



## wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 04:31 pm BST

PDB ID : 7R5H  
EMDB ID : EMD-14320  
Title : In vitro assembled 266/297 - 391 tau filaments with KCl (10b)  
Authors : Lovestam, S.; Scheres, S.H.W.  
Deposited on : 2022-02-10  
Resolution : 2.59 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](mailto: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.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

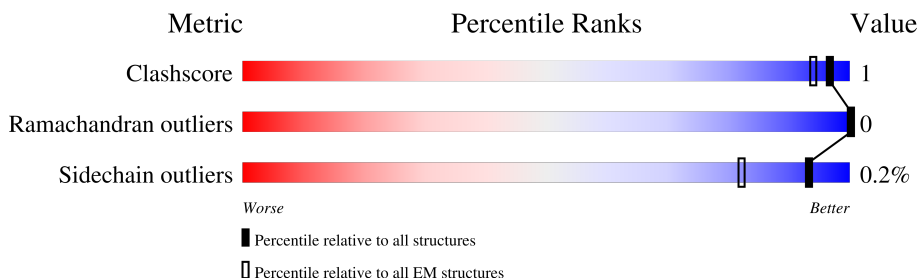
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.59 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  $\geq 3$ , 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	441	<div> <div>18%</div> <div>81%</div> </div>
1	B	441	<div> <div>18%</div> <div>81%</div> </div>
1	C	441	<div> <div>18%</div> <div>81%</div> </div>
1	D	441	<div> <div>17%</div> <div>83%</div> </div>
1	E	441	<div> <div>17%</div> <div>83%</div> </div>
1	F	441	<div> <div>17%</div> <div>83%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7440 atoms, of which 3786 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.

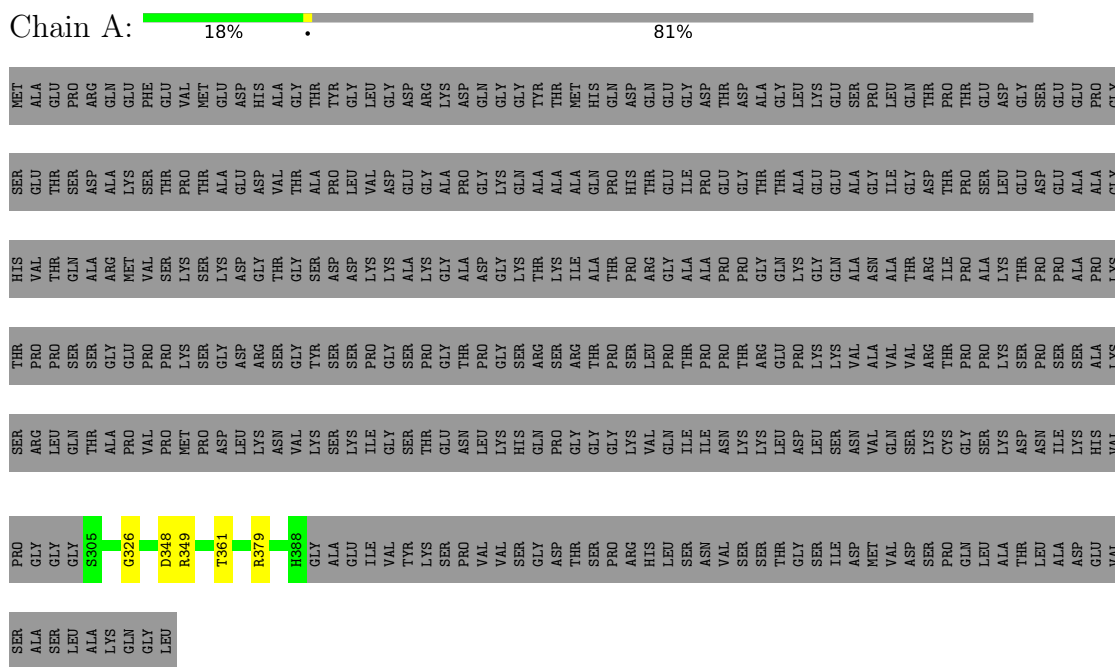
- Molecule 1 is a protein called Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	84	Total	C	H	N	O	S	0	0
			1308	401	664	120	122	1		
1	B	84	Total	C	H	N	O	S	0	0
			1308	401	664	120	122	1		
1	C	84	Total	C	H	N	O	S	0	0
			1308	401	664	120	122	1		
1	D	75	Total	C	H	N	O	S	0	0
			1172	360	598	106	107	1		
1	E	75	Total	C	H	N	O	S	0	0
			1172	360	598	106	107	1		
1	F	75	Total	C	H	N	O	S	0	0
			1172	360	598	106	107	1		

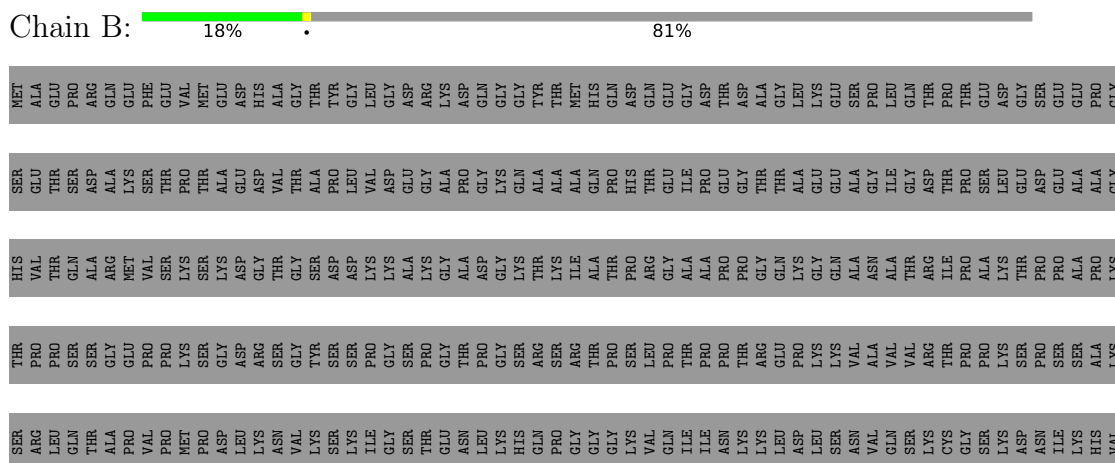
### 3 Residue-property plots

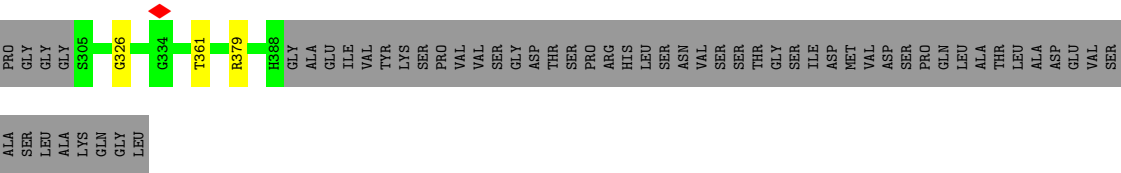
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Microtubule-associated protein tau

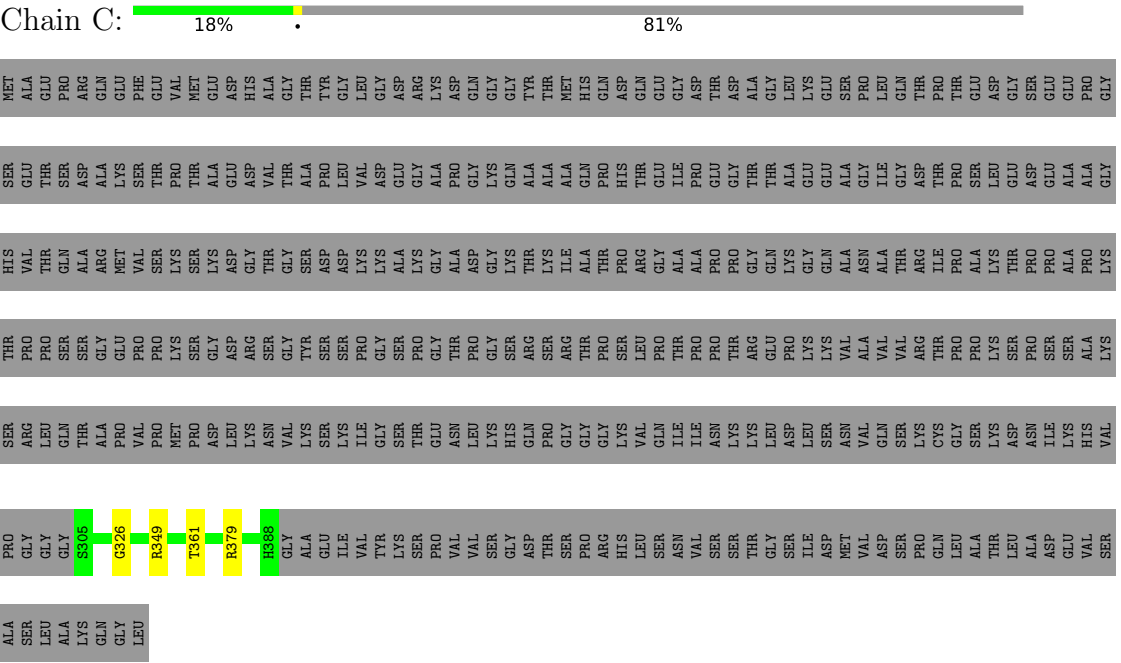


#### • Molecule 1: Microtubule-associated protein tau

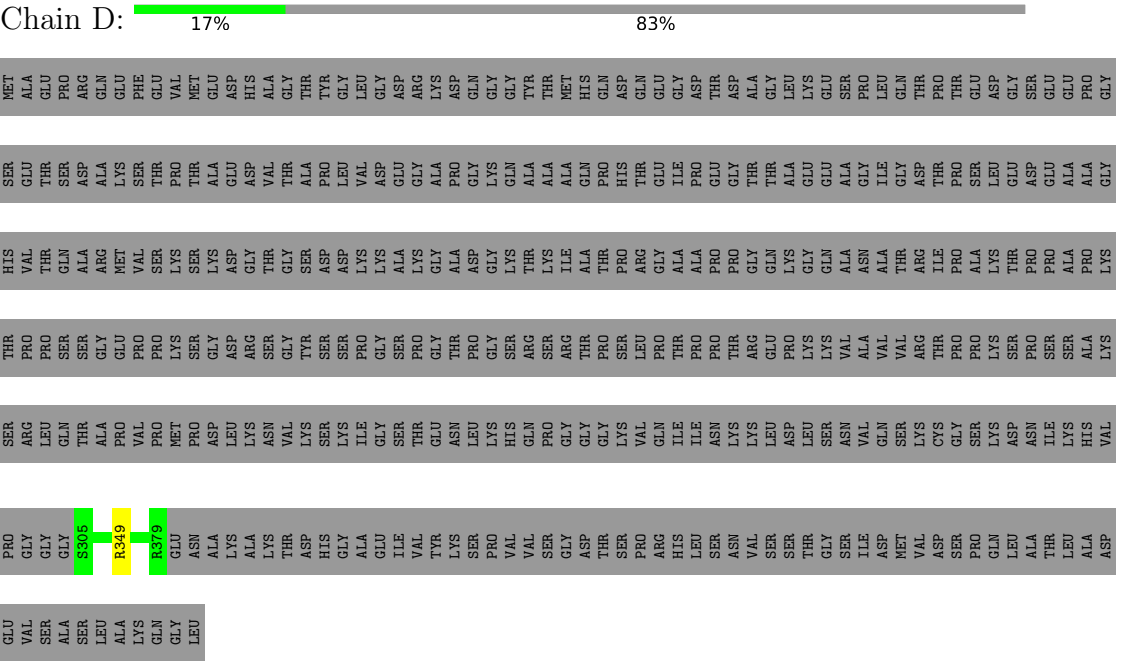




● Molecule 1: Microtubule-associated protein tau



● Molecule 1: Microtubule-associated protein tau



● Molecule 1: Microtubule-associated protein tau

83%

- Molecule 1: Microtubule-associated protein tau

83%

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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-0.88°, rise=4.77 Å, axial sym=C1	Depositor
Number of segments used	111483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00579	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	0/654	0.95	2/875 (0.2%)
1	B	0.53	0/654	0.94	1/875 (0.1%)
1	C	0.53	0/654	0.93	2/875 (0.2%)
1	D	0.54	0/583	0.91	1/780 (0.1%)
1	E	0.53	0/583	0.89	1/780 (0.1%)
1	F	0.53	0/583	0.89	0/780
All	All	0.53	0/3711	0.92	7/4965 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	349	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	379	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	379	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	379	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	349	ARG	NE-CZ-NH1	5.21	122.90	120.30

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	644	664	663	2	0
1	B	644	664	663	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	644	664	663	2	0
1	D	574	598	597	0	0
1	E	574	598	597	0	0
1	F	574	598	597	0	0
All	All	3654	3786	3780	5	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 1.

All (5) 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:A:326:GLY:CA	1:A:361:THR:HG21	2.41	0.50
1:C:326:GLY:HA2	1:C:361:THR:HG21	1.98	0.45
1:A:326:GLY:HA2	1:A:361:THR:HG21	1.98	0.45
1:B:326:GLY:HA3	1:B:361:THR:HG21	1.99	0.44
1:C:326:GLY:CA	1:C:361:THR:HG21	2.50	0.42

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	82/441 (19%)	77 (94%)	5 (6%)	0	100	100
1	B	82/441 (19%)	79 (96%)	3 (4%)	0	100	100
1	C	82/441 (19%)	78 (95%)	4 (5%)	0	100	100
1	D	73/441 (17%)	72 (99%)	1 (1%)	0	100	100
1	E	73/441 (17%)	72 (99%)	1 (1%)	0	100	100
1	F	73/441 (17%)	72 (99%)	1 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	465/2646 (18%)	450 (97%)	15 (3%)	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	73/358 (20%)	72 (99%)	1 (1%)	67	85
1	B	73/358 (20%)	73 (100%)	0	100	100
1	C	73/358 (20%)	73 (100%)	0	100	100
1	D	66/358 (18%)	66 (100%)	0	100	100
1	E	66/358 (18%)	66 (100%)	0	100	100
1	F	66/358 (18%)	66 (100%)	0	100	100
All	All	417/2148 (19%)	416 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	B	327	ASN
1	C	327	ASN

### 5.3.3 RNA ⓘ

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.

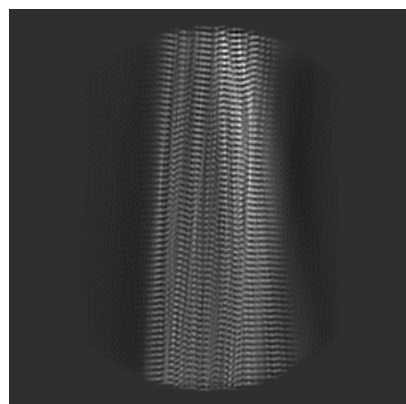
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14320. These allow visual inspection of the internal detail of the map and identification of artifacts.

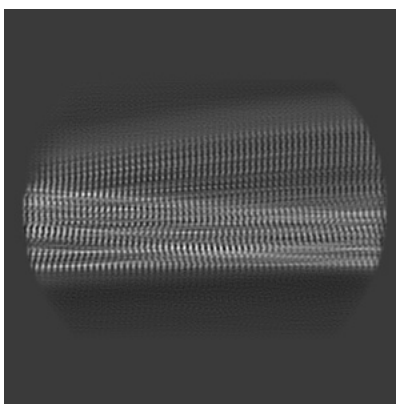
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

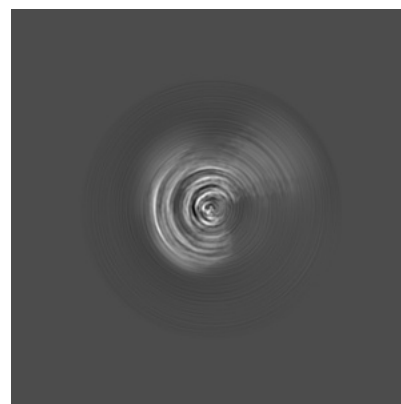
#### 6.1.1 Primary map



X

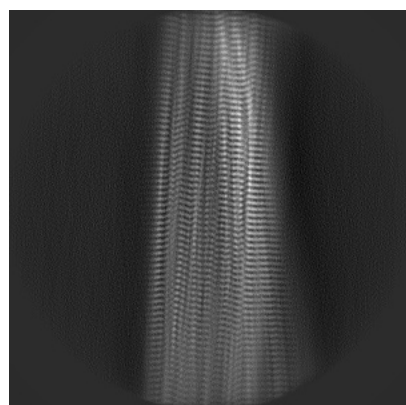


Y

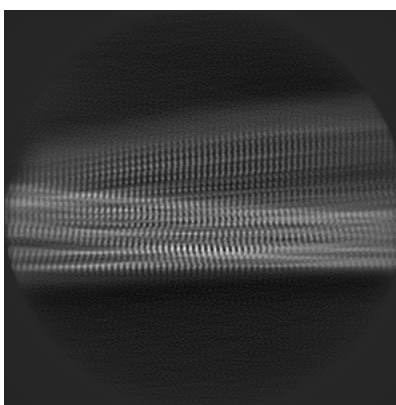


Z

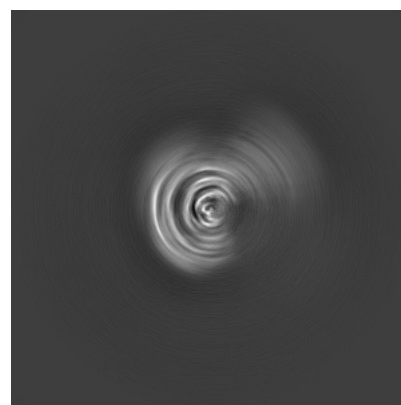
#### 6.1.2 Raw map



X



Y

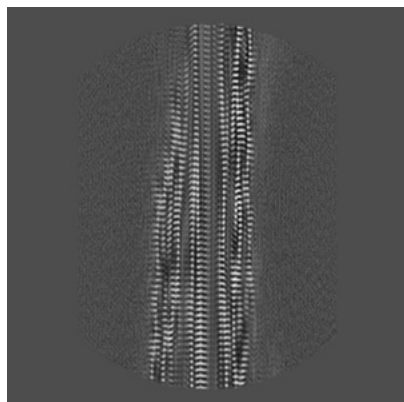


Z

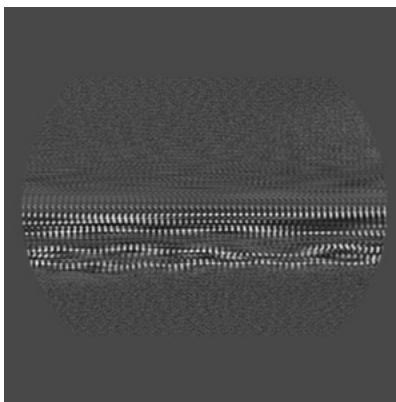
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

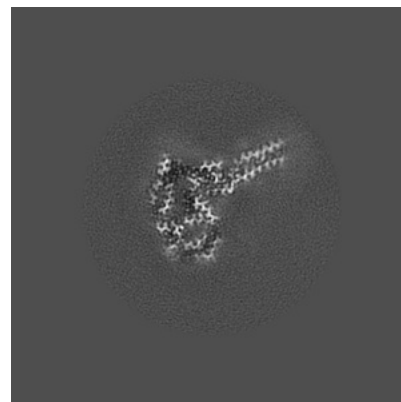
### 6.2.1 Primary map



X Index: 192

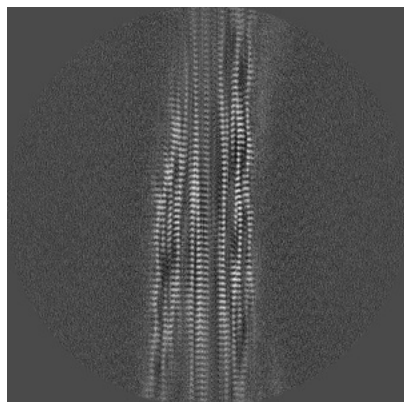


Y Index: 192

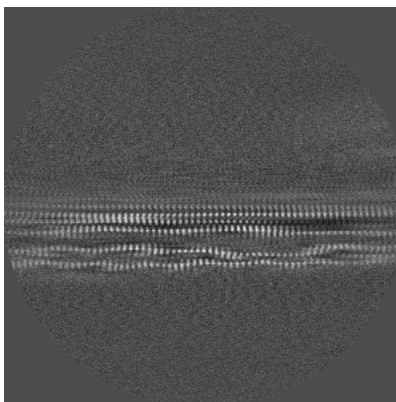


Z Index: 192

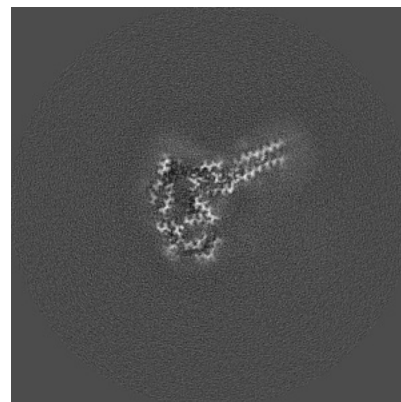
### 6.2.2 Raw map



X Index: 192



Y Index: 192

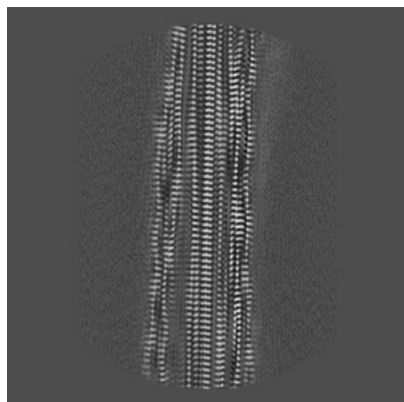


Z Index: 192

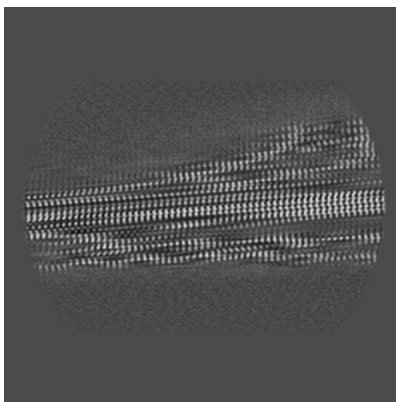
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

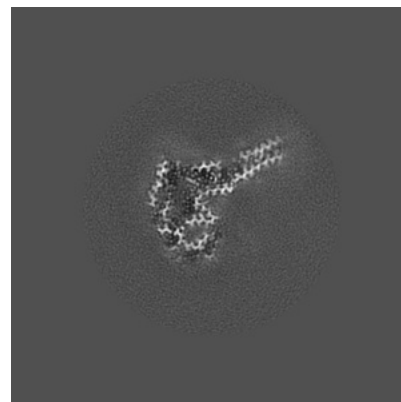
### 6.3.1 Primary map



X Index: 184

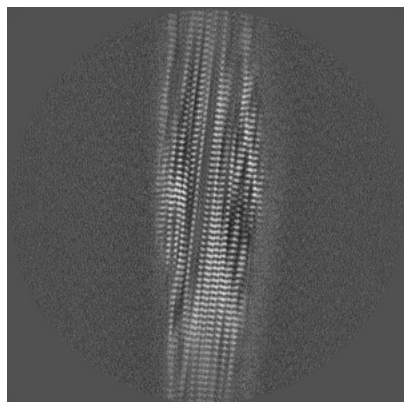


Y Index: 221

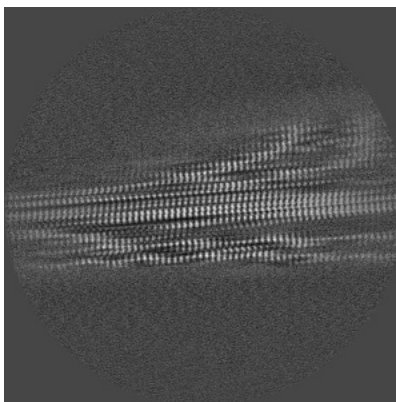


Z Index: 181

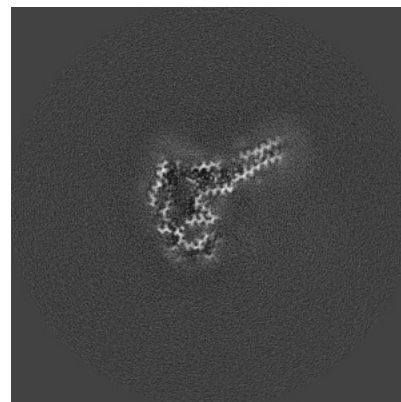
### 6.3.2 Raw map



X Index: 151



Y Index: 221

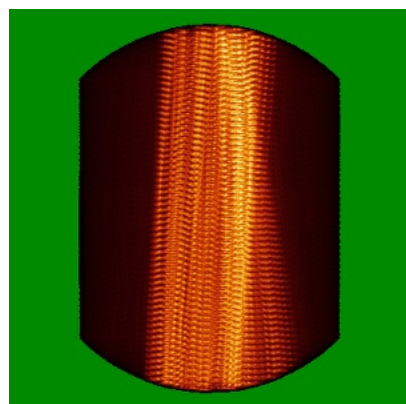


Z Index: 181

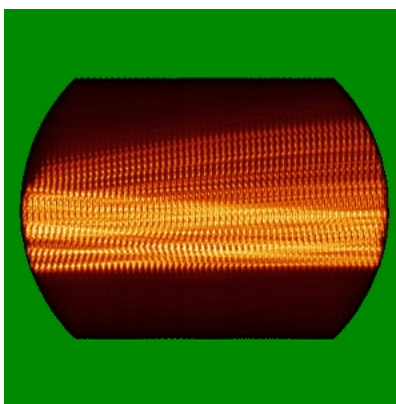
The images above show the largest variance slices of the map in three orthogonal directions.

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

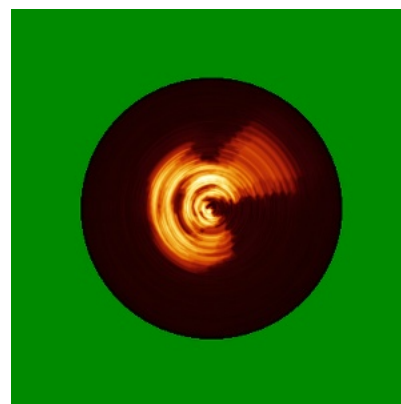
### 6.4.1 Primary map



X

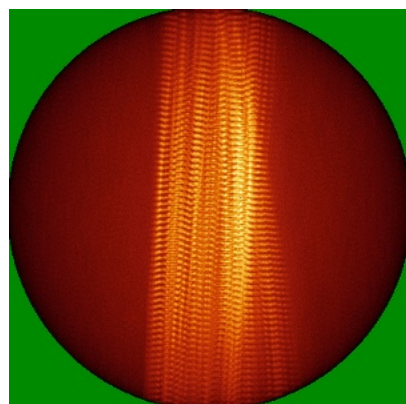


Y

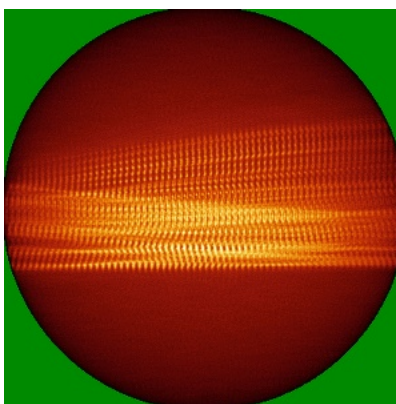


Z

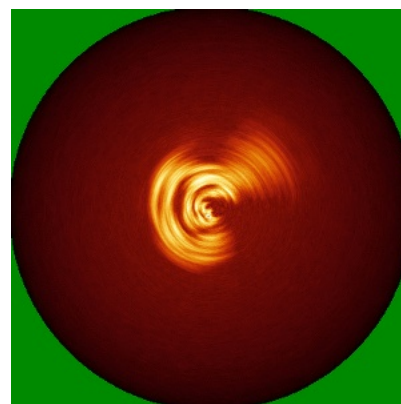
### 6.4.2 Raw map



X



Y

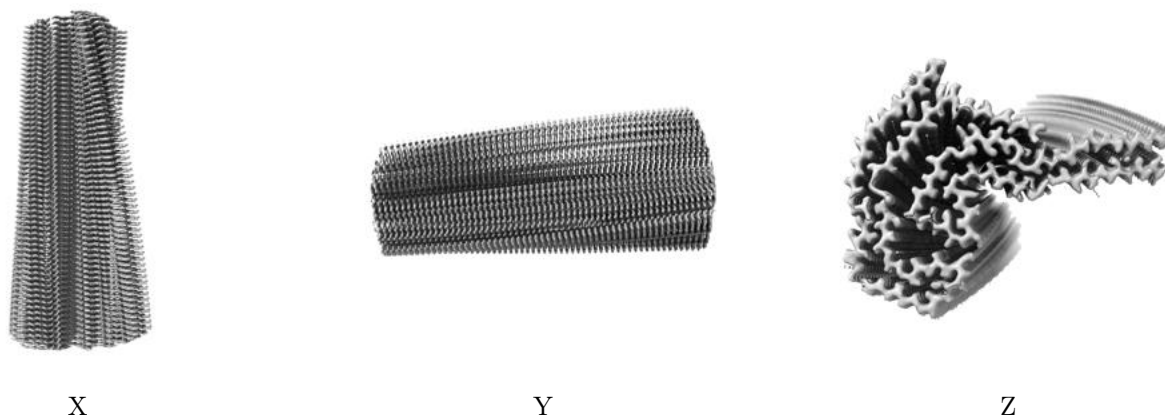


Z

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.

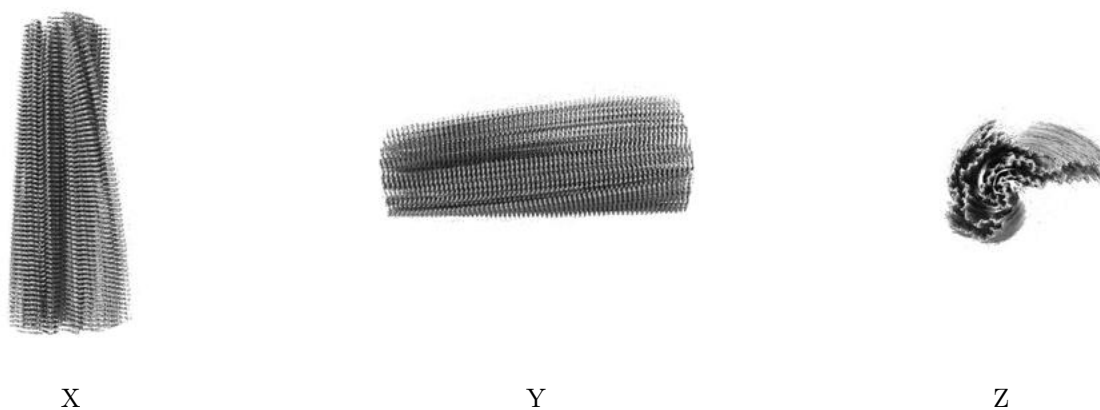
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00579. 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.

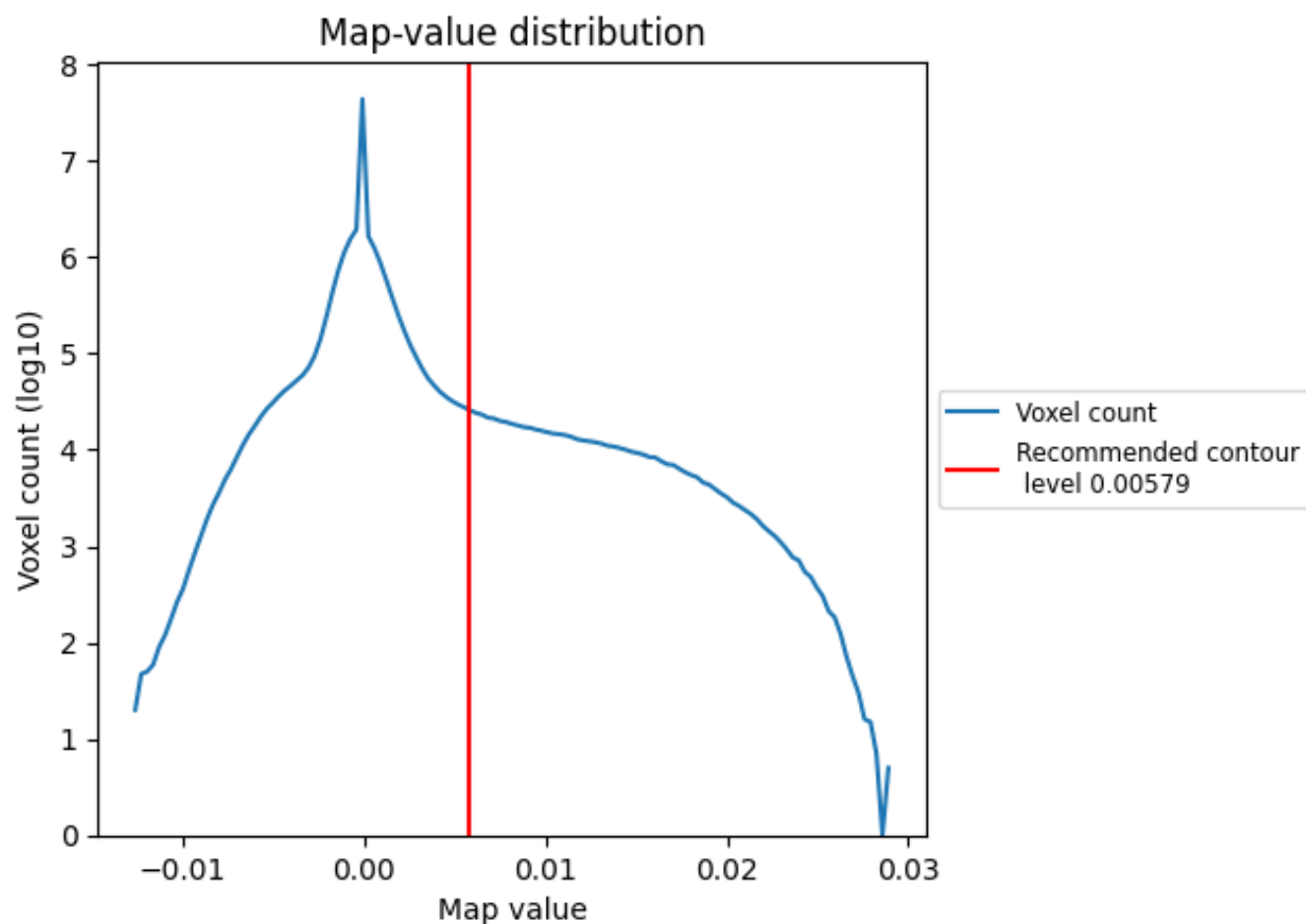
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

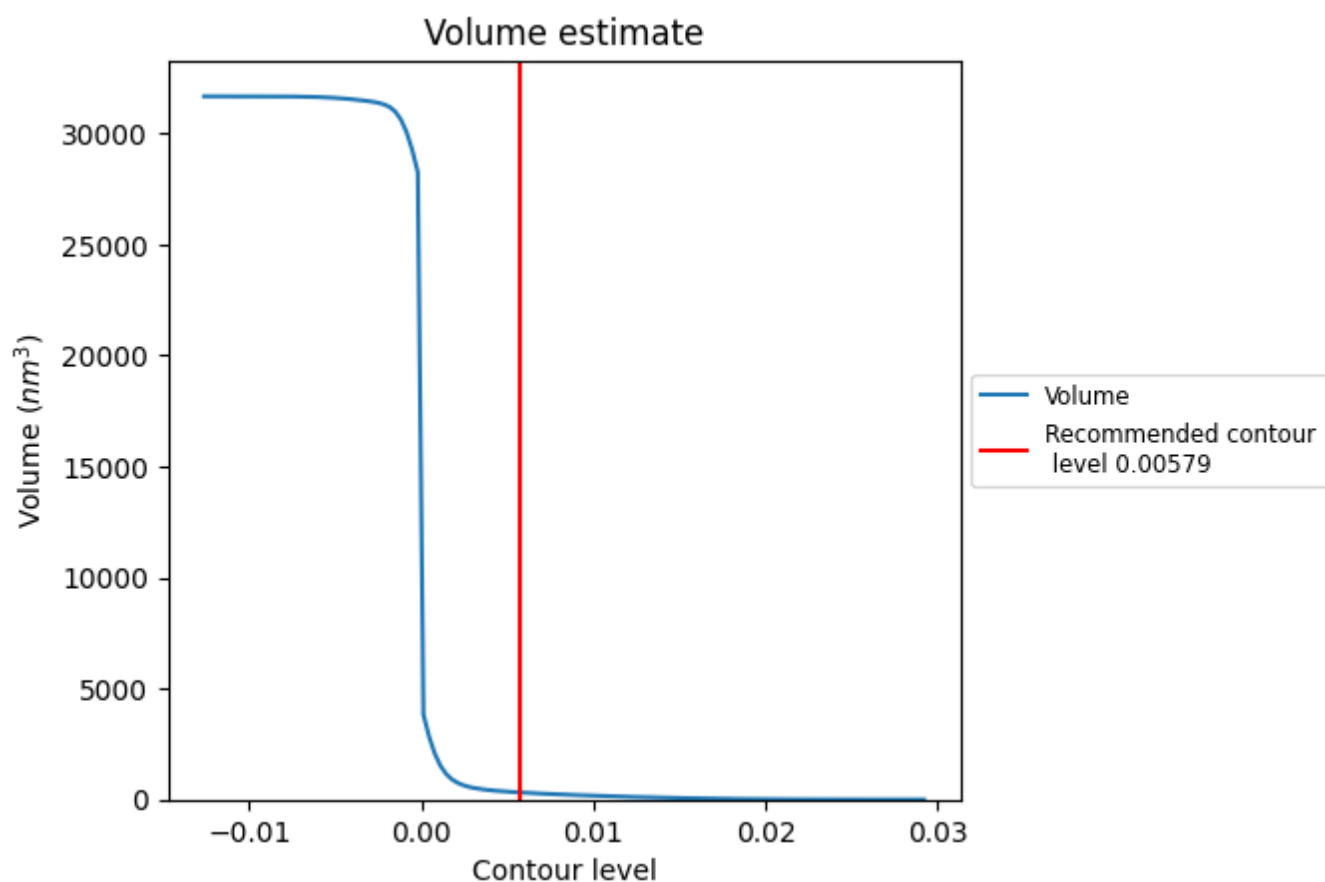
This section contains the results of statistical analysis of the map.

### 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.

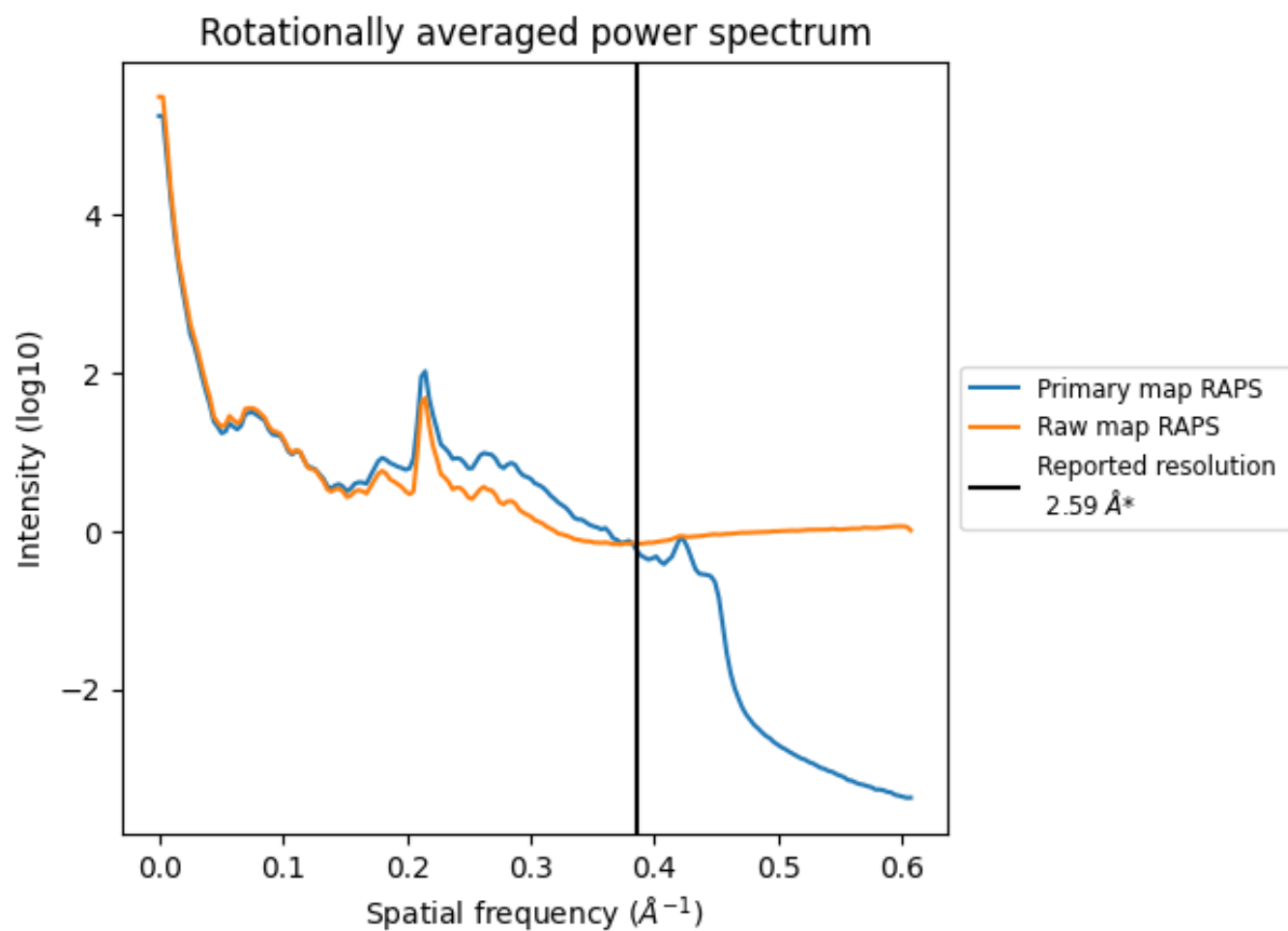
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 318 nm<sup>3</sup>; 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 ⓘ

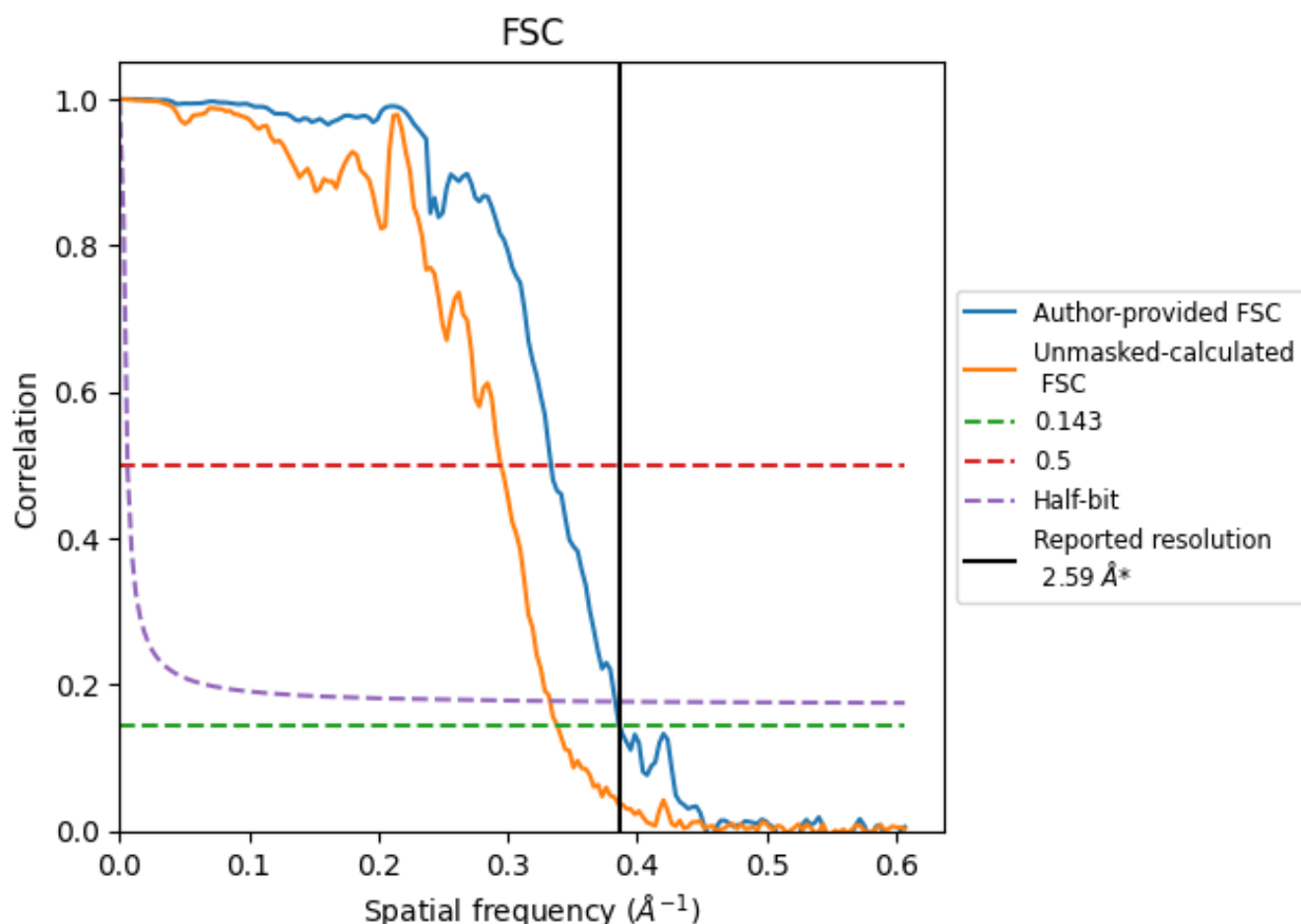


\*Reported resolution corresponds to spatial frequency of 0.386 Å<sup>-1</sup>

## 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 0.386 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	3.00	2.61
Unmasked-calculated*	2.96	3.39	3.01

\*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 2.96 differs from the reported value 2.59 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14320 and PDB model 7R5H. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

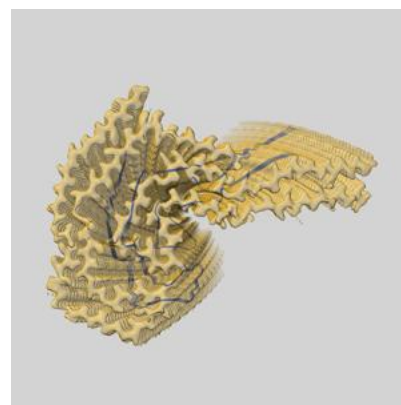
### 9.1 Map-model overlay [i](#)



X



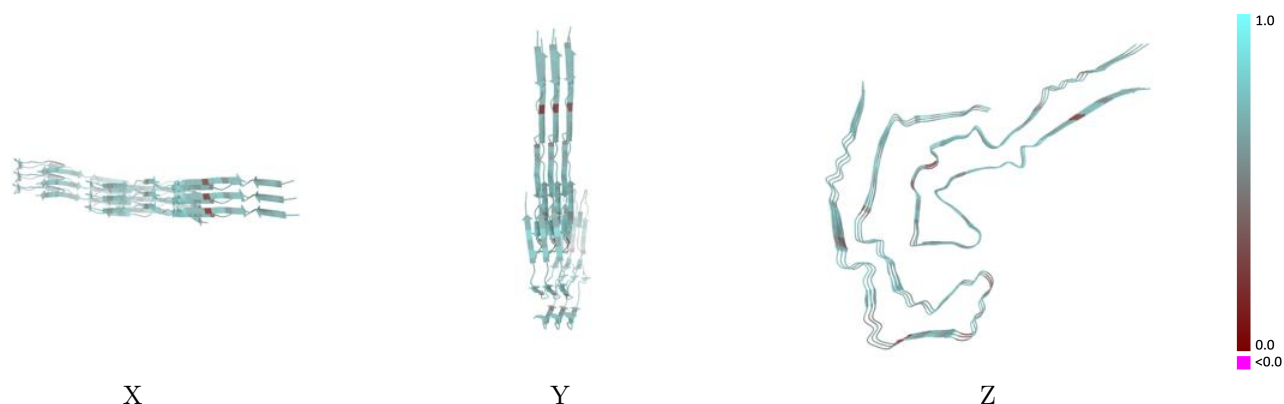
Y



Z

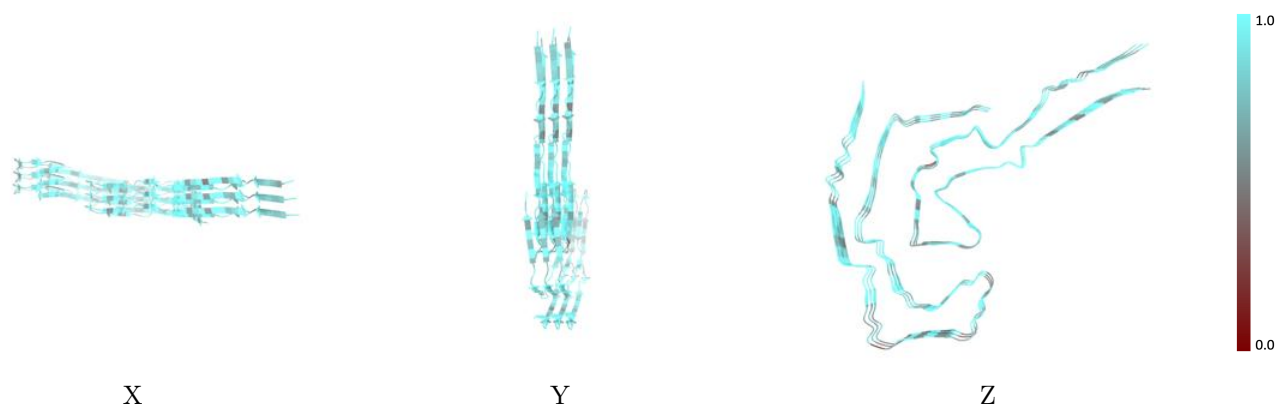
The images above show the 3D surface view of the map at the recommended contour level 0.00579 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



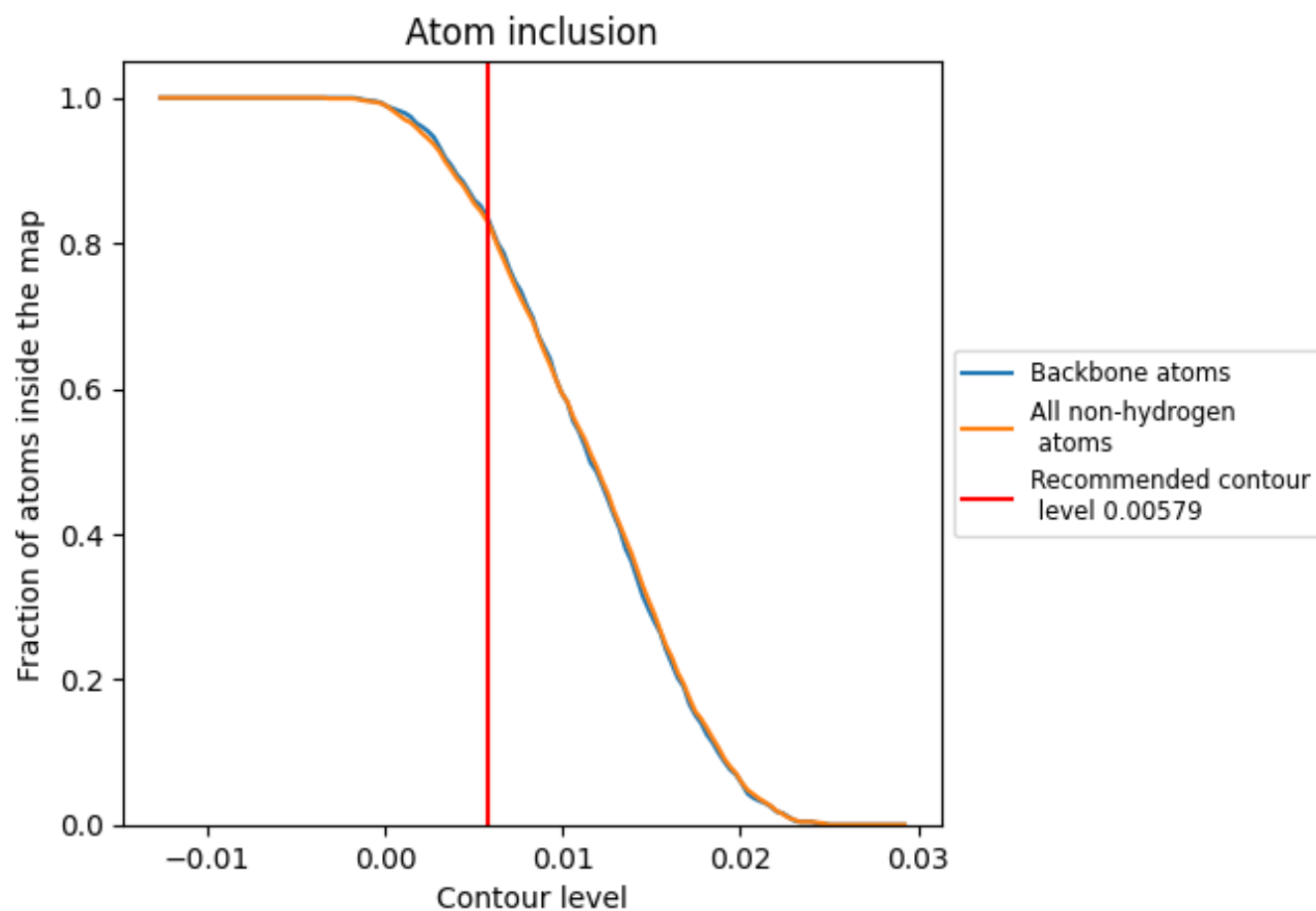
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00579).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.00579) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8290	<div></div> 0.6210
A	<div></div> 0.8230	<div></div> 0.6210
B	<div></div> 0.8250	<div></div> 0.6190
C	<div></div> 0.8280	<div></div> 0.6160
D	<div></div> 0.8280	<div></div> 0.6260
E	<div></div> 0.8260	<div></div> 0.6220
F	<div></div> 0.8240	<div></div> 0.6230

