



## Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 12:31 PM JST

PDB ID : 9VE9 / pdb\_00009ve9  
EMDB ID : EMD-64995  
Title : Hemoglobin amyloid fibril  
Authors : Li, S.; Cao, Q.; Cao, Y.  
Deposited on : 2025-06-09  
Resolution : 3.26 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

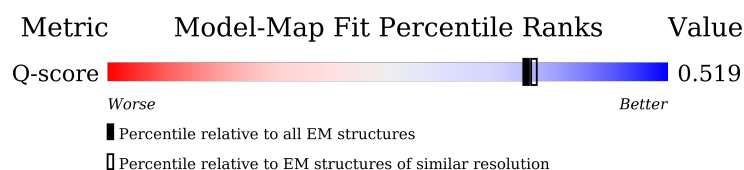
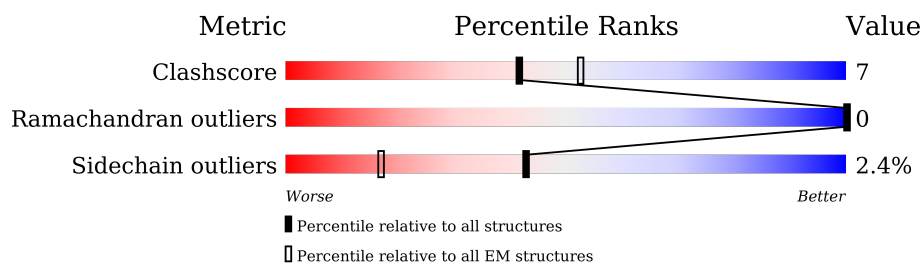
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.26 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	14557 ( 2.76 - 3.76 )

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	145	
1	B	145	
1	C	145	
1	D	145	

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Mol	Chain	Length	Quality of chain
1	E	145	<div><div></div><div>20% . 76%</div></div>
1	F	145	<div><div></div><div>6% . 90%</div></div>
1	G	145	<div><div></div><div>20% . 76%</div></div>
1	H	145	<div><div></div><div>6% . 90%</div></div>
1	I	145	<div><div></div><div>20% . 76%</div></div>
1	J	145	<div><div></div><div>7% . 90%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1900 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.

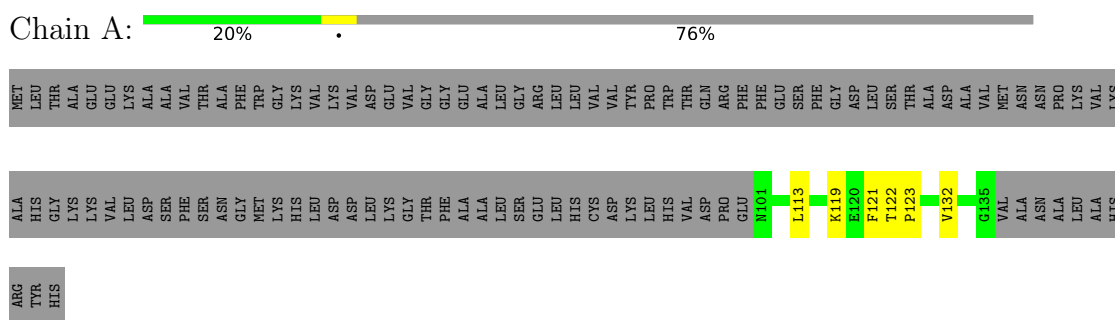
- Molecule 1 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	35	Total	C	N	O	0	0
			271	180	46	45		
1	B	14	Total	C	N	O	0	0
			109	74	17	18		
1	C	35	Total	C	N	O	0	0
			271	180	46	45		
1	D	14	Total	C	N	O	0	0
			109	74	17	18		
1	E	35	Total	C	N	O	0	0
			271	180	46	45		
1	F	14	Total	C	N	O	0	0
			109	74	17	18		
1	G	35	Total	C	N	O	0	0
			271	180	46	45		
1	H	14	Total	C	N	O	0	0
			109	74	17	18		
1	I	35	Total	C	N	O	0	0
			271	180	46	45		
1	J	14	Total	C	N	O	0	0
			109	74	17	18		

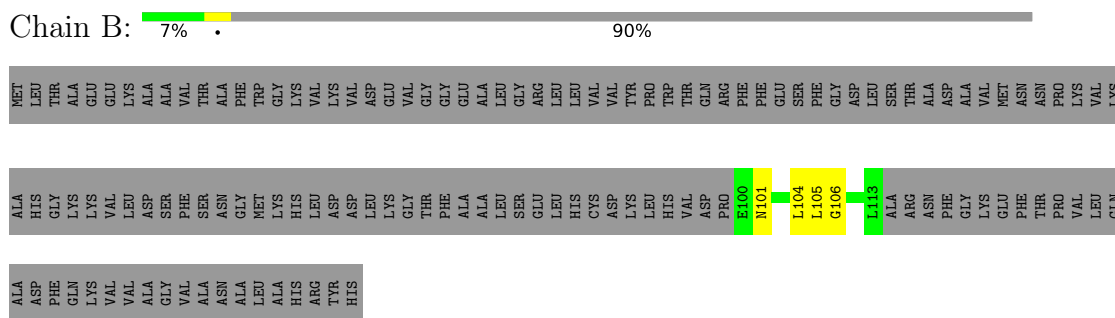
### 3 Residue-property plots

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.

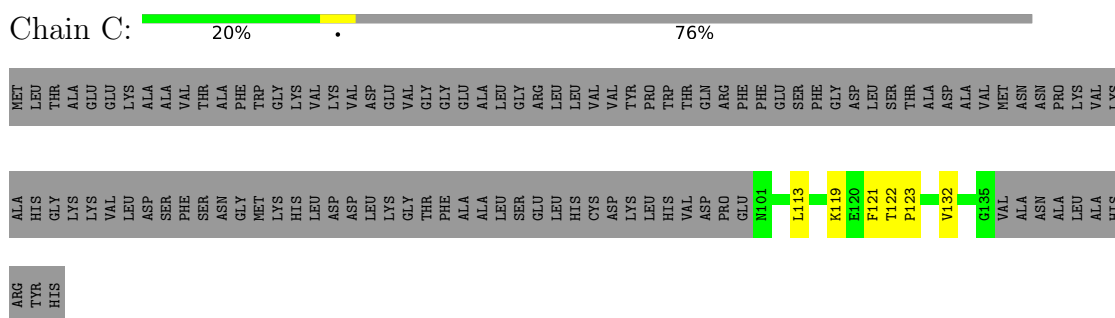
- Molecule 1: Hemoglobin subunit beta



- Molecule 1: Hemoglobin subunit beta



- Molecule 1: Hemoglobin subunit beta



- Molecule 1: Hemoglobin subunit beta

[illegible]

ARG	TYR	HIS
ALA	HIS	GLY
LYS	LYS	VAL
LEU	ASP	SER
PHE	SER	ASN
GLY	MET	LYS
LEU	HIS	ASP
ASP	LEU	LEU
LEU	ASP	GLY
THR	PHE	ALA
ALA	ALA	ALA
LEU	LEU	SER
GLY	SER	GLY
LEU	LEU	LEU
CYS	ASP	LYS
LYS	LYS	HIS
LEU	VAL	ASP
PRO	PRO	GLY
GLU	R101	L113
K119	E120	F121
T122	P123	V132
G135	VAL	ALA
ASN	ASN	ALA
PRO	LYS	LEU
VAL	ALA	HIS

GLN	ALA	MET
ALA	HIS	LEU
ASP	GLY	THR
PHE	LYS	ALA
GLN	LYS	GLU
LYS	VAL	GLU
VAL	LEU	LYS
VAL	ASP	ALA
ALA	SER	ALA
GLY	PHE	VAL
VAL	SER	THR
ALA	ASN	ALA
ASP	GLY	PHE
ALA	MET	TRP
LEU	LYS	GLY
ALA	HIS	LYS
HIS	LEU	VAL
ARG	ASP	LYS
TYR	ASP	VAL
HIS	LEU	ASP
	LYS	GLU
	GLY	VAL
	THR	GLY
	PHE	GLY
	ALA	GLU
	ALA	ALA
	LEU	GLY
	SER	GLY
	GLU	ARG
	LEU	LEU
	HIS	LEU
	CYS	VAL
	ASP	VAL
	LYS	TYR
	LEU	PRO
	HIS	THR
	GLY	TRP
	VAL	THR
	ASP	GLN
	PRO	ARG
	E100	PHE
	M101	PHE
	F102	GLU
	R103	SER
	L104	PHE
	L105	GLY
	G106	ASP
		LEU
		HIS
	I113	SER
	ALA	THR
	ARG	ALA
	ASN	ASP
	PHE	ALA
	GLY	VAL
	LYS	MET
	GLU	ASN
	PHE	ASN
	THR	PRO
	PRO	LYS
	VAL	VAL
	LEU	LYS

[illegible]

Chain H:  6% 90%

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

ALA HIS GLY LYS VAL LYS ASP SER PHE SER ASN GLY MET LYS HIS LYS ASP ASP LEU LYS GLY THR PHE ALA ALA LEU SER GLU LEU HIS CYS ASP TYR PRO HIS TRP THR ASP PRO E100 N101 F102 K103 L104 L105 G106 L113 ALA ARG ASN PHE GLY LYS GLU PHE THR PRO LYS VAL LYS

GLN ALA ASP PHE GLN LYS VAL VAL ALA GLY VAL THR ALA ASN ALA LEU HIS ARG TYR HIS

• Molecule 1: Hemoglobin subunit beta



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

ALA HIS GLY LYS VAL LYS ASP SER PHE SER ASN GLY MET LYS HIS LYS ASP ASP LEU LYS GLY THR PHE ALA ALA LEU SER GLU LEU HIS CYS ASP TYR PRO HIS TRP THR ASP PRO N101 L113 K119 E120 F121 T122 P123 V132 G135 VAL ALA ASN ALA LEU ALA HIS

ARG TYR HIS

• Molecule 1: Hemoglobin subunit beta



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

ALA HIS GLY LYS VAL LYS ASP SER PHE SER ASN GLY MET LYS HIS LYS ASP ASP LEU LYS GLY THR PHE ALA ALA LEU SER GLU LEU HIS CYS ASP TYR PRO HIS TRP THR ASP PRO E100 N101 F102 K103 L104 L105 G106 L113 ALA ARG ASN PHE GLY LYS GLU PHE THR PRO LYS VAL LYS

GLN ALA ASP PHE GLN LYS VAL VAL ALA GLY VAL THR ALA ASN ALA LEU HIS ARG TYR HIS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-1.5912°, rise=4.782 Å, axial sym=C1	Depositor
Number of segments used	31408	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	32.659	Depositor
Minimum map value	-20.263	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (Å)	335.52, 335.52, 335.52	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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	0.28	0/275	0.38	0/371
1	B	0.29	0/109	0.35	0/147
1	C	0.30	0/275	0.45	0/371
1	D	0.30	0/109	0.35	0/147
1	E	0.28	0/275	0.38	0/371
1	F	0.29	0/109	0.35	0/147
1	G	0.30	0/275	0.45	0/371
1	H	0.29	0/109	0.35	0/147
1	I	0.28	0/275	0.38	0/371
1	J	0.29	0/109	0.35	0/147
All	All	0.29	0/1920	0.39	0/2590

There are no bond length outliers.

There are no bond angle outliers.

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	271	0	287	4	0
1	B	109	0	122	3	0
1	C	271	0	287	6	0
1	D	109	0	122	4	0
1	E	271	0	287	6	0
1	F	109	0	122	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	271	0	287	6	0
1	H	109	0	122	4	0
1	I	271	0	287	4	0
1	J	109	0	122	3	0
All	All	1900	0	2045	27	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 7.

All (27) 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:I:113:LEU:HD23	1:I:121:PHE:HD2	1.76	0.51
1:G:113:LEU:HD23	1:G:121:PHE:HD2	1.76	0.51
1:E:113:LEU:HD23	1:E:121:PHE:HD2	1.76	0.50
1:C:113:LEU:HD23	1:C:121:PHE:HD2	1.76	0.50
1:A:113:LEU:HD23	1:A:121:PHE:HD2	1.76	0.50
1:G:122:THR:HG23	1:I:122:THR:O	2.14	0.48
1:E:122:THR:HG23	1:G:122:THR:O	2.14	0.48
1:C:122:THR:HG23	1:E:122:THR:O	2.14	0.47
1:A:122:THR:HG23	1:C:122:THR:O	2.14	0.47
1:D:101:ASN:O	1:F:102:PHE:HD2	1.98	0.45
1:F:101:ASN:O	1:H:102:PHE:HD2	1.98	0.45
1:H:101:ASN:O	1:J:102:PHE:HD2	1.99	0.45
1:B:101:ASN:O	1:D:102:PHE:HD2	1.98	0.45
1:A:132:VAL:HG21	1:B:104:LEU:HD11	1.99	0.43
1:C:132:VAL:HG21	1:D:104:LEU:HD11	1.99	0.43
1:E:132:VAL:HG21	1:F:104:LEU:HD11	1.99	0.43
1:I:132:VAL:HG21	1:J:104:LEU:HD11	1.99	0.43
1:G:132:VAL:HG21	1:H:104:LEU:HD11	1.99	0.43
1:J:105:LEU:HD23	1:J:106:GLY:H	1.85	0.42
1:G:123:PRO:HG2	1:I:123:PRO:HB3	2.02	0.42
1:C:123:PRO:HG2	1:E:123:PRO:HB3	2.02	0.42
1:A:123:PRO:HG2	1:C:123:PRO:HB3	2.02	0.42
1:E:123:PRO:HG2	1:G:123:PRO:HB3	2.02	0.42
1:H:105:LEU:HD23	1:H:106:GLY:H	1.85	0.42
1:B:105:LEU:HD23	1:B:106:GLY:H	1.85	0.41
1:F:105:LEU:HD23	1:F:106:GLY:H	1.85	0.41
1:D:105:LEU:HD23	1:D:106:GLY:H	1.85	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	33/145 (23%)	30 (91%)	3 (9%)	0	100	100
1	B	12/145 (8%)	11 (92%)	1 (8%)	0	100	100
1	C	33/145 (23%)	30 (91%)	3 (9%)	0	100	100
1	D	12/145 (8%)	11 (92%)	1 (8%)	0	100	100
1	E	33/145 (23%)	30 (91%)	3 (9%)	0	100	100
1	F	12/145 (8%)	11 (92%)	1 (8%)	0	100	100
1	G	33/145 (23%)	30 (91%)	3 (9%)	0	100	100
1	H	12/145 (8%)	11 (92%)	1 (8%)	0	100	100
1	I	33/145 (23%)	30 (91%)	3 (9%)	0	100	100
1	J	12/145 (8%)	11 (92%)	1 (8%)	0	100	100
All	All	225/1450 (16%)	205 (91%)	20 (9%)	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	29/118 (25%)	28 (97%)	1 (3%)	32	57
1	B	13/118 (11%)	13 (100%)	0	100	100
1	C	29/118 (25%)	28 (97%)	1 (3%)	32	57
1	D	13/118 (11%)	13 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	29/118 (25%)	28 (97%)	1 (3%)	32	57
1	F	13/118 (11%)	13 (100%)	0	100	100
1	G	29/118 (25%)	28 (97%)	1 (3%)	32	57
1	H	13/118 (11%)	13 (100%)	0	100	100
1	I	29/118 (25%)	28 (97%)	1 (3%)	32	57
1	J	13/118 (11%)	13 (100%)	0	100	100
All	All	210/1180 (18%)	205 (98%)	5 (2%)	43	64

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LYS
1	C	119	LYS
1	E	119	LYS
1	G	119	LYS
1	I	119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

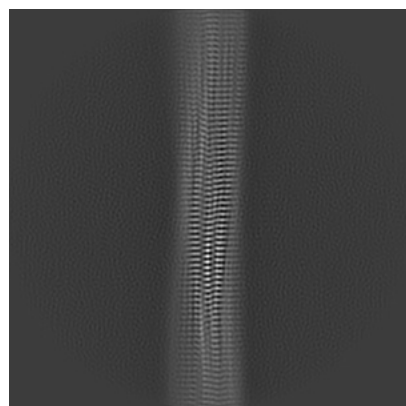
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64995. These allow visual inspection of the internal detail of the map and identification of artifacts.

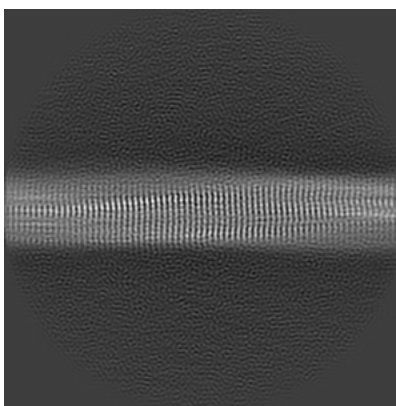
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

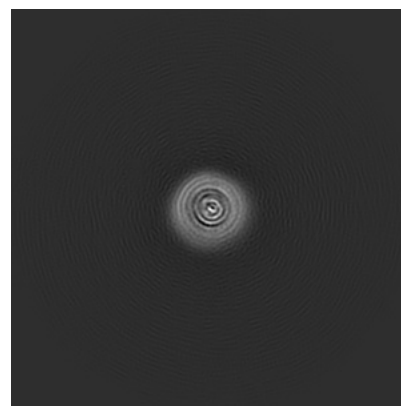
#### 6.1.1 Primary map



X

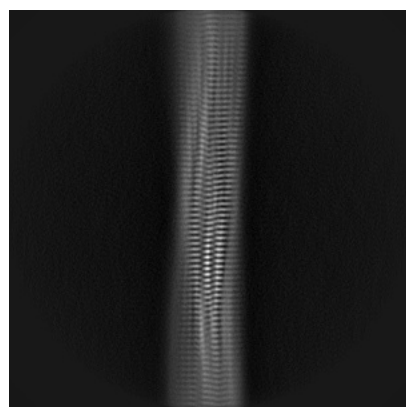


Y

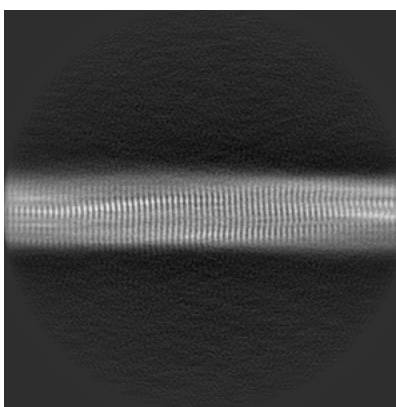


Z

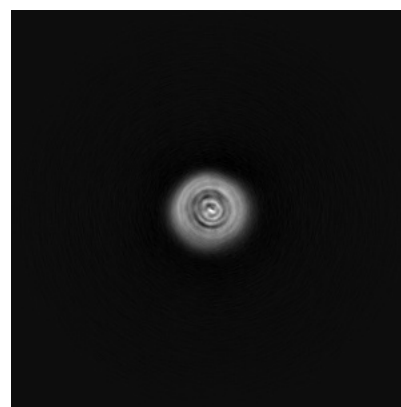
#### 6.1.2 Raw map



X



Y

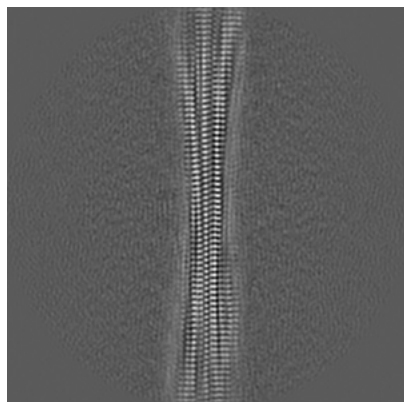


Z

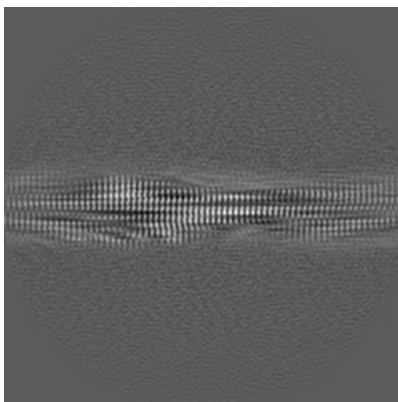
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

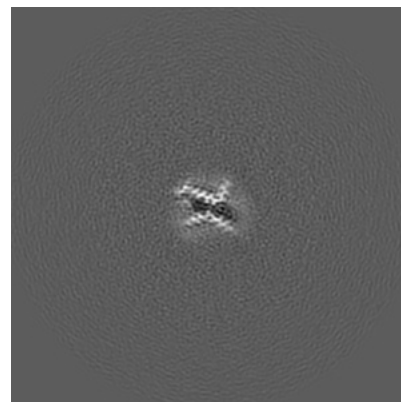
### 6.2.1 Primary map



X Index: 180

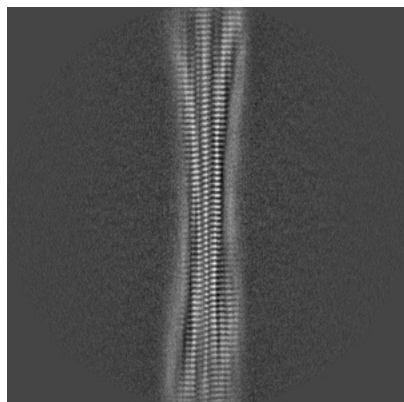


Y Index: 180

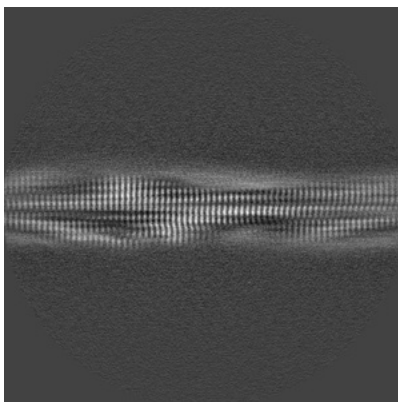


Z Index: 180

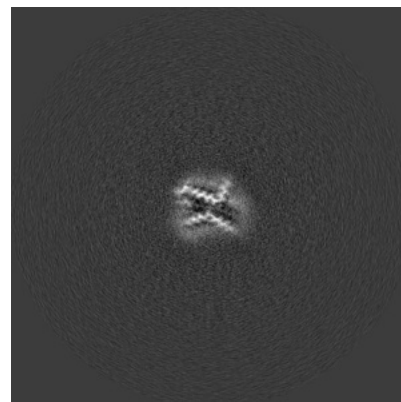
### 6.2.2 Raw map



X Index: 180



Y Index: 180



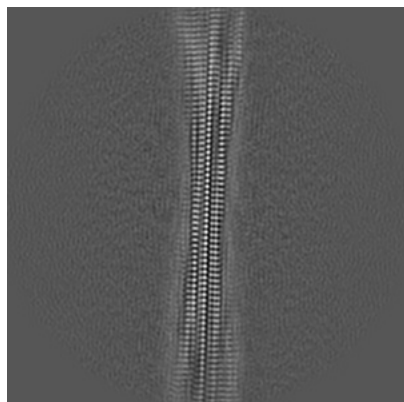
Z Index: 180

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

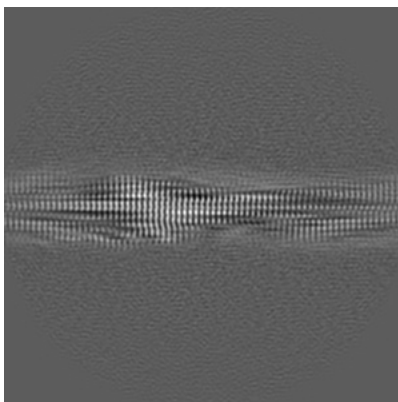


## 6.3 Largest variance slices [i](#)

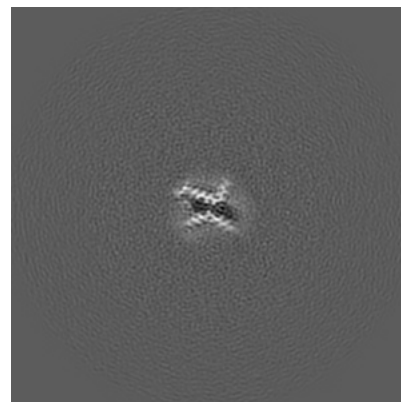
### 6.3.1 Primary map



X Index: 175

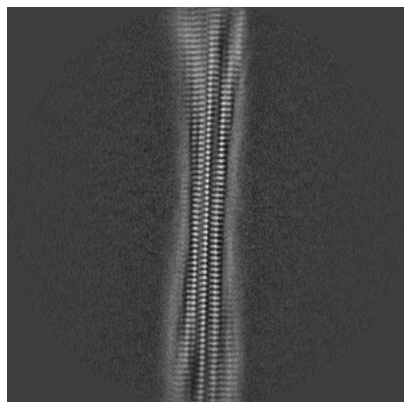


Y Index: 179

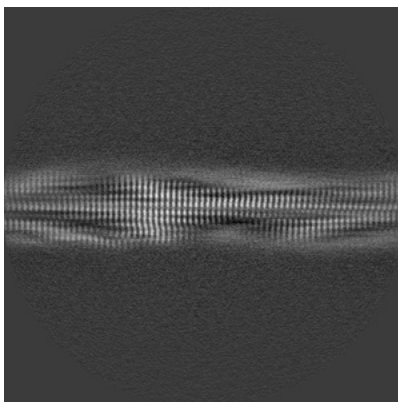


Z Index: 175

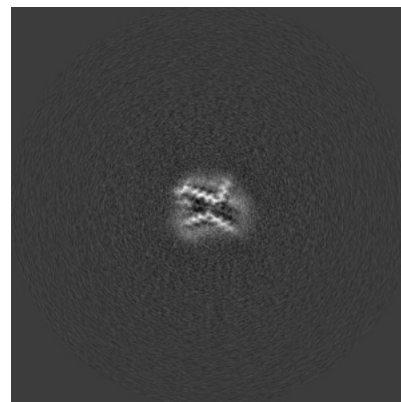
### 6.3.2 Raw map



X Index: 175



Y Index: 178



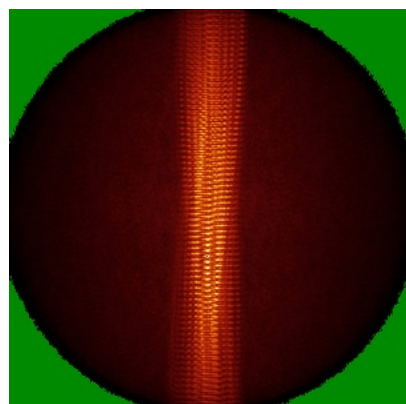
Z Index: 180

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

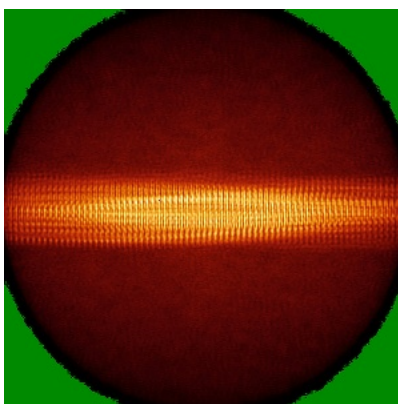


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

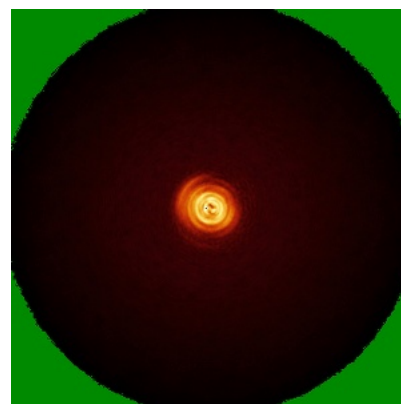
### 6.4.1 Primary map



X

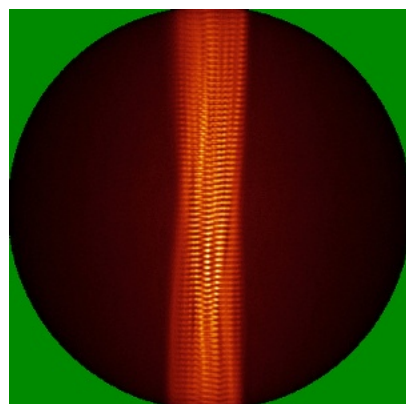


Y

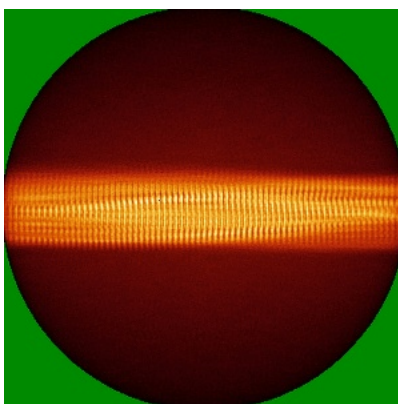


Z

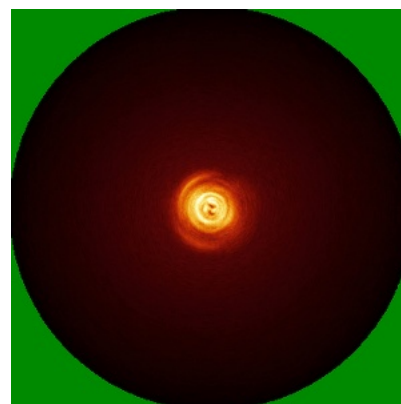
### 6.4.2 Raw map



X



Y

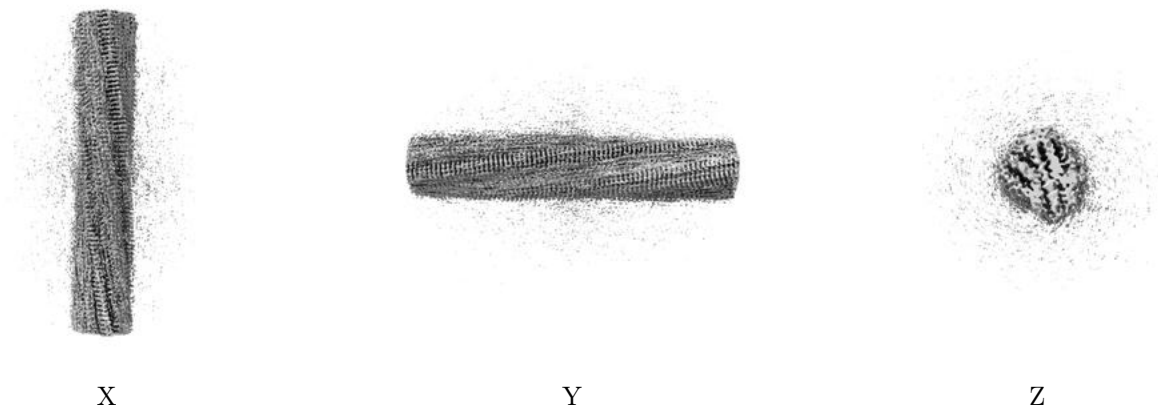


Z

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.

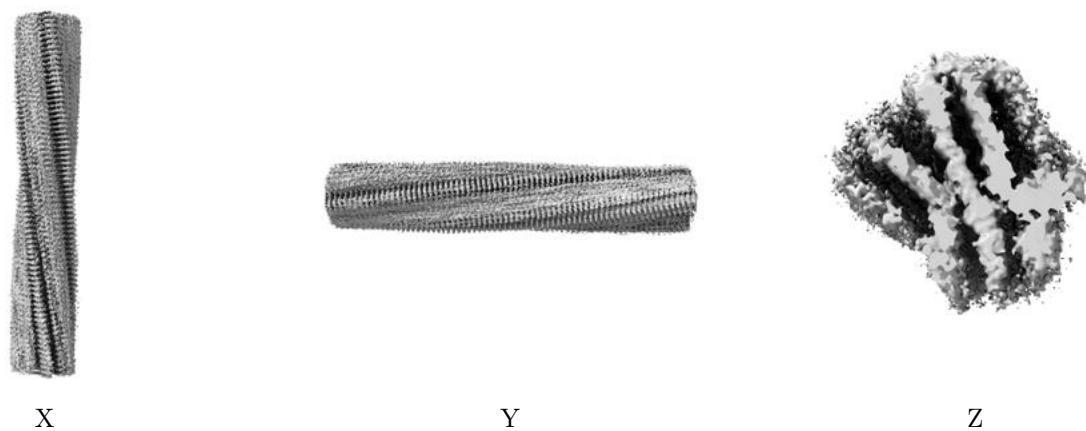
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

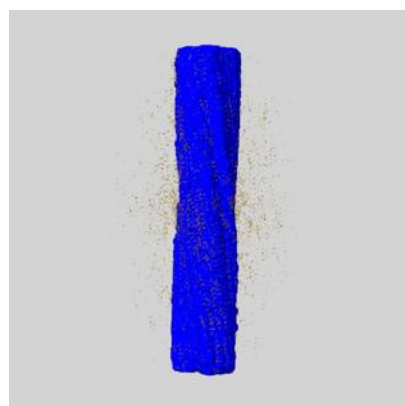
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

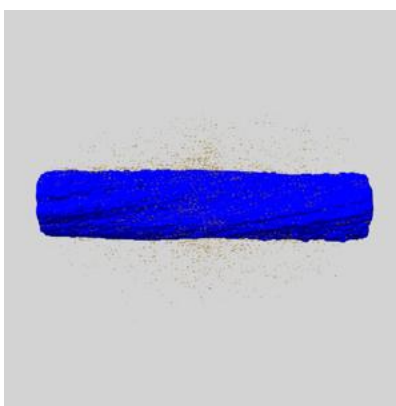
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

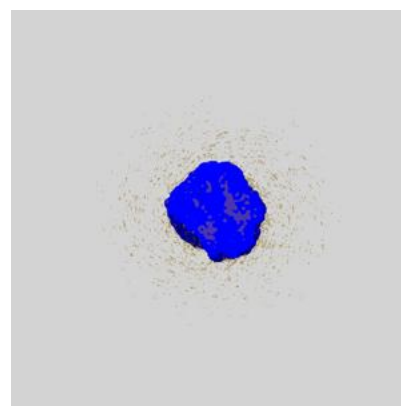
### 6.6.1 emd\_64995\_msk\_1.map [i](#)



X



Y

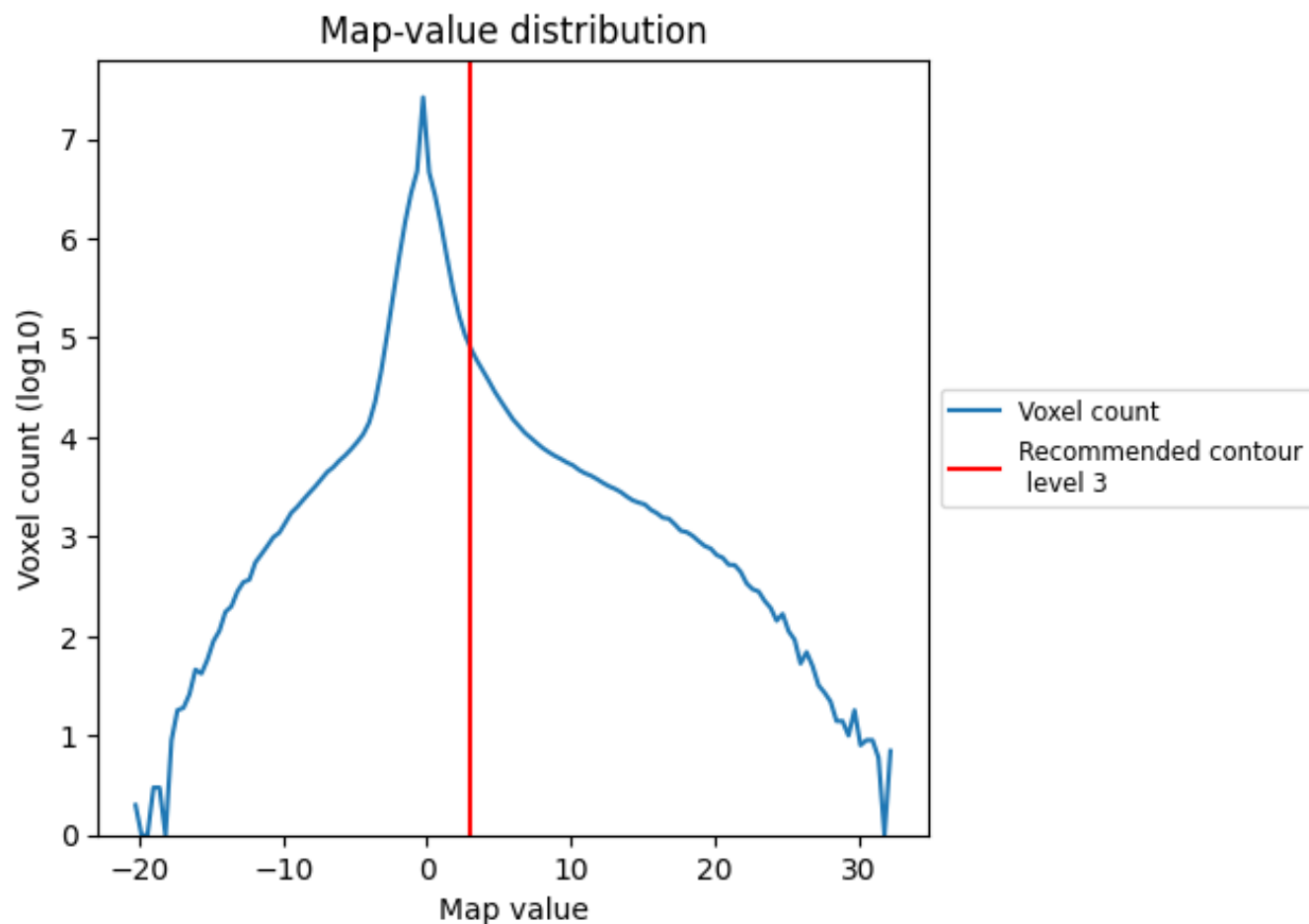


Z

## 7 Map analysis [i](#)

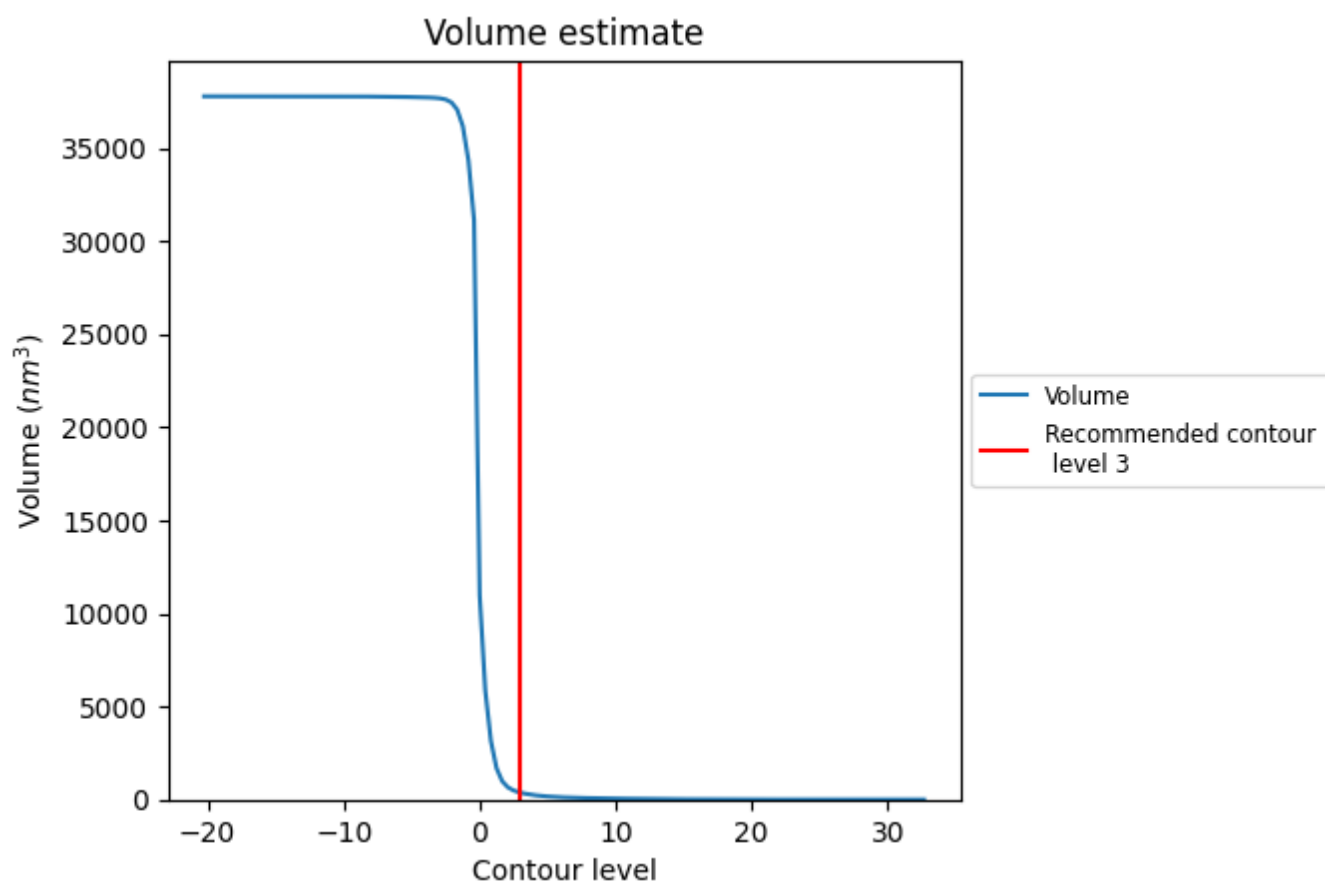
This section contains the results of statistical analysis of the map.

### 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.

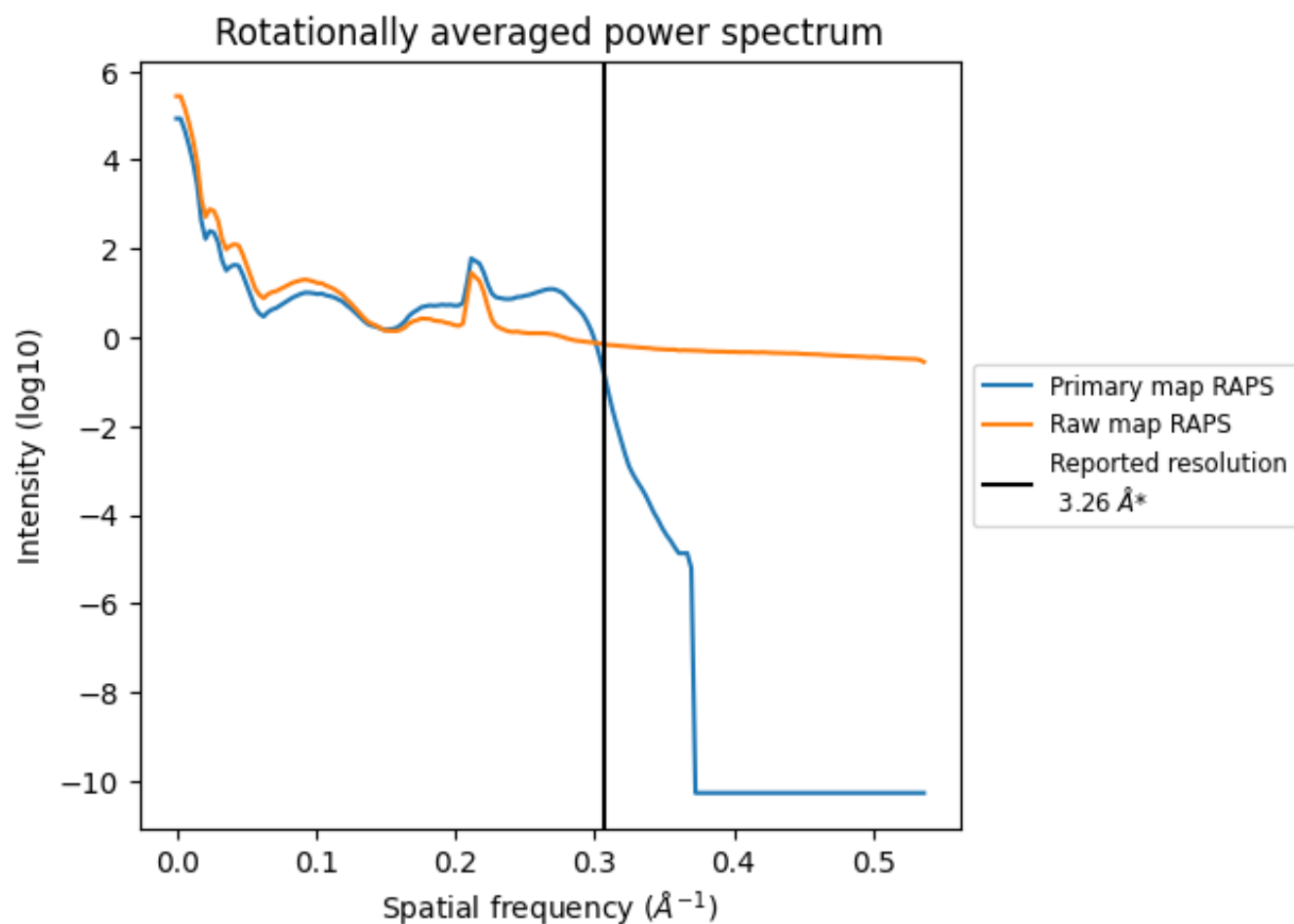
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm<sup>3</sup>; this corresponds to an approximate mass of 336 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 ⓘ

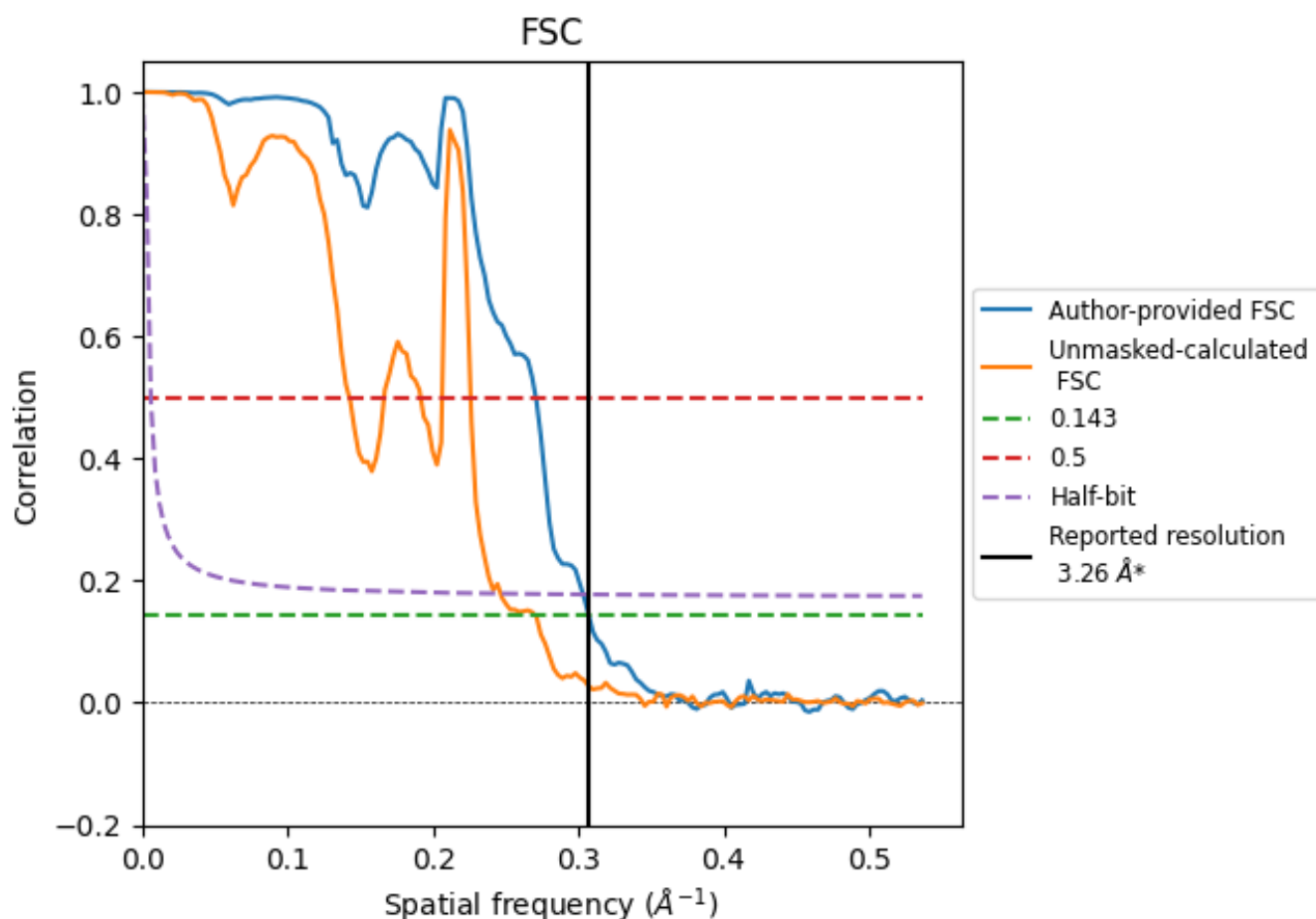


\*Reported resolution corresponds to spatial frequency of 0.307 Å<sup>-1</sup>

## 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  $0.307 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.69	3.30
Unmasked-calculated*	3.70	7.02	4.06

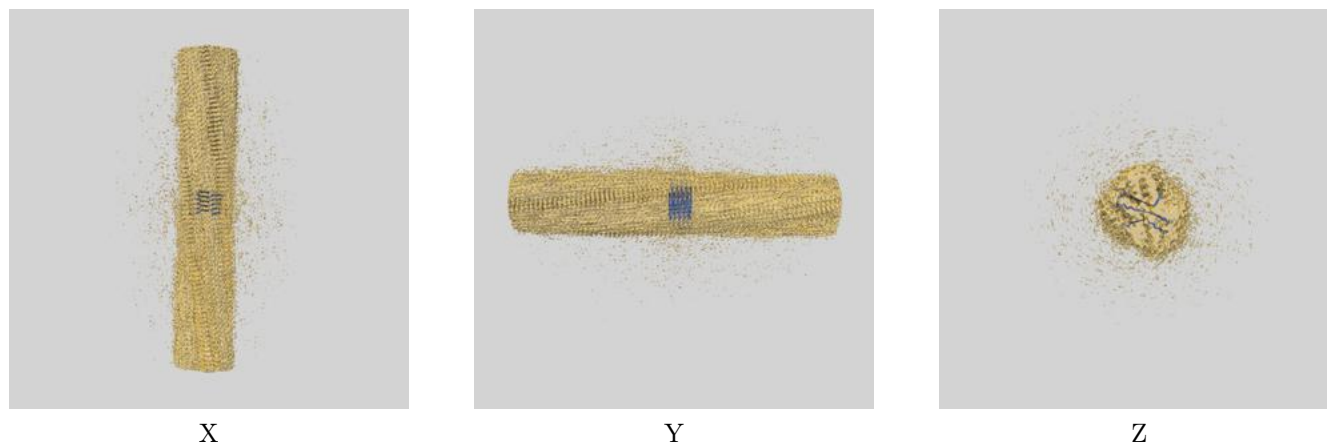
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.26 by more than 10 %



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

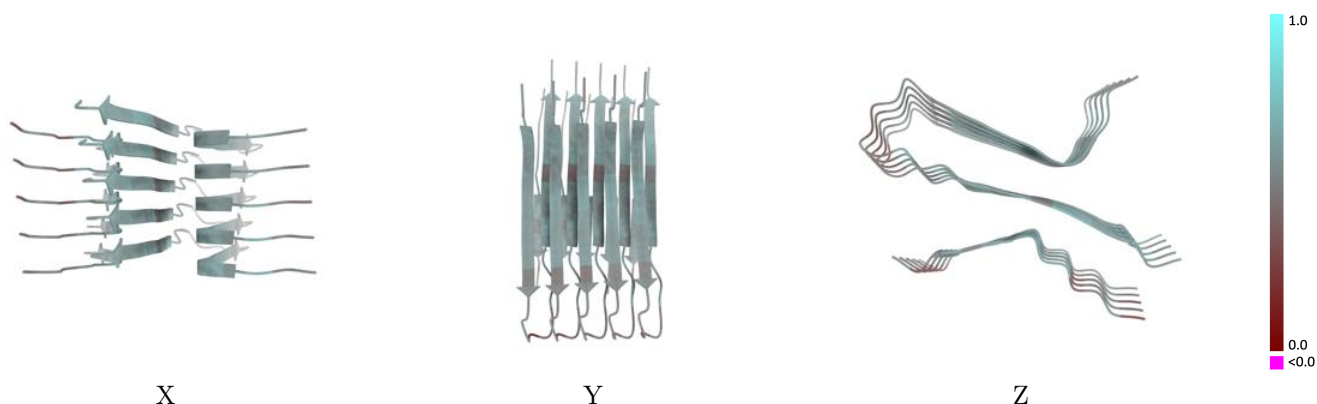
This section contains information regarding the fit between EMDB map EMD-64995 and PDB model 9VE9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



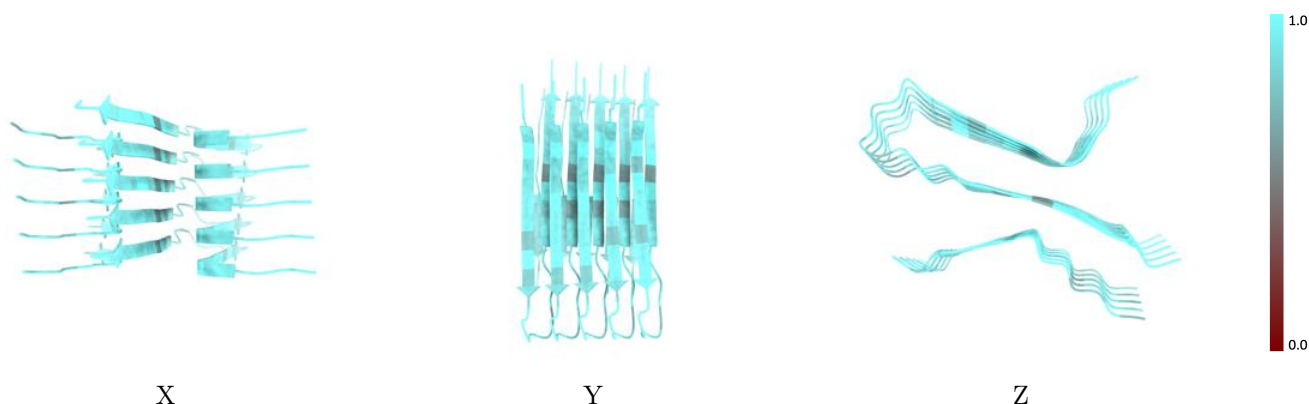
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



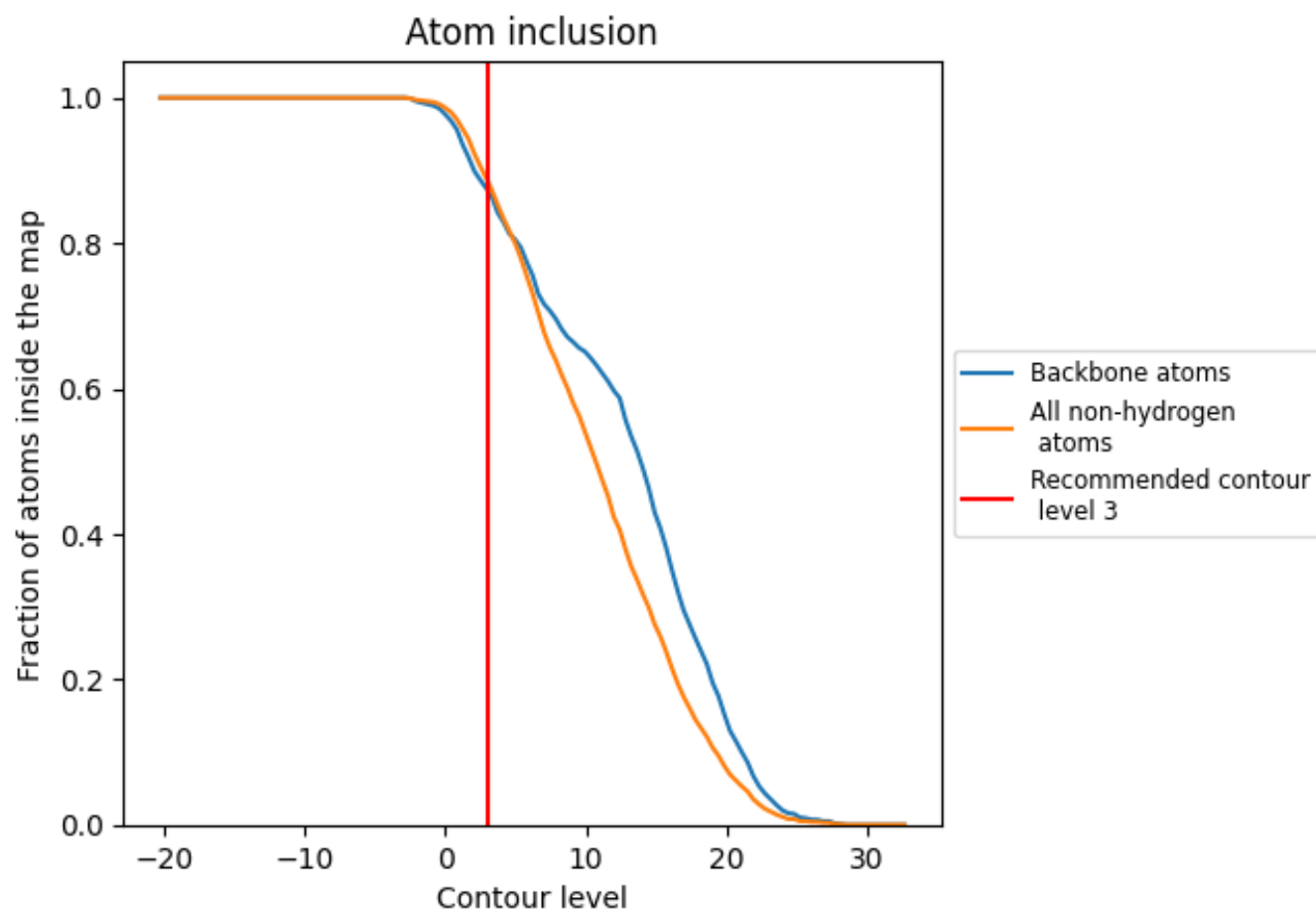
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 89% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8860	<div><div></div></div> 0.5190
A	<div><div></div></div> 0.8770	<div><div></div></div> 0.5260
B	<div><div></div></div> 0.8900	<div><div></div></div> 0.4970
C	<div><div></div></div> 0.8880	<div><div></div></div> 0.5260
D	<div><div></div></div> 0.8810	<div><div></div></div> 0.4960
E	<div><div></div></div> 0.9000	<div><div></div></div> 0.5250
F	<div><div></div></div> 0.8720	<div><div></div></div> 0.4940
G	<div><div></div></div> 0.8880	<div><div></div></div> 0.5290
H	<div><div></div></div> 0.8900	<div><div></div></div> 0.5050
I	<div><div></div></div> 0.8960	<div><div></div></div> 0.5310
J	<div><div></div></div> 0.8530	<div><div></div></div> 0.4940

1.0

0.0

<0.0