D227
E231
N232
G233
D234
I246
P247
V248
N251
I259
S265
F273
D274
V275
D278
E279
G282
R283
M284
I285
L291
V294
A298
Q299
R310
S311
K312
S313
K314
C318
M321
F322
T323
V324
D325
V326
R327
R328
P329
D330
V334
V335
R336
E339
Q340
VAL
THR
PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	630.8, 630.8, 630.8	wwPDB
Map dimensions	664, 664, 664	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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	0.27	0/371	0.51	0/494
1	B	0.25	0/375	0.50	0/499
1	C	0.18	0/271	0.41	0/359
1	D	0.18	0/309	0.38	0/410
1	E	0.26	0/371	0.61	0/494
1	F	0.24	0/371	0.49	0/494
1	G	0.36	0/383	0.44	0/510
2	H	0.33	0/2508	0.55	0/3406
2	I	0.32	0/2500	0.48	0/3395
2	J	0.34	0/2473	0.53	0/3361
2	K	0.34	0/2477	0.52	0/3365
2	L	0.32	0/2574	0.53	0/3496
2	M	0.32	0/2457	0.51	0/3338
2	N	0.33	0/2535	0.51	0/3442
All	All	0.32	0/19975	0.51	0/27063

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

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	365	0	362	8	0
1	B	369	0	365	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	269	0	275	4	0
1	D	305	0	307	6	0
1	E	365	0	362	8	0
1	F	365	0	362	9	0
1	G	377	0	376	6	0
2	H	2460	0	2417	53	0
2	I	2450	0	2408	55	0
2	J	2424	0	2371	63	0
2	K	2428	0	2388	62	0
2	L	2523	0	2484	55	0
2	M	2409	0	2358	66	0
2	N	2485	0	2439	46	0
All	All	19594	0	19274	395	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 10.

The worst 5 of 395 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:M:43:ILE:HG23	2:M:238:ARG:HH21	1.18	1.08
1:F:247:LEU:HD13	2:K:31:GLU:HG3	1.40	1.03
2:M:43:ILE:HG23	2:M:238:ARG:NH2	1.88	0.87
1:E:247:LEU:HA	2:J:31:GLU:HG2	1.63	0.81
2:L:29:ILE:HB	2:L:115:TRP:HB3	1.65	0.77

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	41/286 (14%)	39 (95%)	2 (5%)	0	100	100
1	B	42/286 (15%)	42 (100%)	0	0	100	100
1	C	30/286 (10%)	29 (97%)	1 (3%)	0	100	100
1	D	34/286 (12%)	34 (100%)	0	0	100	100
1	E	41/286 (14%)	40 (98%)	1 (2%)	0	100	100
1	F	41/286 (14%)	41 (100%)	0	0	100	100
1	G	43/286 (15%)	42 (98%)	1 (2%)	0	100	100
2	H	310/343 (90%)	286 (92%)	24 (8%)	0	100	100
2	I	306/343 (89%)	293 (96%)	13 (4%)	0	100	100
2	J	304/343 (89%)	287 (94%)	17 (6%)	0	100	100
2	K	304/343 (89%)	287 (94%)	17 (6%)	0	100	100
2	L	317/343 (92%)	304 (96%)	13 (4%)	0	100	100
2	M	303/343 (88%)	287 (95%)	16 (5%)	0	100	100
2	N	311/343 (91%)	295 (95%)	16 (5%)	0	100	100
All	All	2427/4403 (55%)	2306 (95%)	121 (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	A	37/219 (17%)	37 (100%)	0	100	100
1	B	37/219 (17%)	37 (100%)	0	100	100
1	C	27/219 (12%)	27 (100%)	0	100	100
1	D	30/219 (14%)	30 (100%)	0	100	100
1	E	37/219 (17%)	37 (100%)	0	100	100
1	F	37/219 (17%)	37 (100%)	0	100	100
1	G	38/219 (17%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	266/291 (91%)	266 (100%)	0	100	100
2	I	266/291 (91%)	266 (100%)	0	100	100
2	J	261/291 (90%)	261 (100%)	0	100	100
2	K	263/291 (90%)	263 (100%)	0	100	100
2	L	274/291 (94%)	274 (100%)	0	100	100
2	M	259/291 (89%)	259 (100%)	0	100	100
2	N	268/291 (92%)	268 (100%)	0	100	100
All	All	2100/3570 (59%)	2100 (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 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	237	ASN
2	N	122	ASN
2	N	340	GLN
2	M	219	HIS
2	J	122	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.

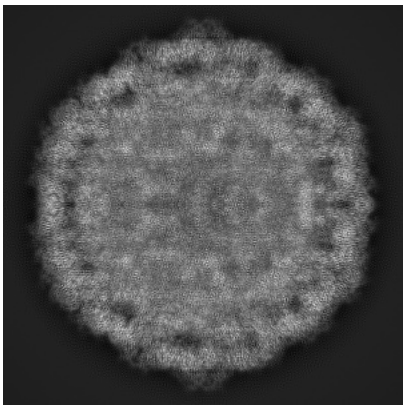
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67032. These allow visual inspection of the internal detail of the map and identification of artifacts.

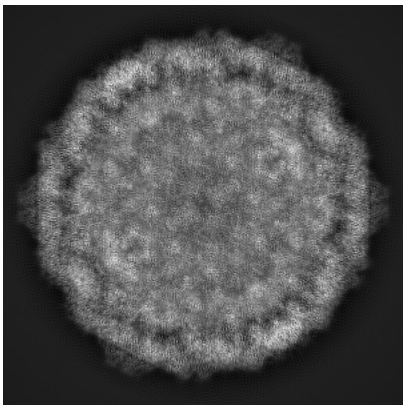
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

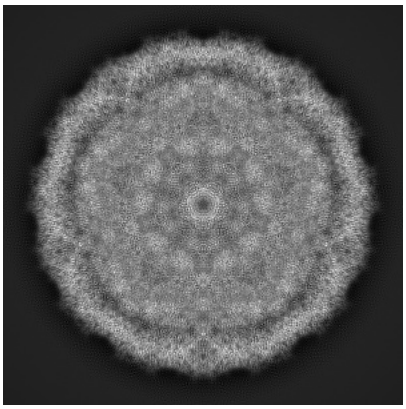
6.1.1 Primary map



X

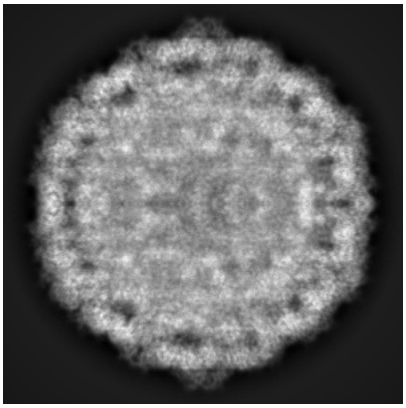


Y

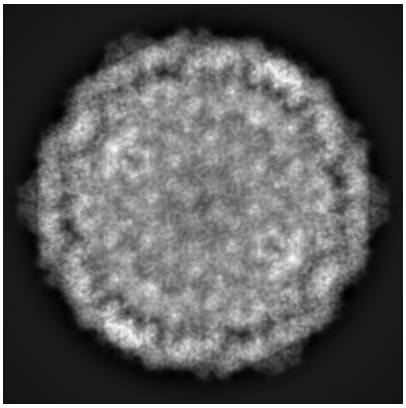


Z

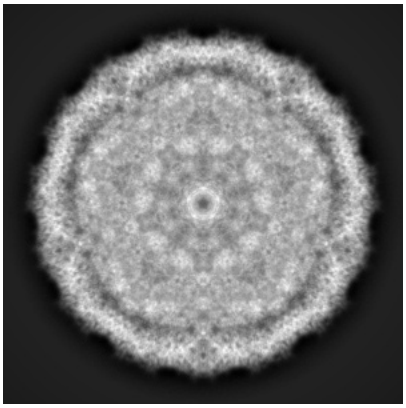
6.1.2 Raw map



X



Y

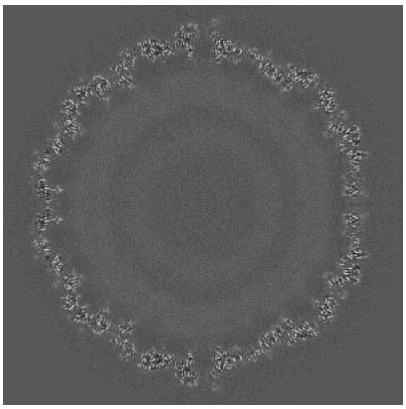


Z

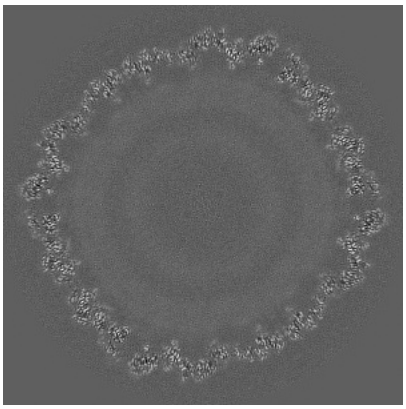
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

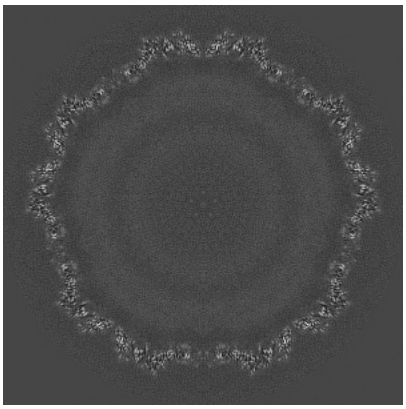
6.2.1 Primary map



X Index: 332

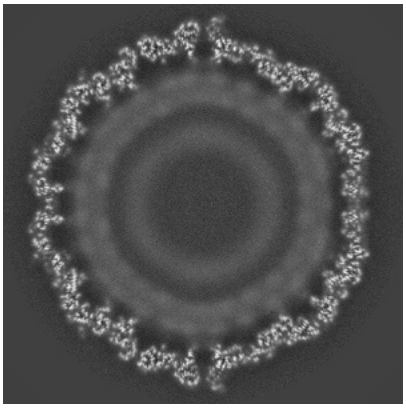


Y Index: 332

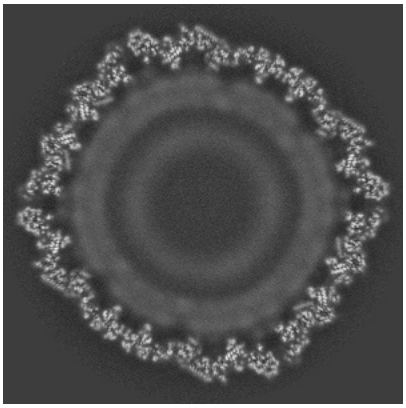


Z Index: 332

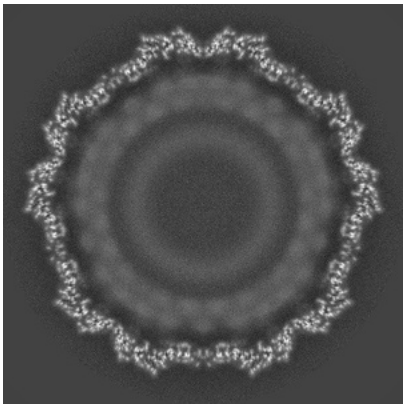
6.2.2 Raw map



X Index: 332



Y Index: 332

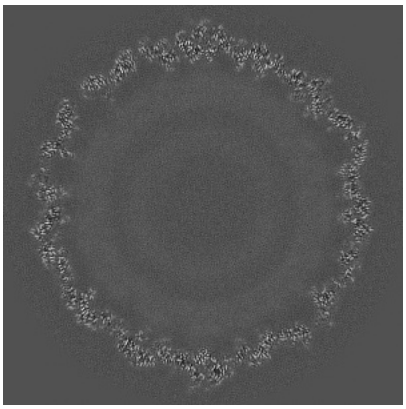


Z Index: 332

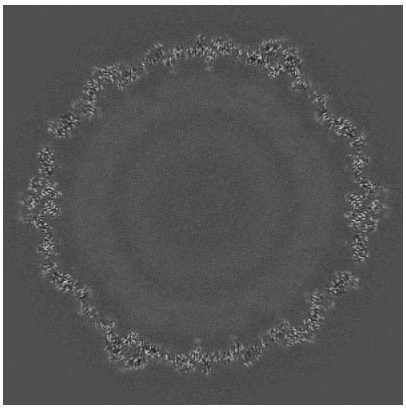
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

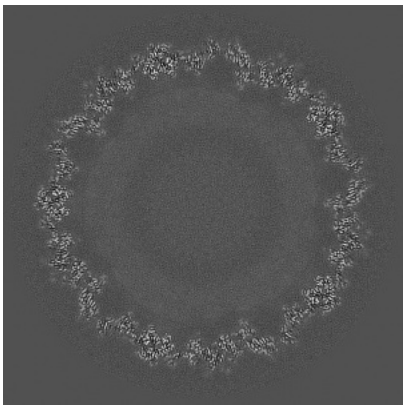
6.3.1 Primary map



X Index: 312

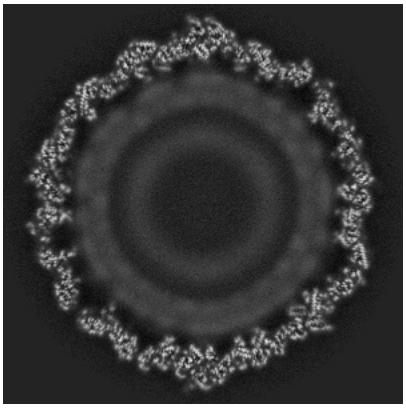


Y Index: 312

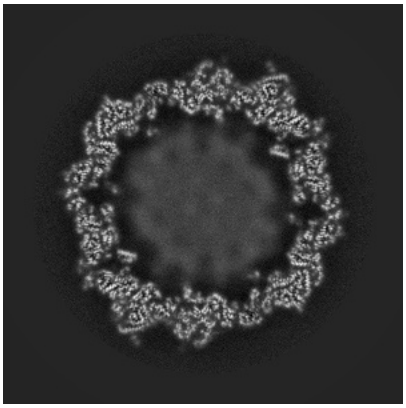


Z Index: 239

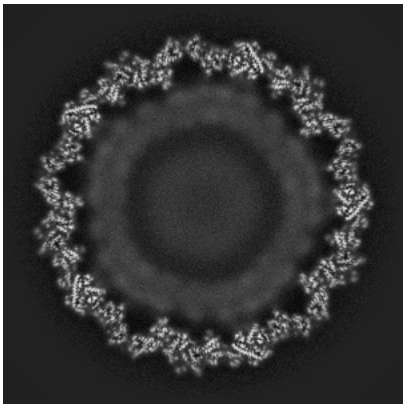
6.3.2 Raw map



X Index: 312



Y Index: 509

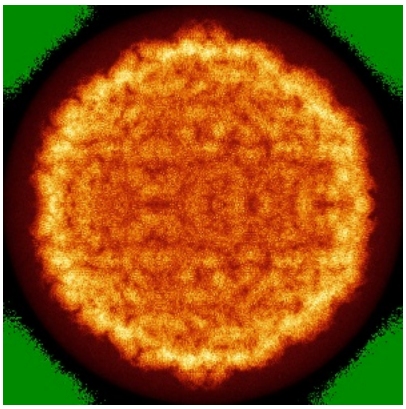


Z Index: 239

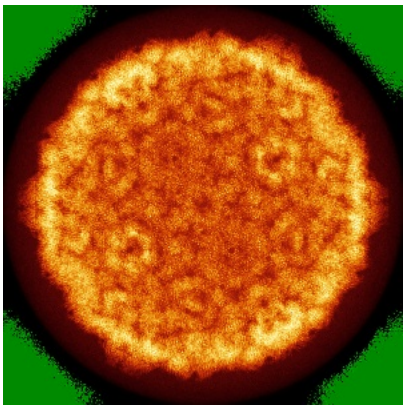
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

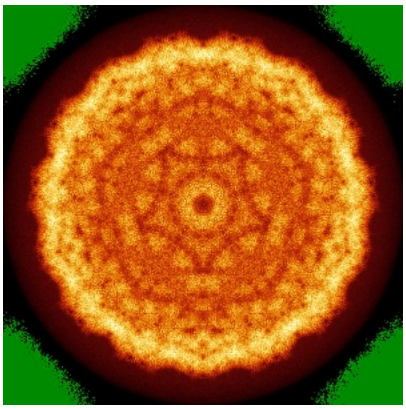
6.4.1 Primary map



X

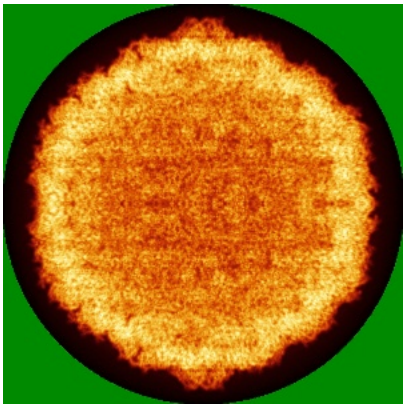


Y

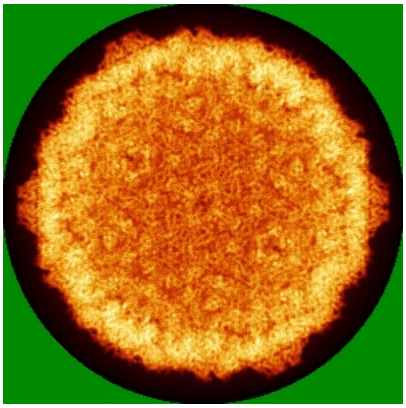


Z

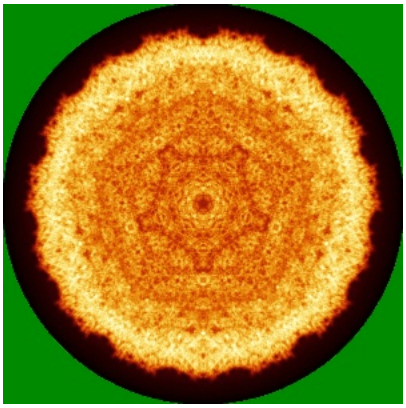
6.4.2 Raw map



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 0.015. 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.

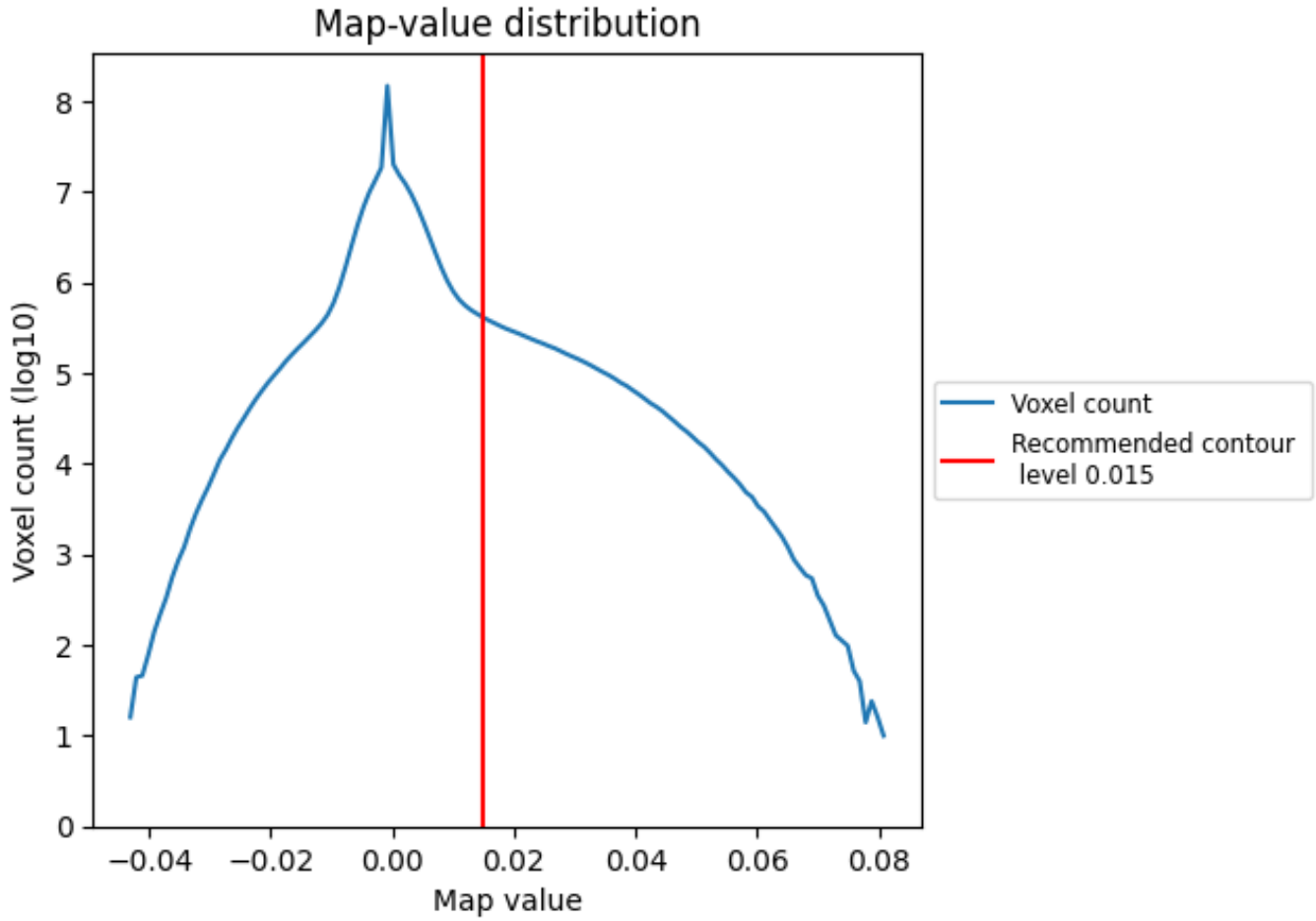
6.6 Mask visualisation (i)

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

7 Map analysis

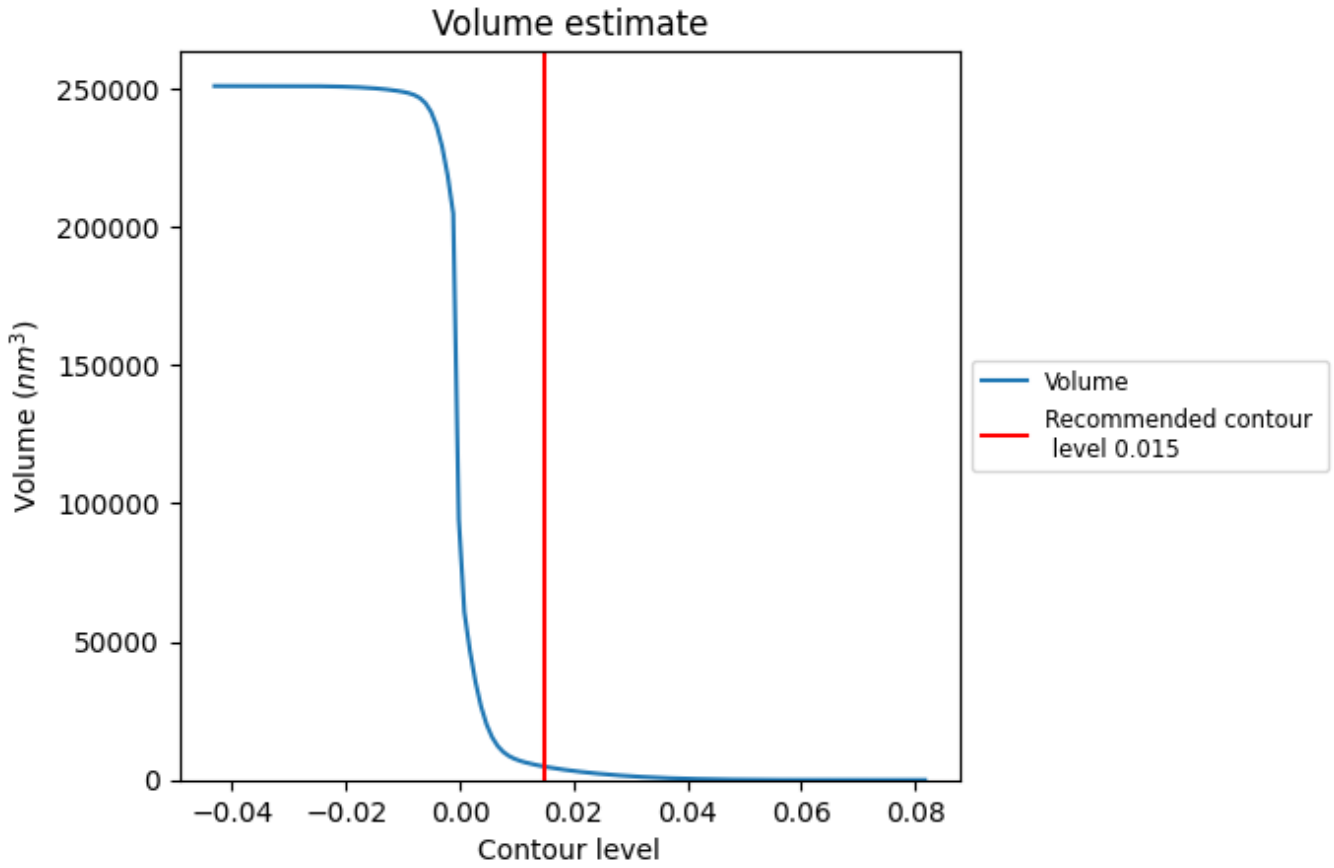
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

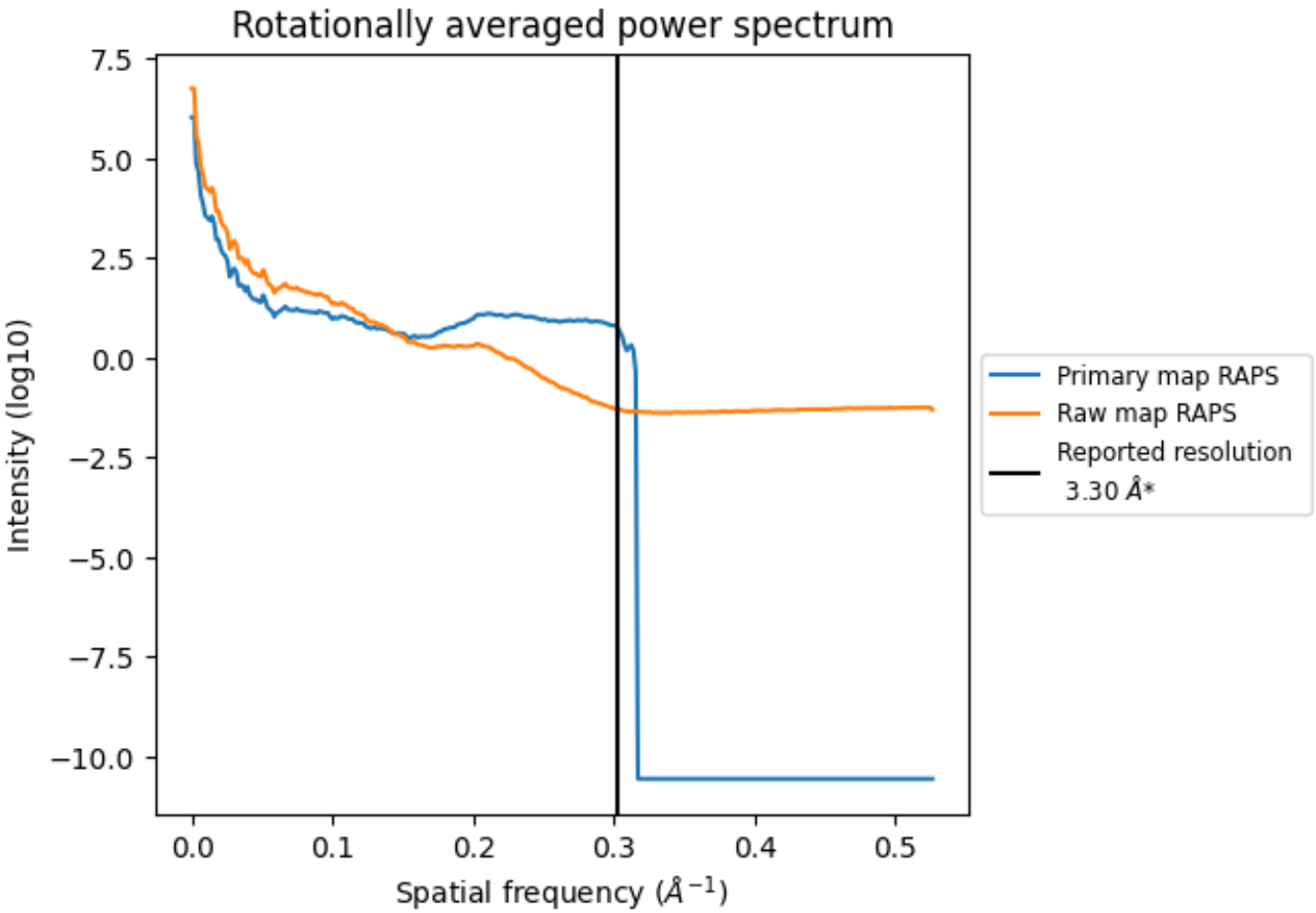
7.2 Volume estimate (i)



The volume at the recommended contour level is 4794 nm^3; this corresponds to an approximate mass of 4330 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)

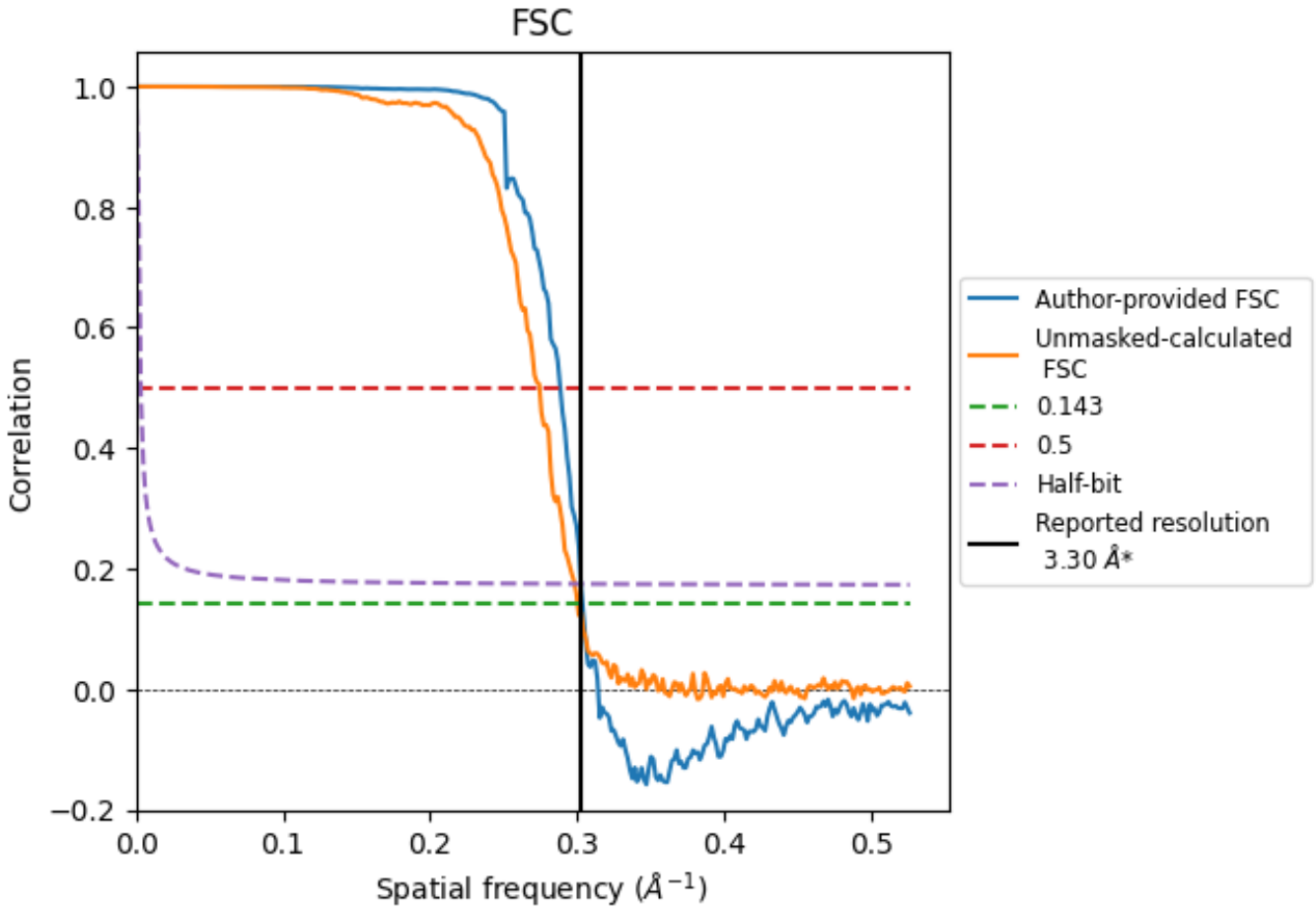


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.47	3.30
Unmasked-calculated*	3.33	3.64	3.35

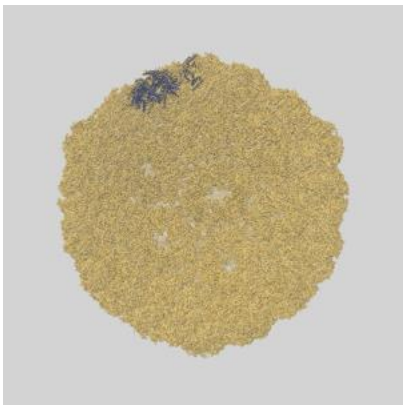
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

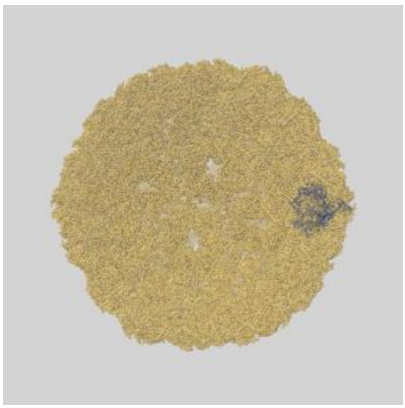
This section contains information regarding the fit between EMDB map EMD-67032 and PDB model 9XMT. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

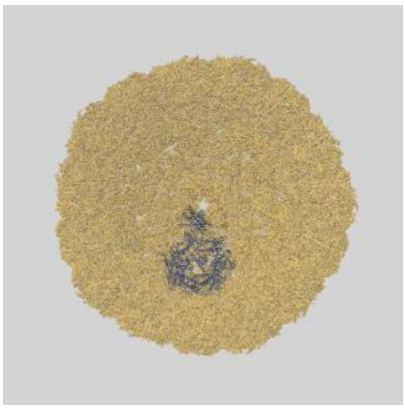
9.1.1 Map-model overlay



X

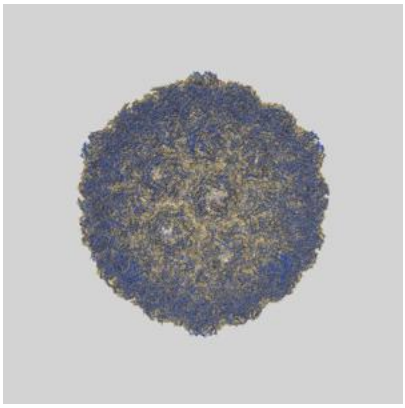


Y

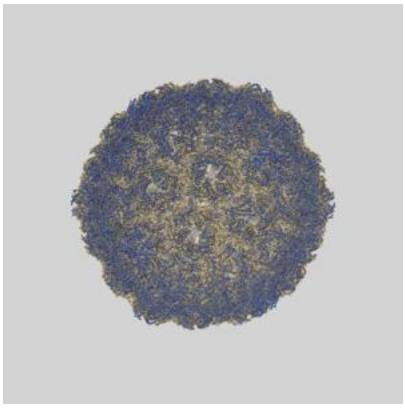


Z

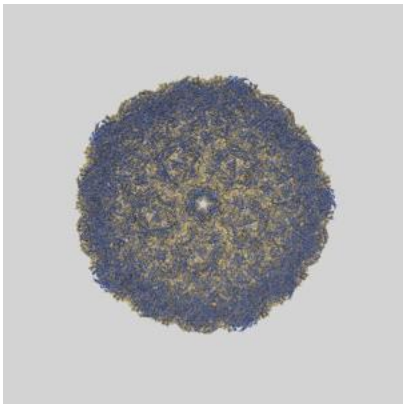
9.1.2 Map-model assembly overlay



X



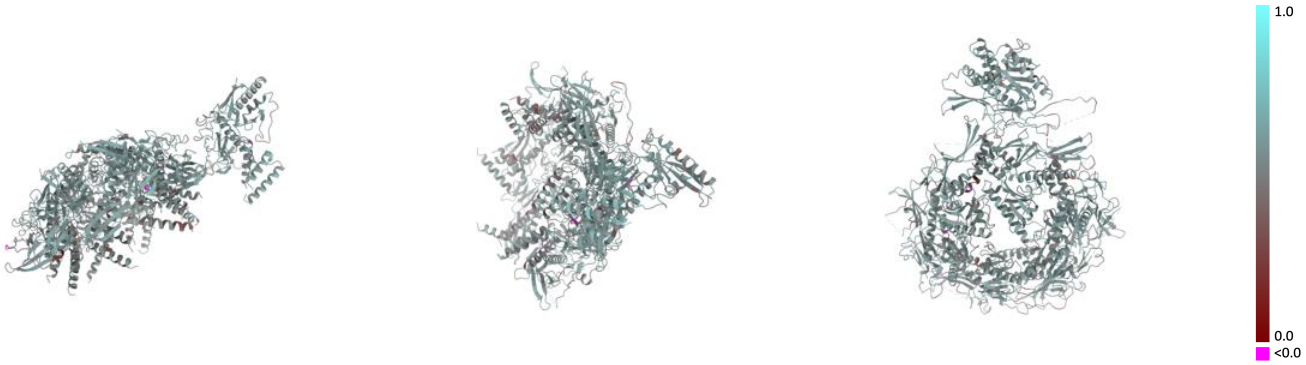
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

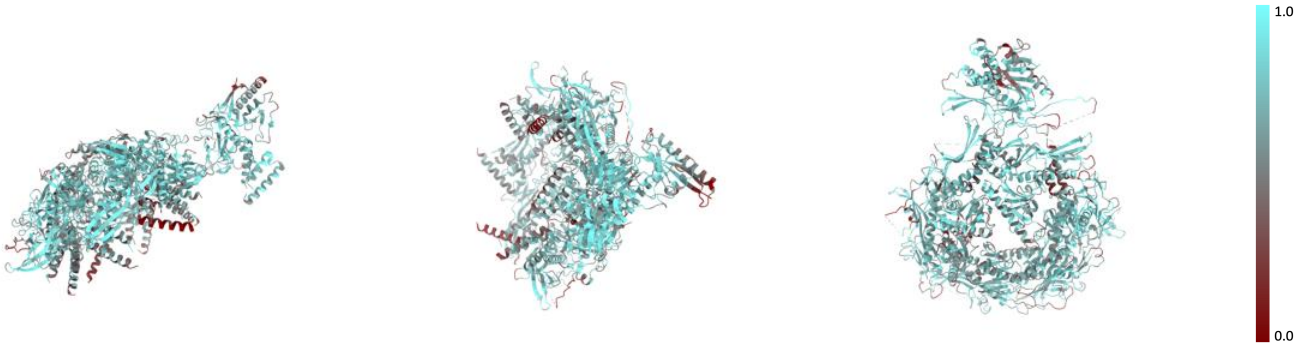
9.2 Q-score mapped to coordinate model



X Y Z

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.

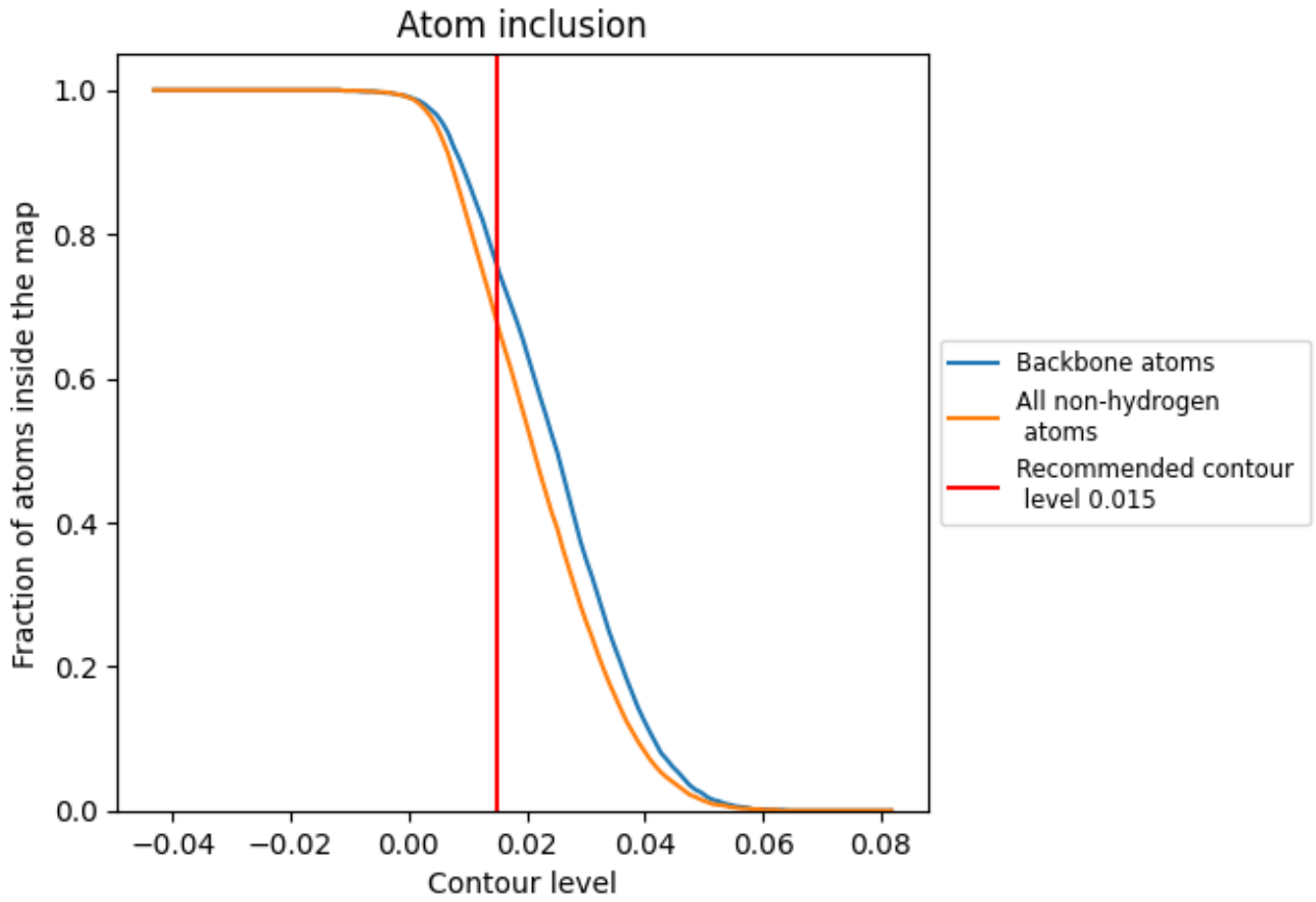
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6750	0.5390
A	0.6050	0.5380
B	0.5920	0.5270
C	0.1810	0.5180
D	0.1700	0.4770
E	0.6130	0.5380
F	0.5880	0.5370
G	0.7700	0.5850
H	0.6820	0.5440
I	0.7170	0.5530
J	0.7150	0.5440
K	0.7040	0.5370
L	0.6750	0.5280
M	0.6880	0.5340
N	0.6930	0.5390

