



Full wwPDB EM Validation Report ⓘ

Oct 2, 2023 – 10:16 PM EDT

PDB ID : 8TU2
EMDB ID : EMD-41616
Title : The Capsid of Rat Bocavirus
Authors : Velez, M.; Mietzsch, M.; McKenna, R.
Deposited on : 2023-08-15
Resolution : 2.52 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev50
MolProbity : **FAILED**
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) : 2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 253980 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	524	4233	2661	735	818	19	0	0
1	B	524	4233	2661	735	818	19	0	0
1	C	524	4233	2661	735	818	19	0	0
1	D	524	4233	2661	735	818	19	0	0
1	E	524	4233	2661	735	818	19	0	0
1	F	524	4233	2661	735	818	19	0	0
1	G	524	4233	2661	735	818	19	0	0
1	H	524	4233	2661	735	818	19	0	0
1	I	524	4233	2661	735	818	19	0	0
1	J	524	4233	2661	735	818	19	0	0
1	K	524	4233	2661	735	818	19	0	0
1	L	524	4233	2661	735	818	19	0	0
1	M	524	4233	2661	735	818	19	0	0
1	N	524	4233	2661	735	818	19	0	0
1	O	524	4233	2661	735	818	19	0	0
1	P	524	4233	2661	735	818	19	0	0
1	Q	524	4233	2661	735	818	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	S	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	T	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	U	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	V	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	W	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	X	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	Y	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	Z	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	1	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	2	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	3	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	4	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	5	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	6	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	a	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	b	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	c	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	d	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	e	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	f	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	h	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	i	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	j	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	k	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	l	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	m	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	n	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	o	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	p	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	q	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	r	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	s	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	t	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	u	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	v	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	w	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	x	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	y	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	z	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		
1	7	524	Total	C	N	O	S	0	0
			4233	2661	735	818	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	524	4233	2661	735	818	19	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9199	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	16.708	Depositor
Minimum map value	-8.411	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (\AA)	386.82, 386.82, 386.82	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.921, 0.921, 0.921	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

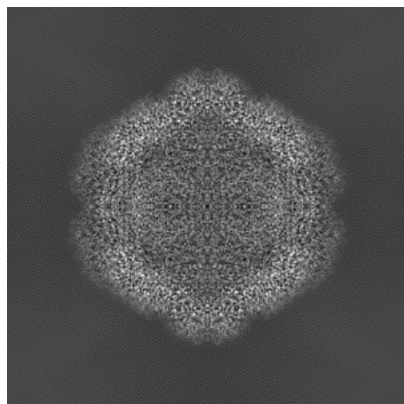
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41616. These allow visual inspection of the internal detail of the map and identification of artifacts.

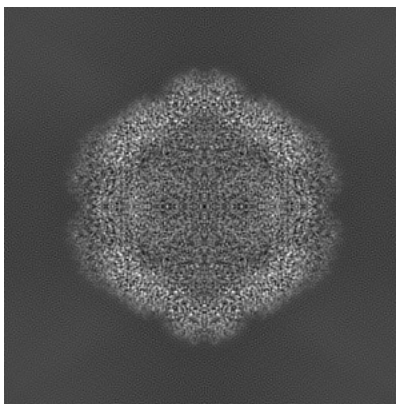
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

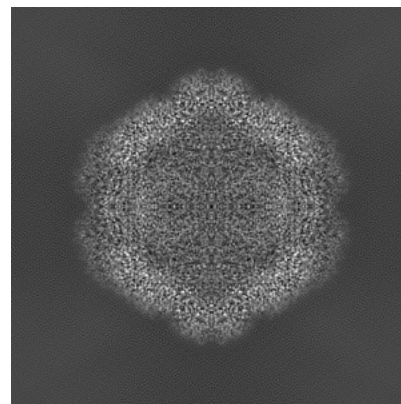
5.1.1 Primary map



X

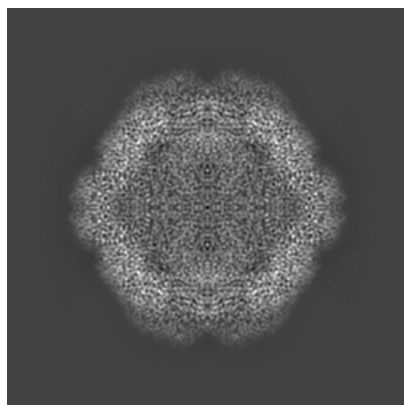


Y

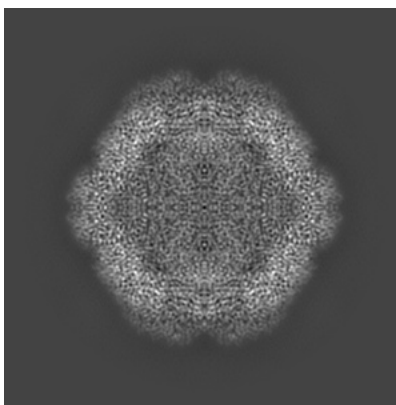


Z

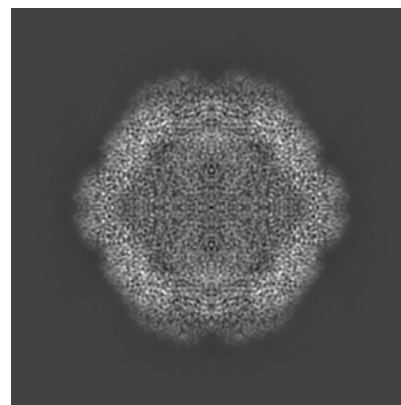
5.1.2 Raw map



X



Y

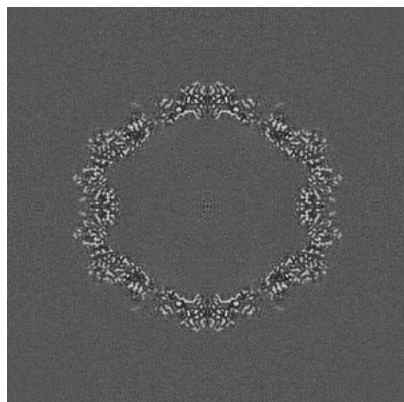


Z

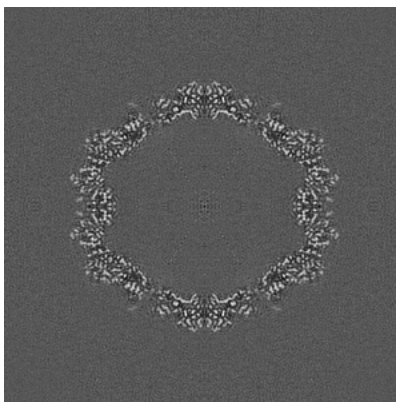
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

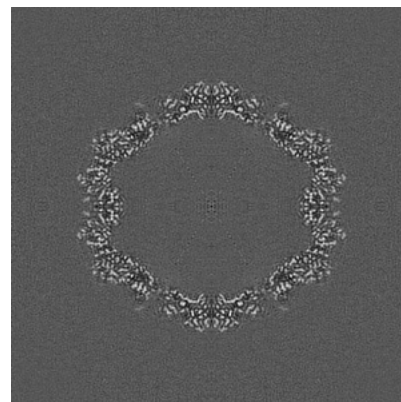
5.2.1 Primary map



X Index: 210

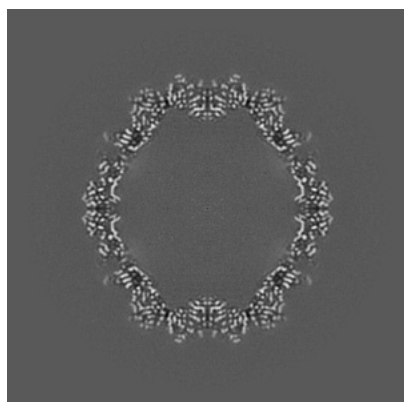


Y Index: 210

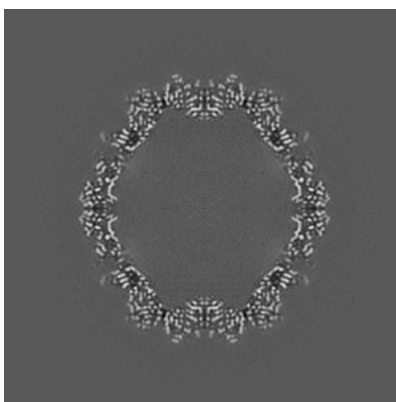


Z Index: 210

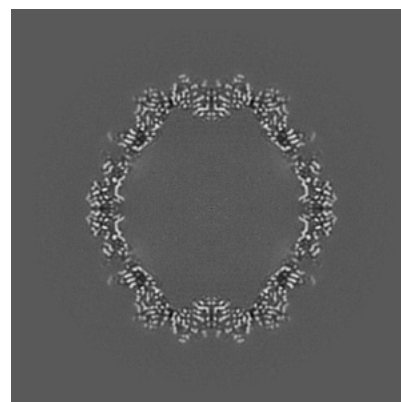
5.2.2 Raw map



X Index: 210



Y Index: 210

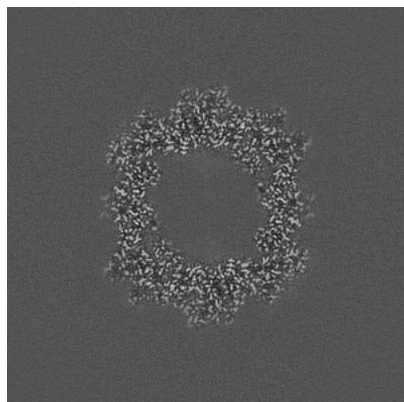


Z Index: 210

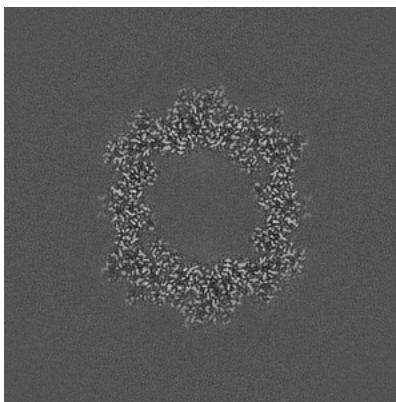
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

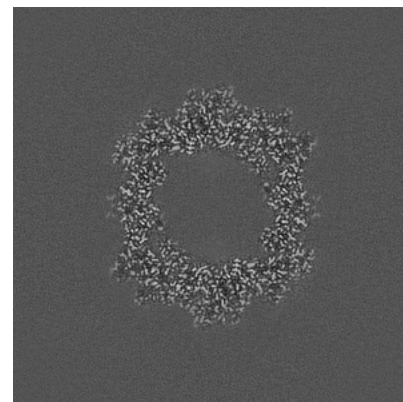
5.3.1 Primary map



X Index: 283

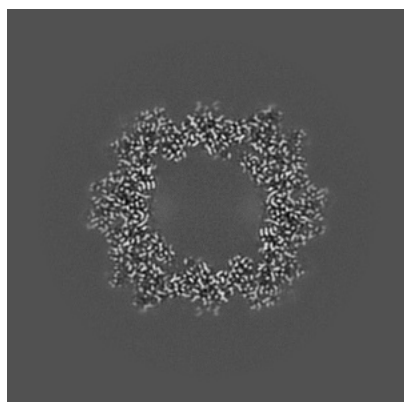


Y Index: 283

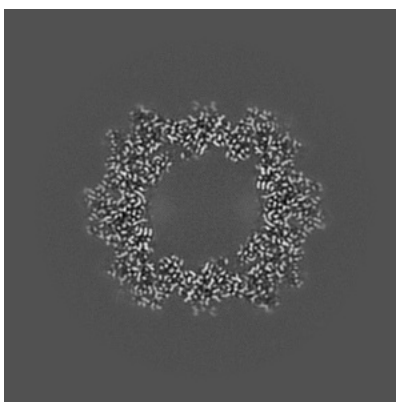


Z Index: 283

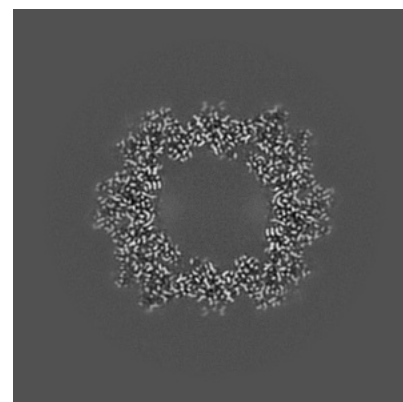
5.3.2 Raw map



X Index: 283



Y Index: 137

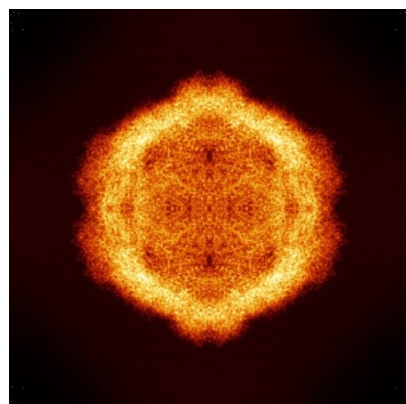


Z Index: 283

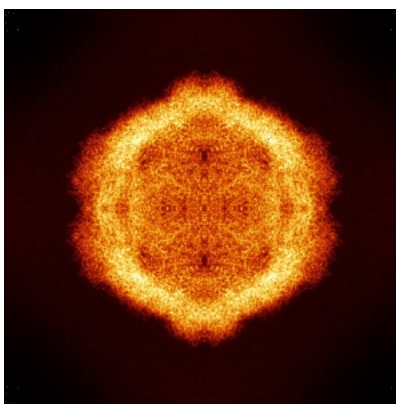
The images above show the largest variance slices of the map in three orthogonal directions.

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

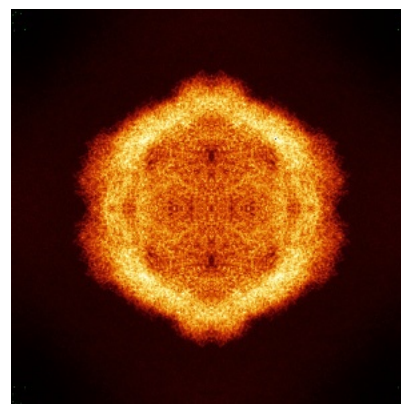
5.4.1 Primary map



X

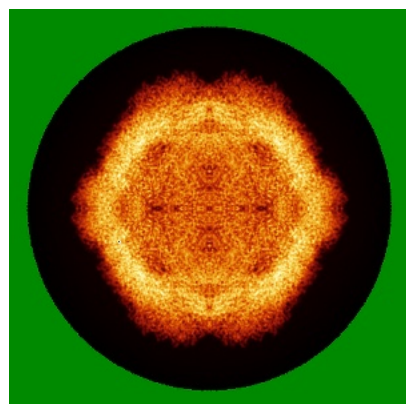


Y

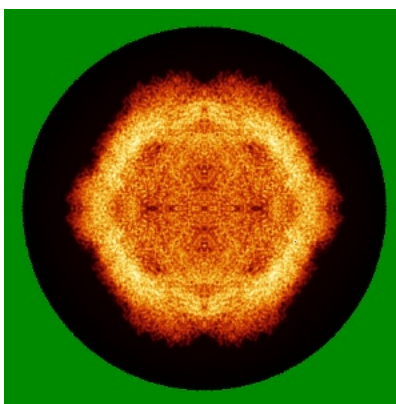


Z

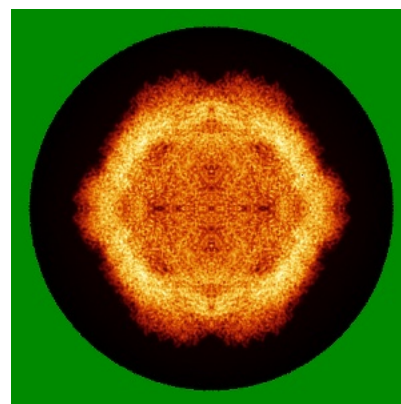
5.4.2 Raw map



X



Y

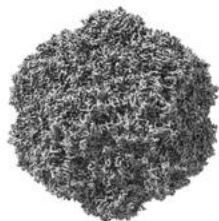


Z

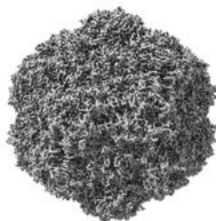
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

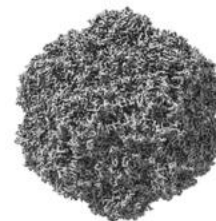
5.5.1 Primary map



X



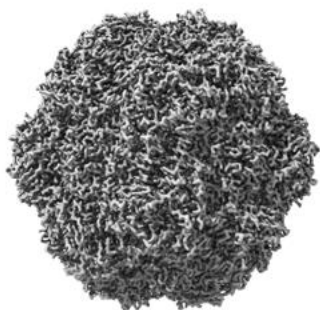
Y



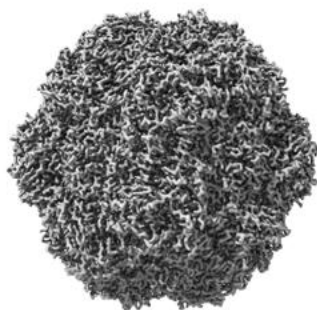
Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

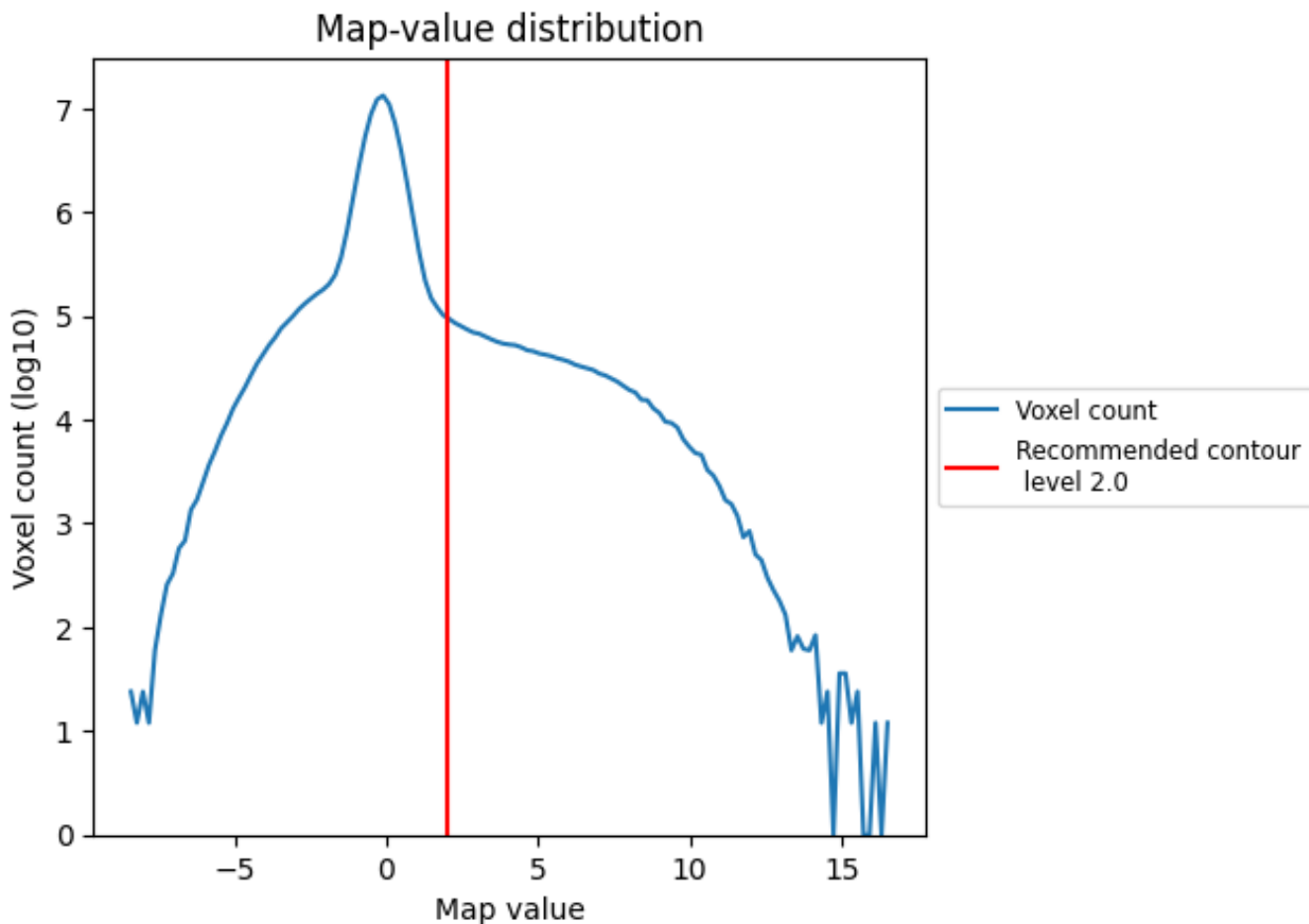
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

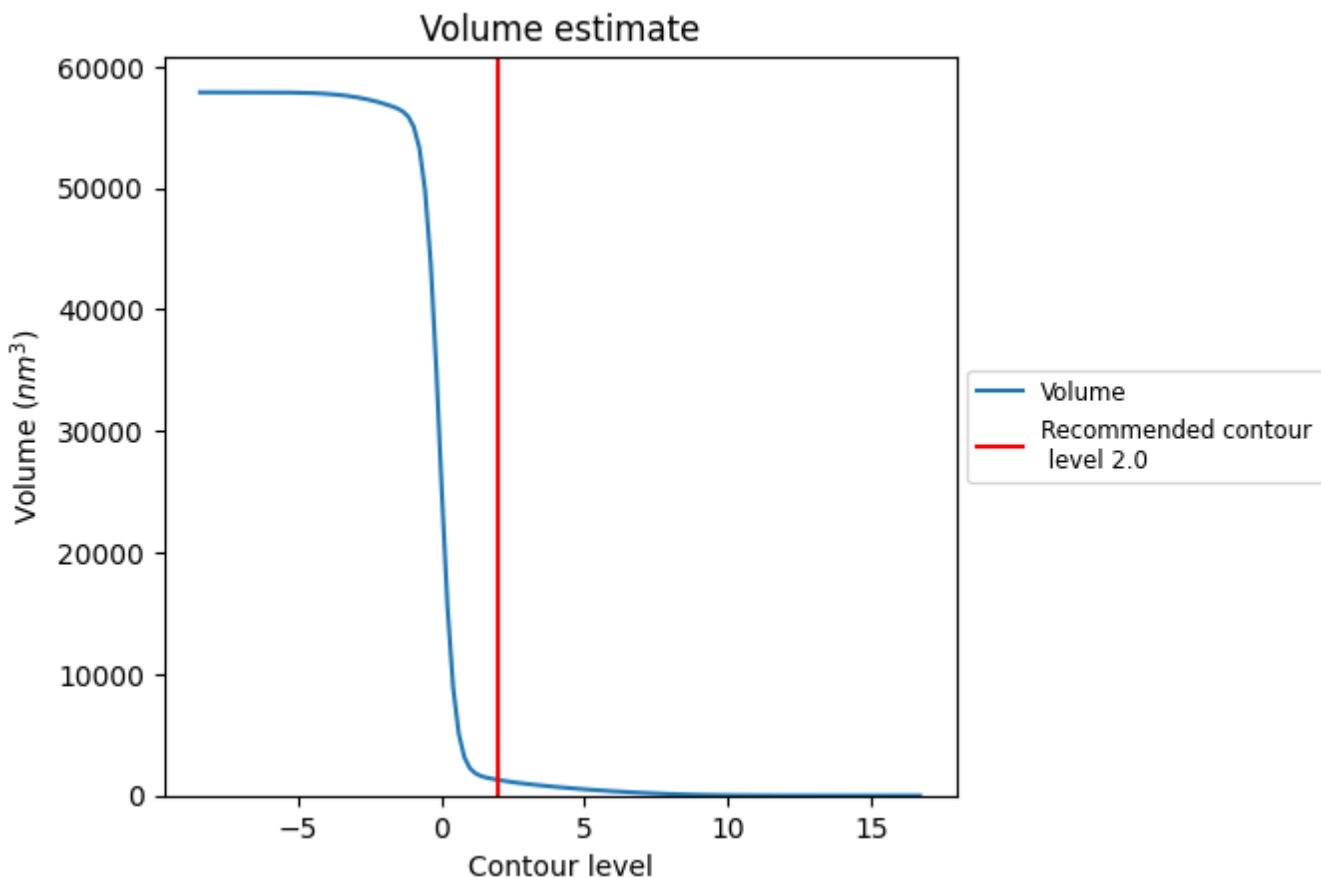
This section contains the results of statistical analysis of the map.

6.1 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.

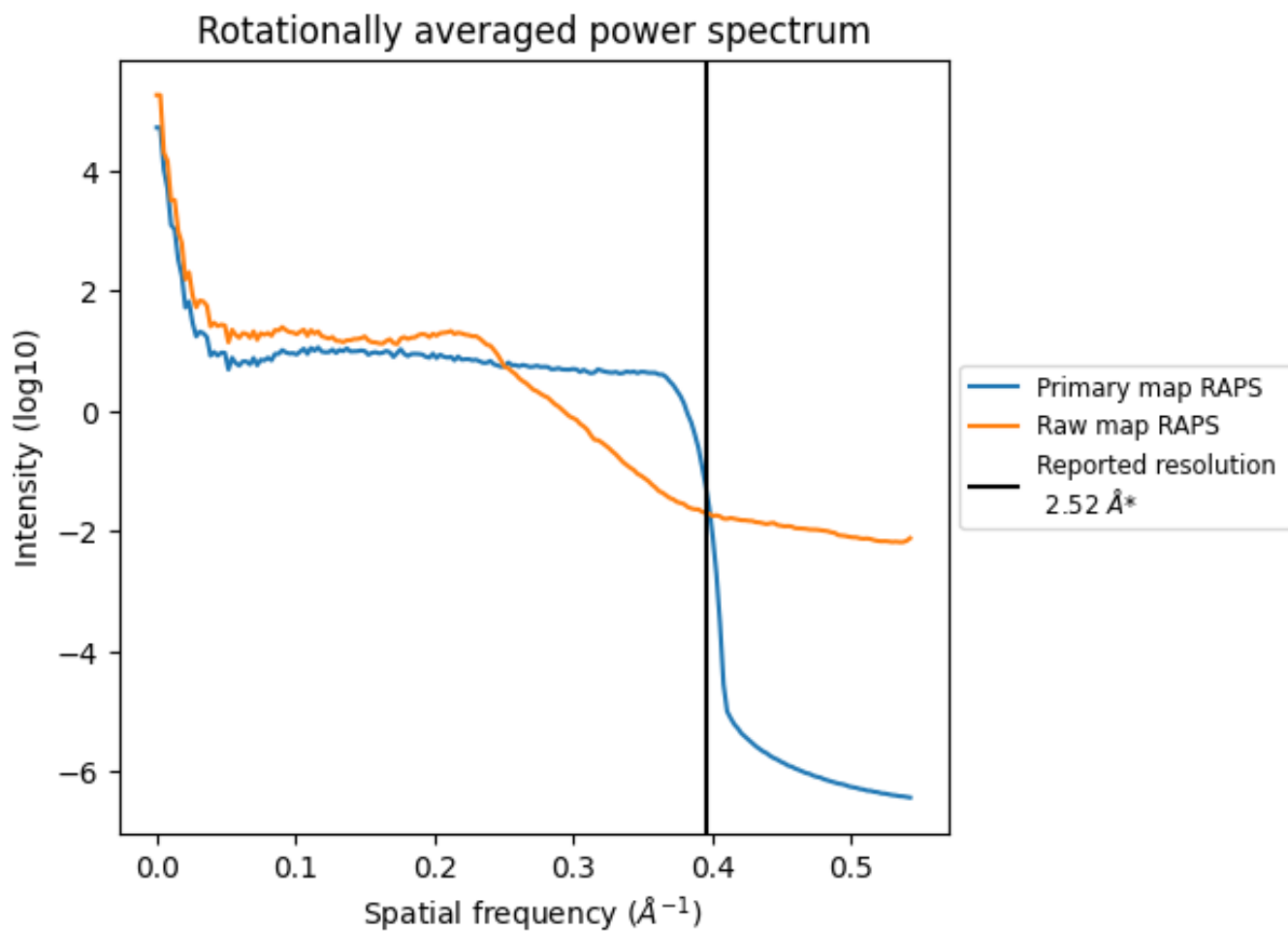
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 1278 nm³; this corresponds to an approximate mass of 1155 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.

6.3 Rotationally averaged power spectrum i

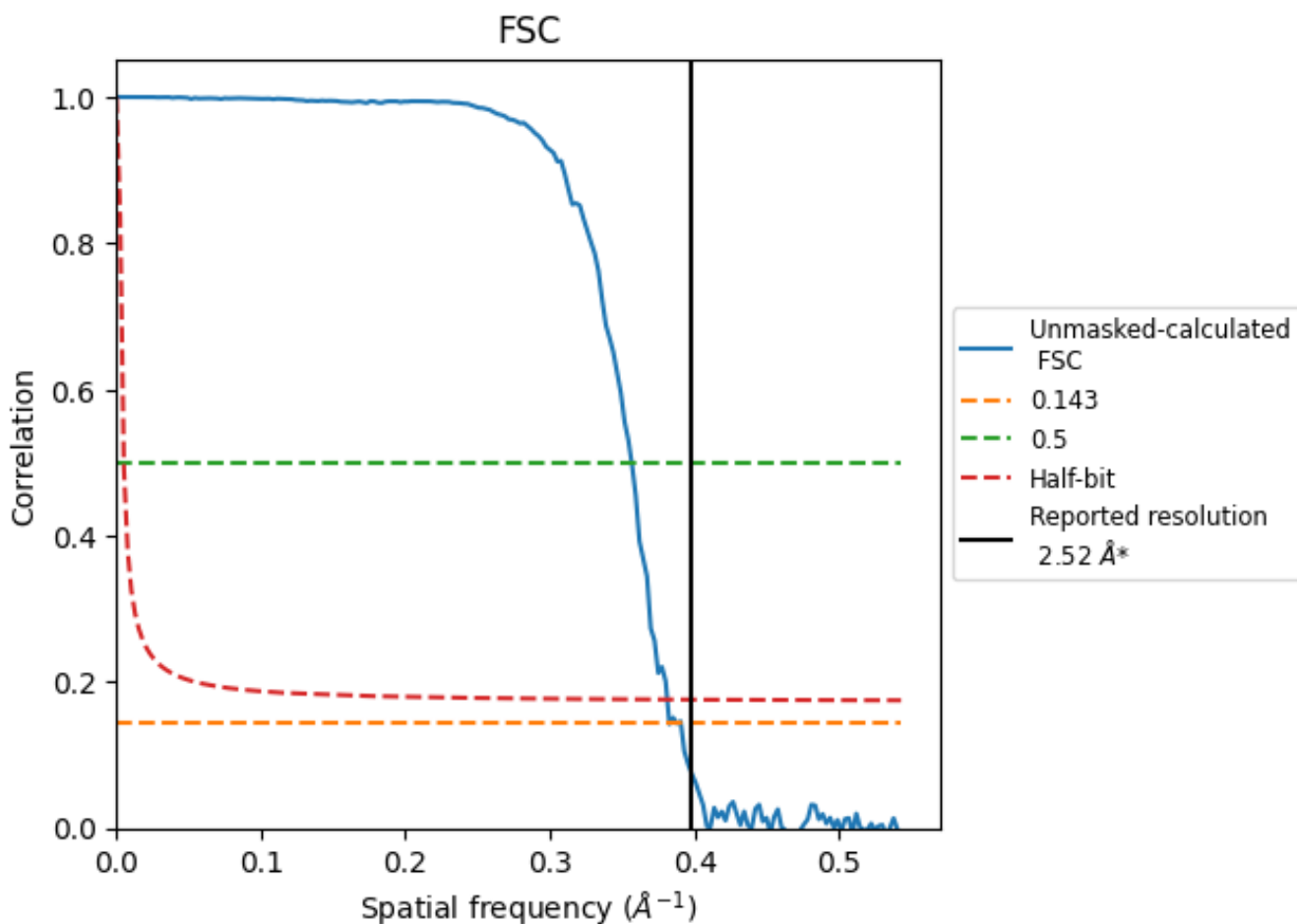


*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.397 \AA^{-1}

7.2 Resolution estimates [i](#)

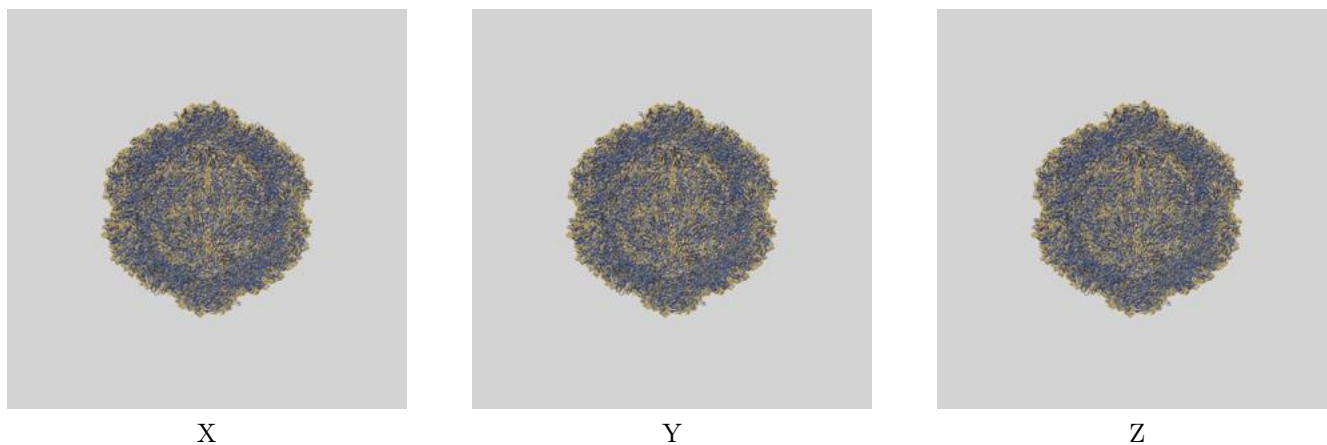
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.61	2.81	2.62

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

8 Map-model fit [i](#)

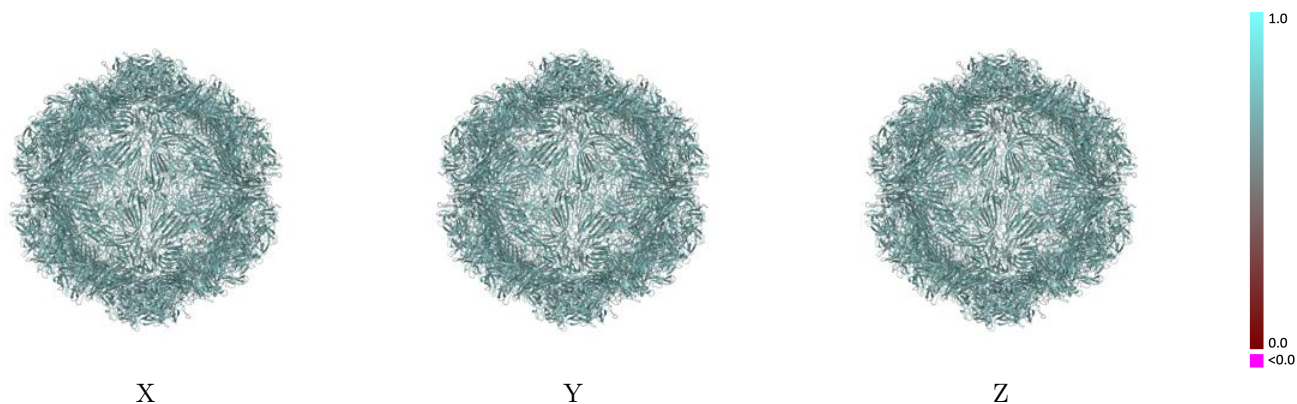
This section contains information regarding the fit between EMDB map EMD-41616 and PDB model 8TU2. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



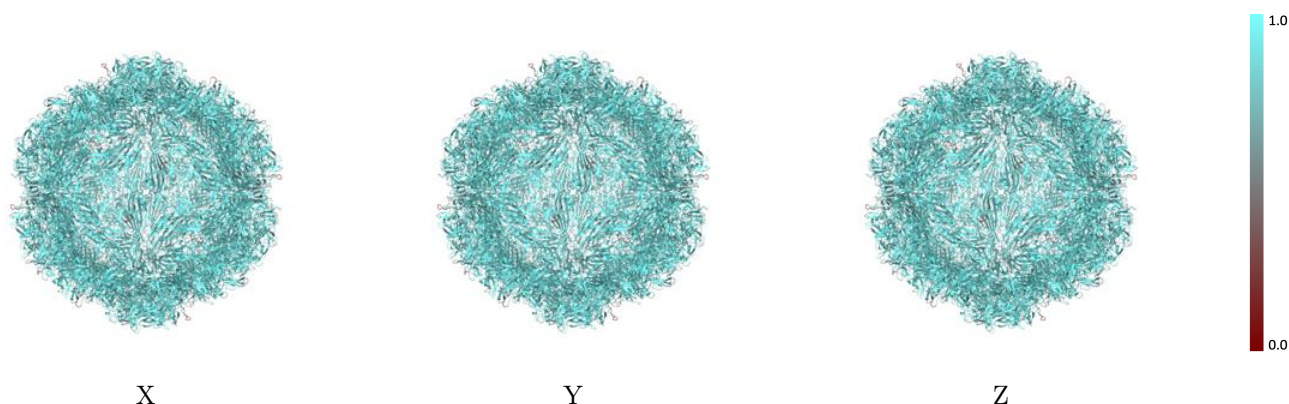
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



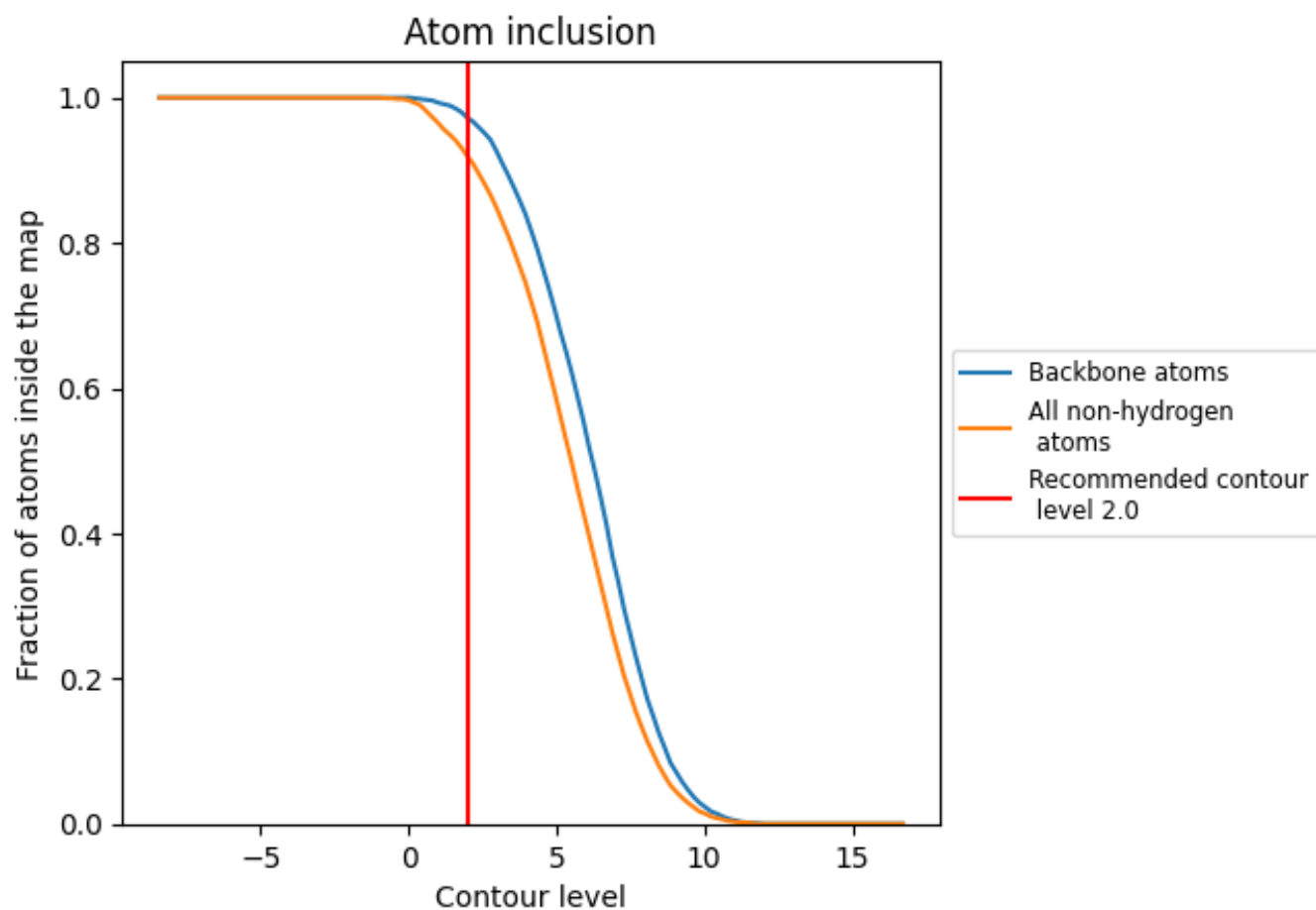
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (2.0).







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary





















































The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.6630
1	 0.9190	 0.6630
2	 0.9190	 0.6630
3	 0.9190	 0.6620
4	 0.9190	 0.6630
5	 0.9190	 0.6630
6	 0.9190	 0.6630
7	 0.9190	 0.6640
8	 0.9180	 0.6640
A	 0.9190	 0.6630
B	 0.9220	 0.6630
C	 0.9190	 0.6630
D	 0.9190	 0.6630
E	 0.9180	 0.6620
F	 0.9190	 0.6630
G	 0.9180	 0.6630
H	 0.9190	 0.6630
I	 0.9190	 0.6630
J	 0.9220	 0.6630
K	 0.9190	 0.6620
L	 0.9220	 0.6630
M	 0.9190	 0.6630
N	 0.9190	 0.6650
O	 0.9180	 0.6630
P	 0.9190	 0.6640
Q	 0.9190	 0.6640
R	 0.9220	 0.6630
S	 0.9220	 0.6630
T	 0.9190	 0.6640
U	 0.9220	 0.6630
V	 0.9190	 0.6630
W	 0.9190	 0.6640
X	 0.9190	 0.6630
Y	 0.9190	 0.6640
Z	 0.9180	 0.6630



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.9190	 0.6630
b	 0.9190	 0.6630
c	 0.9190	 0.6640
d	 0.9190	 0.6630
e	 0.9190	 0.6640
f	 0.9180	 0.6630
g	 0.9190	 0.6640
h	 0.9190	 0.6630
i	 0.9190	 0.6630
j	 0.9190	 0.6640
k	 0.9220	 0.6630
l	 0.9220	 0.6630
m	 0.9220	 0.6620
n	 0.9180	 0.6630
o	 0.9190	 0.6630
p	 0.9190	 0.6630
q	 0.9180	 0.6620
r	 0.9190	 0.6630
s	 0.9190	 0.6630
t	 0.9220	 0.6630
u	 0.9220	 0.6640
v	 0.9220	 0.6630
w	 0.9190	 0.6630
x	 0.9190	 0.6630
y	 0.9190	 0.6630
z	 0.9190	 0.6640