



## wwPDB EM Validation Summary Report ⓘ

Mar 19, 2024 – 06:01 PM JST

PDB ID : 6IDK  
EMDB ID : EMD-9650  
Title : Cryo-EM structure of Immature Dengue virus serotype 3 in complex with human antibody 1H10 Fab at pH 5.0 (Class I particle)  
Authors : Wirawan, M.; Fibriansah, G.; Ng, T.S.; Zhang, Q.; Kostyuchenko, V.A.; Shi, J.; Lok, S.M.  
Deposited on : 2018-09-10  
Resolution : 25.00 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](mailto: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>.

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

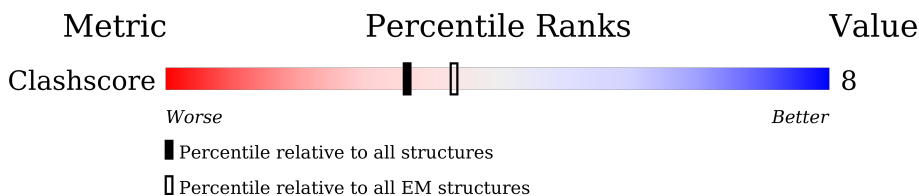
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance

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

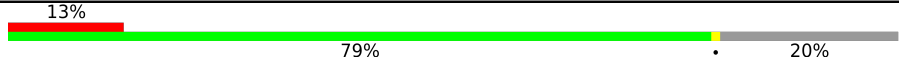



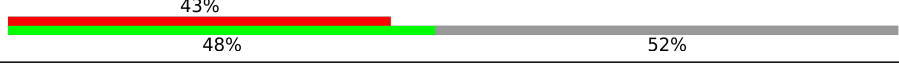

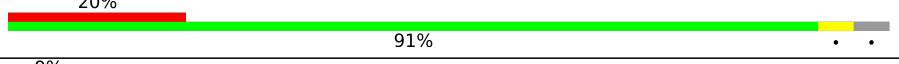
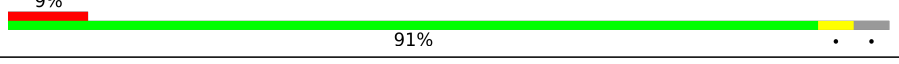
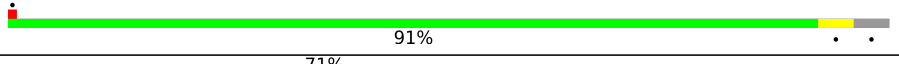
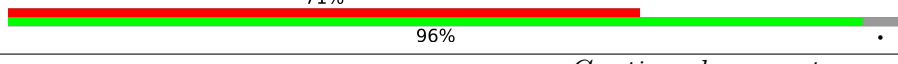
The reported resolution of this entry is 25.00 Å.

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.



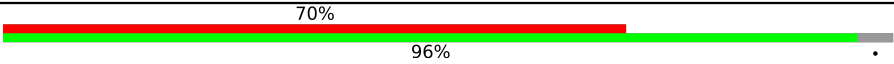
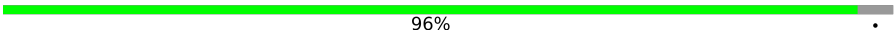
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297

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  $\geq 3$ , 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	493	 13% 79% 20%
1	B	493	 39% 79% 20%
1	C	493	 1% 78% 20%
2	D	166	 40% 48% 52%
2	E	166	 43% 48% 52%
2	F	166	 1% 48% 52%
3	H	137	 20% 91% 2% 5%
3	I	137	 9% 91% 2% 5%
3	M	137	 1% 91% 2% 5%
4	J	116	 71% 96% 1% 5%

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Mol	Chain	Length	Quality of chain
4	L	116	 <p>70% 96%</p>
4	N	116	 <p>96%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2145 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 protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	394	Total C 394 394	0	394
1	B	394	Total C 394 394	0	394
1	C	394	Total C 394 394	0	394

- Molecule 2 is a protein called Premembrane protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	D	79	Total C 79 79	0	79
2	E	79	Total C 79 79	0	79
2	F	79	Total C 79 79	0	79

- Molecule 3 is a protein called Fab 1H10 heavy chain (V-region).

Mol	Chain	Residues	Atoms	AltConf	Trace
3	H	131	Total C 131 131	0	131
3	I	131	Total C 131 131	0	131
3	M	131	Total C 131 131	0	131

- Molecule 4 is a protein called Fab 1H10 light chain (V-region).

Mol	Chain	Residues	Atoms	AltConf	Trace
4	J	111	Total C 111 111	0	111

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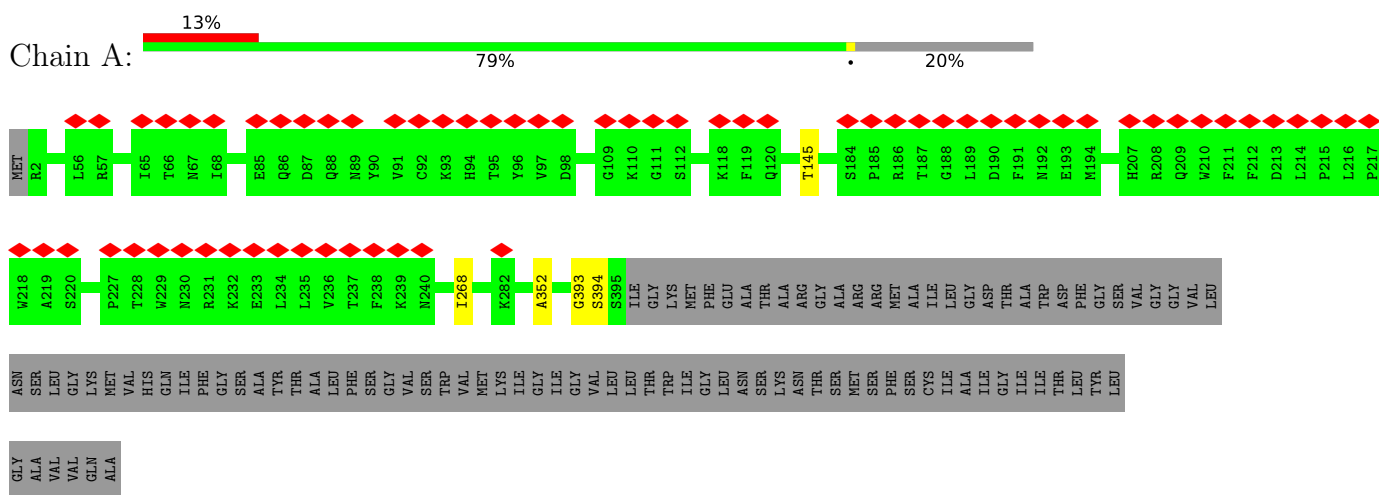
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>	<b>Trace</b>
4	L	111	Total 111	C 111	0	111
4	N	111	Total 111	C 111	0	111

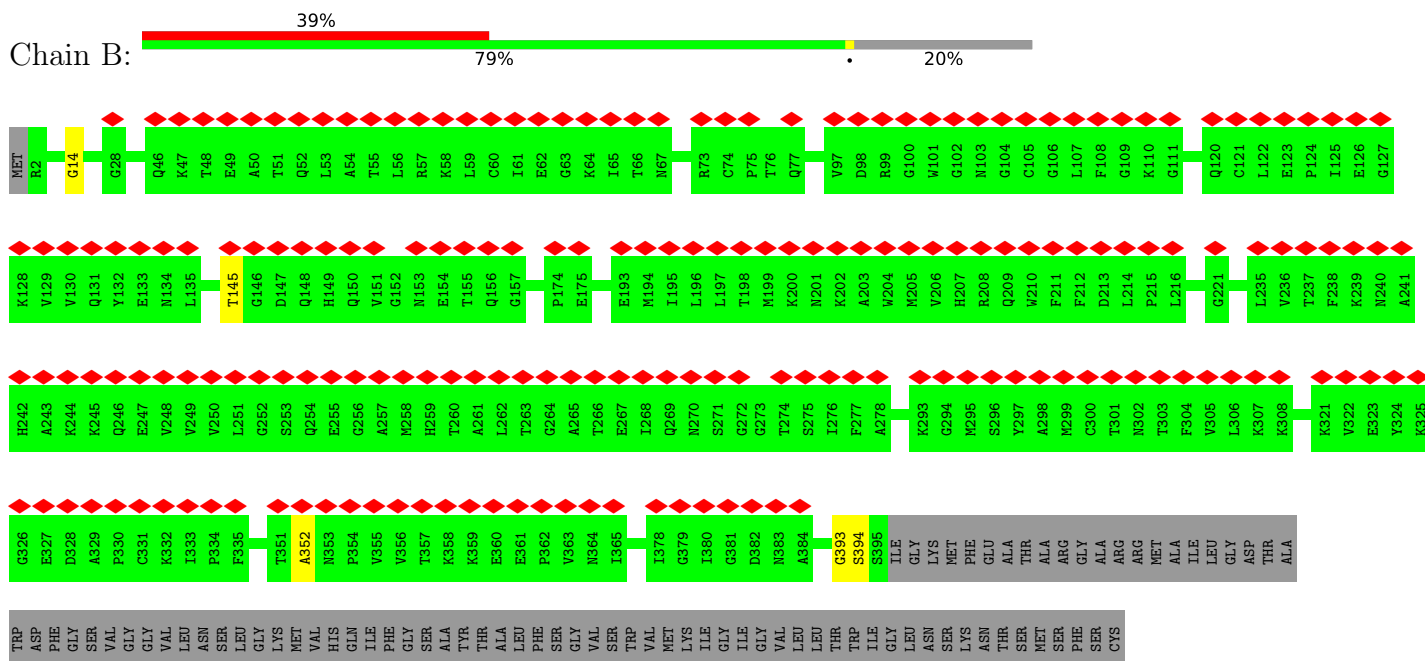
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Envelope protein



- Molecule 1: Envelope protein



ILE  
ALA  
ILE  
GLY  
ILE  
ILE  
THR  
LEU  
TYR  
LEU  
GLY  
ALA  
VAL  
VAL  
GLN  
ALA

• Molecule 1: Envelope protein

Chain C:



MET R2 P75 T76 Q77 G78 E79 G100 H101 G102 G106 L107 F108 G109 K110 T145 I172 L173 Q341 A352 G393 S394 S395 ILE GLY LYS MET PHE GLU THR ALA THR ALA ARG GLY ALA ARG MET MET MET ILE LEU ASP ALA THR ASP PHE GLY SER VAL GLY

GLY VAL LEU ASN SER LEU GLY LYS MET VAL HIS GLN ILE PHE GLY SER TYR THR ALA LEU PHE SER GLY VAL SER TRP VAL MET LYS ILE GLY ILE VAL LEU THR

LEU TYR GLY ALA VAL VAL GLN ALA

• Molecule 2: Premembrane protein

Chain D:



F1 H2 L3 T4 S6 R6 D7 G8 E9 P10 R11 M12 I13 V14 G16 K16 M17 E18 R19 G20 S22 L23 L24 F25 N32 C34 T35 L36 I37 A38 N39 D40 L41 G42 E43 M44 C45 D46 D47 T48 V49 T50 C53 P54 H55 I56 P61 E62 D63 I64 D65 C66 W67 C68 N69

L70 T71 S72 T73 W74 V75 T76 Y77 G78 CYS ASN GLN ALA GLU HIS ARG M17 ASP LYS ARG SER VAL ALA LEU MET PRO HIS VAL GLY LEU LEU MET PRO HIS VAL MET MET THR

HIS PRO GLY PHE THR ILE LEU ALA PHE LEU LEU ALA HIS TYR ILE GLN THR SER GLU THR LEU THR GLN LYS VAL VAL ILE PHE ILE LEU MET LEU VAL THR PRO SER MET MET THR

• Molecule 2: Premembrane protein

Chain E:



F1 G8 E9 P10 R11 M12 V14 G15 K16 M17 E18 R19 G20 K21 S22 L23 L24 F25 K26 T27 A28 S29 G30 I31 N32 N33 C34 T35 L36 I37 A38 N39 D40 L41 G42 E43 M44 C45 D46 D47 T48 V49 T50 Y51 K52 C53 P54 H55 I56 T57 E58 V59 E60 P61 E62 D63 I64 D65

C66 W67 C68 N69 T71 S72 T73 W74 V75 T76 Y77 G78 CYS ASN GLN ALA GLU HIS ARG M17 ASP LYS ARG SER VAL ALA LEU MET PRO HIS VAL MET MET THR

TRP ALA LEU ARG HIS PRO GLY PHE THR ILE LEU LEU ALA PHE LEU LEU ALA HIS TYR ILE GLN THR SER ARG SER VAL THR LYS VAL ILE PHE ILE LEU MET LEU VAL THR PRO SER MET THR

• Molecule 2: Premembrane protein

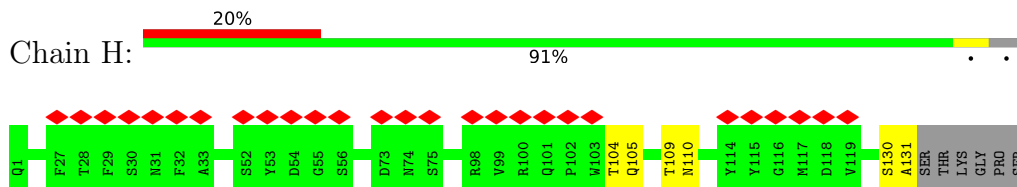
Chain F:



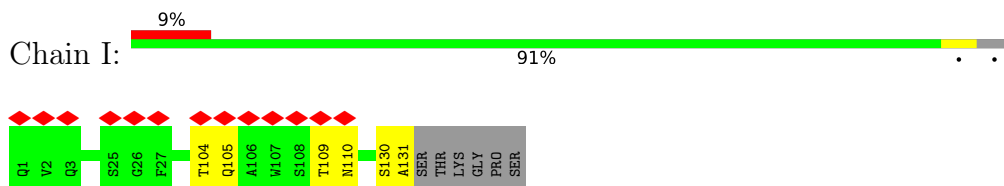
F1 V59 E60 P61 E62 T79 CYS ASN GLN ALA GLU HIS ARG ASP LYS SER VAL THR ALA LEU ALA PRO HIS VAL GLY MET LEU ASP THR ARG ALA GLY MET SER THR TRP MET SER ALA GLY ALA TRP ARG GLN VAL LEU VAL THR TRP ALA LEU ARG HIS

PRO GLY PHE THR ILE LEU ALA LEU PHE LEU ALA HIS TVR ILE GLY THR SER LEU THR GLN LYS VAL VAL ILE PHE ILE LEU MET LEU VAL THR PRO SER MET THR

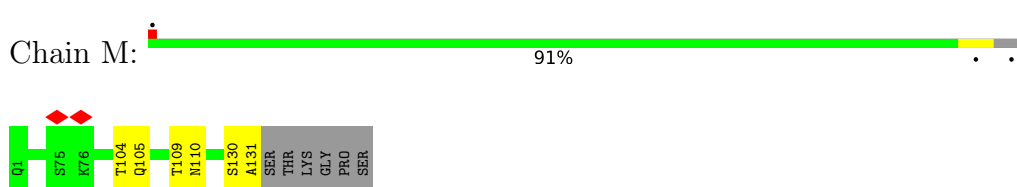
- Molecule 3: Fab 1H10 heavy chain (V-region)



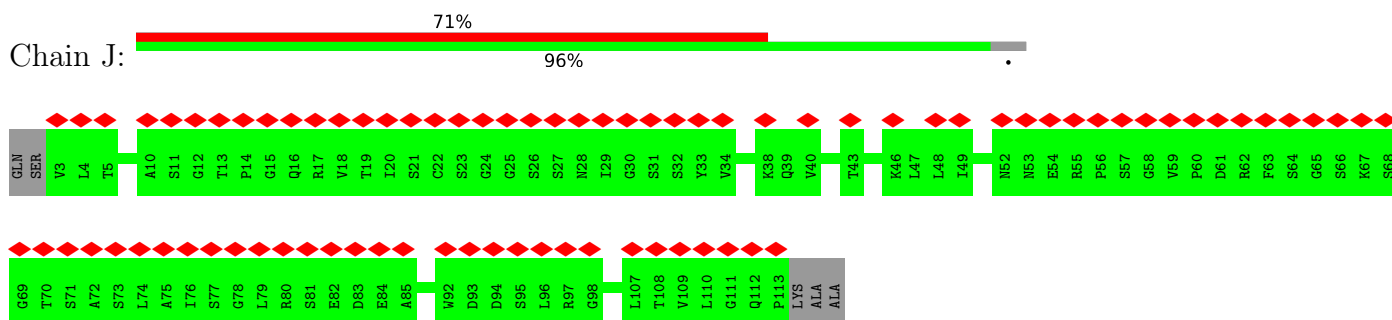
- Molecule 3: Fab 1H10 heavy chain (V-region)



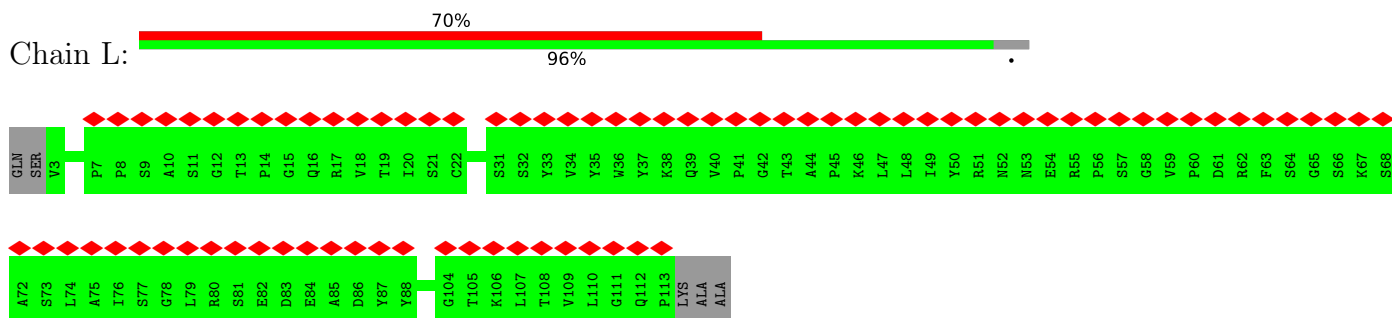
- Molecule 3: Fab 1H10 heavy chain (V-region)



- Molecule 4: Fab 1H10 light chain (V-region)



- Molecule 4: Fab 1H10 light chain (V-region)



- Molecule 4: Fab 1H10 light chain (V-region)



Chain N:  96%

GLN	+	LYS
SER	+	ALA
Y3	+	ALA

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	2216	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	18	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	8.142	Depositor
Minimum map value	-3.555	Depositor
Average map value	0.048	Depositor
Map value standard deviation	0.991	Depositor
Recommended contour level	1.7	Depositor
Map size ( $\text{\AA}$ )	870.4, 870.4, 870.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.7, 1.7, 1.7	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	394	0	0	3	0
1	B	394	0	0	4	0
1	C	394	0	0	5	0
2	D	79	0	0	0	0
2	E	79	0	0	0	0
2	F	79	0	0	0	0
3	H	131	0	0	3	0
3	I	131	0	0	3	0
3	M	131	0	0	3	0
4	J	111	0	0	0	0
4	L	111	0	0	0	0
4	N	111	0	0	0	0
All	All	2145	0	0	18	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 8.

The worst 5 of 18 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:B:14:GLY:CA	1:C:172:ILE:CA	2.49	0.90
1:A:268:ILE:CA	1:C:341:GLN:CA	2.51	0.88
1:B:14:GLY:CA	1:C:173:LEU:CA	2.80	0.60
1:B:145:THR:CA	1:B:352:ALA:CA	2.80	0.59
1:A:145:THR:CA	1:A:352:ALA:CA	2.81	0.59

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

There are no chain breaks in this entry.

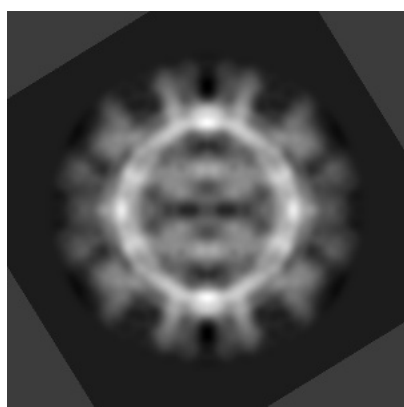
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9650. 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: 256



Y Index: 256

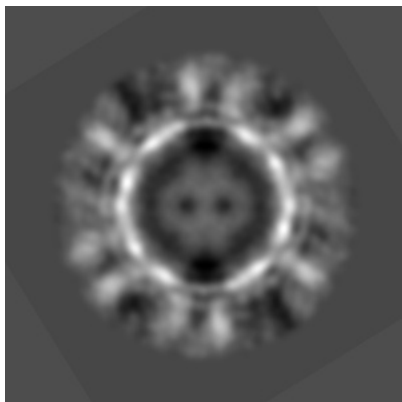


Z Index: 256

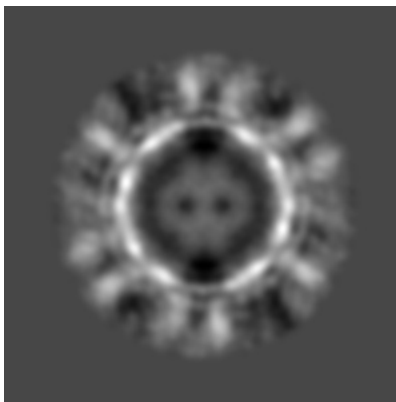
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

### 6.3.1 Primary map



X Index: 212



Y Index: 212

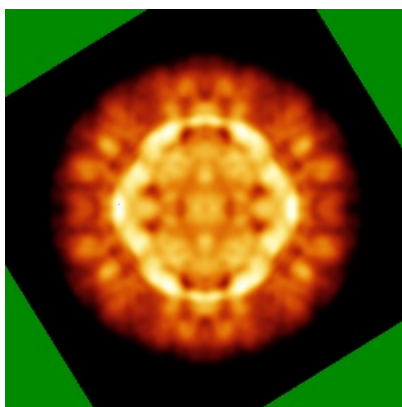


Z Index: 300

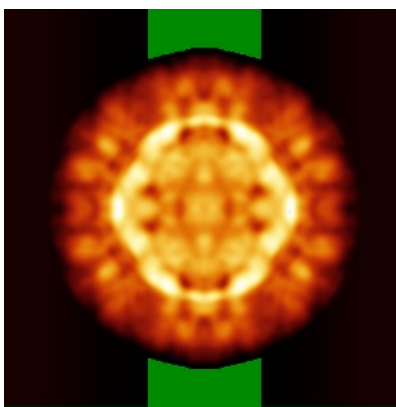
The images above show the largest variance slices of the map in three orthogonal directions.

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

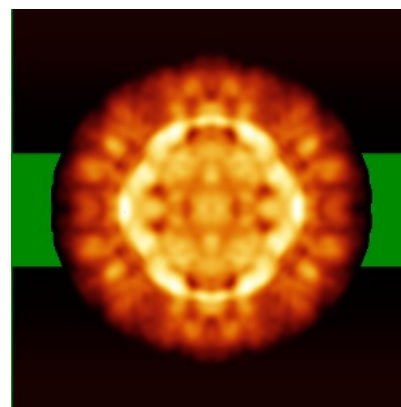
### 6.4.1 Primary map



X



Y

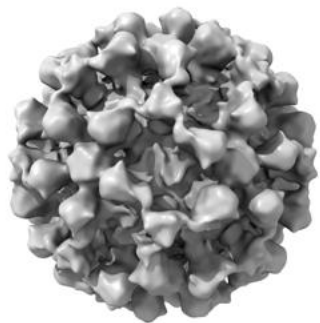


Z

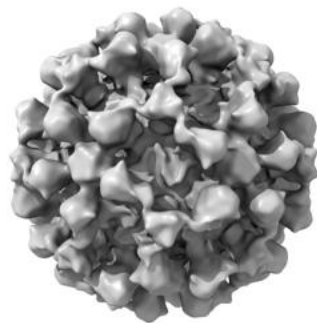
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

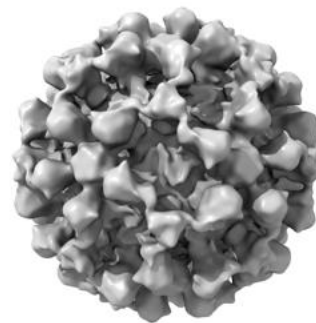
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.7. 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](#)

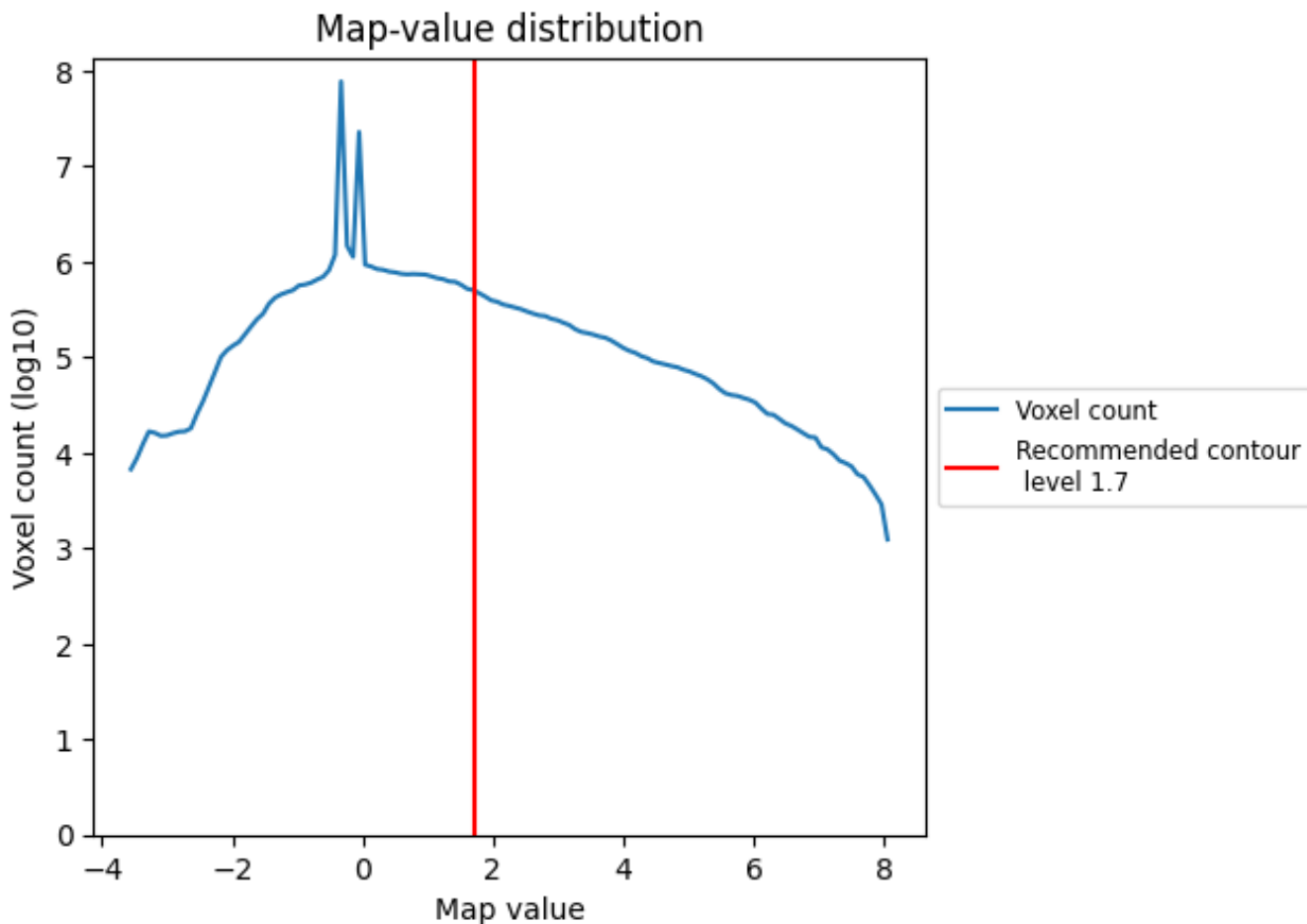
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

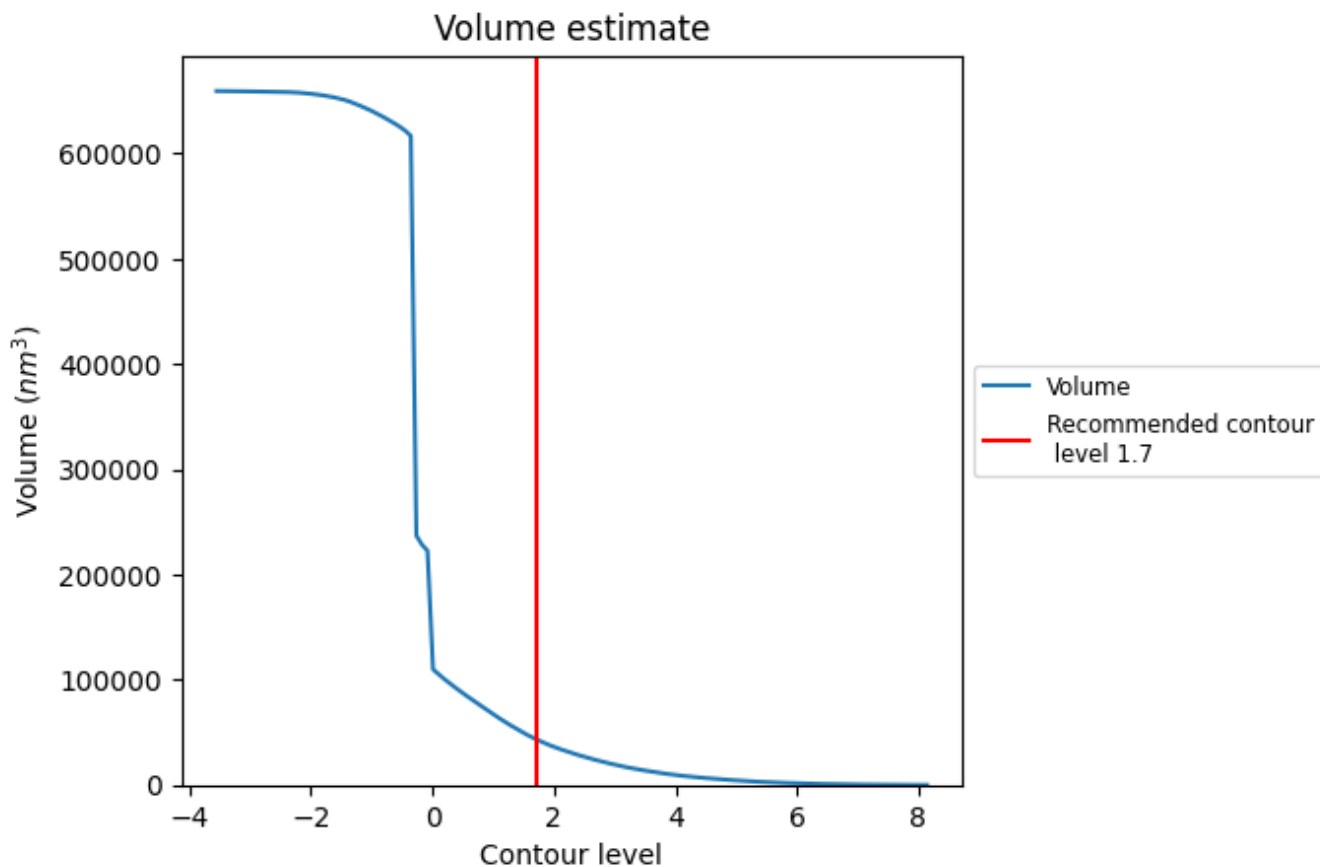
This section contains the results of statistical analysis of the map.

### 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.

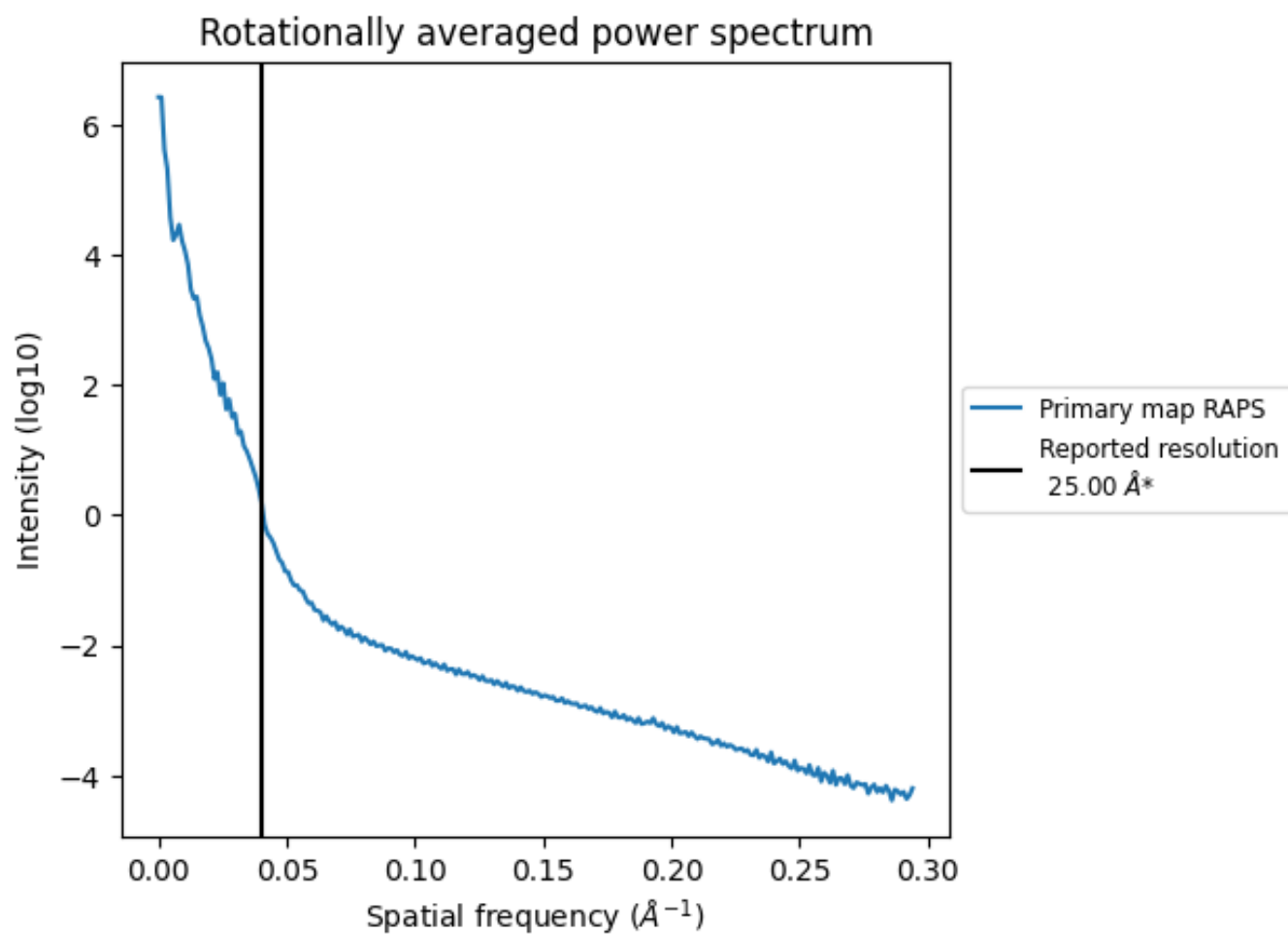
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 43605 nm<sup>3</sup>; this corresponds to an approximate mass of 39390 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](#)

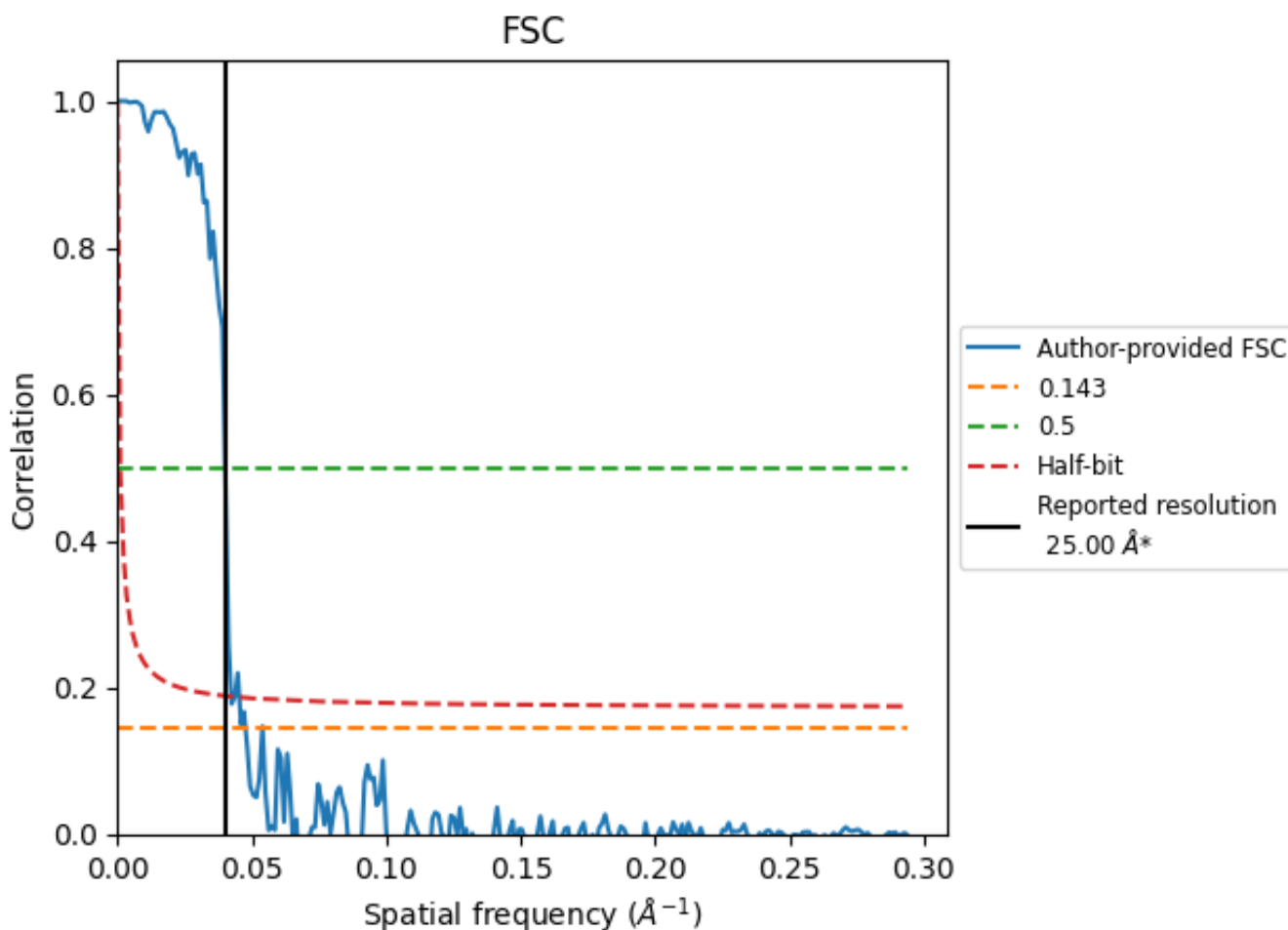


\*Reported resolution corresponds to spatial frequency of 0.040 Å<sup>-1</sup>

## 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 0.040 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	25.00	-
Author-provided FSC curve	20.96	24.88	23.58
Unmasked-calculated*	-	-	-

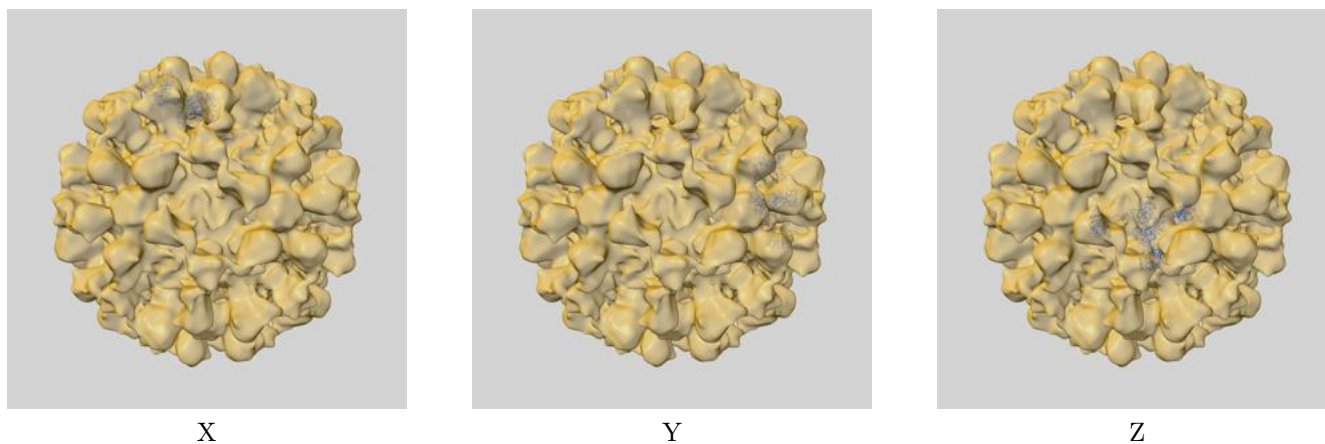
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

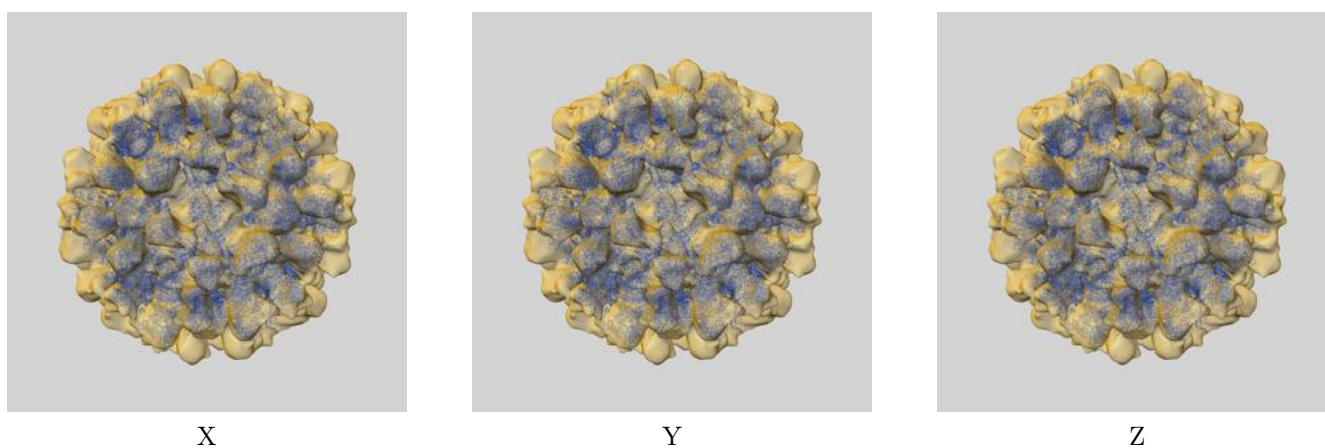
This section contains information regarding the fit between EMDB map EMD-9650 and PDB model 6IDK. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

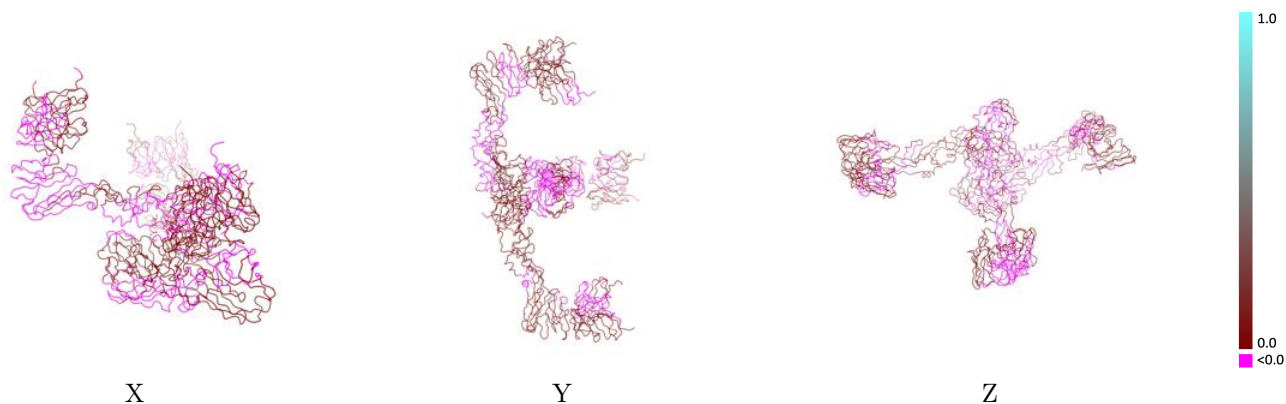


#### 9.1.2 Map-model assembly overlay [i](#)



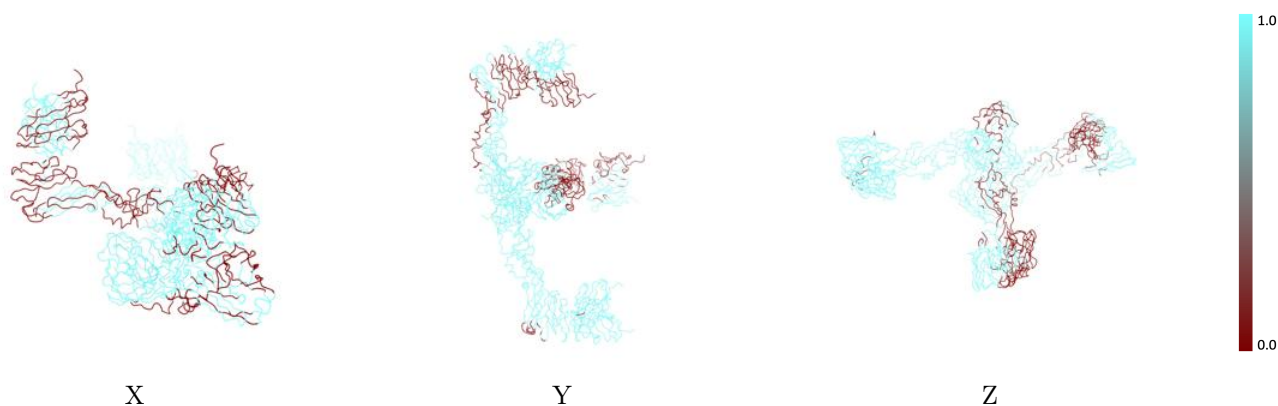
The images above show the 3D surface view of the map at the recommended contour level 1.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



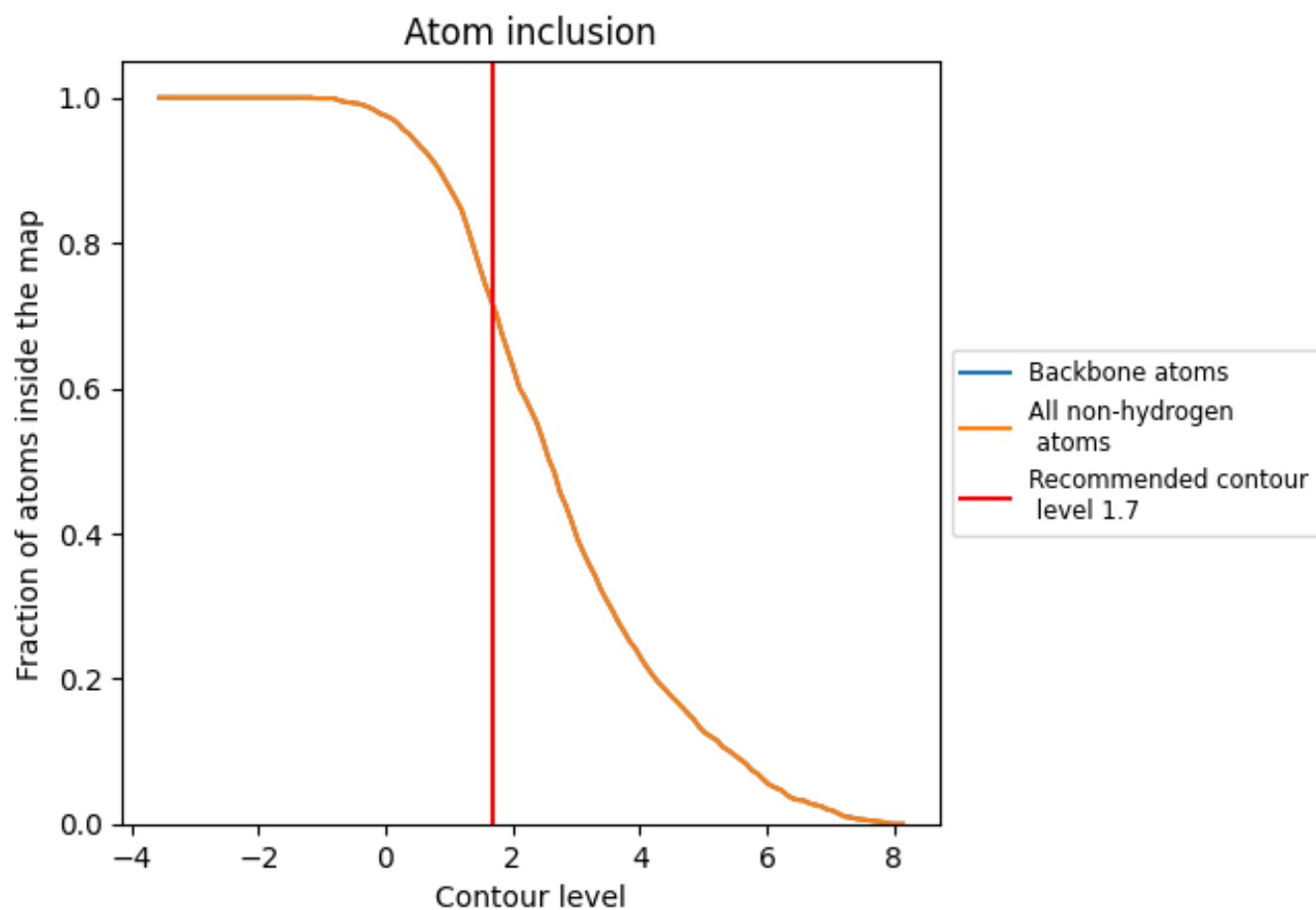
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.7).

## 9.4 Atom inclusion [i](#)





























At the recommended contour level, 71% of all backbone atoms, 71% 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 (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.0180
A	 0.8330	 0.0300
B	 0.5100	 -0.0150
C	 0.9670	 0.0460
D	 0.1650	 -0.0340
E	 0.0890	 -0.0370
F	 0.9620	 0.0420
H	 0.7940	 0.0450
I	 0.9010	 0.0240
J	 0.2610	 -0.0010
L	 0.2700	 0.0320
M	 0.9850	 0.0270
N	 1.0000	 -0.0010

