



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2022 – 04:33 am GMT

PDB ID : 7QKH  
EMDB ID : EMD-14042  
Title : In vitro assembled 258-391 tau filaments with sodium azide, (41a)  
Authors : Lovestam, S.; Scheres, S.H.W.  
Deposited on : 2021-12-17  
Resolution : 3.17 Å (reported)

This is a Full wwPDB EM Validation 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.0.dev97  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

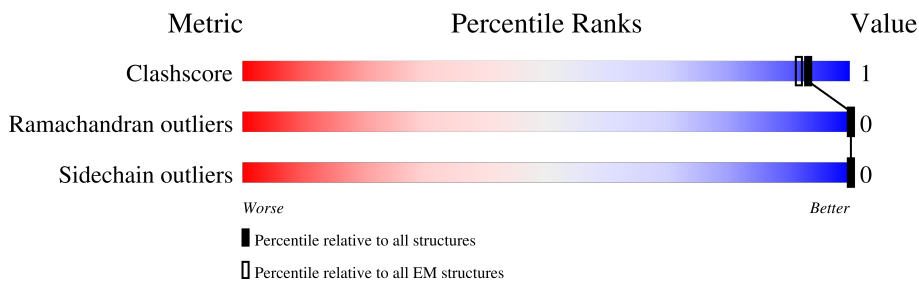
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.17 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	7% 92%
1	B	441	8% 92%
1	C	441	7% 92%
1	D	441	8% 92%
1	E	441	7% 92%
1	G	441	7% 92%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3105 atoms, of which 1593 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.

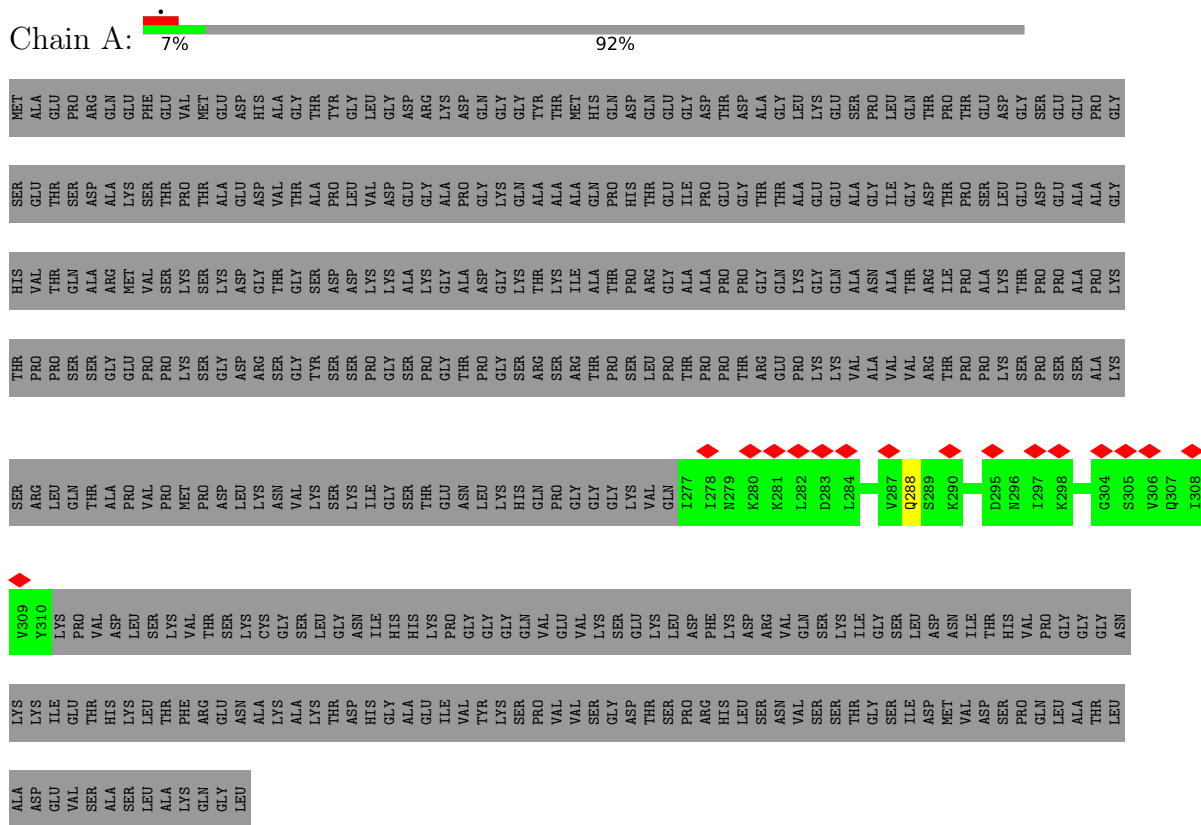
- Molecule 1 is a protein called Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	34	523	159	269	46	48	1	0	0
1	G	34	512	156	262	45	48	1	0	0
1	B	34	523	159	269	46	48	1	0	0
1	C	34	512	156	262	45	48	1	0	0
1	D	34	523	159	269	46	48	1	0	0
1	E	34	512	156	262	45	48	1	0	0

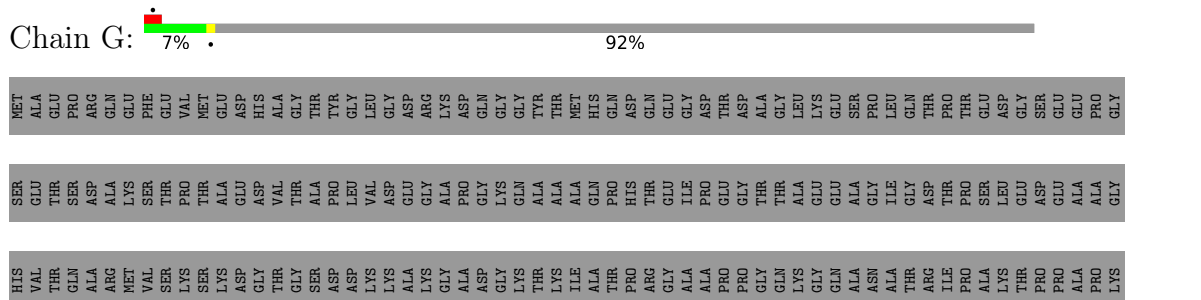
### 3 Residue-property plots [i](#)

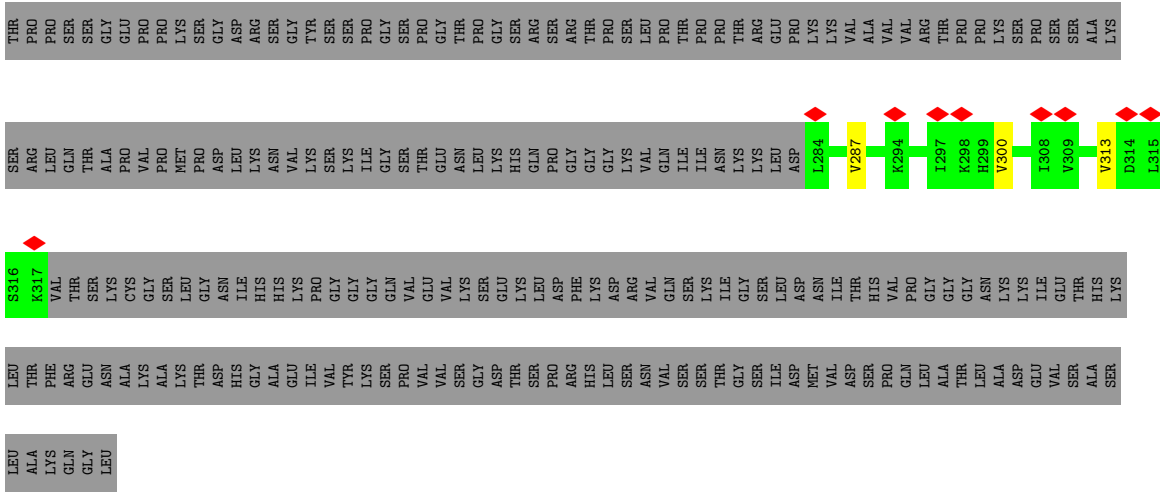
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



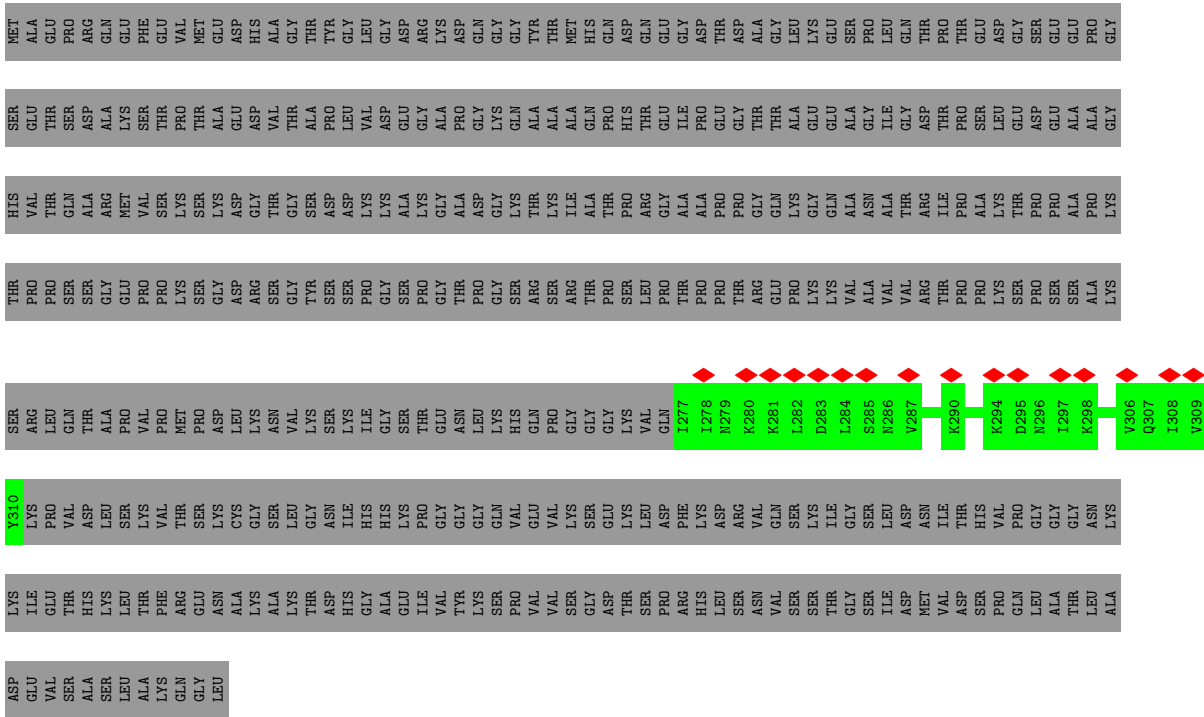
- Molecule 1: Microtubule-associated protein tau





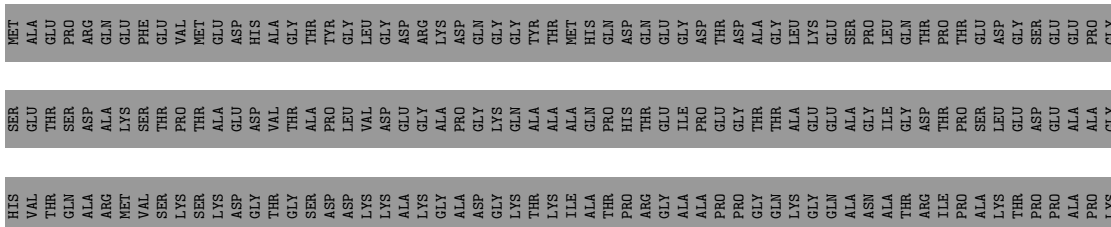
• Molecule 1: Microtubule-associated protein tau

Chain B: 8% 92%



• Molecule 1: Microtubule-associated protein tau

Chain C: 7% 92%





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

THR PRO  
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SER SER  
LYS LYS  
GLY ASP  
ARG ASP  
GLY THR  
SER THR  
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SER SER  
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ALA SER  
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VAL VAL  
MET MET  
SER SER  
ASP ASP  
LEU LEU  
LYS LYS  
ASN ASN  
VAL VAL  
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ILE ILE  
GLY GLY  
THR THR  
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THR THR  
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LEU LEU  
ASP ASP  
L284  
V287  
K284  
I287  
V300  
S305  
I308  
V309  
V313  
D314

L315  
S316  
K317  
VAL THR  
SER SER  
LYS LYS  
CYS CYS  
GLY GLY  
SER SER  
LEU LEU  
GLY ASP  
ASN ASN  
ILE ILE  
HIS HIS  
HIS HIS  
LYS LYS  
PRO PRO  
VAL VAL  
GLY GLY  
GLN GLN  
VAL VAL  
GLU GLU  
VAL VAL  
SER SER  
LYS LYS  
GLU GLU  
THR THR  
LYS LYS  
LEU LEU  
PHE PHE  
LYS LYS  
ASP ASP  
ARG ARG  
VAL VAL  
GLN GLN  
SER SER  
LYS LYS  
ILE ILE  
GLY GLY  
SER SER  
LEU LEU  
ASN ASN  
VAL VAL  
ILE ILE  
THR THR  
HIS HIS  
VAL VAL  
PRO PRO  
GLY GLY  
GLY GLY  
ASN ASN  
GLY GLY  
SER SER  
LYS LYS  
ILE ILE  
THR THR  
HIS HIS  
VAL VAL  
LEU LEU  
ALA ALA  
THR THR  
LEU LEU  
ASP ASP  
GLU GLU  
VAL VAL  
THR THR  
HIS HIS

LYS LEU  
THR THR  
PHE PHE  
ARG ARG  
GLU GLU  
ASN ASN  
ALA ALA  
LYS LYS  
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THR THR  
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ALA ALA  
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VAL VAL  
VAL VAL  
SER SER  
GLY GLY  
THR THR  
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ARG ARG  
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LEU LEU  
SER SER  
ASN ASN  
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LEU LEU  
ALA ALA  
ASP ASP  
GLU GLU  
VAL VAL  
SER SER  
ALA ALA

SER LEU  
LEU ALA  
LYS LYS  
GLN GLY  
LEU LEU

## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-0.807°, rise=4.77 Å, axial sym=C1	Depositor
Number of segments used	26532	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)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0171	Depositor
Map size (Å)	279.168, 279.168, 279.168	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.454, 1.454, 1.454	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	0.52	0/256	1.22	1/342 (0.3%)
1	B	0.50	0/256	1.10	0/342
1	C	0.51	0/253	1.15	1/339 (0.3%)
1	D	0.49	0/256	1.05	0/342
1	E	0.55	0/253	1.31	3/339 (0.9%)
1	G	0.54	0/253	1.38	2/339 (0.6%)
All	All	0.52	0/1527	1.21	7/2043 (0.3%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	313	VAL	CA-CB-CG1	12.10	129.05	110.90
1	G	287	VAL	CA-CB-CG1	11.40	128.00	110.90
1	E	287	VAL	CA-CB-CG1	10.48	126.63	110.90
1	C	287	VAL	CA-CB-CG1	10.19	126.18	110.90
1	E	313	VAL	CA-CB-CG1	9.74	125.52	110.90
1	E	300	VAL	CG1-CB-CG2	-6.04	101.24	110.90
1	A	288	GLN	C-N-CA	5.49	135.41	121.70

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	254	269	268	0	0
1	B	254	269	268	0	0
1	C	250	262	261	1	0
1	D	254	269	268	0	0
1	E	250	262	261	2	0
1	G	250	262	261	4	0
All	All	1512	1593	1587	4	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 (4) 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:G:300:VAL:HG22	1:E:300:VAL:HG12	1.64	0.77
1:G:300:VAL:HG12	1:C:300:VAL:HG22	1.96	0.48
1:G:300:VAL:O	1:G:300:VAL:HG23	2.18	0.42
1:G:300:VAL:HG22	1:E:300:VAL:CG1	2.43	0.40

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	32/441 (7%)	28 (88%)	4 (12%)	0	100	100
1	B	32/441 (7%)	26 (81%)	6 (19%)	0	100	100
1	C	32/441 (7%)	28 (88%)	4 (12%)	0	100	100
1	D	32/441 (7%)	26 (81%)	6 (19%)	0	100	100
1	E	32/441 (7%)	28 (88%)	4 (12%)	0	100	100
1	G	32/441 (7%)	28 (88%)	4 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	192/2646 (7%)	164 (85%)	28 (15%)	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	30/358 (8%)	30 (100%)	0	100	100
1	B	30/358 (8%)	30 (100%)	0	100	100
1	C	30/358 (8%)	30 (100%)	0	100	100
1	D	30/358 (8%)	30 (100%)	0	100	100
1	E	30/358 (8%)	30 (100%)	0	100	100
1	G	30/358 (8%)	30 (100%)	0	100	100
All	All	180/2148 (8%)	180 (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.

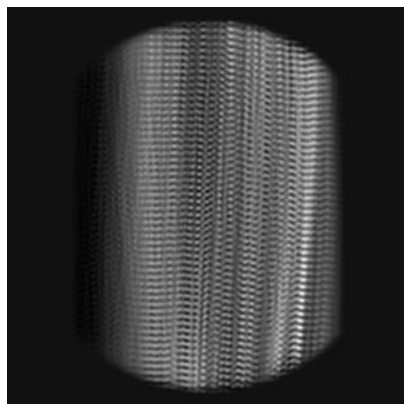
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14042. These allow visual inspection of the internal detail of the map and identification of artifacts.

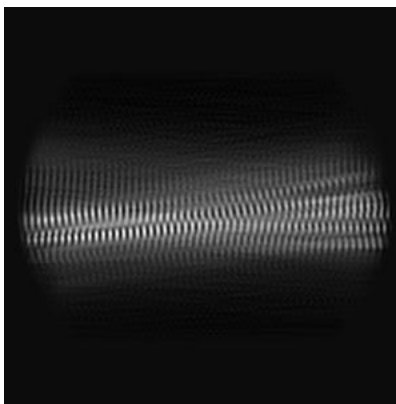
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

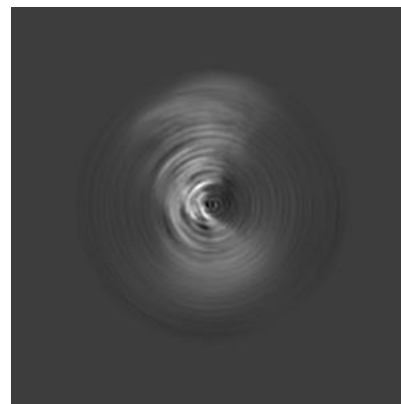
#### 6.1.1 Primary map



X

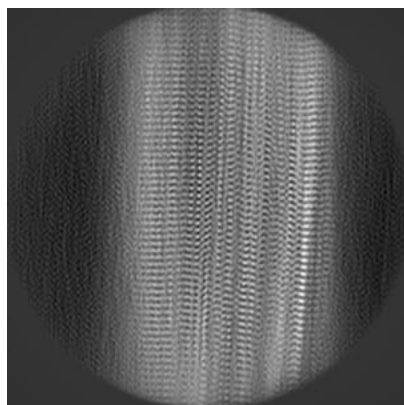


Y

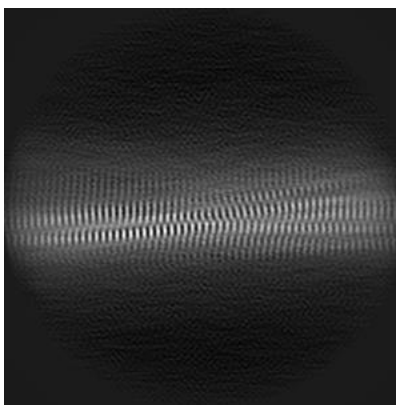


Z

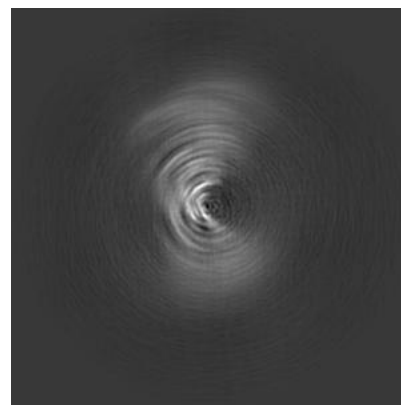
#### 6.1.2 Raw map



X



Y

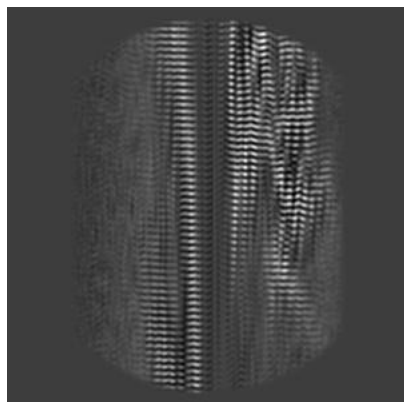


Z

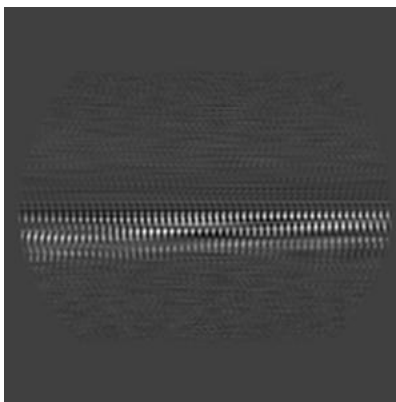
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

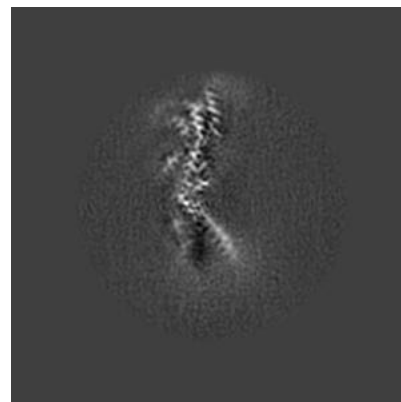
### 6.2.1 Primary map



X Index: 96

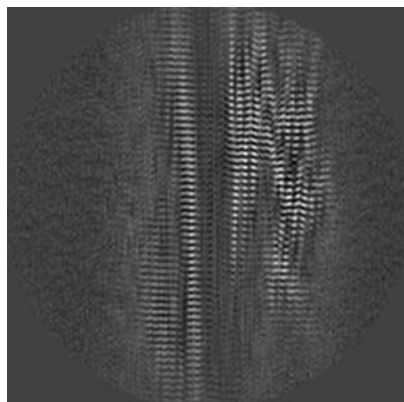


Y Index: 96

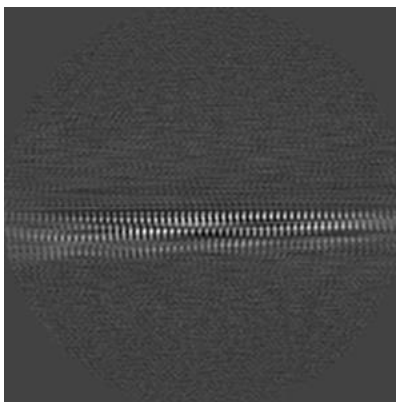


Z Index: 96

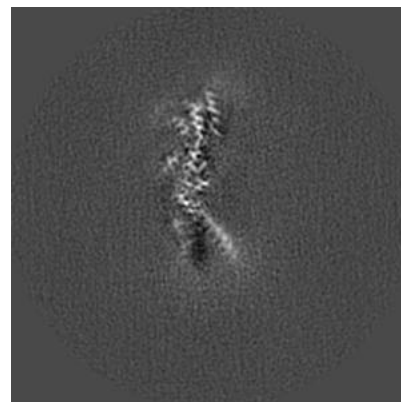
### 6.2.2 Raw map



X Index: 96



Y Index: 96

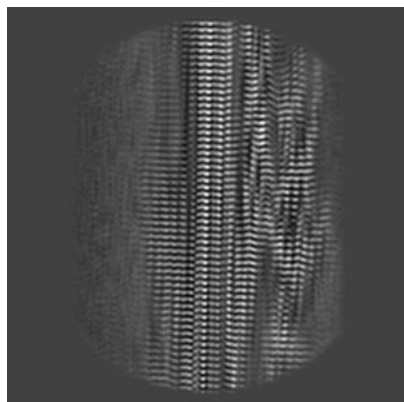


Z Index: 96

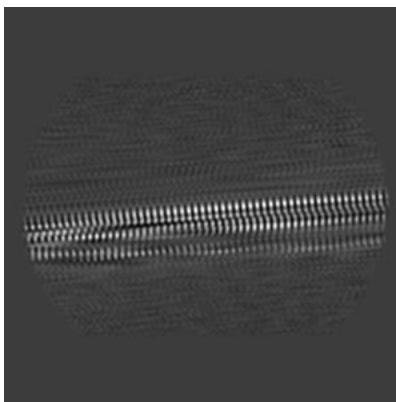
The images above show central slices of the map in three orthogonal directions.

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

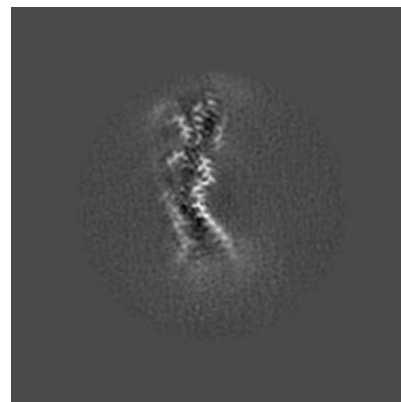
### 6.3.1 Primary map



X Index: 91

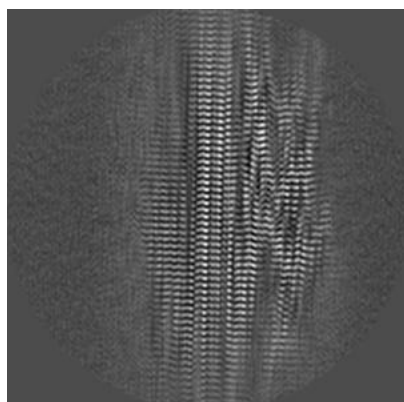


Y Index: 114

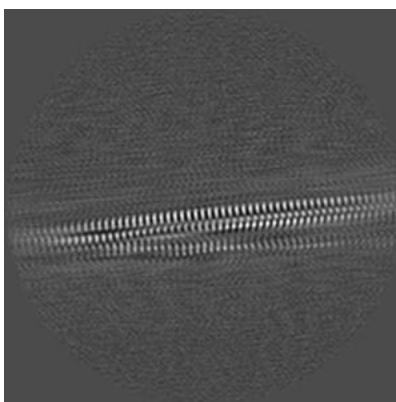


Z Index: 92

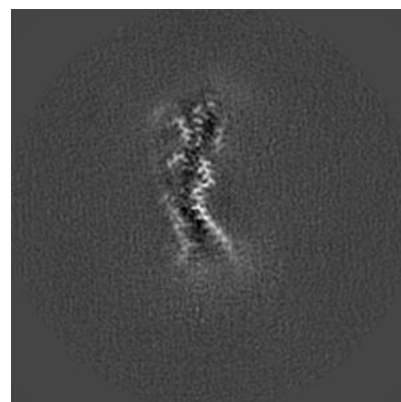
### 6.3.2 Raw map



X Index: 91



Y Index: 118

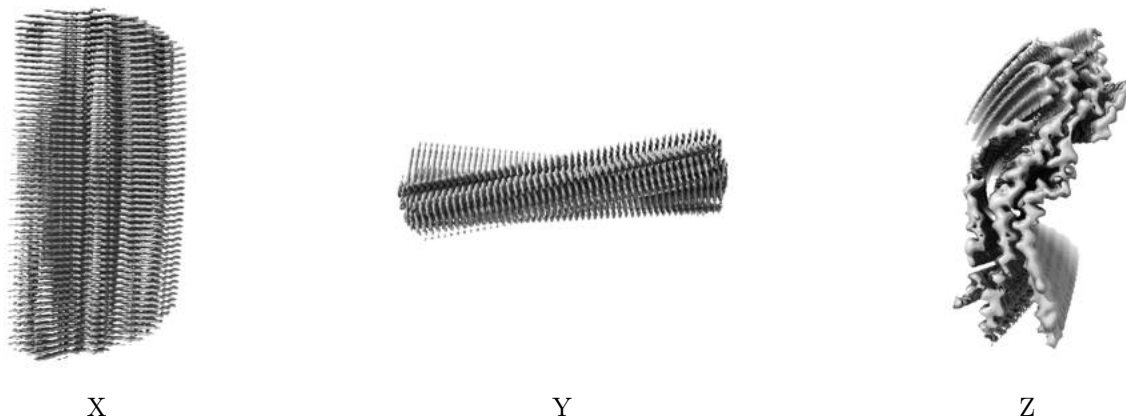


Z Index: 92

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

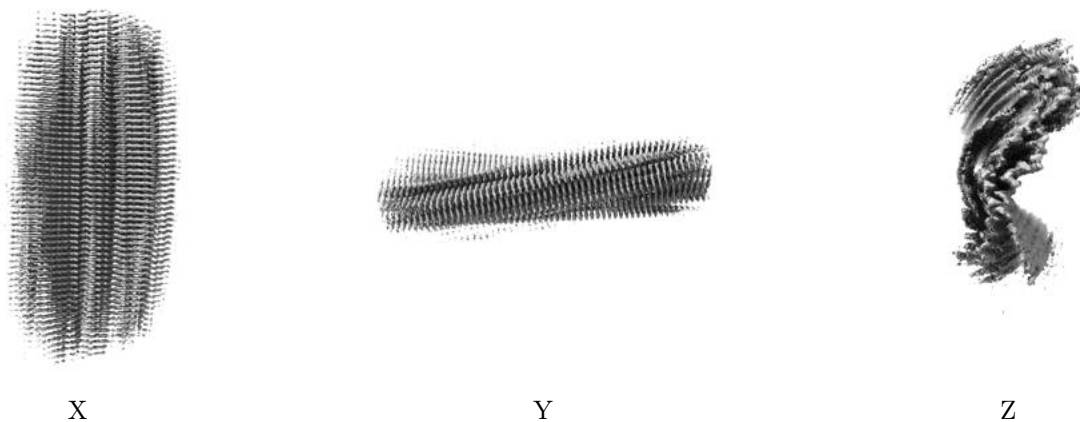
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0171. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

## 6.5 Mask visualisation [i](#)

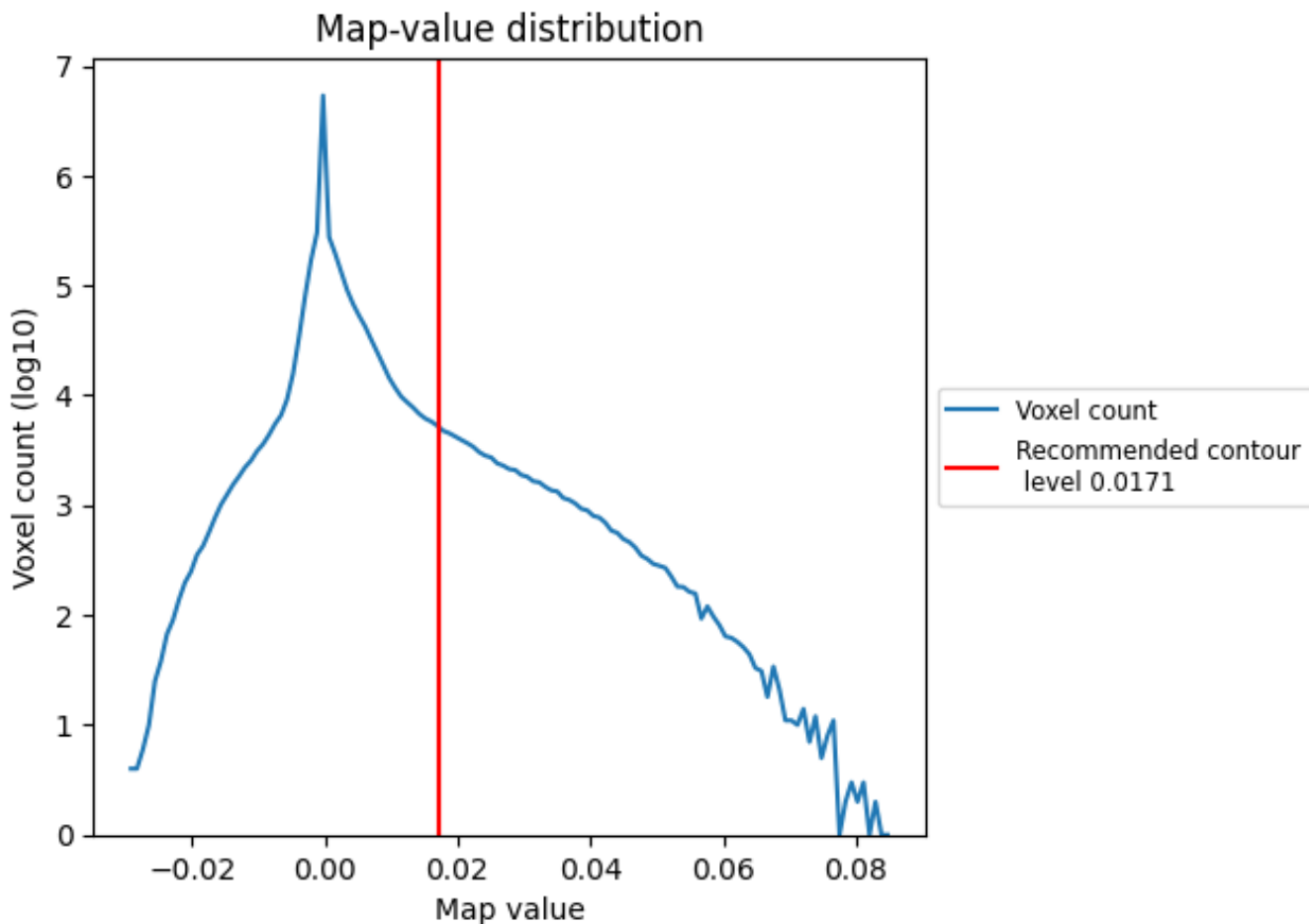
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

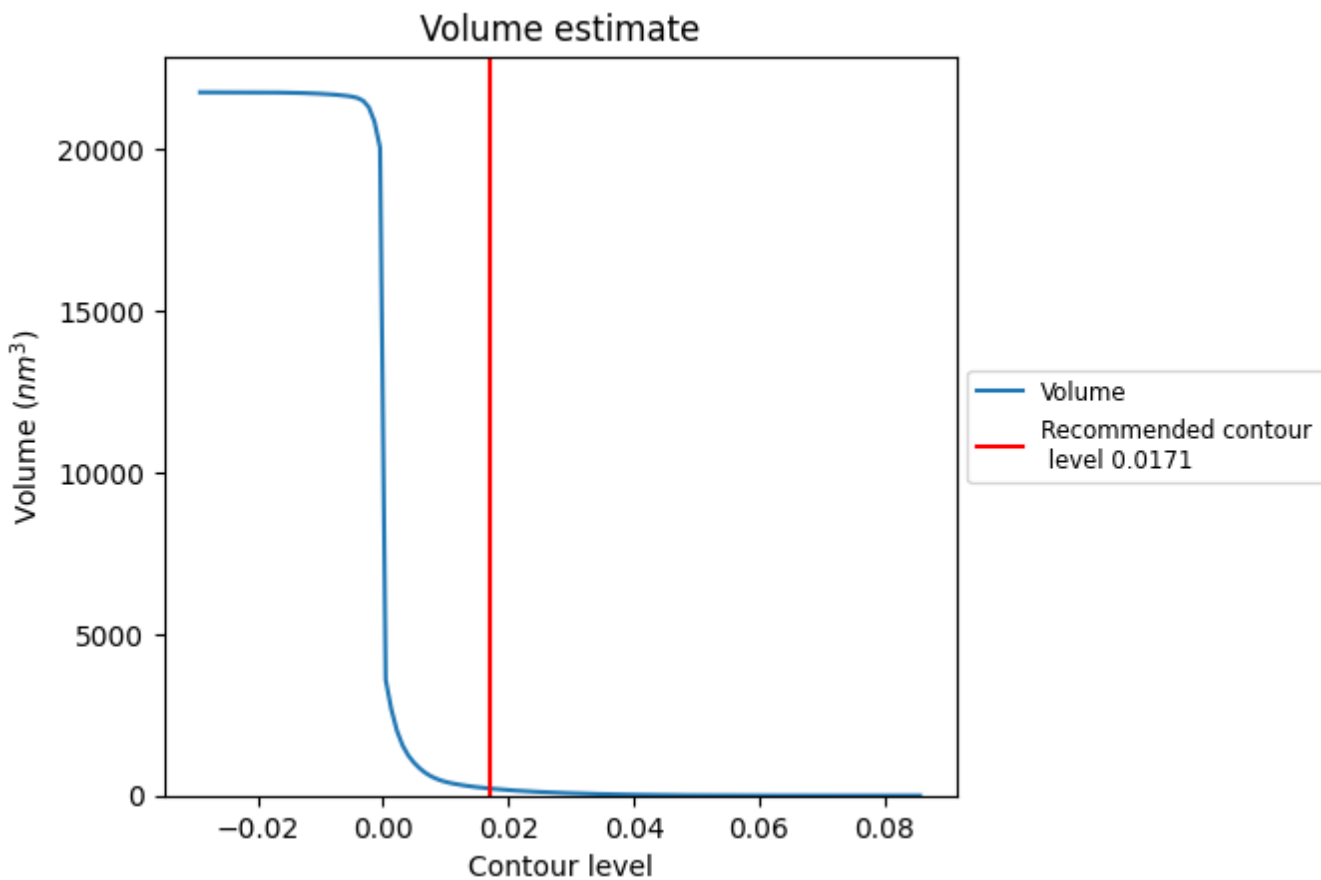
This section contains the results of statistical analysis of the map.

### 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.

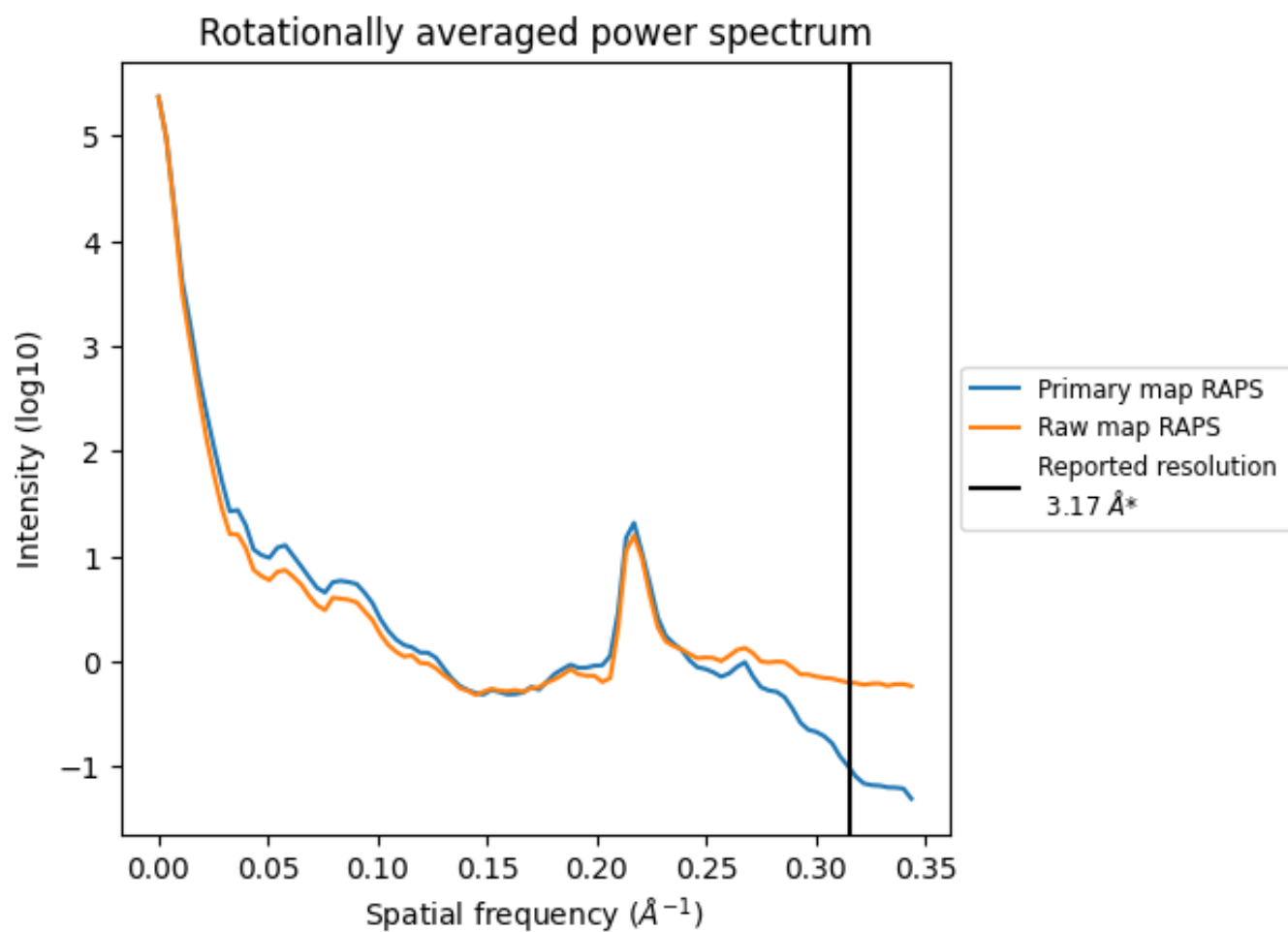
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm<sup>3</sup>; this corresponds to an approximate mass of 197 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

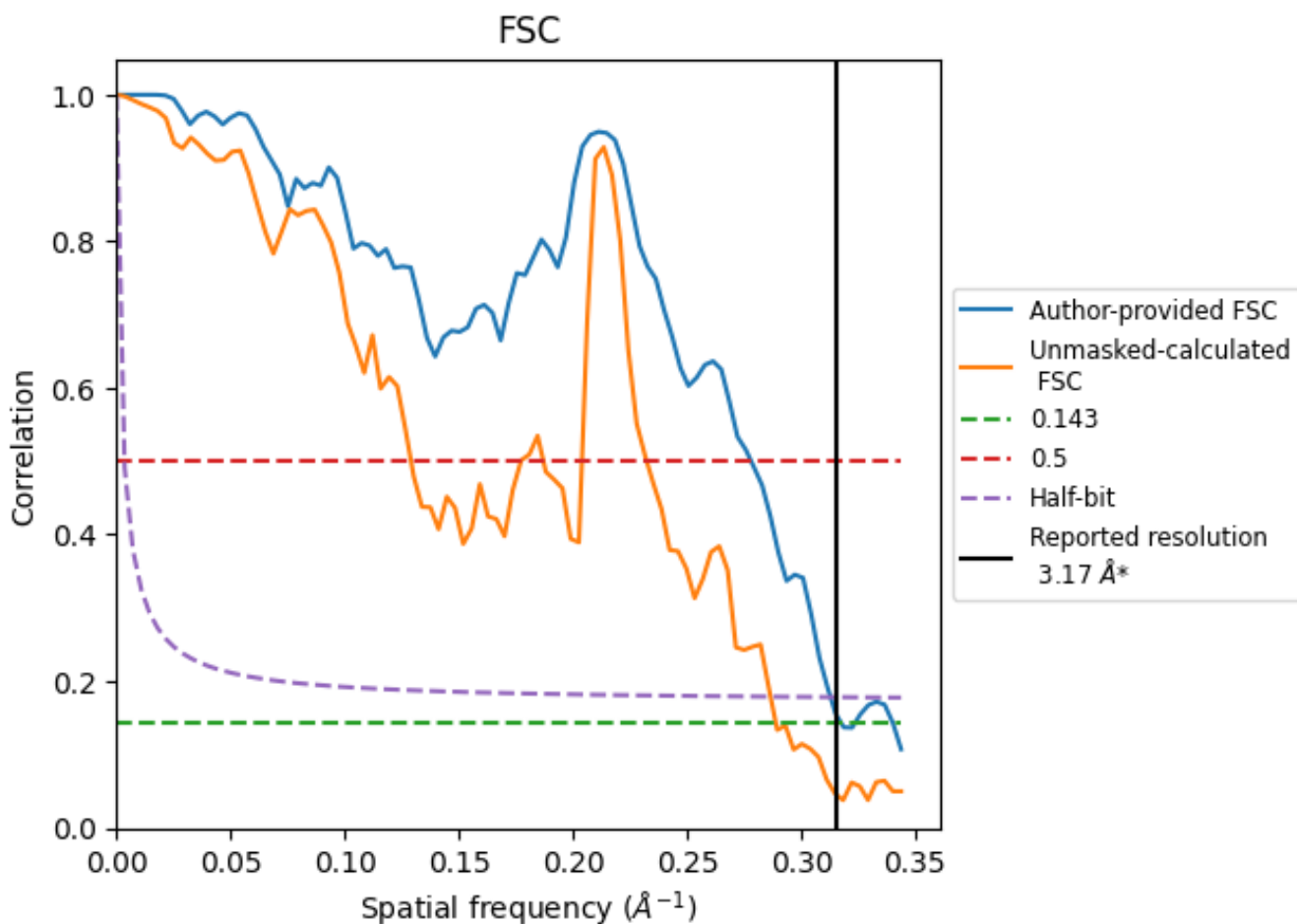


\*Reported resolution corresponds to spatial frequency of  $0.315 \text{ \AA}^{-1}$

## 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 0.315 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

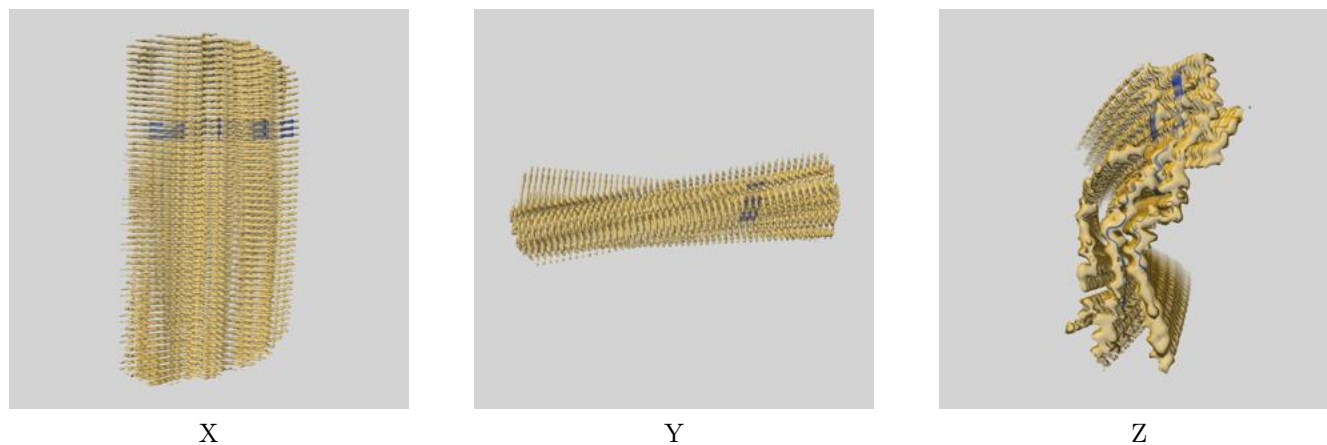
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.15	3.59	3.19
Unmasked-calculated*	3.46	7.75	3.49

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

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

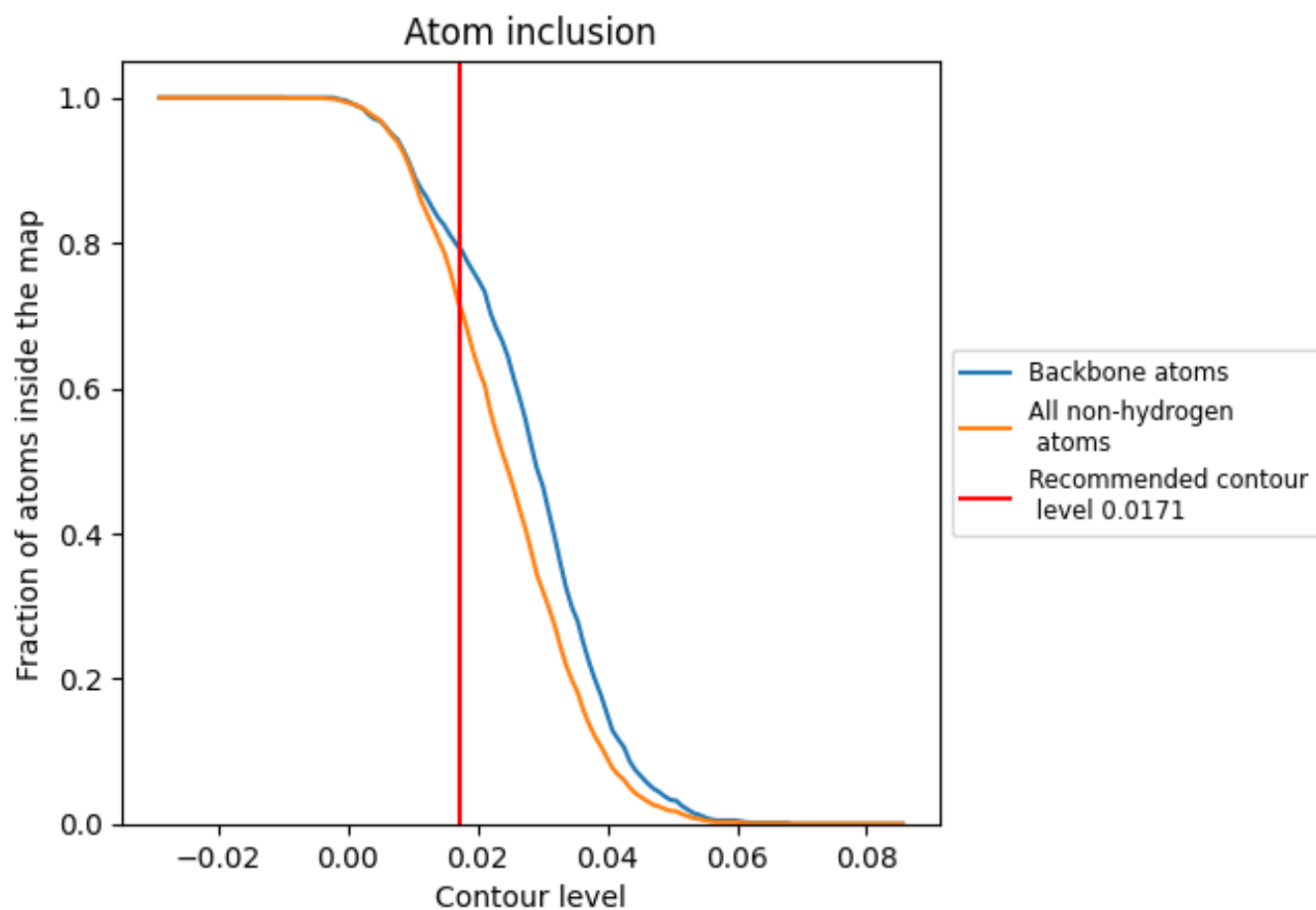
This section contains information regarding the fit between EMDB map EMD-14042 and PDB model 7QKH. Per-residue inclusion information can be found in section [3](#) on page [4](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.0171 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 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.