wwPDB EM Validation Summary Report (i)

Oct 7, 2023 – 01:16 PM EDT

PDB ID	:	7U0F
EMDB ID	:	EMD-26257
Title	:	HIV-1 Rev in complex with tubulin
Authors	:	Eren, E.
Deposited on	:	2022-02-18
Resolution	:	3.53 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.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 (i)

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

The reported resolution of this entry is 3.53 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 are 3 unique types of molecules in this entry. The entry contains 16569 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 Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3419	2161	581	656	21		
1	C	450	Total	C	N	O	S	0	0
			3500	2208	589	682	21		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	428	Total	C	N	O	S	0	0
			3349	2100	575	648	26		
2	D	444	Total	C	N	O	S	0	0
			3482	2178	592	686	26		

- Molecule 3 is a protein called Protein Rev.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	55	Total	C	N	O	0	0
			472	291	103	78		
3	F	55	Total	C	N	O	0	0
			475	294	103	78		
3	G	55	Total	C	N	O	0	0
			475	294	103	78		
3	H	55	Total	C	N	O	0	0
			475	294	103	78		
3	I	55	Total	C	N	O	0	0
			475	294	103	78		
3	J	51	Total	C	N	O	0	0
			447	276	99	72		

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

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C15	Depositor
Number of particles used	34534	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 ($e^-/Å^2$)	73	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	45.739	Depositor
Minimum map value	-28.933	Depositor
Average map value	0.101	Depositor
Map value standard deviation	1.211	Depositor
Recommended contour level	2.7	Depositor
Map size (Å)	556.5, 556.5, 556.5	wwPDB
Map dimensions	525, 525, 525	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

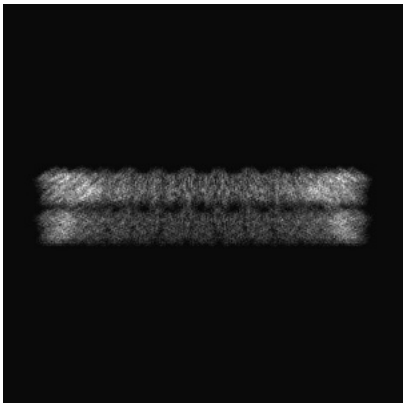
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-26257. These allow visual inspection of the internal detail of the map and identification of artifacts.

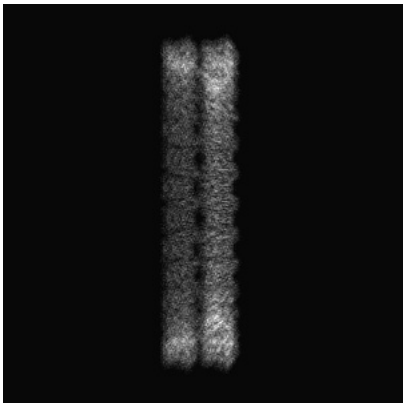
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

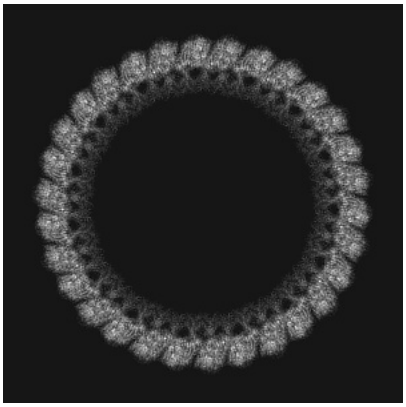
5.1.1 Primary map



X



Y

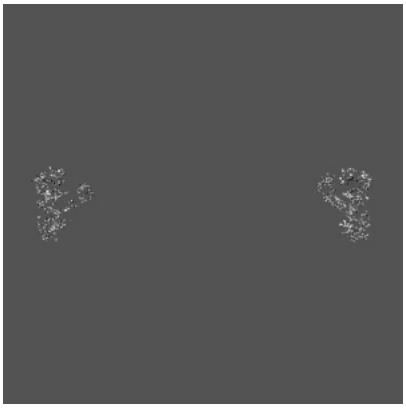


Z

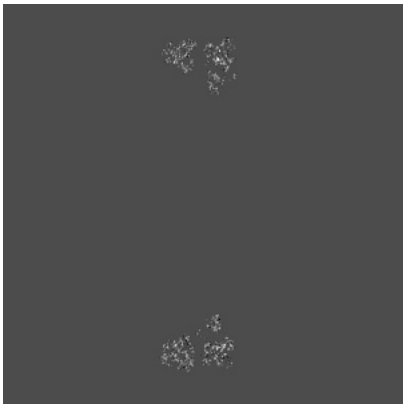
The images above show the map projected in three orthogonal directions.

5.2 Central slices

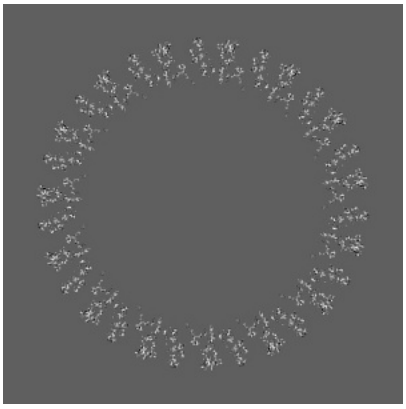
5.2.1 Primary map



X Index: 262



Y Index: 262



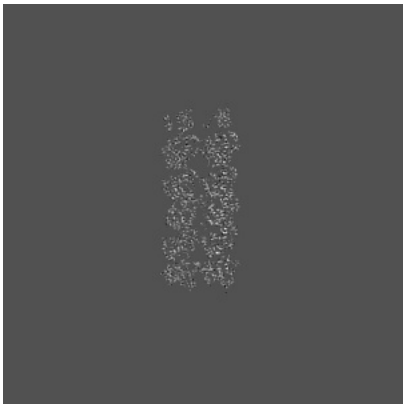
Z Index: 262

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

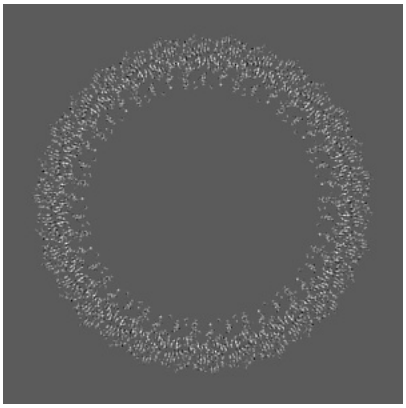
5.3 Largest variance slices (i)

5.3.1 Primary map

X Index: 81



Y Index: 446

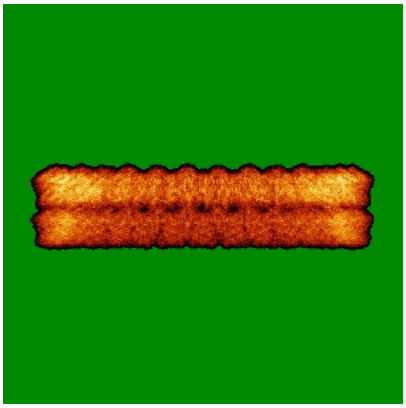


Z Index: 291

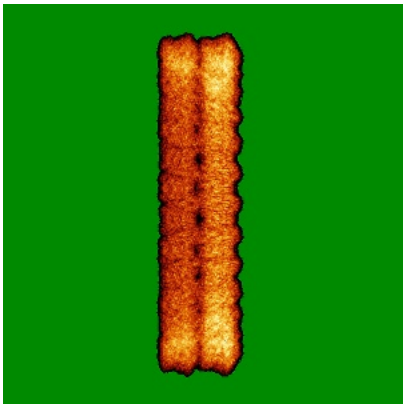
The images above show the largest variance slices of the map in three orthogonal directions.

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

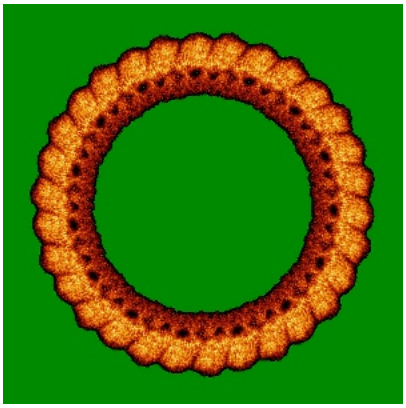
5.4.1 Primary map



X



Y



Z

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

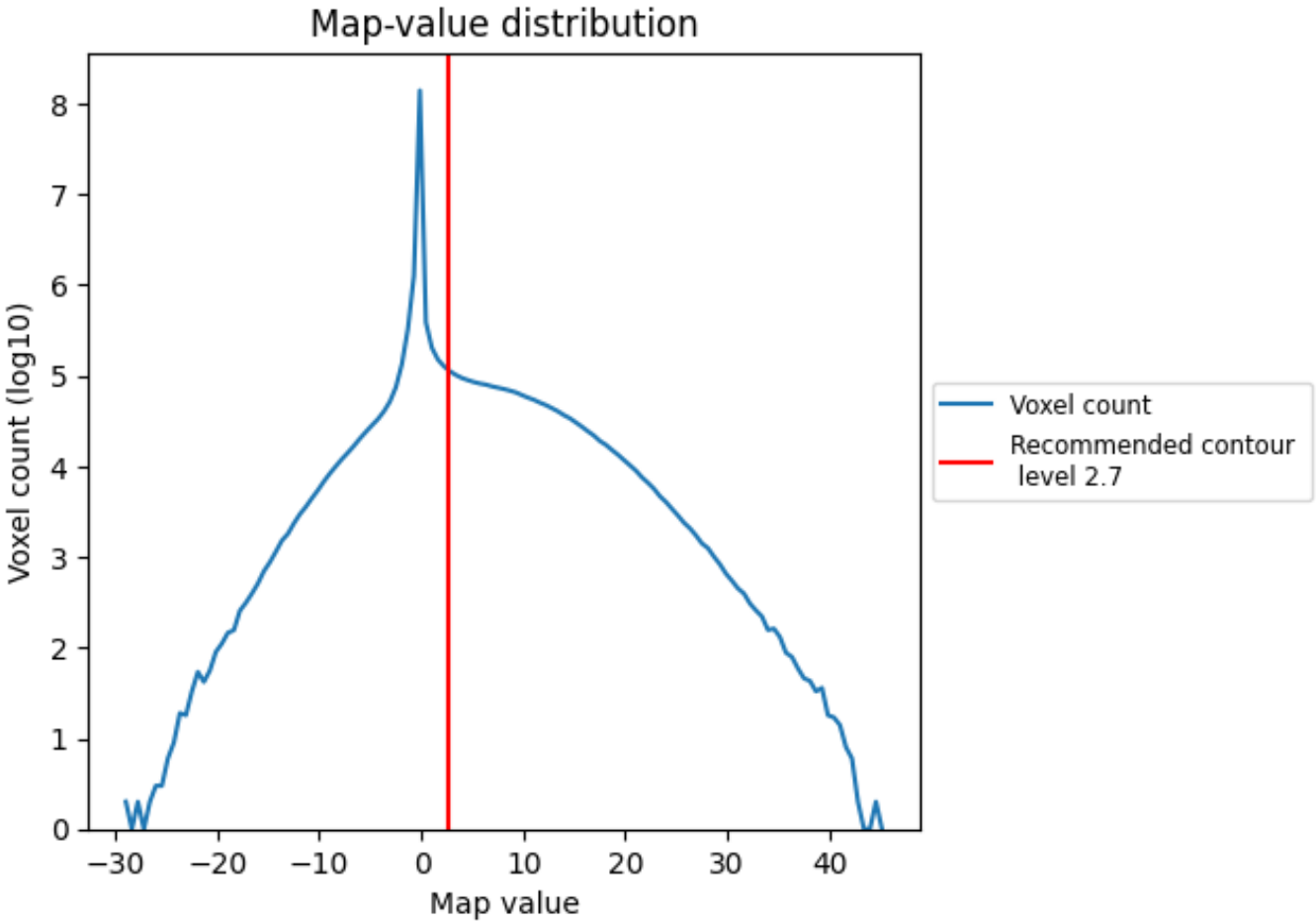
5.6 Mask visualisation (i)

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

6 Map analysis

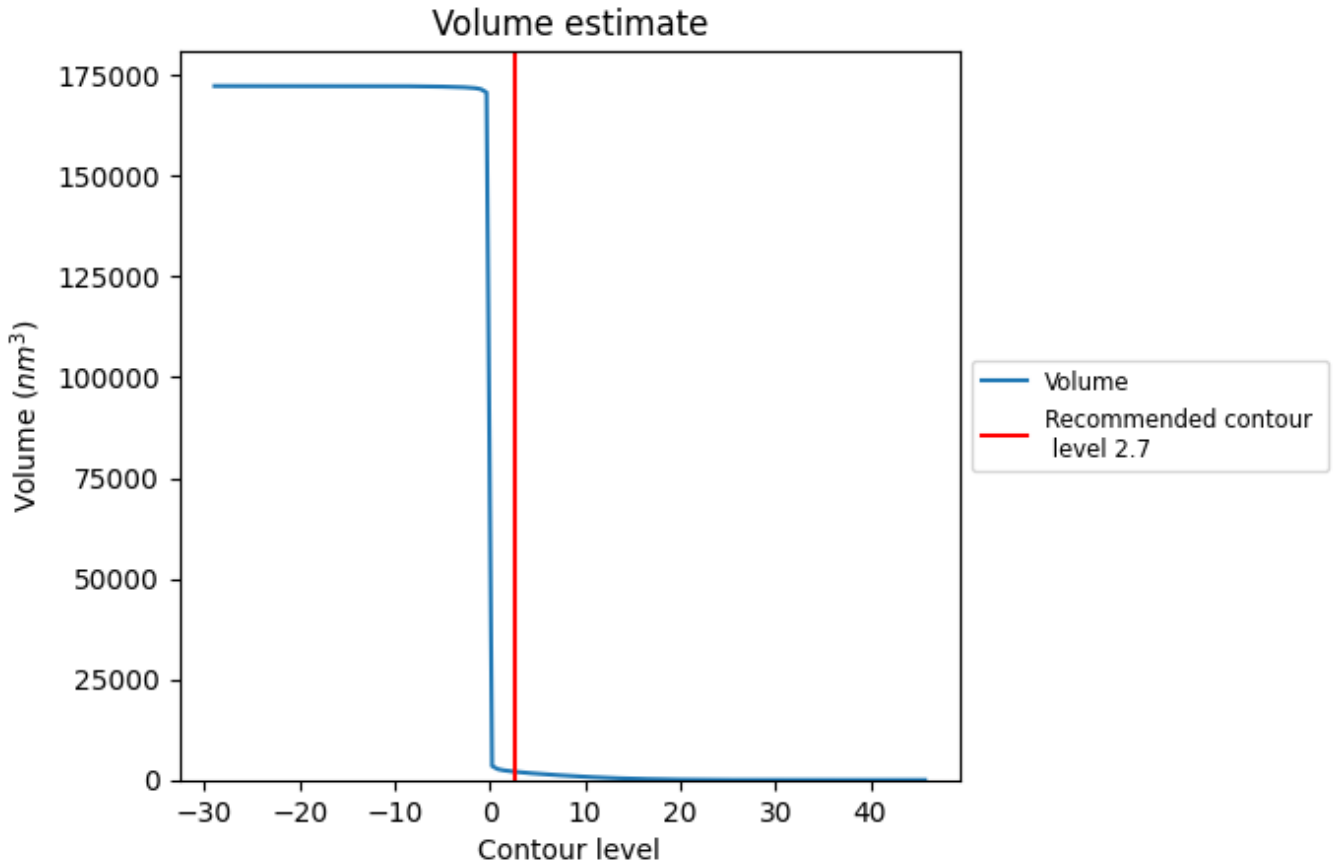
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



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.

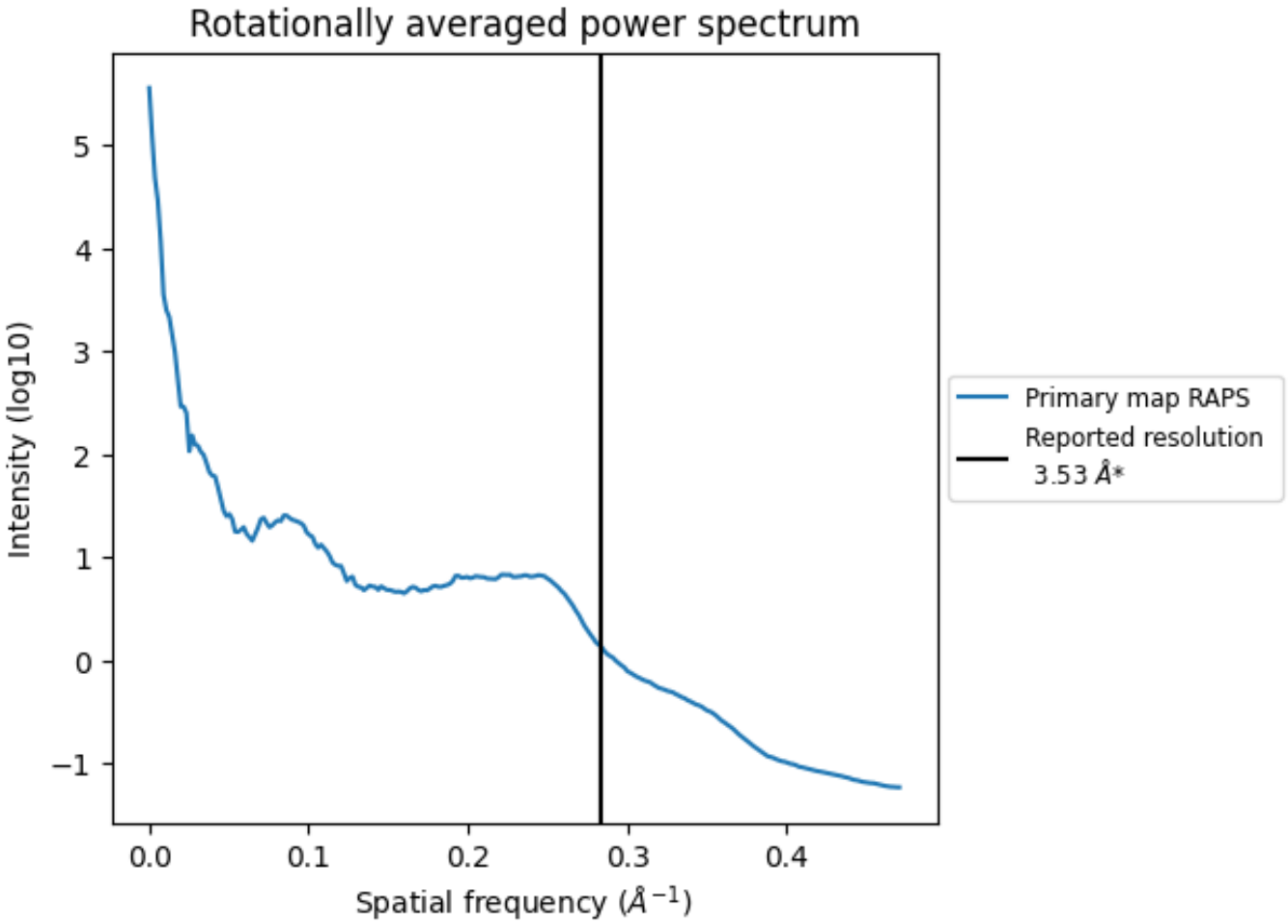
6.2 Volume estimate



The volume at the recommended contour level is 2024 nm^3; this corresponds to an approximate mass of 1828 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)

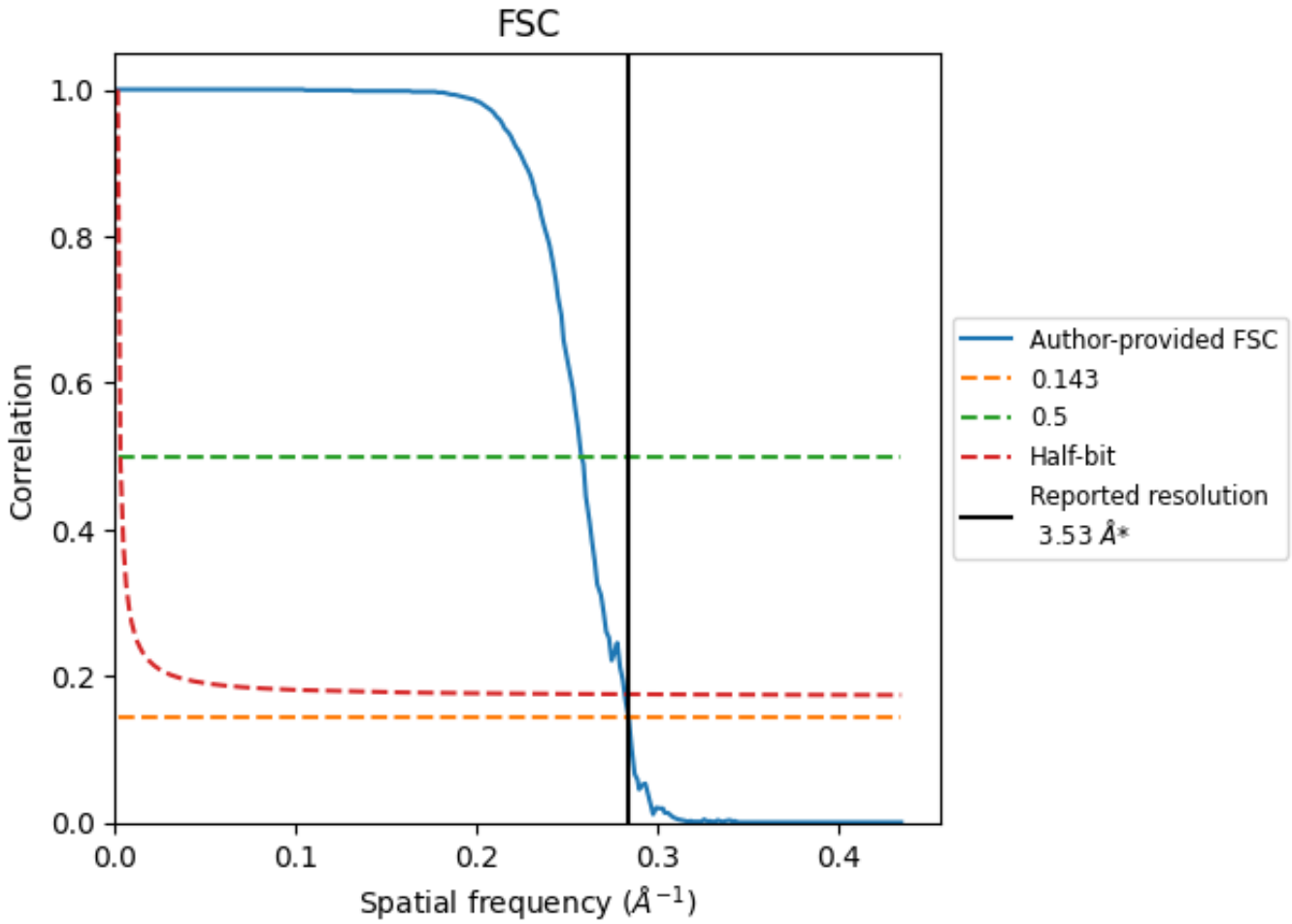


*Reported resolution corresponds to spatial frequency of 0.283 Å^{-1}

7 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.283 Å^{-1}

7.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.52	3.88	3.55
Unmasked-calculated*	-	-	-

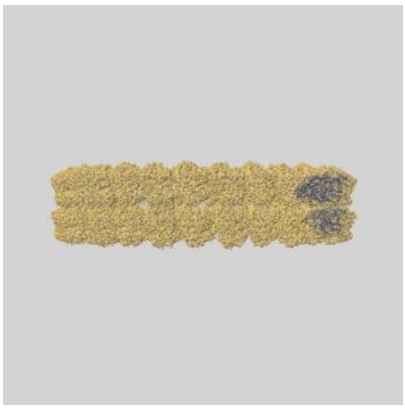
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

8 Map-model fit

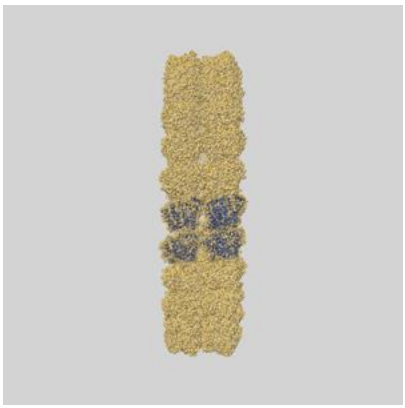
This section contains information regarding the fit between EMDB map EMD-26257 and PDB model 7U0F. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlays

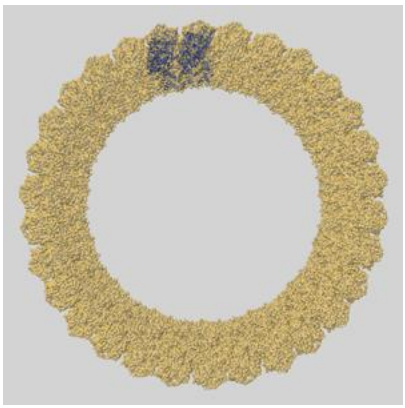
8.1.1 Map-model overlay



X

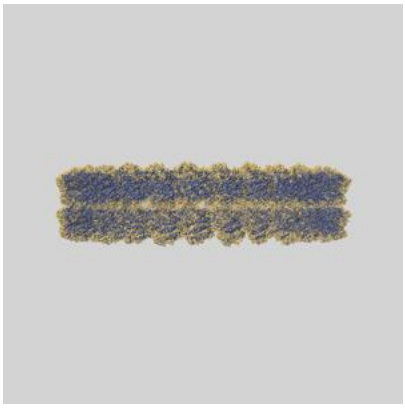


Y

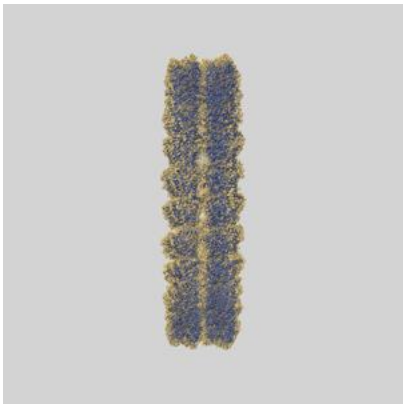


Z

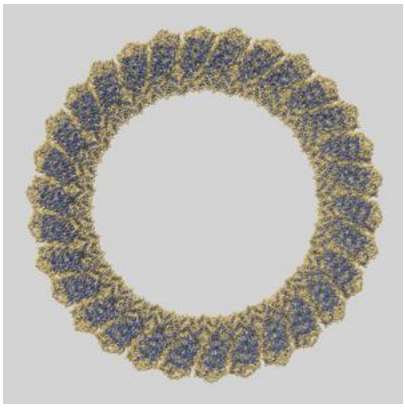
8.1.2 Map-model assembly overlay



X



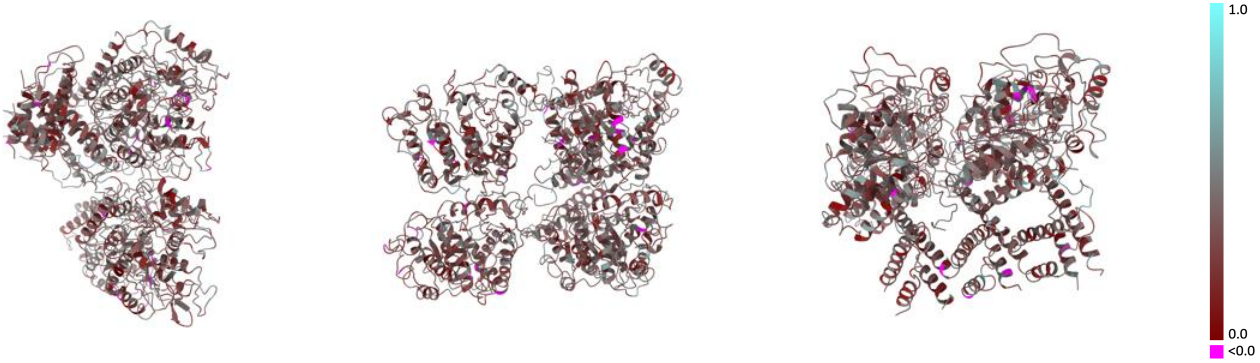
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.7 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.

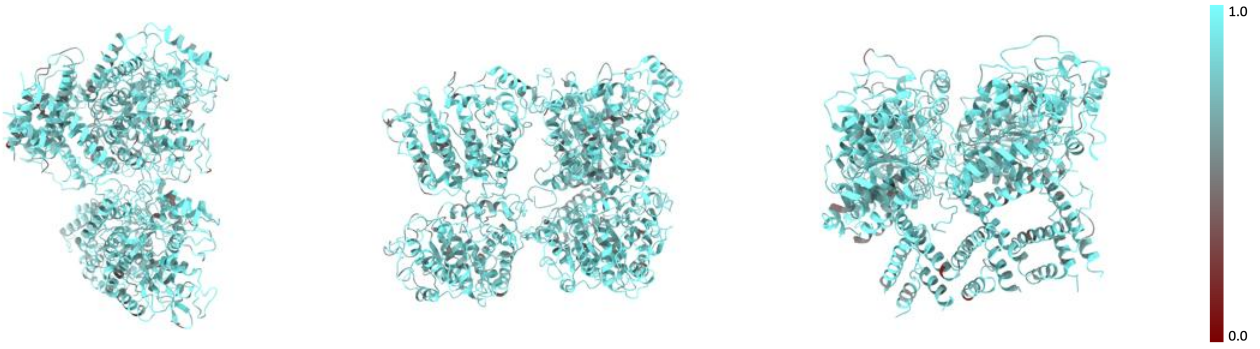
8.2 Q-score mapped to coordinate model (i)



X Y Z

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.

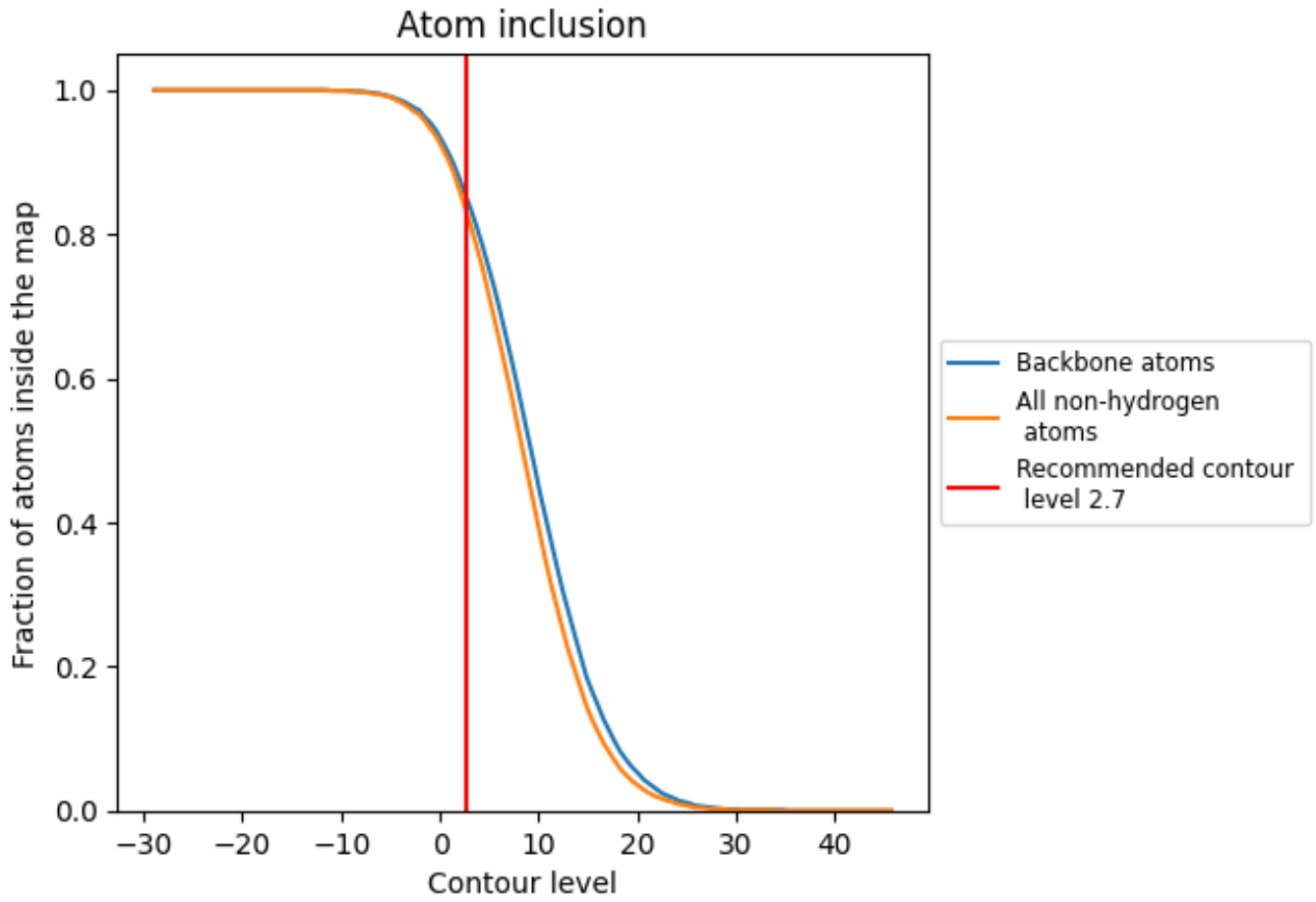
8.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.7).

8.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.3440
A	0.8420	0.3540
B	0.8450	0.3530
C	0.8170	0.3340
D	0.8380	0.3470
E	0.8290	0.3320
F	0.7340	0.3020
G	0.8570	0.3580
H	0.7860	0.3350
I	0.8370	0.3350
J	0.8170	0.3230