



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:57 AM UTC

PDB ID : 9WZI / pdb_00009wzi
EMDB ID : EMD-66403
Title : Full-length Caspase-1-CARD filament
Authors : Xue, D.; Ni, F.; Liu, S.; Yan, H.; Luo, Z.; Fu, G.; Wang, Q.; Ma, J.
Deposited on : 2025-09-29
Resolution : 4.00 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

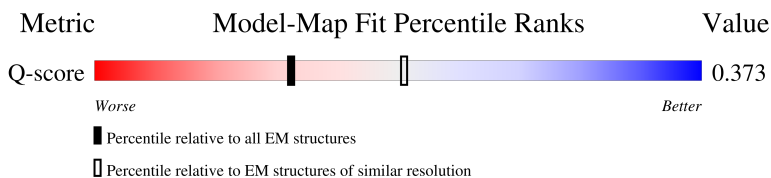
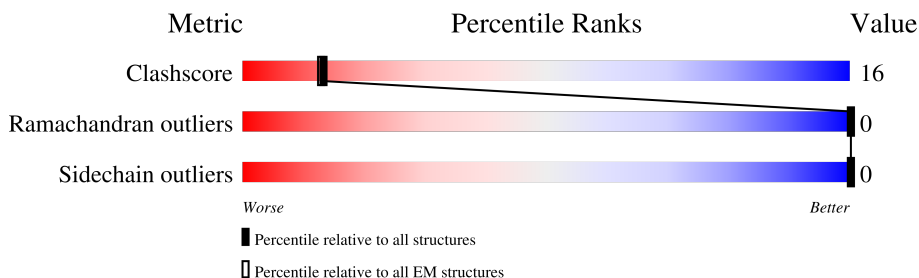
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	404	
1	B	404	
1	C	404	
1	D	404	

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Mol	Chain	Length	Quality of chain
1	E	404	 14% 8% 78%
1	F	404	 15% 7% 78%
1	G	404	 16% 6% 78%
1	H	404	 15% 7% 78%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5544 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.

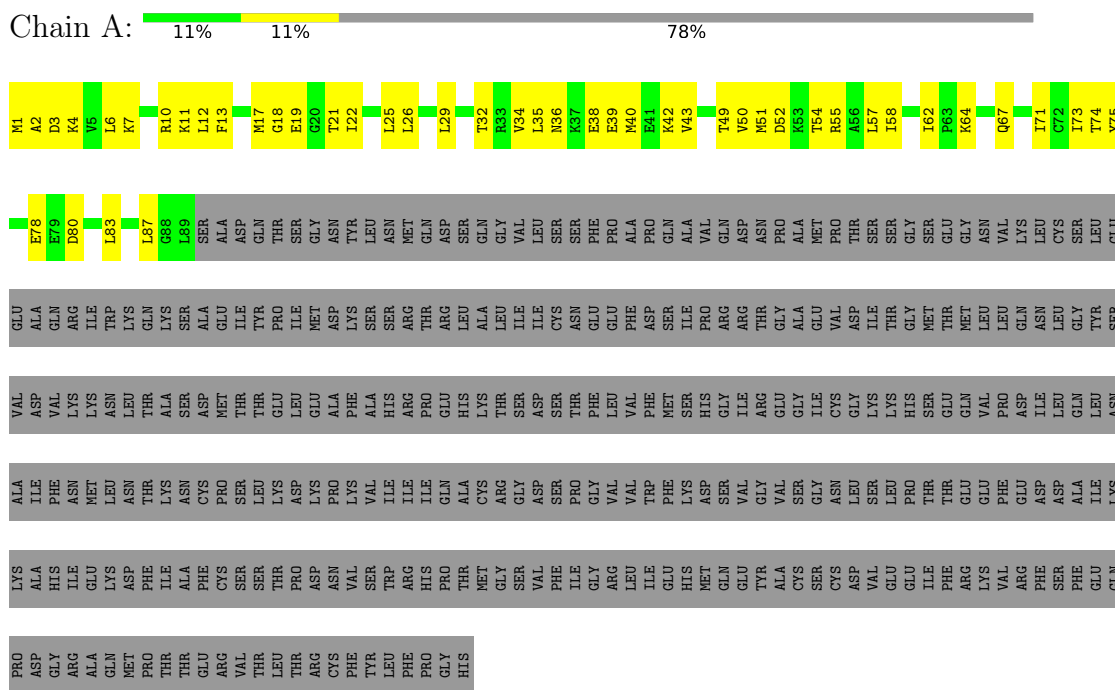
- Molecule 1 is a protein called Caspase-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	89	Total 693	C 433	N 119	O 134	S 7	0	0
1	B	89	Total 693	C 433	N 119	O 134	S 7	0	0
1	C	89	Total 693	C 433	N 119	O 134	S 7	0	0
1	D	89	Total 693	C 433	N 119	O 134	S 7	0	0
1	E	89	Total 693	C 433	N 119	O 134	S 7	0	0
1	F	89	Total 693	C 433	N 119	O 134	S 7	0	0
1	G	89	Total 693	C 433	N 119	O 134	S 7	0	0
1	H	89	Total 693	C 433	N 119	O 134	S 7	0	0

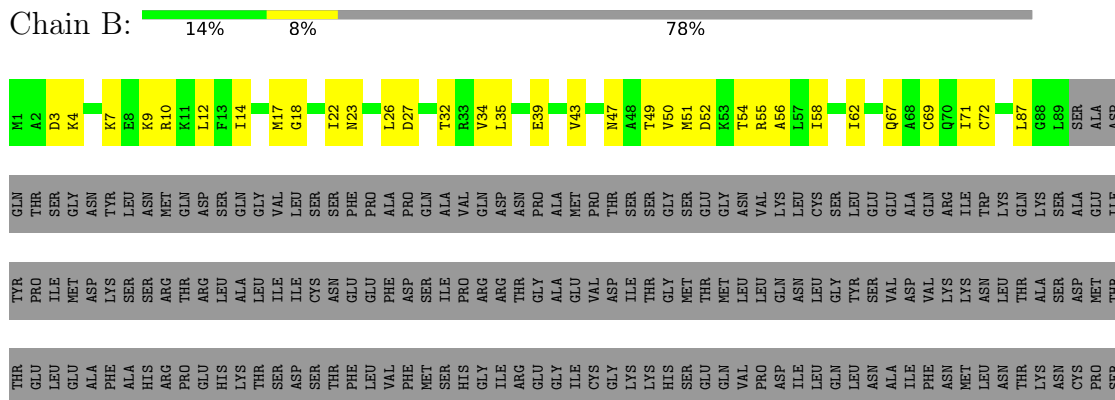
3 Residue-property plots

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: Caspase-1



• Molecule 1: Caspase-1





● Molecule 1: Caspase-1

Chain E:  14% 8% 78%

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● Molecule 1: Caspase-1

Chain F:  15% 7% 78%

M1	A2	D3	K4	K11	G18	E19	G20	T21	I22	T32	R33	V34	M40	E41	V50	M51	D52	K53	T54	I58	I62	Q70	I71	C72	I73	T74	Y75	E79	L83	L87	G88	L89	SER	ALA	ASP	GLN	THR	SER	GLY	ASN	THR	GLN	GLN					
GLY	VAL	LEU	SER	SER	PHE	PRO	ALA	ALA	VAL	GLN	ASP	ASN	PRO	ALA	ALA	MET	PRO	SER	GLY	SER	GLY	LEU	CYS	SER	LEU	TYR	GLU	GLY	ASN	VAL	LYS	LEU	LYS	GLN	ASP	THR	THR	GLN	THR	GLN	THR	ILE	MET	ASP	LYS	THR	ALA	
LEU	ILE	ILE	CYS	ASN	GLU	GLU	PHE	ASP	PHE	ARG	THR	GLY	ALA	GLU	VAL	ASP	ILE	THR	MET	THR	LEU	ASN	GLY	TYR	SER	GLU	VAL	ASP	VAL	LYS	ARG	LYS	ASP	ASP	MET	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
THR	SER	ASP	SER	THR	PHE	LEU	VAL	VAL	PHE	GLY	ARG	GLU	GLY	ILE	CYS	GLY	LYS	HIS	SER	GLY	GLN	VAL	LEU	GLN	LEU	ALA	ASN	ILE	PHE	ASN	MET	LYS	ASN	CYS	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ARG	GLY	ASP	SER	PRO	GLY	VAL	VAL	LYS	ASP	VAL	GLY	VAL	GLY	ASN	LEU	SER	PRO	THR	THR	GLU	PHE	ASP	ALA	ILE	LYS	LYS	ALA	HIS	ILE	GLY	THR	ILE	PHE	CYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLY	SER	VAL	PHE	ILE	GLY	LEU	ARG	HIS	GLN	GLY	TYR	ALA	CYS	CYS	ASP	VAL	GLU	ILE	PHE	ARG	LYS	ARG	PHE	GLU	PRO	GLN	ASP	GLY	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

● Molecule 1: Caspase-1

Chain G:  16% 6% 78%

M1	A2	D3	K4	R10	K11	L12	F13	I14	G18	T21	I22	L26	L29	R33	V34	L35	E39	M40	E41	M51	T54	L57	I58	N61	I62	L63	T86	L87	G88	L89	SER	ALA	ASP	GLN	THR	SER	GLY	ASN	THR	GLN	ASP	SER								
GLY	VAL	LEU	SER	PHE	PRO	ALA	PRO	GLN	VAL	GLN	ASP	PRO	MET	THR	SER	GLY	SER	GLU	GLY	ASN	VAL	LYS	LEU	SER	GLU	ALA	GLN	ARG	ILE	TRP	LYS	GLN	SER	ALA	GLU	ILE	ASP	TYR	THR	PRO	ILE	MET	ASP	LYS	SER	SER	THR	ARG	GLY	ALA

GLY	SER	VAL	PHE	ILE	GLY	ARG	LEU	LEU	GLU	GLU	HIS	MET	GLN	GLU	TYR	ALA	ALA	CYS	SER	CYS	ASP	VAL	GLU	GLU	ILE	PHE	ARG	LYS	VAL	ARG	PHE	SER	PHE	GLU	GLN	ASP	GLY	ARG	ALA	GLN	MET	PRO	THR	THR	GLU	ARG	VAL	THR	THR	ARG	THR	GLU	LEU	PHE	PRO	GLY	HIS
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- Molecule 1: Caspase-1

Chain H: 15% 7% 78%

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

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-100.2°, rise=5.1 Å, axial sym=C3	Depositor
Number of segments used	194125	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 ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	217.6, 217.6, 217.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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	0.21	0/696	0.59	0/930
1	B	0.18	0/696	0.55	0/930
1	C	0.16	0/696	0.47	0/930
1	D	0.18	0/696	0.49	0/930
1	E	0.17	0/696	0.47	0/930
1	F	0.16	0/696	0.44	0/930
1	G	0.16	0/696	0.42	0/930
1	H	0.16	0/696	0.43	0/930
All	All	0.17	0/5568	0.49	0/7440

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	693	0	733	37	0
1	B	693	0	733	26	0
1	C	693	0	733	16	0
1	D	693	0	733	24	0
1	E	693	0	733	28	0
1	F	693	0	733	20	0
1	G	693	0	733	20	0
1	H	693	0	733	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5544	0	5864	185	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 16.

All (185) 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:38:GLU:OE1	1:A:42:LYS:NZ	2.07	0.88
1:E:34:VAL:HG13	1:E:35:LEU:HD12	1.62	0.82
1:B:35:LEU:HD11	1:B:39:GLU:HB2	1.61	0.80
1:E:6:LEU:HD12	1:E:13:PHE:HE2	1.51	0.76
1:D:29:LEU:HD21	1:D:35:LEU:HD13	1.71	0.71
1:B:27:ASP:OD2	1:E:55:ARG:NH2	2.25	0.69
1:G:29:LEU:HD22	1:G:35:LEU:HG	1.77	0.67
1:G:26:LEU:HD21	1:G:40:MET:HB2	1.77	0.67
1:H:36:ASN:N	1:H:39:GLU:OE2	2.26	0.67
1:C:32:THR:HG23	1:C:34:VAL:HG22	1.76	0.66
1:B:4:LYS:HA	1:B:7:LYS:HG2	1.79	0.65
1:G:39:GLU:OE2	1:G:39:GLU:N	2.21	0.64
1:G:22:ILE:HD11	1:G:54:THR:HG22	1.78	0.64
1:E:1:MET:HG3	1:E:2:ALA:H	1.63	0.64
1:B:9:LYS:NZ	1:B:87:LEU:O	2.30	0.63
1:D:25:LEU:HD22	1:D:57:LEU:HD11	1.80	0.63
1:E:3:ASP:OD1	1:E:4:LYS:NZ	2.31	0.63
1:F:22:ILE:HD11	1:F:54:THR:HG22	1.81	0.62
1:A:32:THR:HG23	1:A:34:VAL:HG22	1.83	0.61
1:B:22:ILE:HD11	1:B:54:THR:HG22	1.83	0.61
1:E:26:LEU:HD21	1:E:40:MET:HE2	1.83	0.60
1:G:12:LEU:HB3	1:G:87:LEU:HD22	1.82	0.60
1:F:3:ASP:OD1	1:F:4:LYS:N	2.34	0.60
1:F:3:ASP:OD1	1:F:4:LYS:NZ	2.35	0.60
1:A:75:TYR:HA	1:A:78:GLU:HG3	1.85	0.59
1:E:22:ILE:HD11	1:E:54:THR:HG22	1.83	0.59
1:E:58:ILE:O	1:E:62:ILE:HG12	2.01	0.59
1:D:1:MET:HB3	1:D:4:LYS:HZ1	1.68	0.58
1:E:3:ASP:OD1	1:E:4:LYS:N	2.37	0.58
1:H:22:ILE:HD11	1:H:54:THR:HG22	1.85	0.57
1:G:3:ASP:OD1	1:G:4:LYS:N	2.37	0.57
1:B:4:LYS:O	1:B:7:LYS:N	2.37	0.57
1:G:58:ILE:O	1:G:62:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ASP:OD1	1:D:4:LYS:N	2.38	0.56
1:H:58:ILE:O	1:H:62:ILE:HG12	2.06	0.56
1:F:32:THR:HG23	1:F:34:VAL:HG23	1.86	0.56
1:C:18:GLY:O	1:C:22:ILE:HG12	2.05	0.56
1:H:25:LEU:HD22	1:H:57:LEU:HD11	1.89	0.55
1:A:36:ASN:N	1:A:39:GLU:OE2	2.28	0.55
1:E:84:ALA:O	1:E:88:GLY:N	2.40	0.55
1:A:26:LEU:HD12	1:A:40:MET:HG2	1.87	0.55
1:F:87:LEU:HB3	1:F:89:LEU:HD13	1.88	0.55
1:C:4:LYS:HA	1:C:7:LYS:HE3	1.89	0.55
1:D:18:GLY:O	1:D:22:ILE:HG12	2.07	0.54
1:H:32:THR:HG23	1:H:34:VAL:HG23	1.89	0.53
1:B:17:MET:HG2	1:B:22:ILE:HD11	1.89	0.53
1:G:33:ARG:O	1:G:33:ARG:HG2	2.09	0.53
1:B:58:ILE:O	1:B:62:ILE:HG12	2.09	0.53
1:H:3:ASP:OD1	1:H:4:LYS:N	2.41	0.53
1:A:52:ASP:OD1	1:A:55:ARG:NH1	2.41	0.53
1:F:32:THR:HG21	1:F:71:ILE:HG21	1.90	0.53
1:H:37:LYS:O	1:H:40:MET:HG3	2.10	0.52
1:E:51:MET:HE1	1:E:55:ARG:NH2	2.24	0.52
1:D:58:ILE:O	1:D:62:ILE:HG12	2.09	0.52
1:H:6:LEU:HD13	1:H:13:PHE:HE2	1.75	0.52
1:A:18:GLY:O	1:A:22:ILE:HG12	2.09	0.52
1:C:83:LEU:O	1:C:87:LEU:HB2	2.10	0.52
1:A:17:MET:HE3	1:A:21:THR:OG1	2.10	0.51
1:E:87:LEU:HD22	1:E:89:LEU:HD22	1.90	0.51
1:E:1:MET:HB3	1:E:4:LYS:HZ1	1.75	0.51
1:F:18:GLY:O	1:F:21:THR:OG1	2.27	0.51
1:A:3:ASP:OD1	1:A:4:LYS:N	2.44	0.51
1:E:18:GLY:O	1:E:22:ILE:HG12	2.11	0.51
1:H:33:ARG:O	1:H:33:ARG:HG2	2.10	0.51
1:D:33:ARG:O	1:D:33:ARG:HG2	2.11	0.51
1:B:49:THR:HG23	1:B:52:ASP:H	1.76	0.50
1:E:29:LEU:HD21	1:E:72:CYS:SG	2.51	0.50
1:F:19:GLU:HB3	1:F:50:VAL:HG11	1.94	0.50
1:B:3:ASP:OD1	1:B:4:LYS:N	2.45	0.50
1:C:17:MET:HE3	1:C:18:GLY:O	2.12	0.50
1:G:3:ASP:OD1	1:G:4:LYS:NZ	2.44	0.50
1:D:3:ASP:OD1	1:D:4:LYS:NZ	2.45	0.50
1:E:54:THR:O	1:E:58:ILE:HG12	2.11	0.50
1:E:33:ARG:HG2	1:E:33:ARG:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:MET:O	1:F:54:THR:OG1	2.28	0.49
1:D:1:MET:HG3	1:D:2:ALA:H	1.77	0.49
1:B:43:VAL:HG23	1:B:56:ALA:HB3	1.94	0.49
1:A:58:ILE:O	1:A:62:ILE:HG12	2.12	0.49
1:B:69:CYS:HA	1:B:72:CYS:SG	2.53	0.49
1:E:25:LEU:HD22	1:E:57:LEU:HD11	1.95	0.49
1:H:76:ILE:HD11	1:H:83:LEU:HD23	1.94	0.48
1:G:57:LEU:O	1:G:61:VAL:HG23	2.12	0.48
1:A:64:LYS:HD2	1:A:64:LYS:O	2.14	0.48
1:D:58:ILE:HA	1:D:61:VAL:HG12	1.95	0.48
1:F:33:ARG:HG2	1:F:33:ARG:O	2.14	0.48
1:B:67:GLN:O	1:B:71:ILE:HG12	2.14	0.47
1:F:58:ILE:O	1:F:62:ILE:HG12	2.14	0.47
1:E:51:MET:HE1	1:E:55:ARG:HH22	1.79	0.47
1:G:51:MET:HE2	1:G:51:MET:HB3	1.81	0.47
1:F:18:GLY:O	1:F:22:ILE:HG12	2.15	0.47
1:G:3:ASP:OD1	1:G:4:LYS:HG3	2.15	0.47
1:H:29:LEU:CD2	1:H:35:LEU:HG	2.44	0.47
1:A:51:MET:O	1:A:54:THR:OG1	2.27	0.47
1:B:51:MET:HE1	1:B:55:ARG:HH22	1.79	0.47
1:G:18:GLY:O	1:G:21:THR:OG1	2.31	0.47
1:B:54:THR:O	1:B:58:ILE:HG12	2.15	0.46
1:G:18:GLY:O	1:G:22:ILE:HG12	2.15	0.46
1:D:43:VAL:HG23	1:D:56:ALA:HB3	1.97	0.46
1:C:58:ILE:HA	1:C:61:VAL:HG12	1.98	0.46
1:A:18:GLY:O	1:A:21:THR:OG1	2.23	0.46
1:B:3:ASP:C	1:B:7:LYS:HZ2	2.23	0.46
1:F:11:LYS:HB2	1:F:11:LYS:HE2	1.76	0.46
1:A:6:LEU:HD13	1:A:13:PHE:HE2	1.81	0.46
1:A:39:GLU:HA	1:A:42:LYS:NZ	2.31	0.46
1:B:50:VAL:O	1:B:54:THR:HG23	2.17	0.45
1:C:67:GLN:O	1:C:71:ILE:HG12	2.17	0.45
1:H:18:GLY:O	1:H:22:ILE:HG12	2.15	0.45
1:D:17:MET:HE1	1:D:21:THR:HB	1.98	0.45
1:G:29:LEU:CD2	1:G:34:VAL:HB	2.46	0.45
1:C:52:ASP:OD1	1:C:55:ARG:NH1	2.50	0.45
1:D:3:ASP:OD1	1:D:4:LYS:HG3	2.17	0.45
1:A:29:LEU:HB3	1:A:35:LEU:HD13	1.98	0.45
1:C:35:LEU:HD21	1:C:40:MET:HB3	1.99	0.45
1:F:75:TYR:CE1	1:F:79:GLU:HG3	2.51	0.45
1:F:4:LYS:HE2	1:F:4:LYS:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:LYS:HE2	1:D:11:LYS:HB2	1.60	0.44
1:A:39:GLU:HA	1:A:42:LYS:HZ2	1.82	0.44
1:H:12:LEU:HB3	1:H:87:LEU:HD11	1.99	0.44
1:H:47:ASN:HD22	1:H:52:ASP:C	2.25	0.44
1:A:4:LYS:O	1:A:7:LYS:N	2.51	0.44
1:C:58:ILE:O	1:C:62:ILE:HG12	2.18	0.44
1:D:83:LEU:O	1:D:87:LEU:HD23	2.18	0.44
1:G:29:LEU:HD23	1:G:34:VAL:HB	2.00	0.44
1:H:36:ASN:OD1	1:H:38:GLU:HG3	2.17	0.44
1:A:1:MET:HG3	1:A:2:ALA:H	1.82	0.44
1:E:6:LEU:HD12	1:E:13:PHE:CE2	2.41	0.43
1:E:75:TYR:CZ	1:E:79:GLU:HG3	2.52	0.43
1:F:50:VAL:HA	1:F:53:LYS:HD2	1.99	0.43
1:D:6:LEU:HD13	1:D:13:PHE:HE2	1.82	0.43
1:D:17:MET:HE3	1:D:18:GLY:O	2.17	0.43
1:G:51:MET:SD	1:H:38:GLU:HB2	2.59	0.43
1:A:19:GLU:HB3	1:A:50:VAL:HG11	2.00	0.43
1:A:50:VAL:O	1:A:54:THR:HG23	2.18	0.43
1:D:32:THR:HG23	1:D:34:VAL:HG22	2.01	0.43
1:E:37:LYS:O	1:E:40:MET:HG3	2.19	0.43
1:A:36:ASN:OD1	1:A:38:GLU:HG3	2.18	0.43
1:D:10:ARG:O	1:D:14:ILE:HG12	2.18	0.43
1:B:51:MET:O	1:B:54:THR:OG1	2.27	0.43
1:A:25:LEU:O	1:A:29:LEU:HD23	2.19	0.43
1:D:52:ASP:OD1	1:D:55:ARG:NH1	2.52	0.43
1:E:1:MET:HG3	1:E:2:ALA:N	2.29	0.43
1:C:3:ASP:OD1	1:C:4:LYS:HD2	2.19	0.42
1:C:43:VAL:HG23	1:C:56:ALA:HB3	2.01	0.42
1:B:47:ASN:ND2	1:B:52:ASP:HB3	2.34	0.42
1:H:18:GLY:O	1:H:21:THR:OG1	2.34	0.42
1:A:12:LEU:HB3	1:A:87:LEU:CD1	2.49	0.42
1:B:10:ARG:O	1:B:14:ILE:HG12	2.19	0.42
1:A:10:ARG:HG2	1:A:11:LYS:N	2.35	0.42
1:A:80:ASP:OD2	1:A:83:LEU:HB3	2.20	0.42
1:F:52:ASP:OD1	1:F:53:LYS:N	2.52	0.42
1:G:40:MET:SD	1:G:41:GLU:N	2.92	0.42
1:A:1:MET:HG3	1:A:2:ALA:N	2.35	0.42
1:A:39:GLU:O	1:A:43:VAL:HG23	2.20	0.42
1:A:54:THR:O	1:A:58:ILE:HG12	2.19	0.42
1:B:22:ILE:O	1:B:26:LEU:HD23	2.20	0.42
1:E:44:LYS:HA	1:E:53:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ILE:O	1:C:26:LEU:HD23	2.19	0.41
1:D:19:GLU:HB2	1:D:50:VAL:HG11	2.02	0.41
1:D:69:CYS:HA	1:D:72:CYS:SG	2.61	0.41
1:F:83:LEU:O	1:F:87:LEU:HD23	2.20	0.41
1:A:67:GLN:O	1:A:71:ILE:HG12	2.20	0.41
1:A:13:PHE:O	1:A:17:MET:HB2	2.21	0.41
1:B:32:THR:HG23	1:B:34:VAL:HG12	2.02	0.41
1:A:22:ILE:HD11	1:A:54:THR:HG22	2.03	0.41
1:E:50:VAL:O	1:E:53:LYS:HB2	2.20	0.41
1:A:73:ILE:HG13	1:A:74:THR:N	2.35	0.41
1:B:23:ASN:ND2	1:E:55:ARG:HH12	2.18	0.41
1:E:75:TYR:CE1	1:E:79:GLU:HG3	2.56	0.41
1:A:22:ILE:O	1:A:26:LEU:HD23	2.21	0.41
1:C:47:ASN:HD22	1:C:52:ASP:C	2.29	0.41
1:F:40:MET:SD	1:F:41:GLU:HG2	2.61	0.41
1:G:83:LEU:HA	1:G:86:THR:HG22	2.02	0.41
1:C:44:LYS:HA	1:C:53:LYS:NZ	2.35	0.41
1:D:22:ILE:HD11	1:D:54:THR:HG22	2.02	0.41
1:B:17:MET:HE2	1:B:17:MET:HB2	1.99	0.40
1:B:18:GLY:O	1:B:22:ILE:HG12	2.22	0.40
1:F:70:GLN:HA	1:F:73:ILE:HG22	2.03	0.40
1:G:10:ARG:O	1:G:14:ILE:HG12	2.21	0.40
1:E:19:GLU:HB3	1:E:50:VAL:HG11	2.04	0.40
1:A:3:ASP:OD1	1:A:4:LYS:HD3	2.22	0.40
1:A:49:THR:HG23	1:A:52:ASP:H	1.85	0.40
1:A:25:LEU:HD23	1:A:57:LEU:HD11	2.02	0.40
1:B:12:LEU:HB3	1:B:87:LEU:HD11	2.04	0.40
1:C:73:ILE:HG13	1:C:74:THR:N	2.36	0.40
1:D:13:PHE:O	1:D:17:MET:HB2	2.22	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	87/404 (22%)	85 (98%)	2 (2%)	0	100	100
1	B	87/404 (22%)	86 (99%)	1 (1%)	0	100	100
1	C	87/404 (22%)	84 (97%)	3 (3%)	0	100	100
1	D	87/404 (22%)	87 (100%)	0	0	100	100
1	E	87/404 (22%)	85 (98%)	2 (2%)	0	100	100
1	F	87/404 (22%)	85 (98%)	2 (2%)	0	100	100
1	G	87/404 (22%)	86 (99%)	1 (1%)	0	100	100
1	H	87/404 (22%)	86 (99%)	1 (1%)	0	100	100
All	All	696/3232 (22%)	684 (98%)	12 (2%)	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	77/356 (22%)	77 (100%)	0	100	100
1	B	77/356 (22%)	77 (100%)	0	100	100
1	C	77/356 (22%)	77 (100%)	0	100	100
1	D	77/356 (22%)	77 (100%)	0	100	100
1	E	77/356 (22%)	77 (100%)	0	100	100
1	F	77/356 (22%)	77 (100%)	0	100	100
1	G	77/356 (22%)	77 (100%)	0	100	100
1	H	77/356 (22%)	77 (100%)	0	100	100
All	All	616/2848 (22%)	616 (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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	31	GLN
1	A	47	ASN
1	B	23	ASN
1	B	31	GLN
1	B	47	ASN
1	C	36	ASN
1	C	47	ASN
1	D	47	ASN
1	D	70	GLN
1	E	67	GLN
1	F	47	ASN

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.

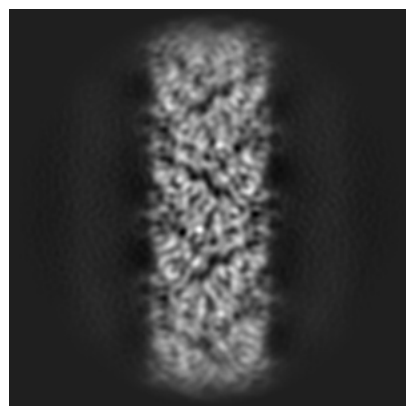
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66403. These allow visual inspection of the internal detail of the map and identification of artifacts.

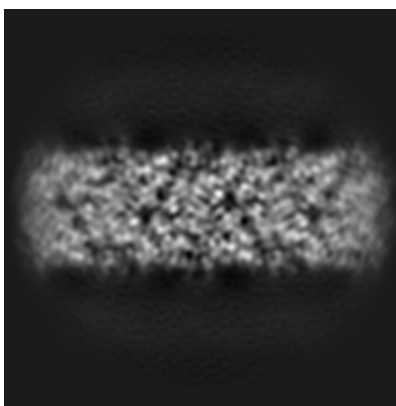
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

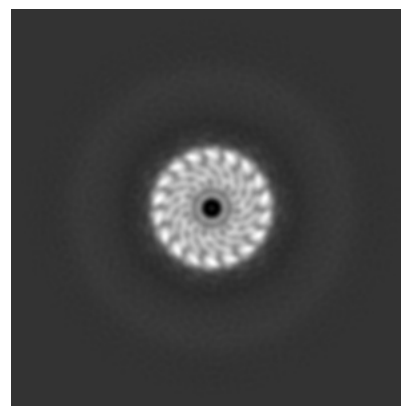
6.1.1 Primary map



X

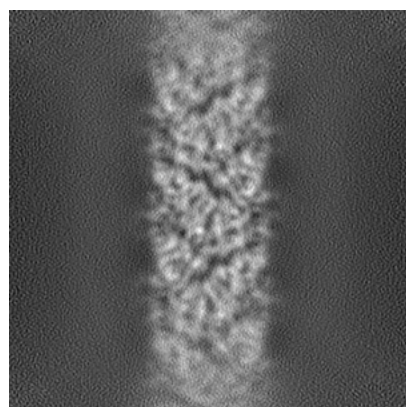


Y

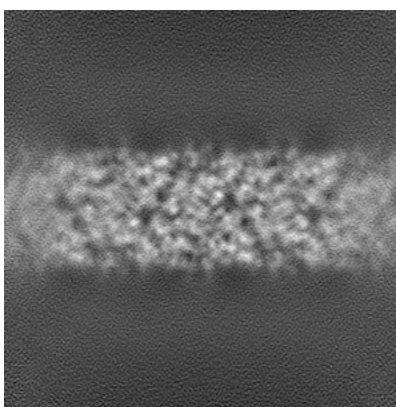


Z

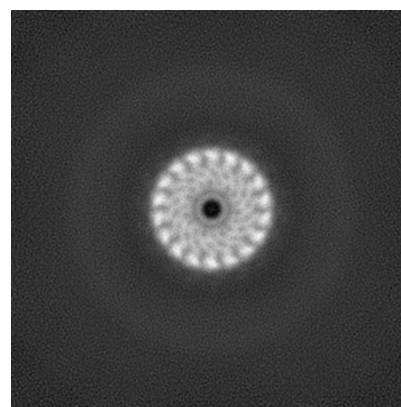
6.1.2 Raw map



X



Y

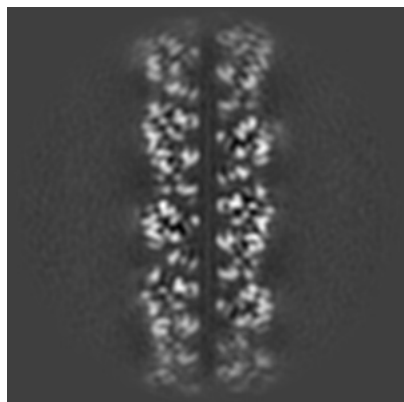


Z

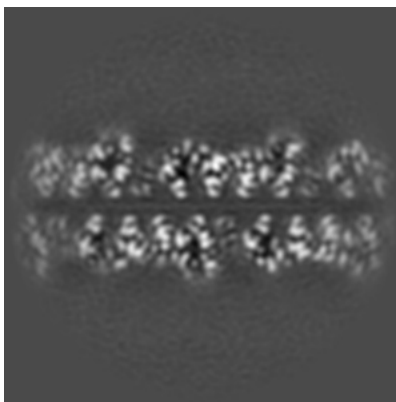
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

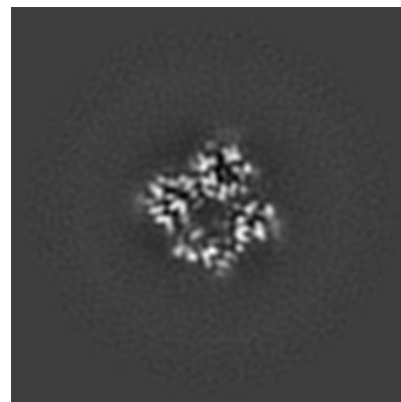
6.2.1 Primary map



X Index: 128

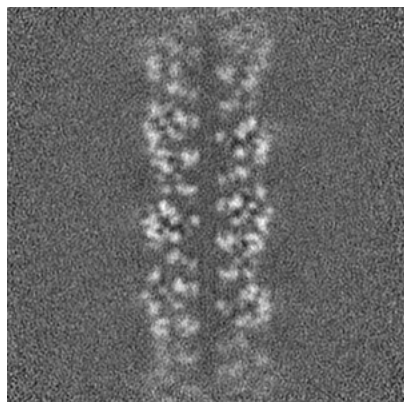


Y Index: 128

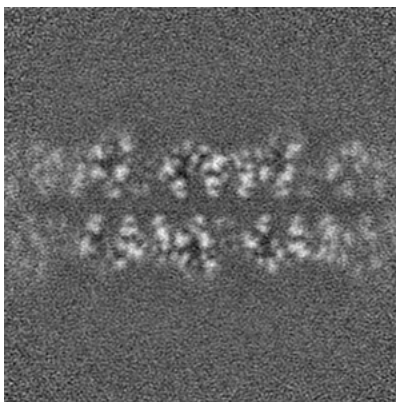


Z Index: 128

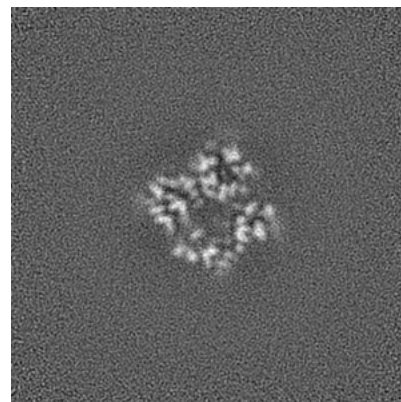
6.2.2 Raw map



X Index: 128



Y Index: 128

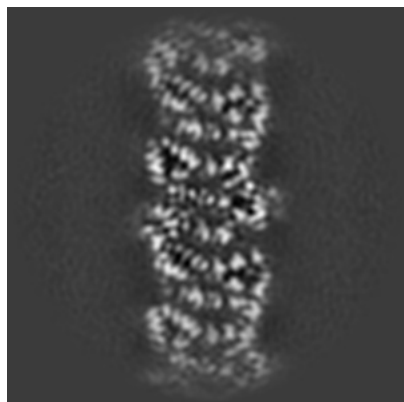


Z Index: 128

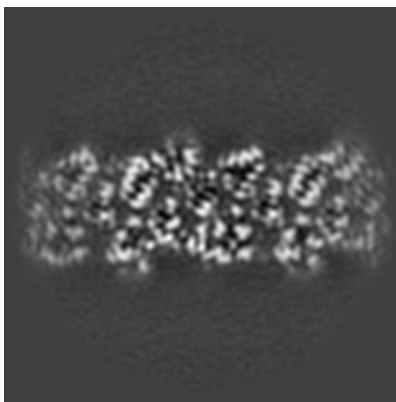
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

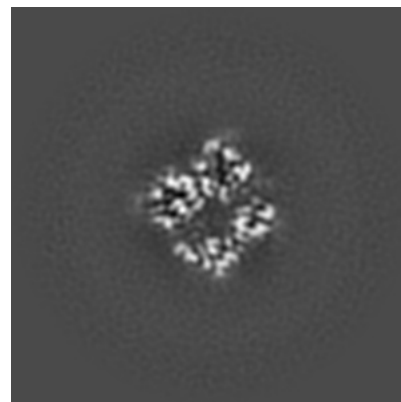
6.3.1 Primary map



X Index: 140

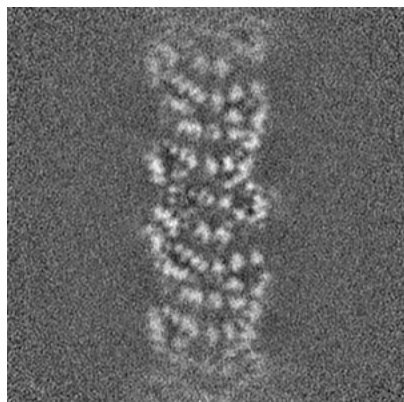


Y Index: 144

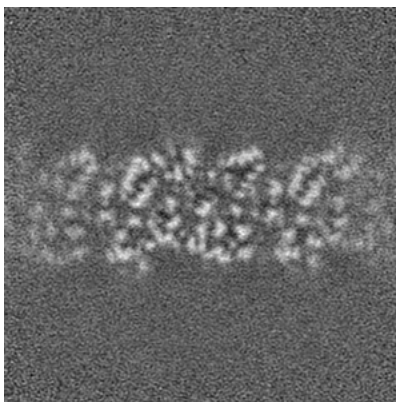


Z Index: 126

6.3.2 Raw map



X Index: 141



Y Index: 144

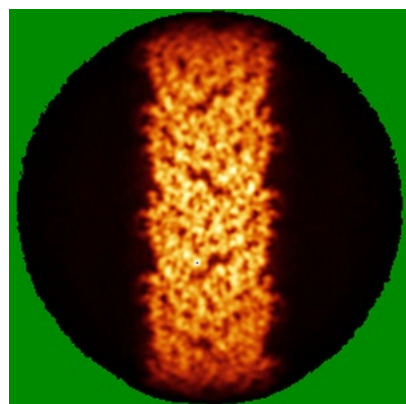


Z Index: 0

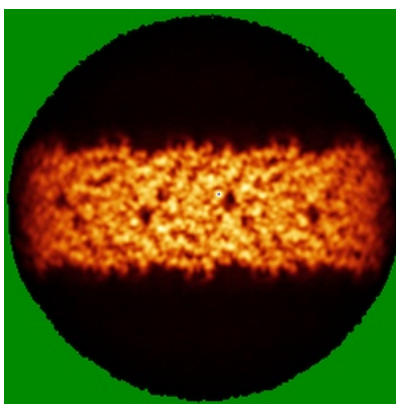
The images above show the largest variance slices of the map in three orthogonal directions.

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

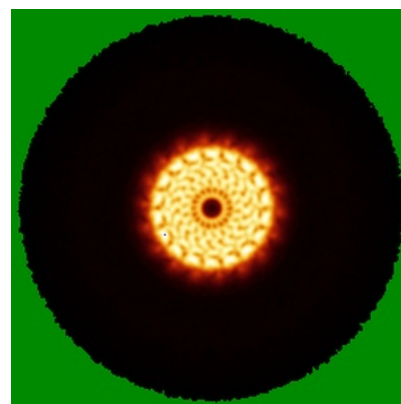
6.4.1 Primary map



X

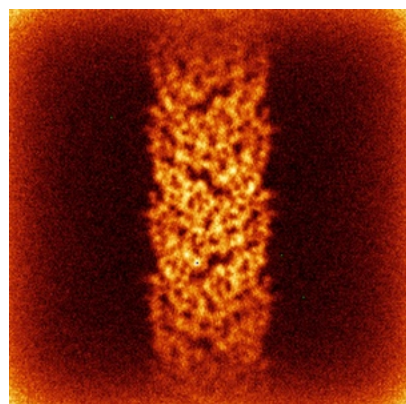


Y

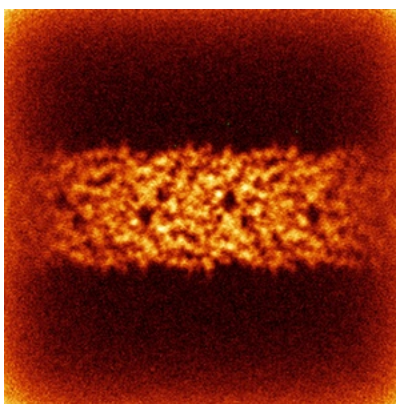


Z

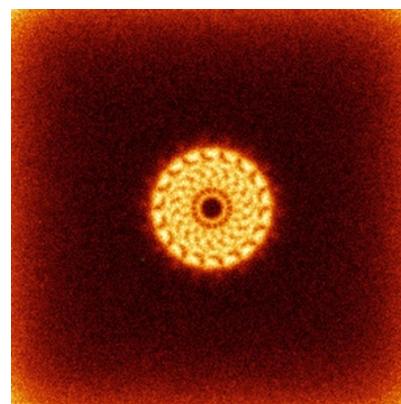
6.4.2 Raw map



X



Y



Z

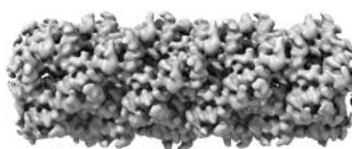
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

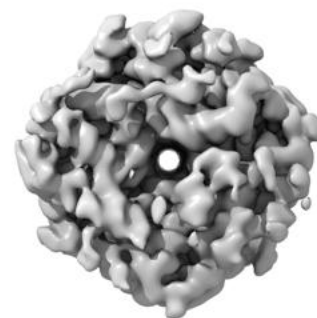
6.5.1 Primary map



X



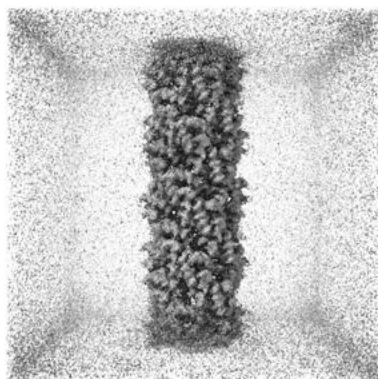
Y



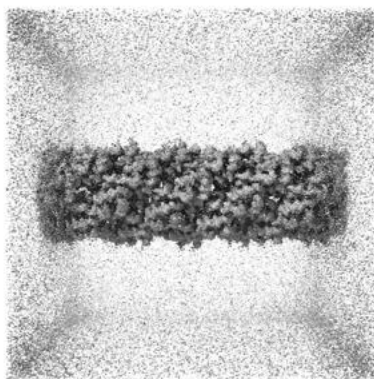
Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

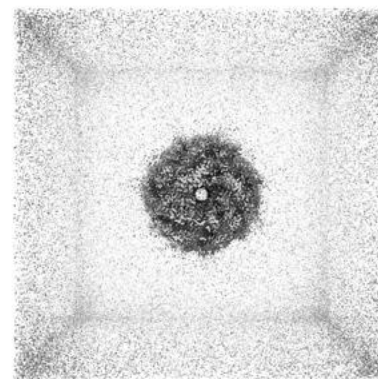
6.5.2 Raw map



X



Y



Z

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.

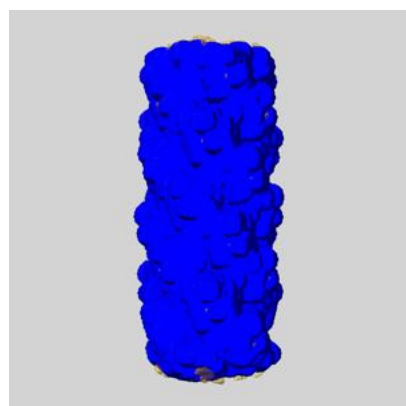
6.6 Mask visualisation [i](#)

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

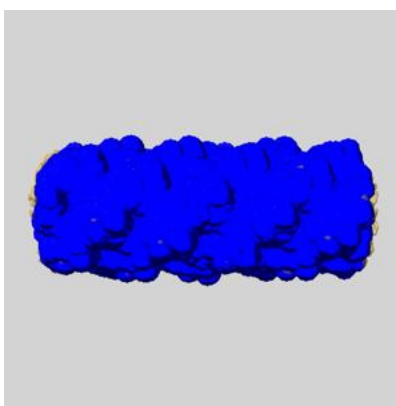
A mask typically either:

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

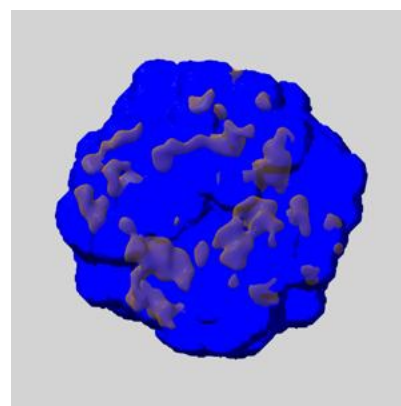
6.6.1 emd_66403_msk_1.map [i](#)



X



Y

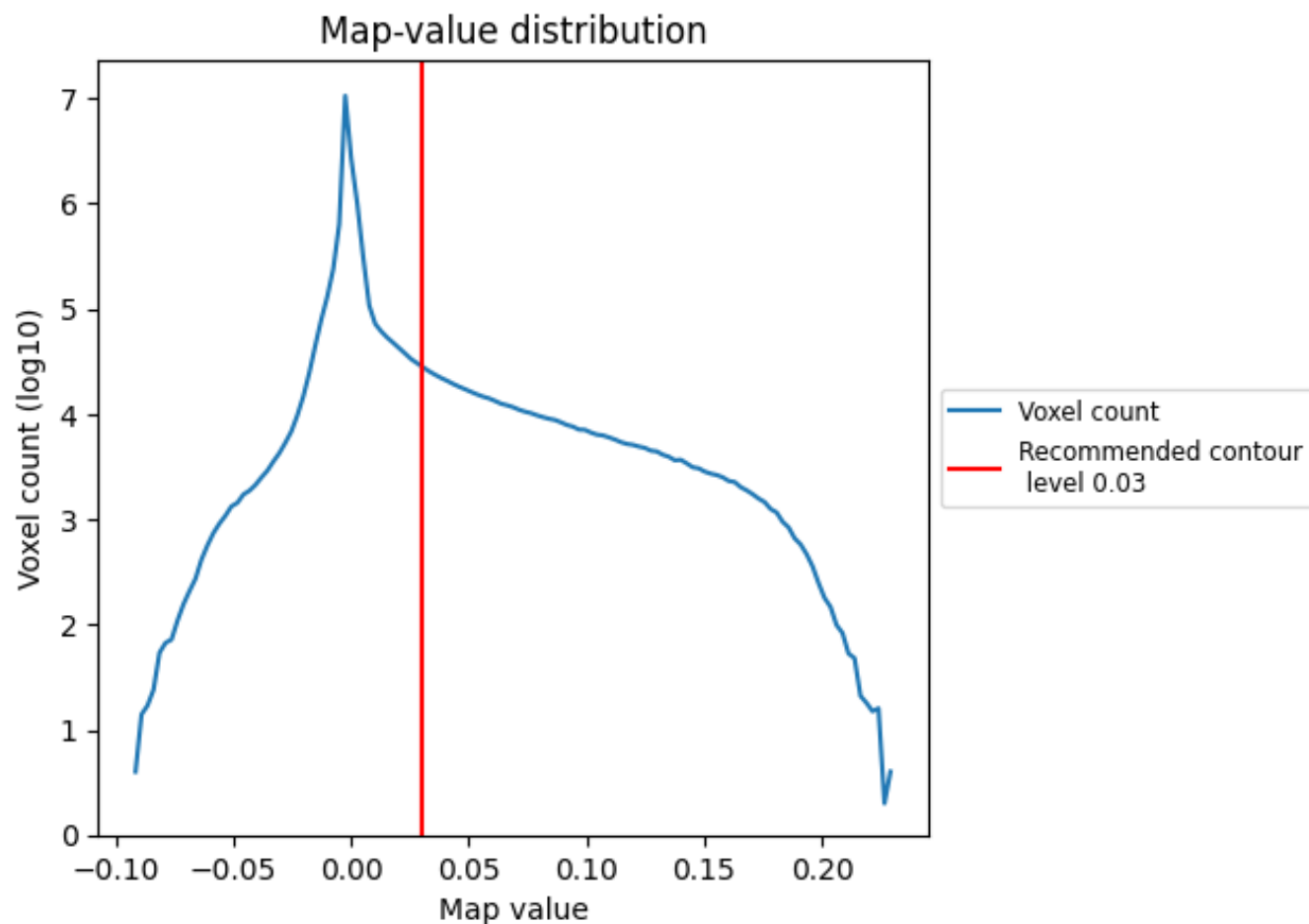


Z

7 Map analysis [i](#)

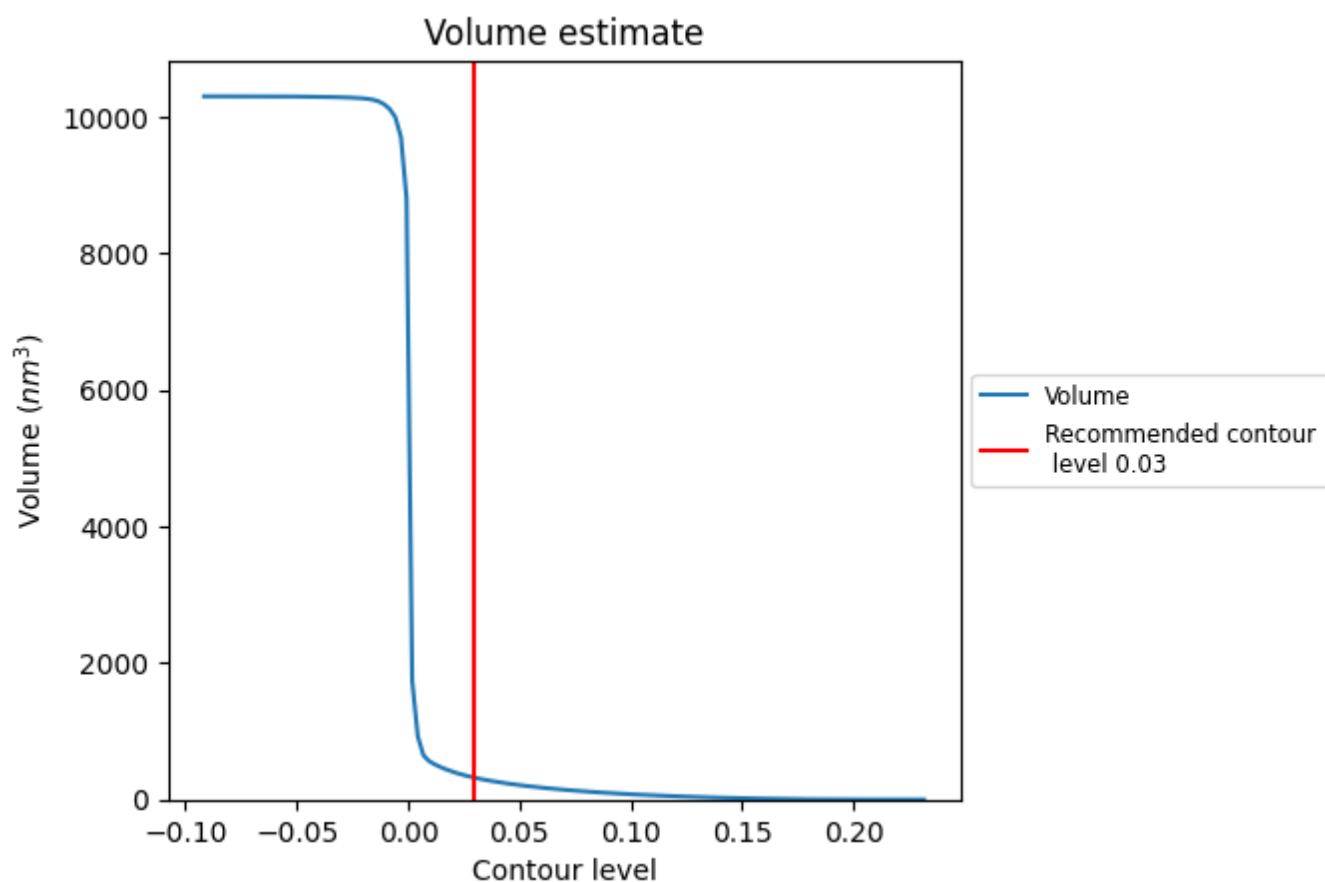
This section contains the results of statistical analysis of the map.

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.

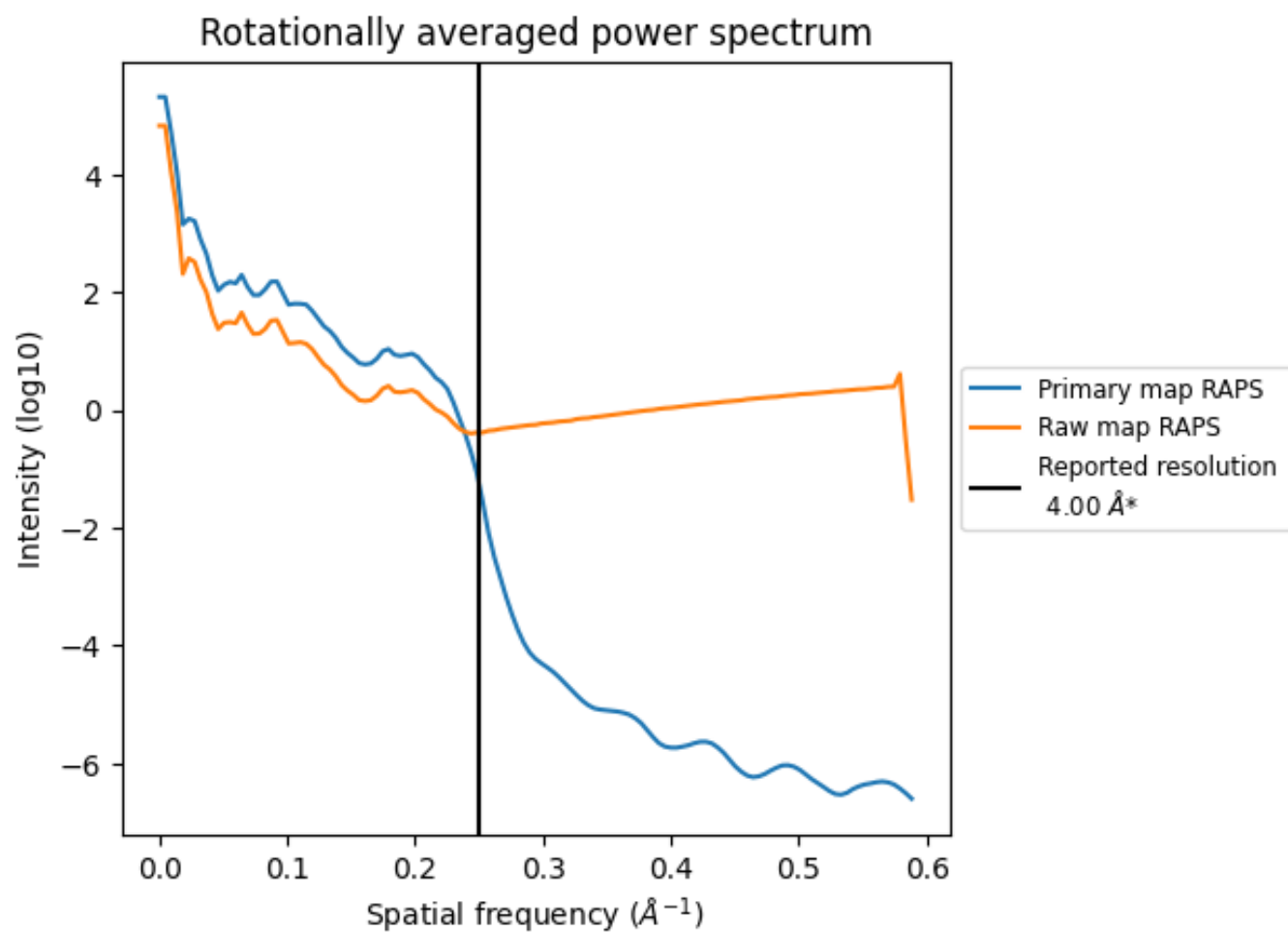
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 319 nm^3 ; this corresponds to an approximate mass of 288 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 ⓘ

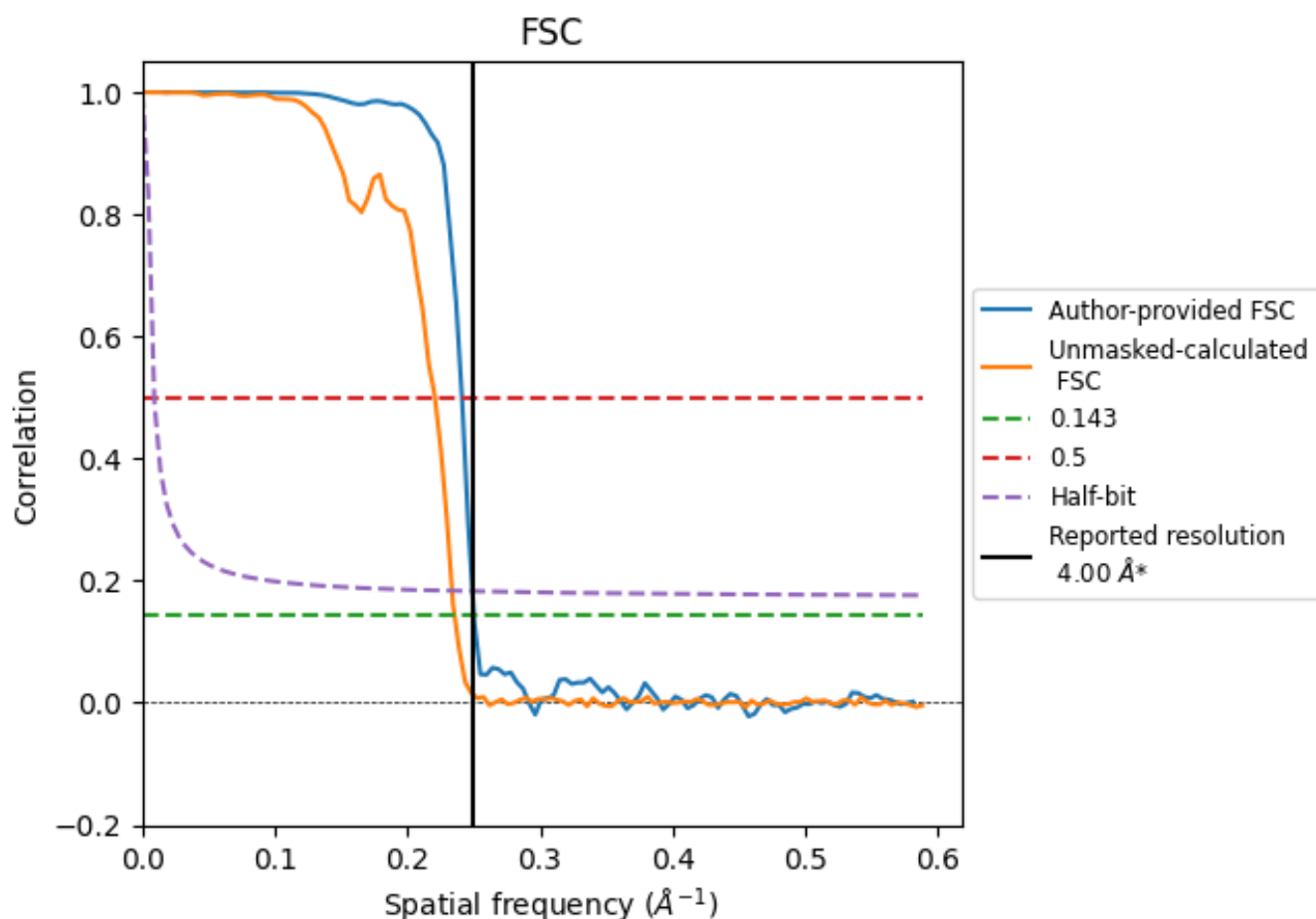


*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

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 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

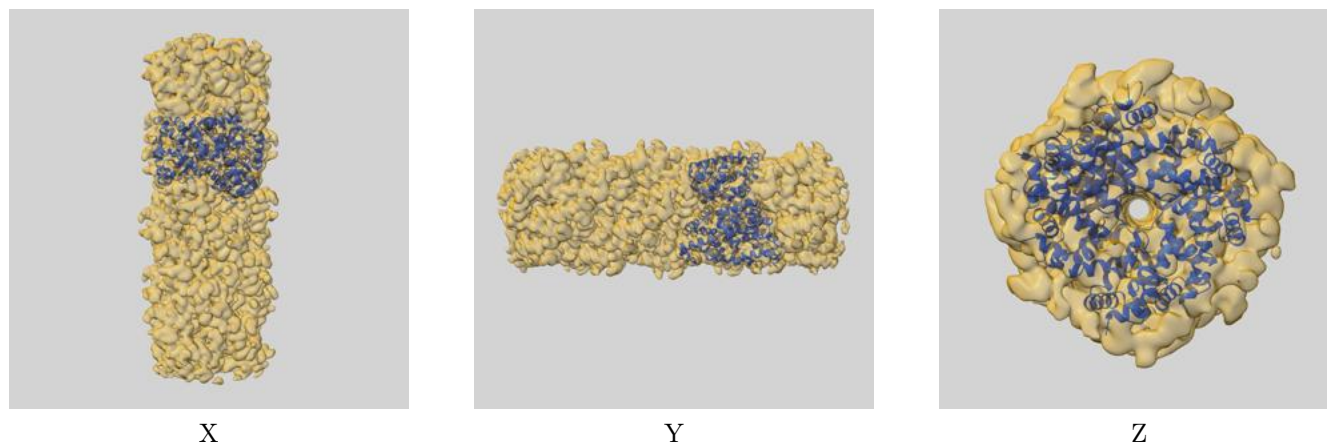
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	4.15	4.02
Unmasked-calculated*	4.24	4.53	4.28

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

9 Map-model fit [i](#)

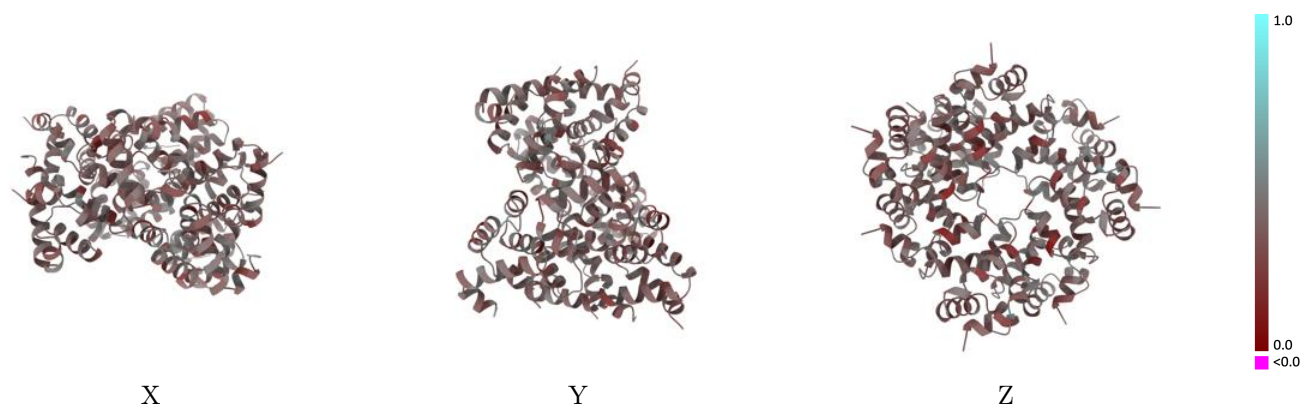
This section contains information regarding the fit between EMDB map EMD-66403 and PDB model 9WZI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



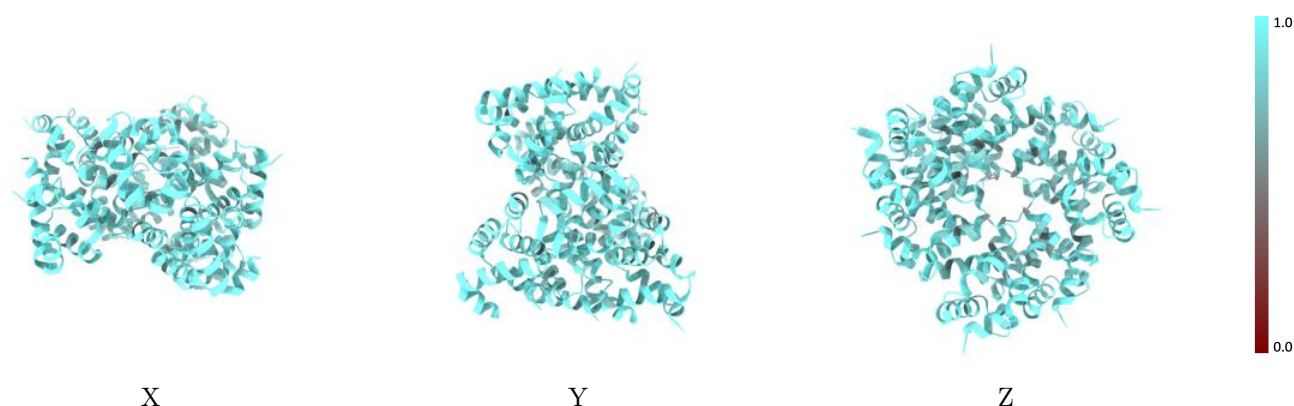
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



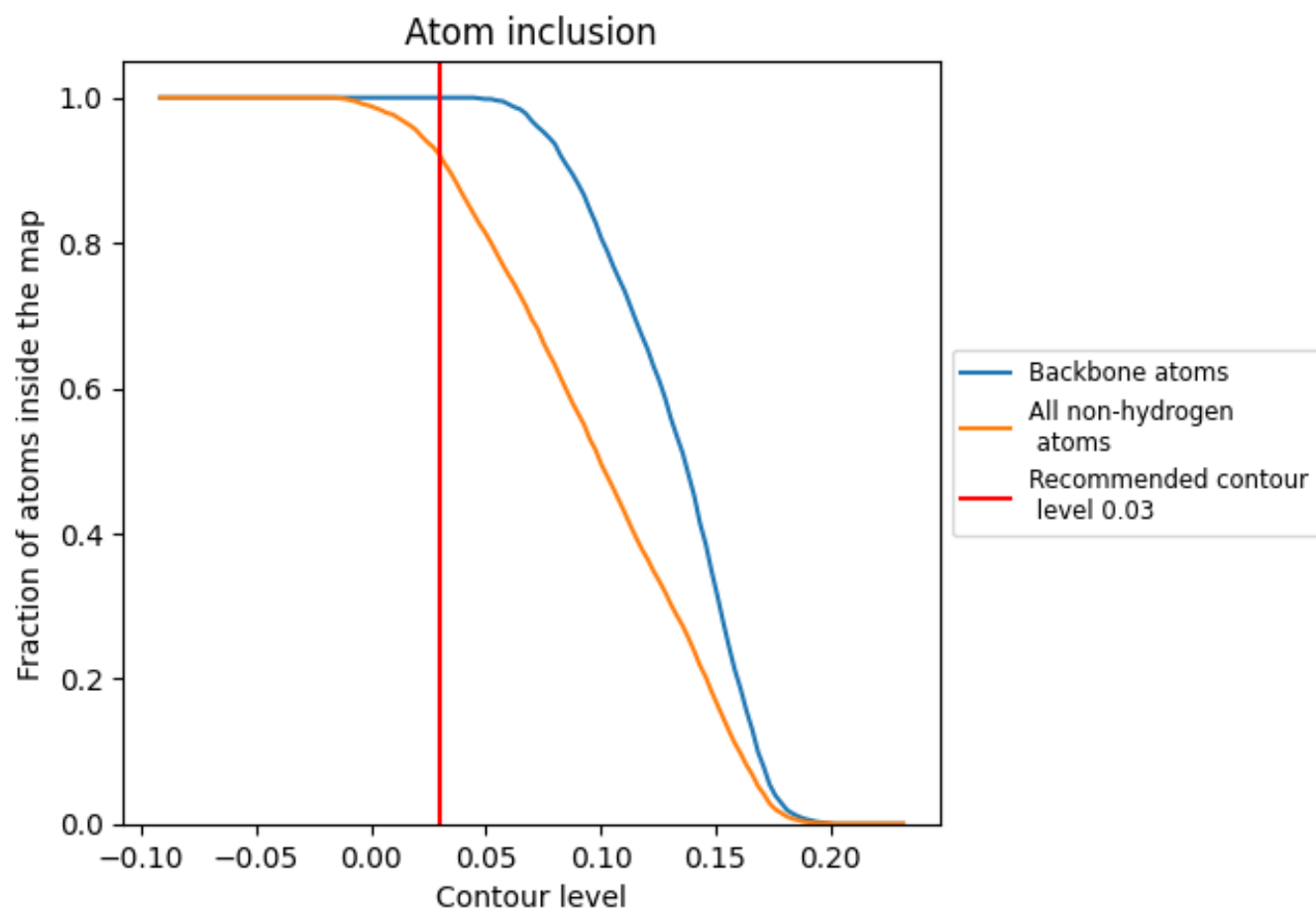
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 92% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9210	<div><div></div></div> 0.3730
A	<div><div></div></div> 0.9180	<div><div></div></div> 0.3490
B	<div><div></div></div> 0.9180	<div><div></div></div> 0.3640
C	<div><div></div></div> 0.9150	<div><div></div></div> 0.3700
D	<div><div></div></div> 0.9120	<div><div></div></div> 0.3730
E	<div><div></div></div> 0.9280	<div><div></div></div> 0.3740
F	<div><div></div></div> 0.9280	<div><div></div></div> 0.3770
G	<div><div></div></div> 0.9310	<div><div></div></div> 0.3900
H	<div><div></div></div> 0.9190	<div><div></div></div> 0.3900

1.0

0.0

<0.0