



wwPDB EM Validation Summary Report ⓘ

Jan 8, 2024 – 06:29 pm GMT

PDB ID : 8Q9C
EMDB ID : EMD-18276
Title : Tau - CTE-MIA14 (tau intermediate amyloid)
Authors : Lovestam, S.; Li, D.; Scheres, S.H.W.; Goedert, M.
Deposited on : 2023-08-20
Resolution : 3.40 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.dev70
MolProbity : 4.02b-467
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) : 2.36

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 3.40 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
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	382	
1	B	382	
1	C	382	
1	D	382	
1	E	382	
1	F	382	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3444 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 Isoform Tau-D of Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	75	574	360	106	107	1	0	0
1	C	75	574	360	106	107	1	0	0
1	D	75	574	360	106	107	1	0	0
1	A	75	574	360	106	107	1	0	0
1	E	75	574	360	106	107	1	0	0
1	F	75	574	360	106	107	1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP P10636
C	?	-	ALA	deletion	UNP P10636
D	?	-	ALA	deletion	UNP P10636
A	?	-	ALA	deletion	UNP P10636
E	?	-	ALA	deletion	UNP P10636
F	?	-	ALA	deletion	UNP P10636

ASP
GLU
VAL
SER
SER
ALA
SER
LEU
LEU
ALA
GLN
GLY
LEU

• Molecule 1: Isoform Tau-D of Microtubule-associated protein tau

Chain D: 19% 80%

MET
ALA
GLU
PRO
PRO
ARG
GLN
GLU
PHE
GLU
VAL
VAL
MET
SER
GLU
ASP
HIS
ALA
GLY
THR
GLY
TVR
SER
GLY
LEU
LEU

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

LYS
THR
PRO
PRO
SER
GLY
GLU
PRO
LYS
SER
ASP
GLY
ASP
ARG
GLY
THR
PRO
PRO
LYS
LYS
GLY
GLN
VAL
VAL
VAL
THR
ARG
THR
LYS
ALA

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

VAL
PRO
GLY
GLY
S395
Y340
D348
R349
R379
ASN
ALA
ALA
LYS
LYS
THR
THR
HIS
ASP
HIS
ALA
ALA
ILE
VAL
TYR
LYS
SER
SER
VAL
VAL
SER
SER
GLY
GLY
VAL
ASP
THR
SER
PRO
ARG
HIS
LYS
SER
ASN
VAL
VAL
SER
SER
THR
THR
SER
ILE
MET
VAL
SER
SER
PRO
PRO
SER
SER
LEU
LEU
ALA

THR
LEU
ALA
ASP
VAL
SER
SER
ALA
SER
LEU
ALA
LYS
GLN
GLY
LEU

• Molecule 1: Isoform Tau-D of Microtubule-associated protein tau

Chain A: 20% 80%

MET
ALA
GLU
PRO
PRO
ARG
GLN
GLU
PHE
GLU
VAL
VAL
MET
SER
GLU
ASP
HIS
ALA
GLY
THR
GLY
TVR
SER
GLY
LEU
LEU

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

LYS
THR
PRO
SER
GLY
GLU
PRO
PRO
SER
GLY
ASP
ARG
GLY
THR
GLY
ASP
GLN
ALA
GLY
GLY
THR
PRO
PRO
ALA
ALA
THR
ALA
THR
PRO
PRO
LYS
LYS
VAL
VAL
VAL
VAL
VAL
THR
ARG
THR
THR
PRO
PRO
LYS
LYS
PRO
PRO
SER
SER
SER
SER
LEU
LEU
LEU
LEU
ALA

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

VAL
PRO
GLY
GLY
S395
D358
R379
ASN
ALA
LYS
LYS
LYS
THR
THR
HIS
GLY
GLY
GLU
ILE
VAL
TYR
LYS
SER
PRO
VAL
VAL
GLY
GLY
THR
THR
HIS
ALA
GLN
ASP
PRO
GLN
ARG
GLY
GLY
ALA
ASP
ALA
PRO
PRO
GLY
GLY
GLN
LYS
LEU
LEU
SER
SER
VAL
VAL
THR
THR
GLY
SER
SER
VAL
VAL
MET
MET
VAL
SER
SER
PRO
PRO
GLN
GLN
LEU
LEU
ALA
LEU
LEU
ALA

ASP
GLU
VAL
SER
SER
ALA
SER
LEU
LEU
ALA
GLN
GLY
LEU

• Molecule 1: Isoform Tau-D of Microtubule-associated protein tau

Chain E: 20% 80%

MET
ALA
GLU
PRO
PRO
ARG
GLN
GLU
PHE
GLU
VAL
VAL
MET
SER
GLU
ASP
HIS
ALA
GLY
THR
GLY
TVR
SER
GLY
LEU
LEU

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

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-1.24°, rise=4.77 Å, axial sym=C1	Depositor
Number of segments used	14186	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 ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00721	Depositor
Map size (Å)	316.41602, 316.41602, 316.41602	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82400006, 0.82400006, 0.82400006	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	0.53	0/583	0.90	0/780
1	B	0.54	0/583	0.99	1/780 (0.1%)
1	C	0.54	0/583	0.97	0/780
1	D	0.54	0/583	0.99	0/780
1	E	0.53	0/583	0.95	0/780
1	F	0.54	0/583	0.93	0/780
All	All	0.54	0/3498	0.95	1/4680 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	ARG	CD-NE-CZ	5.20	130.88	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	TYR	Sidechain
1	D	310	TYR	Sidechain

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	574	0	597	0	0
1	B	574	0	597	0	0
1	C	574	0	597	0	0
1	D	574	0	597	0	0
1	E	574	0	597	0	0
1	F	574	0	597	0	0
All	All	3444	0	3582	0	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 0.

There are no clashes within the asymmetric unit.

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	73/382 (19%)	71 (97%)	2 (3%)	0	100	100
1	B	73/382 (19%)	69 (94%)	4 (6%)	0	100	100
1	C	73/382 (19%)	68 (93%)	5 (7%)	0	100	100
1	D	73/382 (19%)	68 (93%)	5 (7%)	0	100	100
1	E	73/382 (19%)	68 (93%)	5 (7%)	0	100	100
1	F	73/382 (19%)	68 (93%)	5 (7%)	0	100	100
All	All	438/2292 (19%)	412 (94%)	26 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/312 (21%)	66 (100%)	0	100	100
1	B	66/312 (21%)	66 (100%)	0	100	100
1	C	66/312 (21%)	66 (100%)	0	100	100
1	D	66/312 (21%)	66 (100%)	0	100	100
1	E	66/312 (21%)	66 (100%)	0	100	100
1	F	66/312 (21%)	66 (100%)	0	100	100
All	All	396/1872 (21%)	396 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no chain breaks in this entry.

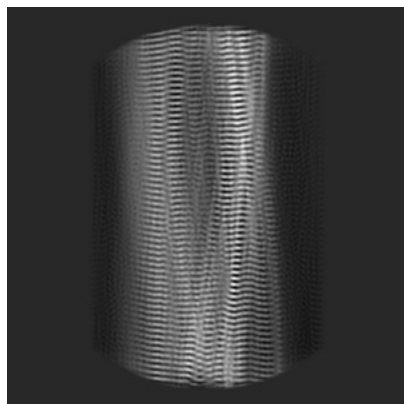
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18276. These allow visual inspection of the internal detail of the map and identification of artifacts.

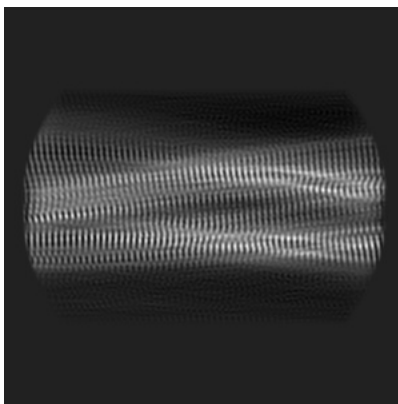
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

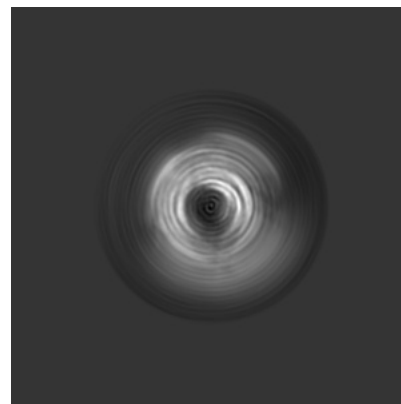
6.1.1 Primary map



X

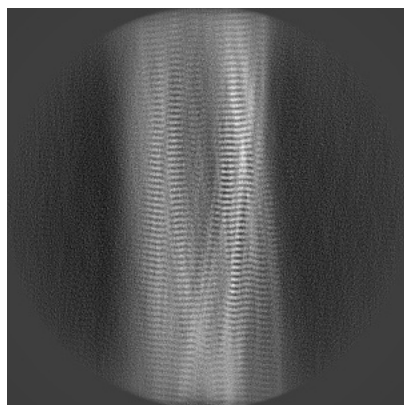


Y

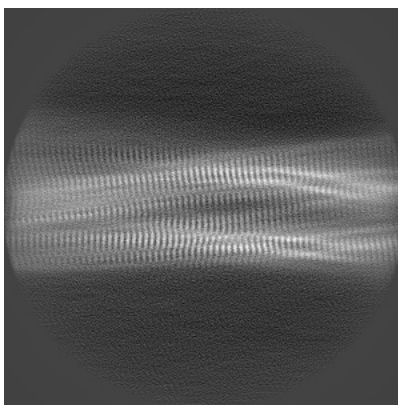


Z

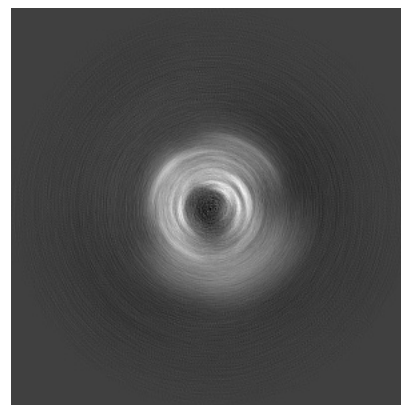
6.1.2 Raw map



X



Y

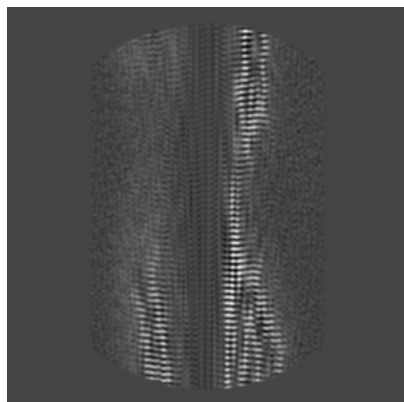


Z

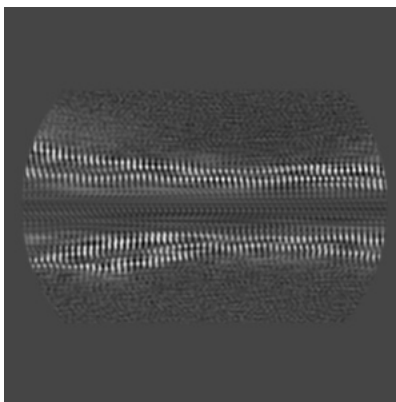
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

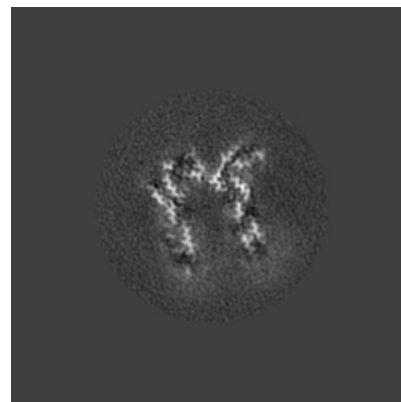
6.2.1 Primary map



X Index: 192

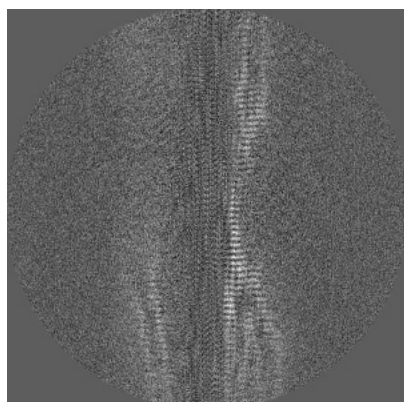


Y Index: 192

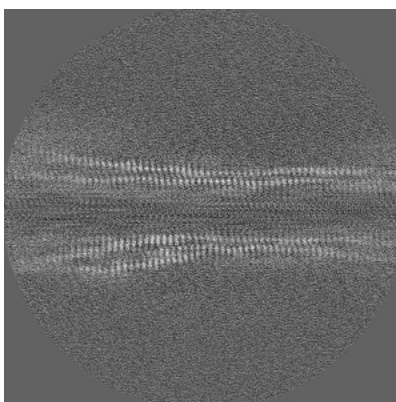


Z Index: 192

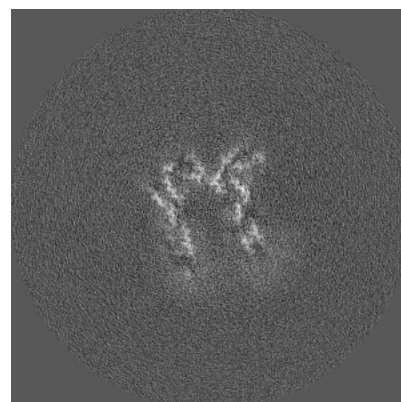
6.2.2 Raw map



X Index: 192



Y Index: 192

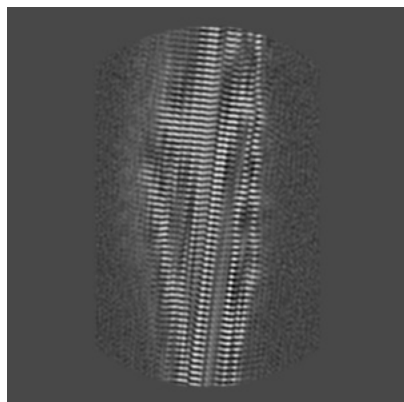


Z Index: 192

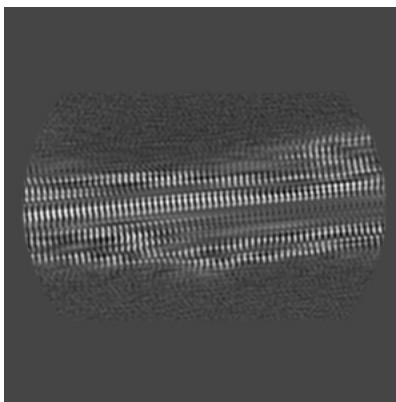
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

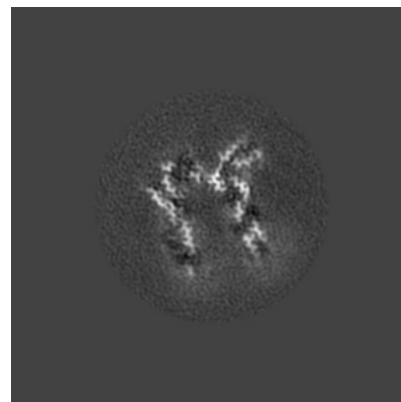
6.3.1 Primary map



X Index: 162

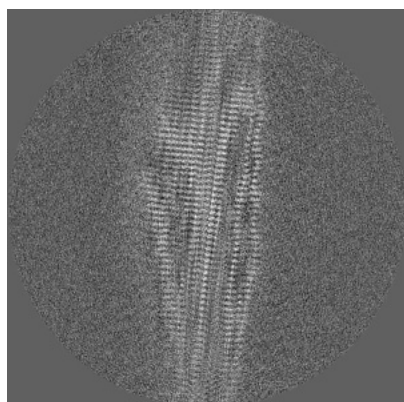


Y Index: 215

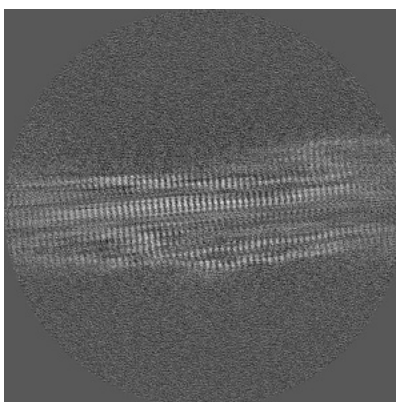


Z Index: 180

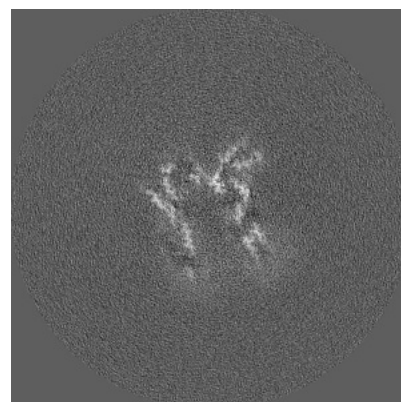
6.3.2 Raw map



X Index: 163



Y Index: 216

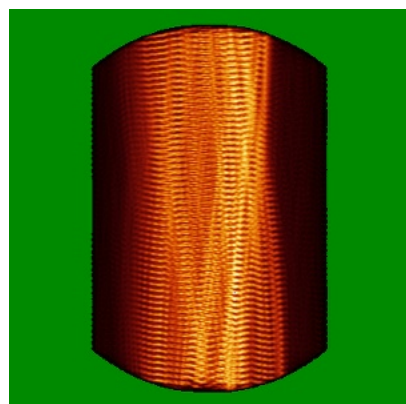


Z Index: 180

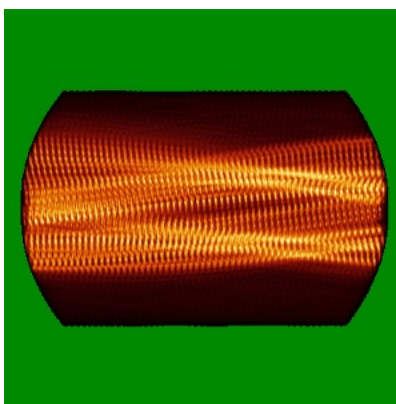
The images above show the largest variance slices of the map in three orthogonal directions.

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

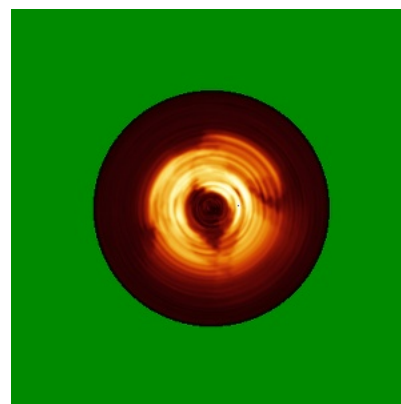
6.4.1 Primary map



X

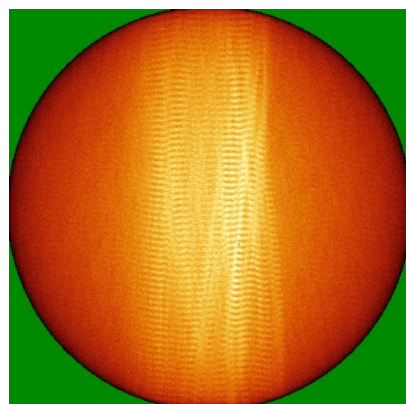


Y

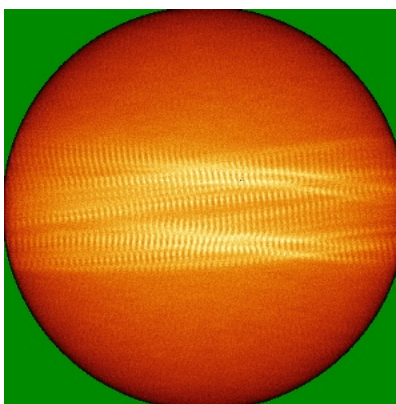


Z

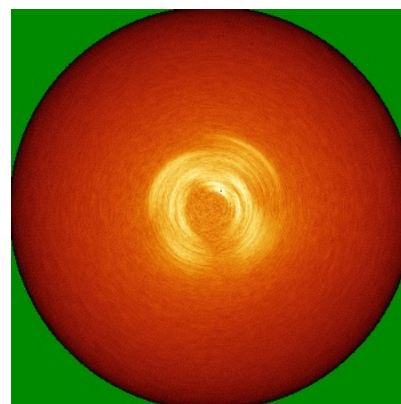
6.4.2 Raw map



X



Y

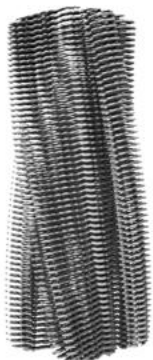


Z

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](#)

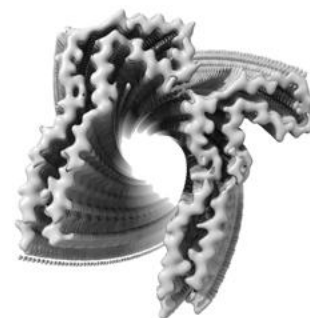
6.5.1 Primary map



X



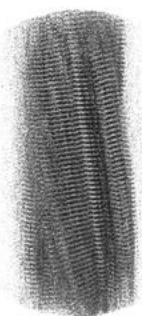
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00721. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

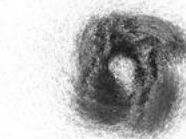
6.5.2 Raw map



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.

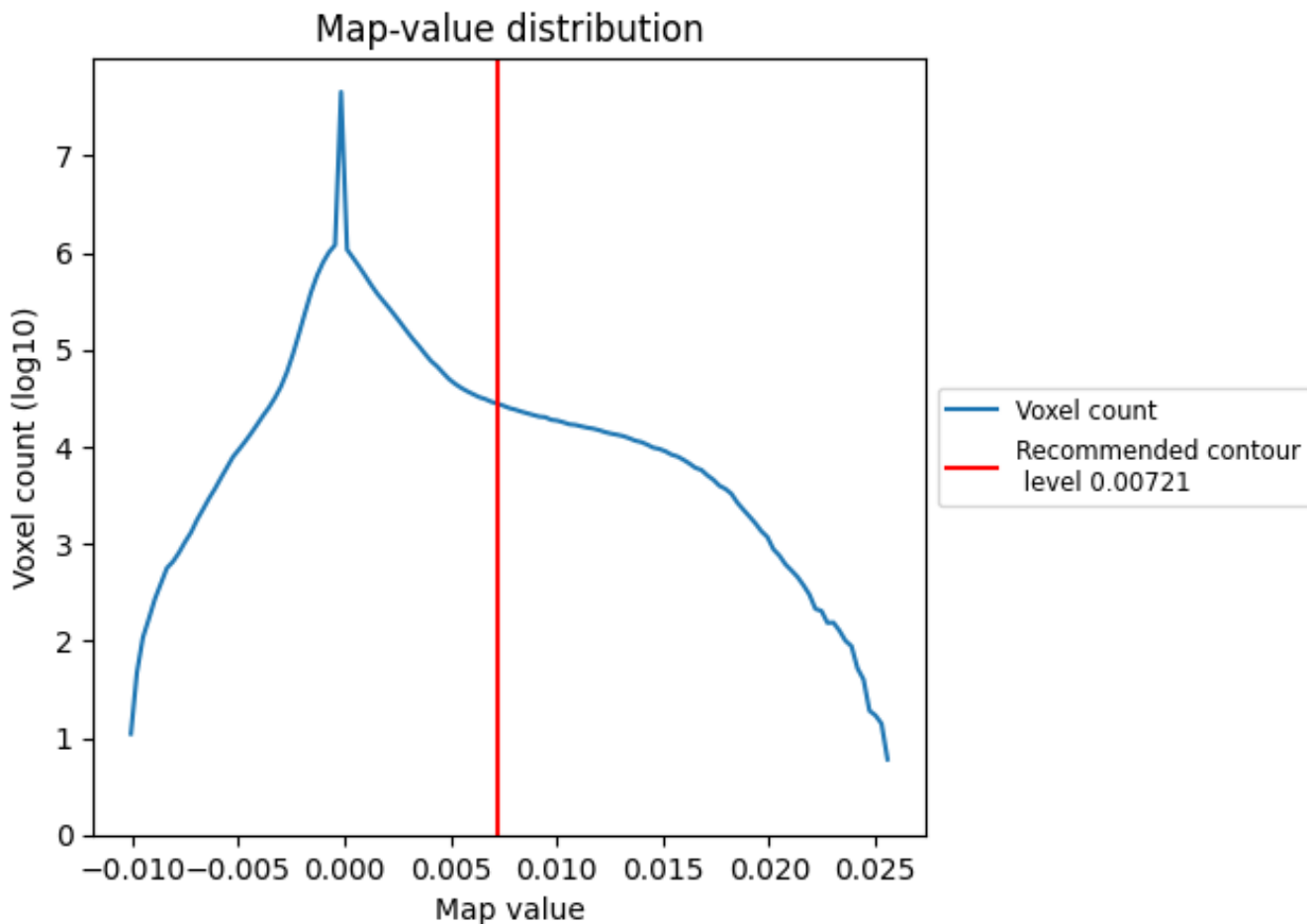
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

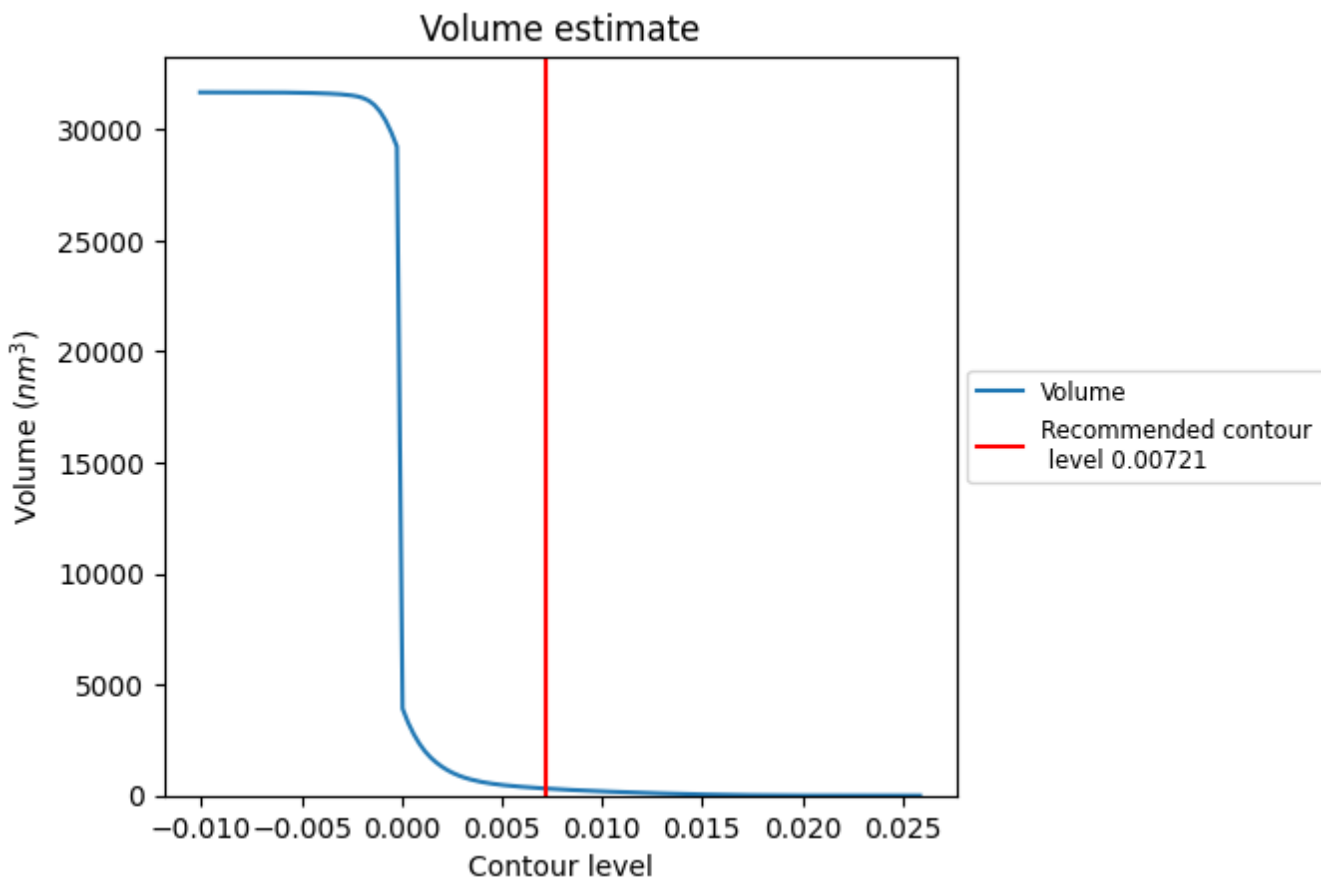
This section contains the results of statistical analysis of the map.

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.

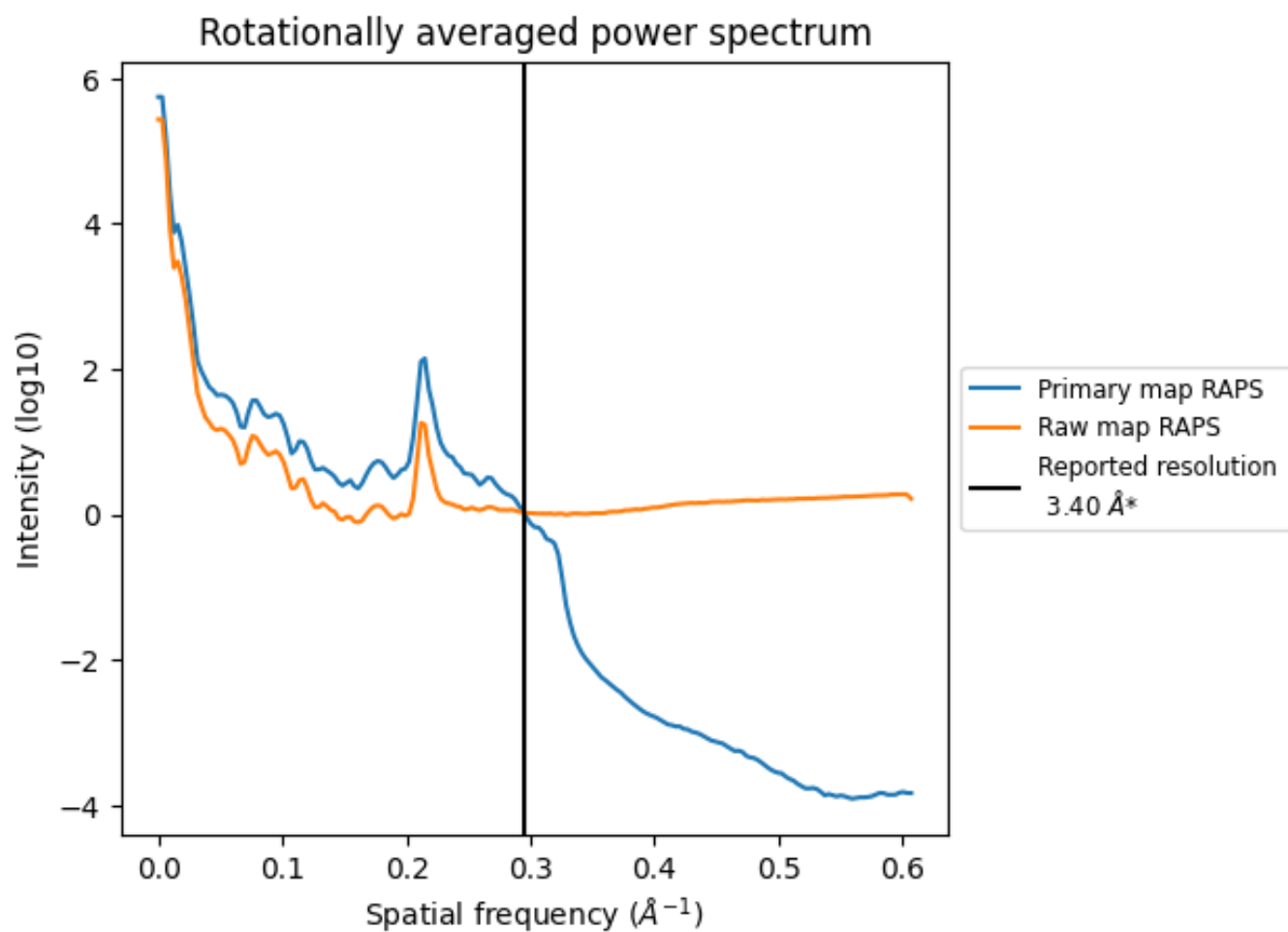
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 317 nm³; this corresponds to an approximate mass of 287 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

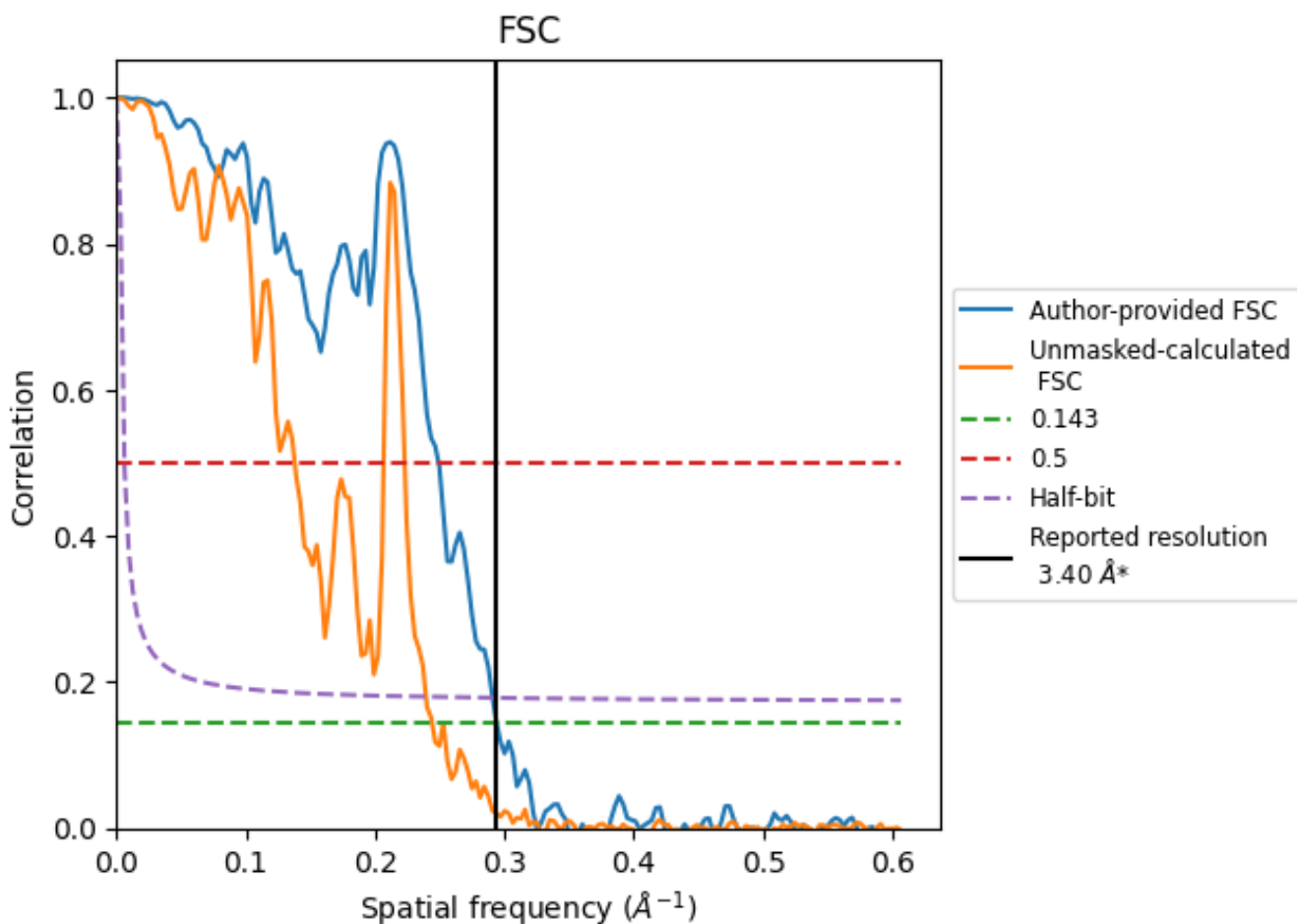


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	4.01	3.44
Unmasked-calculated*	4.10	7.25	4.18

*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 4.10 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

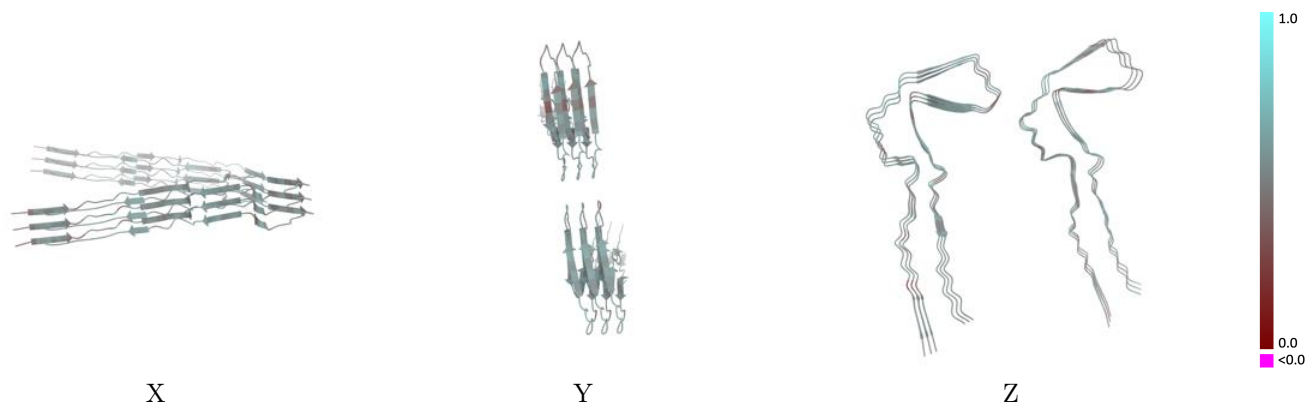
This section contains information regarding the fit between EMDB map EMD-18276 and PDB model 8Q9C. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



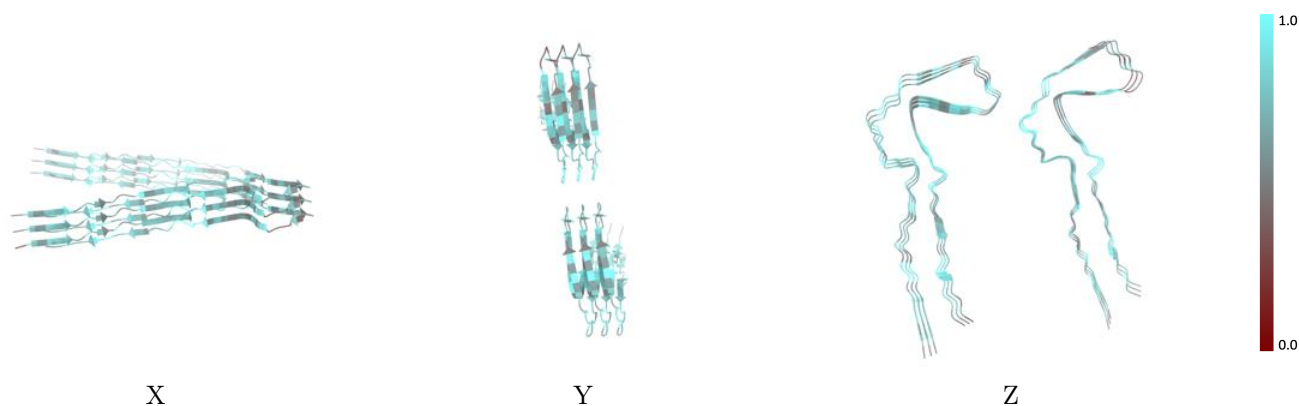
The images above show the 3D surface view of the map at the recommended contour level 0.00721 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



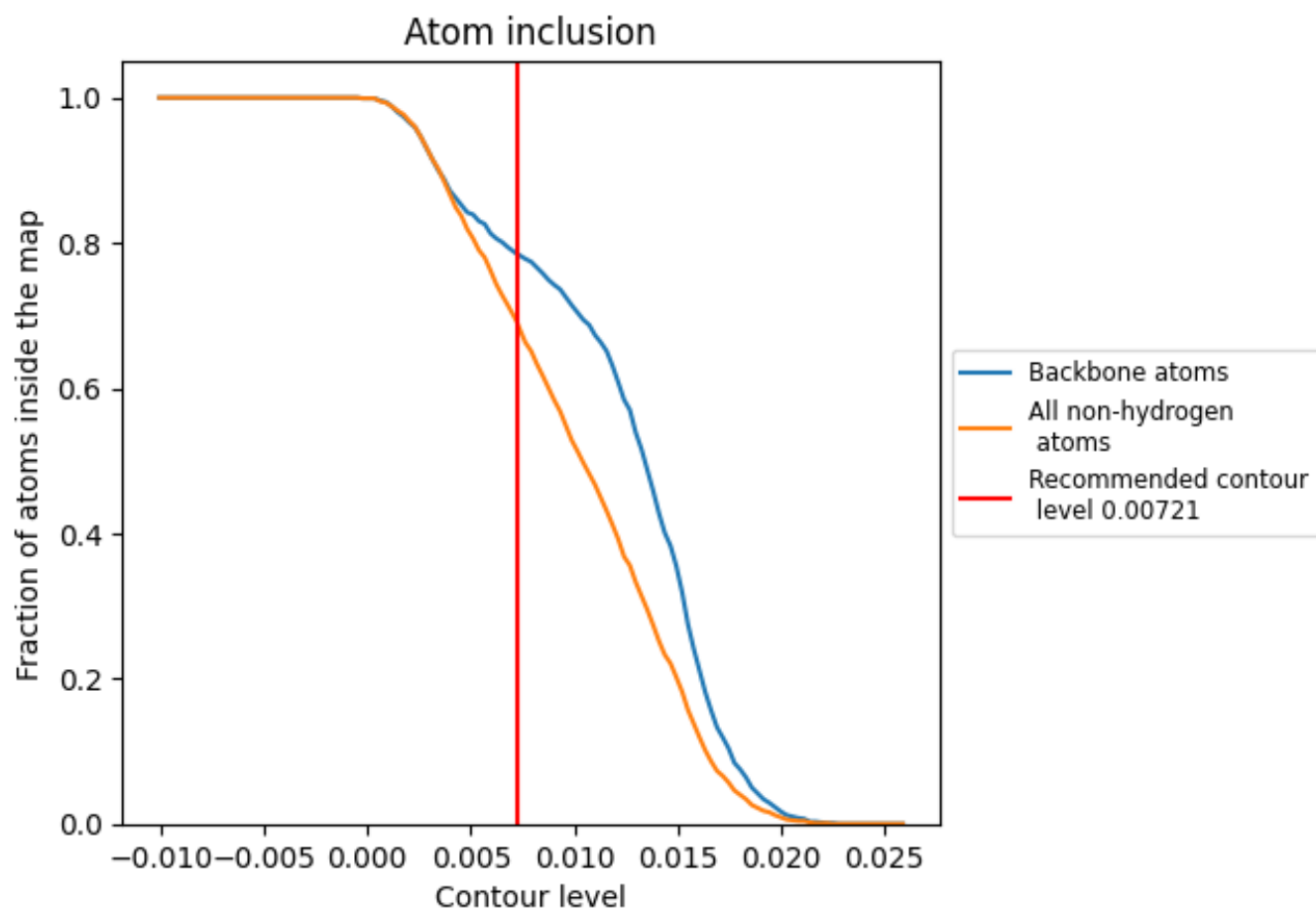
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00721).















9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.00721) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6920	 0.5180
A	 0.6920	 0.5220
B	 0.6840	 0.5110
C	 0.6940	 0.5160
D	 0.6820	 0.5200
E	 0.6980	 0.5160
F	 0.7010	 0.5210

