



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:45 PM UTC

PDB ID : 8KF6 / pdb_00008kf6
EMDB ID : EMD-37200
Title : The cryo-EM structure of AV-45 bound type3 amyloid beta 42 fibril.
Authors : Zhao, Q.Y.; Tao, Y.Q.; Liu, C.; Li, D.
Deposited on : 2023-08-15
Resolution : 3.70 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

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

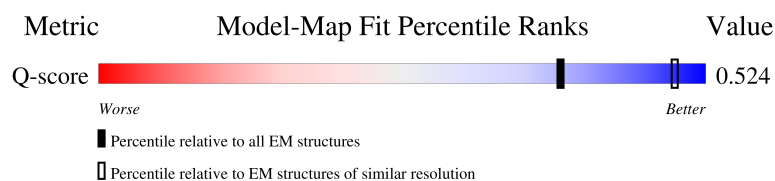
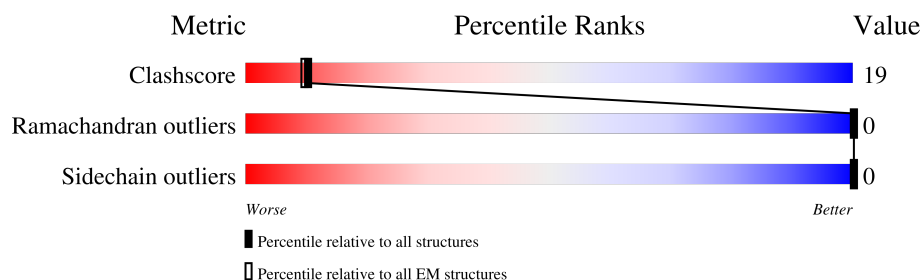
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

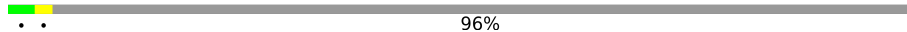
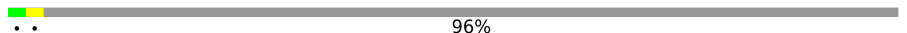
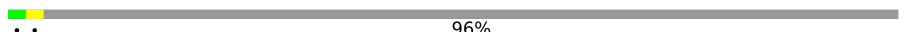
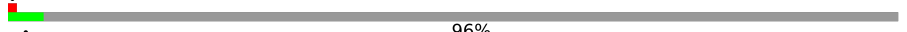
The reported resolution of this entry is 3.70 Å.

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	11569 (3.20 - 4.20)

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	770	 96%
1	B	770	 96%
1	C	770	 96%
1	D	770	 96%

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Mol	Chain	Length	Quality of chain
1	E	770	 96%
1	F	770	 96%
1	G	770	 96%
1	H	770	 96%
1	I	770	 96%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2175 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 P3(40).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	31	Total	C	N	O	S	0	0
			225	147	39	38	1		
1	A	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	G	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	D	31	Total	C	N	O	S	0	0
			225	147	39	38	1		
1	H	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	E	31	Total	C	N	O	S	0	0
			225	147	39	38	1		
1	I	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	B	34	Total	C	N	O	S	0	0
			250	163	42	44	1		
1	C	34	Total	C	N	O	S	0	0
			250	163	42	44	1		

96%

[illegible]

- Molecule 1: P3(40)

96%

[illegible]

VAL	VAL	GLU	VAL	ASP	ALA	ALA	VAL	THR	PRO	GLU	GLU	ARG	HIS	LEU	SER	LYS	MET	GLN	GLN	ASN	GLY	TYR	GLU	ASN	PRO	THR	TYR	LYS	PHE	PHE	GLU	GLN	MET	GLN	ASN
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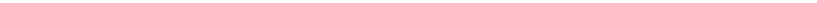
- Molecule 1: P3(40)

Chain H: 96%

[illegible]

VAL	VAL	GLU	VAL	ASP	ALA	ALA	VAL	THR	PRO	GLU	GLU	ARG	HIS	LEU	SER	LYS	MET	GLN	GLN	ASN	GLY	TYR	GLU	ASN	PRO	THR	TYR	LYS	PHE	PHE	GLU	GLN	MET	GLN	ASN
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- Molecule 1: P3(40)

Chain E:  96%

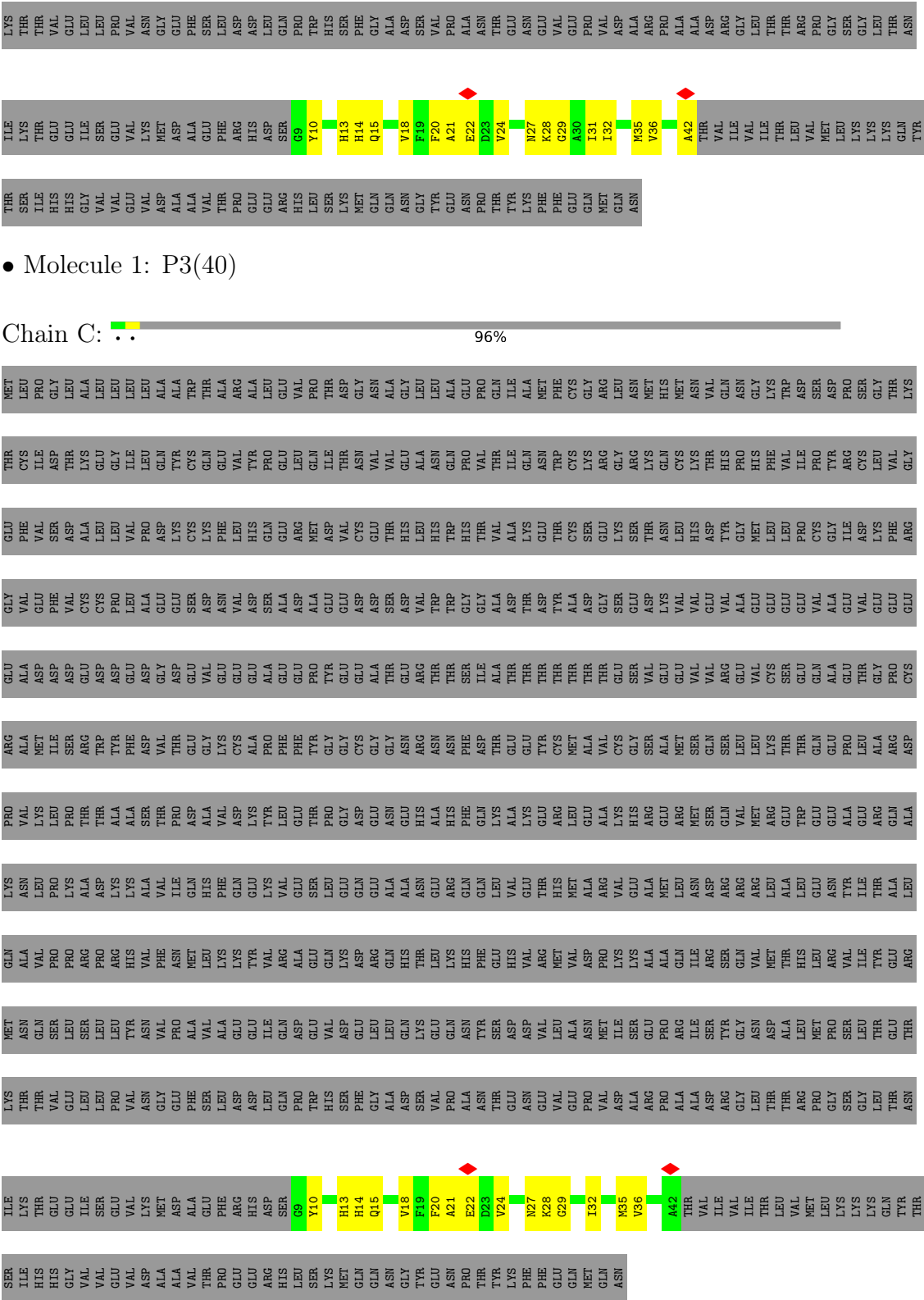


GLY	VAL	GLU	VAL	ASP	ALA	ALA	THR	PRO	GLU	GLU	ARG	HIS	LEU	SER	LYS	MET	GLN	GLN	GLY	GLY	GLU	ASN	PRO	THR	TYR	LYS	PHE	GLU	GLN	MET	GLN	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

- Molecule 1: P3(40)

Chain B: .. 96%

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



● Molecule 1: P3(40)

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-1.92°, rise=4.81 Å, axial sym=C1	Depositor
Number of segments used	18493	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 ($e^-/\text{Å}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00575	Depositor
Map size (Å)	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.24	0/254	0.45	0/341
1	B	0.24	0/254	0.45	0/341
1	C	0.24	0/254	0.45	0/341
1	D	0.17	0/228	0.35	0/306
1	E	0.16	0/228	0.33	0/306
1	F	0.17	0/228	0.41	0/306
1	G	0.23	0/254	0.47	0/341
1	H	0.22	0/254	0.52	0/341
1	I	0.22	0/254	0.49	0/341
All	All	0.21	0/2208	0.44	0/2964

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	250	0	252	27	0
1	B	250	0	252	53	0
1	C	250	0	252	30	0
1	D	225	0	234	2	0
1	E	225	0	234	1	0
1	F	225	0	234	4	0
1	G	250	0	252	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	250	0	252	9	0
1	I	250	0	252	7	0
All	All	2175	0	2214	84	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 19.

All (84) 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:B:20:PHE:CE2	1:C:20:PHE:HE1	1.71	1.07
1:B:20:PHE:HD2	1:C:20:PHE:CD1	1.72	1.04
1:A:20:PHE:CE2	1:B:20:PHE:HE1	1.75	1.02
1:A:20:PHE:HD2	1:B:20:PHE:CD1	1.76	1.02
1:A:10:TYR:HD1	1:B:10:TYR:CD2	1.79	1.00
1:B:10:TYR:HD1	1:C:10:TYR:CD2	1.78	1.00
1:A:10:TYR:CE1	1:B:10:TYR:HE2	1.79	1.00
1:B:20:PHE:CE2	1:C:20:PHE:CE1	2.49	1.00
1:B:20:PHE:CD2	1:C:20:PHE:CD1	2.50	0.99
1:B:10:TYR:CE1	1:C:10:TYR:HE2	1.79	0.99
1:A:10:TYR:HE1	1:B:10:TYR:HE2	0.99	0.97
1:A:10:TYR:CD1	1:B:10:TYR:HD2	1.83	0.96
1:A:10:TYR:HE1	1:B:10:TYR:CE2	1.84	0.96
1:A:10:TYR:HD1	1:B:10:TYR:HD2	0.97	0.96
1:A:20:PHE:CE2	1:B:20:PHE:CE1	2.54	0.95
1:B:20:PHE:HE2	1:C:20:PHE:HE1	1.09	0.95
1:A:20:PHE:CD2	1:B:20:PHE:CD1	2.55	0.94
1:B:10:TYR:HD1	1:C:10:TYR:HD2	0.99	0.94
1:A:10:TYR:CE1	1:B:10:TYR:CE2	2.55	0.94
1:B:10:TYR:HE1	1:C:10:TYR:HE2	1.02	0.93
1:A:10:TYR:CD1	1:B:10:TYR:CD2	2.55	0.93
1:B:10:TYR:CD1	1:C:10:TYR:CD2	2.56	0.93
1:B:10:TYR:CE1	1:C:10:TYR:CE2	2.56	0.93
1:B:10:TYR:CD1	1:C:10:TYR:HD2	1.87	0.92
1:B:20:PHE:HD2	1:C:20:PHE:HD1	1.14	0.91
1:B:10:TYR:HE1	1:C:10:TYR:CE2	1.89	0.90
1:A:20:PHE:HE2	1:B:20:PHE:HE1	1.16	0.88
1:B:20:PHE:HE2	1:C:20:PHE:CE1	1.91	0.87
1:A:20:PHE:HD2	1:B:20:PHE:HD1	1.19	0.87
1:B:20:PHE:CD2	1:C:20:PHE:HD1	1.92	0.85
1:B:21:ALA:HA	1:C:21:ALA:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PHE:CD2	1:C:20:PHE:CE1	2.66	0.81
1:A:20:PHE:HE2	1:B:20:PHE:CE1	1.97	0.81
1:A:20:PHE:CD2	1:B:20:PHE:CE1	2.68	0.80
1:A:20:PHE:CD2	1:B:20:PHE:HD1	1.98	0.79
1:A:21:ALA:HA	1:B:21:ALA:O	1.81	0.79
1:B:24:VAL:O	1:C:24:VAL:HA	1.87	0.73
1:I:32:ILE:HG21	1:I:35:MET:HB2	1.77	0.66
1:A:24:VAL:O	1:B:24:VAL:HA	1.96	0.65
1:H:32:ILE:HG21	1:H:35:MET:HB2	1.80	0.63
1:B:10:TYR:CD1	1:C:10:TYR:CE2	2.82	0.62
1:E:32:ILE:HD11	1:E:40:VAL:HG11	1.83	0.60
1:B:21:ALA:CA	1:C:21:ALA:O	2.52	0.56
1:H:15:GLN:HG2	1:C:36:VAL:O	2.06	0.55
1:B:32:ILE:HG21	1:B:35:MET:HB2	1.89	0.55
1:A:32:ILE:HG21	1:A:35:MET:HB2	1.89	0.55
1:H:36:VAL:HG12	1:B:15:GLN:HB3	1.87	0.55
1:C:32:ILE:HG21	1:C:35:MET:HB2	1.89	0.55
1:I:36:VAL:HG12	1:C:15:GLN:HB3	1.89	0.54
1:G:13:HIS:HD2	1:G:14:HIS:ND1	2.06	0.53
1:G:15:GLN:HG2	1:B:36:VAL:O	2.09	0.53
1:F:26:SER:OG	1:F:27:ASN:N	2.42	0.53
1:G:35:MET:HE1	1:G:40:VAL:HG23	1.92	0.51
1:G:22:GLU:HB3	1:H:22:GLU:O	2.11	0.51
1:H:22:GLU:HB3	1:I:22:GLU:O	2.11	0.50
1:B:13:HIS:O	1:C:13:HIS:HA	2.11	0.49
1:I:13:HIS:HD2	1:I:14:HIS:ND1	2.11	0.49
1:B:13:HIS:HD2	1:B:14:HIS:ND1	2.11	0.49
1:C:13:HIS:HD2	1:C:14:HIS:ND1	2.11	0.49
1:A:13:HIS:HD2	1:A:14:HIS:ND1	2.11	0.48
1:G:32:ILE:HG21	1:G:35:MET:HB2	1.95	0.48
1:G:42:ALA:HB3	1:H:42:ALA:HA	1.95	0.47
1:B:42:ALA:HB1	1:C:29:GLY:HA2	1.96	0.47
1:A:21:ALA:CA	1:B:21:ALA:O	2.57	0.47
1:I:26:SER:OG	1:I:27:ASN:N	2.47	0.47
1:H:26:SER:OG	1:H:27:ASN:N	2.47	0.46
1:D:32:ILE:HD11	1:D:40:VAL:HG11	1.97	0.46
1:I:16:LYS:NZ	1:I:22:GLU:OE2	2.41	0.45
1:C:18:VAL:HG21	1:C:22:GLU:OE1	2.17	0.45
1:A:18:VAL:HG21	1:A:22:GLU:OE1	2.17	0.45
1:B:18:VAL:HG21	1:B:22:GLU:OE1	2.17	0.44
1:I:35:MET:HE1	1:I:40:VAL:HG23	1.99	0.44

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:HIS:HD2	1:H:14:HIS:ND1	2.16	0.43
1:B:28:LYS:O	1:C:28:LYS:HA	2.18	0.43
1:A:13:HIS:O	1:B:13:HIS:HA	2.18	0.42
1:A:15:GLN:HB3	1:G:36:VAL:HG12	2.01	0.42
1:B:31:ILE:HD11	1:C:27:ASN:HD22	1.85	0.42
1:F:22:GLU:HG3	1:F:23:ASP:H	1.85	0.42
1:A:31:ILE:HD11	1:B:27:ASN:HD22	1.85	0.42
1:G:26:SER:OG	1:G:27:ASN:N	2.54	0.41
1:A:42:ALA:HB1	1:B:29:GLY:HA2	2.03	0.41
1:F:21:ALA:HB3	1:D:21:ALA:HA	2.03	0.40
1:F:35:MET:HE2	1:F:35:MET:HB2	1.99	0.40
1:H:35:MET:HE2	1:H:38:GLY:HA3	2.01	0.40

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	32/770 (4%)	24 (75%)	8 (25%)	0	100	100
1	B	32/770 (4%)	24 (75%)	8 (25%)	0	100	100
1	C	32/770 (4%)	24 (75%)	8 (25%)	0	100	100
1	D	29/770 (4%)	28 (97%)	1 (3%)	0	100	100
1	E	29/770 (4%)	27 (93%)	2 (7%)	0	100	100
1	F	29/770 (4%)	27 (93%)	2 (7%)	0	100	100
1	G	32/770 (4%)	28 (88%)	4 (12%)	0	100	100
1	H	32/770 (4%)	24 (75%)	8 (25%)	0	100	100
1	I	32/770 (4%)	25 (78%)	7 (22%)	0	100	100
All	All	279/6930 (4%)	231 (83%)	48 (17%)	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	25/669 (4%)	25 (100%)	0	100	100
1	B	25/669 (4%)	25 (100%)	0	100	100
1	C	25/669 (4%)	25 (100%)	0	100	100
1	D	23/669 (3%)	23 (100%)	0	100	100
1	E	23/669 (3%)	23 (100%)	0	100	100
1	F	23/669 (3%)	23 (100%)	0	100	100
1	G	25/669 (4%)	25 (100%)	0	100	100
1	H	25/669 (4%)	25 (100%)	0	100	100
1	I	25/669 (4%)	25 (100%)	0	100	100
All	All	219/6021 (4%)	219 (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. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	14	HIS
1	F	15	GLN
1	A	13	HIS
1	G	13	HIS
1	H	13	HIS
1	I	13	HIS
1	B	13	HIS
1	C	13	HIS

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 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 [i](#)

There are no chain breaks in this entry.

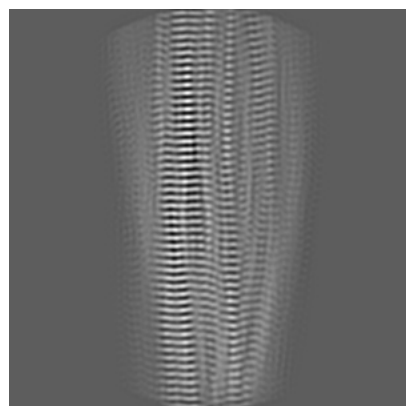
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37200. These allow visual inspection of the internal detail of the map and identification of artifacts.

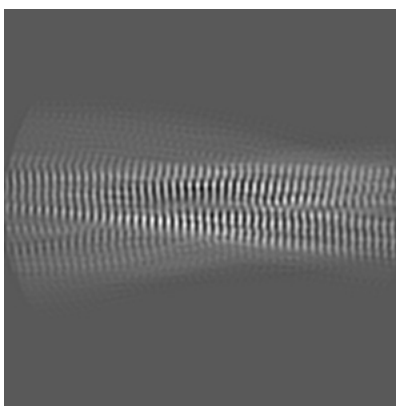
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

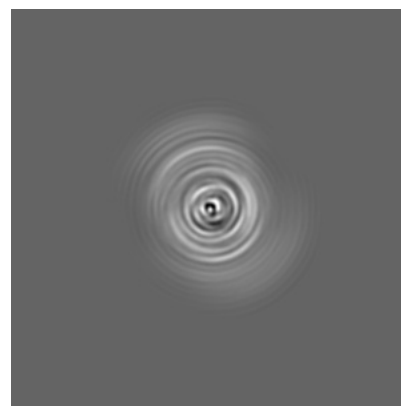
6.1.1 Primary map



X

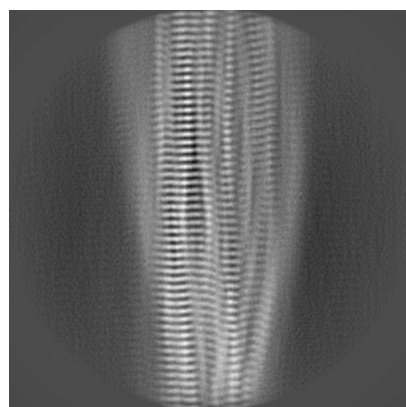


Y

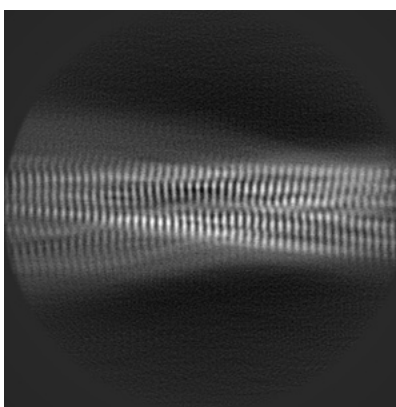


Z

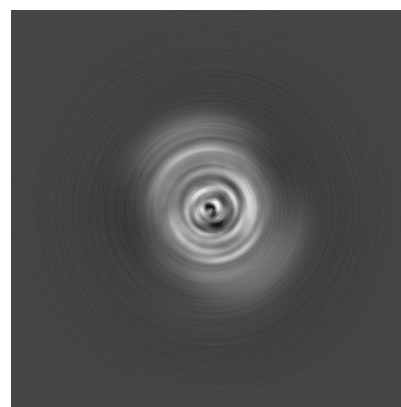
6.1.2 Raw map



X



Y

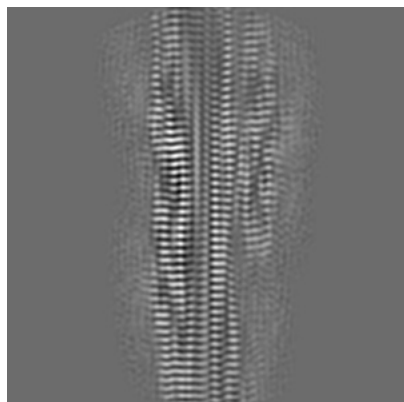


Z

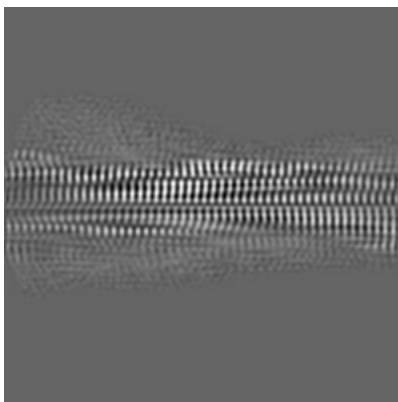
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

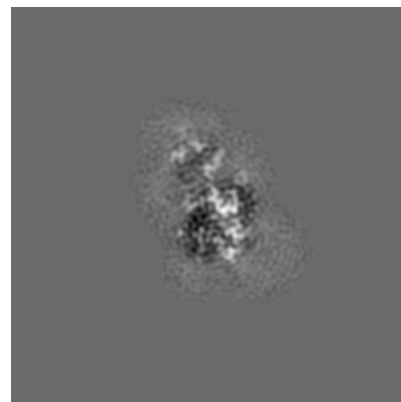
6.2.1 Primary map



X Index: 144

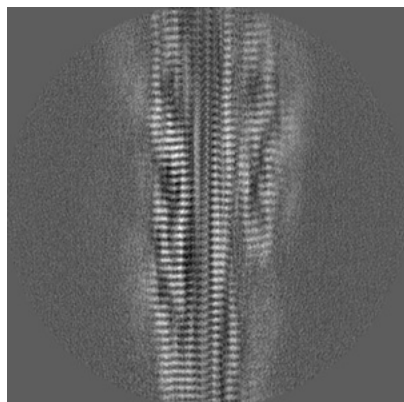


Y Index: 144

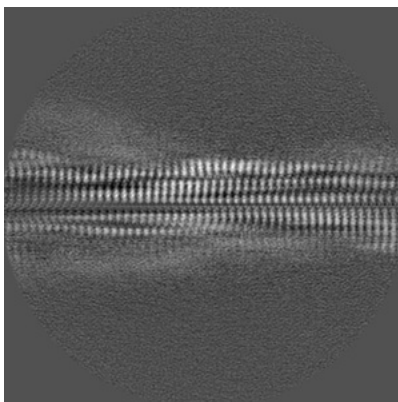


Z Index: 144

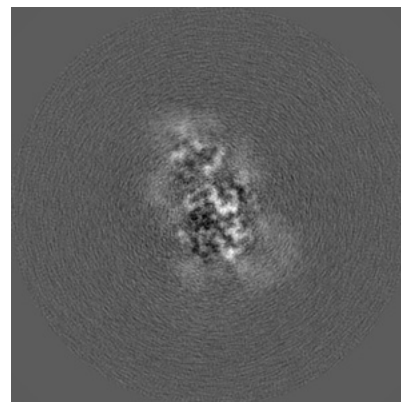
6.2.2 Raw map



X Index: 144



Y Index: 144

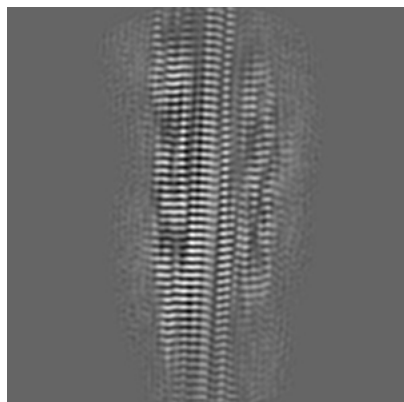


Z Index: 144

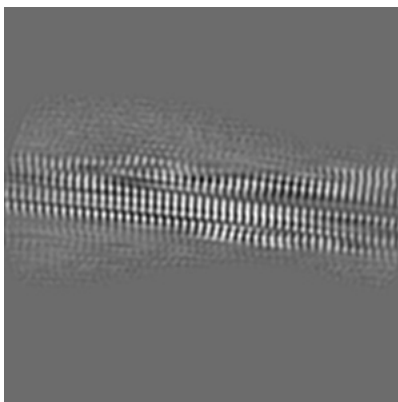
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

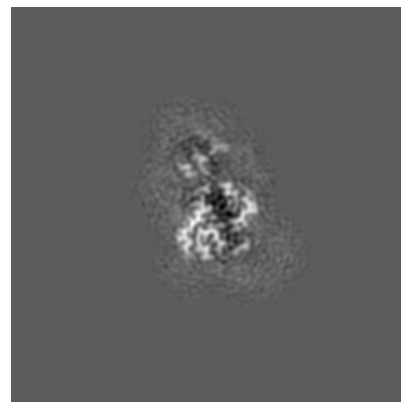
6.3.1 Primary map



X Index: 137

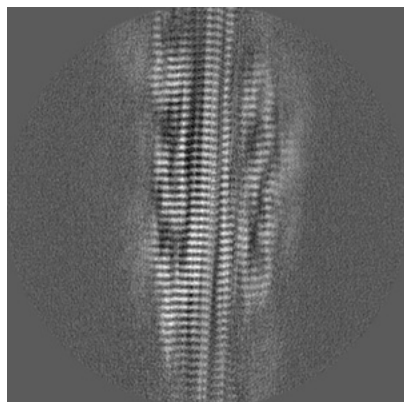


Y Index: 126

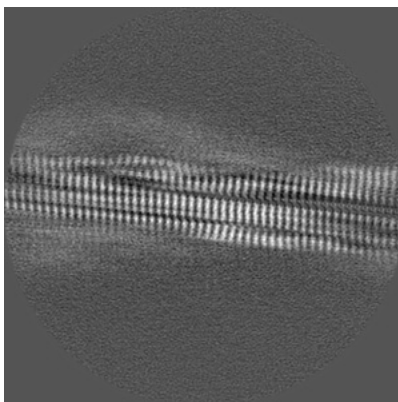


Z Index: 158

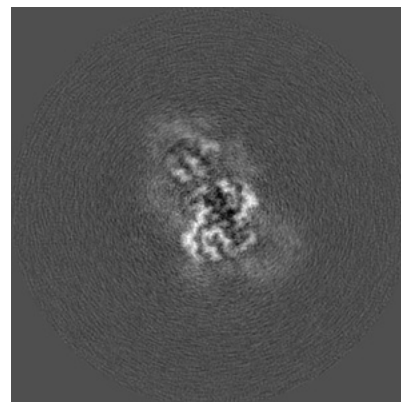
6.3.2 Raw map



X Index: 137



Y Index: 126

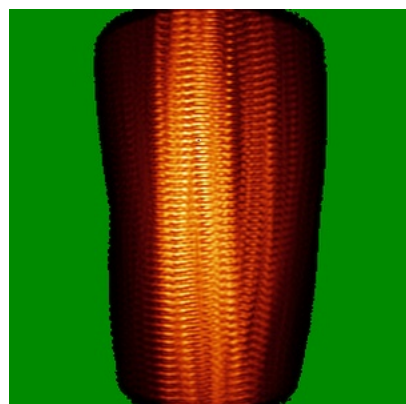


Z Index: 129

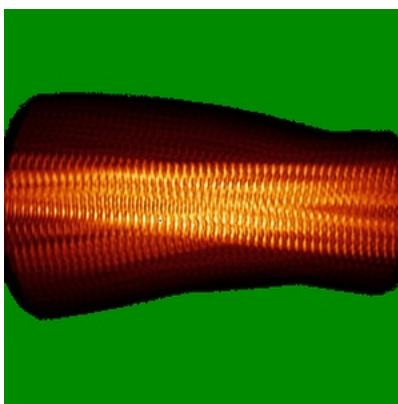
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

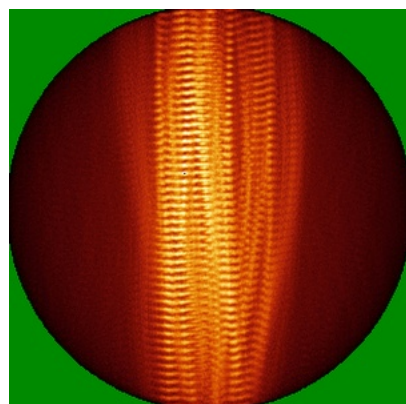


Y

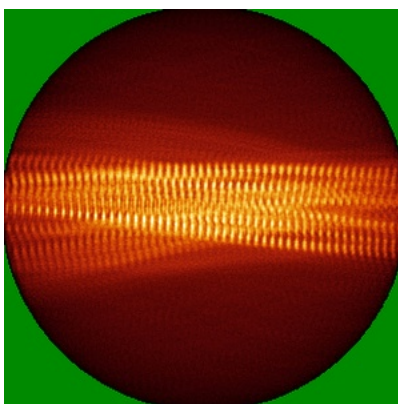


Z

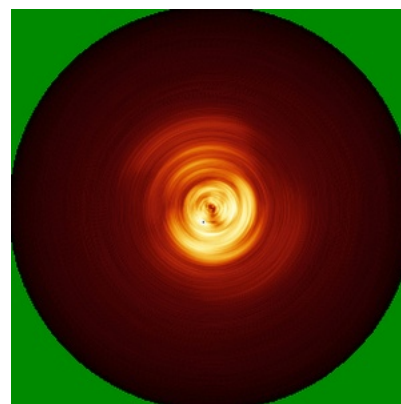
6.4.2 Raw map



X



Y

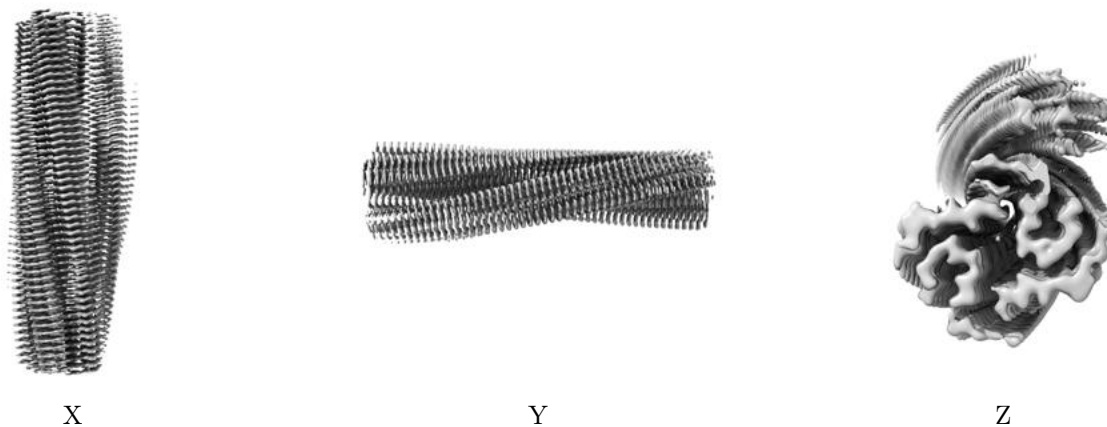


Z

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.

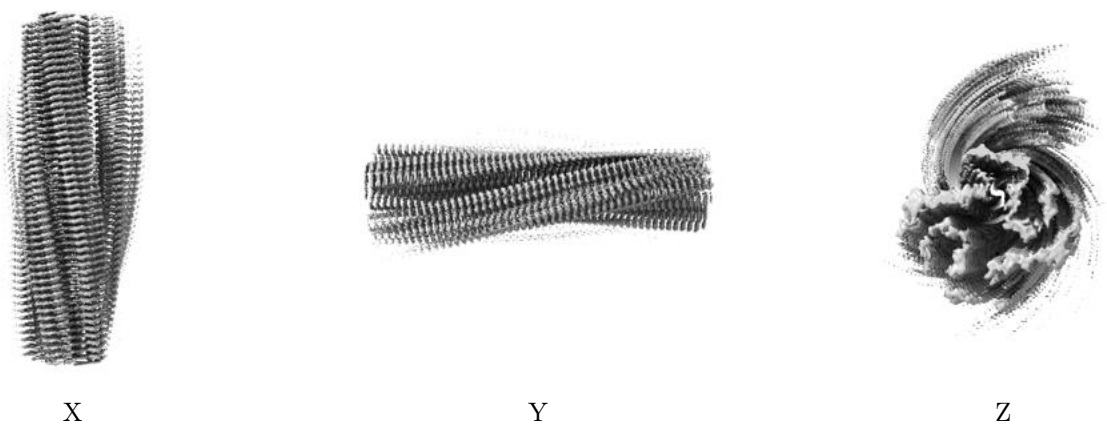
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00575. 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.

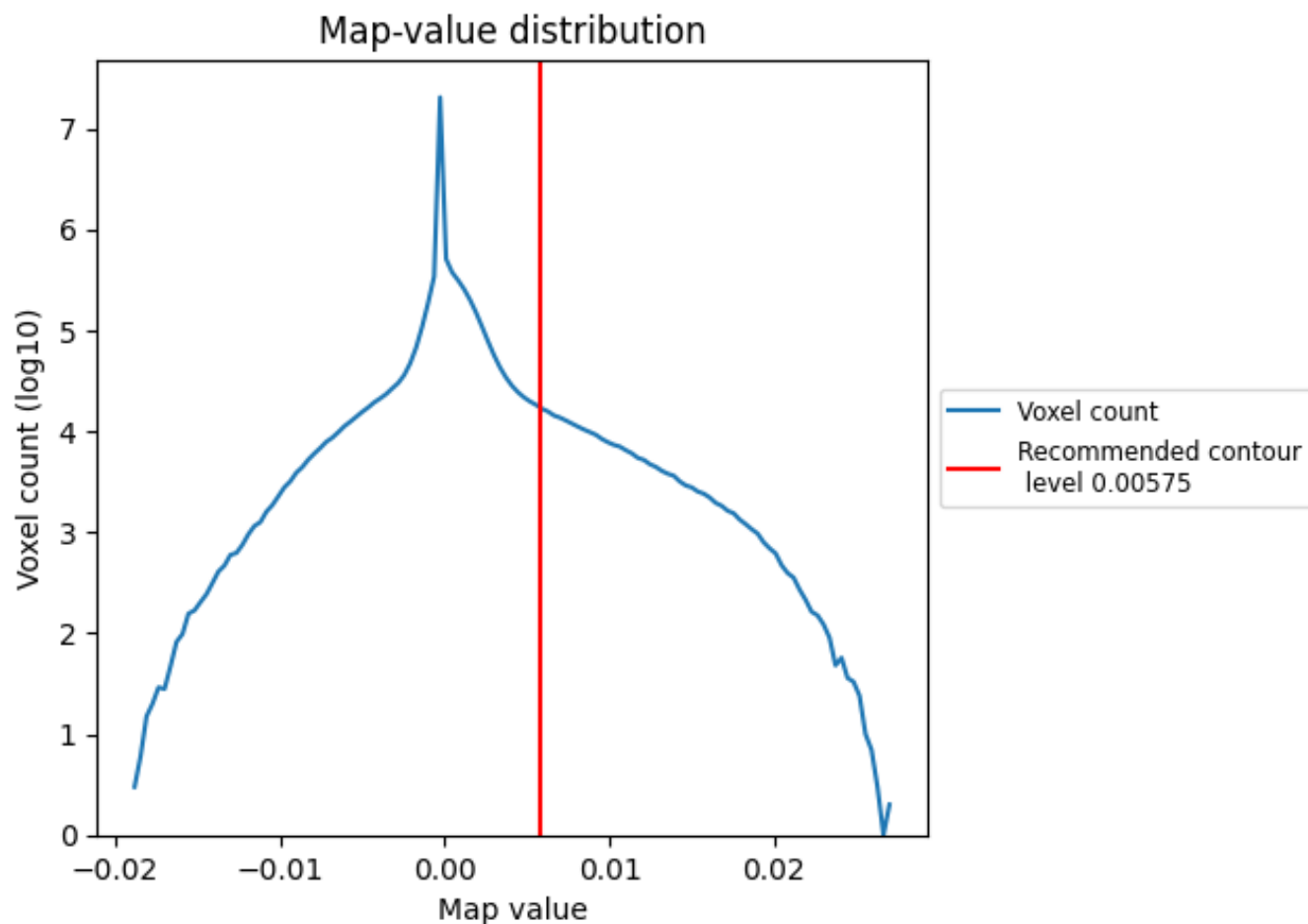
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

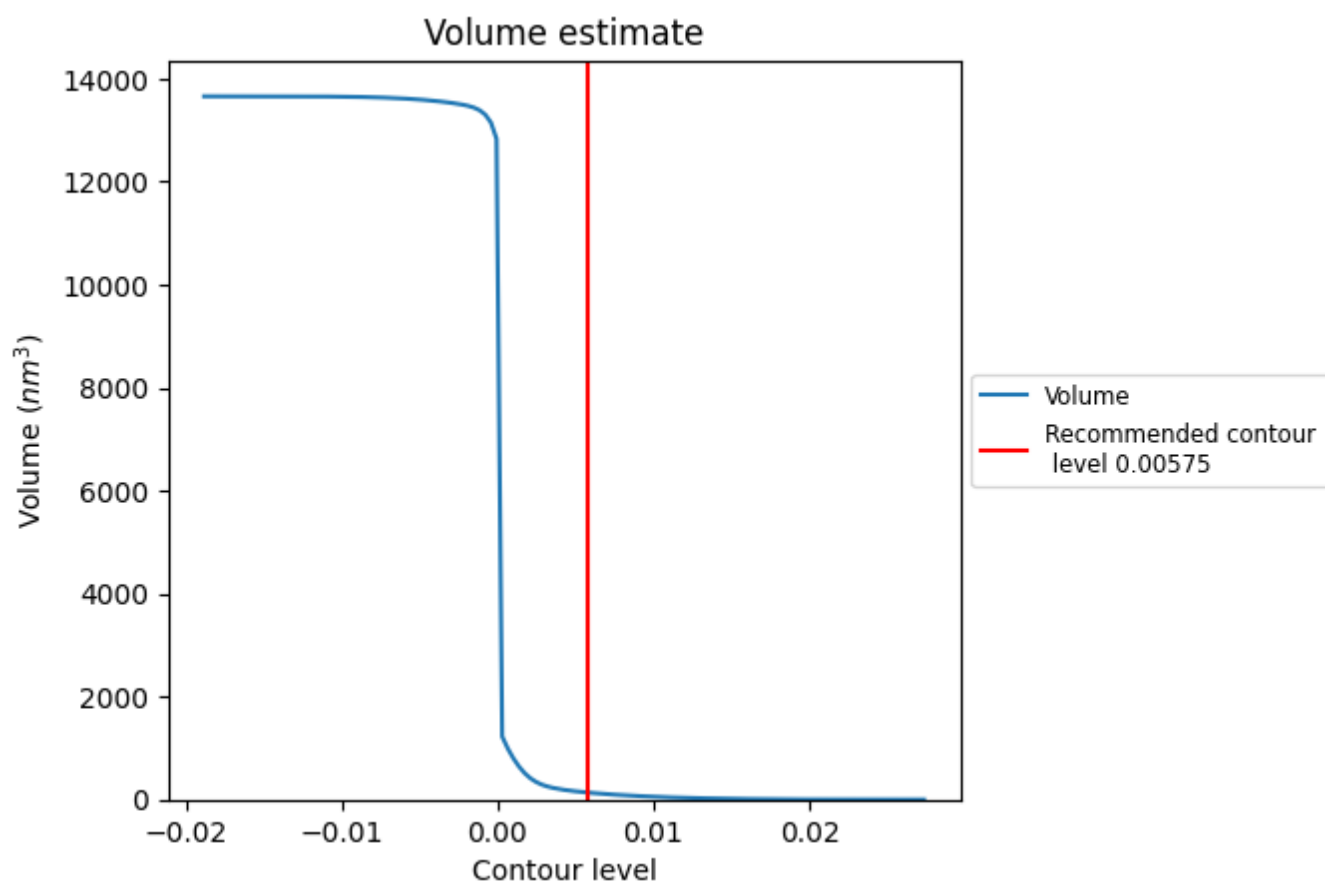
This section contains the results of statistical analysis of the map.

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.

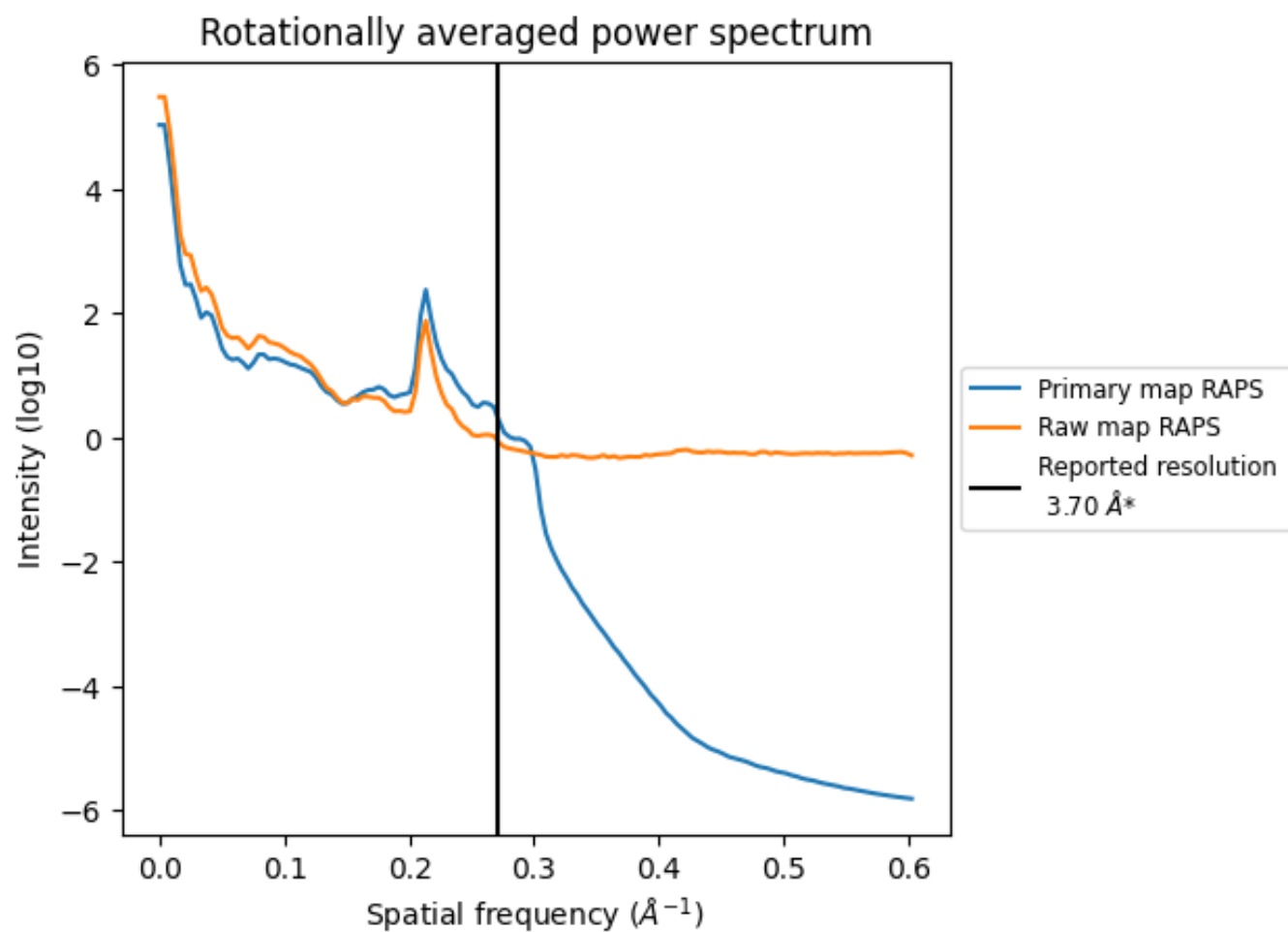
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 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 ⓘ

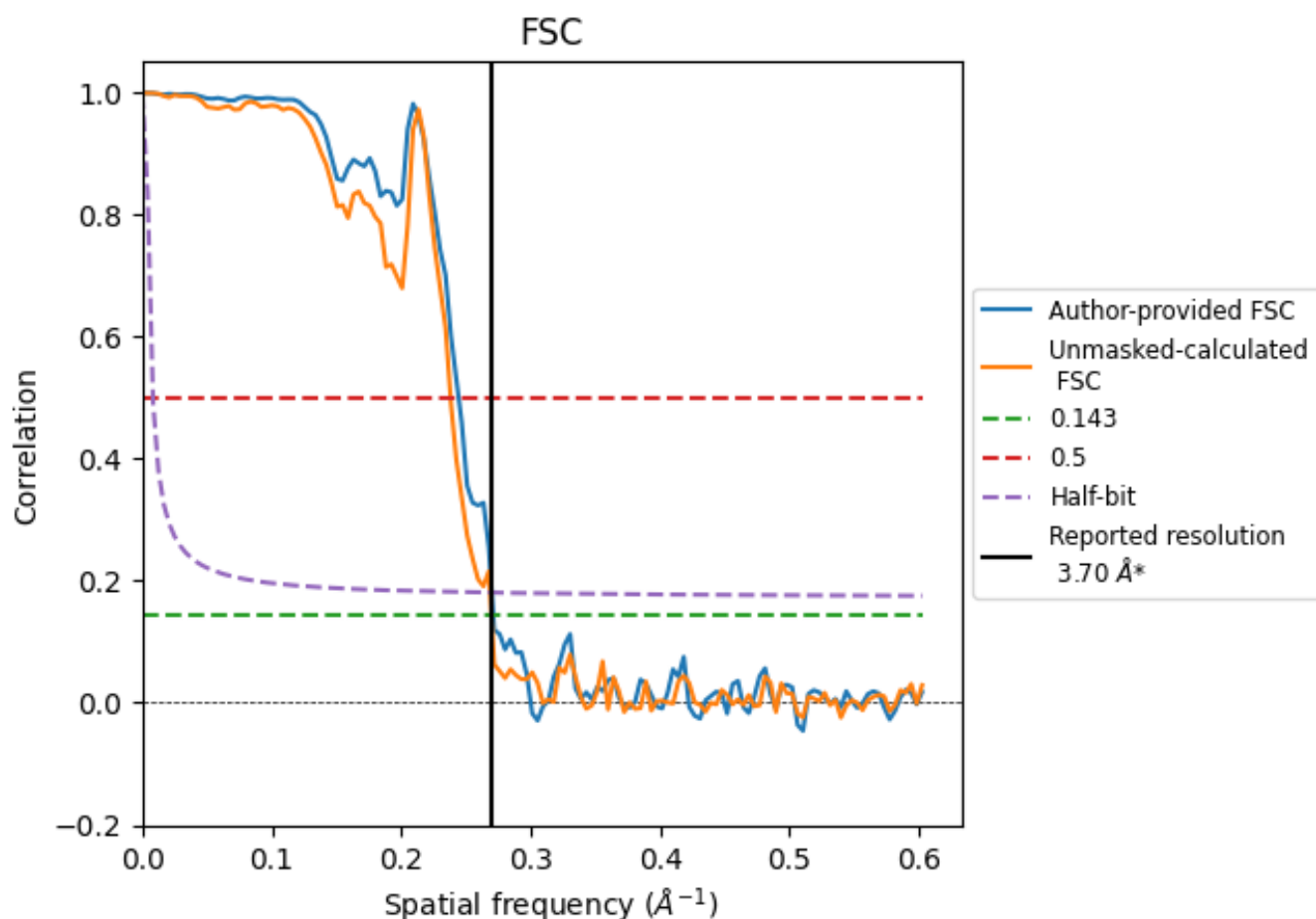


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.69	4.09	3.70
Unmasked-calculated*	3.71	4.20	3.72

*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-37200 and PDB model 8KF6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

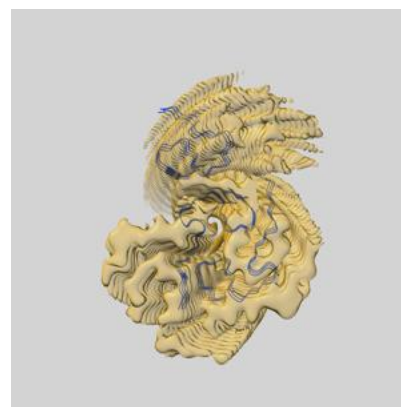
9.1 Map-model overlay [i](#)



X



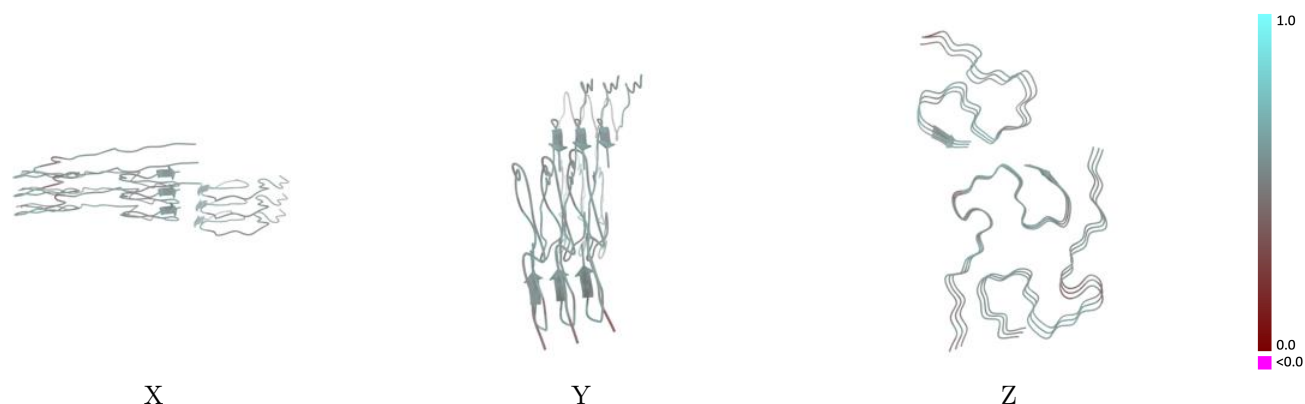
Y



Z

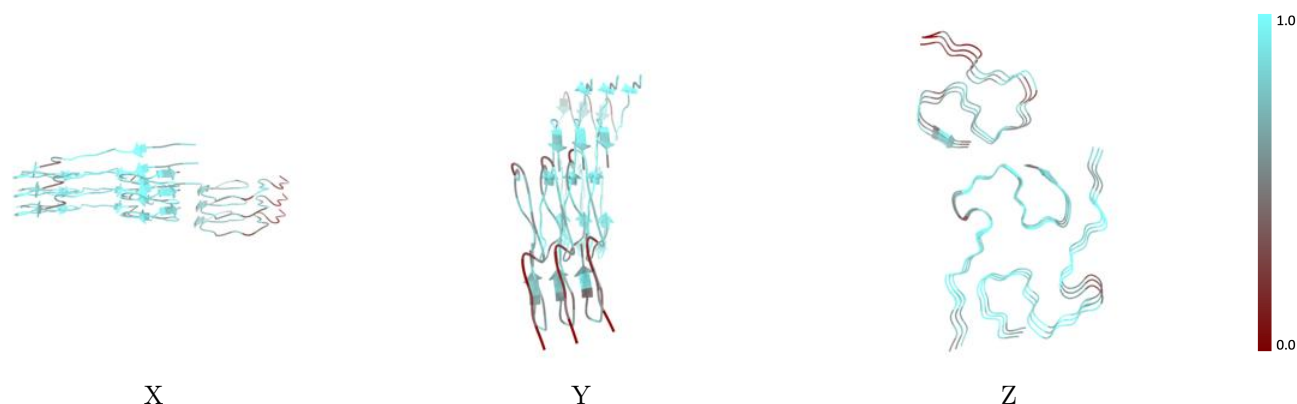
The images above show the 3D surface view of the map at the recommended contour level 0.00575 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



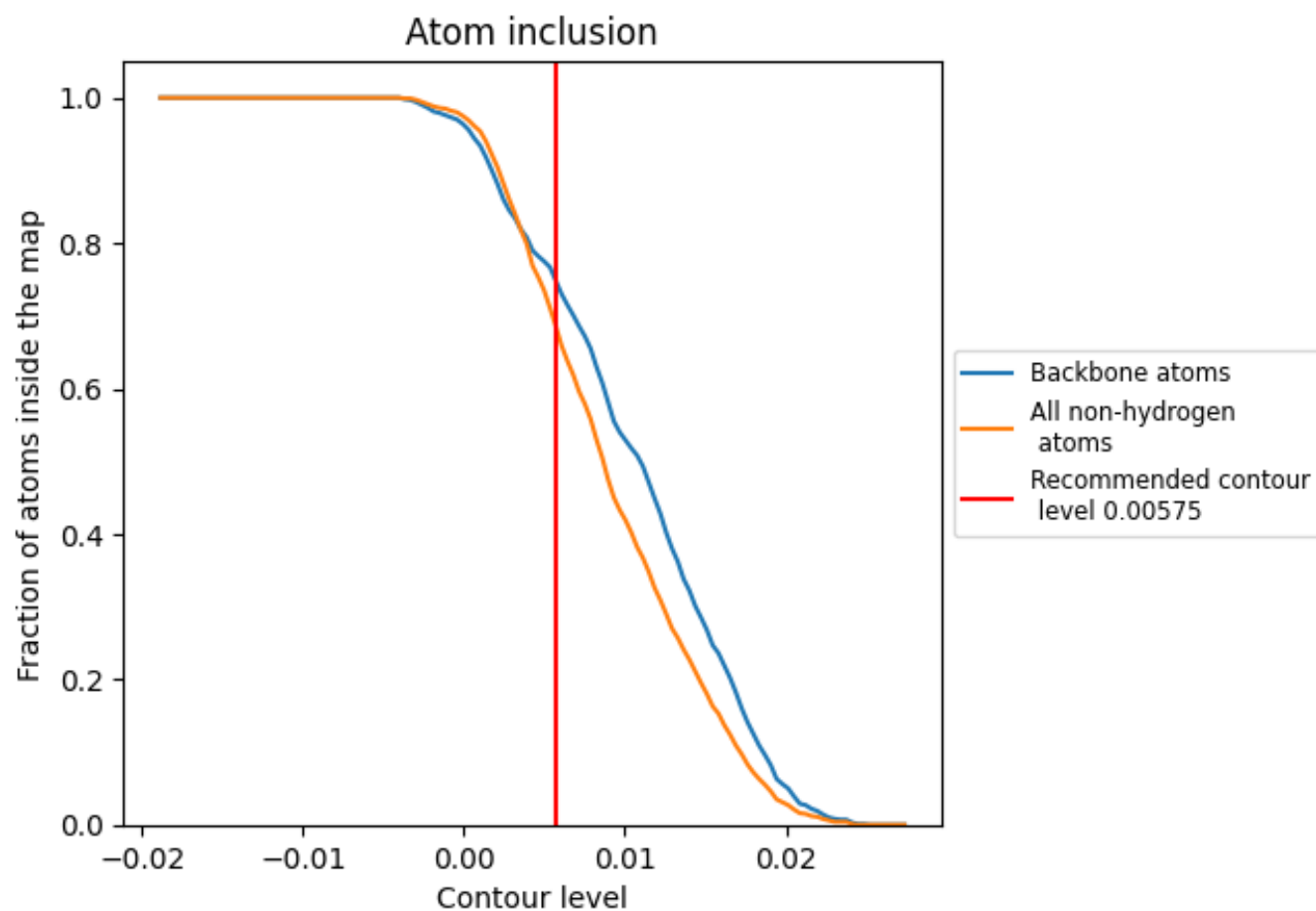
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00575).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.00575) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.5240
A	0.7470	0.5230
B	0.7430	0.5260
C	0.7550	0.5250
D	0.5240	0.5290
E	0.5470	0.5310
F	0.5070	0.5260
G	0.7430	0.5180
H	0.7710	0.5210
I	0.7630	0.5200

1.0

0.0

<0.0