



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:44 AM UTC

PDB ID : 8QXA / pdb_00008qxa
EMDB ID : EMD-18716
Title : TDP-43 amyloid fibrils: Morphology-1b
Authors : Sharma, K.; Shenoy, J.; Loquet, A.; Schmidt, M.; Faendrich, M.
Deposited on : 2023-10-24
Resolution : 4.05 Å(reported)

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

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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:

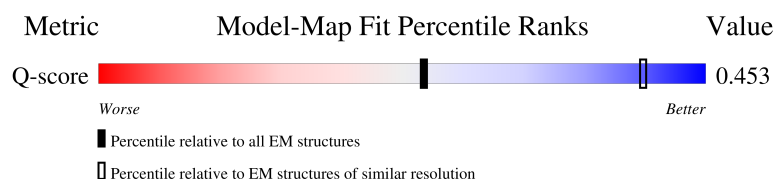
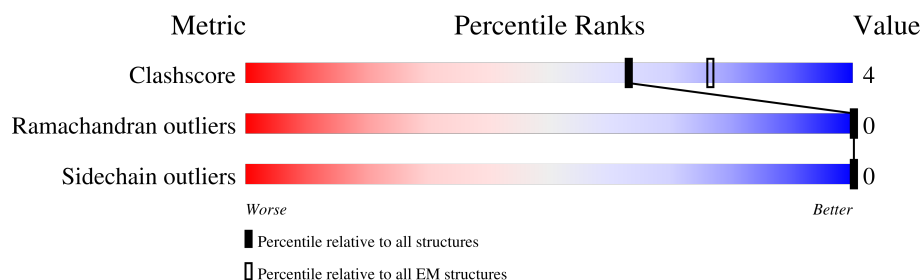
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.05 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6569 (3.55 - 4.55)

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	414	
1	B	414	
1	C	414	
1	D	414	

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Mol	Chain	Length	Quality of chain
1	E	414	 9% . 89%
1	F	414	 10% . 89%
1	G	414	 9% . 89%
1	H	414	 10% . 89%
1	I	414	 9% . 89%
1	J	414	 10% . 89%
1	K	414	 9% . 89%
1	L	414	 10% . 89%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3696 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.

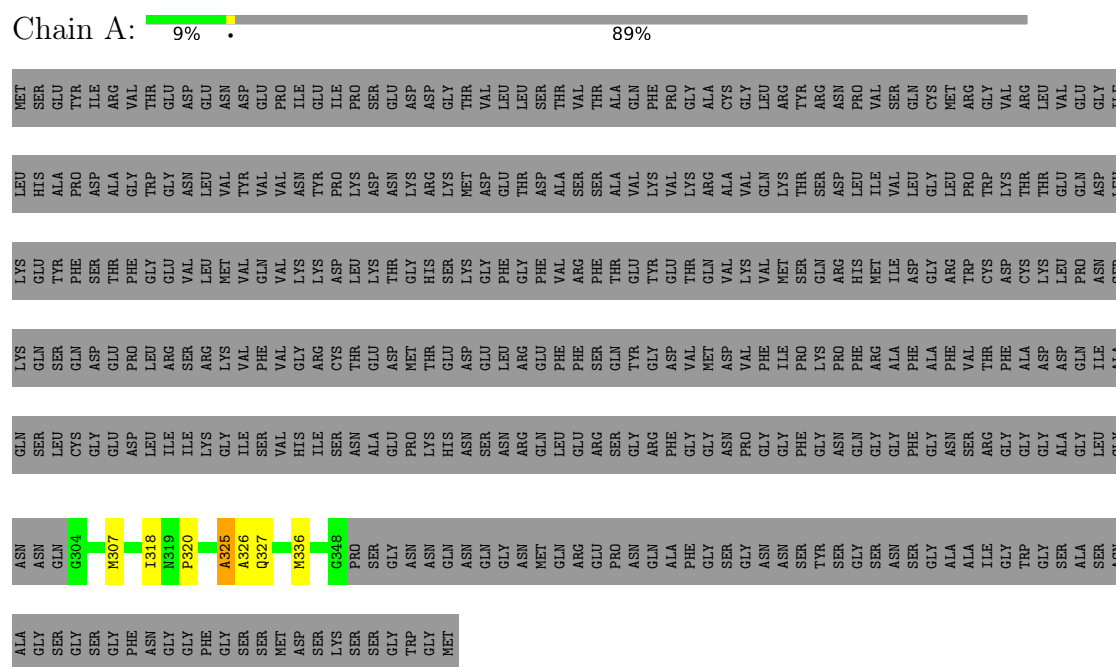
- Molecule 1 is a protein called TAR DNA-binding protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	B	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	C	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	D	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	E	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	F	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	G	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	H	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	I	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	J	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	K	45	Total	C	N	O	S	0	0
			308	186	55	60	7		
1	L	45	Total	C	N	O	S	0	0
			308	186	55	60	7		

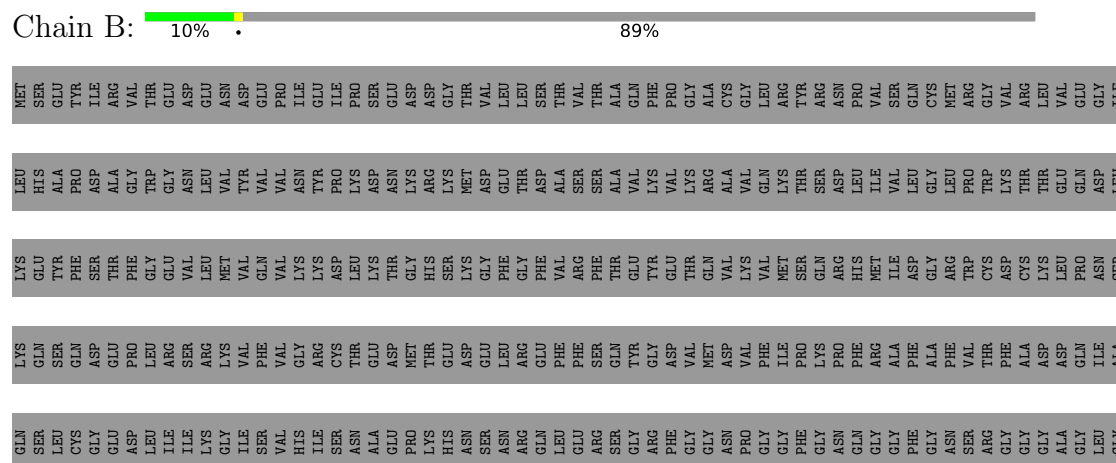
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TAR DNA-binding protein 43

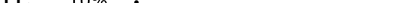


• Molecule 1: TAR DNA-binding protein 43



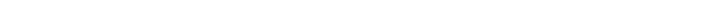
GLY	ASN	GLN	LYS	LEU
SER	ASN	SER	GLN	HIS
GLY	ASN	LEU	GLN	ALA
PHE	G304	CYS	GLN	PRO
GLY	H307	GLU	ASP	ASP
GLY		ASP	GLU	THR
PHE	A326	LEU	LEU	PHE
GLY	A326	ILE	ARG	GLY
SER	Q327	ILE	SER	GLY
SER		LYS	ARG	ASN
MET	H336	GLY	LYS	LEU
ASP	H337	ILE	VAL	VAL
SER	G348	SER	PHE	TYR
LYS	PRO	VAL	GLY	VAL
SER	SER	HIS	GLY	VAL
SER	GLY	ILE	ARG	ASN
GLY	ASN	SER	CYS	PRO
TRP	ASN	ASN	THR	ASP
GLY	ASN	ALA	LYS	LEU
MET	GLN	GLU	LYS	ASP
	ASN	ASP	THR	LYS
	ASN	PRO	MET	GLY
	GLN	LYS	HIS	LYS
	GLY	HIS	THR	ARG
	ASN	ASN	GLU	LYS
	ASN	ASN	ASP	LYS
	GLN	SER	GLU	MET
	GLN	ARG	LEU	GLY
	ARG	GLN	ARG	PHE
	GLU	GLN	GLU	ASP
	PRO	LEU	PHE	ALA
	ASN	GLU	PHE	ALA
	GLN	ARG	SER	SER
	ALA	SER	GLN	ALA
	PHE	GLY	TVR	VAL
	GLY	ARG	GLY	VAL
	SER	PHE	ASP	GLN
	GLY	GLY	VAL	LYS
	ASN	ASN	MET	VAL
	ASN	ASN	GLN	ARG
	SER	ASN	ASP	ALA
	ASN	GLN	VAL	VAL
	TVR	GLY	VAL	GLN
	SER	GLY	MET	LYS
	GLY	PHE	SER	THR
	GLY	SER	GLN	SER
	ASN	SER	ARG	ASP
	SER	GLN	PHE	LEU
	GLY	GLY	ARG	ILE
	ALA	PHE	ALA	VAL
	ALA	GLY	GLY	GLY
	ILE	GLY	ARG	LEU
	GLY	ASN	PHE	LEU
	TRP	SER	VAL	TRP
	GLY	ARG	THR	CYS
	SER	GLY	PHE	ASP
	ALA	GLY	ALA	LYS
	SER	GLY	ASP	THR
	ASN	ALA	ASP	THR
	ALA	GLY	LEU	GLY
	GLY	LEU	PRO	GLN
	C	C	ASN	ASP

- Molecule 1: TAR DNA-binding protein 43

Chain H:  10% . 89%

[illegible]

- Molecule 1: TAR DNA-binding protein 43

Chain I:  9% . 89%

[illegible]



GLY
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GLY
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● Molecule 1: TAR DNA-binding protein 43

Chain L: 10% . 89%

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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-1.802°, rise=4.792 Å, axial sym=C1	Depositor
Number of segments used	26881	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 ($e^-/\text{Å}^2$)	52.08	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	239.2, 239.2, 239.2	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.99	0/312	1.53	5/415 (1.2%)
1	B	1.03	0/312	1.46	1/415 (0.2%)
1	C	0.99	0/312	1.53	5/415 (1.2%)
1	D	1.03	0/312	1.46	1/415 (0.2%)
1	E	0.99	0/312	1.53	5/415 (1.2%)
1	F	1.03	0/312	1.46	1/415 (0.2%)
1	G	0.99	0/312	1.53	5/415 (1.2%)
1	H	1.03	0/312	1.46	1/415 (0.2%)
1	I	0.99	0/312	1.53	5/415 (1.2%)
1	J	1.03	0/312	1.46	1/415 (0.2%)
1	K	0.99	0/312	1.53	5/415 (1.2%)
1	L	1.03	0/312	1.46	1/415 (0.2%)
All	All	1.01	0/3744	1.49	36/4980 (0.7%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	327	GLN	N-CA-C	-9.57	100.17	112.23
1	A	327	GLN	N-CA-C	-9.56	100.18	112.23
1	I	327	GLN	N-CA-C	-9.56	100.18	112.23
1	G	327	GLN	N-CA-C	-9.56	100.19	112.23
1	C	327	GLN	N-CA-C	-9.55	100.20	112.23

There are no chirality outliers.

There are no planarity outliers.

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	308	0	288	3	0
1	B	308	0	288	3	0
1	C	308	0	288	5	0
1	D	308	0	288	5	0
1	E	308	0	288	5	0
1	F	308	0	288	5	0
1	G	308	0	288	4	0
1	H	308	0	288	5	0
1	I	308	0	288	4	0
1	J	308	0	288	5	0
1	K	308	0	288	3	0
1	L	308	0	288	3	0
All	All	3696	0	3456	30	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 4.

The worst 5 of 30 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)
1:C:307:MET:HE2	1:E:337:MET:HE2	1.83	0.59
1:A:307:MET:HE2	1:C:337:MET:HE2	1.83	0.59
1:E:307:MET:HE2	1:G:337:MET:HE2	1.83	0.59
1:I:307:MET:HE2	1:K:337:MET:HE2	1.83	0.59
1:G:307:MET:HE2	1:I:337:MET:HE2	1.83	0.59

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	43/414 (10%)	42 (98%)	1 (2%)	0	100	100
1	B	43/414 (10%)	41 (95%)	2 (5%)	0	100	100
1	C	43/414 (10%)	42 (98%)	1 (2%)	0	100	100
1	D	43/414 (10%)	41 (95%)	2 (5%)	0	100	100
1	E	43/414 (10%)	42 (98%)	1 (2%)	0	100	100
1	F	43/414 (10%)	41 (95%)	2 (5%)	0	100	100
1	G	43/414 (10%)	42 (98%)	1 (2%)	0	100	100
1	H	43/414 (10%)	41 (95%)	2 (5%)	0	100	100
1	I	43/414 (10%)	42 (98%)	1 (2%)	0	100	100
1	J	43/414 (10%)	41 (95%)	2 (5%)	0	100	100
1	K	43/414 (10%)	42 (98%)	1 (2%)	0	100	100
1	L	43/414 (10%)	41 (95%)	2 (5%)	0	100	100
All	All	516/4968 (10%)	498 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	29/333 (9%)	29 (100%)	0	100	100
1	B	29/333 (9%)	29 (100%)	0	100	100
1	C	29/333 (9%)	29 (100%)	0	100	100
1	D	29/333 (9%)	29 (100%)	0	100	100
1	E	29/333 (9%)	29 (100%)	0	100	100
1	F	29/333 (9%)	29 (100%)	0	100	100
1	G	29/333 (9%)	29 (100%)	0	100	100
1	H	29/333 (9%)	29 (100%)	0	100	100
1	I	29/333 (9%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	29/333 (9%)	29 (100%)	0	100	100
1	K	29/333 (9%)	29 (100%)	0	100	100
1	L	29/333 (9%)	29 (100%)	0	100	100
All	All	348/3996 (9%)	348 (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. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	345	ASN
1	I	327	GLN
1	L	345	ASN
1	H	345	ASN
1	I	344	GLN

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 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 ⓘ

There are no chain breaks in this entry.

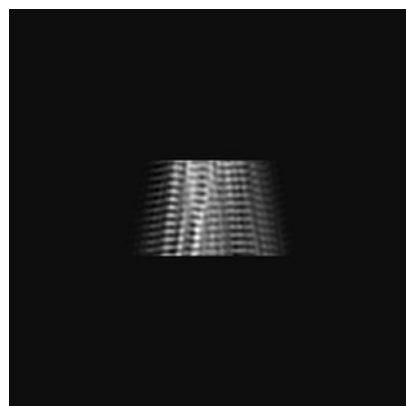
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18716. These allow visual inspection of the internal detail of the map and identification of artifacts.

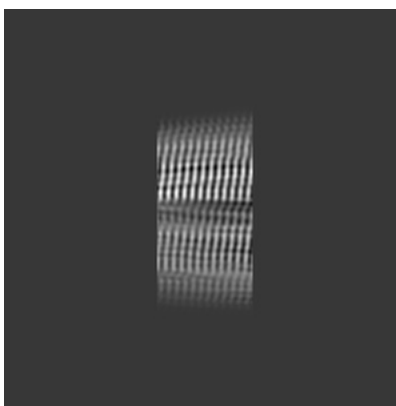
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

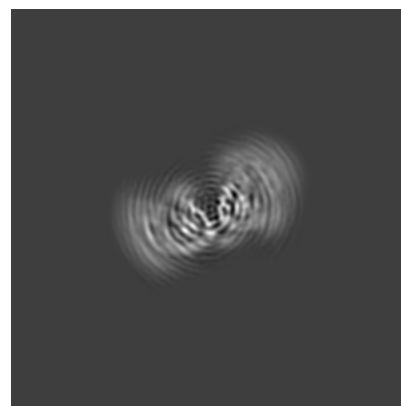
6.1.1 Primary map



X

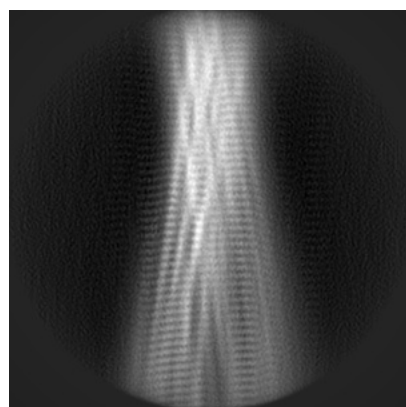


Y

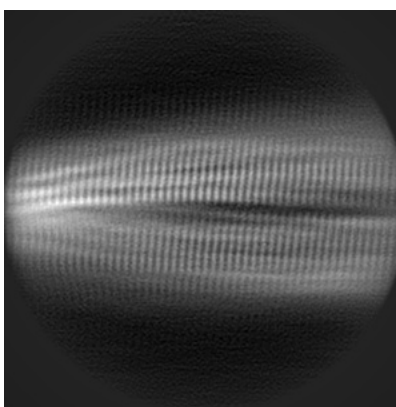


Z

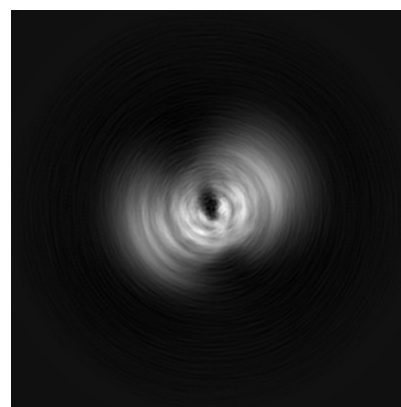
6.1.2 Raw map



X



Y

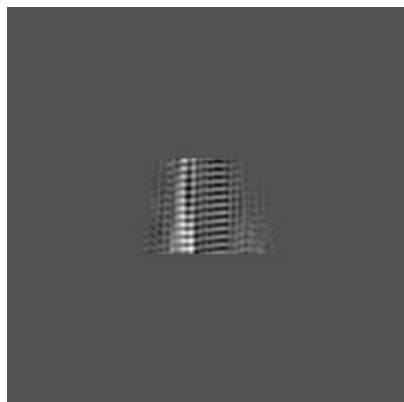


Z

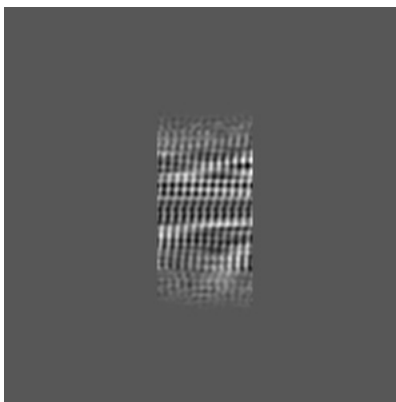
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

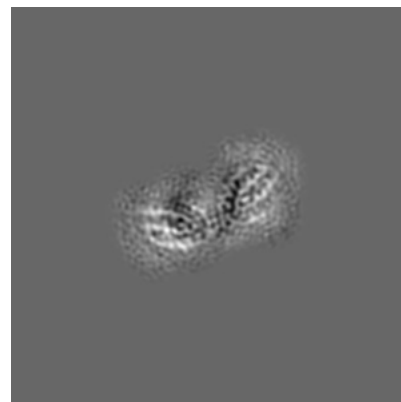
6.2.1 Primary map



X Index: 115

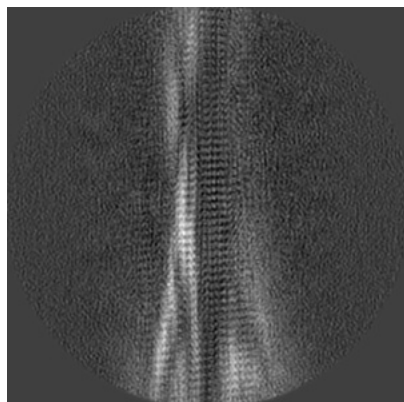


Y Index: 115

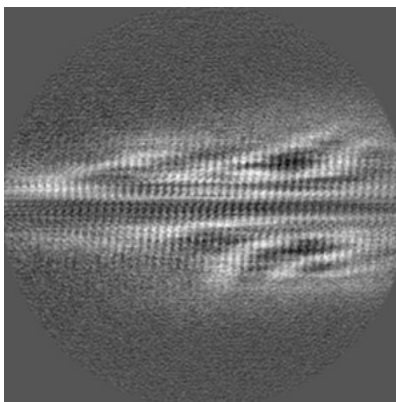


Z Index: 115

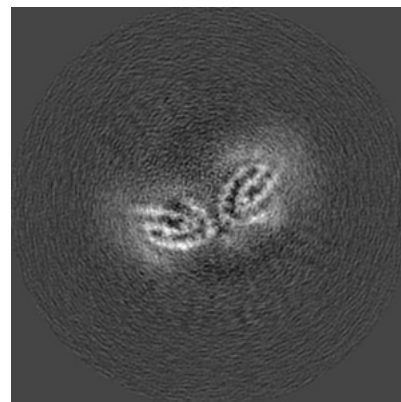
6.2.2 Raw map



X Index: 115



Y Index: 115

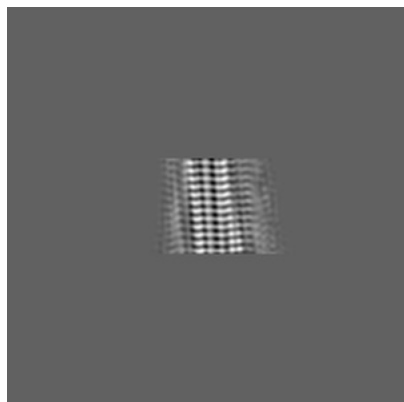


Z Index: 115

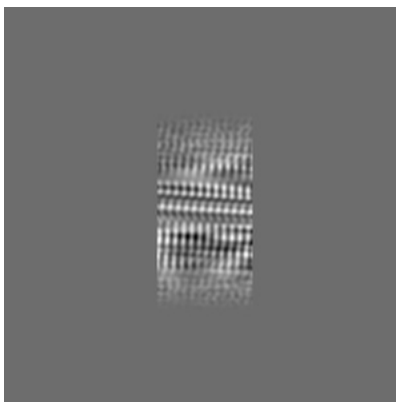
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

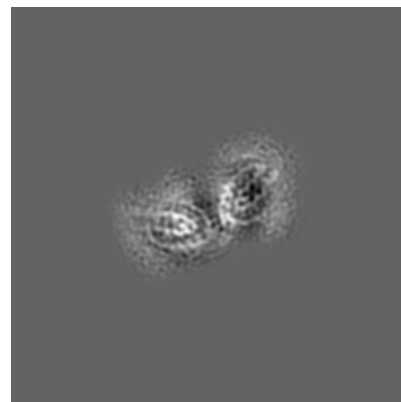
6.3.1 Primary map



X Index: 125

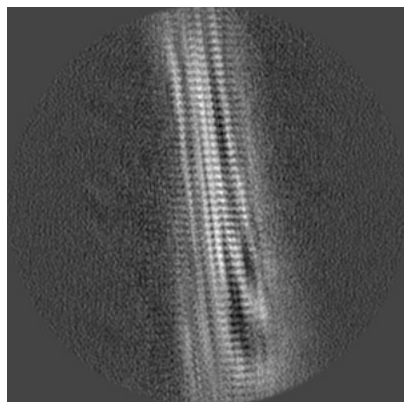


Y Index: 106

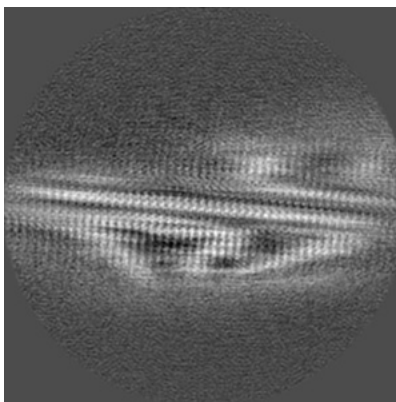


Z Index: 112

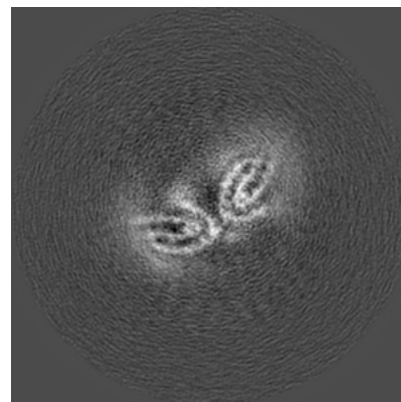
6.3.2 Raw map



X Index: 133



Y Index: 102

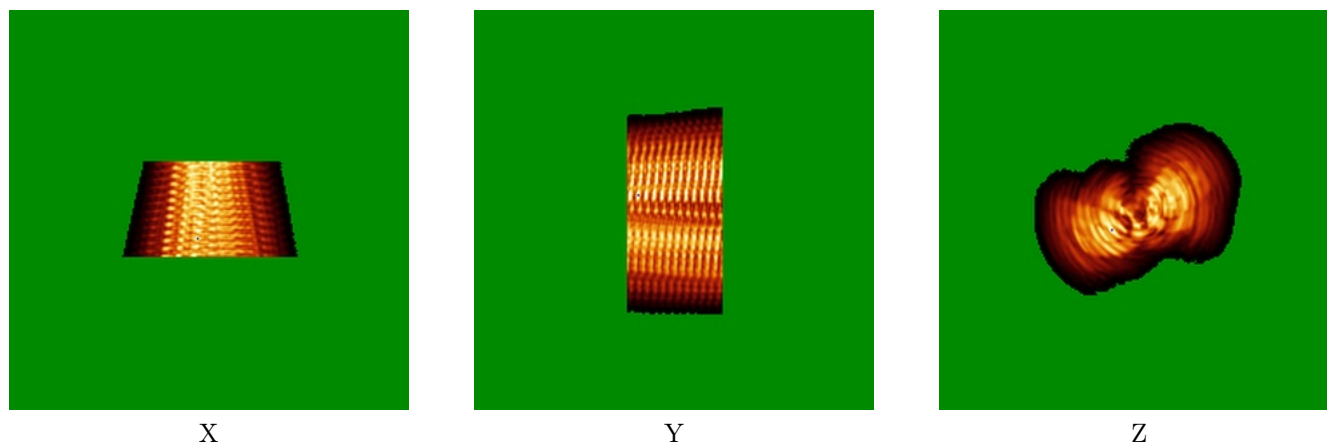


Z Index: 95

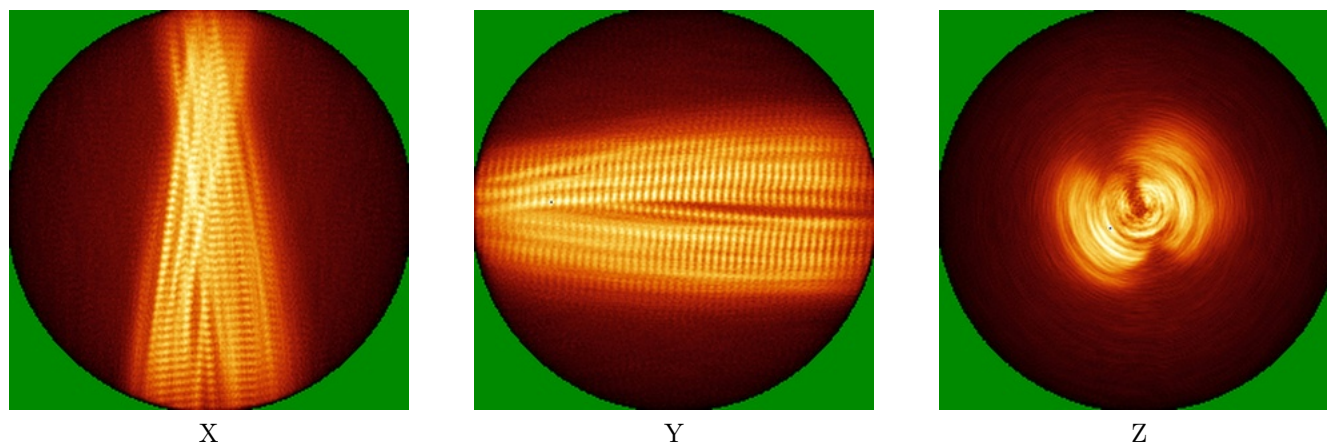
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

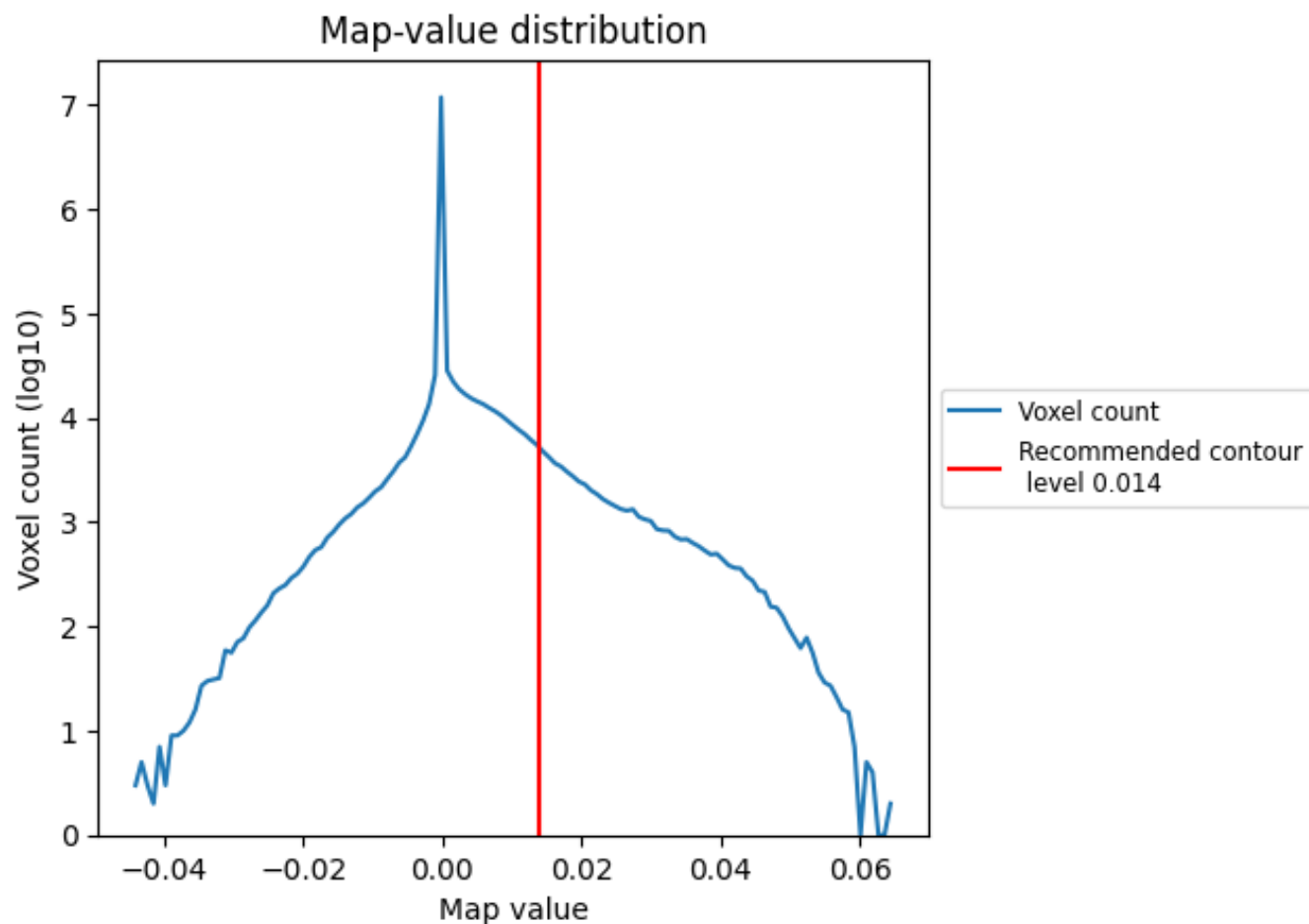
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

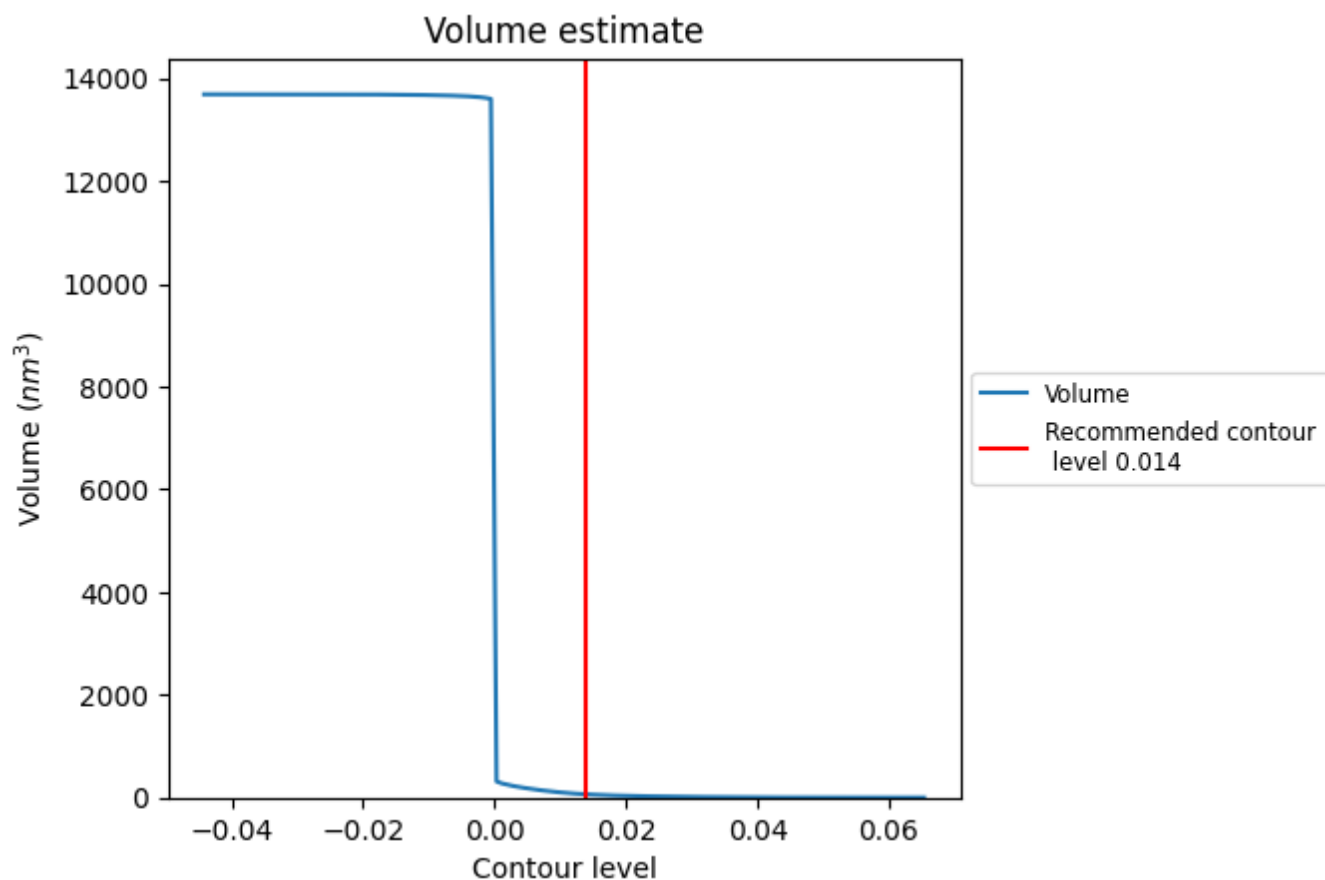
This section contains the results of statistical analysis of the map.

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.

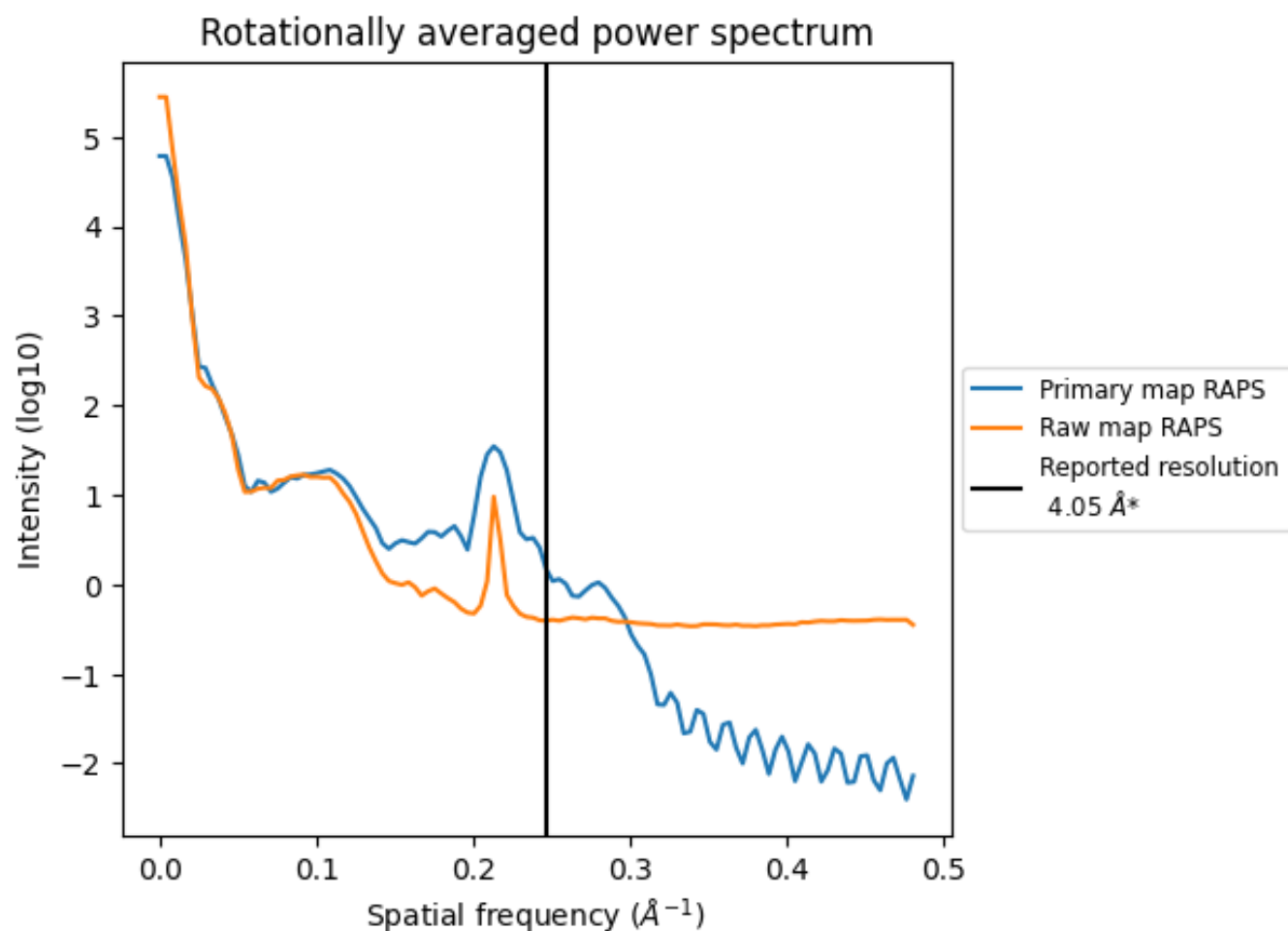
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm³; this corresponds to an approximate mass of 57 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 ⓘ

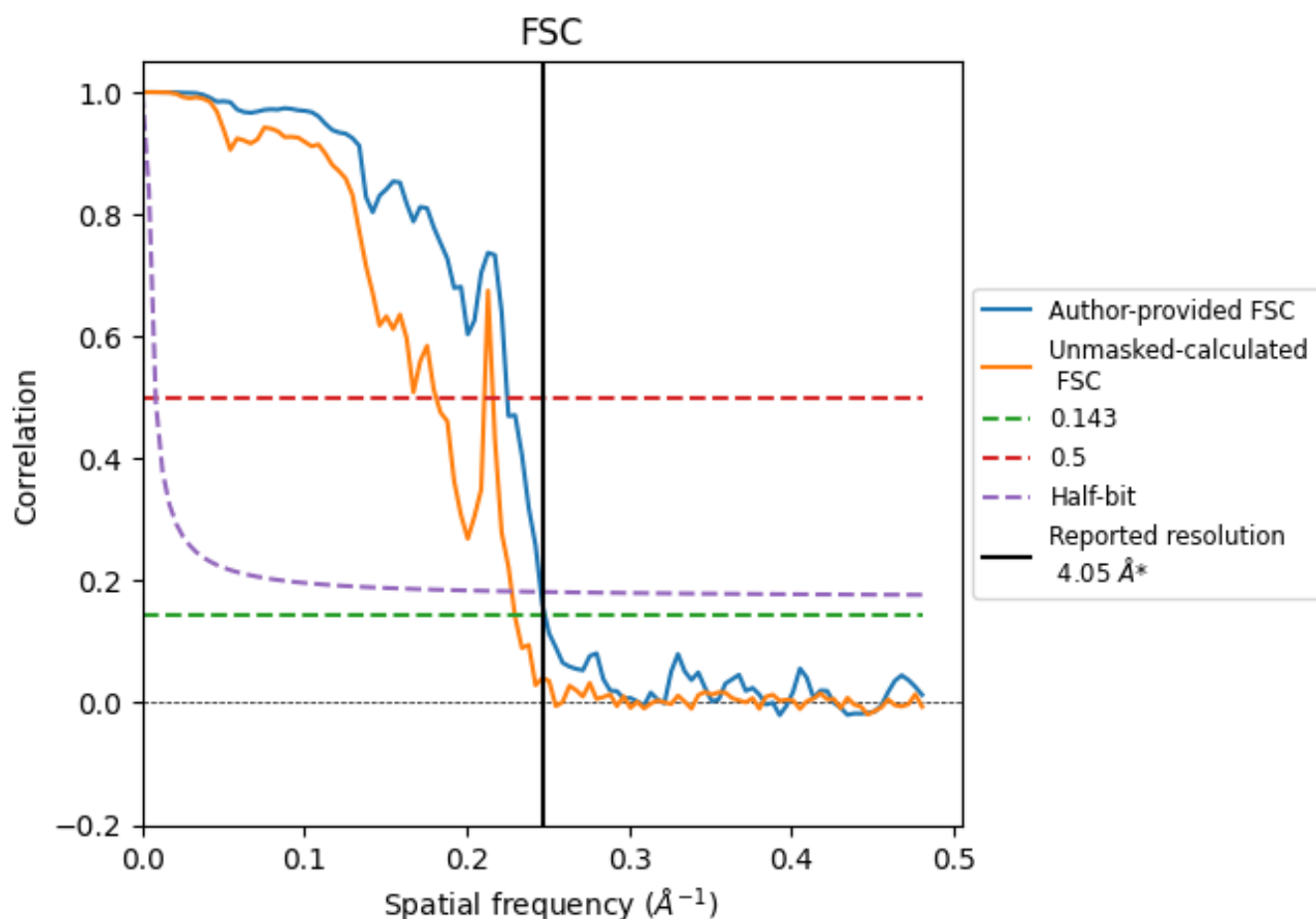


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

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 0.247 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.03	4.44	4.07
Unmasked-calculated*	4.35	5.52	4.39

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

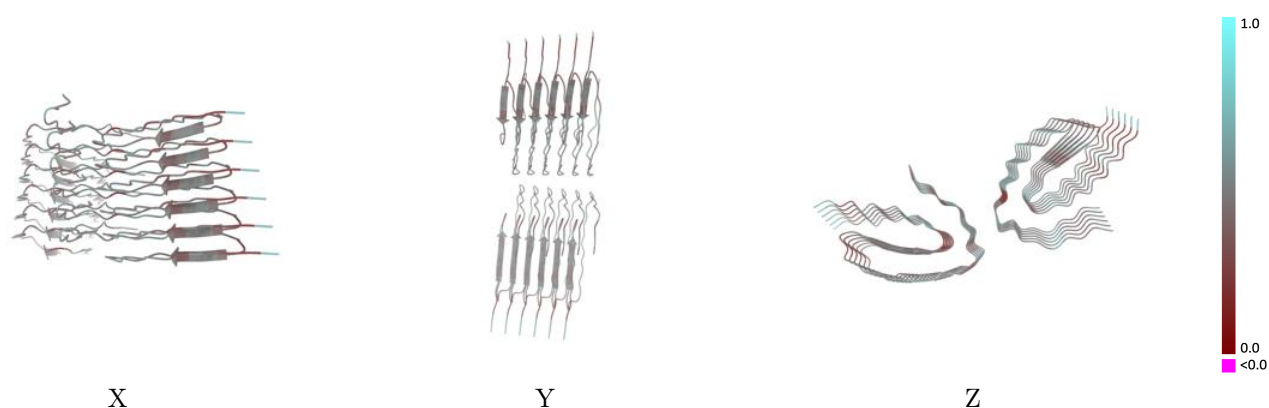
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18716 and PDB model 8QXA. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)

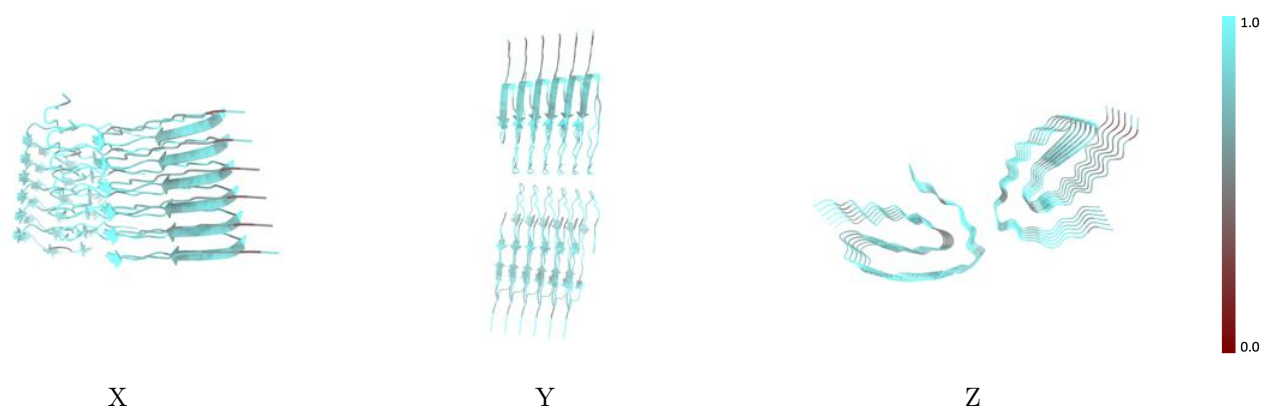
This section was not generated.

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



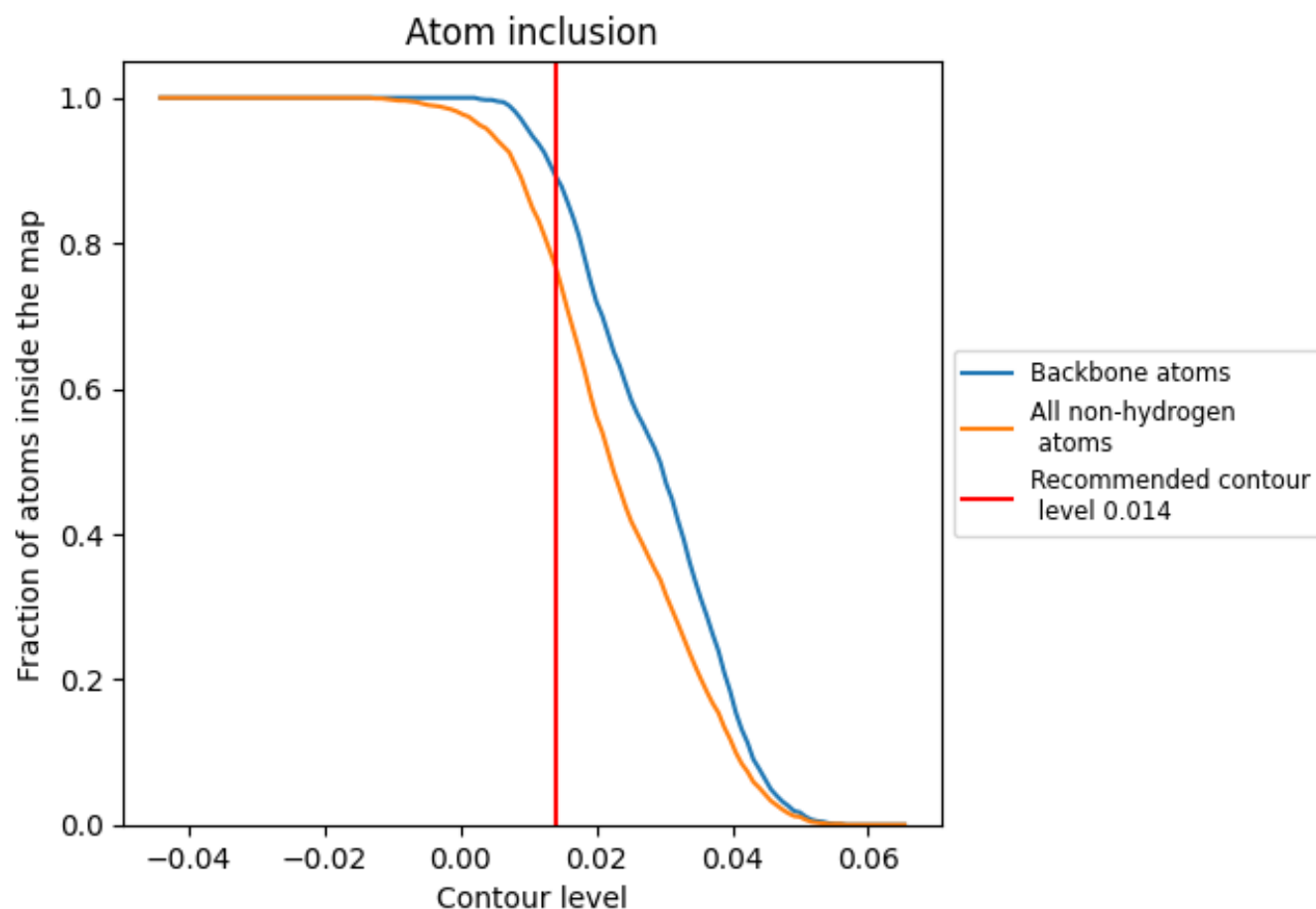
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 77% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.4530
A	0.7850	0.4520
B	0.7490	0.4540
C	0.7880	0.4520
D	0.7520	0.4510
E	0.7910	0.4540
F	0.7490	0.4540
G	0.7780	0.4540
H	0.7490	0.4540
I	0.7850	0.4500
J	0.7430	0.4500
K	0.7850	0.4530
L	0.7460	0.4530

1.0

0.0

<0.0