wwPDB EM Validation Summary Report (i)

May 4, 2024 – 11:29 am BST

PDB ID	:	5LK7
EMDB ID	:	EMD-4063
Title	:	Single particle reconstruction of slow bee paralysis virus virion at pH 5.5
Authors	:	Kalynych, S.; Fuzik, T.; Plevka, P.
Deposited on	:	2016-07-21
Resolution	:	3.42 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 (i) 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 (i)) were used in the production of this report:

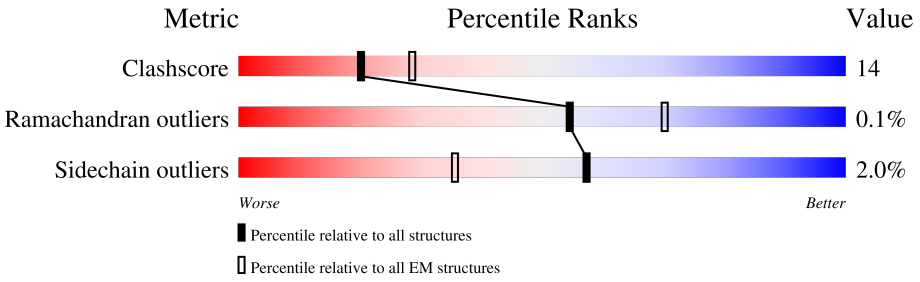
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.42 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 <=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	266	38%; 56%; 30%; • ; 12%
2	B	261	31%; 70%; 26%; • •
3	C	430	17%; 44%; 14%; • ; 41%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5866 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
			Total	C	N	O	S		
1	A	233	1856	1194	321	332	9	0	0

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	252	2032	1308	338	372	14	0	0

- Molecule 3 is a protein called VP3.

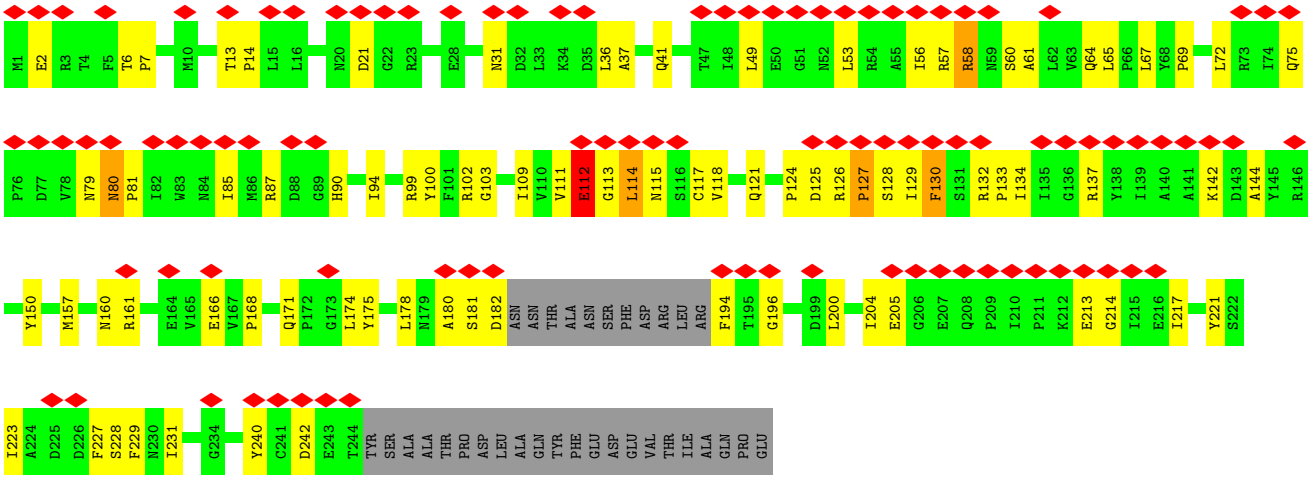
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	254	1978	1276	331	364	7	0	0

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.

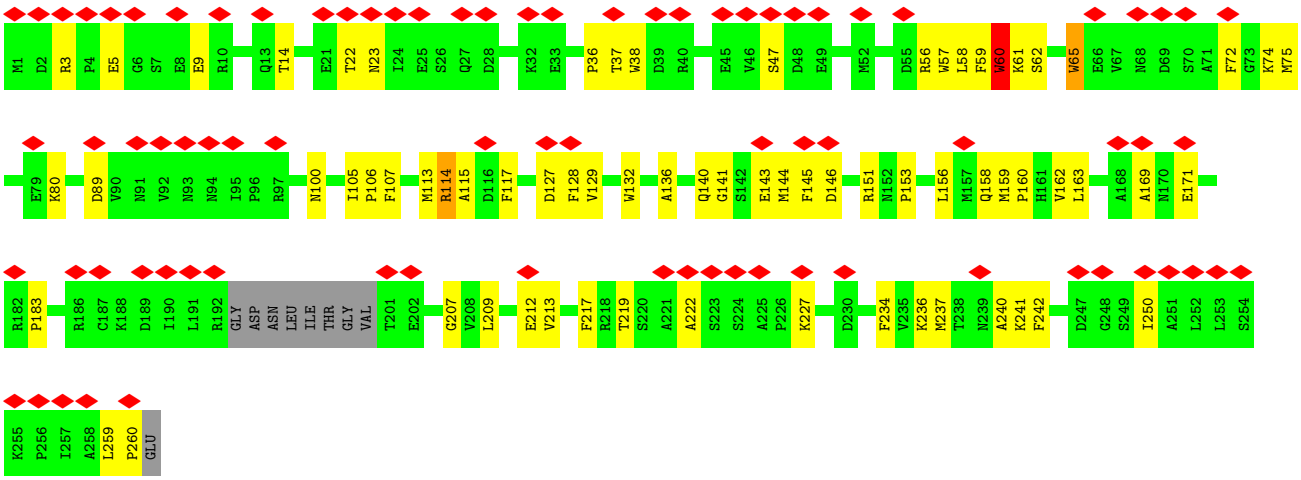
- Molecule 1: VP1

Chain A:



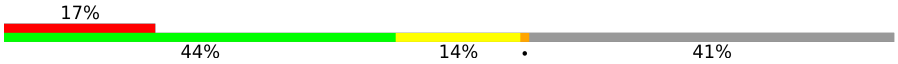
- Molecule 2: VP2

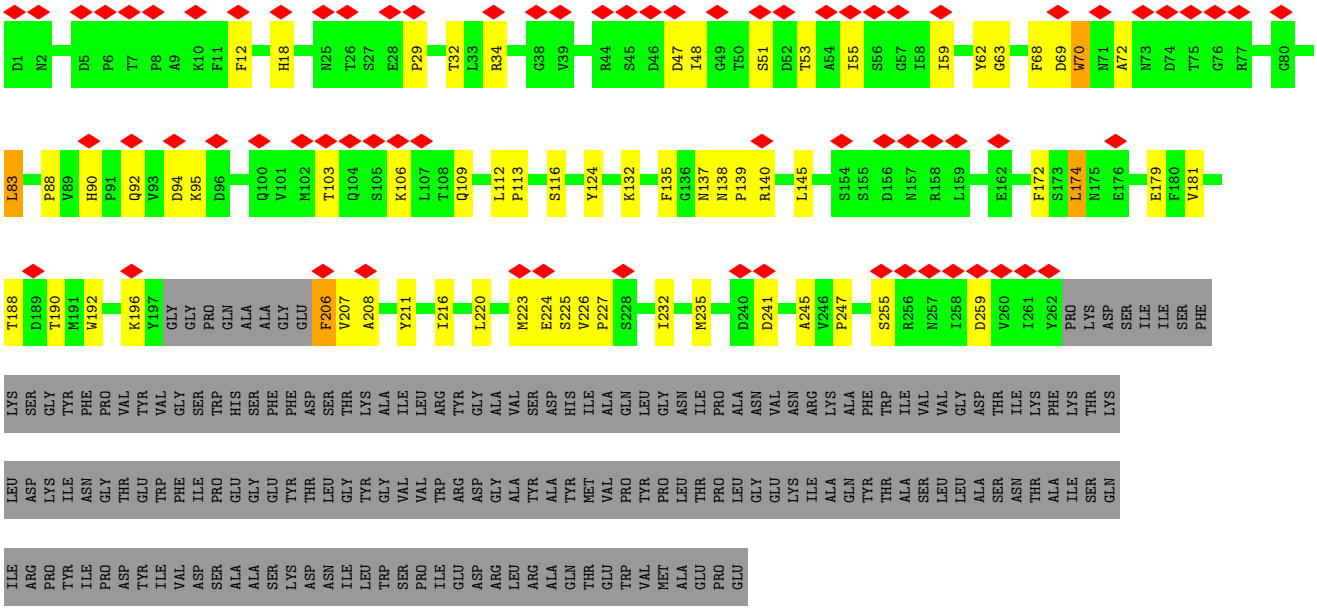
Chain B:



- Molecule 3: VP3

Chain C:


17%
44%
14%
41%


D1 N2 D5 P6 T7 P8 A9 K10 F11 F12 H18 N25 T26 S27 E28 P29 T32 L33 R34 G38 V39 R44 S45 D46 D47 I48 G49 T50 S51 D52 T53 A54 I55 S56 G57 I58 I59 Y62 G63 F68 D69 W70 N71 A72 N73 D74 T75 G76 R77 G80
L83 P88 V89 H90 P91 Q92 V93 D94 K95 D96 Q100 V101 M102 T103 Q104 S105 K106 L107 T108 Q109 L112 P113 S116 Y124 K132 F135 G136 N137 N138 P139 R140 L145 S154 S155 D156 N157 R158 L159 E162 F172 S173 L174 N175 E176 E179 F180 V181
T188 D189 T190 M191 W192 K196 Y197 GLY GLY PRO GLN ALA ALA GLY GLU F206 V207 A208 Y211 I216 L220 M223 E224 S225 V226 P227 S228 I232 M235 D240 D241 A245 V246 P247 S255 R256 N257 I258 D259 V260 I261 Y262 PRO LYS ASP SER ILE ILE SER PHE
LYS SER GLY TYR PHE PRO VAL TYR VAL GLY SER TRP HIS SER PHE PHE ASP SER THR LYS ALA ILE LEU ARG TYR GLY ALA VAL SER ASP HIS ILE ALA GLN LEU GLY ASN ILE PRO ALA ASN VAL ASN ARG LYS ALA PHE TRP ILE VAL VAL GLY ASP THR ILE LYS PHE LYS THR LYS
LEU ASP LYS ILE ASN GLY THR GLU TRP PHE ILE PRO GLU GLY GLU TYR THR LEU GLY TYR GLY VAL VAL TRP ARG ASP GLY ALA TYR ALA TYR MET VAL PRO TYR PRO LEU THR PRO LEU GLY GLU LYS ILE ALA GLN TYR THR ALA SER LEU LEU ALA SER ASN THR ALA ILE SER GLN
ILE ARG PRO TYR ILE PRO ASP TYR ILE VAL ASP SER ALA ALA SER LYS ASP ASN ILE LEU TRP SER PRO ILE GLU ASP ARG LEU ARG ALA GLN THR GLU TRP VAL MET ALA GLU PRO GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10350	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 ($e^-/Å^2$)	21	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	14.482	Depositor
Minimum map value	-9.695	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.66	Depositor
Map size (Å)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.73	2/1908 (0.1%)	0.84	2/2599 (0.1%)
2	B	0.71	0/2084	0.75	2/2830 (0.1%)
3	C	0.68	1/2036 (0.0%)	0.77	3/2790 (0.1%)
All	All	0.71	3/6028 (0.0%)	0.78	7/8219 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	70	TRP	CB-CG	-7.02	1.37	1.50
1	A	75	GLN	C-N	-5.77	1.23	1.34
1	A	112	GLU	CB-CG	5.75	1.63	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	LEU	CA-CB-CG	6.10	129.34	115.30
2	B	60	TRP	CA-CB-CG	6.10	125.28	113.70
1	A	113	GLY	N-CA-C	-5.94	98.25	113.10
3	C	174	LEU	CA-CB-CG	5.91	128.88	115.30
3	C	83	LEU	CA-CB-CG	5.80	128.64	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	GLU	Peptide
1	A	58	ARG	Peptide
3	C	69	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1856	0	1808	71	0
2	B	2032	0	2017	54	0
3	C	1978	0	1953	54	0
All	All	5866	0	5778	159	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 14.

The worst 5 of 159 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:121:GLN:HE21	1:A:150:TYR:HB2	1.22	1.02
1:A:223:ILE:HG23	1:A:227:PHE:HB3	1.66	0.76
1:A:115:ASN:HA	1:A:157:MET:HB2	1.68	0.76
3:C:188:THR:HG22	3:C:190:THR:H	1.52	0.74
1:A:132:ARG:HD3	1:A:133:PRO:HD2	1.68	0.74

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	229/266 (86%)	206 (90%)	22 (10%)	1 (0%)	34	69
2	B	248/261 (95%)	235 (95%)	13 (5%)	0	100	100
3	C	250/430 (58%)	234 (94%)	16 (6%)	0	100	100
All	All	727/957 (76%)	675 (93%)	51 (7%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	PRO

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	198/230 (86%)	191 (96%)	7 (4%)	36	67
2	B	227/234 (97%)	223 (98%)	4 (2%)	59	81
3	C	221/366 (60%)	219 (99%)	2 (1%)	78	90
All	All	646/830 (78%)	633 (98%)	13 (2%)	57	79

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	37	THR
2	B	60	TRP
3	C	206	PHE
2	B	65	TRP
3	C	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
2	B	158	GLN
3	C	109	GLN

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)

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.

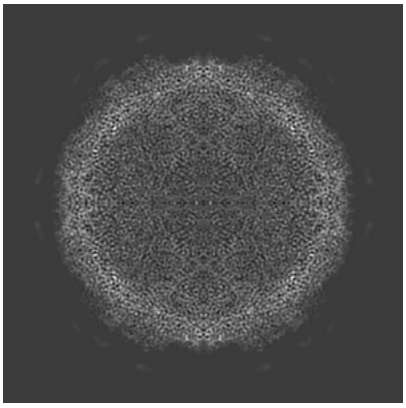
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4063. These allow visual inspection of the internal detail of the map and identification of artifacts.

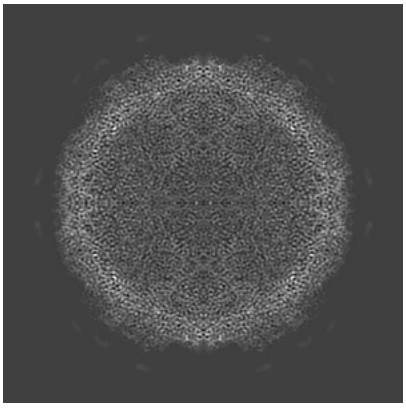
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

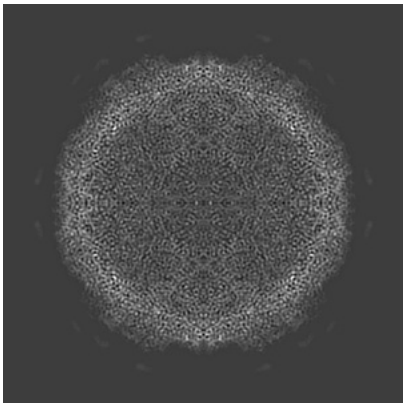
6.1.1 Primary map



X



Y

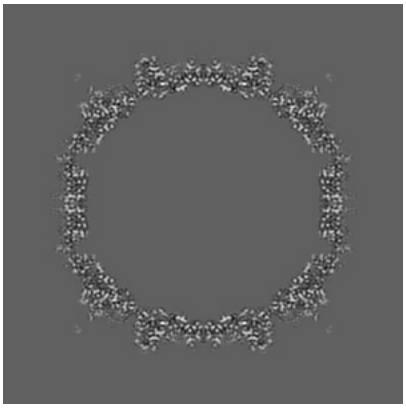


Z

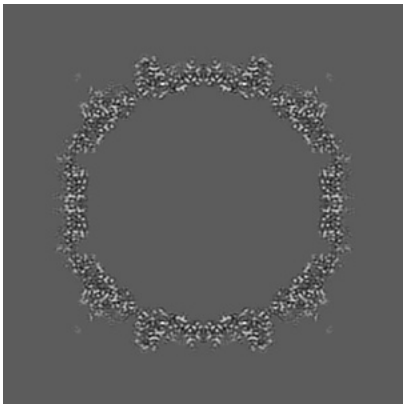
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

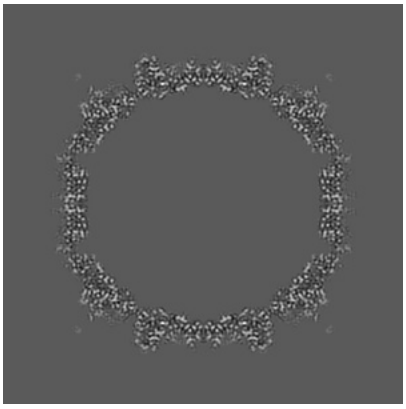
6.2.1 Primary map



X Index: 190



Y Index: 190

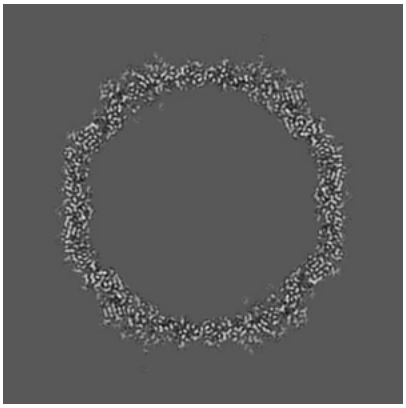


Z Index: 190

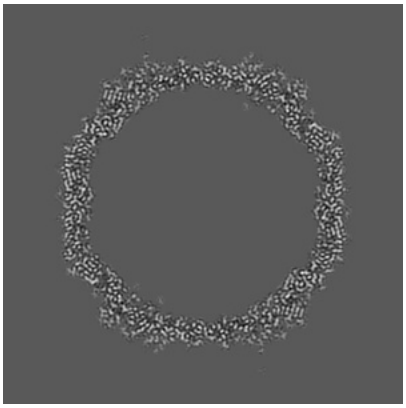
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

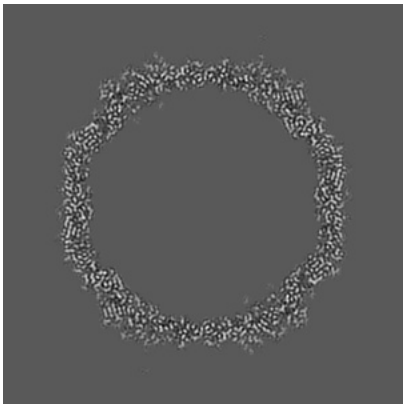
6.3.1 Primary map



X Index: 174



Y Index: 206

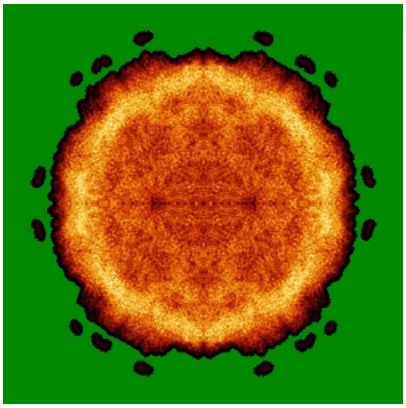


Z Index: 174

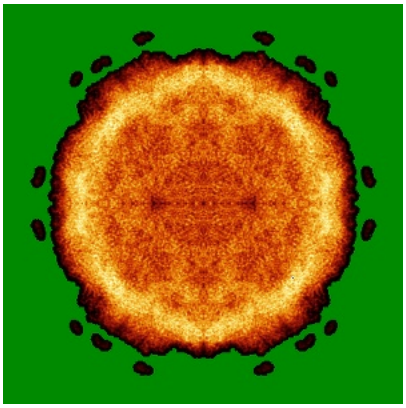
The images above show the largest variance slices of the map in three orthogonal directions.

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

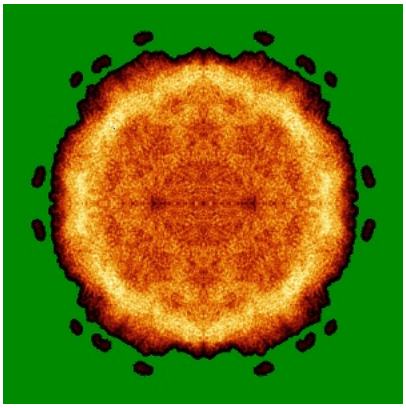
6.4.1 Primary map



X



Y

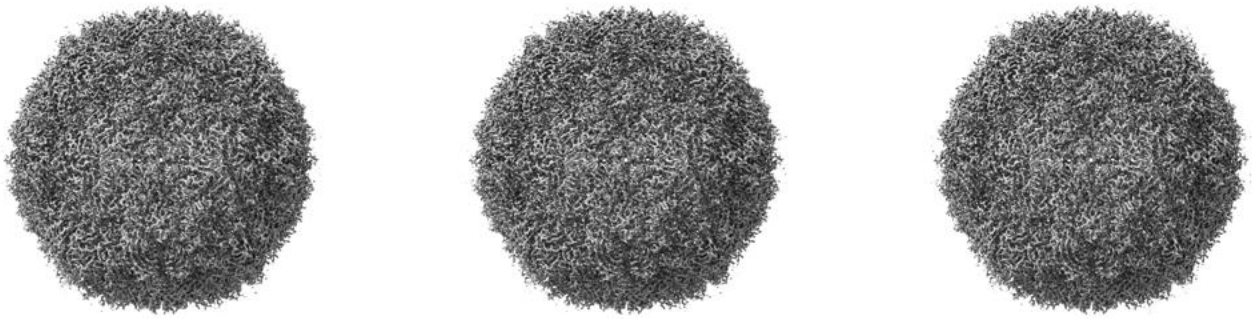


Z

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

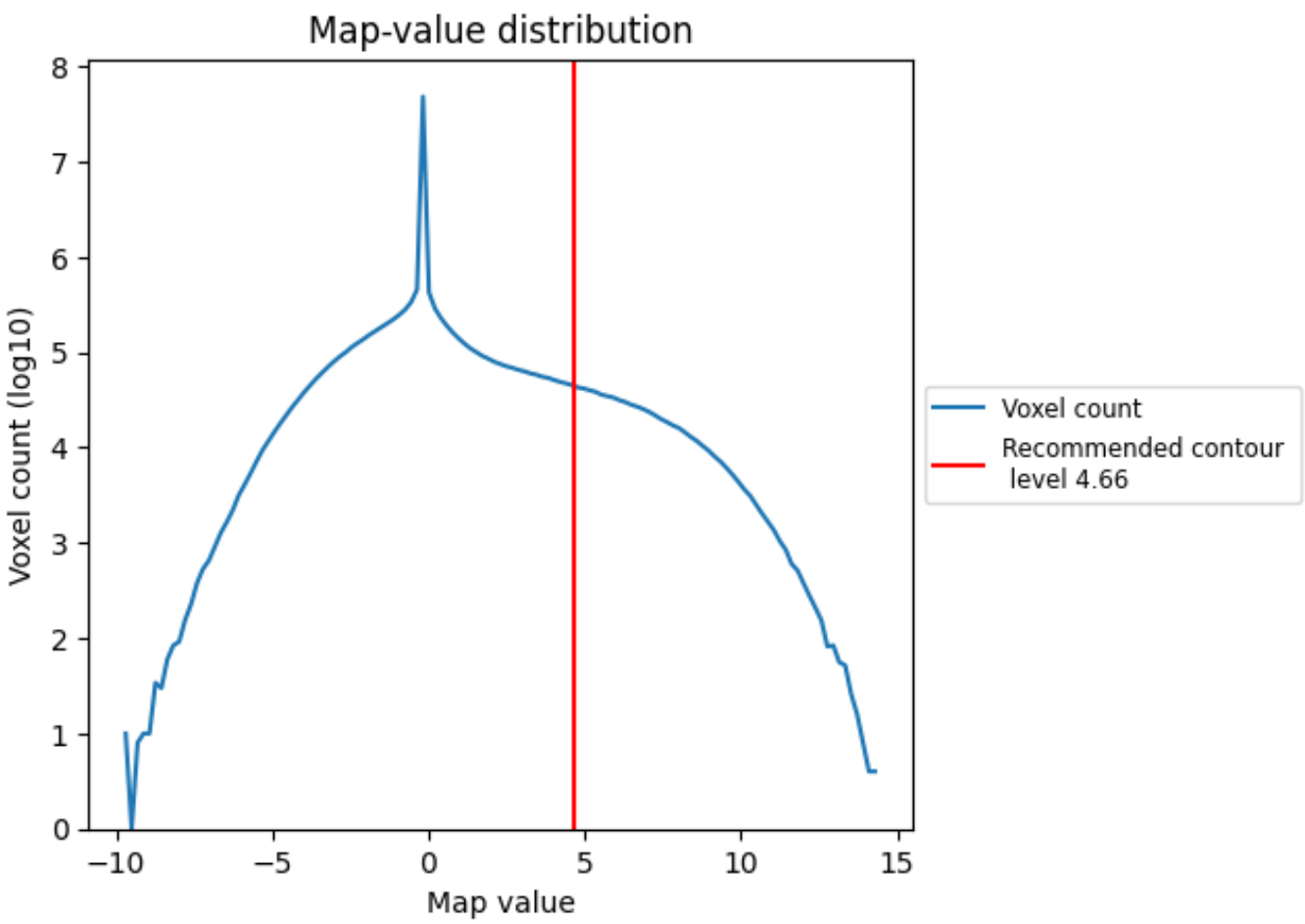
6.6 Mask visualisation (i)

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

7 Map analysis (i)

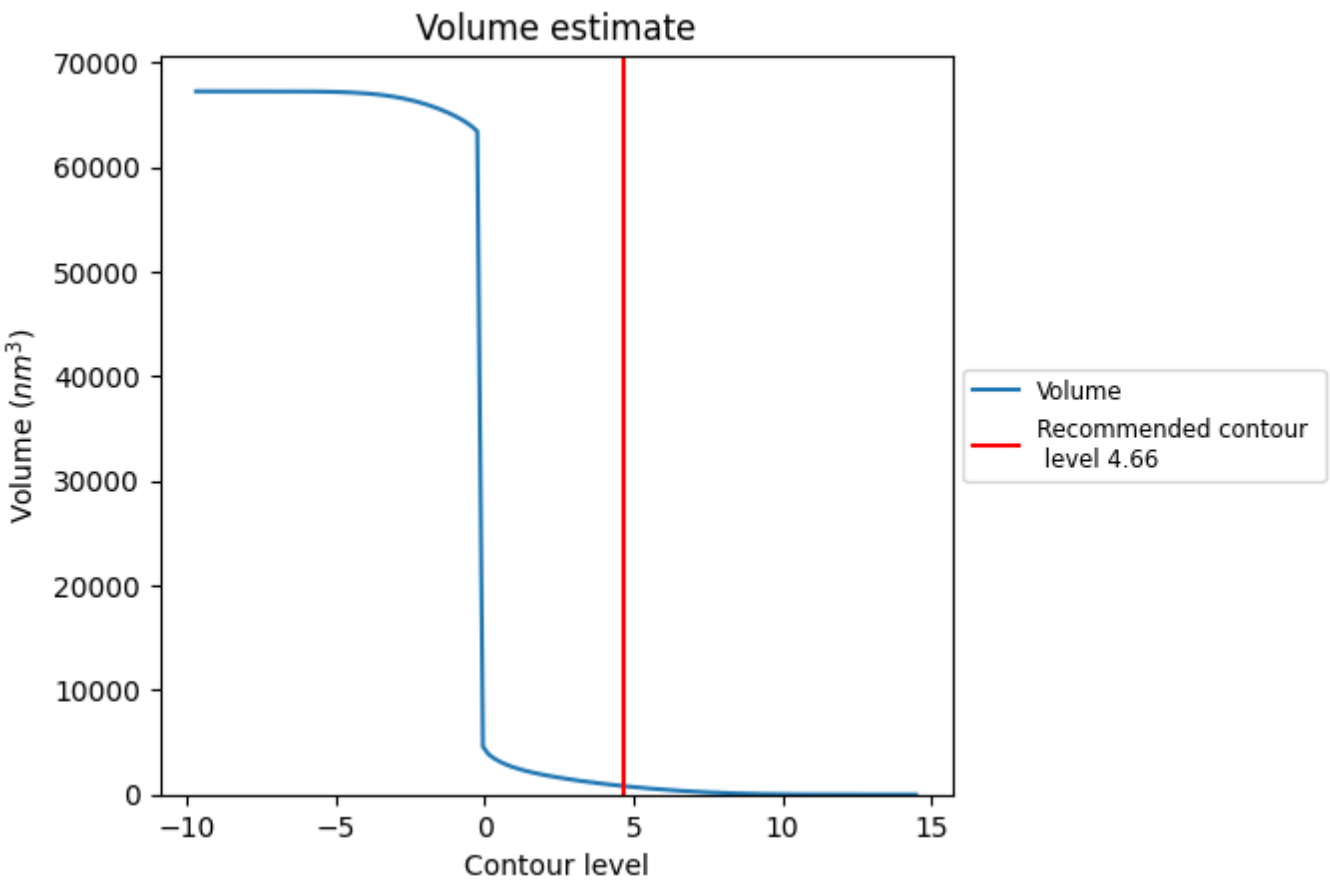
This section contains the results of statistical analysis of the map.

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.

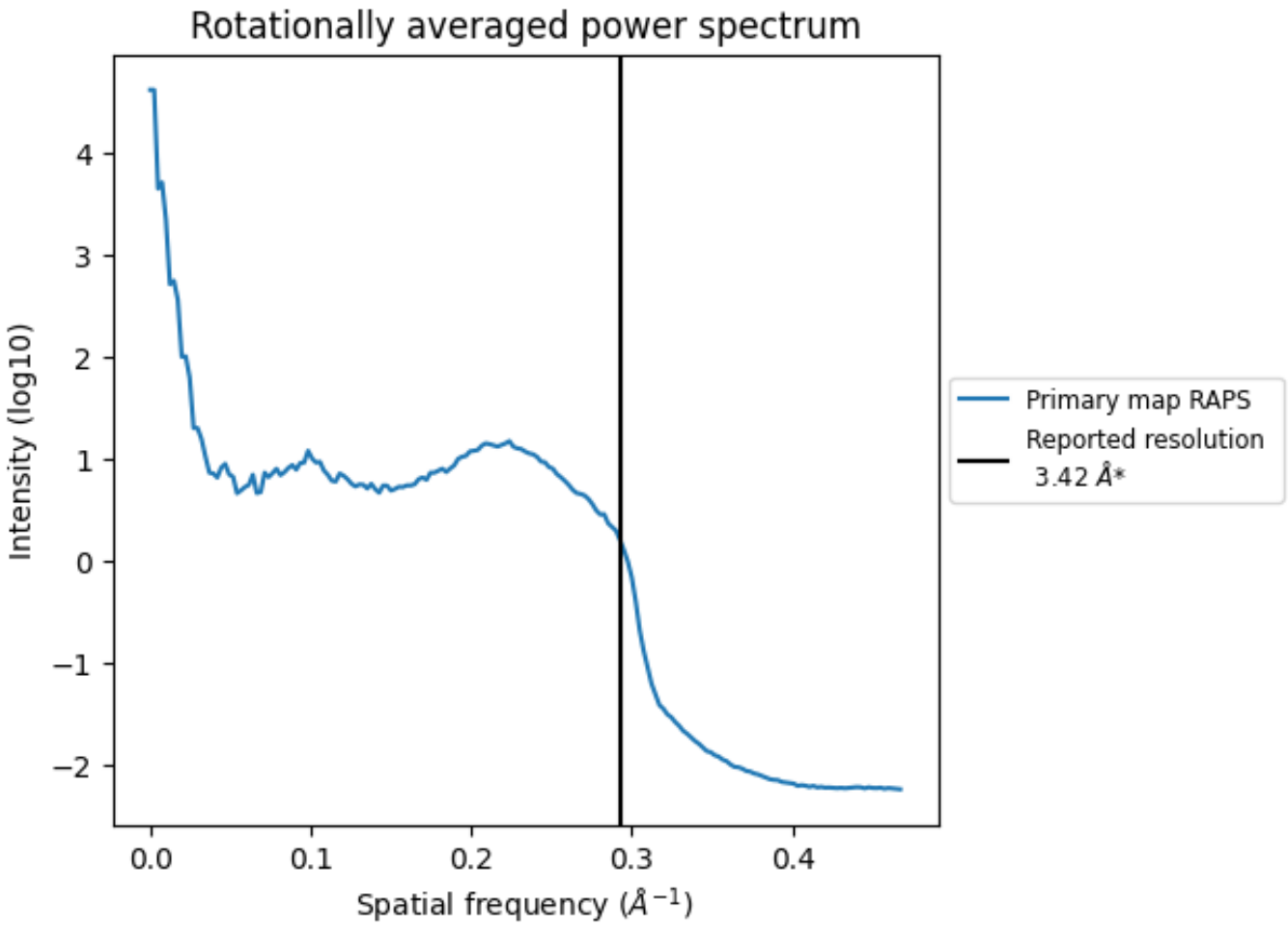
7.2 Volume estimate (i)



The volume at the recommended contour level is 811 nm^3; this corresponds to an approximate mass of 732 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)

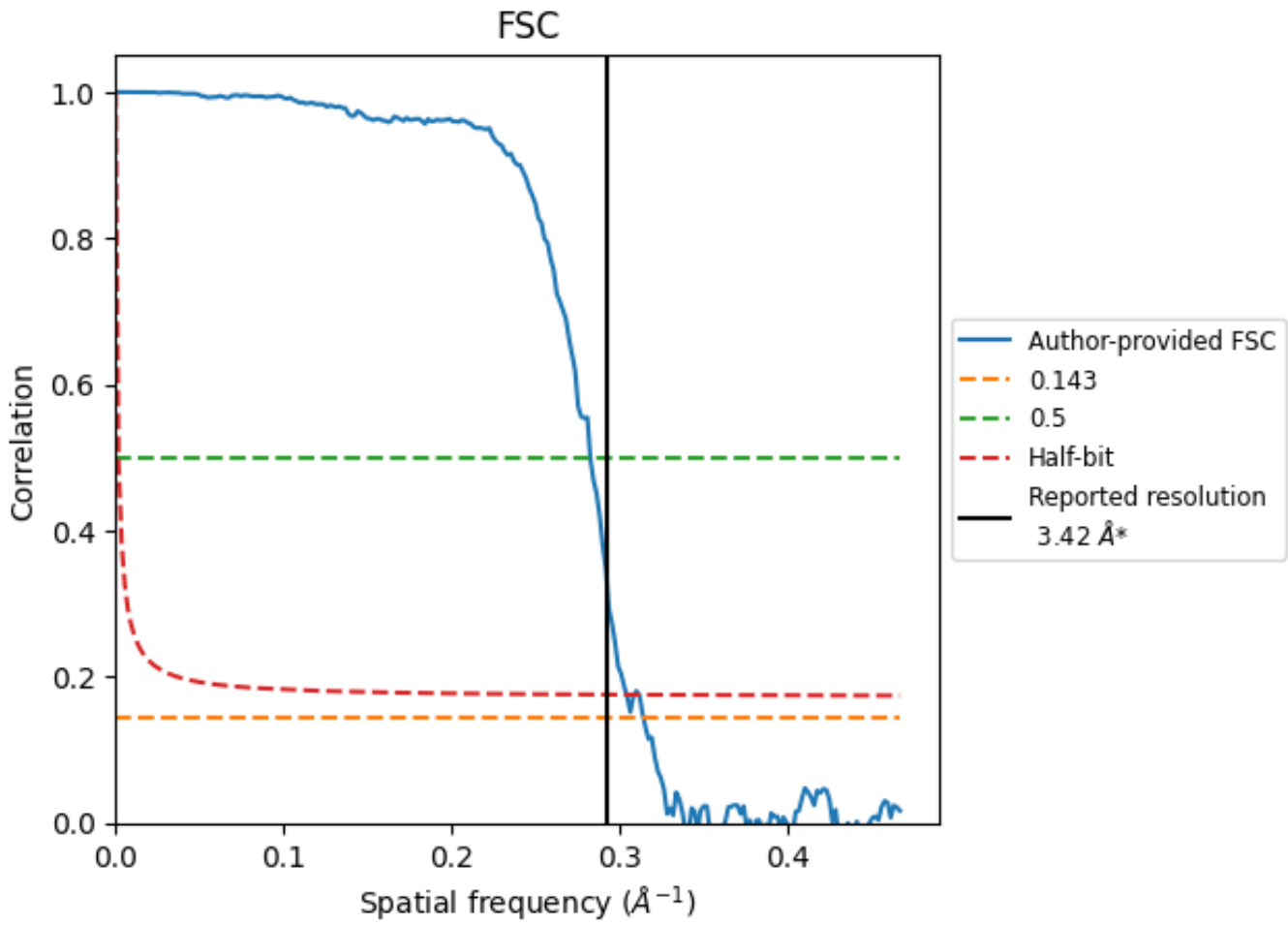


*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

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 0.292 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.18	3.54	3.29
Unmasked-calculated*	-	-	-

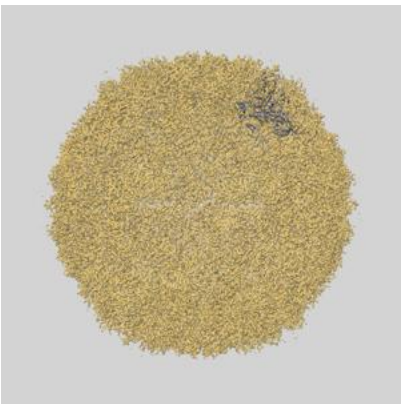
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

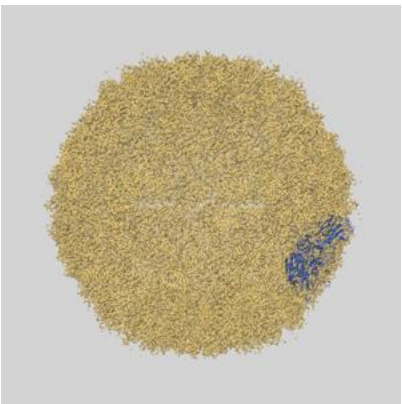
This section contains information regarding the fit between EMDB map EMD-4063 and PDB model 5LK7. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

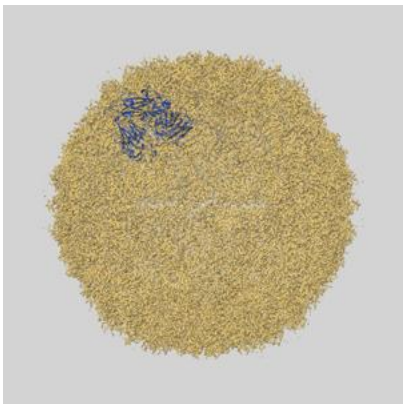
9.1.1 Map-model overlay (i)



X

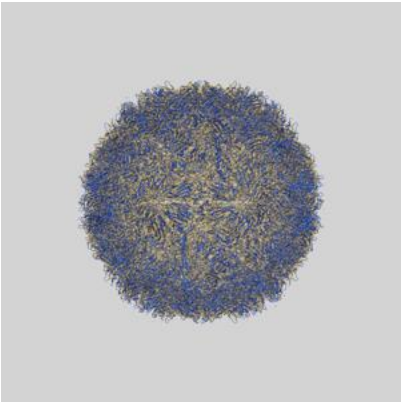


Y

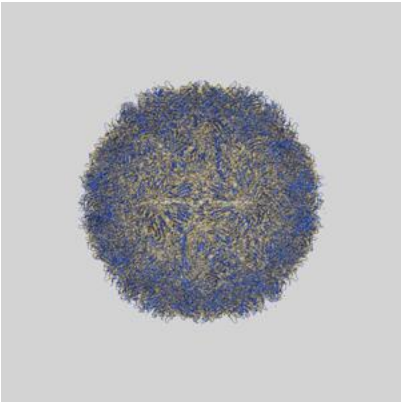


Z

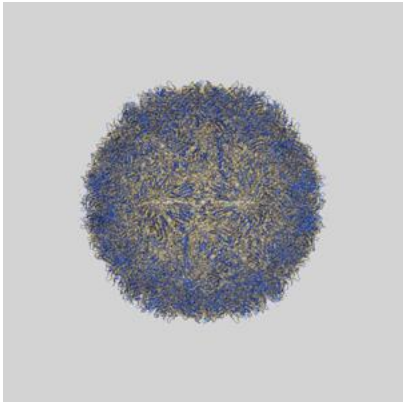
9.1.2 Map-model assembly overlay (i)



X



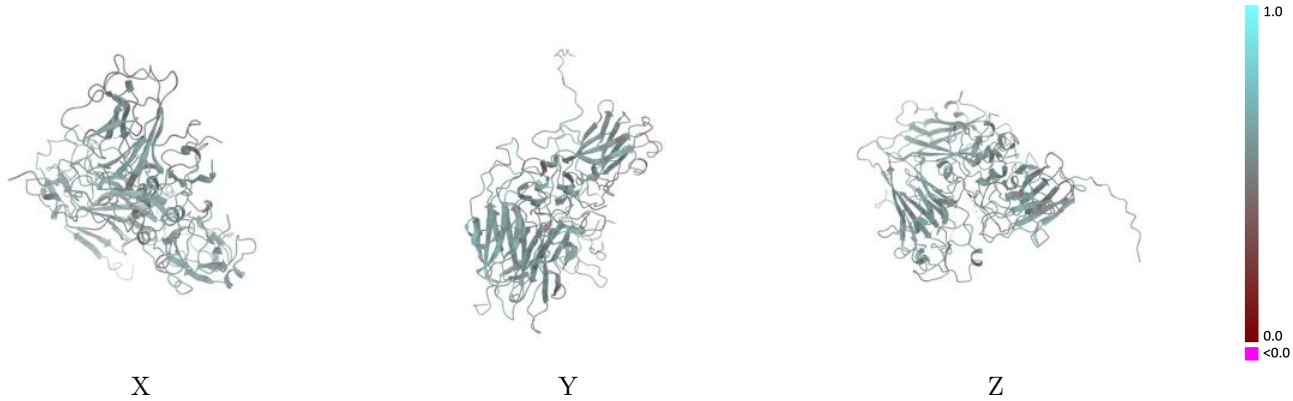
Y



Z

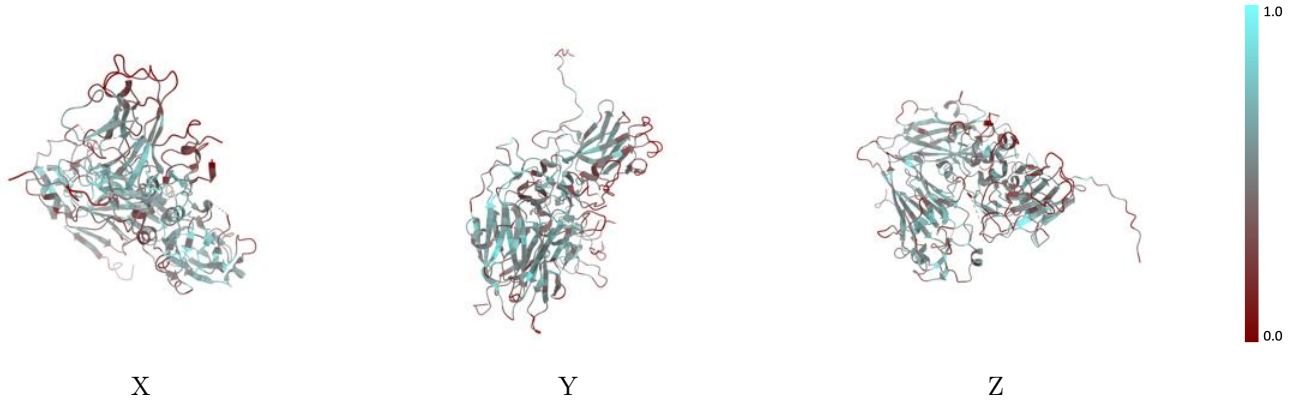
The images above show the 3D surface view of the map at the recommended contour level 4.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



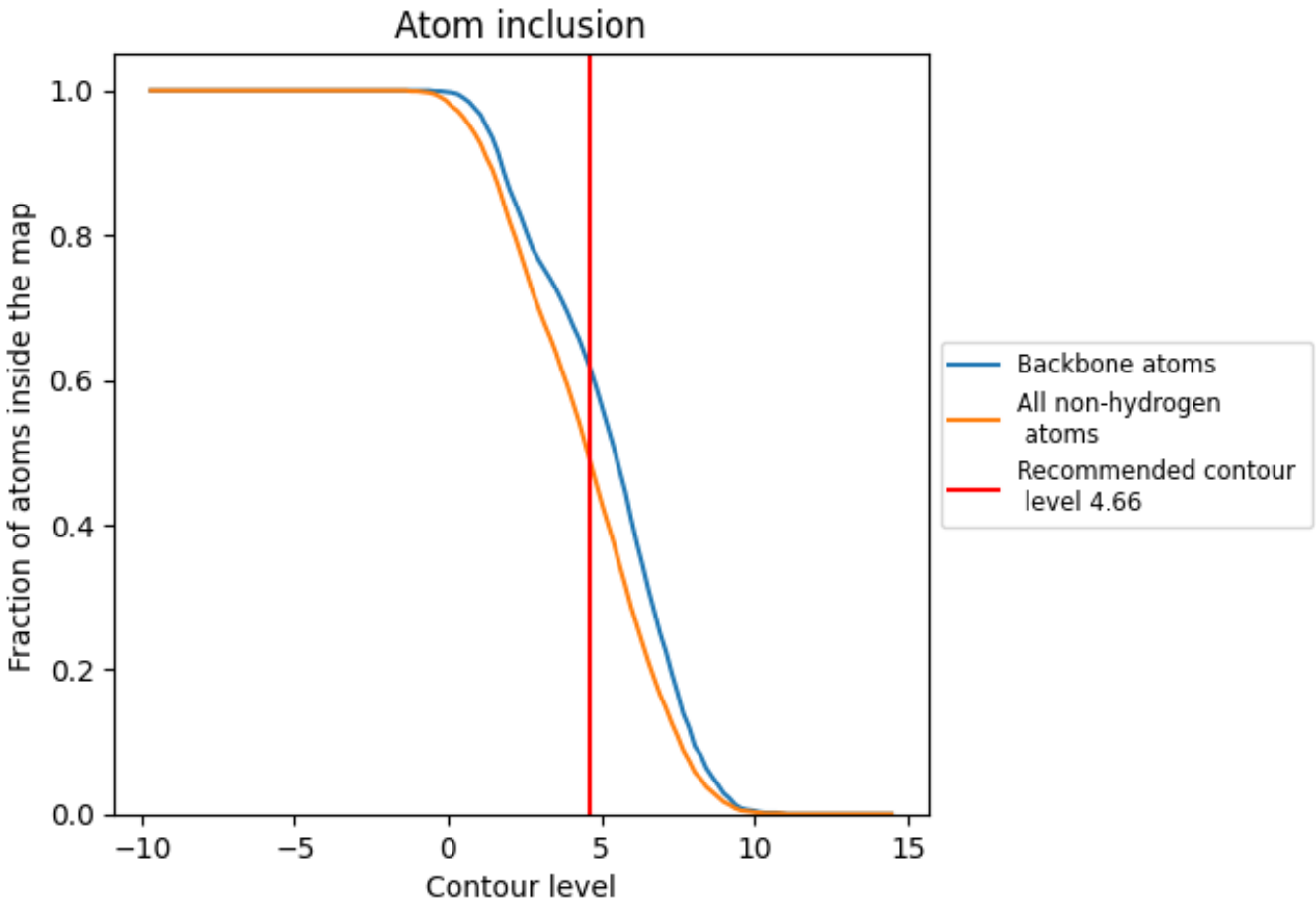
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.66).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 48% 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 (4.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4850	0.5550
A	0.4410	0.5420
B	0.5060	0.5580
C	0.5050	0.5630