Full wwPDB EM Validation Report (i)

Dec 16, 2023 – 11:30 AM EST

PDB ID	:	2OF6
EMDB ID	:	EMD-1314
Title	:	Structure of immature West Nile virus
Authors	:	Zhang, Y.; Kaufmann, B.; Chipman, P.R.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2007-01-02
Resolution	:	24.00 Å(reported)
Based on initial model	:	2HG0

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 (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:

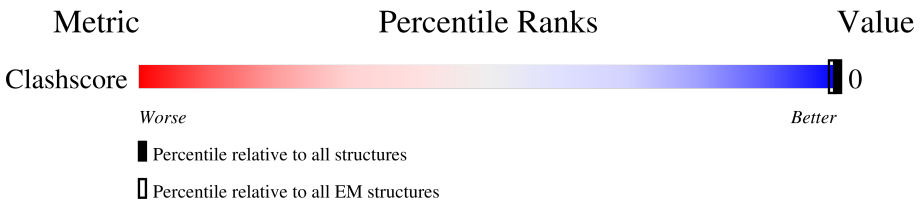
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 24.00 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

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	400	42% 100%
1	B	400	39% 100%
1	C	400	35% 100%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1200 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 envelope glycoprotein E.

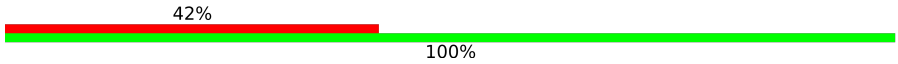
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
1	A	400	400	400	0	400
1	B	400	400	400	0	400
1	C	400	400	400	0	400

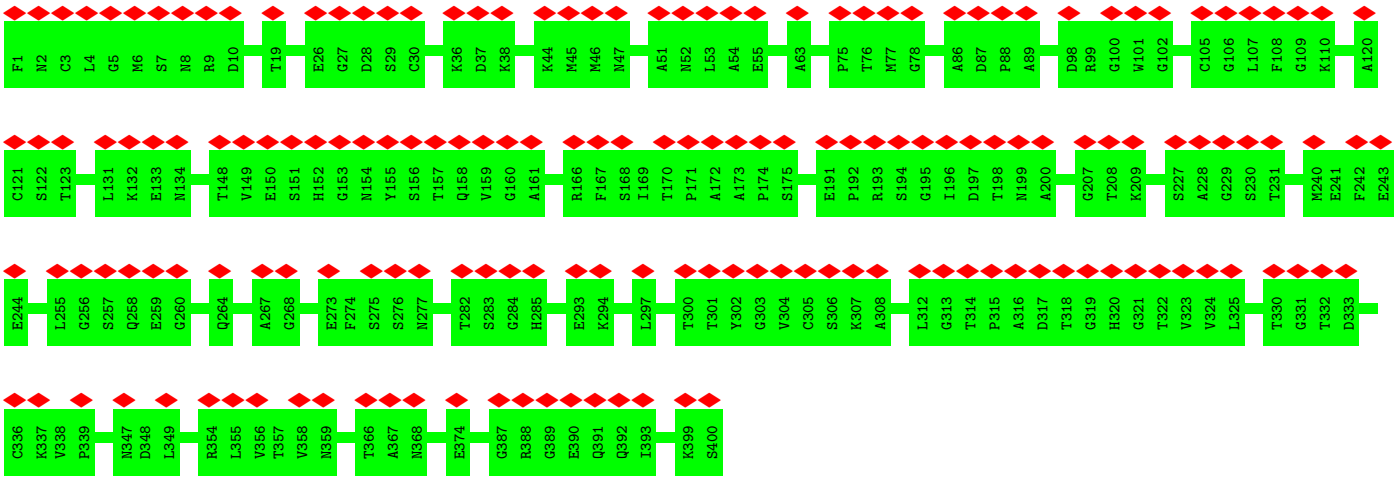
3 Residue-property plots (i)

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: envelope glycoprotein E

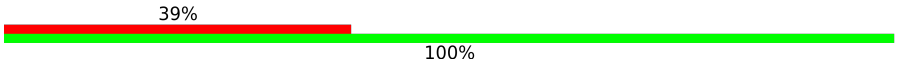
Chain A:

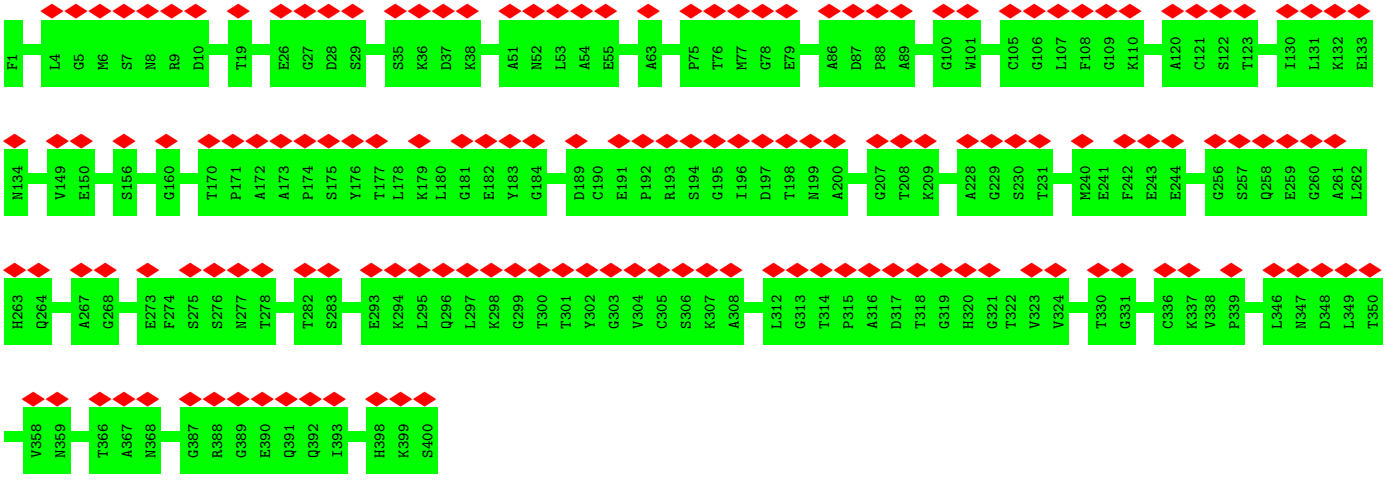




- Molecule 1: envelope glycoprotein E

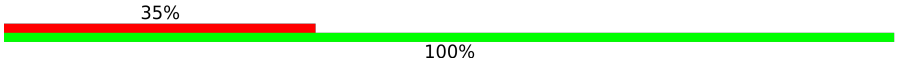
Chain B:

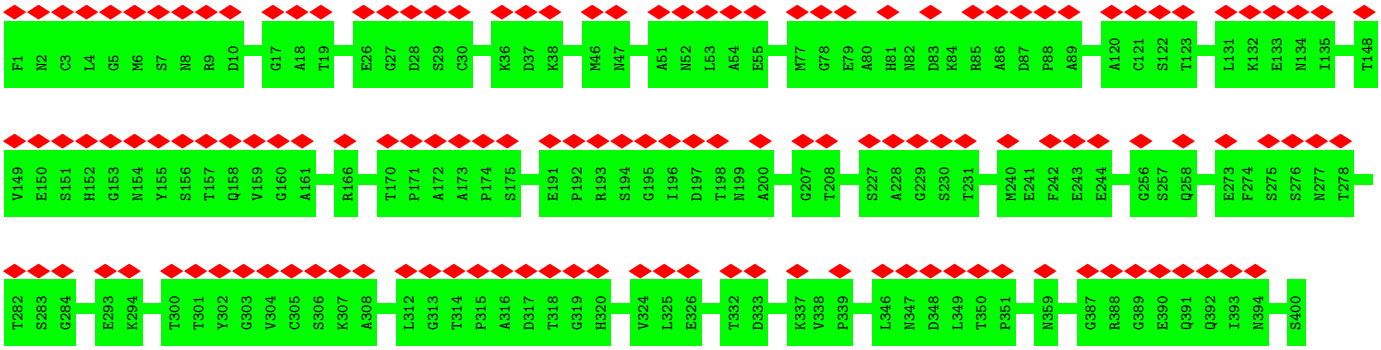




- Molecule 1: envelope glycoprotein E

Chain C:


35%
100%


F1 N2 C3 L4 G5 M6 S7 N8 R9 D10 G17 A18 T19 E26 G27 D28 S29 C30 K36 D37 K38 M46 N47 A51 N52 L53 A54 E55 M77 G78 E79 A80 H81 N82 D83 K84 R85 A86 D87 P88 A89 A120 C121 S122 T123 L131 K132 E133 N134 I135 T148
V149 E150 S151 H152 G153 N154 Y155 S156 T157 Q158 V159 G160 A161 R166 T170 P171 A172 A173 P174 S175 E191 P192 R193 S194 G195 I196 D197 T198 N199 A200 G207 T208 S227 A228 G229 S230 T231 M240 E241 F242 E243 E244 G256 S257 Q258 E273 F274 S275 S276 N277 T278
T282 S283 G284 E293 K294 T300 T301 Y302 G303 V304 C305 S306 K307 A308 L312 G313 T314 P315 A316 D317 T318 G319 H320 V324 L325 E326 T332 D333 K337 V338 P339 L346 N347 D348 L349 T350 P351 N359 G387 R388 G389 E390 Q391 Q392 I393 N394 S400

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	341	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF correction of each particle	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	22	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	47400	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	297.944	Depositor
Minimum map value	-159.534	Depositor
Average map value	-28.515	Depositor
Map value standard deviation	72.980	Depositor
Recommended contour level	156.0	Depositor
Map size (Å)	722.75, 722.75, 722.75	wwPDB
Map dimensions	245, 245, 245	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.95, 2.95, 2.95	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	400	0	0	0	0
1	B	400	0	0	0	0
1	C	400	0	0	0	0
All	All	1200	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

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.

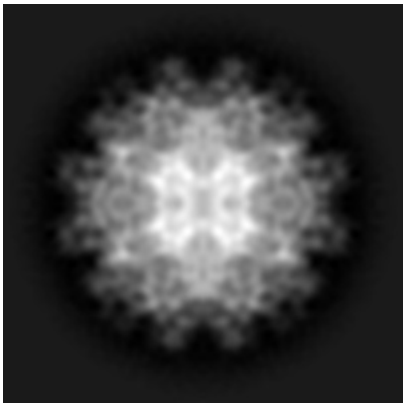
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1314. These allow visual inspection of the internal detail of the map and identification of artifacts.

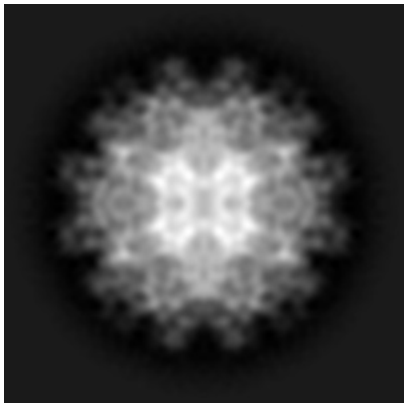
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

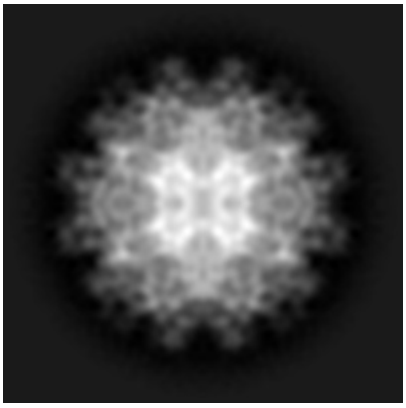
6.1.1 Primary map



X



Y

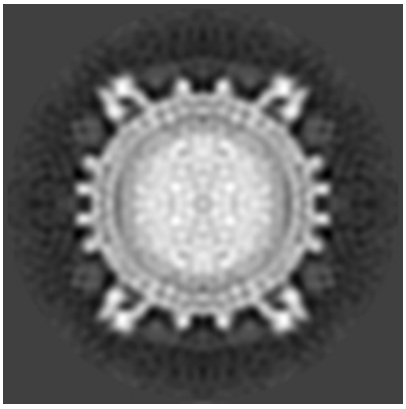


Z

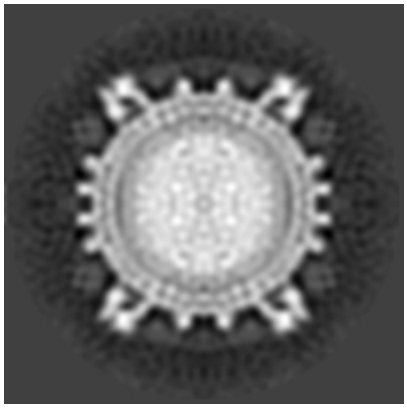
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

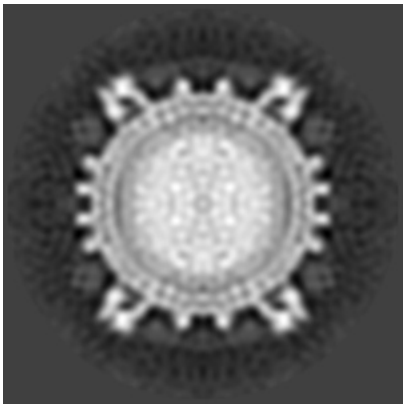
6.2.1 Primary map



X Index: 122



Y Index: 122

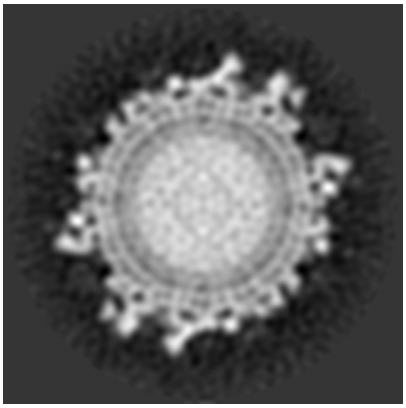


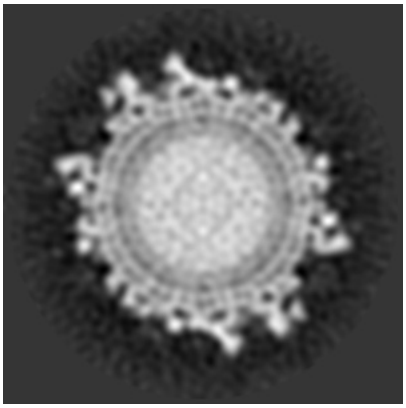
Z Index: 122

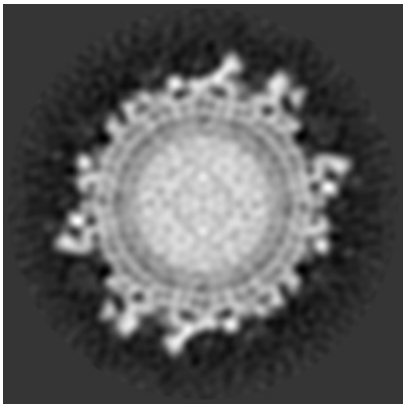
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 113

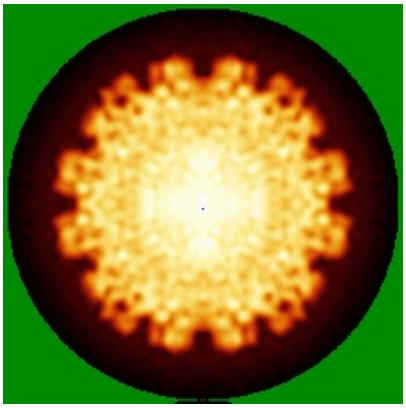

Y Index: 131

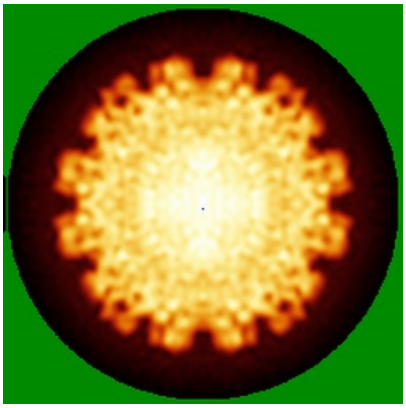

Z Index: 113

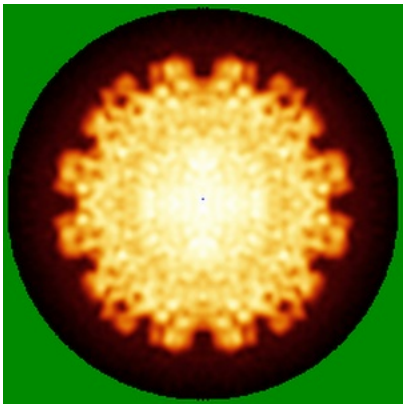
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

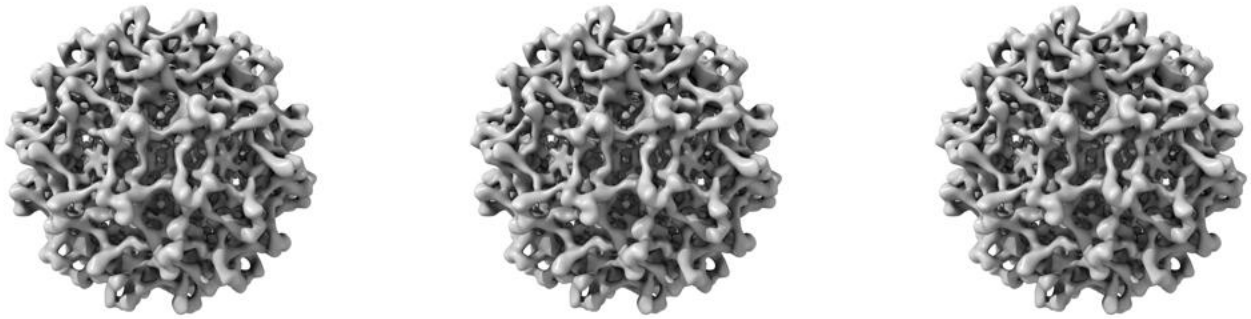

Y


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

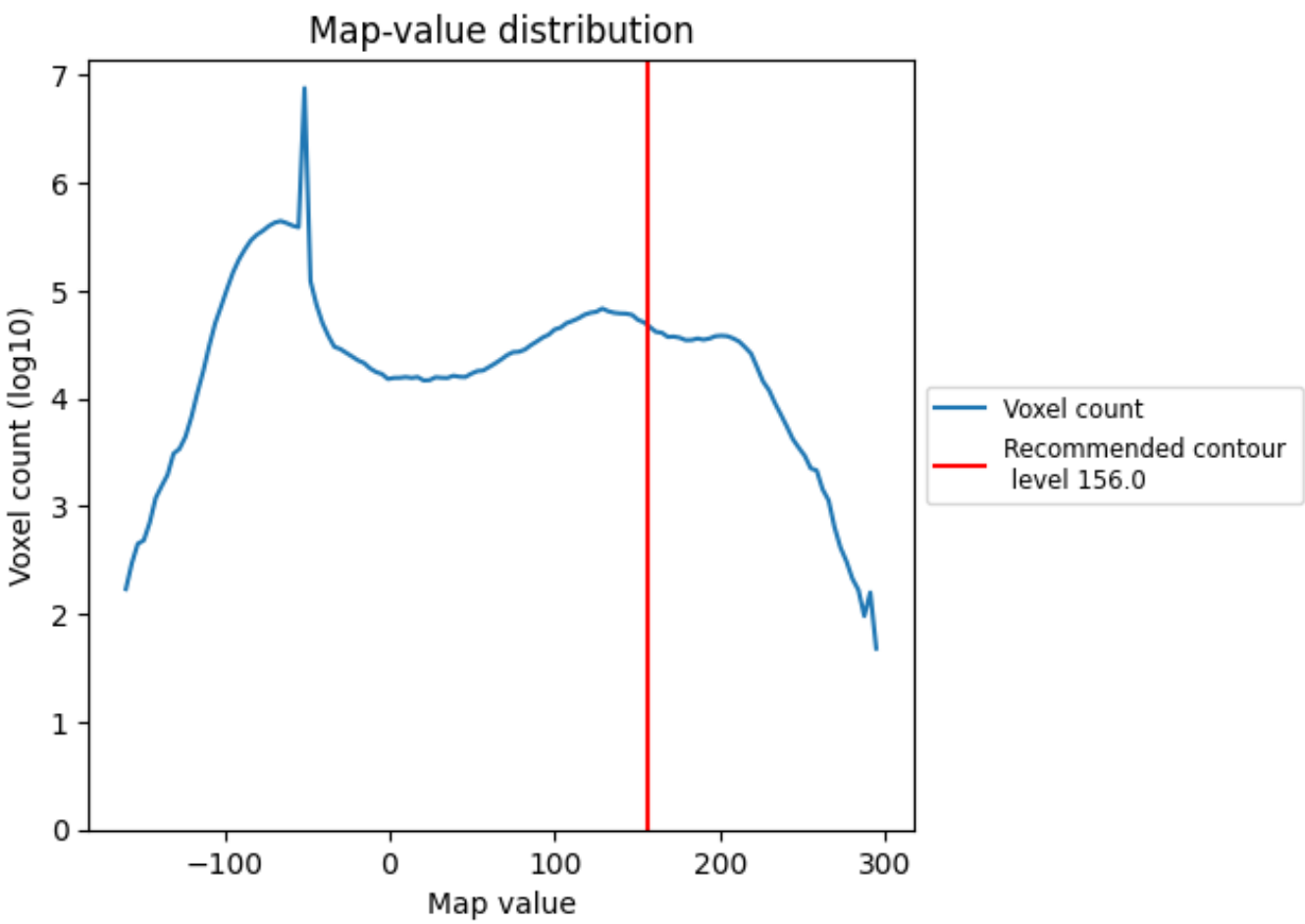
6.6 Mask visualisation (i)

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

7 Map analysis (i)

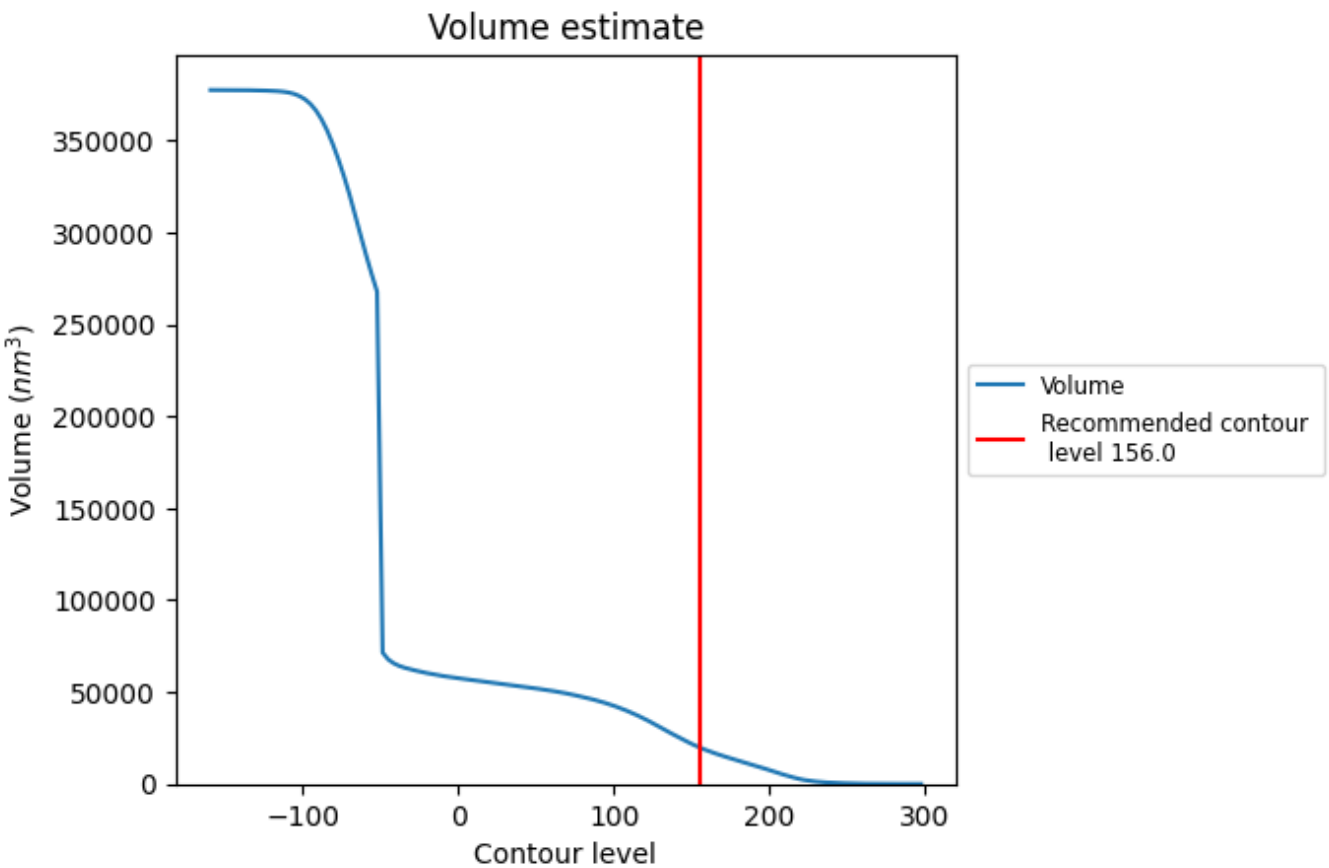
This section contains the results of statistical analysis of the map.

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.

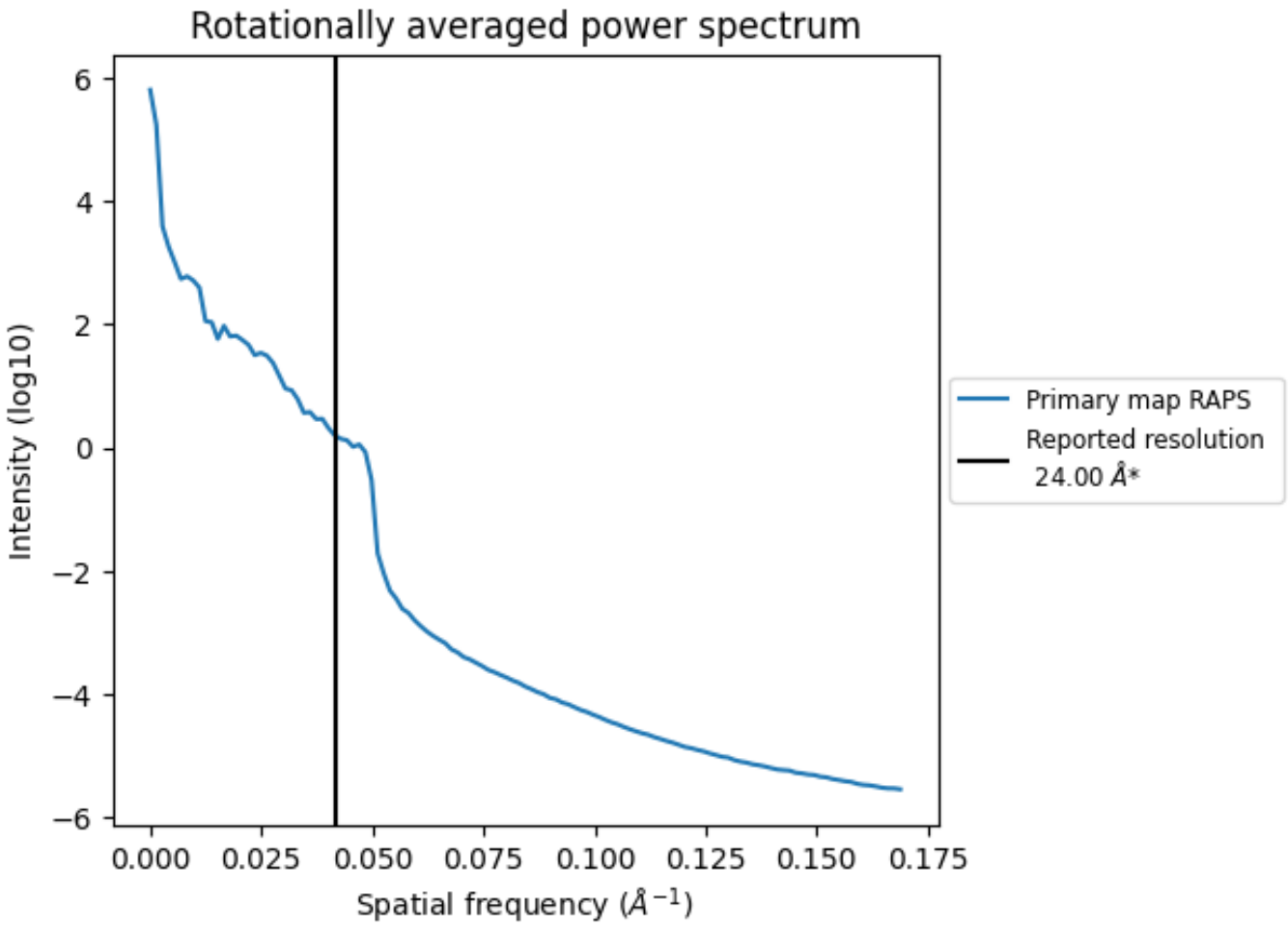
7.2 Volume estimate (i)



The volume at the recommended contour level is 19626 nm^3; this corresponds to an approximate mass of 17729 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 0.042 Å^{-1}

8 Fourier-Shell correlation (i)

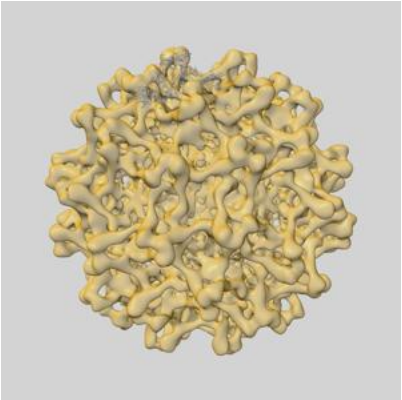
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

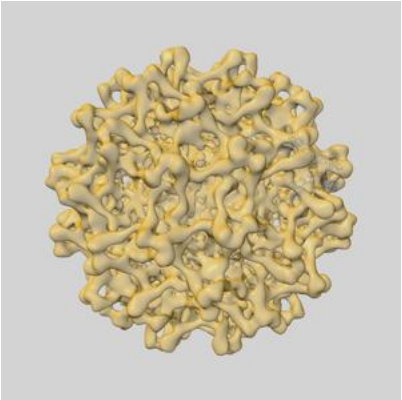
This section contains information regarding the fit between EMDB map EMD-1314 and PDB model 2OF6. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

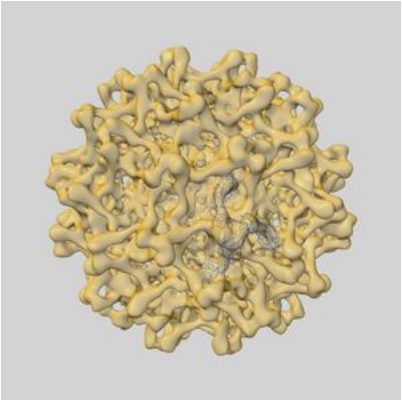
9.1.1 Map-model overlay (i)



X

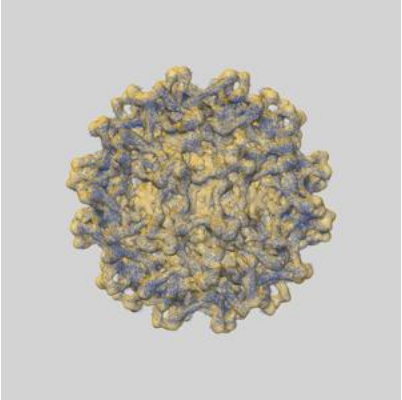


Y

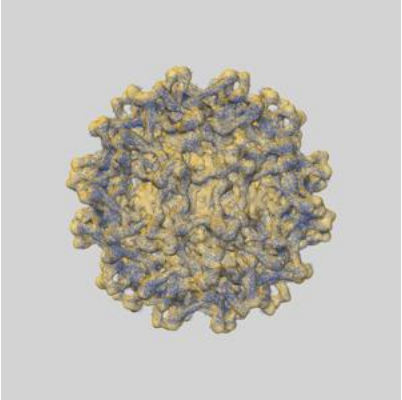


Z

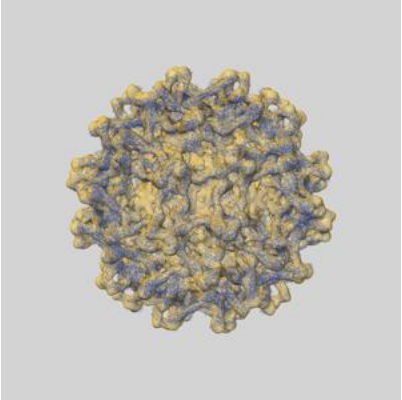
9.1.2 Map-model assembly overlay (i)



X



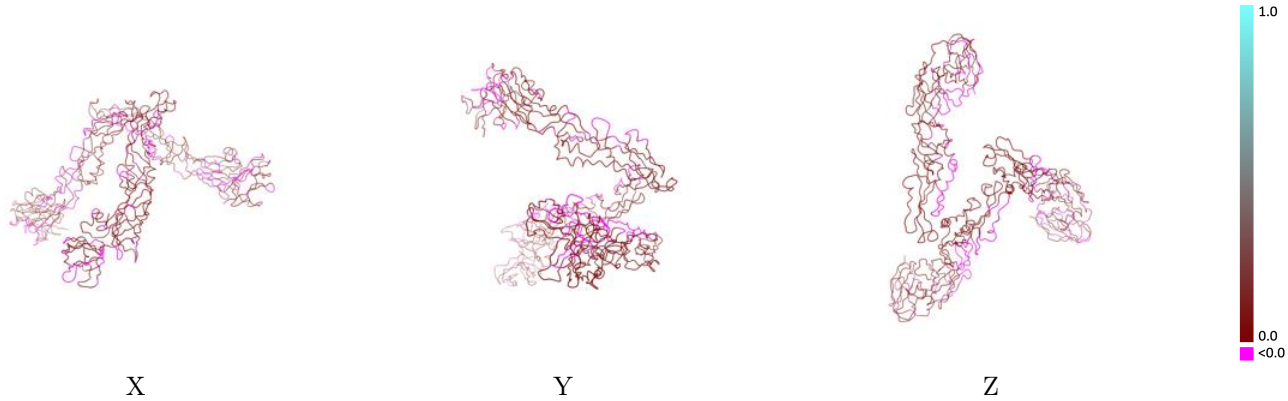
Y



Z

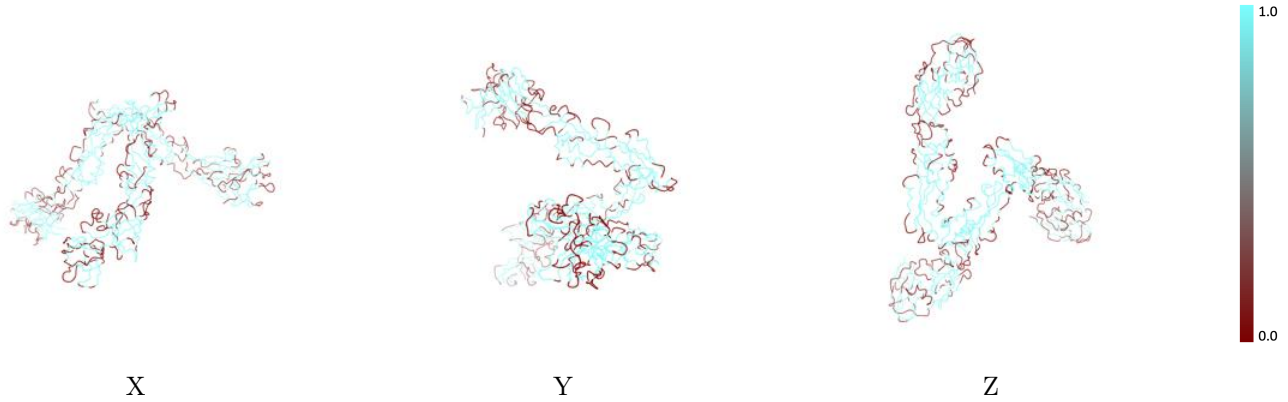
The images above show the 3D surface view of the map at the recommended contour level 156.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



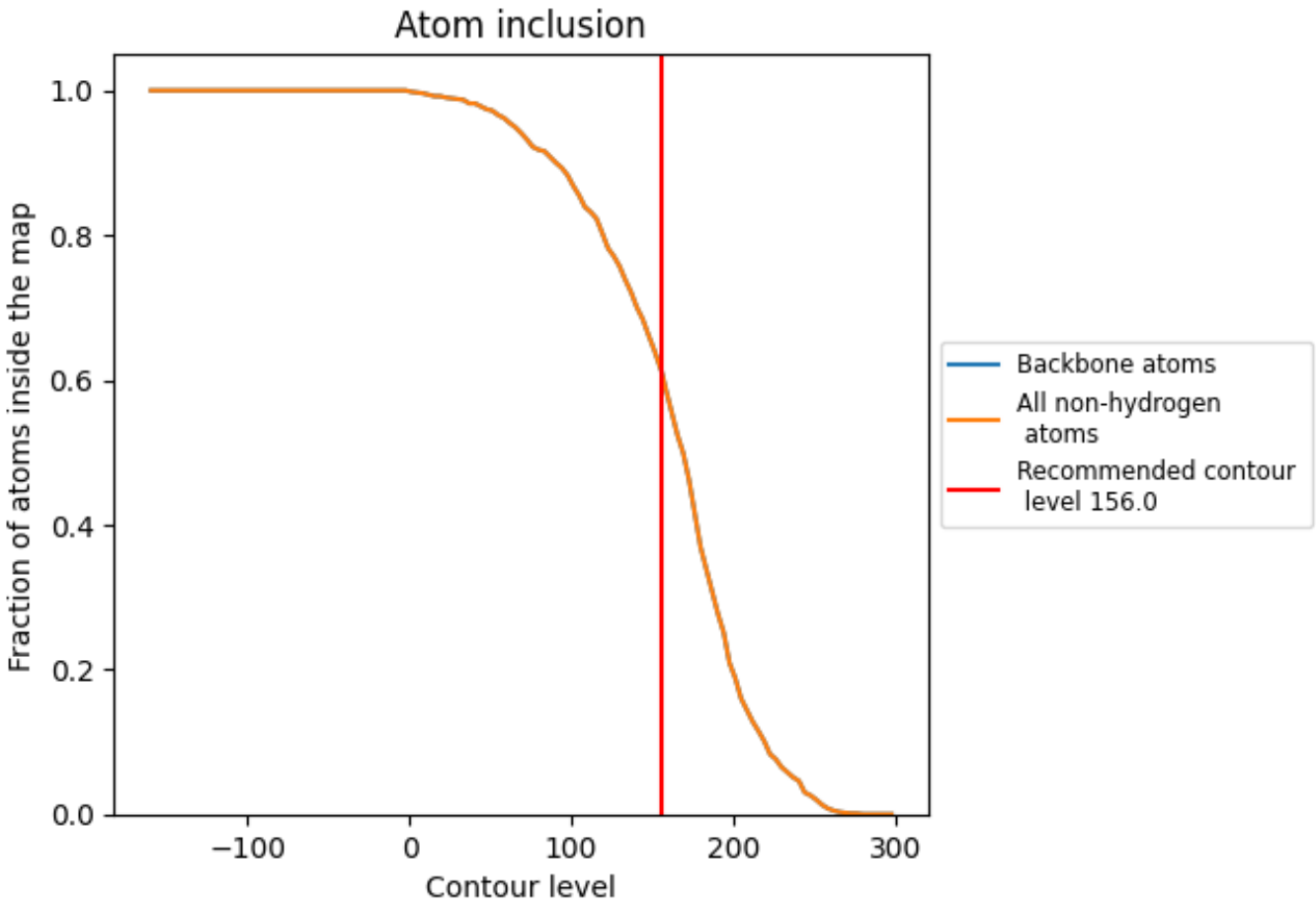
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (156.0).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 61% 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 (156.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6110	0.0520
A	0.5750	0.0480
B	0.6080	0.0530
C	0.6500	0.0570