



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 07:40 pm BST

PDB ID : 9SKK / pdb_00009skk
EMDB ID : EMD-54967
Title : Polysaccharide co-polymerase FepE open 9 subunit complex
Authors : Wiseman, B.; Hogbom, M.
Deposited on : 2025-09-02
Resolution : 3.30 Å(reported)
Based on initial model : .

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

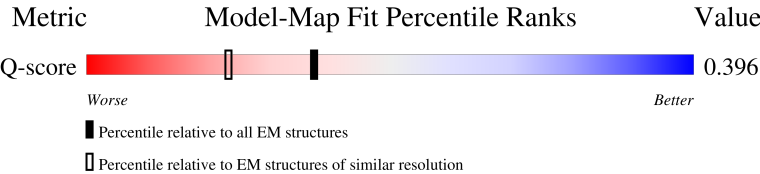
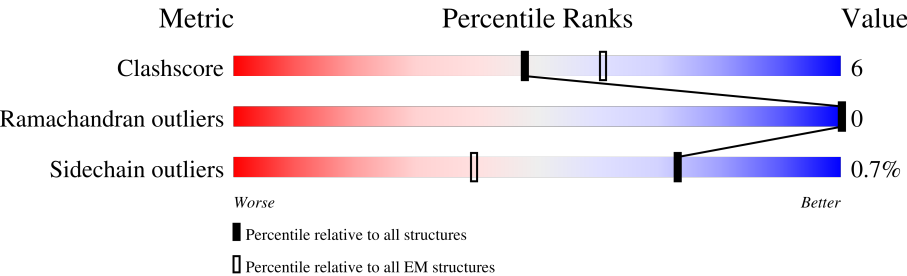
1 Overall quality at a glance

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	392	 6% 58% 22% 20%
1	B	392	 1% 70% 15% 16%
1	C	392	 1% 78% 7% 16%
1	D	392	 1% 76% 8% 16%

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Mol	Chain	Length	Quality of chain
1	E	392	
1	F	392	
1	G	392	
1	H	392	
1	I	392	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22904 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 Ferric enterobactin transport protein FepE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	313	Total	C	N	O	S	0	0
			2468	1585	409	468	6		
1	B	330	Total	C	N	O	S	0	0
			2599	1667	431	495	6		
1	C	330	Total	C	N	O	S	0	0
			2599	1667	431	495	6		
1	D	330	Total	C	N	O	S	0	0
			2599	1667	431	495	6		
1	E	330	Total	C	N	O	S	0	0
			2599	1667	431	495	6		
1	F	330	Total	C	N	O	S	0	0
			2599	1667	431	495	6		
1	G	330	Total	C	N	O	S	0	0
			2599	1667	431	495	6		
1	H	330	Total	C	N	O	S	0	0
			2599	1667	431	495	6		
1	I	280	Total	C	N	O	S	0	0
			2243	1429	374	438	2		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	GLU	-	expression tag	UNP P26266
A	379	PHE	-	expression tag	UNP P26266
A	380	ARG	-	expression tag	UNP P26266
A	381	VAL	-	expression tag	UNP P26266
A	382	PRO	-	expression tag	UNP P26266
A	383	GLY	-	expression tag	UNP P26266
A	384	SER	-	expression tag	UNP P26266
A	385	HIS	-	expression tag	UNP P26266
A	386	HIS	-	expression tag	UNP P26266
A	387	HIS	-	expression tag	UNP P26266
A	388	HIS	-	expression tag	UNP P26266
A	389	HIS	-	expression tag	UNP P26266

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Chain	Residue	Modelled	Actual	Comment	Reference
A	390	HIS	-	expression tag	UNP P26266
A	391	HIS	-	expression tag	UNP P26266
A	392	HIS	-	expression tag	UNP P26266
B	378	GLU	-	expression tag	UNP P26266
B	379	PHE	-	expression tag	UNP P26266
B	380	ARG	-	expression tag	UNP P26266
B	381	VAL	-	expression tag	UNP P26266
B	382	PRO	-	expression tag	UNP P26266
B	383	GLY	-	expression tag	UNP P26266
B	384	SER	-	expression tag	UNP P26266
B	385	HIS	-	expression tag	UNP P26266
B	386	HIS	-	expression tag	UNP P26266
B	387	HIS	-	expression tag	UNP P26266
B	388	HIS	-	expression tag	UNP P26266
B	389	HIS	-	expression tag	UNP P26266
B	390	HIS	-	expression tag	UNP P26266
B	391	HIS	-	expression tag	UNP P26266
B	392	HIS	-	expression tag	UNP P26266
C	378	GLU	-	expression tag	UNP P26266
C	379	PHE	-	expression tag	UNP P26266
C	380	ARG	-	expression tag	UNP P26266
C	381	VAL	-	expression tag	UNP P26266
C	382	PRO	-	expression tag	UNP P26266
C	383	GLY	-	expression tag	UNP P26266
C	384	SER	-	expression tag	UNP P26266
C	385	HIS	-	expression tag	UNP P26266
C	386	HIS	-	expression tag	UNP P26266
C	387	HIS	-	expression tag	UNP P26266
C	388	HIS	-	expression tag	UNP P26266
C	389	HIS	-	expression tag	UNP P26266
C	390	HIS	-	expression tag	UNP P26266
C	391	HIS	-	expression tag	UNP P26266
C	392	HIS	-	expression tag	UNP P26266
D	378	GLU	-	expression tag	UNP P26266
D	379	PHE	-	expression tag	UNP P26266
D	380	ARG	-	expression tag	UNP P26266
D	381	VAL	-	expression tag	UNP P26266
D	382	PRO	-	expression tag	UNP P26266
D	383	GLY	-	expression tag	UNP P26266
D	384	SER	-	expression tag	UNP P26266
D	385	HIS	-	expression tag	UNP P26266
D	386	HIS	-	expression tag	UNP P26266

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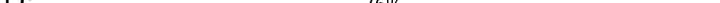
Chain	Residue	Modelled	Actual	Comment	Reference
D	387	HIS	-	expression tag	UNP P26266
D	388	HIS	-	expression tag	UNP P26266
D	389	HIS	-	expression tag	UNP P26266
D	390	HIS	-	expression tag	UNP P26266
D	391	HIS	-	expression tag	UNP P26266
D	392	HIS	-	expression tag	UNP P26266
E	378	GLU	-	expression tag	UNP P26266
E	379	PHE	-	expression tag	UNP P26266
E	380	ARG	-	expression tag	UNP P26266
E	381	VAL	-	expression tag	UNP P26266
E	382	PRO	-	expression tag	UNP P26266
E	383	GLY	-	expression tag	UNP P26266
E	384	SER	-	expression tag	UNP P26266
E	385	HIS	-	expression tag	UNP P26266
E	386	HIS	-	expression tag	UNP P26266
E	387	HIS	-	expression tag	UNP P26266
E	388	HIS	-	expression tag	UNP P26266
E	389	HIS	-	expression tag	UNP P26266
E	390	HIS	-	expression tag	UNP P26266
E	391	HIS	-	expression tag	UNP P26266
E	392	HIS	-	expression tag	UNP P26266
F	378	GLU	-	expression tag	UNP P26266
F	379	PHE	-	expression tag	UNP P26266
F	380	ARG	-	expression tag	UNP P26266
F	381	VAL	-	expression tag	UNP P26266
F	382	PRO	-	expression tag	UNP P26266
F	383	GLY	-	expression tag	UNP P26266
F	384	SER	-	expression tag	UNP P26266
F	385	HIS	-	expression tag	UNP P26266
F	386	HIS	-	expression tag	UNP P26266
F	387	HIS	-	expression tag	UNP P26266
F	388	HIS	-	expression tag	UNP P26266
F	389	HIS	-	expression tag	UNP P26266
F	390	HIS	-	expression tag	UNP P26266
F	391	HIS	-	expression tag	UNP P26266
F	392	HIS	-	expression tag	UNP P26266
G	378	GLU	-	expression tag	UNP P26266
G	379	PHE	-	expression tag	UNP P26266
G	380	ARG	-	expression tag	UNP P26266
G	381	VAL	-	expression tag	UNP P26266
G	382	PRO	-	expression tag	UNP P26266
G	383	GLY	-	expression tag	UNP P26266

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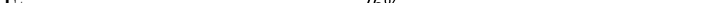
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Chain	Residue	Modelled	Actual	Comment	Reference
G	384	SER	-	expression tag	UNP P26266
G	385	HIS	-	expression tag	UNP P26266
G	386	HIS	-	expression tag	UNP P26266
G	387	HIS	-	expression tag	UNP P26266
G	388	HIS	-	expression tag	UNP P26266
G	389	HIS	-	expression tag	UNP P26266
G	390	HIS	-	expression tag	UNP P26266
G	391	HIS	-	expression tag	UNP P26266
G	392	HIS	-	expression tag	UNP P26266
H	378	GLU	-	expression tag	UNP P26266
H	379	PHE	-	expression tag	UNP P26266
H	380	ARG	-	expression tag	UNP P26266
H	381	VAL	-	expression tag	UNP P26266
H	382	PRO	-	expression tag	UNP P26266
H	383	GLY	-	expression tag	UNP P26266
H	384	SER	-	expression tag	UNP P26266
H	385	HIS	-	expression tag	UNP P26266
H	386	HIS	-	expression tag	UNP P26266
H	387	HIS	-	expression tag	UNP P26266
H	388	HIS	-	expression tag	UNP P26266
H	389	HIS	-	expression tag	UNP P26266
H	390	HIS	-	expression tag	UNP P26266
H	391	HIS	-	expression tag	UNP P26266
H	392	HIS	-	expression tag	UNP P26266
I	378	GLU	-	expression tag	UNP P26266
I	379	PHE	-	expression tag	UNP P26266
I	380	ARG	-	expression tag	UNP P26266
I	381	VAL	-	expression tag	UNP P26266
I	382	PRO	-	expression tag	UNP P26266
I	383	GLY	-	expression tag	UNP P26266
I	384	SER	-	expression tag	UNP P26266
I	385	HIS	-	expression tag	UNP P26266
I	386	HIS	-	expression tag	UNP P26266
I	387	HIS	-	expression tag	UNP P26266
I	388	HIS	-	expression tag	UNP P26266
I	389	HIS	-	expression tag	UNP P26266
I	390	HIS	-	expression tag	UNP P26266
I	391	HIS	-	expression tag	UNP P26266
I	392	HIS	-	expression tag	UNP P26266

V263	K264	F269	L273	L278	E297	L298	I341	L344	V352	A353	C354	G355	G356	VAL	LEU	LEU	ARG	TYR	I27	D28	L29	L30	M44	P74	W79	M128	K135	L139	M152	D164	E165	S175	I213	E220	R239	S258	Q261	A262
SER	SER	LEU	ASN	ILE	LYS	GLN	SER	ASP	ALA	HIS	PHE	PRO	ASP	TYR	PRO	PRO	ASN	GLU	I27	D28	L29	L30	M44	P74	W79	M128	K135	L139	M152	D164	E165	S175	I213	E220	R239	S258	Q261	A262

- Chain D:  76% 8% 16%

Protein	Category	Score
VAL	HIS	M128
PRO	GLY	K132
SER	SER	L139
HIS	HIS	E150
HIS	HIS	A154
HIS	HIS	K163
HIS	HIS	V207
HIS	HIS	I237
HIS	HIS	S243
HIS	HIS	P255
HIS	HIS	V256
HIS	HIS	Y257
HIS	HIS	S258
HIS	HIS	K264
HIS	HIS	K286
HIS	HIS	V313
HIS	HIS	I348
HIS	HIS	V352
HIS	HIS	A353
HIS	HIS	C354
HIS	HIS	G355
HIS	HIS	G356
HIS	HIS	VAL
HIS	HIS	LEU
HIS	HIS	ARG
HIS	HIS	TYR
HIS	HIS	ALA
HIS	HIS	ALA
HIS	HIS	SER
HIS	HIS	ARG
HIS	HIS	LYS
HIS	HIS	GLN
HIS	HIS	ASP
HIS	HIS	ALA
HIS	HIS	MET
HIS	HIS	MET
HIS	HIS	ALA
HIS	HIS	ASP
HIS	HIS	HIS
HIS	HIS	LEU
HIS	HIS	VAL
HIS	HIS	GLU
HIS	HIS	PHE
HIS	HIS	MET
HIS	HIS	SER
HIS	HIS	LEU
HIS	HIS	ASN
HIS	HIS	ILE
HIS	HIS	LYS
HIS	HIS	GLN
HIS	HIS	GLY
HIS	HIS	SER
HIS	HIS	ASP
HIS	HIS	ALA
HIS	HIS	HIS
HIS	HIS	PHE
HIS	HIS	ASP
HIS	HIS	TYR
HIS	HIS	PRO
HIS	HIS	LEU
HIS	HIS	ALA
HIS	HIS	SER
HIS	HIS	PRO
HIS	HIS	ASN
HIS	HIS	ASN
HIS	HIS	GLU
HIS	HIS	I27
HIS	HIS	L30
HIS	HIS	N31
HIS	HIS	L32
HIS	HIS	K41
HIS	HIS	M44
HIS	HIS	A45
HIS	HIS	F48
HIS	HIS	L56
HIS	HIS	I57
HIS	HIS	L60
HIS	HIS	L61
HIS	HIS	P62
HIS	HIS	V77
HIS	HIS	L82
HIS	HIS	L89
HIS	HIS	R90
HIS	HIS	V91
HIS	HIS	I96
HIS	HIS	K97
HIS	HIS	I98
HIS	HIS	F111

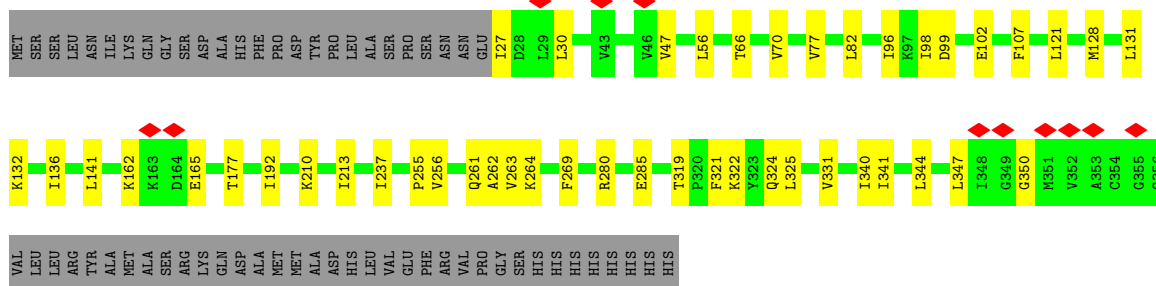
- Chain E:  76% 8% 16%

Protein	Position	Residue	Score	Conservation	Annotations
P00001	1	ARG	0.85	High	
	2	VAL	0.75	Medium	
	3	PRO	0.65	Low	
	4	GLY	0.55	Low	
	5	SER	0.45	Low	
	6	HIS	0.35	Low	
	7	HIS	0.25	Low	
	8	HIS	0.15	Low	
	9	HIS	0.05	Low	
	10	HIS	0.00	Low	
P00002	11	ASP	0.90	High	
	12	VAL	0.80	High	
	13	GLY	0.70	Medium	
	14	SER	0.60	Medium	
	15	ASP	0.50	Medium	
	16	ALA	0.40	Low	
	17	HIS	0.30	Low	
	18	ASP	0.20	Low	
	19	PRO	0.10	Low	
	20	ASP	0.00	Low	
P00003	21	ASP	0.95	High	
	22	PRO	0.85	High	
	23	TYR	0.75	Medium	
	24	PRO	0.65	Medium	
	25	LEU	0.55	Medium	
	26	ALA	0.45	Low	
	27	SER	0.35	Low	
	28	PRO	0.25	Low	
	29	SER	0.15	Low	
	30	ASN	0.05	Low	
P00004	31	ASN	0.90	High	
	32	GLU	0.80	High	
	33	PRO	0.70	Medium	
	34	ASP	0.60	Medium	
	35	TYR	0.50	Medium	
	36	PRO	0.40	Low	
	37	LEU	0.30	Low	
	38	ALA	0.20	Low	
	39	SER	0.10	Low	
	40	PRO	0.00	Low	
P00005	41	ASP	0.95	High	
	42	PRO	0.85	High	
	43	LEU	0.75	Medium	
	44	ALA	0.65	Medium	
	45	SER	0.55	Medium	
	46	PRO	0.45	Low	
	47	SER	0.35	Low	
	48	ASN	0.25	Low	
	49	ASN	0.15	Low	
	50	GLU	0.05	Low	
P00006	51	ASP	0.90	High	
	52	PRO	0.80	High	
	53	LEU	0.70	Medium	
	54	ALA	0.60	Medium	
	55	SER	0.50	Medium	
	56	PRO	0.40	Low	
	57	SER	0.30	Low	
	58	ASN	0.20	Low	
	59	ASN	0.10	Low	
	60	GLU	0.00	Low	
P00007	61	ASP	0.95	High	
	62	PRO	0.85	High	
	63	LEU	0.75	Medium	
	64	ALA	0.65	Medium	
	65	SER	0.55	Medium	
	66	PRO	0.45	Low	
	67	SER	0.35	Low	
	68	ASN	0.25	Low	
	69	ASN	0.15	Low	
	70	GLU	0.05	Low	
P00008	71	ASP	0.90	High	
	72	PRO	0.80	High	
	73	LEU	0.70	Medium	
	74	ALA	0.60	Medium	
	75	SER	0.50	Medium	
	76	PRO	0.40	Low	
	77	SER	0.30	Low	
	78	ASN	0.20	Low	
	79	ASN	0.10	Low	
	80	GLU	0.00	Low	
P00009	81	ASP	0.95	High	
	82	PRO	0.85	High	
	83	LEU	0.75	Medium	
	84	ALA	0.65	Medium	
	85	SER	0.55	Medium	
	86	PRO	0.45	Low	
	87	SER	0.35	Low	
	88	ASN	0.25	Low	

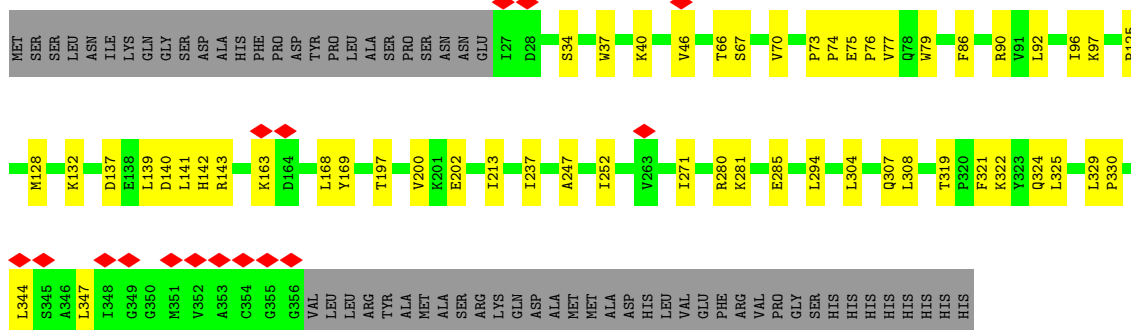
- Chain F: 76% 8% 16%

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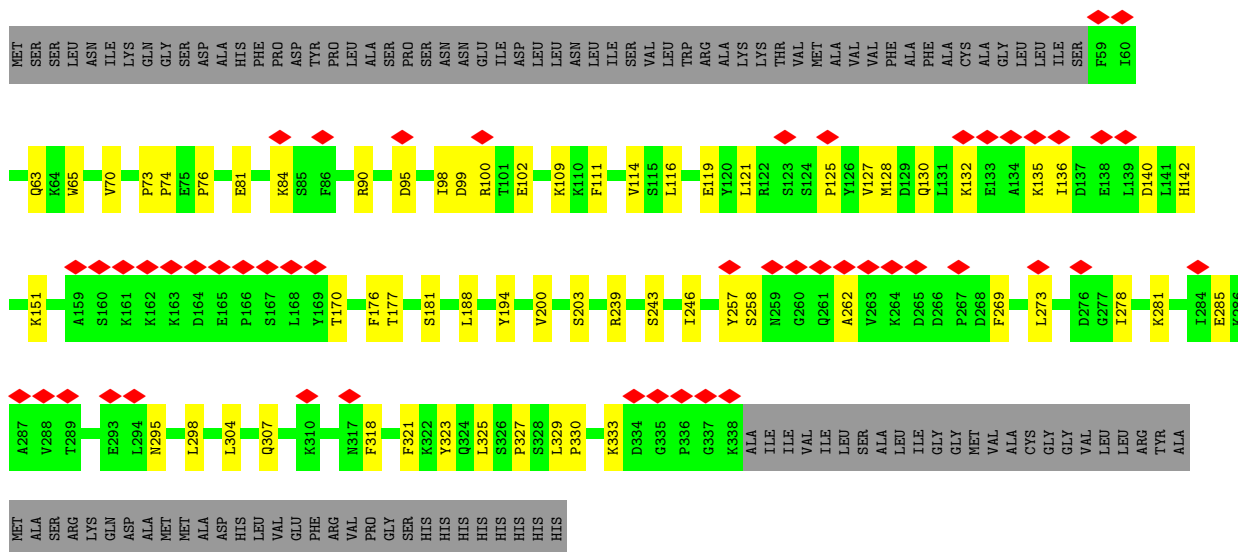
Chain G:



Chain H:



Chain I:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	226507	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.389	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	372.6, 372.6, 372.6	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.828, 0.828, 0.828	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	0/2507	0.37	0/3390
1	B	0.09	0/2642	0.26	0/3575
1	C	0.16	0/2642	0.31	0/3575
1	D	0.14	0/2642	0.29	0/3575
1	E	0.13	0/2642	0.31	0/3575
1	F	0.09	0/2642	0.24	0/3575
1	G	0.15	0/2642	0.31	0/3575
1	H	0.20	0/2642	0.37	0/3575
1	I	0.09	0/2282	0.27	0/3086
All	All	0.14	0/23283	0.31	0/31501

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	2468	0	2552	58	0
1	B	2599	0	2683	39	0
1	C	2599	0	2683	19	0
1	D	2599	0	2683	23	0
1	E	2599	0	2683	23	0
1	F	2599	0	2683	21	0
1	G	2599	0	2683	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2599	0	2683	44	0
1	I	2243	0	2282	41	0
All	All	22904	0	23615	274	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 6.

All (274) 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:H:324:GLN:HE22	1:I:109:LYS:HG3	1.39	0.88
1:A:271:ILE:HD13	1:A:280:ARG:HH12	1.51	0.76
1:A:222:LEU:HA	1:A:301:ARG:HH12	1.51	0.75
1:A:162:LYS:HG3	1:A:164:ASP:H	1.53	0.73
1:E:94:LEU:HD13	1:E:214:LYS:HD3	1.71	0.71
1:D:41:LYS:HA	1:D:44:MET:HE1	1.70	0.71
1:D:264:LYS:HA	1:D:264:LYS:HE2	1.71	0.71
1:H:294:LEU:HB3	1:I:239:ARG:HH21	1.56	0.70
1:B:273:LEU:HB2	1:B:278:ILE:HG13	1.73	0.70
1:B:237:ILE:HD12	1:B:286:LYS:HG3	1.74	0.69
1:I:257:TYR:HA	1:I:262:ALA:H	1.57	0.69
1:H:325:LEU:HD13	1:I:114:VAL:HB	1.75	0.67
1:I:128:MET:H	1:I:128:MET:HE3	1.60	0.66
1:H:140:ASP:O	1:H:143:ARG:N	2.29	0.65
1:D:91:VAL:HG23	1:E:221:LYS:HD3	1.79	0.65
1:G:255:PRO:HG2	1:H:252:ILE:HD11	1.78	0.64
1:H:97:LYS:HE3	1:H:97:LYS:HA	1.78	0.64
1:I:243:SER:HA	1:I:246:ILE:HD12	1.80	0.64
1:A:164:ASP:HA	1:B:163:LYS:HE3	1.81	0.63
1:D:82:LEU:HD21	1:D:98:ILE:HD12	1.81	0.63
1:D:256:VAL:HG12	1:D:258:SER:H	1.63	0.62
1:E:99:ASP:HB3	1:E:102:GLU:HB2	1.82	0.62
1:C:128:MET:HE2	1:C:128:MET:HA	1.82	0.62
1:E:41:LYS:HA	1:E:44:MET:HE2	1.84	0.60
1:A:218:GLU:HB3	1:A:305:VAL:HG22	1.84	0.60
1:I:63:GLN:HE21	1:I:333:LYS:HB2	1.66	0.60
1:I:70:VAL:HB	1:I:325:LEU:HB2	1.84	0.60
1:D:237:ILE:HD11	1:D:286:LYS:HD3	1.83	0.60
1:H:140:ASP:O	1:H:141:LEU:C	2.45	0.60
1:I:295:ASN:HB3	1:I:298:LEU:HG	1.84	0.58
1:H:280:ARG:HH22	1:I:246:ILE:HG23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ALA:HB1	1:F:43:VAL:HG23	1.86	0.58
1:A:39:ALA:HB1	1:A:43:VAL:HB	1.85	0.58
1:C:164:ASP:O	1:C:165:GLU:C	2.46	0.57
1:H:96:ILE:HD12	1:H:96:ILE:O	2.04	0.57
1:A:204:LEU:HB3	1:A:208:ARG:HH12	1.70	0.57
1:G:70:VAL:HB	1:G:324:GLN:HB3	1.87	0.57
1:G:192:ILE:HG13	1:G:321:PHE:CZ	2.40	0.56
1:A:99:ASP:HB3	1:A:102:GLU:HB2	1.86	0.56
1:E:257:TYR:HB3	1:F:256:VAL:HG21	1.88	0.56
1:H:92:LEU:HD13	1:H:307:GLN:HE22	1.70	0.56
1:A:294:LEU:HB3	1:B:239:ARG:HH21	1.68	0.55
1:I:121:LEU:HA	1:I:127:VAL:HG11	1.88	0.55
1:I:99:ASP:HB3	1:I:102:GLU:OE2	2.07	0.55
1:G:331:VAL:HA	1:H:143:ARG:HH12	1.72	0.55
1:I:90:ARG:HH22	1:I:95:ASP:HA	1.71	0.55
1:A:292:ALA:HB1	1:A:299:ARG:HG2	1.88	0.54
1:C:258:SER:HB2	1:C:262:ALA:HB2	1.89	0.54
1:H:237:ILE:HD11	1:H:285:GLU:HB3	1.89	0.54
1:I:304:LEU:HA	1:I:307:GLN:HE21	1.72	0.54
1:C:273:LEU:HD23	1:C:278:ILE:HD13	1.89	0.54
1:I:76:PRO:HA	1:I:100:ARG:HE	1.74	0.53
1:A:197:THR:O	1:A:201:LYS:HG2	2.08	0.53
1:A:240:LEU:O	1:A:244:LEU:HG	2.08	0.53
1:E:94:LEU:HG	1:E:96:ILE:HD11	1.90	0.53
1:B:30:LEU:HD12	1:B:33:ILE:HD12	1.89	0.53
1:A:113:SER:HB3	1:A:116:LEU:HB2	1.91	0.53
1:H:34:SER:HA	1:H:37:TRP:HD1	1.73	0.53
1:I:132:LYS:HA	1:I:136:ILE:HB	1.89	0.53
1:H:140:ASP:HB3	1:H:143:ARG:HB2	1.90	0.53
1:E:51:ALA:HB2	1:E:346:ALA:HB2	1.91	0.53
1:A:121:LEU:HD12	1:A:145:ILE:HG23	1.91	0.52
1:I:273:LEU:HB3	1:I:278:ILE:HG13	1.91	0.52
1:E:94:LEU:HD21	1:E:211:LEU:HA	1.90	0.52
1:B:259:ASN:HA	1:C:261:GLN:HB2	1.90	0.52
1:I:140:ASP:HA	1:I:142:HIS:CE1	2.44	0.52
1:C:239:ARG:HG3	1:C:269:PHE:HD1	1.75	0.52
1:I:125:PRO:HA	1:I:128:MET:HE1	1.91	0.52
1:G:340:ILE:HG13	1:G:341:ILE:HD12	1.92	0.51
1:G:82:LEU:HD11	1:G:98:ILE:HD12	1.92	0.51
1:A:122:ARG:HA	1:A:122:ARG:NE	2.25	0.51
1:A:217:PHE:O	1:A:221:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LYS:HG3	1:B:164:ASP:H	1.76	0.51
1:E:70:VAL:HB	1:E:324:GLN:HB3	1.92	0.51
1:F:139:LEU:HD23	1:F:139:LEU:H	1.75	0.51
1:G:77:VAL:HG21	1:H:202:GLU:HG2	1.92	0.51
1:I:176:PHE:HB2	1:I:188:LEU:HD13	1.92	0.51
1:B:82:LEU:HD21	1:B:98:ILE:HD12	1.92	0.51
1:A:27:ILE:HG22	1:A:29:LEU:HG	1.92	0.51
1:A:106:LEU:HD22	1:A:199:VAL:HG13	1.92	0.51
1:G:96:ILE:HG22	1:G:210:LYS:HD2	1.92	0.51
1:B:253:LYS:HA	1:B:275:ALA:HB3	1.93	0.51
1:B:50:PHE:HB2	1:B:346:ALA:HA	1.93	0.51
1:F:161:LYS:HG3	1:F:164:ASP:HB2	1.92	0.51
1:H:76:PRO:HA	1:H:79:TRP:HB2	1.93	0.50
1:I:323:TYR:HE1	1:I:327:PRO:HD3	1.76	0.50
1:A:217:PHE:O	1:A:220:GLU:HG2	2.12	0.50
1:C:29:LEU:HD23	1:C:29:LEU:H	1.77	0.50
1:F:72:THR:HG23	1:F:322:LYS:HB3	1.92	0.50
1:F:114:VAL:O	1:F:118:GLU:HG2	2.11	0.50
1:H:319:THR:HG22	1:H:321:PHE:H	1.77	0.49
1:H:344:LEU:HA	1:H:347:LEU:HD12	1.92	0.49
1:A:74:PRO:HG2	1:A:100:ARG:HB3	1.93	0.49
1:A:139:LEU:O	1:A:143:ARG:HG2	2.12	0.49
1:A:156:ASP:HB3	1:A:159:ALA:HB3	1.94	0.49
1:I:90:ARG:O	1:I:90:ARG:HD3	2.12	0.49
1:G:165:GLU:HB2	1:H:163:LYS:HG2	1.95	0.49
1:I:200:VAL:HG12	1:I:318:PHE:CE1	2.47	0.49
1:D:77:VAL:HG21	1:E:202:GLU:HG2	1.93	0.49
1:A:142:HIS:O	1:A:146:VAL:HG22	2.13	0.48
1:G:319:THR:HG22	1:G:321:PHE:H	1.77	0.48
1:H:137:ASP:C	1:H:139:LEU:H	2.22	0.48
1:I:151:LYS:HB2	1:I:176:PHE:HE2	1.78	0.48
1:A:178:ALA:HB3	1:A:184:ALA:HB2	1.94	0.48
1:G:237:ILE:HD11	1:G:285:GLU:HB3	1.94	0.48
1:H:281:LYS:HE3	1:I:269:PHE:HE2	1.77	0.48
1:D:139:LEU:HD22	1:D:139:LEU:H	1.77	0.48
1:A:70:VAL:HG12	1:A:325:LEU:HB3	1.96	0.48
1:G:162:LYS:HE3	1:G:165:GLU:HB3	1.95	0.48
1:F:70:VAL:HB	1:F:324:GLN:HB3	1.95	0.47
1:H:168:LEU:HG	1:H:169:TYR:HD1	1.78	0.47
1:D:61:LEU:HD12	1:D:62:PRO:HD2	1.95	0.47
1:B:168:LEU:H	1:B:168:LEU:HD23	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ALA:HB2	1:C:261:GLN:HG3	1.96	0.47
1:B:35:VAL:HA	1:B:38:ARG:HG2	1.97	0.47
1:A:233:LEU:O	1:A:237:ILE:HG13	2.14	0.47
1:A:34:SER:HA	1:A:37:TRP:HD1	1.80	0.47
1:F:126:TYR:HE2	1:F:183:GLU:HG3	1.80	0.47
1:D:255:PRO:HG2	1:E:252:ILE:HD11	1.97	0.47
1:A:240:LEU:HB3	1:A:281:LYS:HZ3	1.78	0.47
1:A:169:TYR:HE2	1:B:109:LYS:HA	1.81	0.46
1:B:98:ILE:HD13	1:B:203:SER:HB3	1.97	0.46
1:B:164:ASP:O	1:B:166:PRO:HD3	2.15	0.46
1:B:128:MET:HE1	1:B:145:ILE:HD11	1.97	0.46
1:C:297:GLU:OE2	1:C:298:LEU:HD23	2.16	0.46
1:D:128:MET:HE2	1:D:128:MET:HA	1.96	0.46
1:F:180:THR:HG23	1:F:183:GLU:H	1.79	0.46
1:E:47:VAL:HG13	1:E:346:ALA:HB1	1.97	0.46
1:H:75:GLU:HB2	1:H:77:VAL:HG12	1.97	0.46
1:E:211:LEU:O	1:E:215:THR:HG22	2.15	0.46
1:C:264:LYS:HA	1:C:264:LYS:HD3	1.59	0.46
1:A:116:LEU:HA	1:A:119:GLU:OE2	2.16	0.46
1:A:310:LYS:HA	1:A:310:LYS:HD2	1.71	0.46
1:B:55:LEU:HD23	1:B:56:LEU:HD22	1.97	0.46
1:D:150:GLU:H	1:D:150:GLU:HG2	1.60	0.46
1:I:116:LEU:HA	1:I:119:GLU:HG2	1.98	0.46
1:A:29:LEU:O	1:A:33:ILE:HG12	2.17	0.45
1:A:33:ILE:HD13	1:A:36:LEU:HD12	1.99	0.45
1:A:136:ILE:HG22	1:A:140:ASP:HB3	1.98	0.45
1:A:91:VAL:HG21	1:B:220:GLU:HB3	1.97	0.45
1:B:323:TYR:CE1	1:B:327:PRO:HD3	2.51	0.45
1:D:256:VAL:C	1:D:258:SER:H	2.25	0.45
1:A:132:LYS:HB3	1:A:132:LYS:HE3	1.54	0.45
1:A:230:LYS:HE2	1:A:230:LYS:HB3	1.76	0.45
1:B:91:VAL:HG21	1:C:220:GLU:HB3	1.98	0.45
1:H:75:GLU:OE1	1:H:322:LYS:HE3	2.16	0.45
1:C:29:LEU:HG	1:C:30:LEU:HD12	1.99	0.45
1:G:331:VAL:HA	1:H:143:ARG:NH1	2.30	0.45
1:E:63:GLN:HG3	1:E:65:TRP:HE1	1.82	0.45
1:I:98:ILE:HD13	1:I:203:SER:HB3	1.99	0.45
1:D:89:LEU:HD11	1:D:313:VAL:HG22	1.98	0.44
1:F:163:LYS:HA	1:F:163:LYS:HD3	1.60	0.44
1:A:201:LYS:O	1:A:205:GLU:HG2	2.16	0.44
1:H:125:PRO:HA	1:H:128:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:258:SER:H	1:I:262:ALA:HA	1.82	0.44
1:E:102:GLU:OE1	1:E:102:GLU:HA	2.18	0.44
1:E:261:GLN:HG3	1:F:263:VAL:HG12	1.99	0.44
1:H:141:LEU:HG	1:H:142:HIS:N	2.32	0.44
1:I:65:TRP:HE3	1:I:330:PRO:HB2	1.81	0.44
1:H:308:LEU:HD23	1:H:308:LEU:HA	1.86	0.44
1:F:50:PHE:HB2	1:F:346:ALA:HA	1.99	0.44
1:F:343:ILE:HG13	1:F:344:LEU:N	2.32	0.44
1:G:256:VAL:HB	1:G:263:VAL:HG21	2.00	0.44
1:I:73:PRO:HG2	1:I:170:THR:HG23	1.99	0.44
1:A:135:LYS:HA	1:A:135:LYS:HD2	1.74	0.44
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.90	0.44
1:C:152:MET:HE3	1:C:152:MET:HB2	1.83	0.44
1:E:264:LYS:HD2	1:E:264:LYS:HA	1.71	0.44
1:G:47:VAL:HG13	1:G:350:GLY:HA3	1.98	0.44
1:G:131:LEU:HD23	1:G:131:LEU:HA	1.88	0.44
1:A:138:GLU:HA	1:A:141:LEU:HD12	1.99	0.44
1:A:219:LYS:HB3	1:A:219:LYS:HE2	1.90	0.44
1:I:74:PRO:HD3	1:I:321:PHE:HA	2.00	0.44
1:D:96:ILE:HG21	1:D:207:VAL:HG13	2.00	0.44
1:F:161:LYS:HD2	1:F:165:GLU:HB2	1.99	0.44
1:H:143:ARG:HD3	1:H:143:ARG:HA	1.73	0.44
1:A:207:VAL:HA	1:A:210:LYS:HE2	1.99	0.43
1:I:135:LYS:HA	1:I:135:LYS:HD2	1.75	0.43
1:B:344:LEU:HD12	1:B:345:SER:N	2.33	0.43
1:F:82:LEU:HD23	1:F:82:LEU:HA	1.84	0.43
1:H:329:LEU:HD12	1:H:330:PRO:HD2	2.01	0.43
1:A:152:MET:HE2	1:A:152:MET:HA	2.01	0.43
1:A:325:LEU:HD13	1:B:114:VAL:HB	2.01	0.43
1:B:216:GLN:HA	1:B:219:LYS:HB3	2.00	0.43
1:G:132:LYS:HD2	1:G:132:LYS:HA	1.78	0.43
1:G:344:LEU:HA	1:G:347:LEU:HD12	2.01	0.43
1:A:141:LEU:O	1:A:145:ILE:HG12	2.19	0.43
1:D:111:PHE:CE2	1:D:154:ALA:HB2	2.54	0.43
1:G:141:LEU:HD12	1:G:141:LEU:H	1.83	0.43
1:D:30:LEU:HD23	1:D:30:LEU:HA	1.88	0.43
1:H:247:ALA:HB2	1:H:271:ILE:HD11	2.00	0.43
1:B:95:ASP:O	1:B:96:ILE:HD13	2.18	0.43
1:B:237:ILE:HD11	1:B:285:GLU:HB3	2.01	0.43
1:B:242:TYR:O	1:B:246:ILE:HG12	2.18	0.43
1:B:264:LYS:HB2	1:B:264:LYS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:SER:HB2	1:I:330:PRO:HG2	2.00	0.43
1:A:70:VAL:HG13	1:A:324:GLN:HB3	2.01	0.43
1:B:135:LYS:HD2	1:B:135:LYS:HA	1.80	0.43
1:E:254:LYS:HD3	1:E:254:LYS:HA	1.87	0.43
1:F:29:LEU:HG	1:F:32:LEU:HD12	2.01	0.43
1:B:161:LYS:H	1:B:161:LYS:HG2	1.66	0.43
1:C:74:PRO:HG2	1:C:79:TRP:HE1	1.84	0.43
1:D:163:LYS:HD2	1:D:163:LYS:HA	1.66	0.43
1:G:99:ASP:HB3	1:G:102:GLU:HG2	2.01	0.43
1:D:27:ILE:HD13	1:D:30:LEU:HD12	2.01	0.42
1:F:108:ILE:HD13	1:F:108:ILE:HA	1.85	0.42
1:A:204:LEU:HB3	1:A:208:ARG:NH1	2.32	0.42
1:A:209:ASN:O	1:A:213:ILE:HG22	2.20	0.42
1:A:323:TYR:CE1	1:A:327:PRO:HD3	2.54	0.42
1:B:341:ILE:HA	1:B:344:LEU:HG	2.00	0.42
1:A:228:LYS:HA	1:A:228:LYS:HD3	1.78	0.42
1:B:213:ILE:HD13	1:B:213:ILE:HA	1.91	0.42
1:H:213:ILE:HD13	1:H:213:ILE:HA	1.86	0.42
1:E:152:MET:HE2	1:E:176:PHE:CD1	2.54	0.42
1:I:281:LYS:O	1:I:285:GLU:HG2	2.20	0.42
1:A:225:ASP:O	1:A:229:THR:HG22	2.20	0.42
1:E:293:GLU:HG2	1:F:238:GLN:HG2	2.02	0.42
1:F:61:LEU:HD23	1:F:62:PRO:HD2	2.02	0.42
1:G:136:ILE:HD12	1:G:136:ILE:HA	1.83	0.42
1:I:194:TYR:C	1:I:194:TYR:CD1	2.96	0.42
1:B:32:LEU:HD22	1:B:32:LEU:H	1.85	0.42
1:C:341:ILE:HA	1:C:344:LEU:HD12	2.02	0.42
1:G:70:VAL:HG23	1:G:325:LEU:HB3	2.01	0.42
1:H:66:THR:O	1:H:330:PRO:HB3	2.20	0.42
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.91	0.42
1:G:30:LEU:HD12	1:G:30:LEU:HA	1.91	0.42
1:A:195:ILE:O	1:A:199:VAL:HG23	2.20	0.41
1:H:73:PRO:HA	1:H:74:PRO:HD3	1.88	0.41
1:I:151:LYS:HB3	1:I:177:THR:HG23	2.02	0.41
1:B:153:LYS:HE2	1:B:153:LYS:HB2	1.87	0.41
1:B:247:ALA:HA	1:B:271:ILE:HD11	2.03	0.41
1:E:323:TYR:CE1	1:E:327:PRO:HD3	2.56	0.41
1:F:169:TYR:HD1	1:F:171:SER:HB3	1.85	0.41
1:G:27:ILE:HD12	1:G:27:ILE:HA	1.96	0.41
1:H:67:SER:HB2	1:H:330:PRO:HD3	2.02	0.41
1:H:304:LEU:HD12	1:H:307:GLN:HE21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:CE2	1:A:184:ALA:HA	2.55	0.41
1:A:40:LYS:HE2	1:A:40:LYS:HB3	1.89	0.41
1:B:239:ARG:HD2	1:B:268:ASP:O	2.21	0.41
1:G:261:GLN:HG2	1:G:262:ALA:H	1.85	0.41
1:I:130:GLN:H	1:I:130:GLN:HG3	1.68	0.41
1:E:91:VAL:C	1:E:93:ASP:H	2.29	0.41
1:H:132:LYS:HD2	1:H:132:LYS:HA	1.87	0.41
1:C:135:LYS:HA	1:C:135:LYS:HD2	1.70	0.41
1:G:121:LEU:O	1:G:128:MET:HE3	2.20	0.41
1:I:304:LEU:HA	1:I:307:GLN:NE2	2.36	0.41
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.93	0.41
1:C:139:LEU:H	1:C:139:LEU:HD22	1.85	0.41
1:D:57:ILE:HA	1:D:60:ILE:HG22	2.03	0.41
1:E:257:TYR:HB3	1:F:263:VAL:HG21	2.03	0.41
1:G:213:ILE:HD13	1:G:213:ILE:HA	1.87	0.41
1:H:70:VAL:HB	1:H:324:GLN:HB3	2.01	0.41
1:A:52:CYS:O	1:A:55:LEU:HG	2.21	0.41
1:D:256:VAL:O	1:D:257:TYR:HB3	2.21	0.41
1:G:322:LYS:HA	1:G:322:LYS:HD2	1.73	0.41
1:H:34:SER:HA	1:H:37:TRP:CD1	2.54	0.41
1:H:40:LYS:HE3	1:H:40:LYS:HB3	1.95	0.41
1:H:163:LYS:HA	1:H:163:LYS:HD2	1.79	0.41
1:C:44:MET:H	1:C:44:MET:HE3	1.86	0.41
1:H:86:PHE:HB2	1:H:90:ARG:HH21	1.86	0.41
1:I:81:GLU:HA	1:I:84:LYS:HE3	2.02	0.41
1:B:254:LYS:HD2	1:B:254:LYS:HA	1.84	0.40
1:C:213:ILE:HD13	1:C:213:ILE:HA	1.91	0.40
1:D:132:LYS:HA	1:D:132:LYS:HD3	1.88	0.40
1:G:107:PHE:CE1	1:G:321:PHE:HE1	2.39	0.40
1:I:329:LEU:HD12	1:I:330:PRO:HD2	2.03	0.40
1:G:107:PHE:HZ	1:G:192:ILE:HD11	1.85	0.40
1:H:197:THR:HA	1:H:200:VAL:HG12	2.02	0.40
1:I:140:ASP:HA	1:I:142:HIS:HE1	1.86	0.40
1:A:122:ARG:NH1	1:A:145:ILE:HG13	2.36	0.40
1:A:194:TYR:CE2	1:A:198:LEU:HD11	2.57	0.40
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.85	0.40
1:G:66:THR:HG22	1:G:177:THR:HG23	2.04	0.40
1:H:168:LEU:H	1:H:168:LEU:HD23	1.86	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	309/392 (79%)	293 (95%)	16 (5%)	0	100	100
1	B	328/392 (84%)	316 (96%)	12 (4%)	0	100	100
1	C	328/392 (84%)	316 (96%)	12 (4%)	0	100	100
1	D	328/392 (84%)	314 (96%)	14 (4%)	0	100	100
1	E	328/392 (84%)	312 (95%)	16 (5%)	0	100	100
1	F	328/392 (84%)	319 (97%)	9 (3%)	0	100	100
1	G	328/392 (84%)	301 (92%)	27 (8%)	0	100	100
1	H	328/392 (84%)	308 (94%)	20 (6%)	0	100	100
1	I	278/392 (71%)	268 (96%)	10 (4%)	0	100	100
All	All	2883/3528 (82%)	2747 (95%)	136 (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	274/343 (80%)	269 (98%)	5 (2%)	51	70
1	B	289/343 (84%)	287 (99%)	2 (1%)	76	80
1	C	289/343 (84%)	288 (100%)	1 (0%)	86	86
1	D	289/343 (84%)	287 (99%)	2 (1%)	76	80
1	E	289/343 (84%)	288 (100%)	1 (0%)	86	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	289/343 (84%)	287 (99%)	2 (1%)	76	80
1	G	289/343 (84%)	285 (99%)	4 (1%)	59	73
1	H	289/343 (84%)	288 (100%)	1 (0%)	86	86
1	I	252/343 (74%)	251 (100%)	1 (0%)	84	84
All	All	2549/3087 (83%)	2530 (99%)	19 (1%)	73	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
1	A	119	GLU
1	A	155	VAL
1	A	323	TYR
1	A	342	VAL
1	B	66	THR
1	B	196	SER
1	C	175	SER
1	D	32	LEU
1	D	243	SER
1	E	168	LEU
1	F	155	VAL
1	F	344	LEU
1	G	56	LEU
1	G	264	LYS
1	G	269	PHE
1	G	280	ARG
1	H	46	VAL
1	I	111	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	B	238	GLN
1	B	317	ASN
1	C	112	GLN
1	C	158	ASN
1	C	259	ASN
1	C	261	GLN
1	C	295	ASN

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Mol	Chain	Res	Type
1	C	300	ASN
1	C	312	HIS
1	D	31	ASN
1	D	78	GLN
1	D	224	GLN
1	D	261	GLN
1	D	300	ASN
1	F	31	ASN
1	F	142	HIS
1	F	314	ASN
1	G	238	GLN
1	H	31	ASN
1	H	307	GLN
1	I	112	GLN
1	I	185	GLN
1	I	238	GLN

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 ⓘ

There are no chain breaks in this entry.

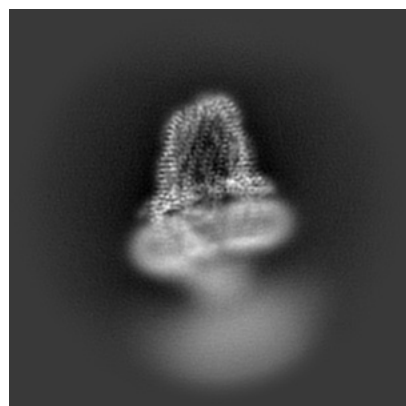
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54967. These allow visual inspection of the internal detail of the map and identification of artifacts.

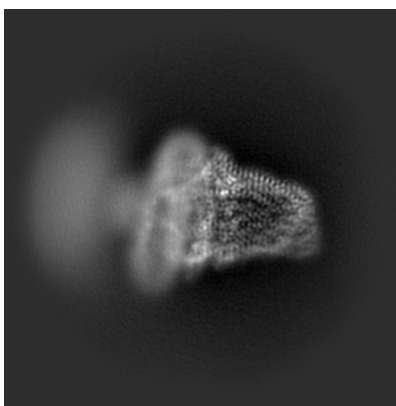
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

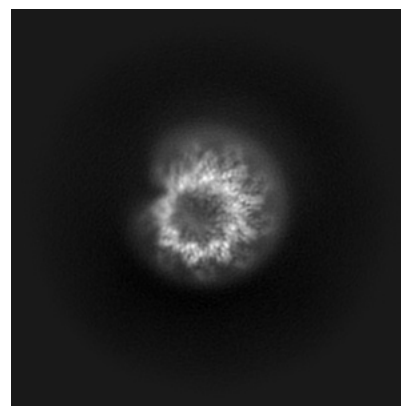
6.1.1 Primary map



X

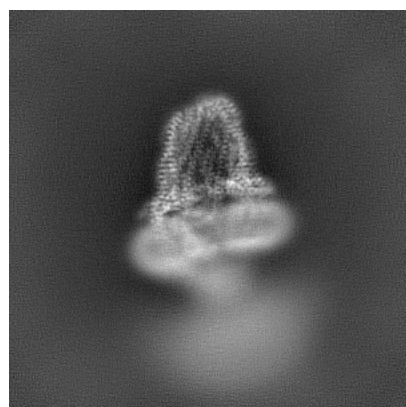


Y

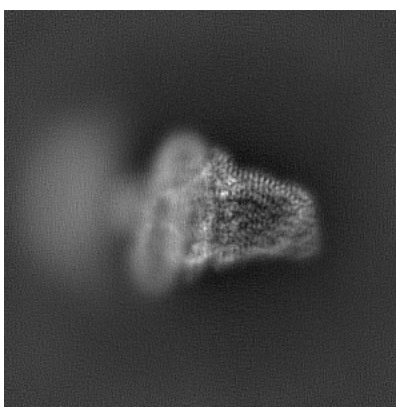


Z

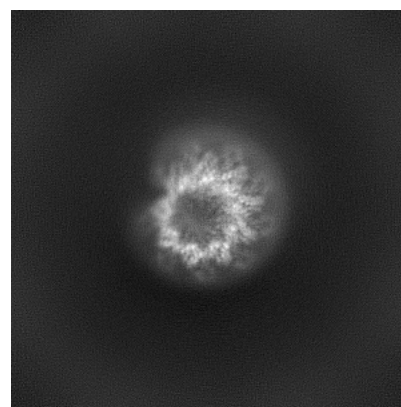
6.1.2 Raw map



X



Y

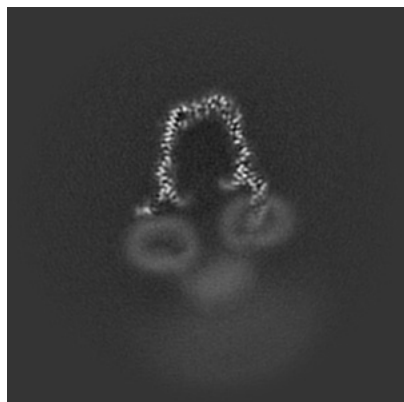


Z

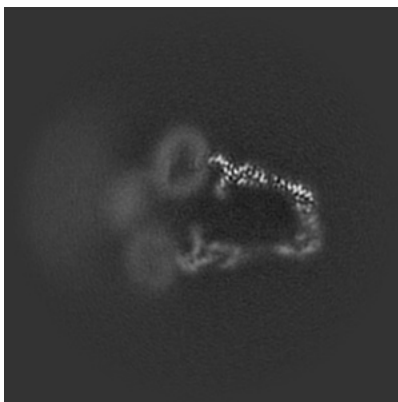
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

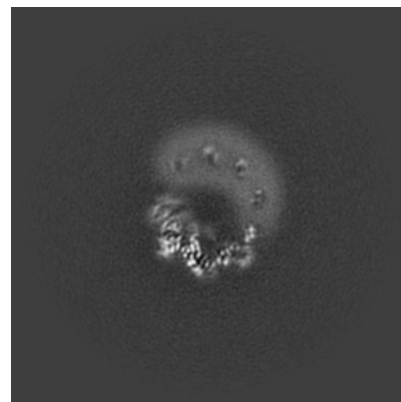
6.2.1 Primary map



X Index: 225



Y Index: 225



Z Index: 225

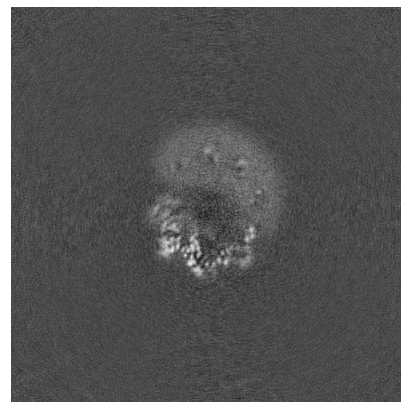
6.2.2 Raw map



X Index: 225



Y Index: 225

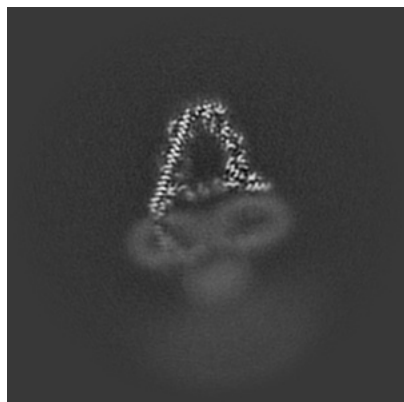


Z Index: 225

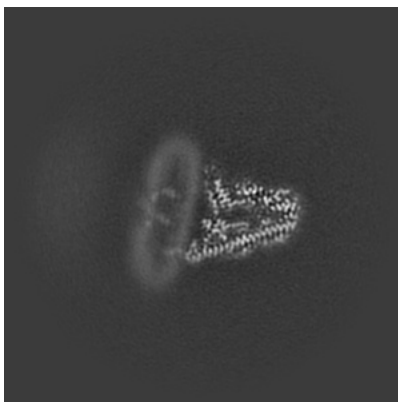
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

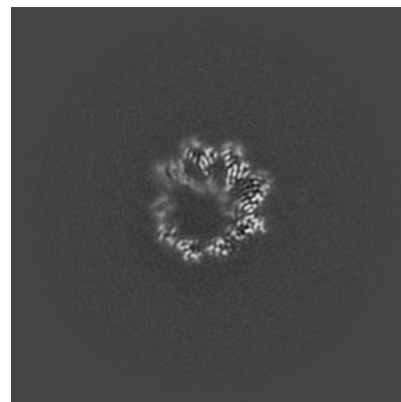
6.3.1 Primary map



X Index: 243

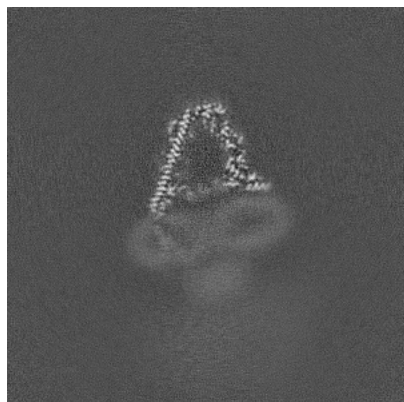


Y Index: 184

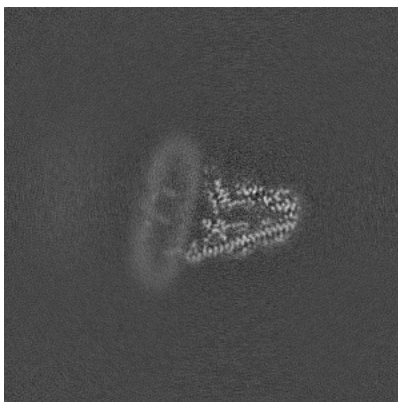


Z Index: 249

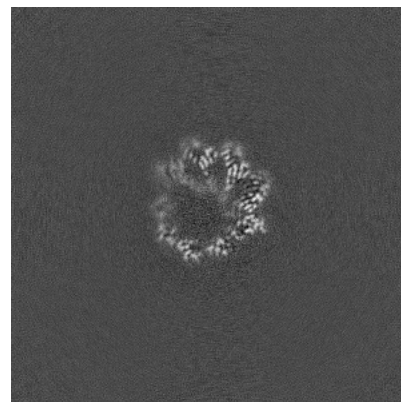
6.3.2 Raw map



X Index: 243



Y Index: 184

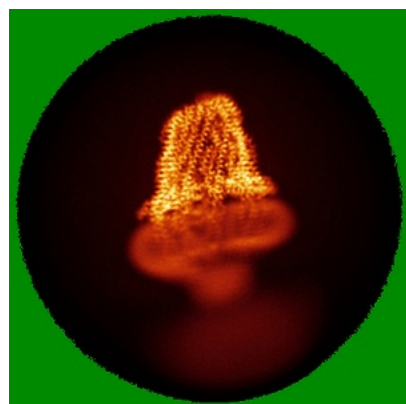


Z Index: 249

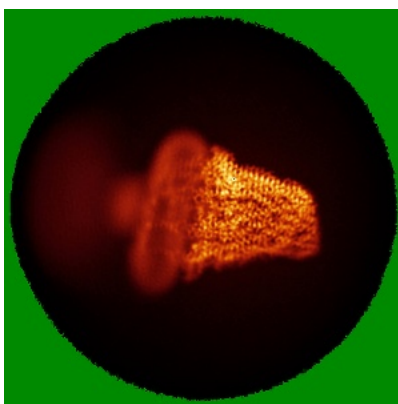
The images above show the largest variance slices of the map in three orthogonal directions.

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

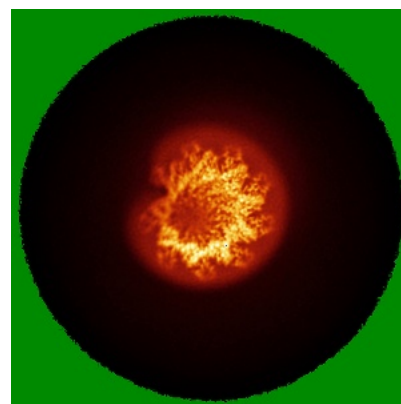
6.4.1 Primary map



X

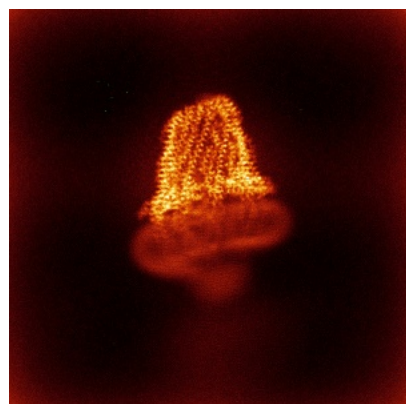


Y

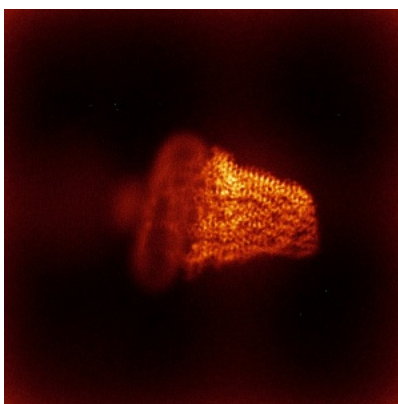


Z

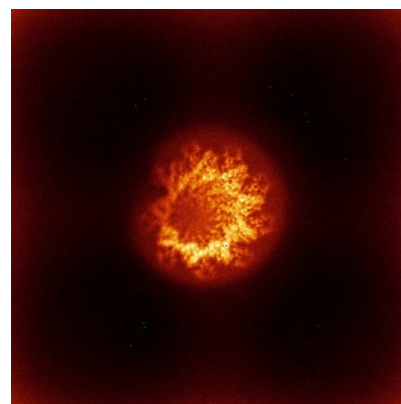
6.4.2 Raw map



X



Y

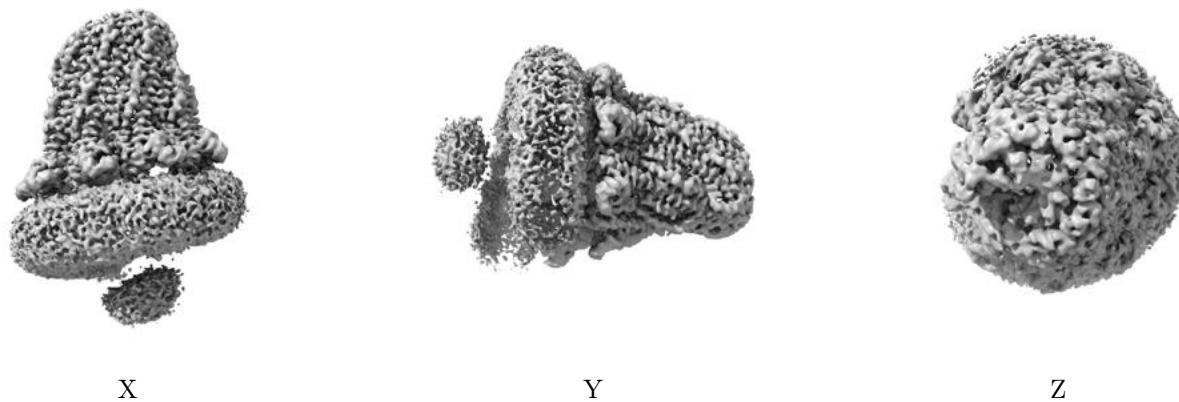


Z

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.

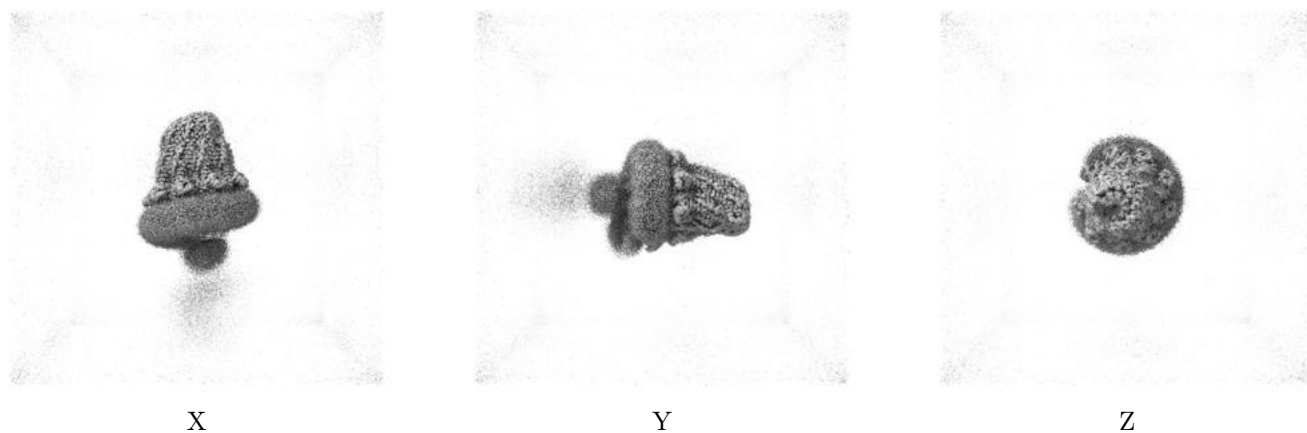
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

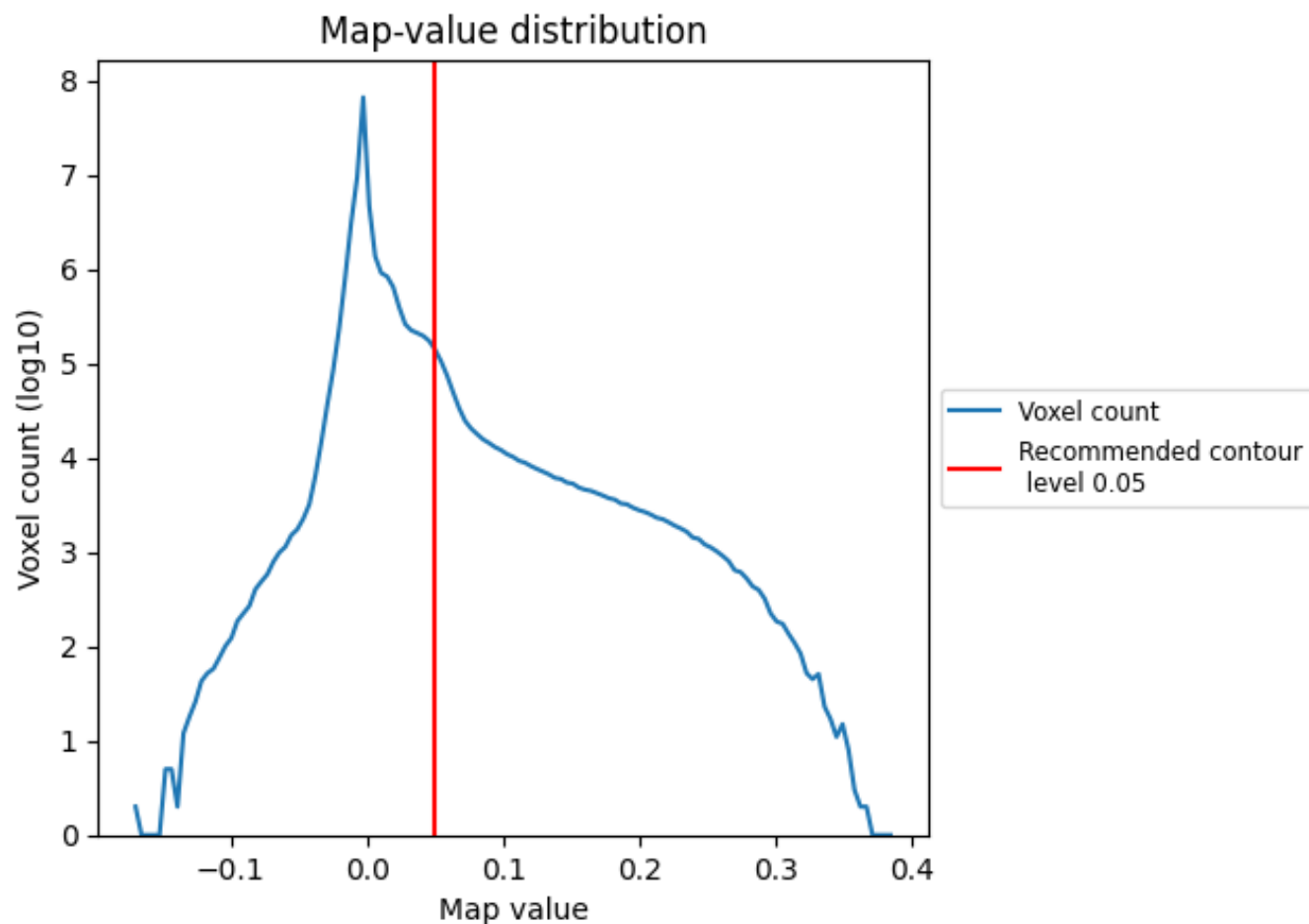
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

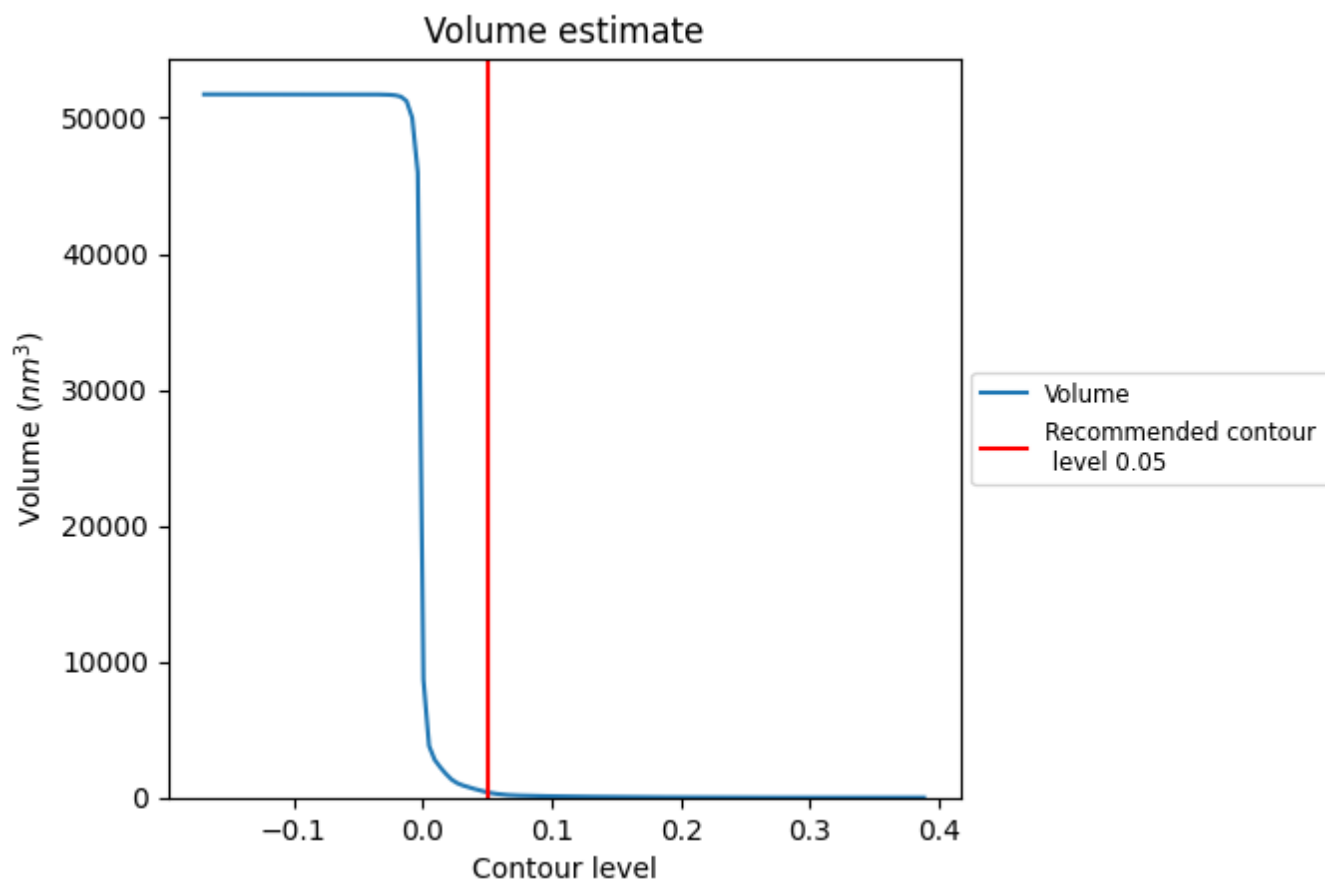
This section contains the results of statistical analysis of the map.

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.

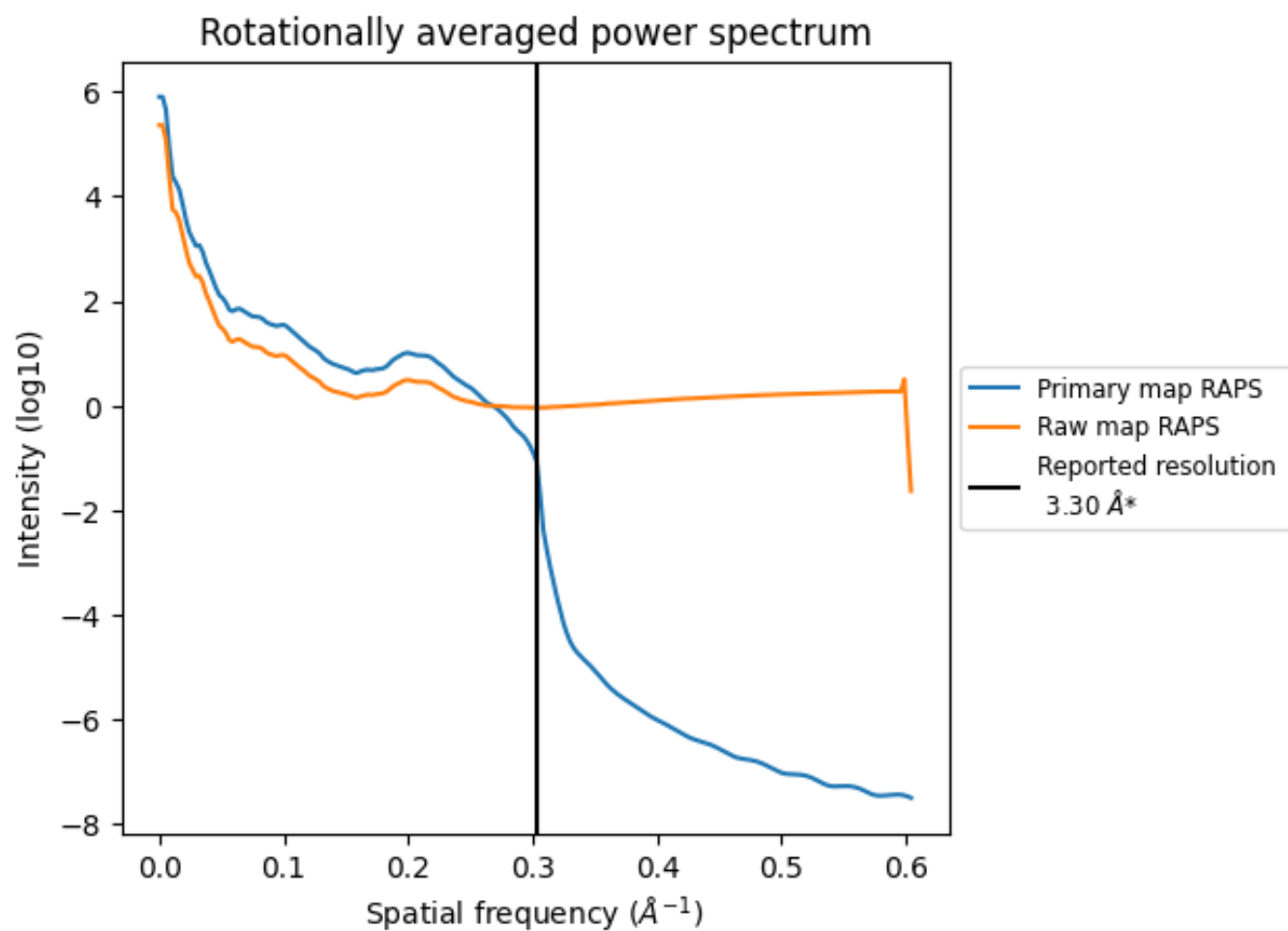
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 393 nm³; this corresponds to an approximate mass of 355 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 ⓘ

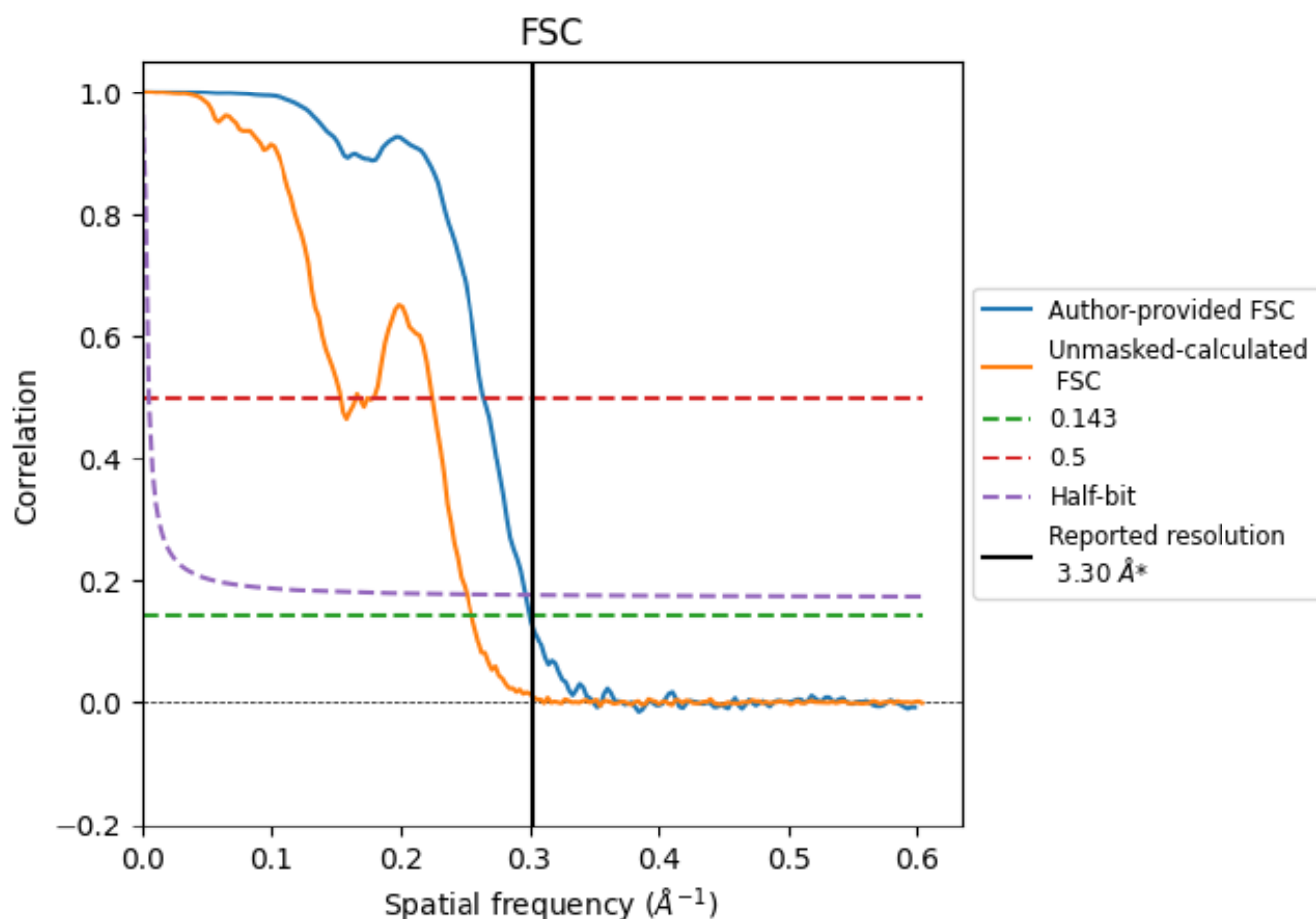


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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](#)

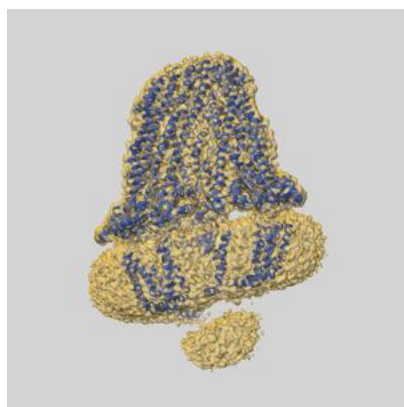
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.78	3.37
Unmasked-calculated*	3.92	6.51	3.98

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

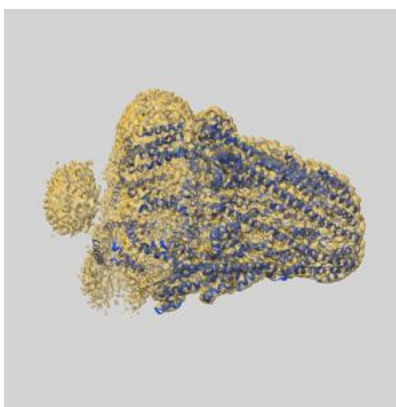
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54967 and PDB model 9SKK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

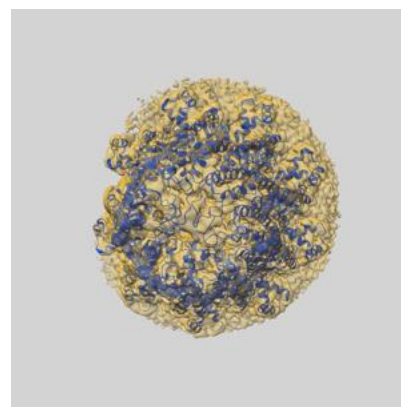
9.1 Map-model overlay [i](#)



X



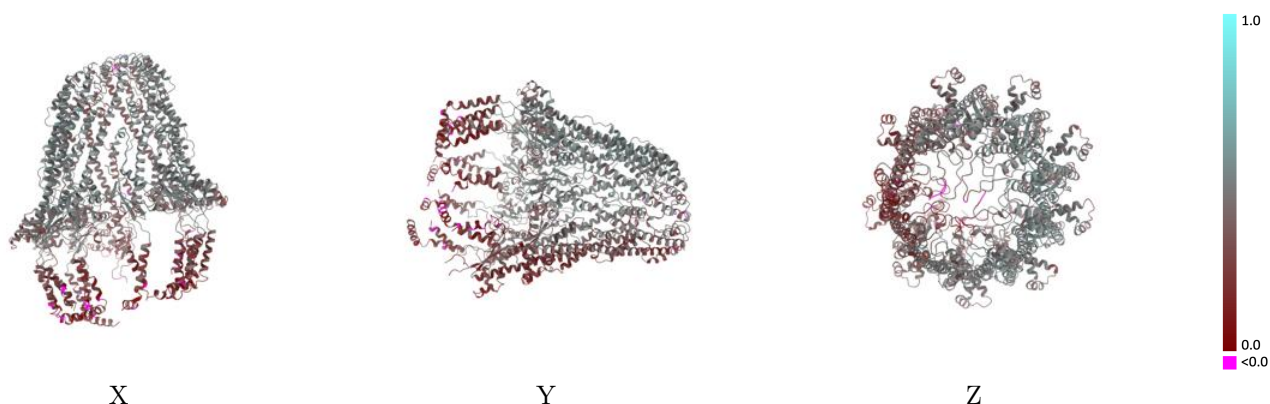
Y



Z

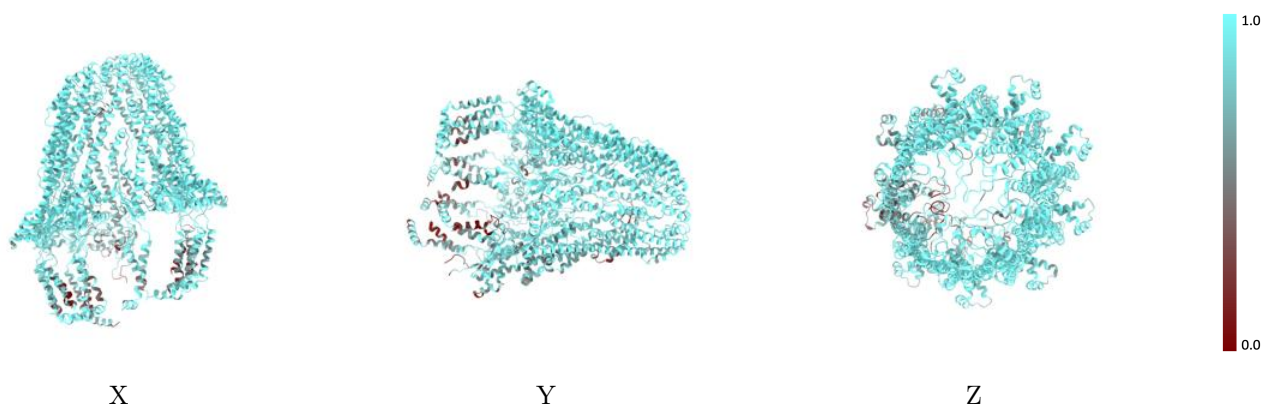
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



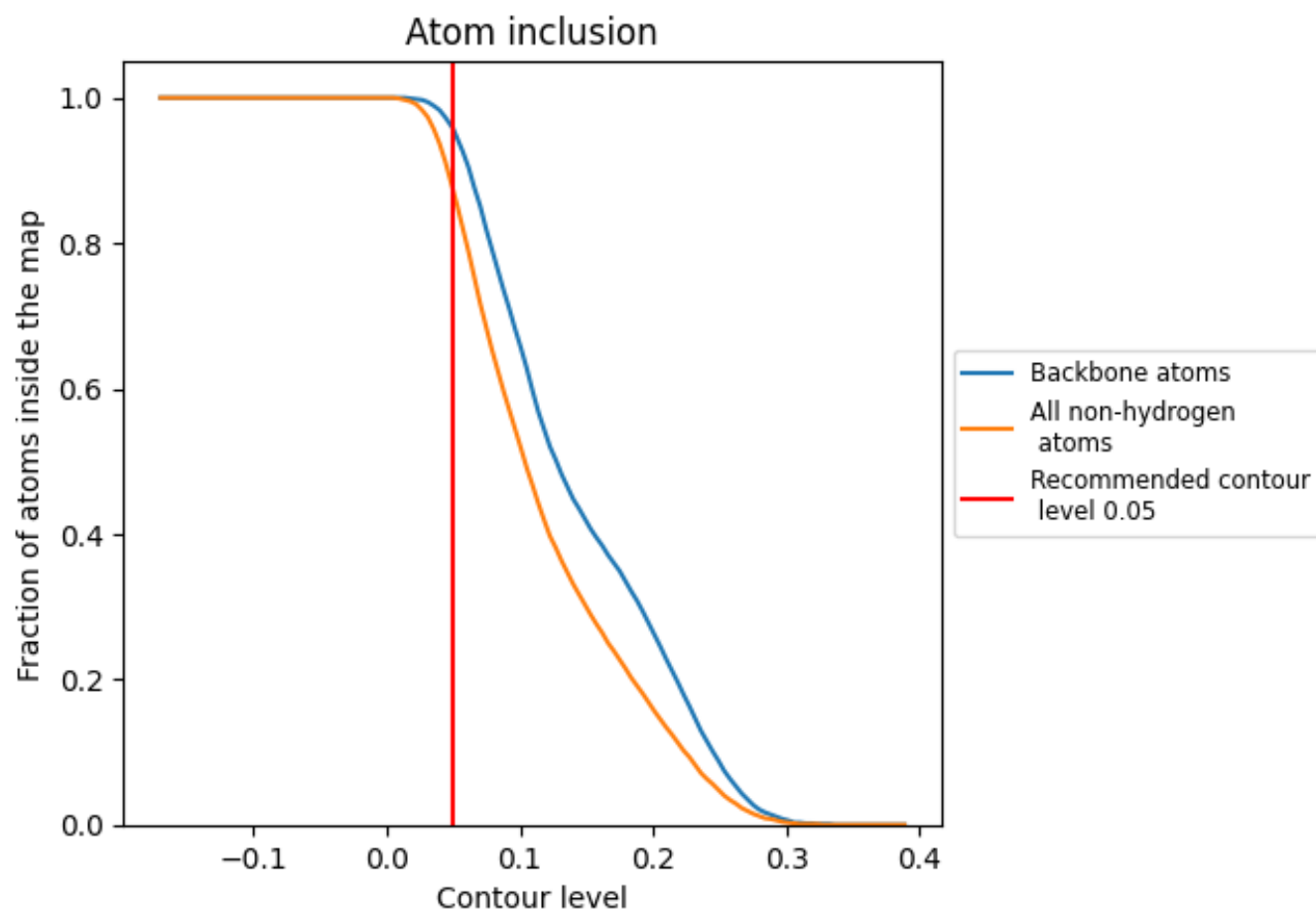
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8720	<div></div> 0.3960
A	<div></div> 0.8070	<div></div> 0.3180
B	<div></div> 0.9040	<div></div> 0.4150
C	<div></div> 0.9200	<div></div> 0.4410
D	<div></div> 0.9270	<div></div> 0.4500
E	<div></div> 0.9200	<div></div> 0.4470
F	<div></div> 0.9130	<div></div> 0.4360
G	<div></div> 0.9020	<div></div> 0.4200
H	<div></div> 0.8600	<div></div> 0.3700
I	<div></div> 0.6670	<div></div> 0.2400

1.0

0.0

<0.0