



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:46 AM UTC

PDB ID : 9PHB / pdb_00009phb
EMDB ID : EMD-71644
Title : CryoEM structure of filament of Bacillus subtilis TIR domain protein SpbK
Authors : Mishra, B.P.; Ve, T.
Deposited on : 2025-07-09
Resolution : 3.30 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:

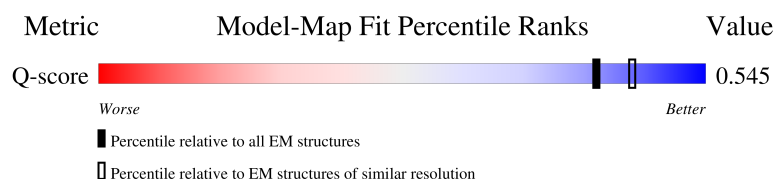
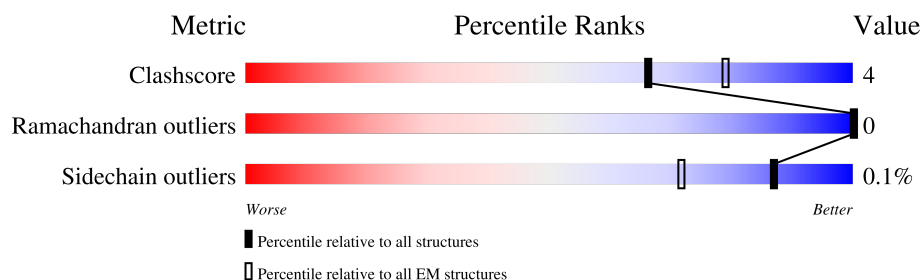
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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	15087 (2.80 - 3.80)

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	290	
1	B	290	
1	C	290	
1	D	290	

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Mol	Chain	Length	Quality of chain
1	E	290	<div><div><div></div><div></div><div></div></div><div>49%5%46%</div></div>
1	F	290	<div><div><div></div><div></div><div></div></div><div>48%6%46%</div></div>
1	G	290	<div><div><div></div><div></div><div></div></div><div>50%.46%</div></div>
1	H	290	<div><div><div></div><div></div><div></div></div><div>6%49%5%46%</div></div>
1	I	290	<div><div><div></div><div></div><div></div></div><div>51%.46%</div></div>
1	J	290	<div><div><div></div><div></div><div></div></div><div>47%7%46%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25560 atoms, of which 12760 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 SpbK.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	I	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	B	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	E	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	D	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	A	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	F	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	H	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	J	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		
1	C	156	Total	C	H	N	O	S	0	0
			2556	833	1276	199	242	6		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-23	MET	-	expression tag	UNP P96648
G	-22	HIS	-	expression tag	UNP P96648
G	-21	HIS	-	expression tag	UNP P96648
G	-20	HIS	-	expression tag	UNP P96648
G	-19	HIS	-	expression tag	UNP P96648
G	-18	HIS	-	expression tag	UNP P96648
G	-17	HIS	-	expression tag	UNP P96648
G	-16	SER	-	expression tag	UNP P96648
G	-15	SER	-	expression tag	UNP P96648
G	-14	GLY	-	expression tag	UNP P96648

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	VAL	-	expression tag	UNP P96648
G	-12	ASP	-	expression tag	UNP P96648
G	-11	LEU	-	expression tag	UNP P96648
G	-10	GLY	-	expression tag	UNP P96648
G	-9	THR	-	expression tag	UNP P96648
G	-8	GLU	-	expression tag	UNP P96648
G	-7	ASN	-	expression tag	UNP P96648
G	-6	LEU	-	expression tag	UNP P96648
G	-5	TYR	-	expression tag	UNP P96648
G	-4	PHE	-	expression tag	UNP P96648
G	-3	GLN	-	expression tag	UNP P96648
G	-2	SER	-	expression tag	UNP P96648
G	-1	ASN	-	expression tag	UNP P96648
G	0	ALA	-	expression tag	UNP P96648
I	-23	MET	-	expression tag	UNP P96648
I	-22	HIS	-	expression tag	UNP P96648
I	-21	HIS	-	expression tag	UNP P96648
I	-20	HIS	-	expression tag	UNP P96648
I	-19	HIS	-	expression tag	UNP P96648
I	-18	HIS	-	expression tag	UNP P96648
I	-17	HIS	-	expression tag	UNP P96648
I	-16	SER	-	expression tag	UNP P96648
I	-15	SER	-	expression tag	UNP P96648
I	-14	GLY	-	expression tag	UNP P96648
I	-13	VAL	-	expression tag	UNP P96648
I	-12	ASP	-	expression tag	UNP P96648
I	-11	LEU	-	expression tag	UNP P96648
I	-10	GLY	-	expression tag	UNP P96648
I	-9	THR	-	expression tag	UNP P96648
I	-8	GLU	-	expression tag	UNP P96648
I	-7	ASN	-	expression tag	UNP P96648
I	-6	LEU	-	expression tag	UNP P96648
I	-5	TYR	-	expression tag	UNP P96648
I	-4	PHE	-	expression tag	UNP P96648
I	-3	GLN	-	expression tag	UNP P96648
I	-2	SER	-	expression tag	UNP P96648
I	-1	ASN	-	expression tag	UNP P96648
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B	-23	MET	-	expression tag	UNP P96648
B	-22	HIS	-	expression tag	UNP P96648
B	-21	HIS	-	expression tag	UNP P96648
B	-20	HIS	-	expression tag	UNP P96648

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Chain	Residue	Modelled	Actual	Comment	Reference
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B	-18	HIS	-	expression tag	UNP P96648
B	-17	HIS	-	expression tag	UNP P96648
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B	-15	SER	-	expression tag	UNP P96648
B	-14	GLY	-	expression tag	UNP P96648
B	-13	VAL	-	expression tag	UNP P96648
B	-12	ASP	-	expression tag	UNP P96648
B	-11	LEU	-	expression tag	UNP P96648
B	-10	GLY	-	expression tag	UNP P96648
B	-9	THR	-	expression tag	UNP P96648
B	-8	GLU	-	expression tag	UNP P96648
B	-7	ASN	-	expression tag	UNP P96648
B	-6	LEU	-	expression tag	UNP P96648
B	-5	TYR	-	expression tag	UNP P96648
B	-4	PHE	-	expression tag	UNP P96648
B	-3	GLN	-	expression tag	UNP P96648
B	-2	SER	-	expression tag	UNP P96648
B	-1	ASN	-	expression tag	UNP P96648
B	0	ALA	-	expression tag	UNP P96648
E	-23	MET	-	expression tag	UNP P96648
E	-22	HIS	-	expression tag	UNP P96648
E	-21	HIS	-	expression tag	UNP P96648
E	-20	HIS	-	expression tag	UNP P96648
E	-19	HIS	-	expression tag	UNP P96648
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E	-17	HIS	-	expression tag	UNP P96648
E	-16	SER	-	expression tag	UNP P96648
E	-15	SER	-	expression tag	UNP P96648
E	-14	GLY	-	expression tag	UNP P96648
E	-13	VAL	-	expression tag	UNP P96648
E	-12	ASP	-	expression tag	UNP P96648
E	-11	LEU	-	expression tag	UNP P96648
E	-10	GLY	-	expression tag	UNP P96648
E	-9	THR	-	expression tag	UNP P96648
E	-8	GLU	-	expression tag	UNP P96648
E	-7	ASN	-	expression tag	UNP P96648
E	-6	LEU	-	expression tag	UNP P96648
E	-5	TYR	-	expression tag	UNP P96648
E	-4	PHE	-	expression tag	UNP P96648
E	-3	GLN	-	expression tag	UNP P96648
E	-2	SER	-	expression tag	UNP P96648

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Chain	Residue	Modelled	Actual	Comment	Reference
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E	0	ALA	-	expression tag	UNP P96648
D	-23	MET	-	expression tag	UNP P96648
D	-22	HIS	-	expression tag	UNP P96648
D	-21	HIS	-	expression tag	UNP P96648
D	-20	HIS	-	expression tag	UNP P96648
D	-19	HIS	-	expression tag	UNP P96648
D	-18	HIS	-	expression tag	UNP P96648
D	-17	HIS	-	expression tag	UNP P96648
D	-16	SER	-	expression tag	UNP P96648
D	-15	SER	-	expression tag	UNP P96648
D	-14	GLY	-	expression tag	UNP P96648
D	-13	VAL	-	expression tag	UNP P96648
D	-12	ASP	-	expression tag	UNP P96648
D	-11	LEU	-	expression tag	UNP P96648
D	-10	GLY	-	expression tag	UNP P96648
D	-9	THR	-	expression tag	UNP P96648
D	-8	GLU	-	expression tag	UNP P96648
D	-7	ASN	-	expression tag	UNP P96648
D	-6	LEU	-	expression tag	UNP P96648
D	-5	TYR	-	expression tag	UNP P96648
D	-4	PHE	-	expression tag	UNP P96648
D	-3	GLN	-	expression tag	UNP P96648
D	-2	SER	-	expression tag	UNP P96648
D	-1	ASN	-	expression tag	UNP P96648
D	0	ALA	-	expression tag	UNP P96648
A	-23	MET	-	expression tag	UNP P96648
A	-22	HIS	-	expression tag	UNP P96648
A	-21	HIS	-	expression tag	UNP P96648
A	-20	HIS	-	expression tag	UNP P96648
A	-19	HIS	-	expression tag	UNP P96648
A	-18	HIS	-	expression tag	UNP P96648
A	-17	HIS	-	expression tag	UNP P96648
A	-16	SER	-	expression tag	UNP P96648
A	-15	SER	-	expression tag	UNP P96648
A	-14	GLY	-	expression tag	UNP P96648
A	-13	VAL	-	expression tag	UNP P96648
A	-12	ASP	-	expression tag	UNP P96648
A	-11	LEU	-	expression tag	UNP P96648
A	-10	GLY	-	expression tag	UNP P96648
A	-9	THR	-	expression tag	UNP P96648
A	-8	GLU	-	expression tag	UNP P96648

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASN	-	expression tag	UNP P96648
A	-6	LEU	-	expression tag	UNP P96648
A	-5	TYR	-	expression tag	UNP P96648
A	-4	PHE	-	expression tag	UNP P96648
A	-3	GLN	-	expression tag	UNP P96648
A	-2	SER	-	expression tag	UNP P96648
A	-1	ASN	-	expression tag	UNP P96648
A	0	ALA	-	expression tag	UNP P96648
F	-23	MET	-	expression tag	UNP P96648
F	-22	HIS	-	expression tag	UNP P96648
F	-21	HIS	-	expression tag	UNP P96648
F	-20	HIS	-	expression tag	UNP P96648
F	-19	HIS	-	expression tag	UNP P96648
F	-18	HIS	-	expression tag	UNP P96648
F	-17	HIS	-	expression tag	UNP P96648
F	-16	SER	-	expression tag	UNP P96648
F	-15	SER	-	expression tag	UNP P96648
F	-14	GLY	-	expression tag	UNP P96648
F	-13	VAL	-	expression tag	UNP P96648
F	-12	ASP	-	expression tag	UNP P96648
F	-11	LEU	-	expression tag	UNP P96648
F	-10	GLY	-	expression tag	UNP P96648
F	-9	THR	-	expression tag	UNP P96648
F	-8	GLU	-	expression tag	UNP P96648
F	-7	ASN	-	expression tag	UNP P96648
F	-6	LEU	-	expression tag	UNP P96648
F	-5	TYR	-	expression tag	UNP P96648
F	-4	PHE	-	expression tag	UNP P96648
F	-3	GLN	-	expression tag	UNP P96648
F	-2	SER	-	expression tag	UNP P96648
F	-1	ASN	-	expression tag	UNP P96648
F	0	ALA	-	expression tag	UNP P96648
H	-23	MET	-	expression tag	UNP P96648
H	-22	HIS	-	expression tag	UNP P96648
H	-21	HIS	-	expression tag	UNP P96648
H	-20	HIS	-	expression tag	UNP P96648
H	-19	HIS	-	expression tag	UNP P96648
H	-18	HIS	-	expression tag	UNP P96648
H	-17	HIS	-	expression tag	UNP P96648
H	-16	SER	-	expression tag	UNP P96648
H	-15	SER	-	expression tag	UNP P96648
H	-14	GLY	-	expression tag	UNP P96648

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Chain	Residue	Modelled	Actual	Comment	Reference
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H	-12	ASP	-	expression tag	UNP P96648
H	-11	LEU	-	expression tag	UNP P96648
H	-10	GLY	-	expression tag	UNP P96648
H	-9	THR	-	expression tag	UNP P96648
H	-8	GLU	-	expression tag	UNP P96648
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H	-2	SER	-	expression tag	UNP P96648
H	-1	ASN	-	expression tag	UNP P96648
H	0	ALA	-	expression tag	UNP P96648
J	-23	MET	-	expression tag	UNP P96648
J	-22	HIS	-	expression tag	UNP P96648
J	-21	HIS	-	expression tag	UNP P96648
J	-20	HIS	-	expression tag	UNP P96648
J	-19	HIS	-	expression tag	UNP P96648
J	-18	HIS	-	expression tag	UNP P96648
J	-17	HIS	-	expression tag	UNP P96648
J	-16	SER	-	expression tag	UNP P96648
J	-15	SER	-	expression tag	UNP P96648
J	-14	GLY	-	expression tag	UNP P96648
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J	-12	ASP	-	expression tag	UNP P96648
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J	-5	TYR	-	expression tag	UNP P96648
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J	-3	GLN	-	expression tag	UNP P96648
J	-2	SER	-	expression tag	UNP P96648
J	-1	ASN	-	expression tag	UNP P96648
J	0	ALA	-	expression tag	UNP P96648
C	-23	MET	-	expression tag	UNP P96648
C	-22	HIS	-	expression tag	UNP P96648
C	-21	HIS	-	expression tag	UNP P96648
C	-20	HIS	-	expression tag	UNP P96648

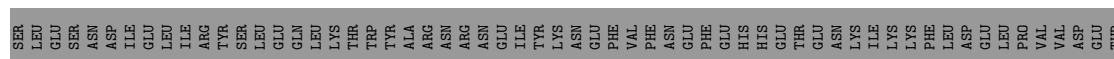
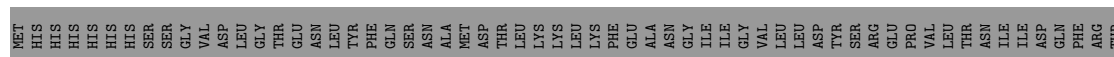
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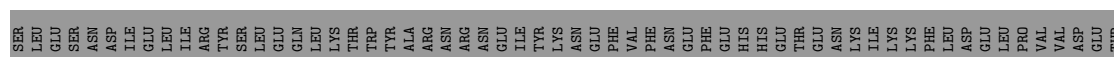
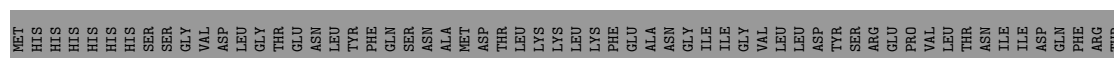
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	HIS	-	expression tag	UNP P96648
C	-18	HIS	-	expression tag	UNP P96648
C	-17	HIS	-	expression tag	UNP P96648
C	-16	SER	-	expression tag	UNP P96648
C	-15	SER	-	expression tag	UNP P96648
C	-14	GLY	-	expression tag	UNP P96648
C	-13	VAL	-	expression tag	UNP P96648
C	-12	ASP	-	expression tag	UNP P96648
C	-11	LEU	-	expression tag	UNP P96648
C	-10	GLY	-	expression tag	UNP P96648
C	-9	THR	-	expression tag	UNP P96648
C	-8	GLU	-	expression tag	UNP P96648
C	-7	ASN	-	expression tag	UNP P96648
C	-6	LEU	-	expression tag	UNP P96648
C	-5	TYR	-	expression tag	UNP P96648
C	-4	PHE	-	expression tag	UNP P96648
C	-3	GLN	-	expression tag	UNP P96648
C	-2	SER	-	expression tag	UNP P96648
C	-1	ASN	-	expression tag	UNP P96648
C	0	ALA	-	expression tag	UNP P96648



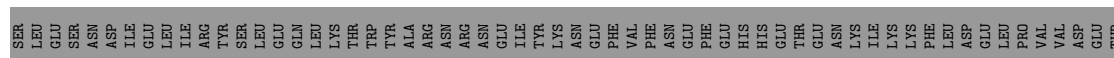
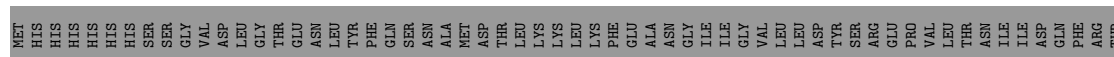
• Molecule 1: SpbK



• Molecule 1: SpbK



• Molecule 1: SpbK



• Molecule 1: SpbK

Chain F: 

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

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

GLU LYS SER SER THR HIS PHE SER SER ASP ASP GLN ASN ARG E111 E112 E113 V132 E133 E134 E135 S142 I145 I146 H153 V187 M191 A195 T196 W197 V198 K212 G213 E214 E230 D233 I241 I242 R243 E250 D251 E255 K258 N262 T263

K264 L265 K266

• Molecule 1: SpbK

Chain H: 

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

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

GLU LYS SER SER THR HIS PHE SER SER ASP ASP GLN ASN ARG E111 L112 E113 K114 K123 E133 L134 D137 S150 H153 K167 F176 Y177 M178 V187 M191 K212 G213 K221 S227 E230 D233 D243 D246 E250 D251 K252 K253 W254

E255 F261 L265 K266

• Molecule 1: SpbK

Chain J: 

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

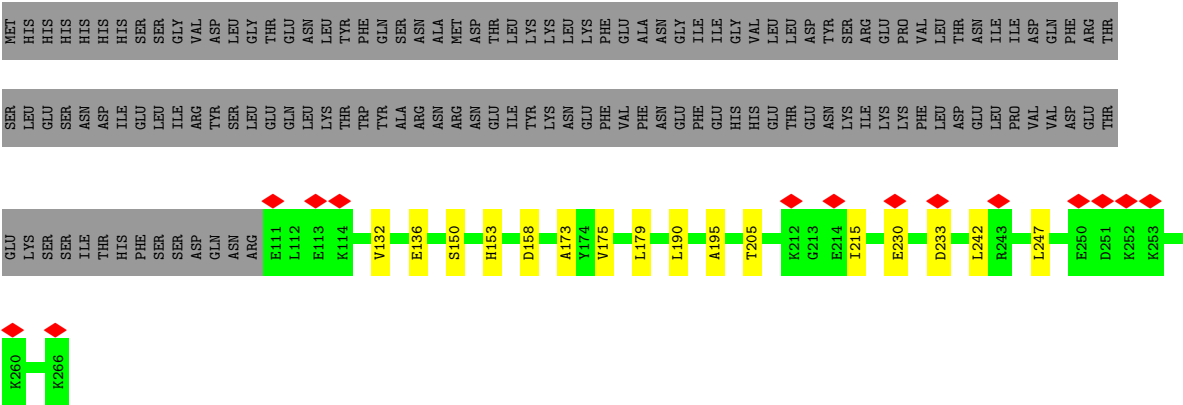
SER LEU GLU SER SER ASN ASP ILE ILE GLU SER SER ILE VAL TYR SER LEU GLU GLN THR TRP TYR PHE THR LYS LYS LEU ASN GLU PHE VAL PHE ALA ASN ASN GLY ILE ILE TYR LYS LYS ASN GLU PHE VAL PHE ALA ASN ASN GLY ILE ILE GLU HIS VAL LEU LEU ASP THR TYR SER ILE ARG GLU PRO VAL LEU THR ASP LEU ASN ILE LEU PRO VAL ASP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

GLU LYS SER SER THR HIS PHE SER SER ASP ASP GLN ASN ARG E111 E112 E113 I118 C128 V132 E133 L134 I145 I146 Y147 A173 Y174 V175 I207 F211 K212 E229 E230 D233 K240 R243 M244 E250 D251 K252 K253 K258 F261 N262 T263 K264

L265 K266

• Molecule 1: SpbK

Chain C: 



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=79.3°, rise=8.9 Å, axial sym=D1	Depositor
Number of segments used	116455	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.880	Depositor
Minimum map value	-0.588	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	389.12, 389.12, 389.12	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9728, 0.9728, 0.9728	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	0.13	0/1309	0.28	0/1758
1	B	0.13	0/1309	0.27	0/1758
1	C	0.12	0/1309	0.28	0/1758
1	D	0.12	0/1309	0.26	0/1758
1	E	0.13	0/1309	0.29	0/1758
1	F	0.14	0/1309	0.31	0/1758
1	G	0.13	0/1309	0.30	0/1758
1	H	0.13	0/1309	0.29	0/1758
1	I	0.14	0/1309	0.29	0/1758
1	J	0.13	0/1309	0.29	0/1758
All	All	0.13	0/13090	0.29	0/17580

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	1280	1276	1275	15	0
1	B	1280	1276	1275	17	0
1	C	1280	1276	1275	12	0
1	D	1280	1276	1275	11	0
1	E	1280	1276	1275	10	0
1	F	1280	1276	1275	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1280	1276	1275	7	0
1	H	1280	1276	1275	8	0
1	I	1280	1276	1275	4	0
1	J	1280	1276	1275	13	0
All	All	12800	12760	12750	99	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 4.

All (99) 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:177:TYR:HH	1:A:196:THR:HG1	1.24	0.80
1:J:134:LEU:HD12	1:J:261:PHE:CD2	2.17	0.80
1:C:179:LEU:HD12	1:C:205:THR:HG23	1.63	0.79
1:B:261:PHE:HE2	1:B:265:LEU:HD11	1.51	0.75
1:E:198:VAL:HG21	1:F:195:ALA:HB1	1.67	0.73
1:E:195:ALA:HB1	1:F:198:VAL:HG21	1.74	0.69
1:I:158:ASP:OD2	1:J:240:LYS:NZ	2.29	0.65
1:A:134:LEU:HD12	1:A:261:PHE:CD2	2.31	0.65
1:F:146:ILE:O	1:F:146:ILE:HG22	1.98	0.63
1:J:146:ILE:O	1:J:146:ILE:HG22	1.98	0.62
1:B:261:PHE:CE2	1:B:265:LEU:HD11	2.34	0.62
1:F:258:LYS:O	1:F:262:ASN:ND2	2.33	0.61
1:J:258:LYS:O	1:J:262:ASN:OD1	2.19	0.60
1:J:134:LEU:HD12	1:J:261:PHE:HD2	1.65	0.60
1:J:118:ILE:HD12	1:J:145:ILE:HG23	1.84	0.58
1:D:198:VAL:HG21	1:C:195:ALA:HB1	1.85	0.58
1:B:186:SER:OG	1:B:189:CYS:SG	2.64	0.56
1:B:150:SER:OG	1:B:153:HIS:ND1	2.33	0.56
1:J:145:ILE:HG22	1:J:147:TYR:H	1.71	0.56
1:A:145:ILE:HG22	1:A:147:TYR:H	1.71	0.56
1:A:132:VAL:HG23	1:A:145:ILE:HD13	1.87	0.55
1:A:146:ILE:HG22	1:A:146:ILE:O	2.05	0.55
1:G:218:VAL:O	1:G:218:VAL:HG22	2.07	0.54
1:F:133:GLU:OE1	1:F:264:LYS:NZ	2.37	0.53
1:J:173:ALA:O	1:J:175:VAL:HG23	2.09	0.53
1:D:198:VAL:HG21	1:C:195:ALA:CB	2.39	0.53
1:H:261:PHE:CZ	1:H:265:LEU:HD11	2.45	0.52
1:B:133:GLU:OE1	1:B:264:LYS:NZ	2.37	0.52
1:J:133:GLU:OE1	1:J:264:LYS:NZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:TRP:CE3	1:E:198:VAL:HG23	2.45	0.52
1:C:215:ILE:HG22	1:C:215:ILE:O	2.10	0.51
1:F:132:VAL:HG23	1:F:145:ILE:HG21	1.93	0.51
1:F:142:SER:OG	1:F:153:HIS:NE2	2.42	0.51
1:E:230:GLU:N	1:E:233:ASP:OD2	2.39	0.50
1:D:145:ILE:HG22	1:D:147:TYR:H	1.77	0.50
1:C:230:GLU:N	1:C:233:ASP:OD2	2.43	0.50
1:J:118:ILE:HD13	1:J:132:VAL:HG22	1.93	0.50
1:F:187:VAL:O	1:F:191:ASN:OD1	2.30	0.49
1:D:197:TRP:CE3	1:D:198:VAL:HG23	2.47	0.49
1:C:179:LEU:HD12	1:C:205:THR:CG2	2.38	0.49
1:B:253:LYS:O	1:B:257:ILE:HG13	2.12	0.49
1:J:128:CYS:O	1:J:132:VAL:HG23	2.12	0.49
1:A:129:ASN:O	1:A:132:VAL:HG12	2.13	0.48
1:E:133:GLU:OE1	1:E:264:LYS:NZ	2.41	0.48
1:E:218:VAL:HG22	1:F:191:ASN:HD22	1.77	0.48
1:E:132:VAL:HG23	1:E:145:ILE:HG21	1.95	0.48
1:B:240:LYS:NZ	1:C:158:ASP:OD2	2.47	0.48
1:J:240:LYS:HE3	1:J:244:MET:HE2	1.96	0.48
1:B:191:ASN:HD22	1:A:218:VAL:HG22	1.80	0.47
1:H:134:LEU:HD12	1:H:261:PHE:CD2	2.50	0.47
1:D:134:LEU:HD12	1:D:261:PHE:CG	2.50	0.47
1:H:133:GLU:O	1:H:137:ASP:OD2	2.33	0.47
1:E:251:ASP:O	1:E:255:GLU:HG2	2.15	0.47
1:D:134:LEU:HD12	1:D:261:PHE:CD1	2.50	0.47
1:H:187:VAL:O	1:H:191:ASN:OD1	2.32	0.47
1:F:251:ASP:O	1:F:255:GLU:HG2	2.16	0.46
1:I:199:ASN:O	1:I:200:SER:OG	2.27	0.45
1:I:251:ASP:O	1:I:255:GLU:HG2	2.16	0.45
1:A:178:MET:CE	1:A:208:LEU:HD21	2.46	0.45
1:H:176:PHE:HB3	1:H:178:MET:HE2	1.99	0.45
1:G:251:ASP:O	1:G:255:GLU:HG2	2.17	0.44
1:B:197:TRP:CE2	1:B:218:VAL:HG21	2.51	0.44
1:G:133:GLU:OE1	1:G:264:LYS:NZ	2.45	0.44
1:B:251:ASP:O	1:B:255:GLU:OE2	2.36	0.44
1:B:128:CYS:O	1:B:132:VAL:HG23	2.18	0.44
1:A:132:VAL:CG2	1:A:145:ILE:HD13	2.47	0.44
1:A:192:GLU:O	1:A:196:THR:HG23	2.18	0.44
1:A:259:ALA:O	1:A:263:THR:HG22	2.17	0.44
1:G:132:VAL:HG13	1:G:145:ILE:HG21	1.99	0.44
1:E:176:PHE:HB3	1:E:178:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:O	1:B:118:ILE:HG22	2.18	0.43
1:D:215:ILE:HG23	1:D:219:ILE:HD11	2.00	0.43
1:C:150:SER:OG	1:C:153:HIS:ND1	2.41	0.43
1:D:132:VAL:HG13	1:D:145:ILE:HD13	2.01	0.43
1:A:180:SER:OG	1:A:181:ASP:N	2.51	0.43
1:B:134:LEU:C	1:B:134:LEU:HD23	2.44	0.42
1:D:116:ILE:HD11	1:D:245:TYR:HE2	1.84	0.42
1:D:133:GLU:OE1	1:D:264:LYS:NZ	2.42	0.42
1:B:258:LYS:O	1:B:262:ASN:ND2	2.49	0.42
1:E:195:ALA:CB	1:F:198:VAL:HG21	2.47	0.42
1:C:132:VAL:O	1:C:136:GLU:HG3	2.20	0.42
1:F:197:TRP:CE3	1:F:198:VAL:HG23	2.54	0.42
1:H:150:SER:OG	1:H:153:HIS:ND1	2.43	0.42
1:G:197:TRP:CD2	1:G:218:VAL:HG21	2.54	0.42
1:G:187:VAL:O	1:G:191:ASN:OD1	2.38	0.41
1:A:251:ASP:O	1:A:255:GLU:HG2	2.20	0.41
1:I:133:GLU:OE1	1:I:264:LYS:NZ	2.39	0.41
1:C:173:ALA:O	1:C:175:VAL:HG23	2.20	0.41
1:G:199:ASN:O	1:G:200:SER:OG	2.30	0.41
1:F:135:LEU:HD23	1:F:241:ILE:HD13	2.02	0.41
1:D:190:LEU:HD12	1:C:190:LEU:HD13	2.02	0.41
1:H:227:SER:O	1:H:233:ASP:HB3	2.20	0.41
1:J:207:ILE:HG23	1:J:211:PHE:HB3	2.02	0.41
1:H:251:ASP:O	1:H:255:GLU:HG2	2.20	0.41
1:C:242:LEU:HD23	1:C:247:LEU:HB2	2.03	0.41
1:B:148:THR:HG21	1:B:165:LEU:HD21	2.03	0.40
1:B:190:LEU:HD12	1:A:190:LEU:HD13	2.04	0.40
1:A:186:SER:OG	1:A:189:CYS:SG	2.78	0.40
1:B:251:ASP:OD1	1:B:251:ASP:N	2.55	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	154/290 (53%)	146 (95%)	8 (5%)	0	100	100
1	B	154/290 (53%)	147 (96%)	7 (4%)	0	100	100
1	C	154/290 (53%)	148 (96%)	6 (4%)	0	100	100
1	D	154/290 (53%)	145 (94%)	9 (6%)	0	100	100
1	E	154/290 (53%)	147 (96%)	7 (4%)	0	100	100
1	F	154/290 (53%)	144 (94%)	10 (6%)	0	100	100
1	G	154/290 (53%)	146 (95%)	8 (5%)	0	100	100
1	H	154/290 (53%)	149 (97%)	5 (3%)	0	100	100
1	I	154/290 (53%)	147 (96%)	7 (4%)	0	100	100
1	J	154/290 (53%)	144 (94%)	10 (6%)	0	100	100
All	All	1540/2900 (53%)	1463 (95%)	77 (5%)	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	143/270 (53%)	143 (100%)	0	100	100
1	B	143/270 (53%)	143 (100%)	0	100	100
1	C	143/270 (53%)	143 (100%)	0	100	100
1	D	143/270 (53%)	142 (99%)	1 (1%)	76	80
1	E	143/270 (53%)	143 (100%)	0	100	100
1	F	143/270 (53%)	143 (100%)	0	100	100
1	G	143/270 (53%)	143 (100%)	0	100	100
1	H	143/270 (53%)	143 (100%)	0	100	100
1	I	143/270 (53%)	143 (100%)	0	100	100
1	J	143/270 (53%)	142 (99%)	1 (1%)	76	80
All	All	1430/2700 (53%)	1428 (100%)	2 (0%)	87	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	263	THR
1	J	174	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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.

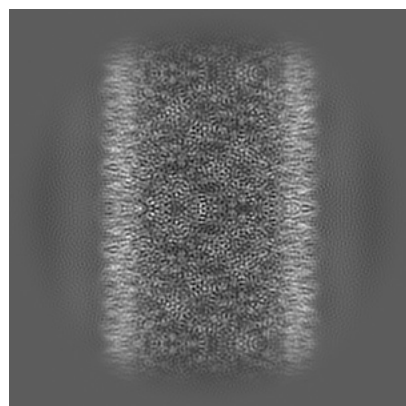
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71644. These allow visual inspection of the internal detail of the map and identification of artifacts.

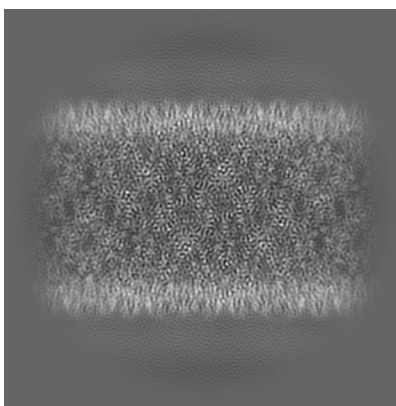
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

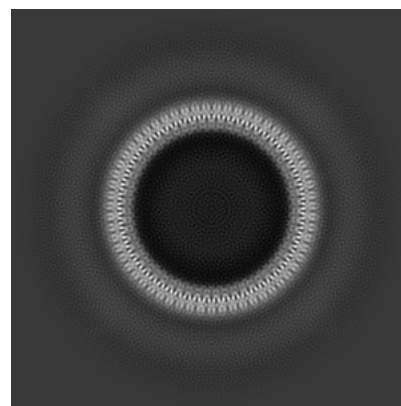
6.1.1 Primary map



X

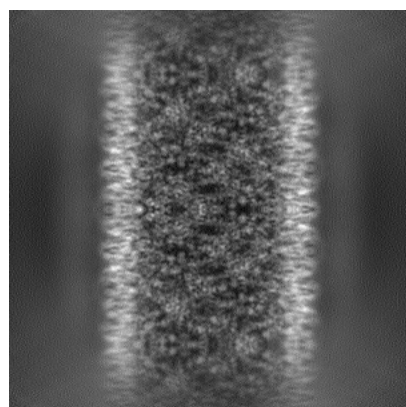


Y

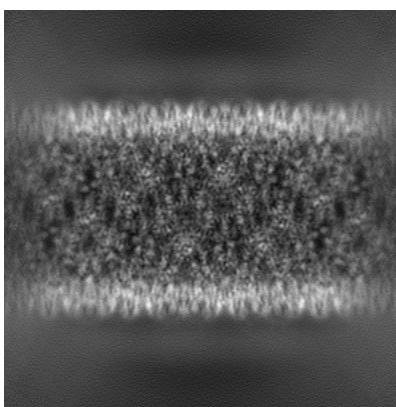


Z

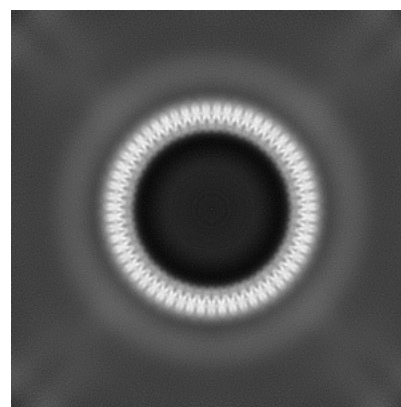
6.1.2 Raw map



X



Y

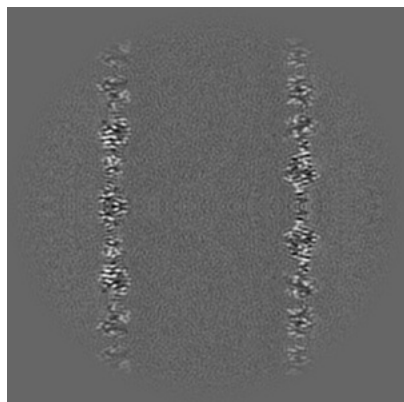


Z

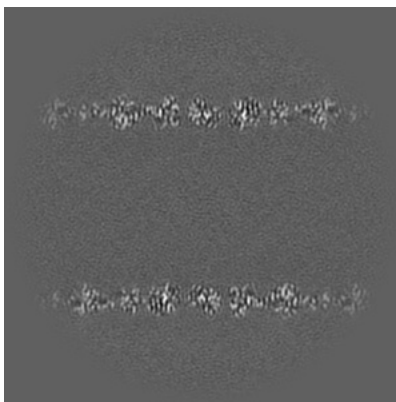
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

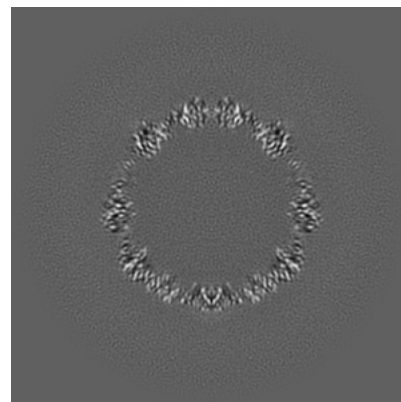
6.2.1 Primary map



X Index: 200

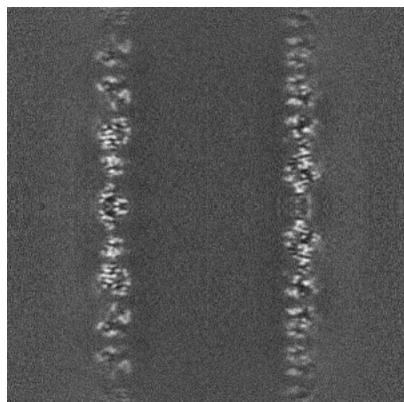


Y Index: 200

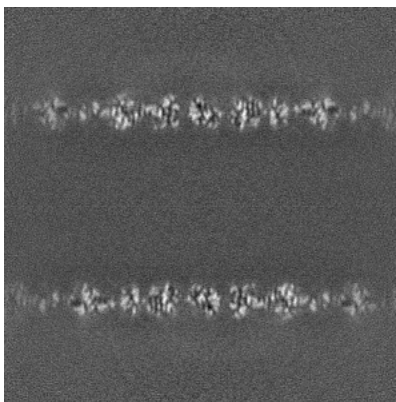


Z Index: 200

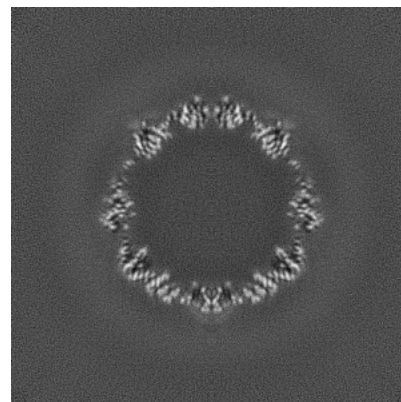
6.2.2 Raw map



X Index: 200



Y Index: 200

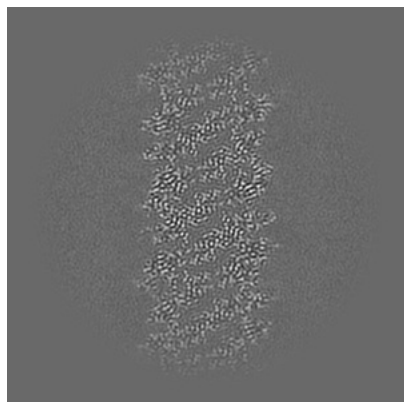


Z Index: 200

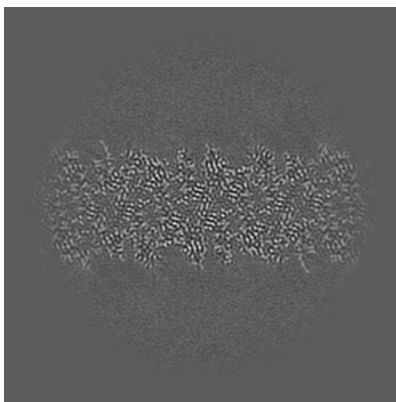
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

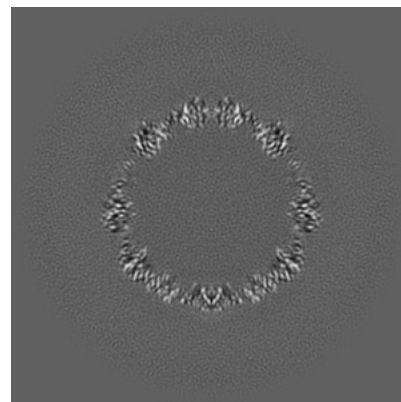
6.3.1 Primary map



X Index: 113

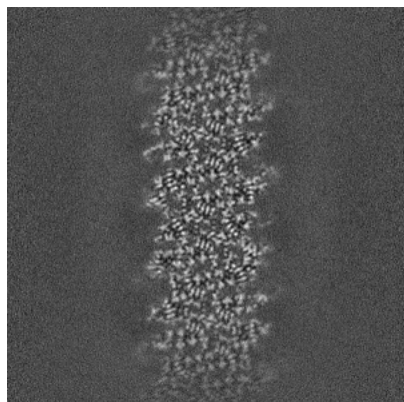


Y Index: 110

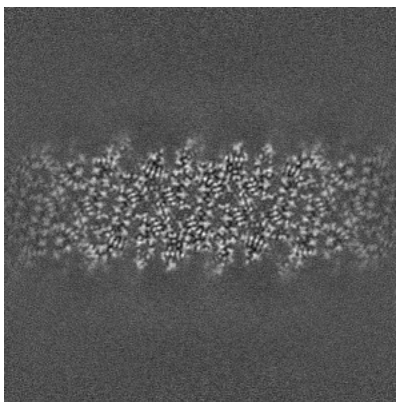


Z Index: 200

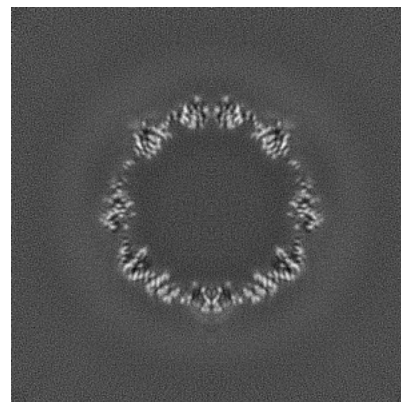
6.3.2 Raw map



X Index: 109



Y Index: 290

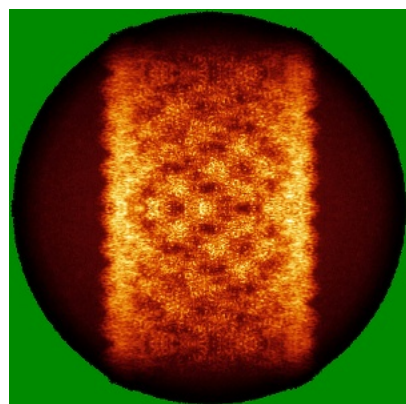


Z Index: 200

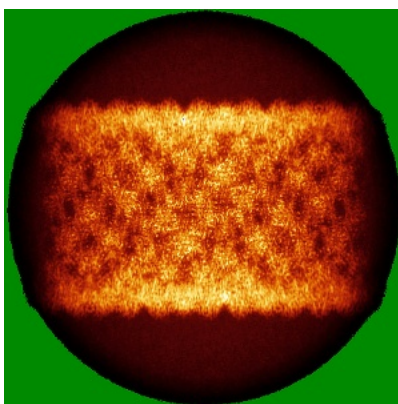
The images above show the largest variance slices of the map in three orthogonal directions.

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

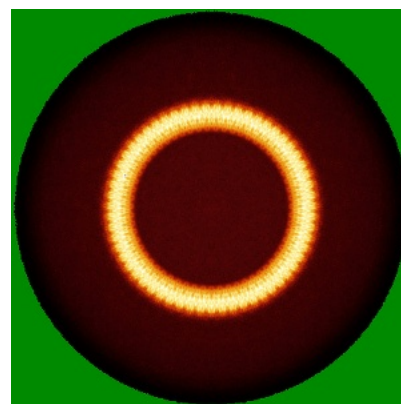
6.4.1 Primary map



X

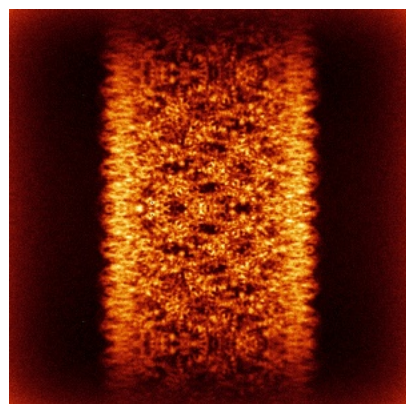


Y

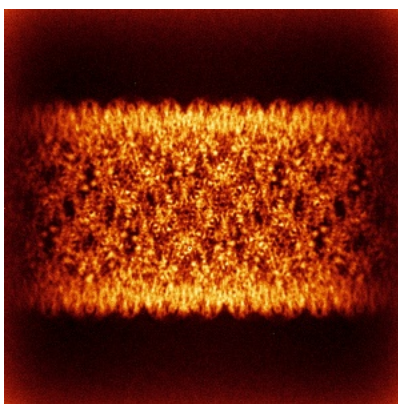


Z

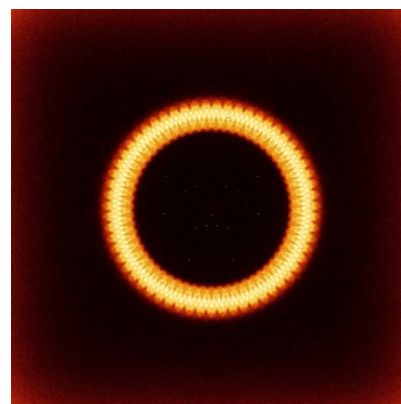
6.4.2 Raw map



X



Y

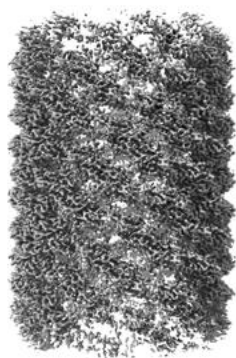


Z

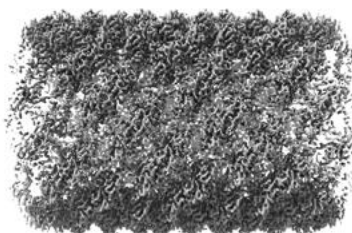
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

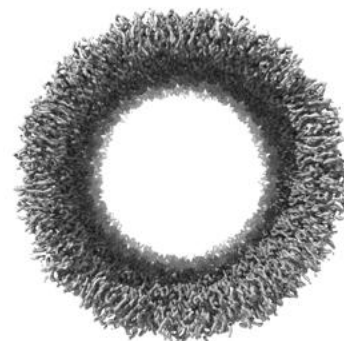
6.5.1 Primary map



X



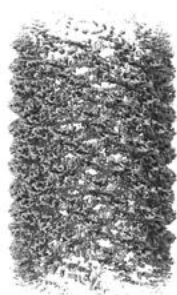
Y



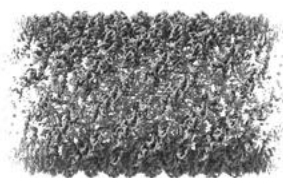
Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

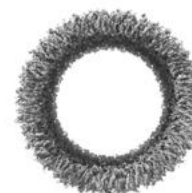
6.5.2 Raw map



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.

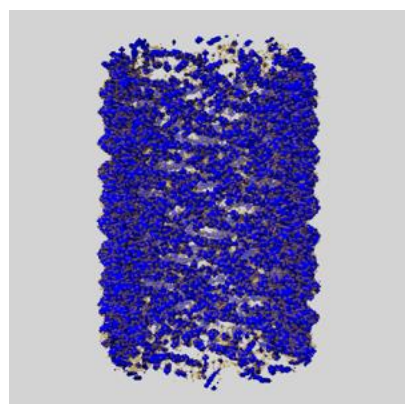
6.6 Mask visualisation [i](#)

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

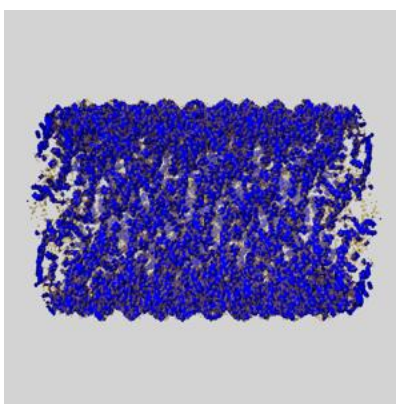
A mask typically either:

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

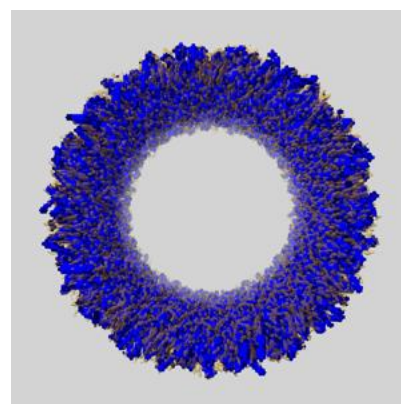
6.6.1 emd_71644_msk_1.map [i](#)



X



Y

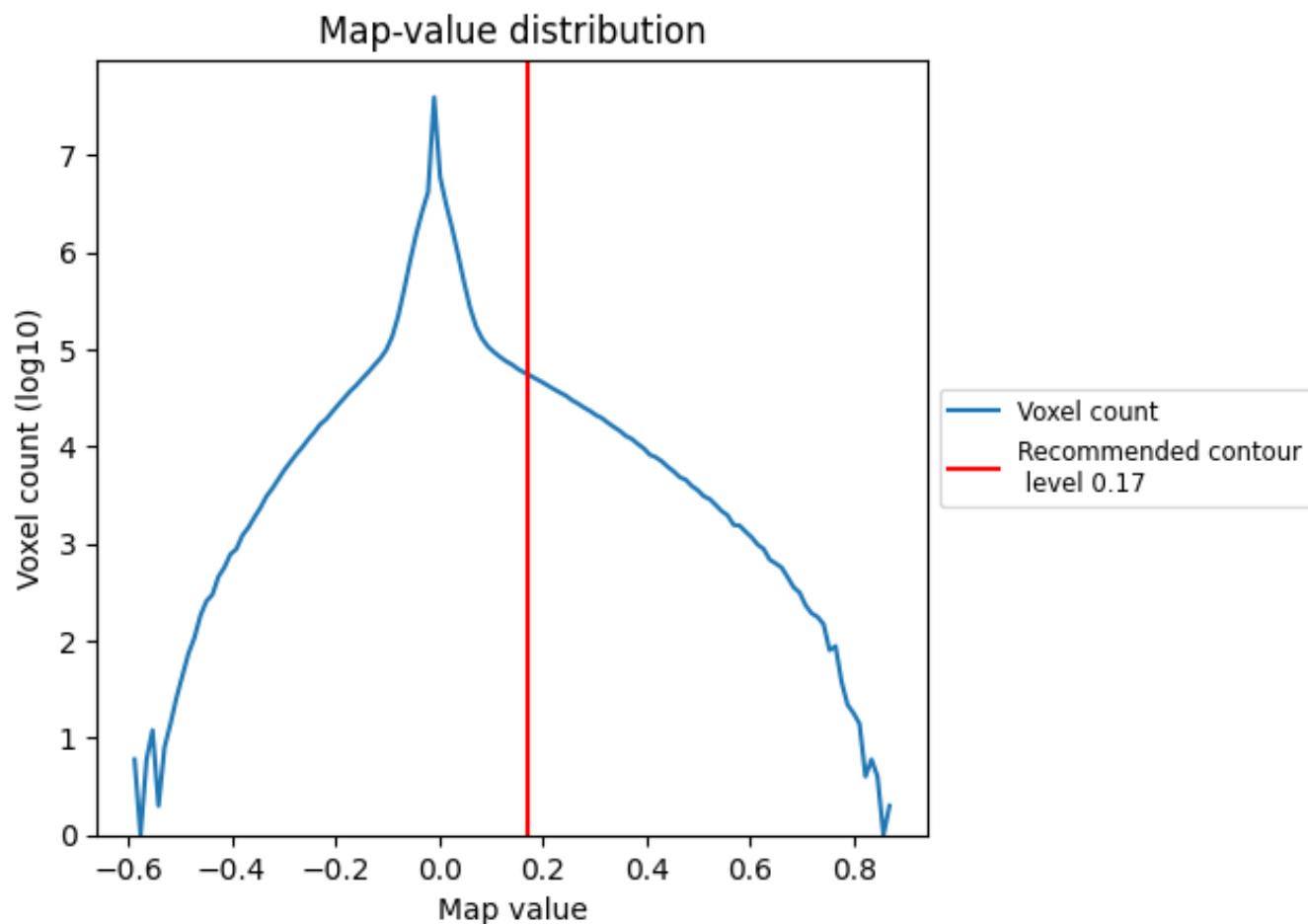


Z

7 Map analysis [i](#)

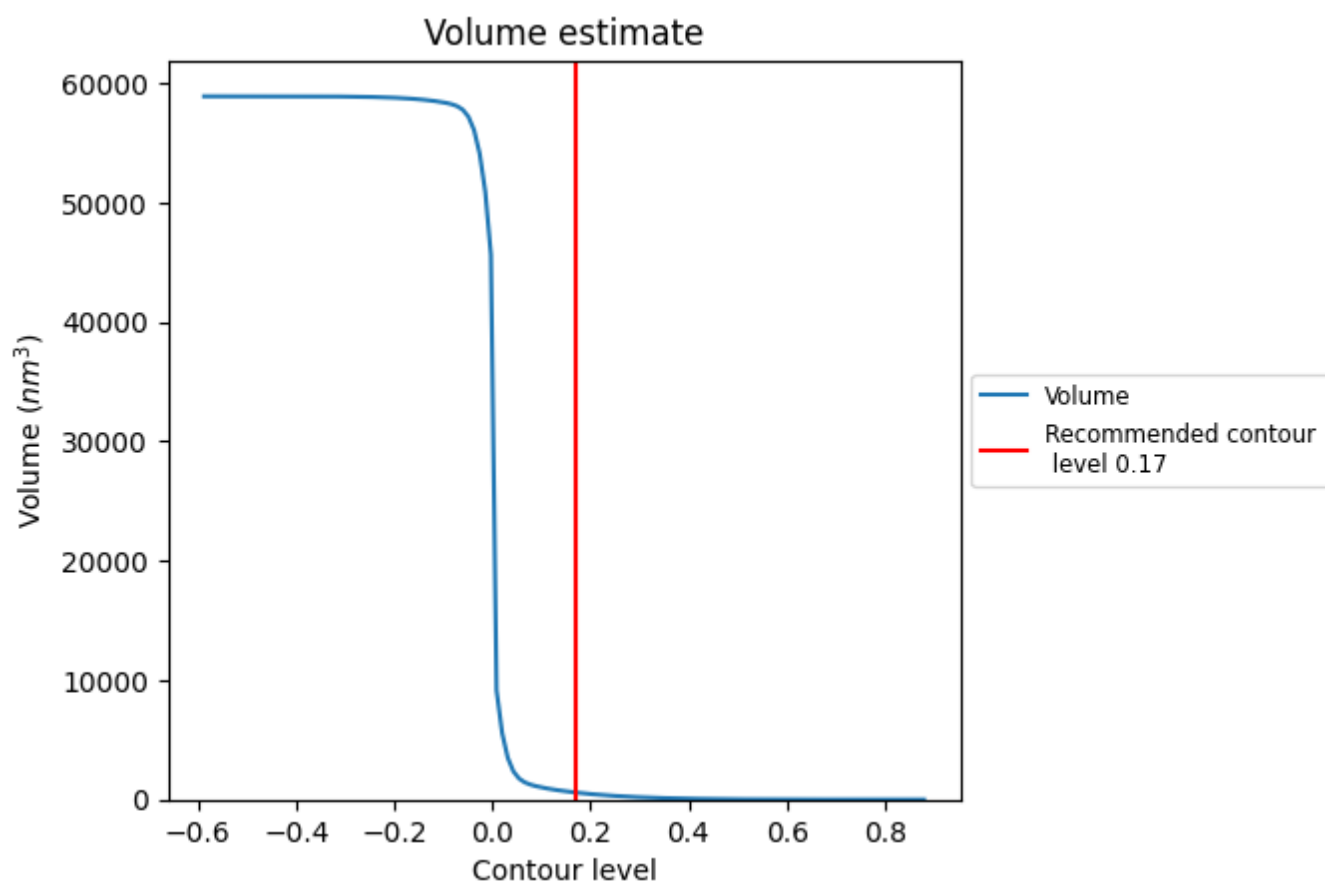
This section contains the results of statistical analysis of the map.

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.

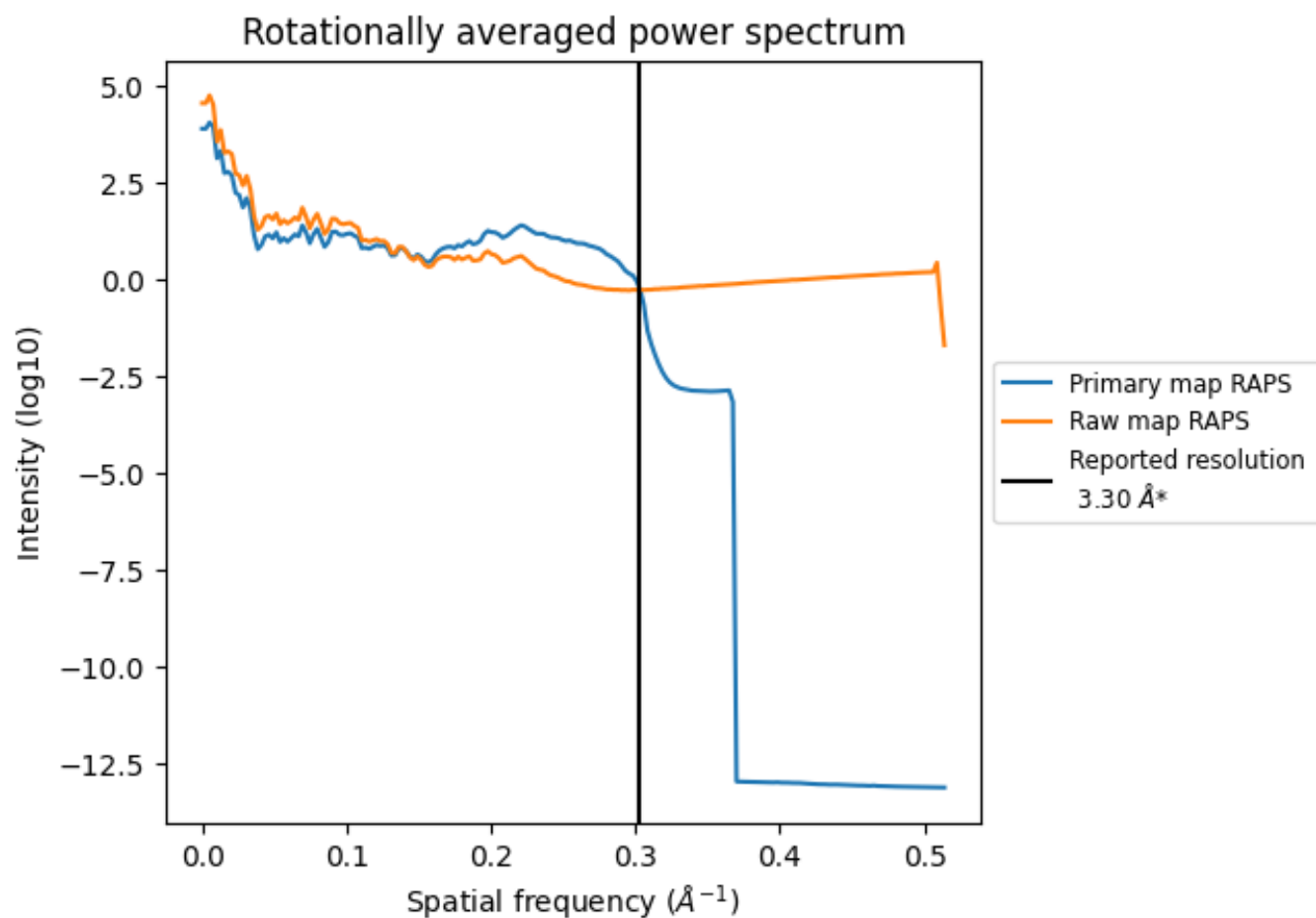
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 590 nm³; this corresponds to an approximate mass of 533 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 ⓘ

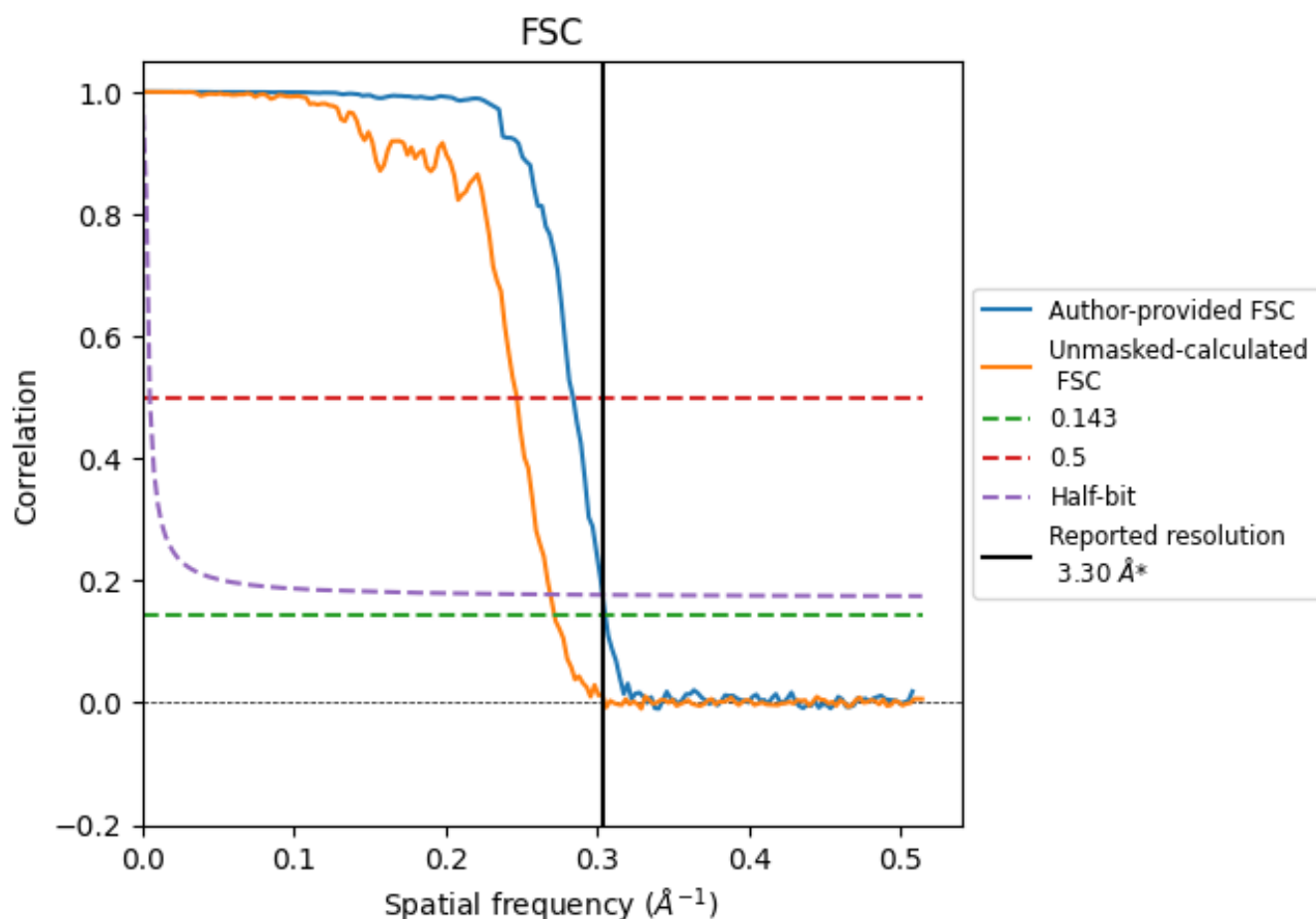


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

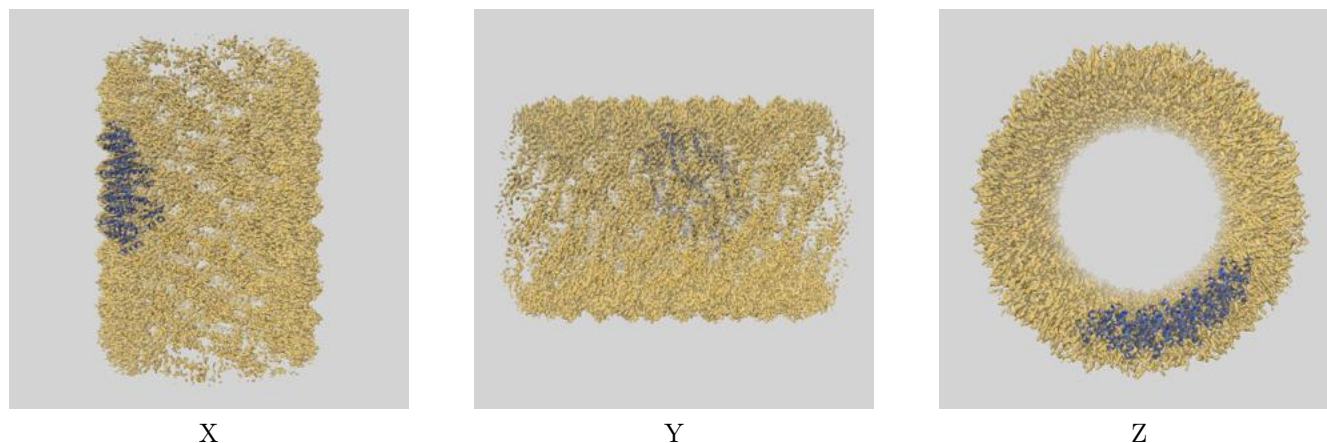
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.52	3.30
Unmasked-calculated*	3.68	4.05	3.72

*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 3.68 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

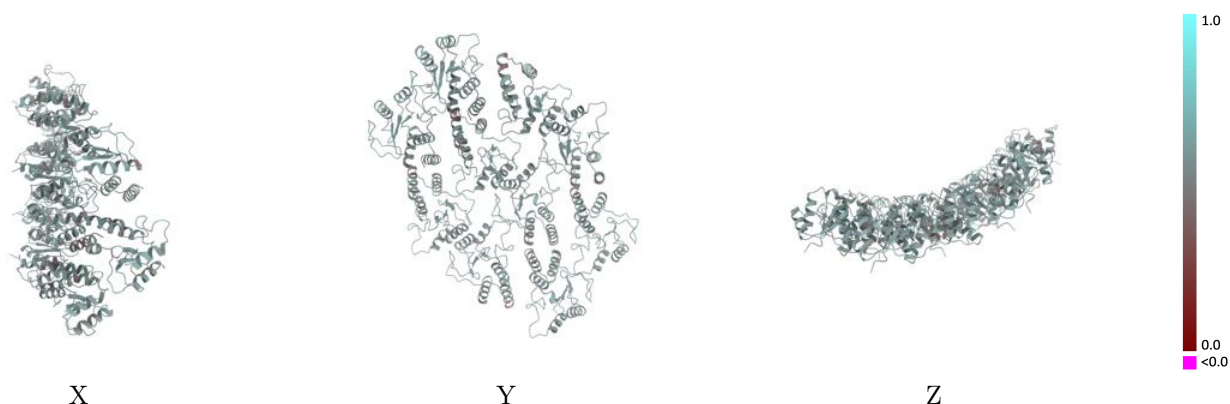
This section contains information regarding the fit between EMDB map EMD-71644 and PDB model 9PHB. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



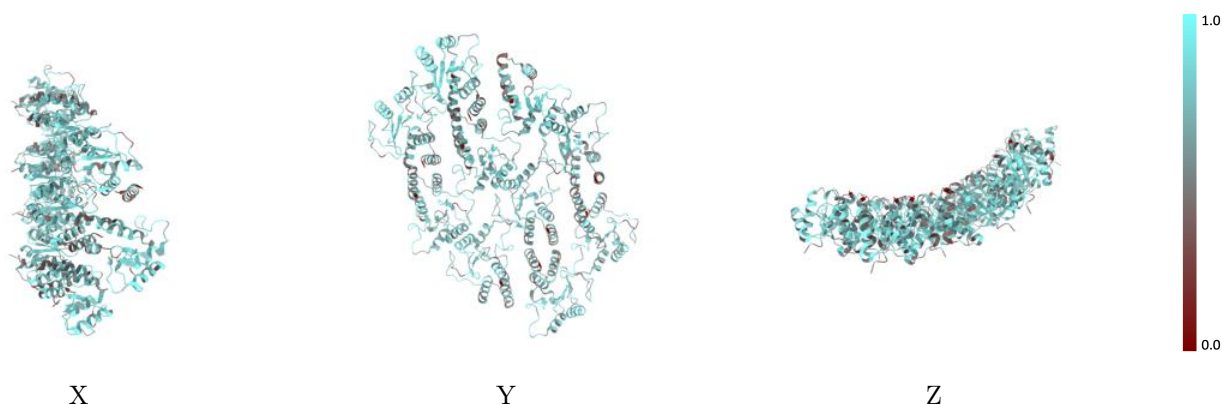
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



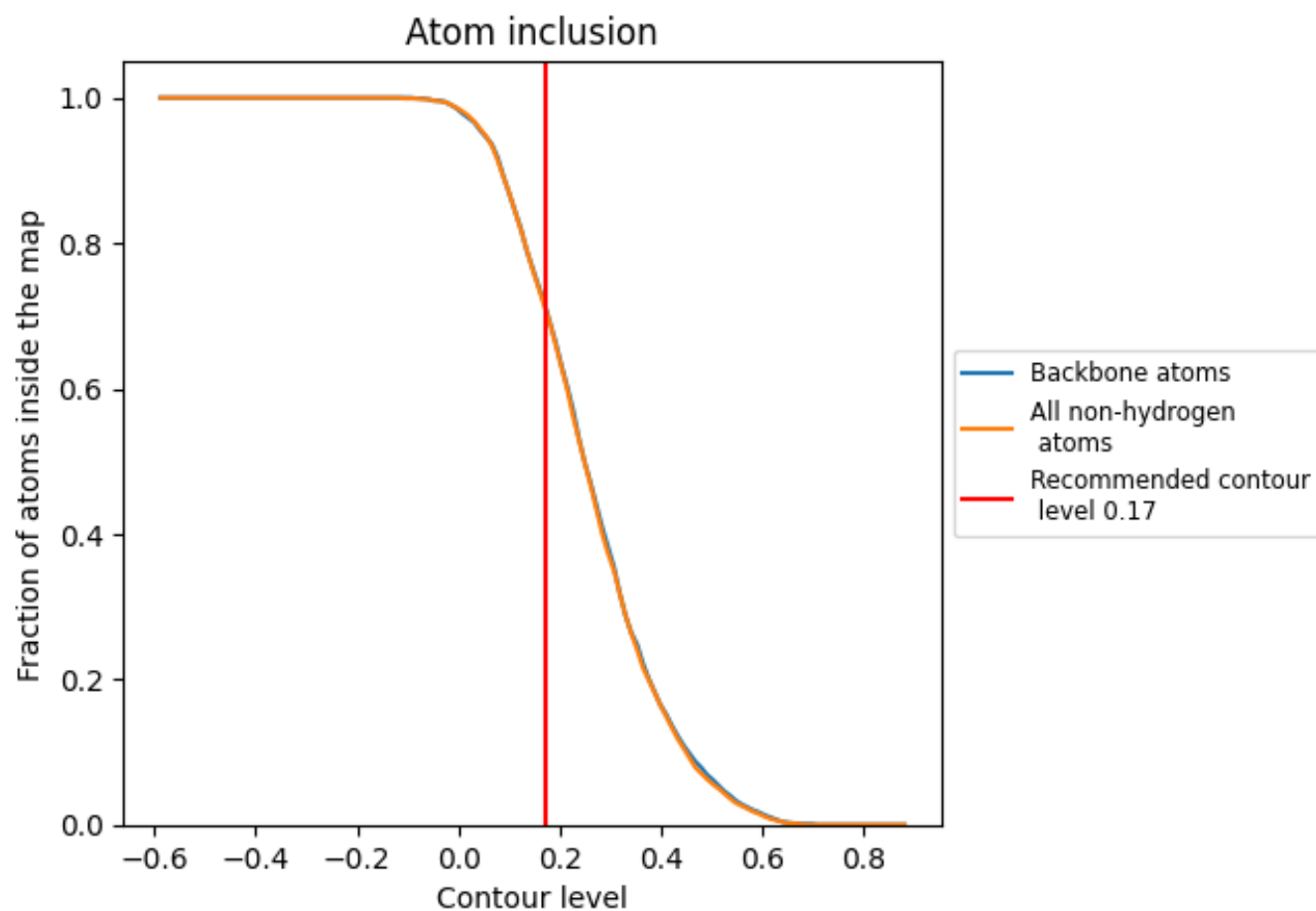
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7120	<div><div></div></div> 0.5450
A	<div><div></div></div> 0.7210	<div><div></div></div> 0.5470
B	<div><div></div></div> 0.7230	<div><div></div></div> 0.5460
C	<div><div></div></div> 0.7190	<div><div></div></div> 0.5490
D	<div><div></div></div> 0.6890	<div><div></div></div> 0.5420
E	<div><div></div></div> 0.7250	<div><div></div></div> 0.5460
F	<div><div></div></div> 0.7290	<div><div></div></div> 0.5450
G	<div><div></div></div> 0.6950	<div><div></div></div> 0.5440
H	<div><div></div></div> 0.6800	<div><div></div></div> 0.5430
I	<div><div></div></div> 0.7260	<div><div></div></div> 0.5470
J	<div><div></div></div> 0.7290	<div><div></div></div> 0.5440

1.0

0.0

<0.0