



wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 06:50 PM EDT

PDB ID : 8USN
EMDB ID : EMD-42509
Title : Intracellular cryo-tomography structure of EBOV nucleocapsid at 8.9 Angstrom
Authors : Watanabe, R.; Zyla, D.; Saphire, E.O.
Deposited on : 2023-10-27
Resolution : 8.90 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:

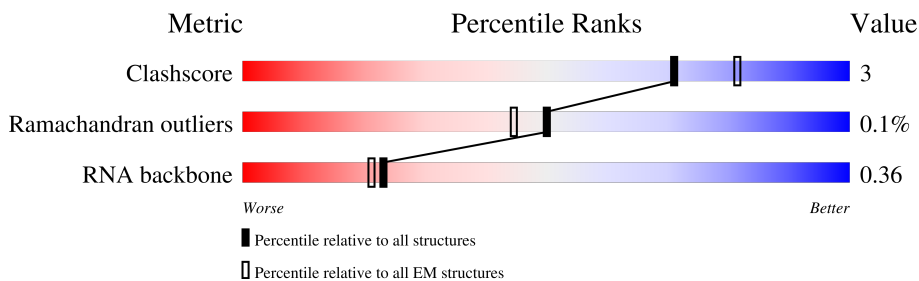
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 8.90 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	210492	15764
Ramachandran outliers	207382	16835
RNA backbone	6643	2191

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 $\leq 5\%$. 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	739	
1	B	739	
1	E	739	
2	C	6	
2	D	6	
3	I	251	
3	J	251	
4	F	340	

Continued on next page...

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Mol	Chain	Length	Quality of chain
4	K	340	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '35%' and a grey segment on the right labeled '65%'. There is a small red square at the beginning of the green segment and a small black dot at the end of the grey segment.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6954 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 Nucleoprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	387	Total	C	N	O	0	0
			1548	774	387	387		
1	B	387	Total	C	N	O	0	0
			1548	774	387	387		
1	E	318	Total	C	N	O	0	0
			1272	636	318	318		

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C	6	Total	C	N	O	P	0	0
			129	60	30	34	5		
2	D	6	Total	C	N	O	P	0	0
			129	60	30	34	5		

- Molecule 3 is a protein called Membrane-associated protein VP24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	I	217	Total	C	N	O	0	0
			868	434	217	217		
3	J	217	Total	C	N	O	0	0
			868	434	217	217		

- Molecule 4 is a protein called Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	K	120	Total	C	N	O	0	0
			480	240	120	120		
4	F	28	Total	C	N	O	0	0
			112	56	28	28		

THR VAL
ASP PRO
GLN GLN
SER SER
VAL VAL
ARG ARG
GLU GLU
ALA ALA
ASN ASN
LEU LEU
SER SER
THR THR
SER SER
LEU LEU
THR THR
GLU GLU
GLU GLU
SER SER
ASN ASN
PHE PHE
GLY GLY
LYS LYS
PRO PRO
ILE ILE
ASP ASP
ILE ILE
SER SER
THR THR
ALA ALA
LYS LYS
ASP ASP
VAL VAL
LEU LEU
ARG ARG
ILE ILE
ASN ASN
PHE PHE
ILE ILE
MET MET
TYR TYR
ASP ASP
ALA ALA
HIS HIS
LEU LEU
PRO PRO
GLY GLY
PHE PHE
GLY GLY
HIS HIS
THR THR
ALA ALA
PHE PHE
HIS HIS
GLN GLN
LEU LEU
VAL VAL
GLN GLN
VAL VAL
CYS CYS
LYS LYS
LEU LEU
GLY GLY

LYS ASP
SER SER
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PRO PRO
LEU LEU
ASP ASP
ILE ILE
HIS HIS
PHE PHE
ALA ALA
ASN ASN
GLU GLU
PHE PHE
GLN GLN
ALA ALA
SER SER
THR THR
LEU LEU
PHE PHE
GLU GLU
GLY GLY
ASP ASP
SER SER
PRO PRO
GLN GLN
CYS CYS
ALA ALA
LEU LEU
ILE ILE
ASP ASP
ILE ILE
GLN GLN
ILE ILE
SER SER
THR THR
ALA ALA
LYS LYS
ASP ASP
VAL VAL
PRO PRO
ARG ARG
ILE ILE
ASN ASN
PHE PHE
ILE ILE
GLN GLN
SER SER
PHE PHE
HIS HIS
GLY GLY
LEU LEU
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PRO PRO
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VAL VAL
ARG ARG
ALA ALA
CYS CYS
LYS LYS
LEU LEU
SER SER

LEU ARG
PRO PRO
VAL VAL
PRO PRO
SER SER
PRO PRO
LYS LYS
ILE ILE
ASP ASP
ARG ARG
GLY GLY
TRP TRP
VAL VAL
CYS CYS
PHE PHE
VAL VAL
GLN GLN
LEU LEU
GLN GLN
ASN ASN
GLY GLY
LYS LYS
THR THR
LEU LEU
GLY GLY
LEU LEU
LYS LYS
ILE ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	28000	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 ($e^-/\text{\AA}^2$)	160	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0037	Depositor
Map size (\AA)	481.37598, 481.37598, 481.37598	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.149, 2.149, 2.149	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1547	0.42	0/1932
1	B	0.26	0/1547	0.42	0/1932
1	E	0.25	0/1271	0.44	0/1587
2	C	0.50	0/146	0.72	0/226
2	D	0.50	0/146	0.73	0/226
3	I	0.26	0/867	0.45	0/1082
3	J	0.26	0/867	0.45	0/1082
4	F	0.23	0/111	0.46	0/137
4	K	0.26	0/479	0.44	0/597
All	All	0.27	0/6981	0.46	0/8801

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
4	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	80	PHE	Peptide
4	F	27	VAL	Peptide

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	1548	0	428	3	0
1	B	1548	0	428	3	0
1	E	1272	0	353	4	0
2	C	129	0	68	4	0
2	D	129	0	68	4	0
3	I	868	0	230	6	0
3	J	868	0	230	5	0
4	F	112	0	31	0	0
4	K	480	0	125	1	0
All	All	6954	0	1961	29	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 3.

The worst 5 of 29 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)
3:J:23:LEU:O	3:J:28:ASN:N	2.21	0.73
3:I:23:LEU:O	3:I:28:ASN:N	2.21	0.72
3:J:27:CYS:O	3:J:134:PHE:N	2.25	0.69
3:I:27:CYS:O	3:I:134:PHE:N	2.25	0.68
3:I:66:ALA:O	3:I:70:SER:N	2.27	0.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/739 (52%)	348 (90%)	36 (9%)	1 (0%)	37	73
1	B	385/739 (52%)	348 (90%)	36 (9%)	1 (0%)	37	73
1	E	316/739 (43%)	299 (95%)	17 (5%)	0	100	100
3	I	215/251 (86%)	198 (92%)	17 (8%)	0	100	100
3	J	215/251 (86%)	198 (92%)	17 (8%)	0	100	100
4	F	26/340 (8%)	21 (81%)	5 (19%)	0	100	100
4	K	118/340 (35%)	113 (96%)	5 (4%)	0	100	100
All	All	1660/3399 (49%)	1525 (92%)	133 (8%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	B	138	PRO

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](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	5/6 (83%)	0	0
2	D	5/6 (83%)	0	0
All	All	10/12 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 oligosaccharides 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.

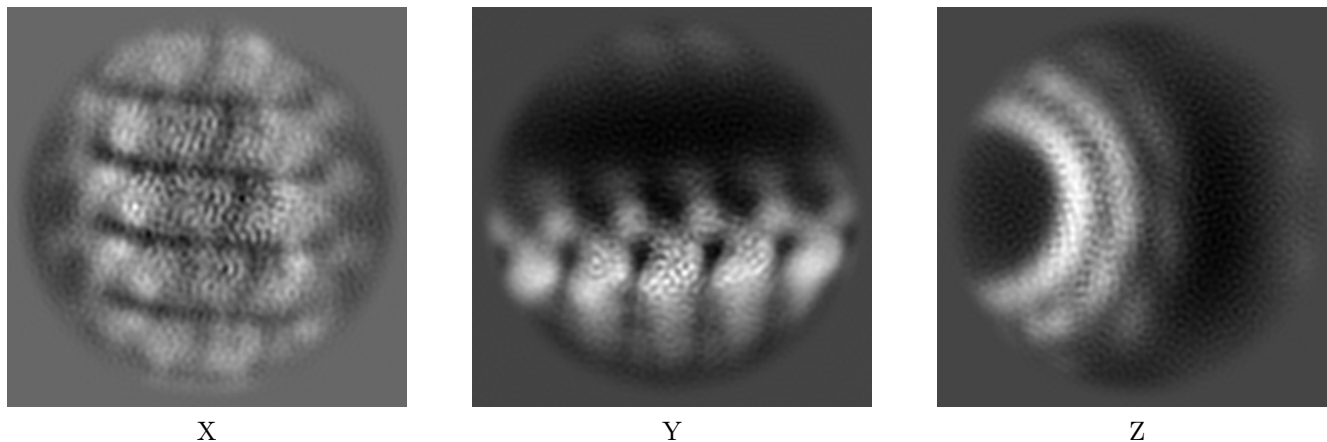
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42509. These allow visual inspection of the internal detail of the map and identification of artifacts.

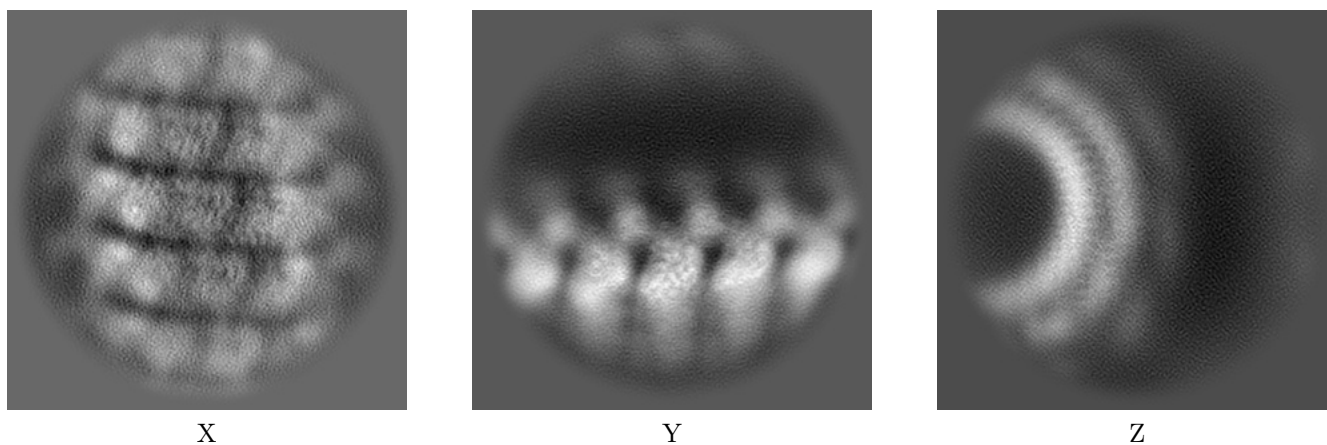
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



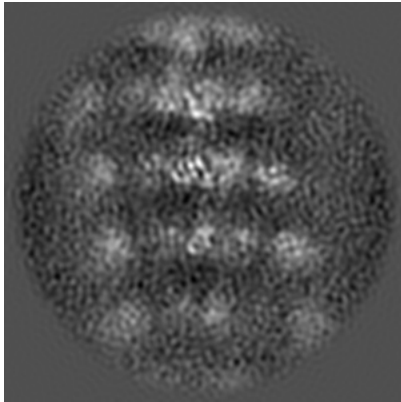
6.1.2 Raw map



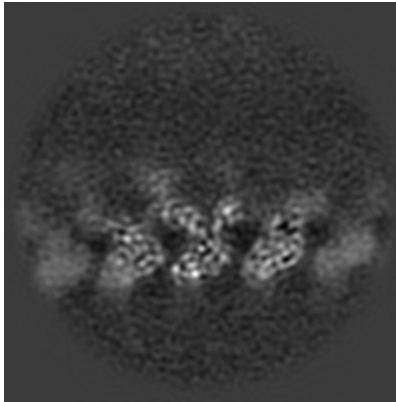
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

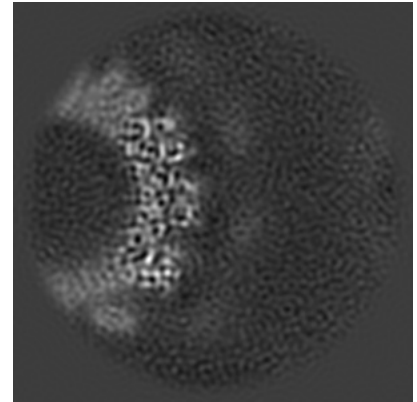
6.2.1 Primary map



X Index: 112

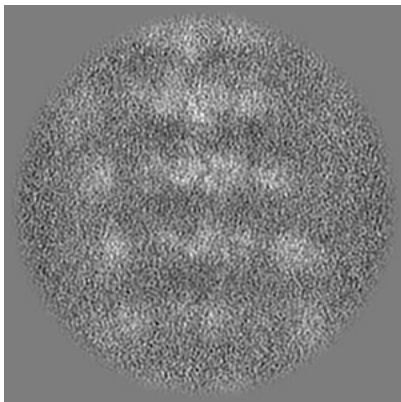


Y Index: 112

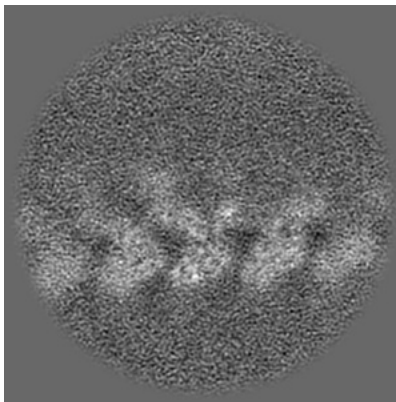


Z Index: 112

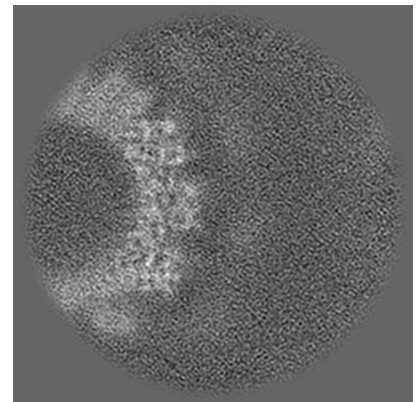
6.2.2 Raw map



X Index: 112



Y Index: 112

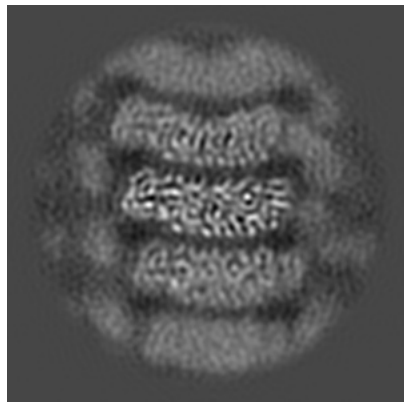


Z Index: 112

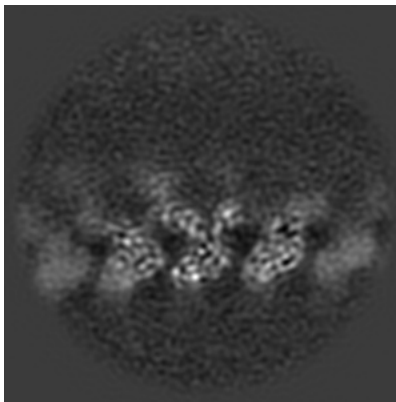
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

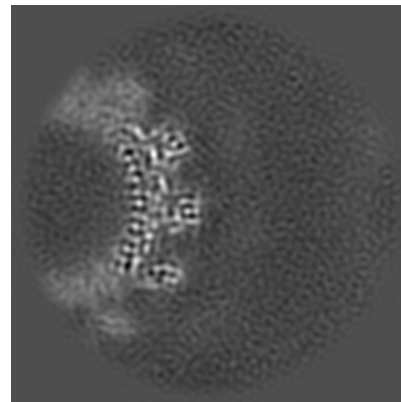
6.3.1 Primary map



X Index: 75

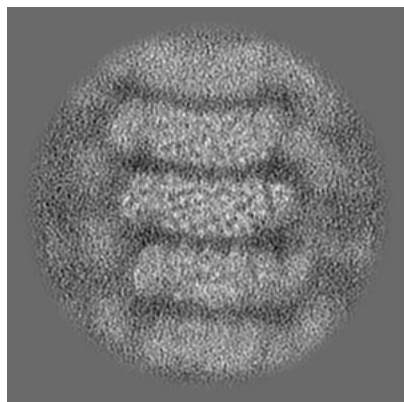


Y Index: 112

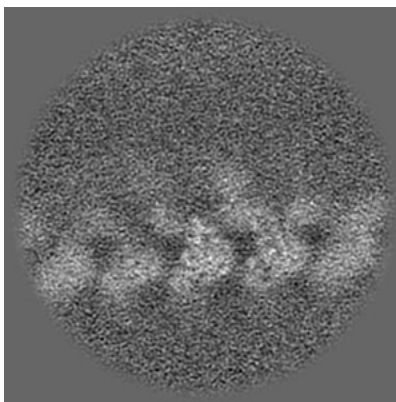


Z Index: 108

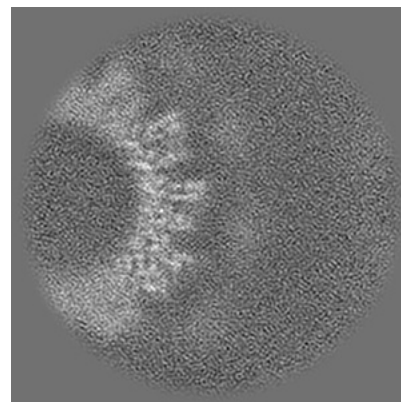
6.3.2 Raw map



X Index: 78



Y Index: 103

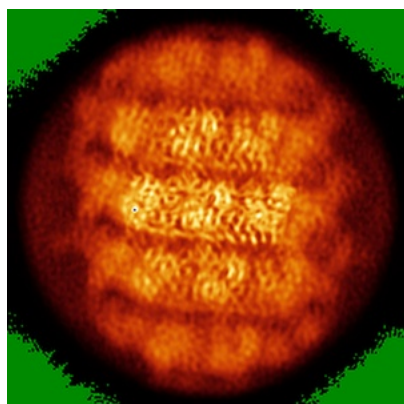


Z Index: 116

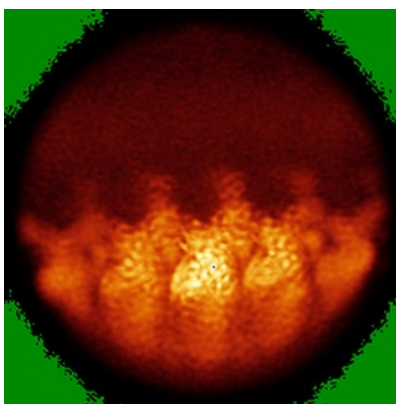
The images above show the largest variance slices of the map in three orthogonal directions.

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

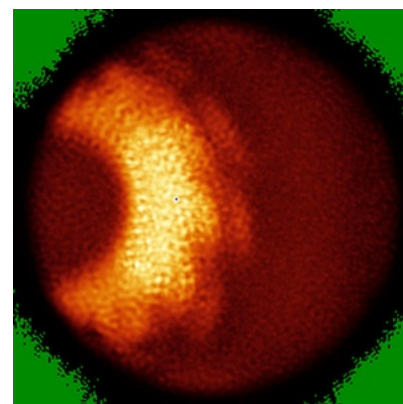
6.4.1 Primary map



X

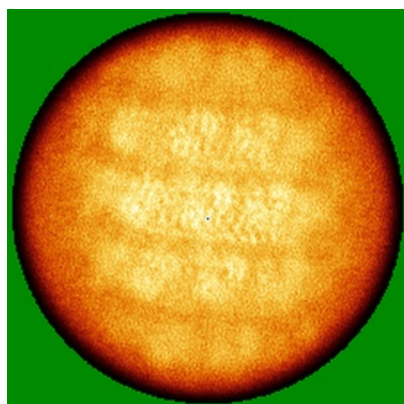


Y

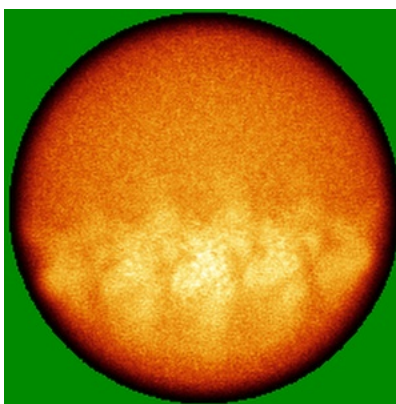


Z

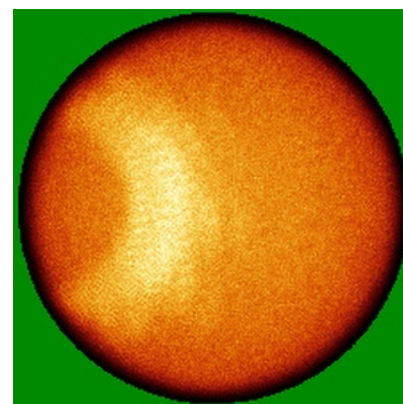
6.4.2 Raw map



X



Y

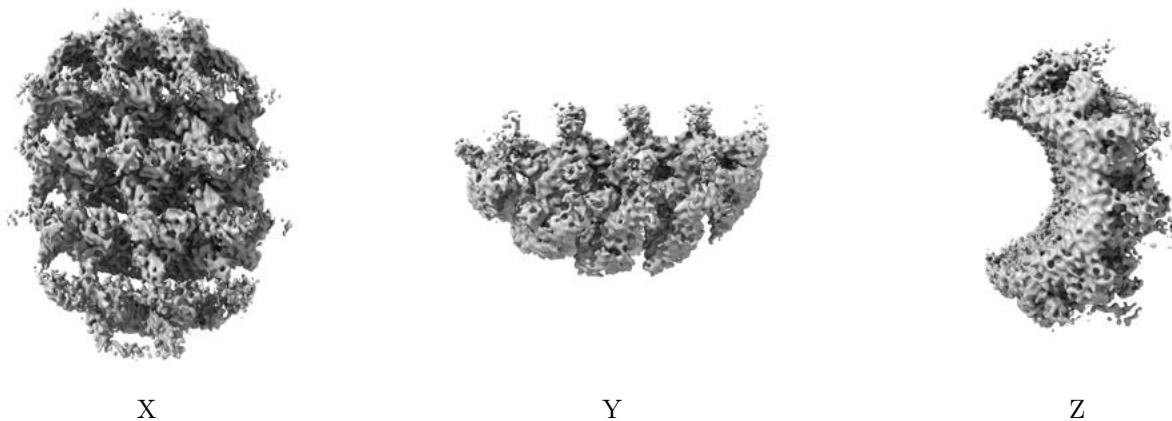


Z

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.

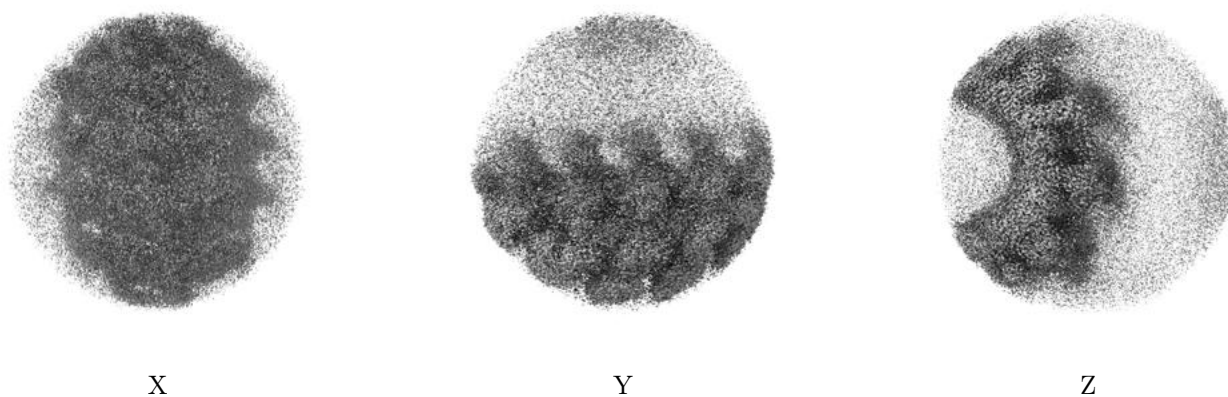
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

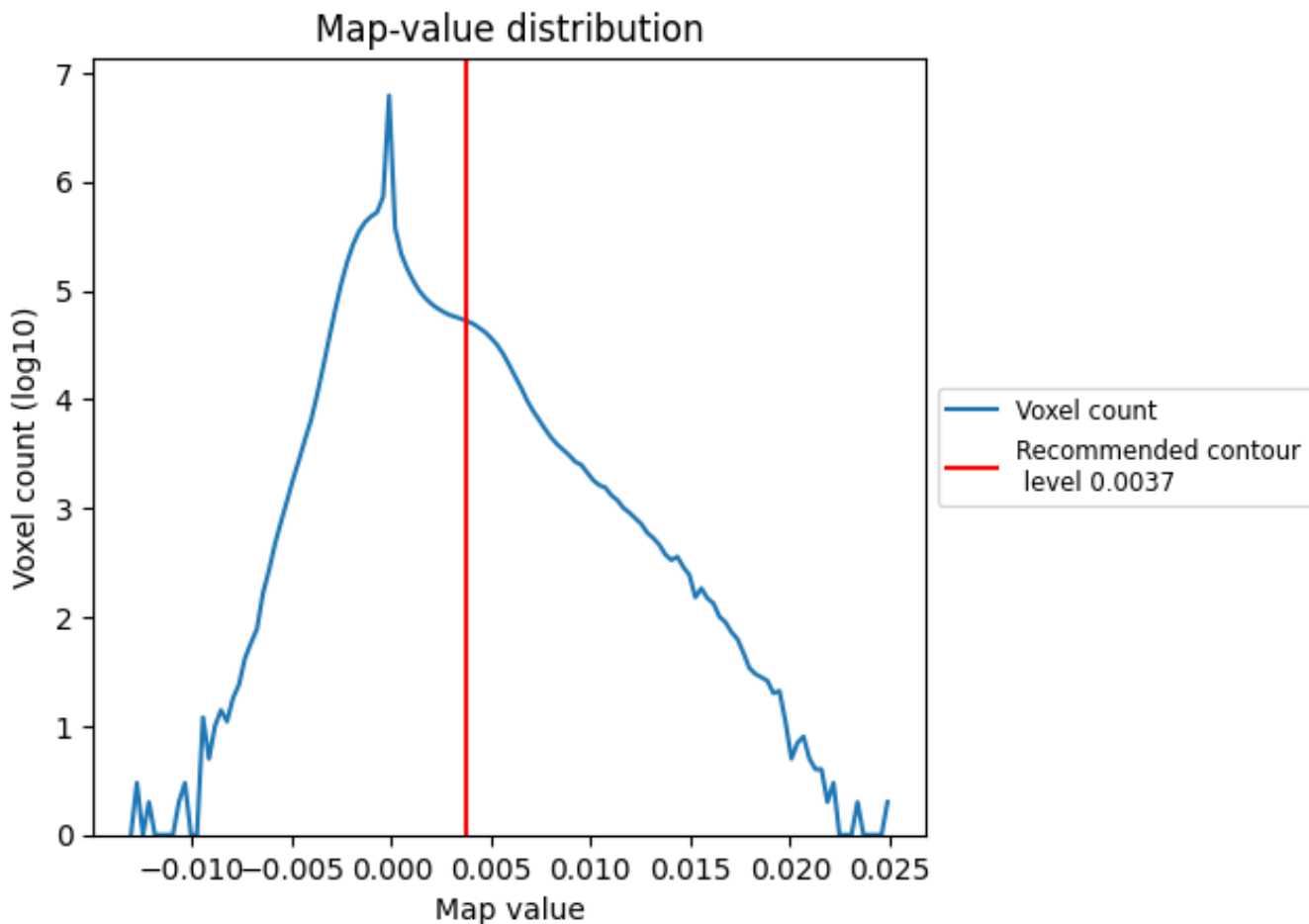
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

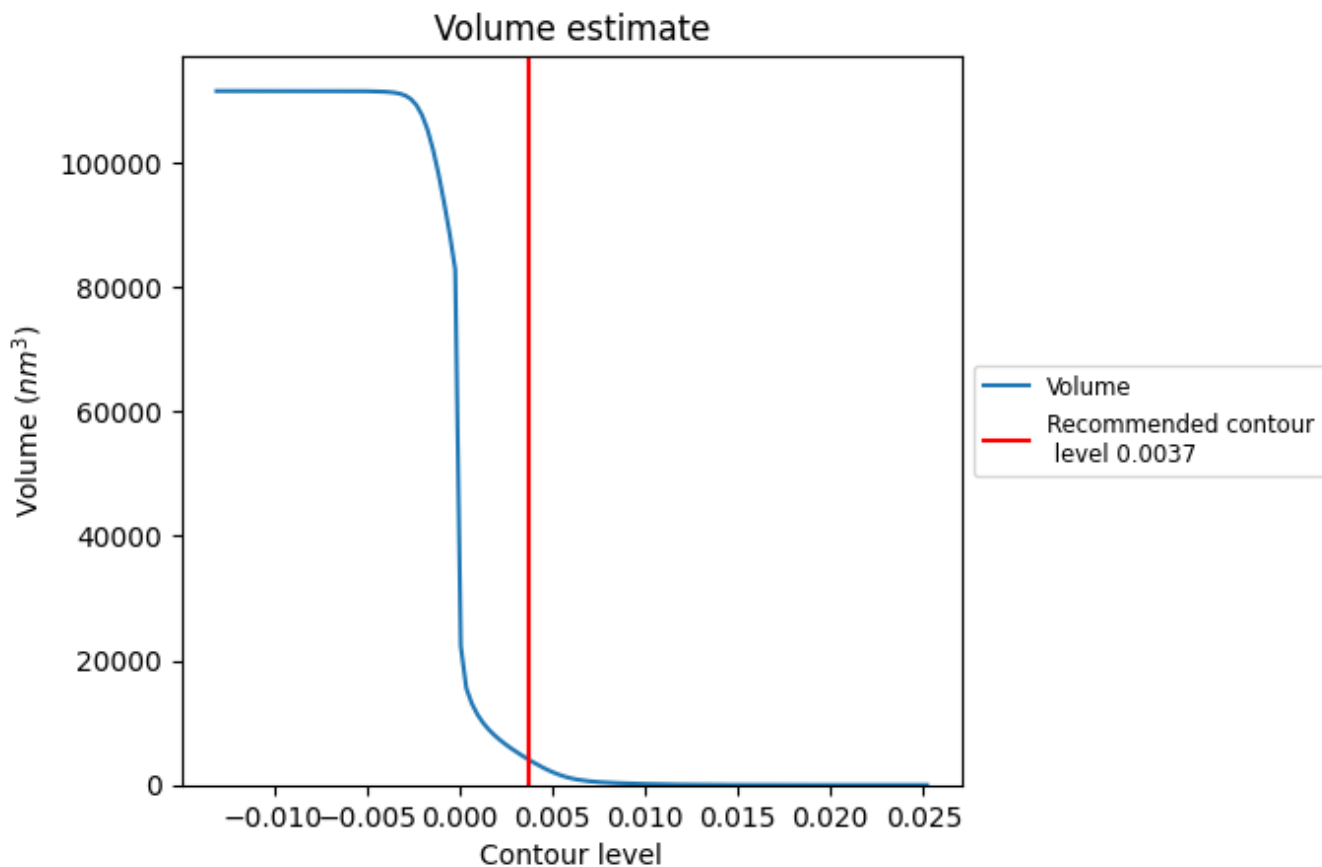
This section contains the results of statistical analysis of the map.

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.

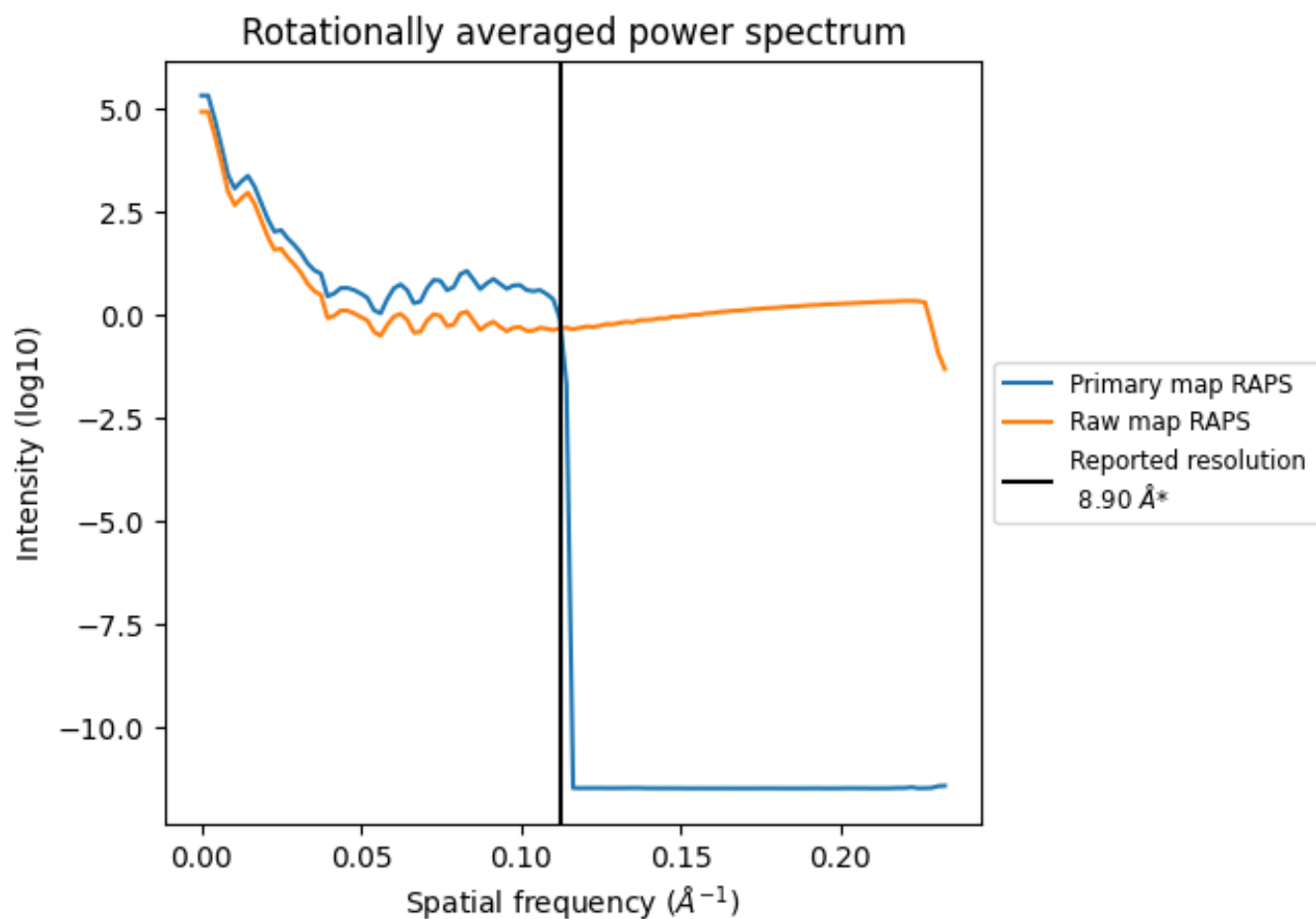
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 41420 nm^3 ; this corresponds to an approximate mass of 3742 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](#)

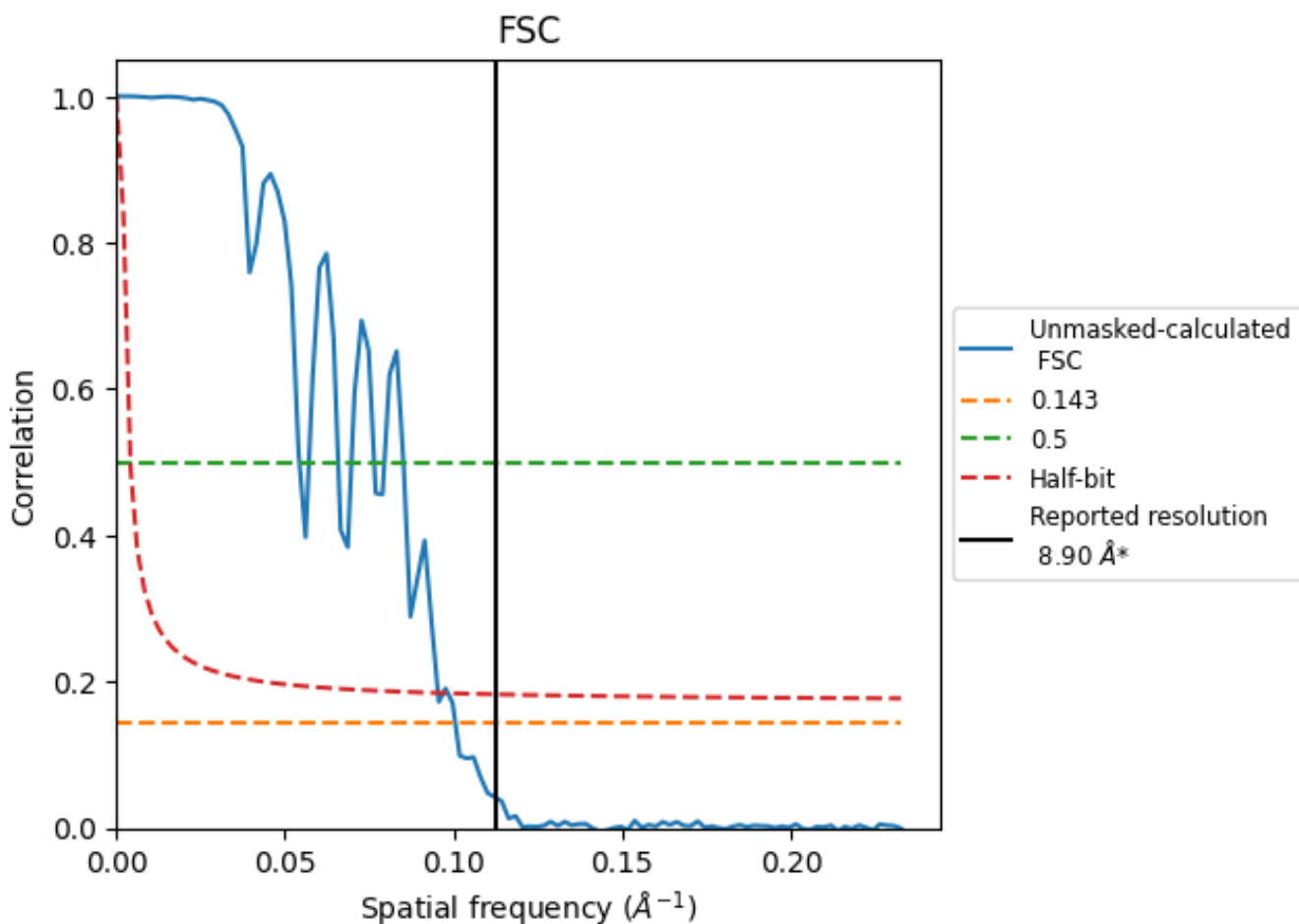


*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

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 0.112 Å⁻¹

8.2 Resolution estimates [i](#)

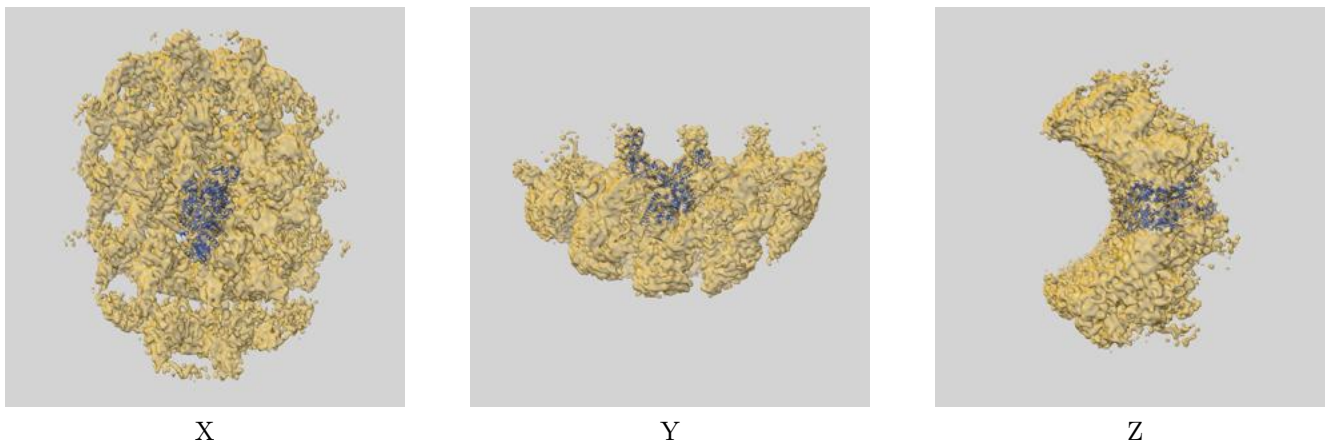
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.95	18.42	10.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.95 differs from the reported value 8.9 by more than 10 %

9 Map-model fit [i](#)

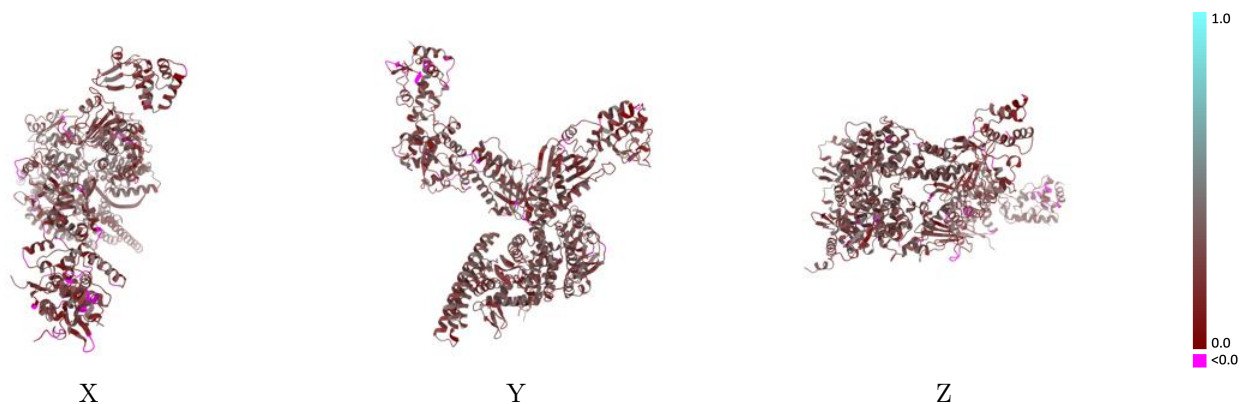
This section contains information regarding the fit between EMDB map EMD-42509 and PDB model 8USN. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



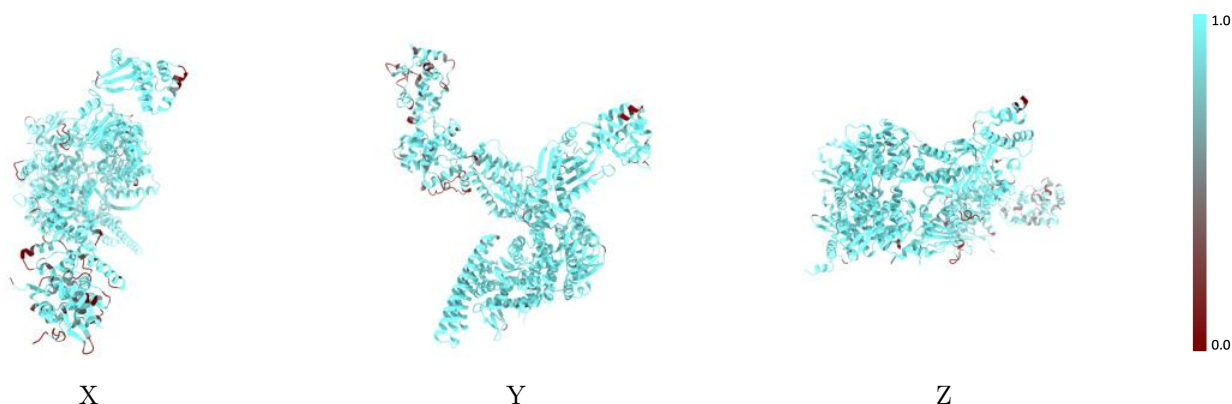
The images above show the 3D surface view of the map at the recommended contour level 0.0037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



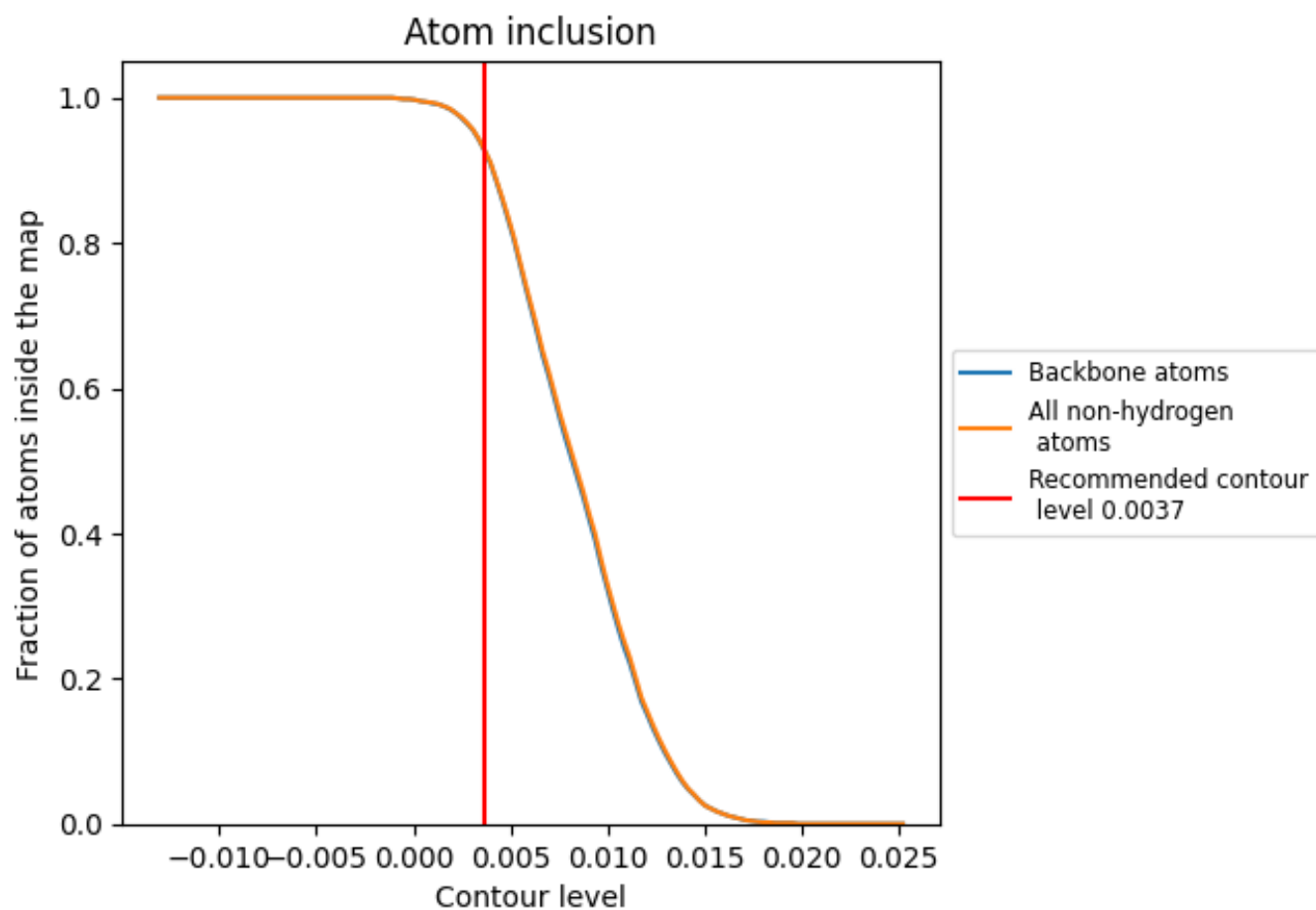
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0037).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% 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 (0.0037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.2510
A	 0.9880	 0.2770
B	 0.9820	 0.2760
C	 0.9850	 0.2510
D	 0.9540	 0.2270
E	 0.7990	 0.2250
F	 0.5360	 0.1660
I	 0.9410	 0.2360
J	 0.9420	 0.2460
K	 0.8940	 0.2230

