



wwPDB EM Validation Summary Report ⓘ

Sep 21, 2022 – 04:20 am BST

PDB ID : 7OZL
EMDB ID : EMD-13128
Title : CryoEM structure of human enterovirus 70 in complex with WIN51711
Authors : Fuzik, T.; Plevka, P.; Moravcova, J.
Deposited on : 2021-06-28
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.30

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 2.74 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

There are 6 unique types of molecules in this entry. The entry contains 6455 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	297	2331	1480	402	436	13	0	0

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	239	1859	1186	315	346	12	0	0

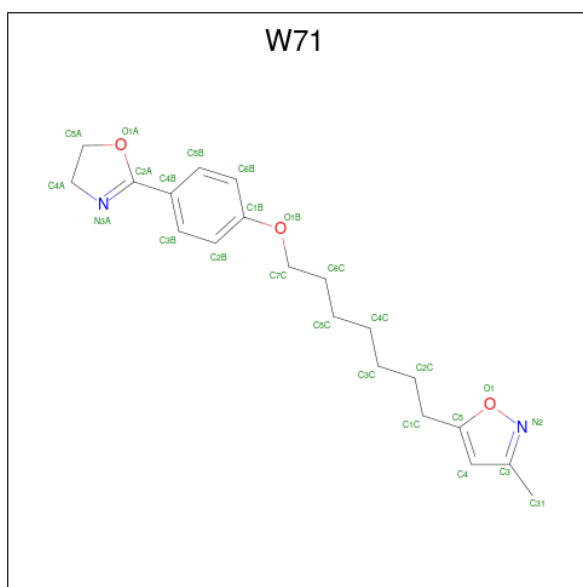
- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	243	1866	1181	311	355	19	0	0

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	40	305	195	48	62	0	0

- Molecule 5 is 5-(7-(4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (three-letter code: W71) (formula: C₂₀H₂₆N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	25	20	2	3	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	34	Total	O	0
			34	34	
6	B	19	Total	O	0
			19	19	
6	C	13	Total	O	0
			13	13	
6	D	3	Total	O	0
			3	3	

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, I	Depositor
Number of particles used	17054	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 ($e^-/\text{\AA}^2$)	48	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	12.744	Depositor
Minimum map value	-8.785	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.67	Depositor
Map size (Å)	339.52, 339.52, 339.52	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	W71	A	401	-	24,27,27	4.14	7 (29%)	29,34,34	2.18	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	W71	A	401	-	-	7/14/22/22	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	W71	C2A-N3A	16.66	1.49	1.27
5	A	401	W71	C4A-N3A	-7.94	1.33	1.47
5	A	401	W71	C5A-C4A	5.10	1.64	1.52
5	A	401	W71	O1B-C1B	3.17	1.45	1.37
5	A	401	W71	O1A-C5A	3.14	1.53	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	W71	O1A-C2A-N3A	-8.53	110.90	118.23
5	A	401	W71	O1A-C2A-C4B	3.65	120.69	115.85
5	A	401	W71	C4A-N3A-C2A	3.65	110.03	106.77
5	A	401	W71	C31-C3-N2	3.08	126.16	120.06
5	A	401	W71	C4B-C2A-N3A	-2.87	121.03	125.71

There are no chirality outliers.

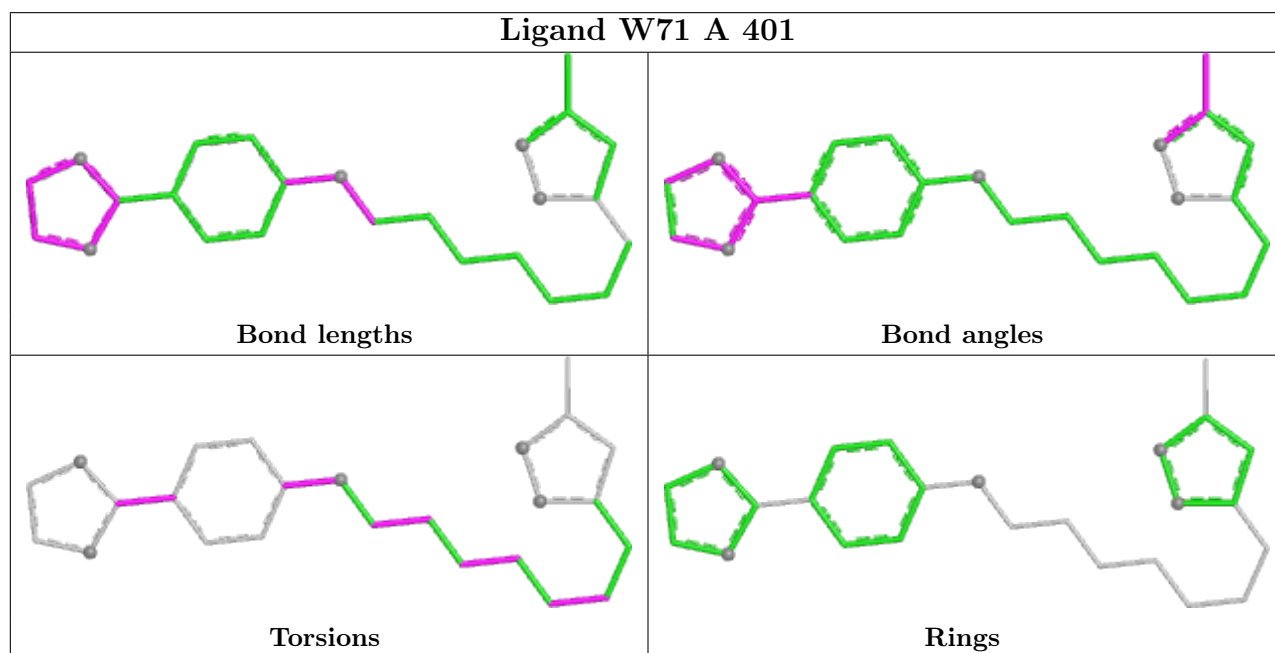
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	W71	C5C-C6C-C7C-O1B
5	A	401	W71	C1C-C2C-C3C-C4C
5	A	401	W71	C2B-C1B-O1B-C7C
5	A	401	W71	C6B-C1B-O1B-C7C
5	A	401	W71	C3C-C4C-C5C-C6C

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

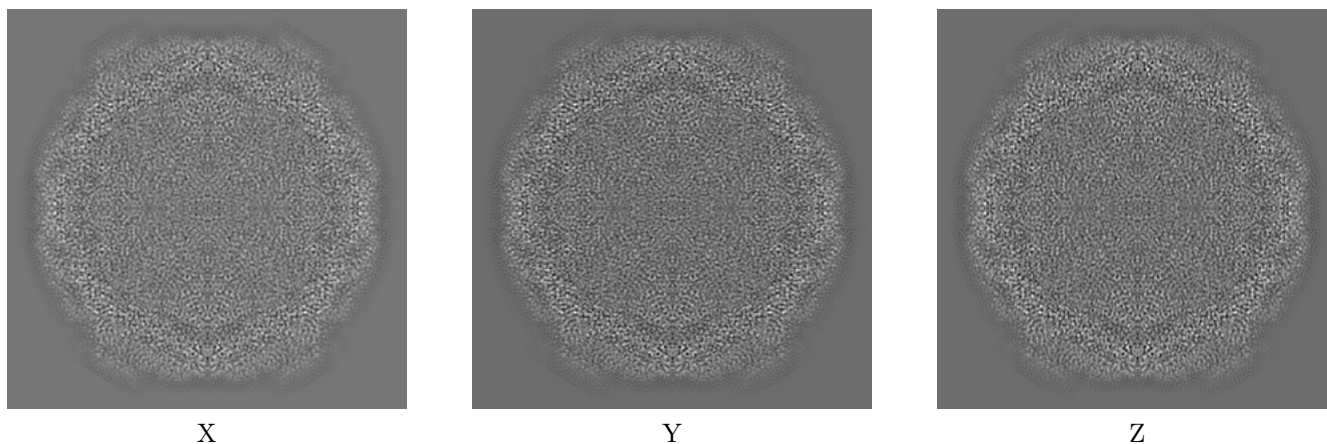
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13128. These allow visual inspection of the internal detail of the map and identification of artifacts.

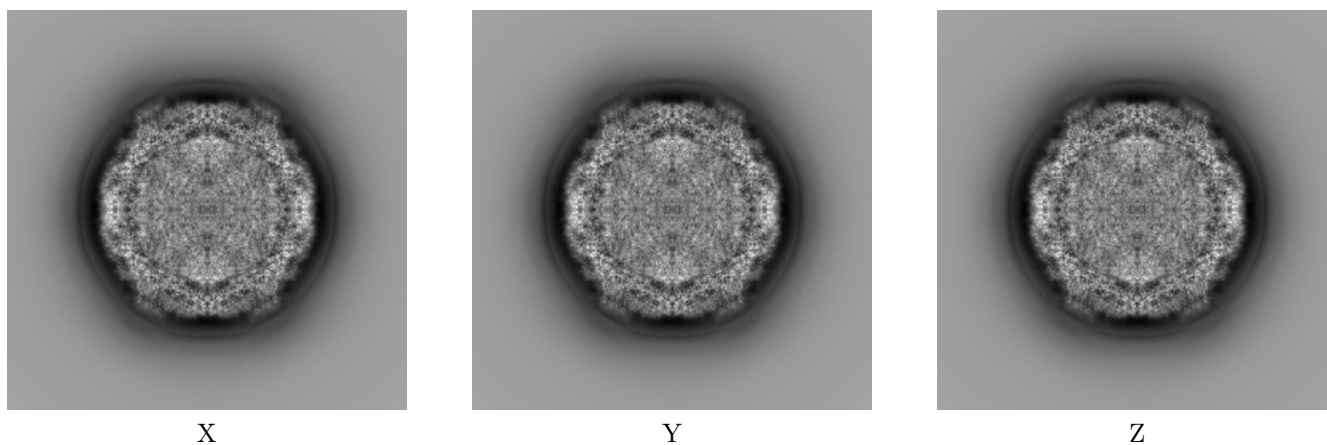
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

5.1.1 Primary map



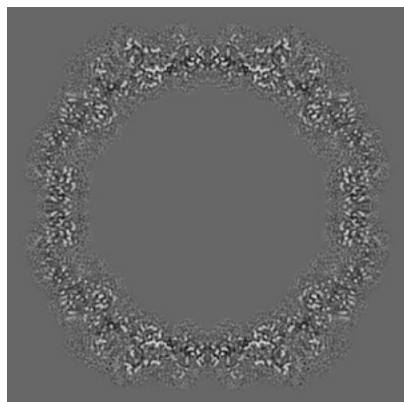
5.1.2 Raw map



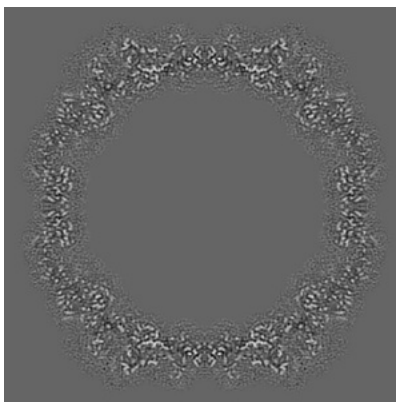
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

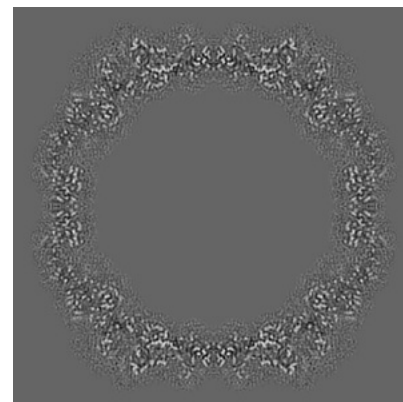
5.2.1 Primary map



X Index: 160

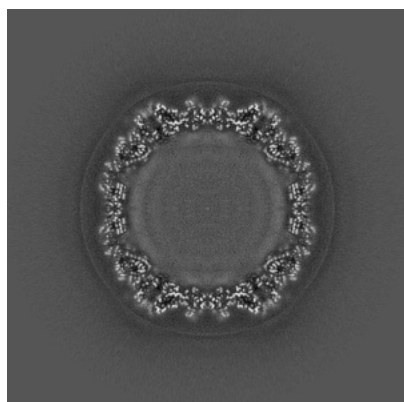


Y Index: 160

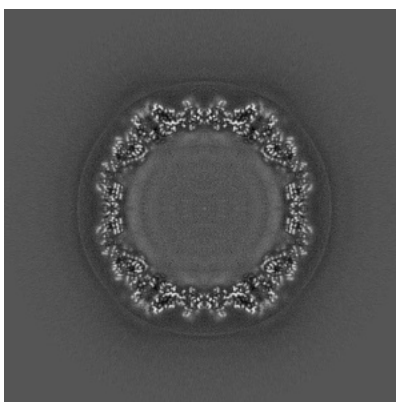


Z Index: 160

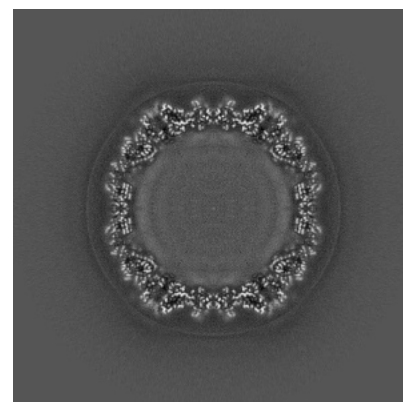
5.2.2 Raw map



X Index: 256



Y Index: 256

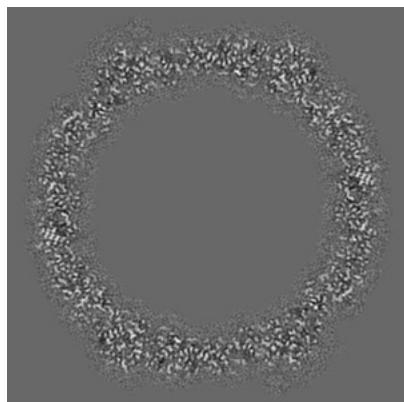


Z Index: 256

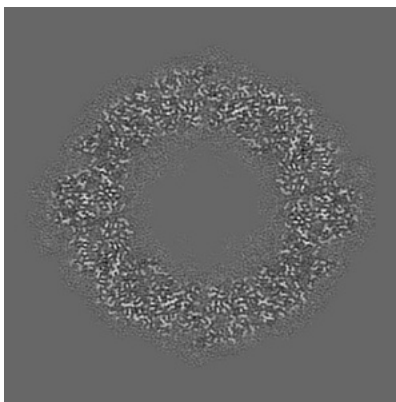
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

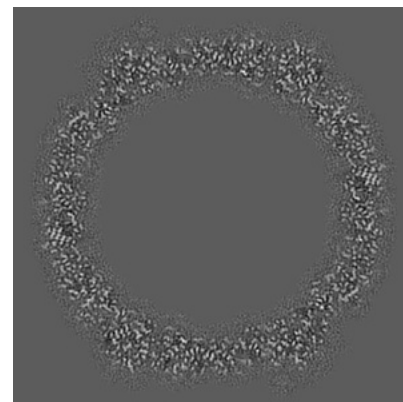
5.3.1 Primary map



X Index: 145

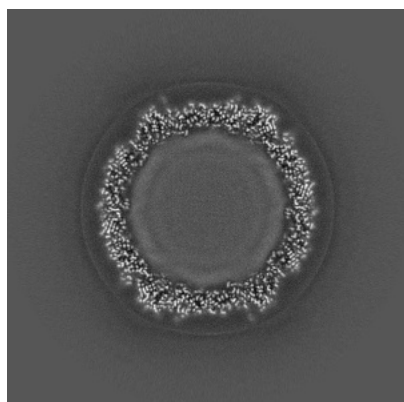


Y Index: 243

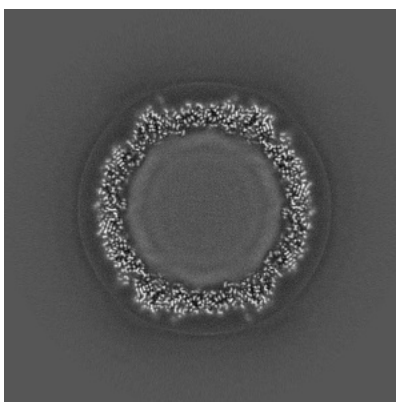


Z Index: 145

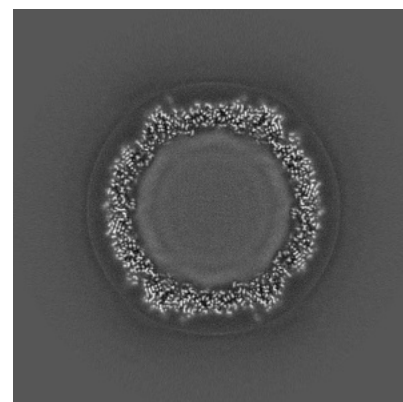
5.3.2 Raw map



X Index: 240



Y Index: 240

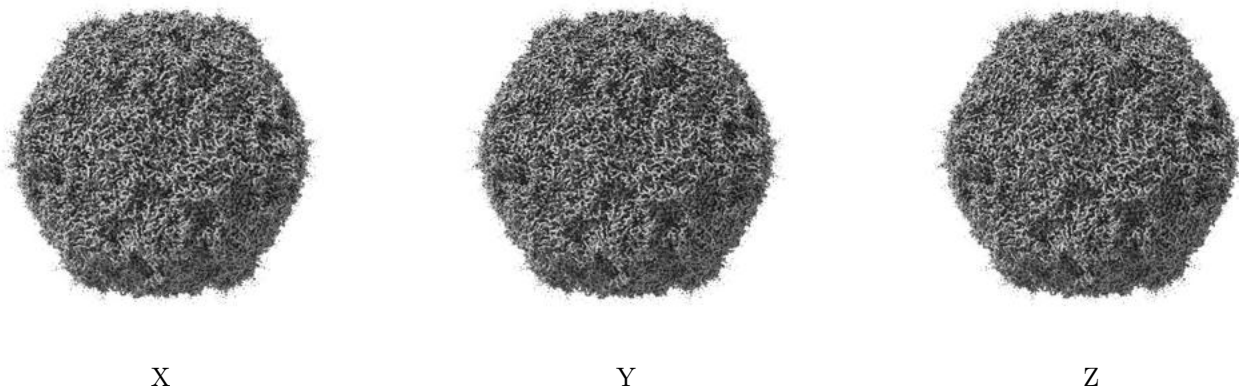


Z Index: 240

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

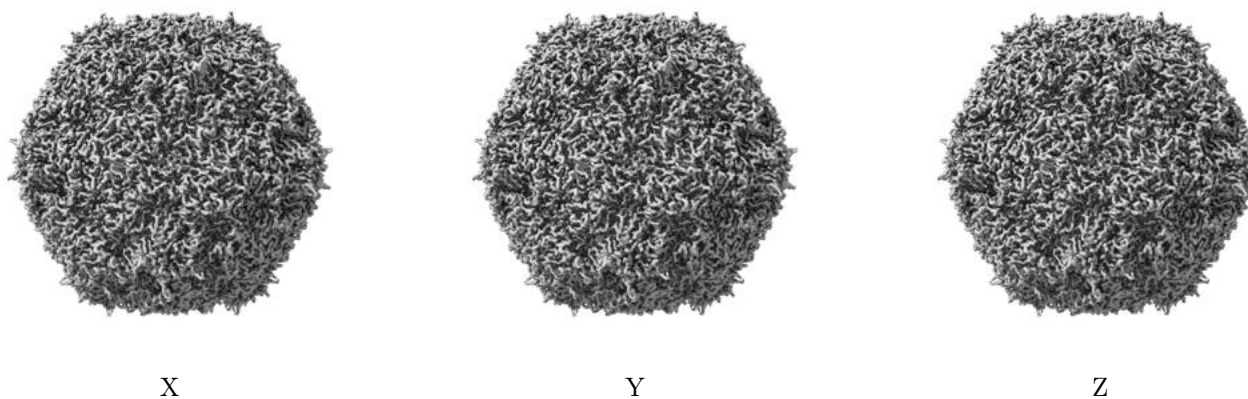
5.4 Orthogonal surface views [i](#)

5.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.67. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.4.2 Raw map



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.

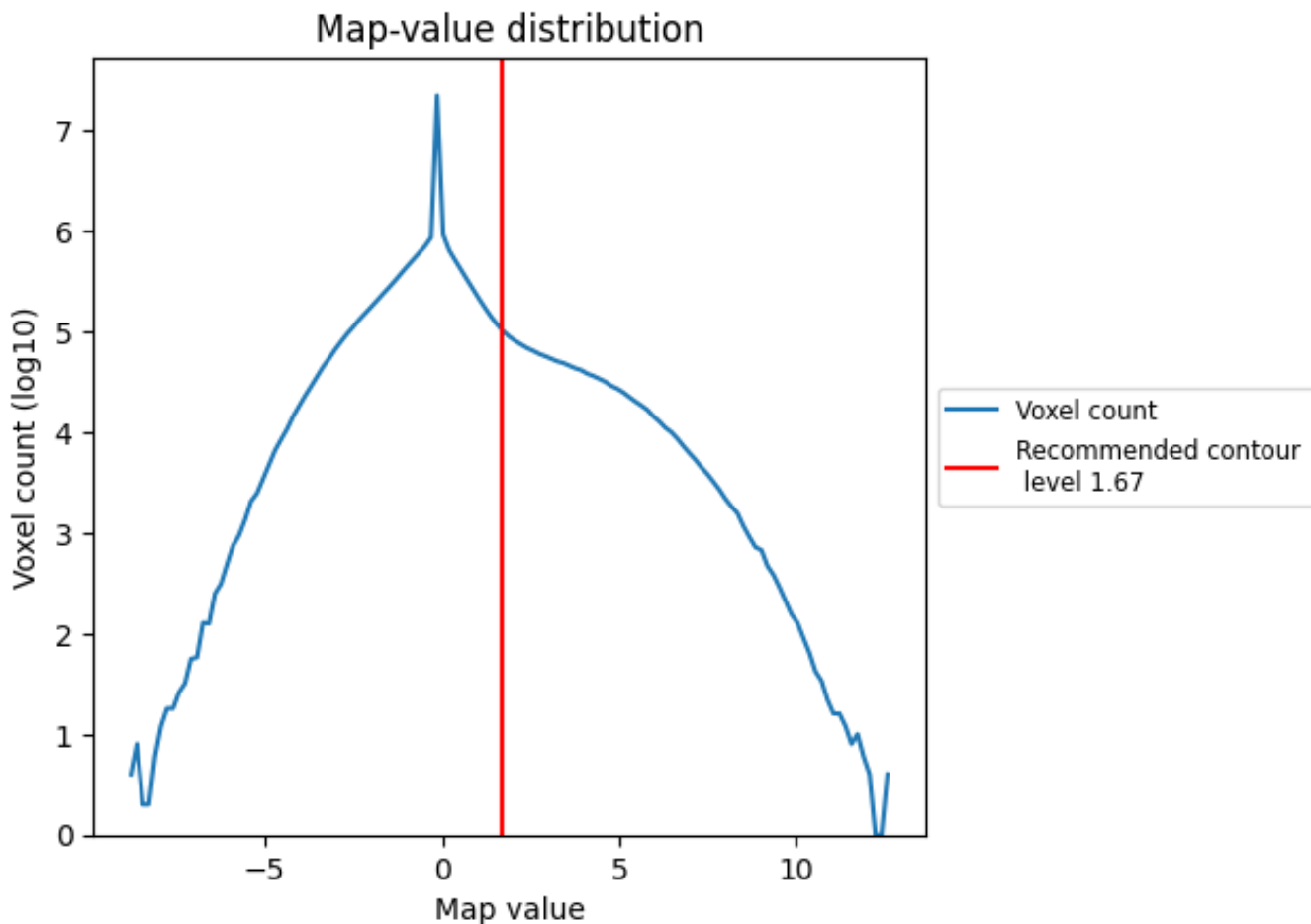
5.5 Mask visualisation [i](#)

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

6 Map analysis [i](#)

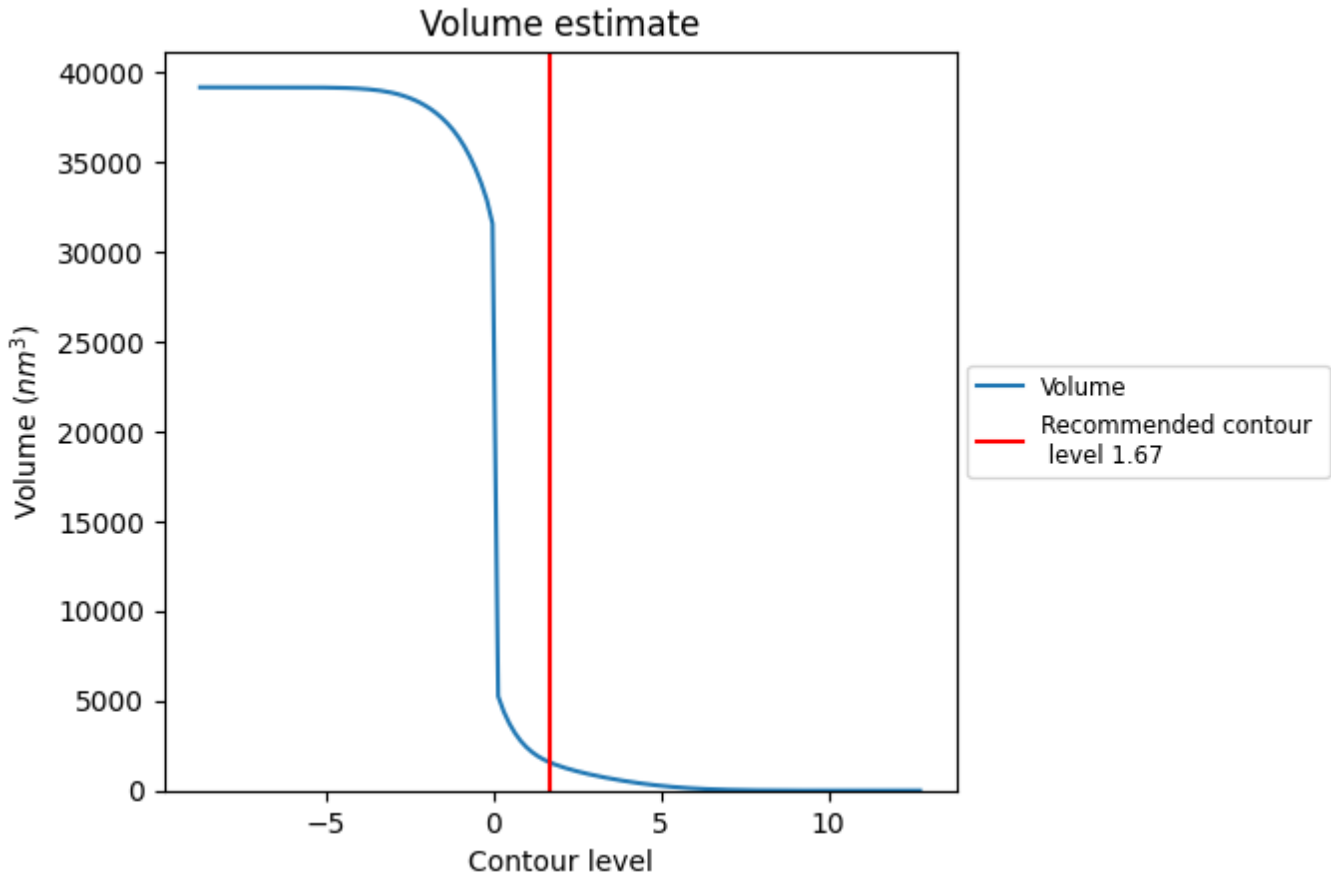
This section contains the results of statistical analysis of the map.

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.

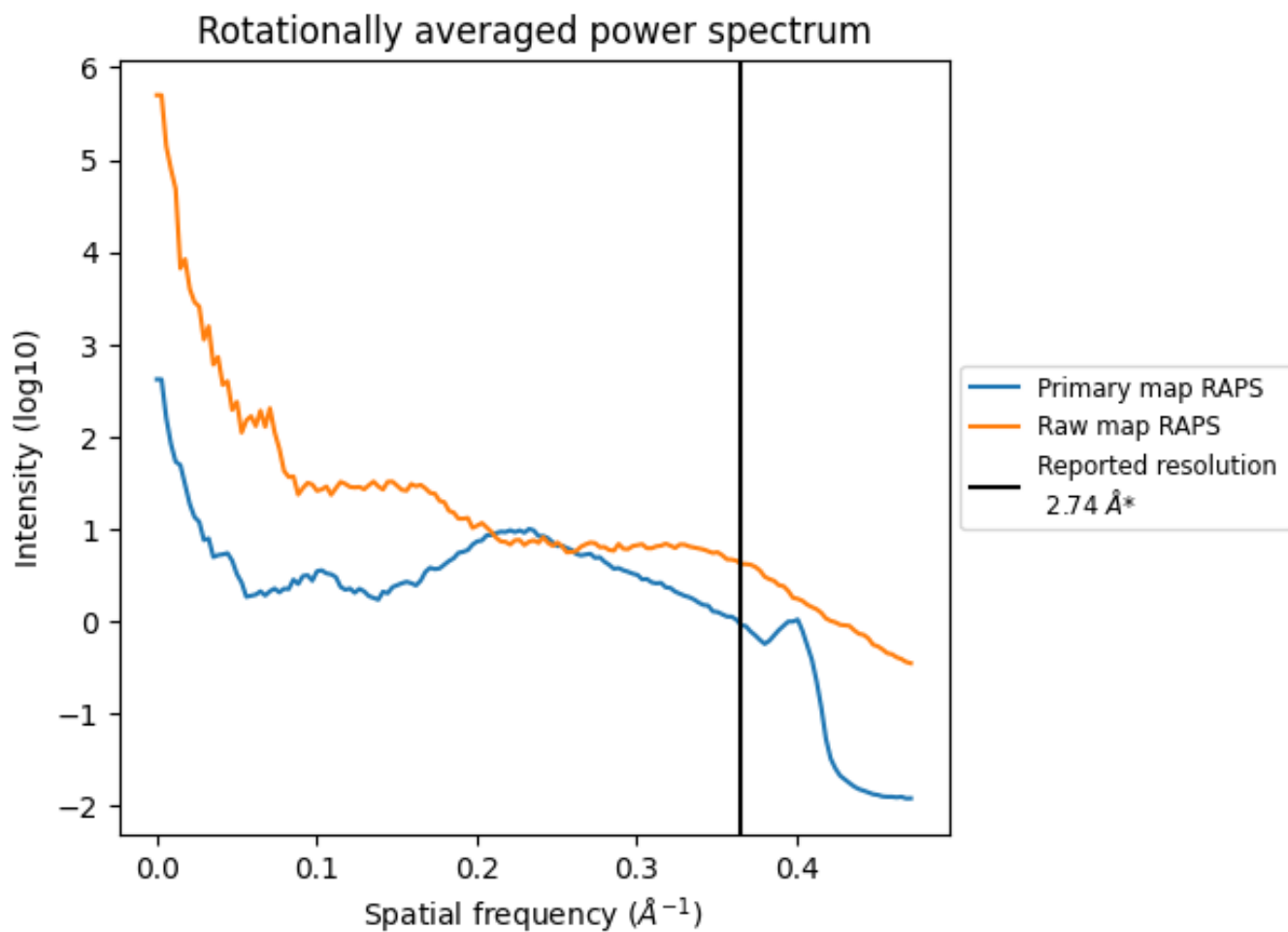
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 1571 nm³; this corresponds to an approximate mass of 1419 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

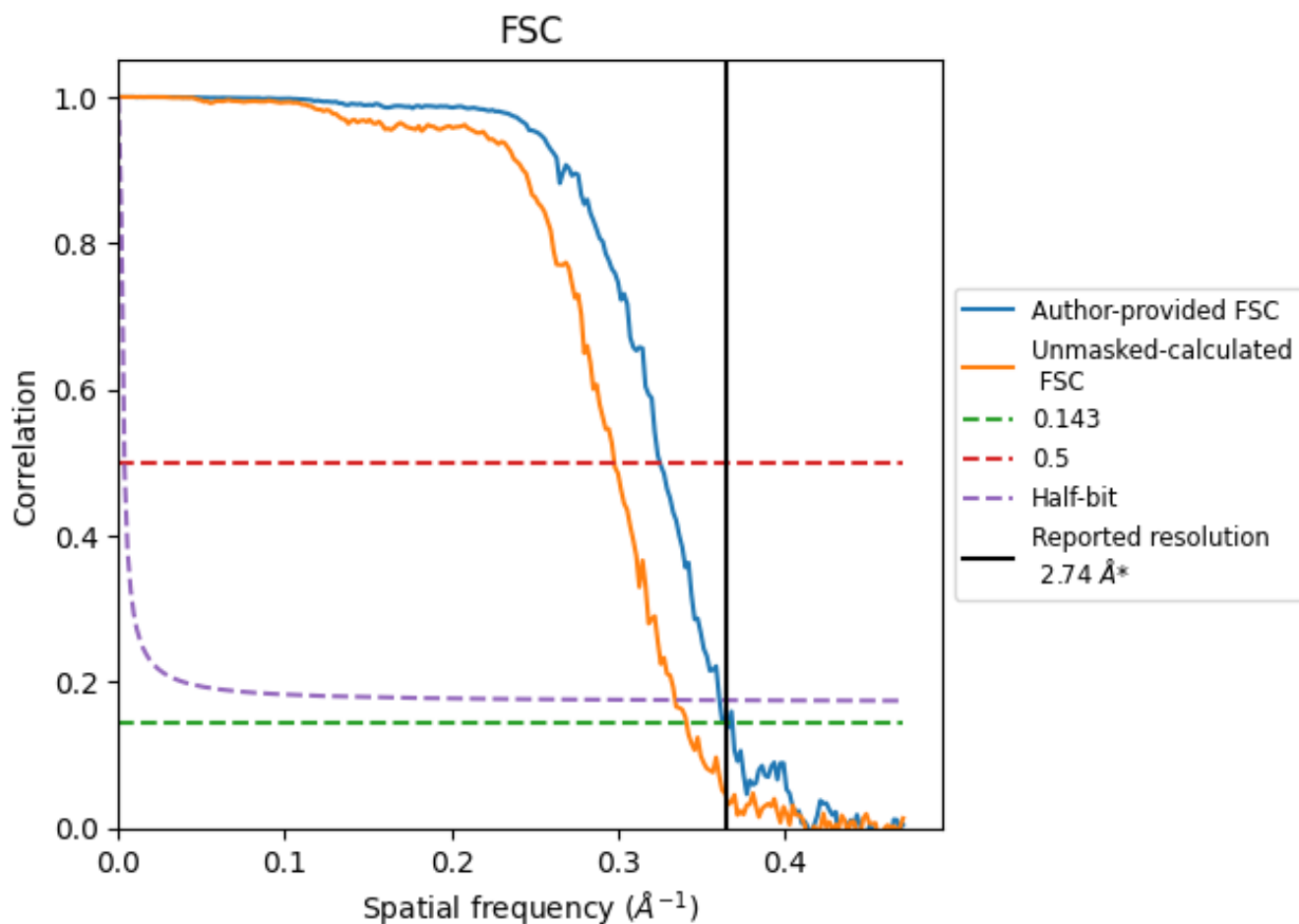


*Reported resolution corresponds to spatial frequency of 0.365 \AA^{-1}

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 0.365 Å⁻¹

7.2 Resolution estimates [i](#)

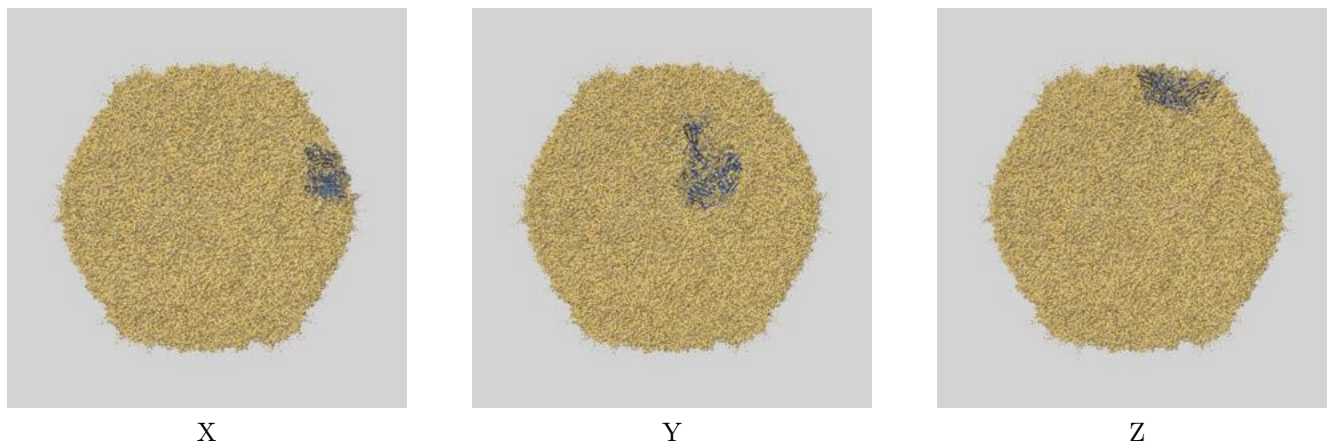
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	3.08	2.77
Unmasked-calculated*	2.93	3.36	2.99

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

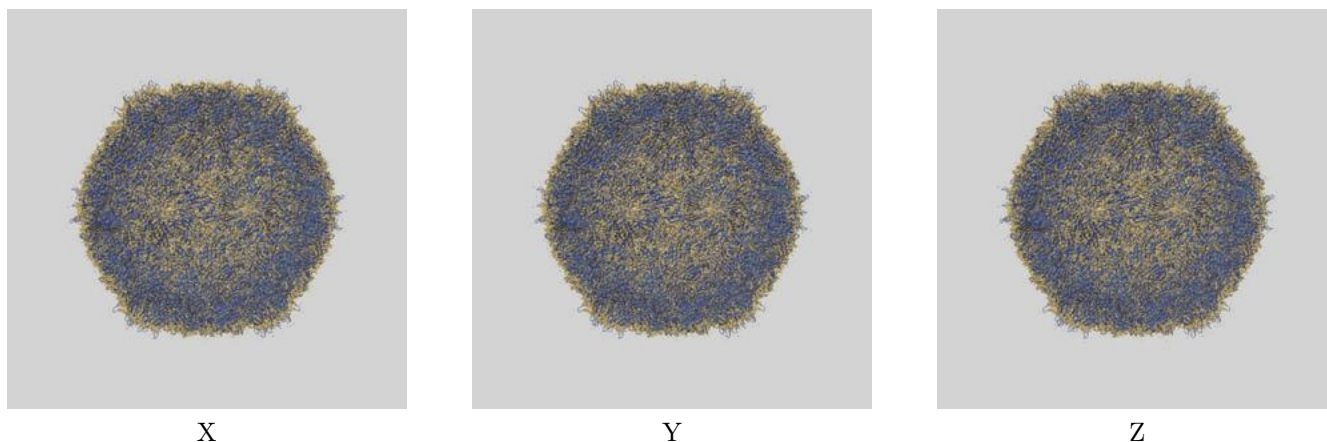
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13128 and PDB model 7OZL. Per-residue inclusion information can be found in section ?? on page ??.

8.0.1 Map-model overlay [i](#)

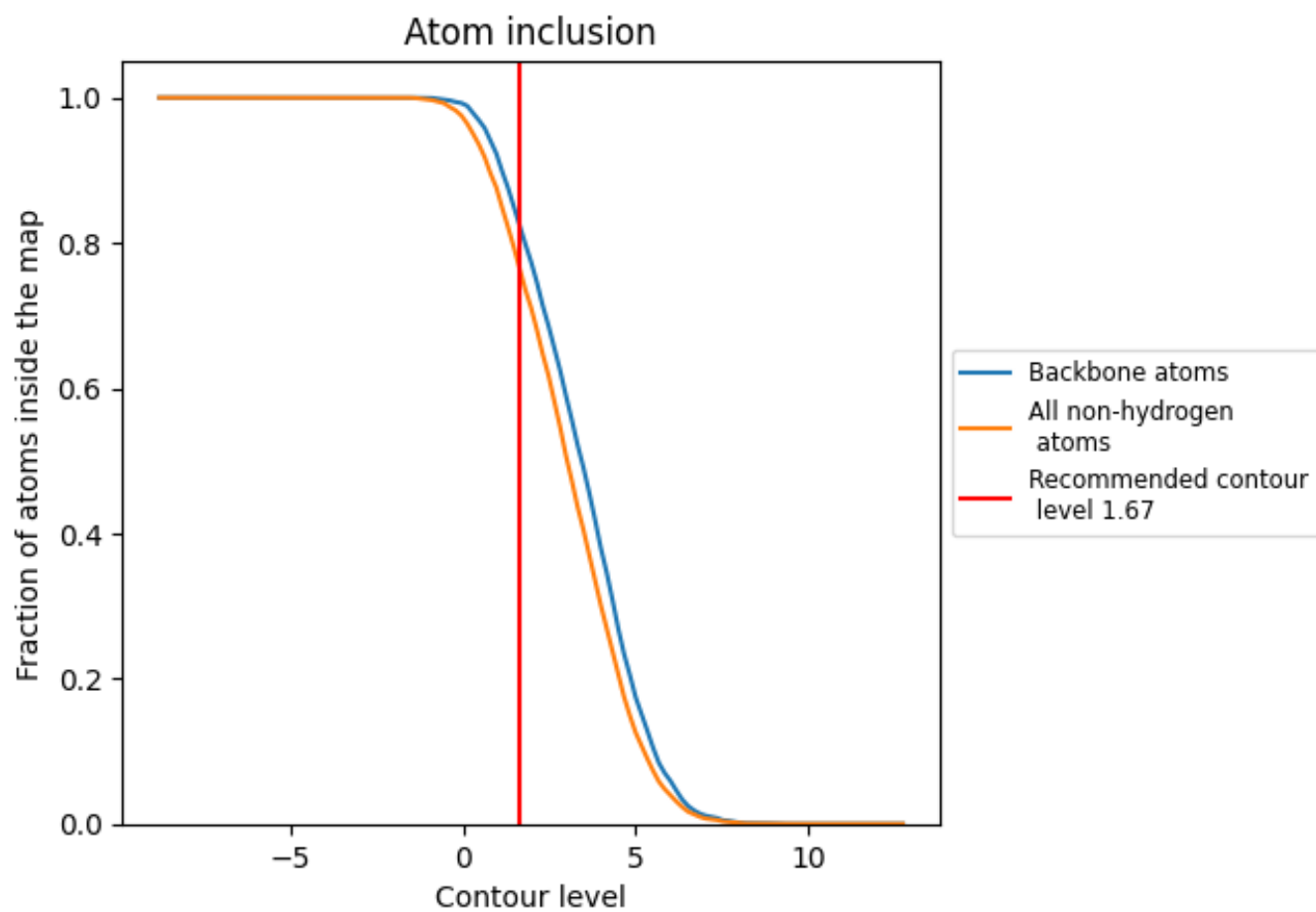


8.0.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.67 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.

8.1 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.