



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 01:10 AM UTC

PDB ID : 9FMV / pdb_00009fmv
EMDB ID : EMD-50571
Title : Cryo-EM structure of the c-di-GMP-free synthase:pEtN transferase complex (BcsA-Bct-G3) from the E. coli cellulose secretion macrocomplex
Authors : Anso, I.; Krasteva, P.V.
Deposited on : 2024-06-07
Resolution : 3.43 Å(reported)
Based on initial model : .

This is a wwPDB EM Validation Summary 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:

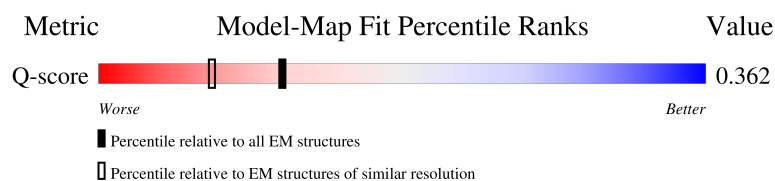
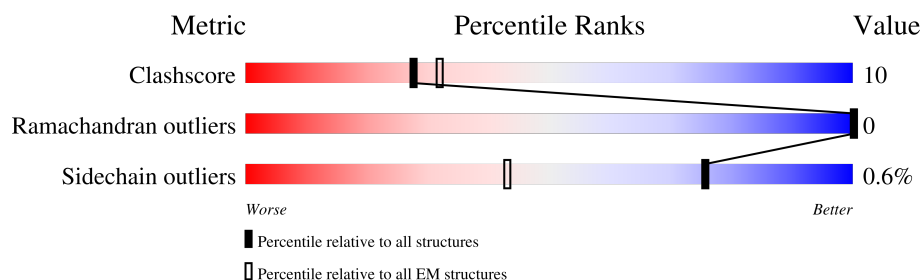
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.43 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	13927 (2.93 - 3.93)

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	908	
2	B	536	
2	C	536	
2	D	536	

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Mol	Chain	Length	Quality of chain
3	E	754	5% • 94%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10272 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 Cellulose synthase catalytic subunit [UDP-forming].

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	777	Total	C	N	O	S	0	0
			6272	4099	1093	1046	34		

- Molecule 2 is a protein called Cellulose biosynthesis protein BcsG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1205	829	192	181	3		
2	C	144	Total	C	N	O	S	0	0
			1205	829	192	181	3		
2	D	144	Total	C	N	O	S	0	0
			1205	829	192	181	3		

- Molecule 3 is a protein called Cyclic di-GMP-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	45	Total	C	N	O	0	0
			385	262	71	52		

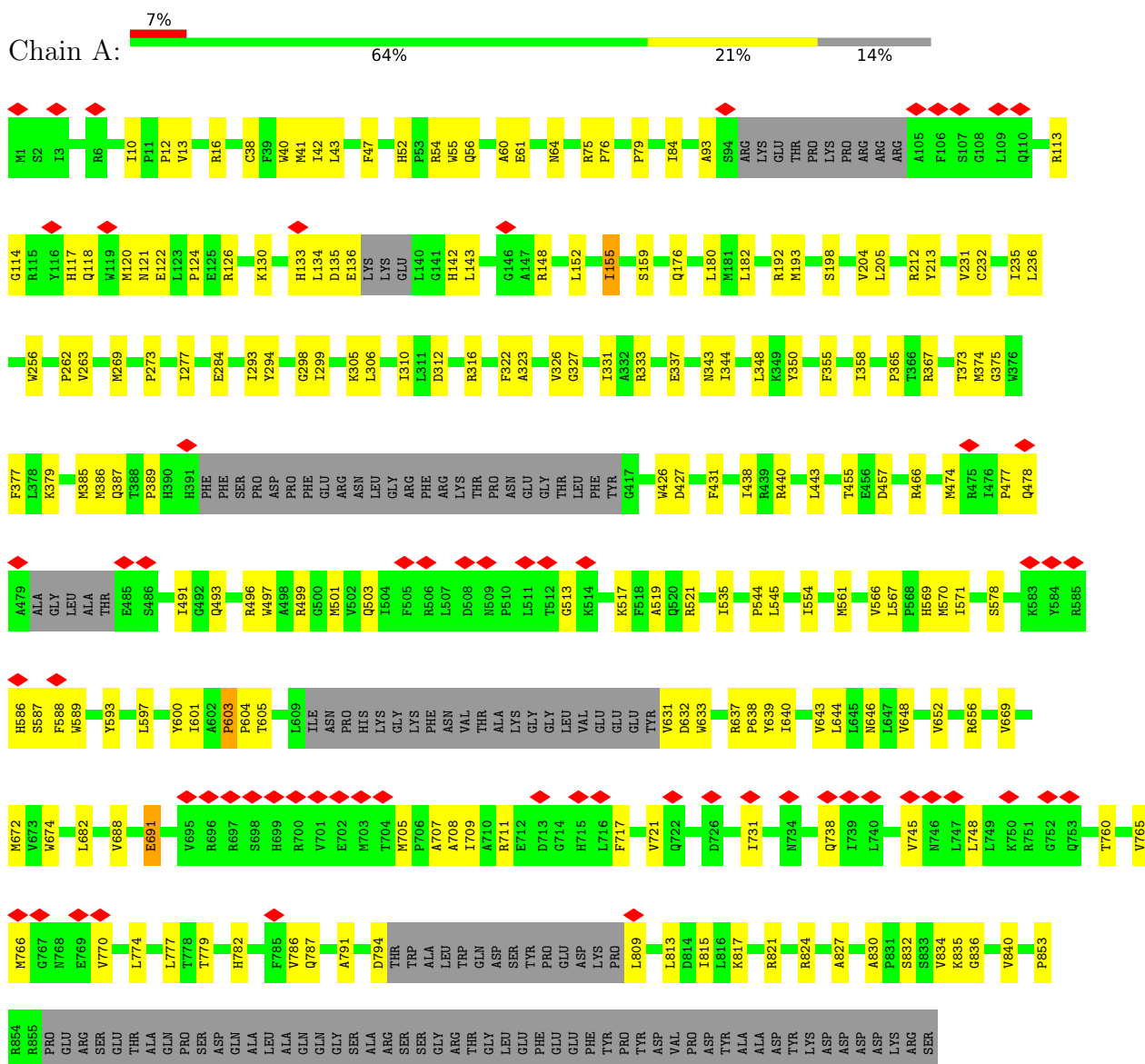
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-147	ALA	THR	conflict	UNP A0A193LYZ8
E	-101	ILE	VAL	conflict	UNP A0A193LYZ8
E	-53	ARG	GLN	conflict	UNP A0A193LYZ8
E	51	ILE	VAL	conflict	UNP A0A193LYZ8

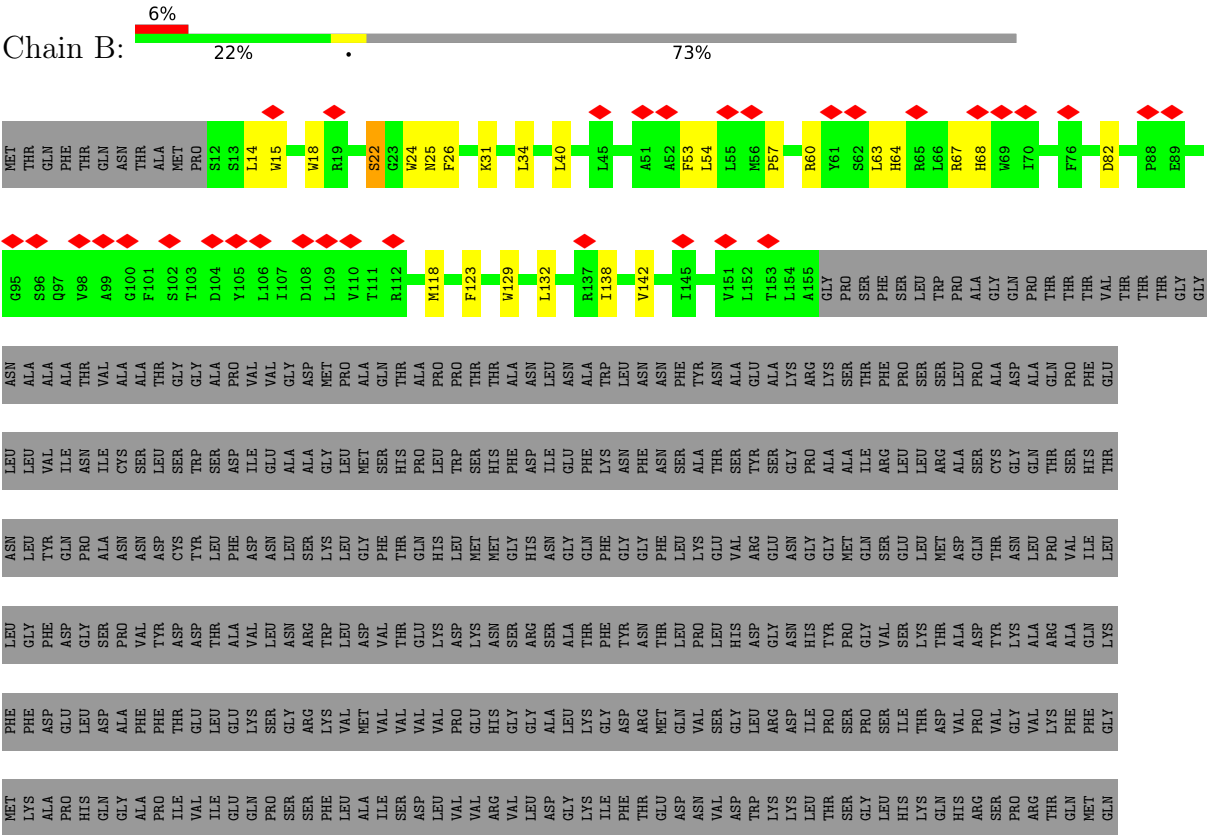
3 Residue-property plots

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.

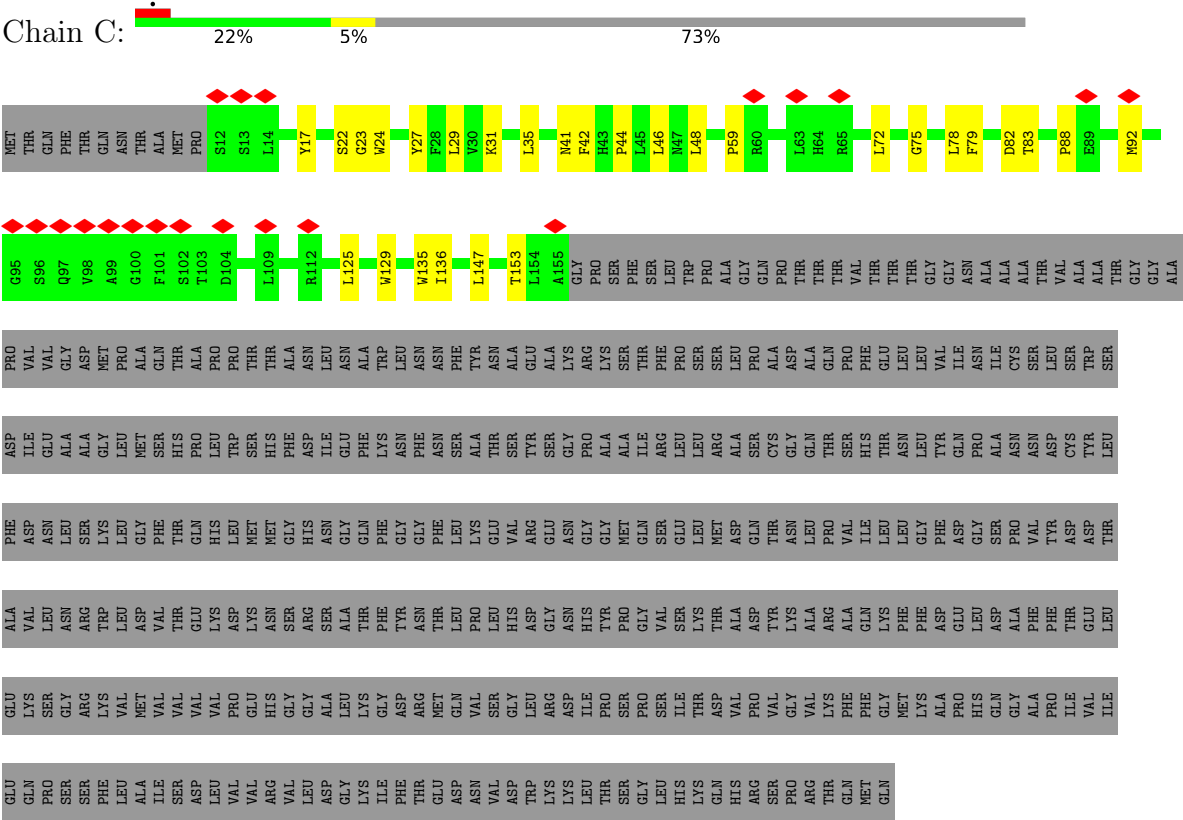
- Molecule 1: Cellulose synthase catalytic subunit [UDP-forming]



- Molecule 2: Cellulose biosynthesis protein BcsG



• Molecule 2: Cellulose biosynthesis protein BcsG



Chain D: 21% 6% 73%



R66	ARG	SER	THR	VAL
R67	GLY	TRP	LEU	GLN
R68	TYR	VAL	LEU	ASN
L69	GLU	LYS	ASN	HIS
M70	MET	THR	THR	VAL
PRO	LEU	PRO	VAL	VAL
ASN	MET	MET	GLY	ILE
ASN	ARG	ARG	PHE	GLY
ASN	ALA	GLN	ILE	ASP
GLU	VAL	THR	GLY	ASP
	ASN	PRO	ALA	SER
	ASP	PHE	GLN	THR
	SER	PRO	THR	ILE
	GLY	GLY	PHE	ILE
	LYS	ILE	GLY	PHE
	ARG	VAL	PRO	SER
	ALA	PRO	ALA	LYS
	THR	ASP	ILE	TYR
	MET	GLU	ASN	TYR
	PHE	SER	LEU	HIS
	GLY	ASP	THR	PHE
	SER	ARG	VAL	ILE
	VAL	ALA	THR	PRO
	ALA	ALA	ASP	MET
	VAL	GLU	ASP	PRO
	ILE	THR	GLY	LEU
	ARG	ARG	SER	ALA
	GLU	SER	THR	GLY
	SER	THR	ILE	ALA
	GLY	LEU	GLN	ALA
	ILE	THR	GLY	ASN
	ASN	SER	LYS	GLY
	SER	SER	ALA	ALA
	LEU	GLY	ASP	PHE
	ARG	ALA	ILE	PRO
	VAL	GLY	ILE	GLY
	TYR	ILE	GLY	ALA
	VAL	VAL	ILE	ASP
	VAL	VAL	ILE	GLN
	TYR	ILE	GLY	THR
	VAL	PHE	ILE	ILE
	GLY	GLN	PRO	THR
	HIS	SER	ASP	VAL
	LEU	PRO	LYS	VAL
P26	TYR	TYR	LEU	THR
	ASN	ASN	LYS	ILE
I40	ASP	ASP	ASP	THR
	GLN	GLN	ASP	VAL
V50	ARG	GLN	LYS	VAL
I51	SER	ARG	GLN	PRO
L52	VAL	VAL	ILE	LYS
L53	ILE	ILE	ASP	ALA
	ALA	ALA	LEU	PRO
V66	LEU	LEU	LEU	ASN
	LEU	LEU	VAL	GLY
L61	ALA	ALA	GLN	ALA
R62	ASP	ASP	ALA	GLN
I63	SER	SER	THR	GLN
	PRO	PRO	THR	CTR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	314979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; cryoSPARC V.4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.35	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.059	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	419.5, 419.5, 419.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.839, 0.839, 0.839	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	0.17	0/6444	0.38	1/8760 (0.0%)
2	B	0.12	0/1254	0.29	1/1720 (0.1%)
2	C	0.15	0/1254	0.27	0/1720
2	D	0.14	0/1254	0.35	1/1720 (0.1%)
3	E	0.17	0/397	0.35	0/543
All	All	0.16	0/10603	0.35	3/14463 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	603	PRO	N-CA-C	6.47	118.59	110.70
2	D	22	SER	CB-CA-C	-5.13	110.25	117.23
2	B	22	SER	CB-CA-C	-5.01	110.41	117.23

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	6272	0	6377	147	0
2	B	1205	0	1212	15	0
2	C	1205	0	1212	20	0
2	D	1205	0	1212	19	0
3	E	385	0	418	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10272	0	10431	200	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 10.

The worst 5 of 200 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:600:TYR:HH	1:A:631:VAL:N	1.64	0.93
1:A:603:PRO:HD2	1:A:604:PRO:CD	2.11	0.80
1:A:832:SER:HA	1:A:835:LYS:HB2	1.65	0.77
1:A:93:ALA:HA	2:D:137:ARG:HG2	1.67	0.75
2:D:56:MET:O	2:D:67:ARG:NH1	2.20	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	763/908 (84%)	738 (97%)	25 (3%)	0	100	100
2	B	142/536 (26%)	138 (97%)	4 (3%)	0	100	100
2	C	142/536 (26%)	138 (97%)	4 (3%)	0	100	100
2	D	142/536 (26%)	135 (95%)	7 (5%)	0	100	100
3	E	43/754 (6%)	43 (100%)	0	0	100	100
All	All	1232/3270 (38%)	1192 (97%)	40 (3%)	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	671/783 (86%)	668 (100%)	3 (0%)	84	82
2	B	125/453 (28%)	125 (100%)	0	100	100
2	C	125/453 (28%)	125 (100%)	0	100	100
2	D	125/453 (28%)	122 (98%)	3 (2%)	43	64
3	E	39/649 (6%)	39 (100%)	0	100	100
All	All	1085/2791 (39%)	1079 (99%)	6 (1%)	76	80

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	70	ILE
2	D	92	MET
2	D	147	LEU
1	A	569	HIS
1	A	155	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	68	HIS
2	B	150	ASN
1	A	371	GLN
1	A	390	HIS
1	A	478	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

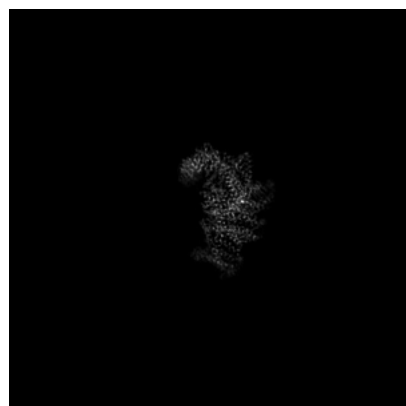
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50571. These allow visual inspection of the internal detail of the map and identification of artifacts.

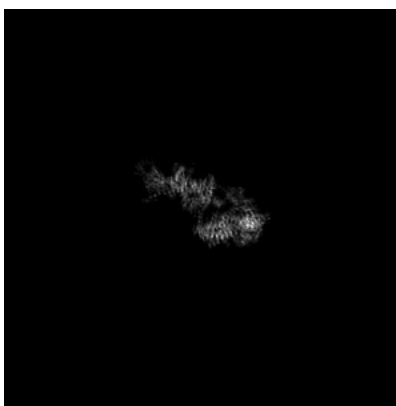
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

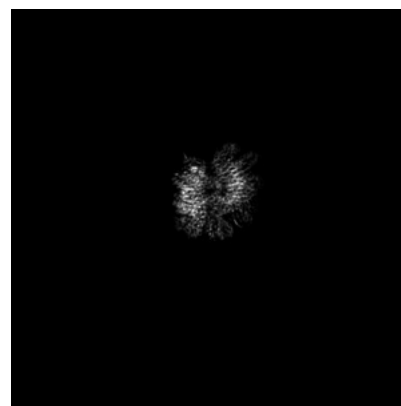
6.1.1 Primary map



X

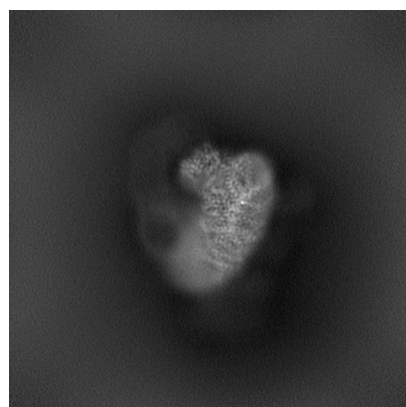


Y

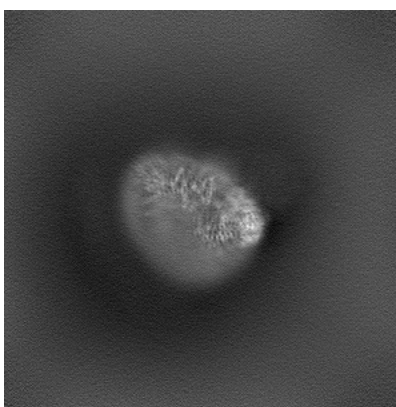


Z

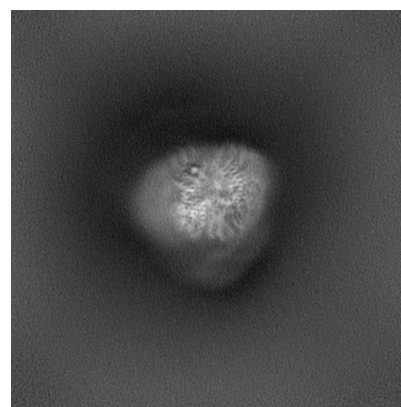
6.1.2 Raw map



X



Y

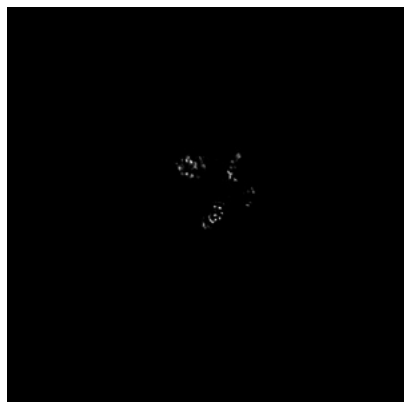


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 250



Y Index: 250

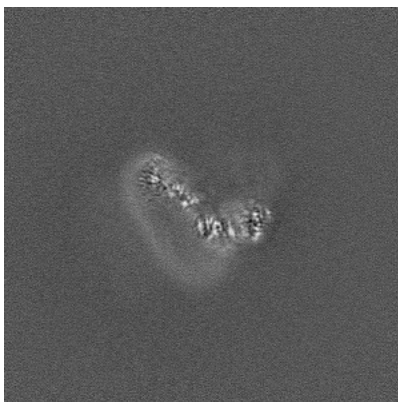


Z Index: 250

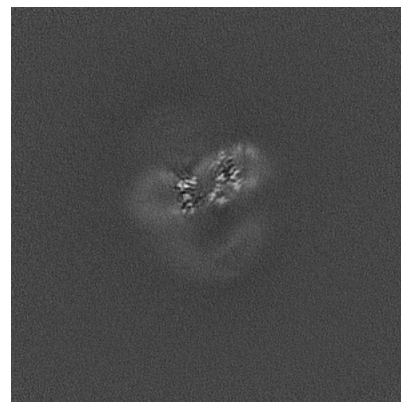
6.2.2 Raw map



X Index: 250



Y Index: 250

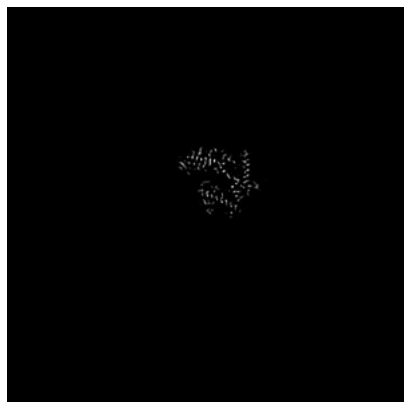


Z Index: 250

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: 229

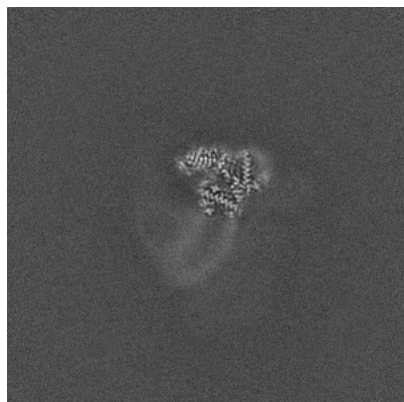


Y Index: 280

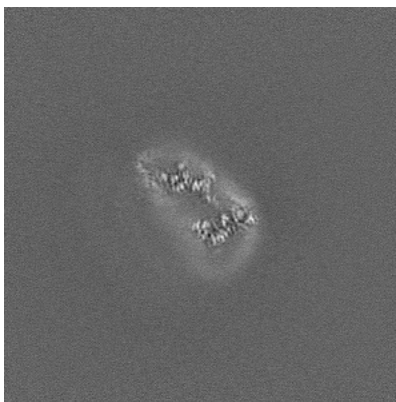


Z Index: 258

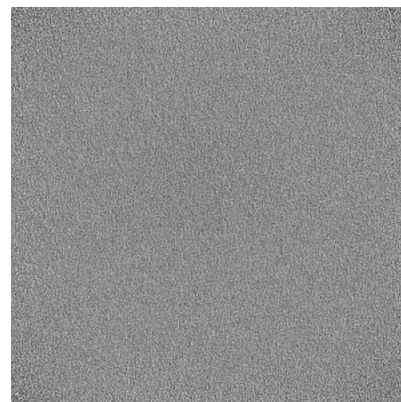
6.3.2 Raw map



X Index: 228



Y Index: 280

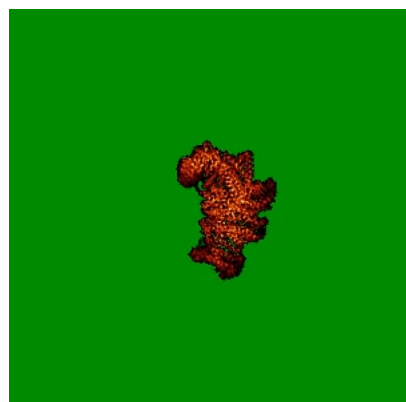


Z Index: 499

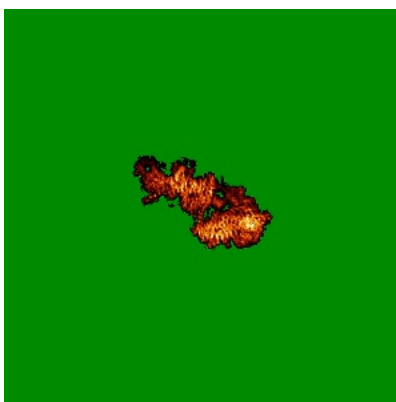
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

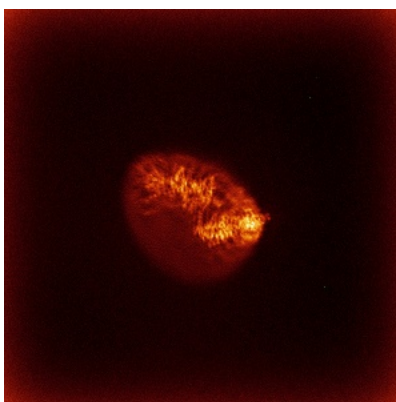


Z

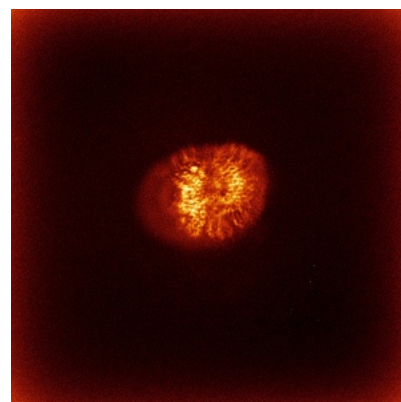
6.4.2 Raw map



X



Y

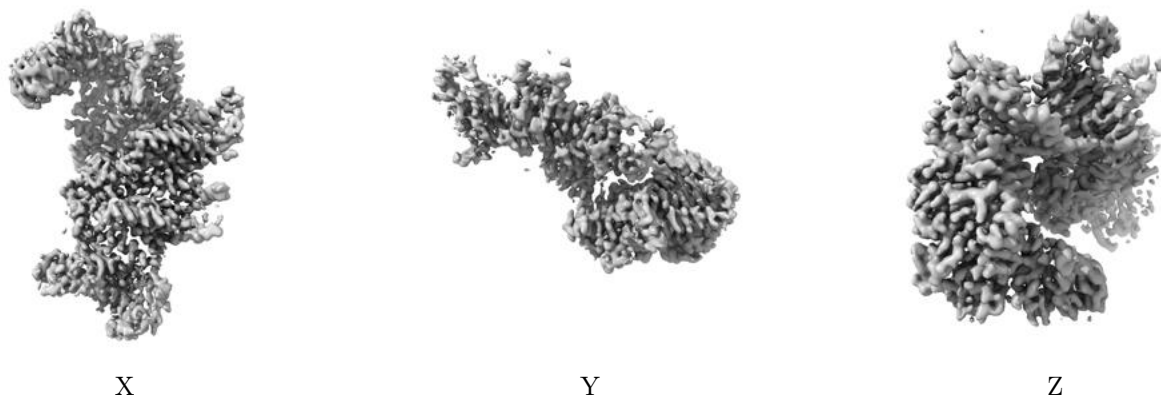


Z

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.

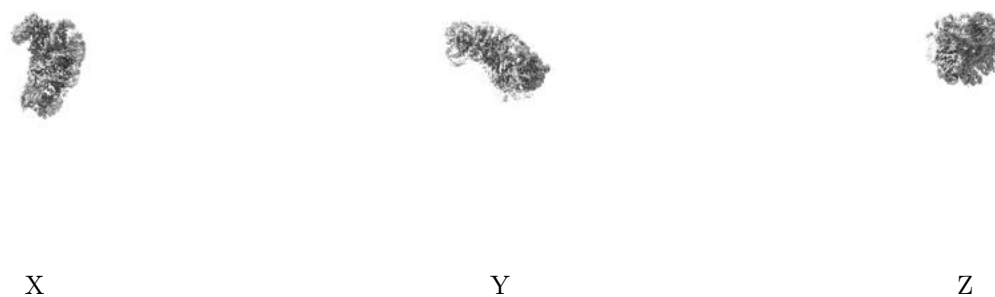
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. 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.

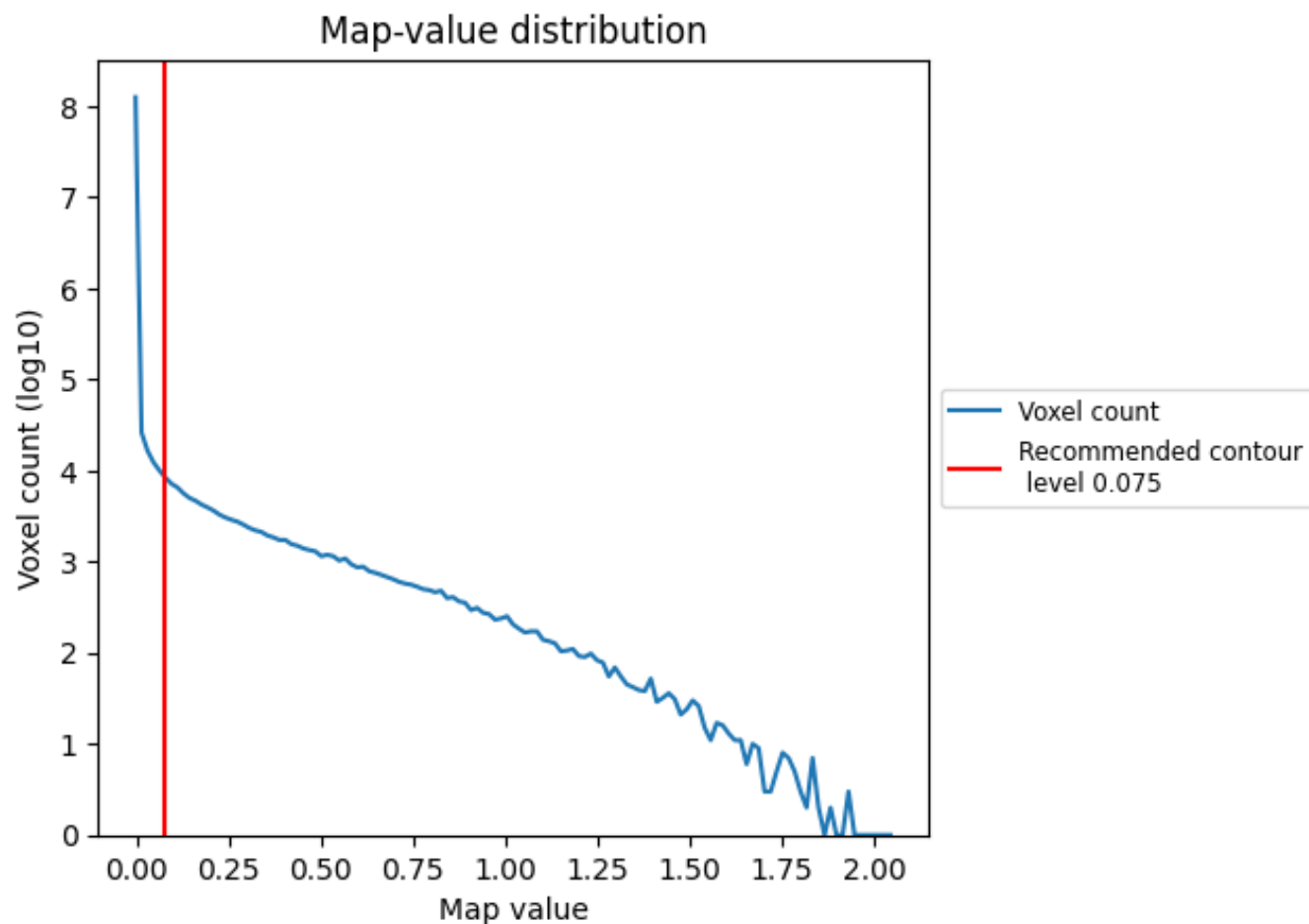
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

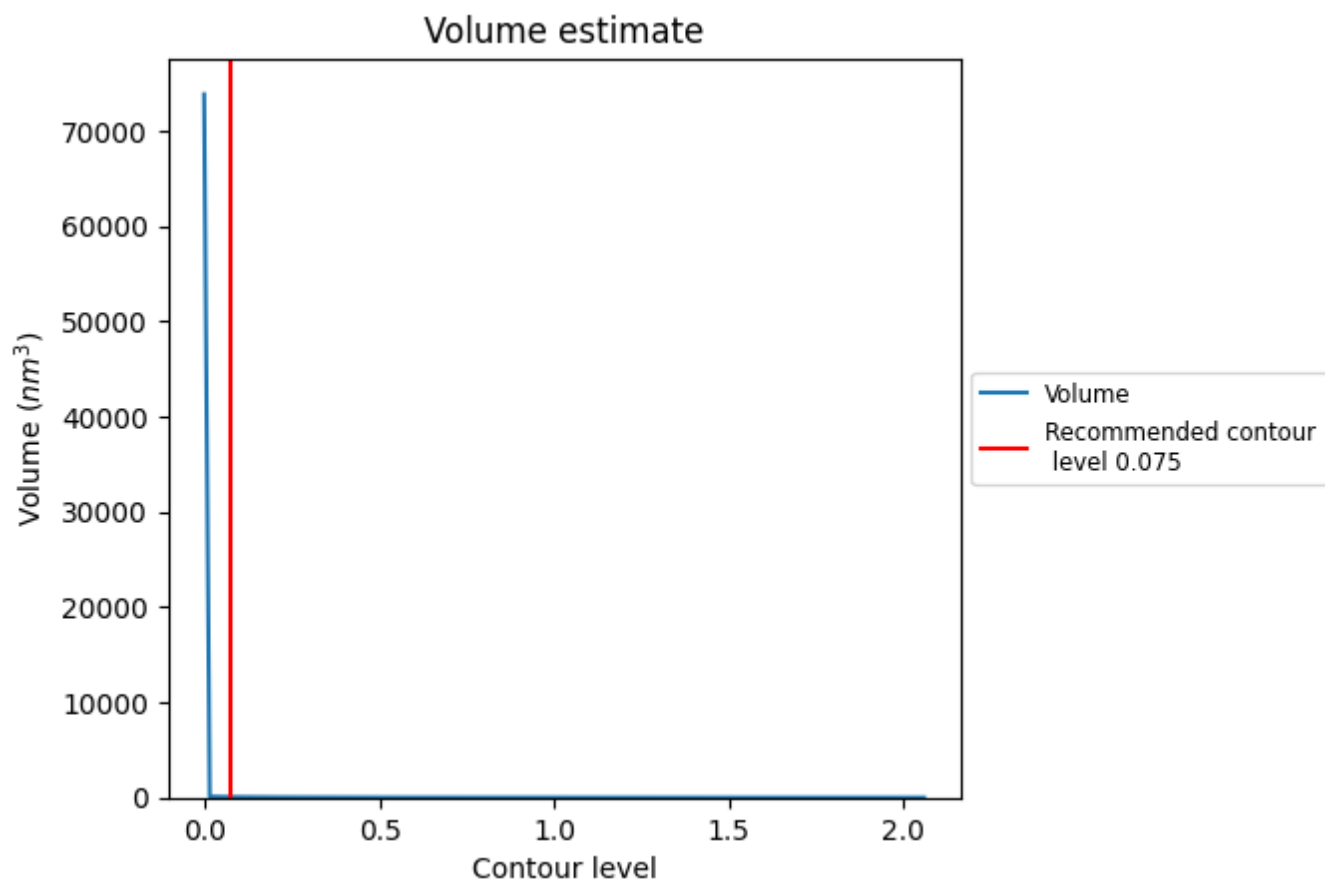
This section contains the results of statistical analysis of the map.

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.

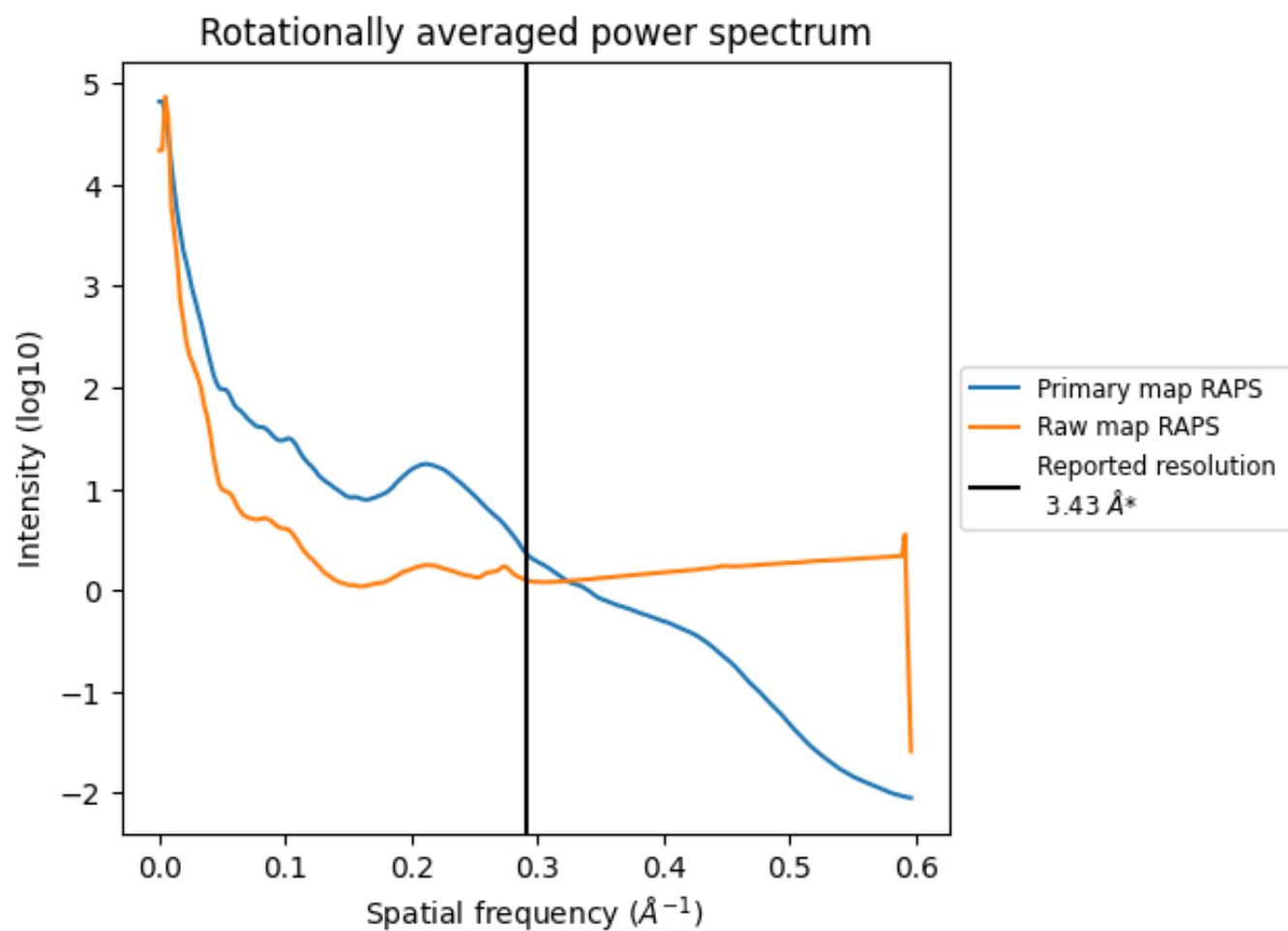
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm^3 ; this corresponds to an approximate mass of 58 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 ⓘ

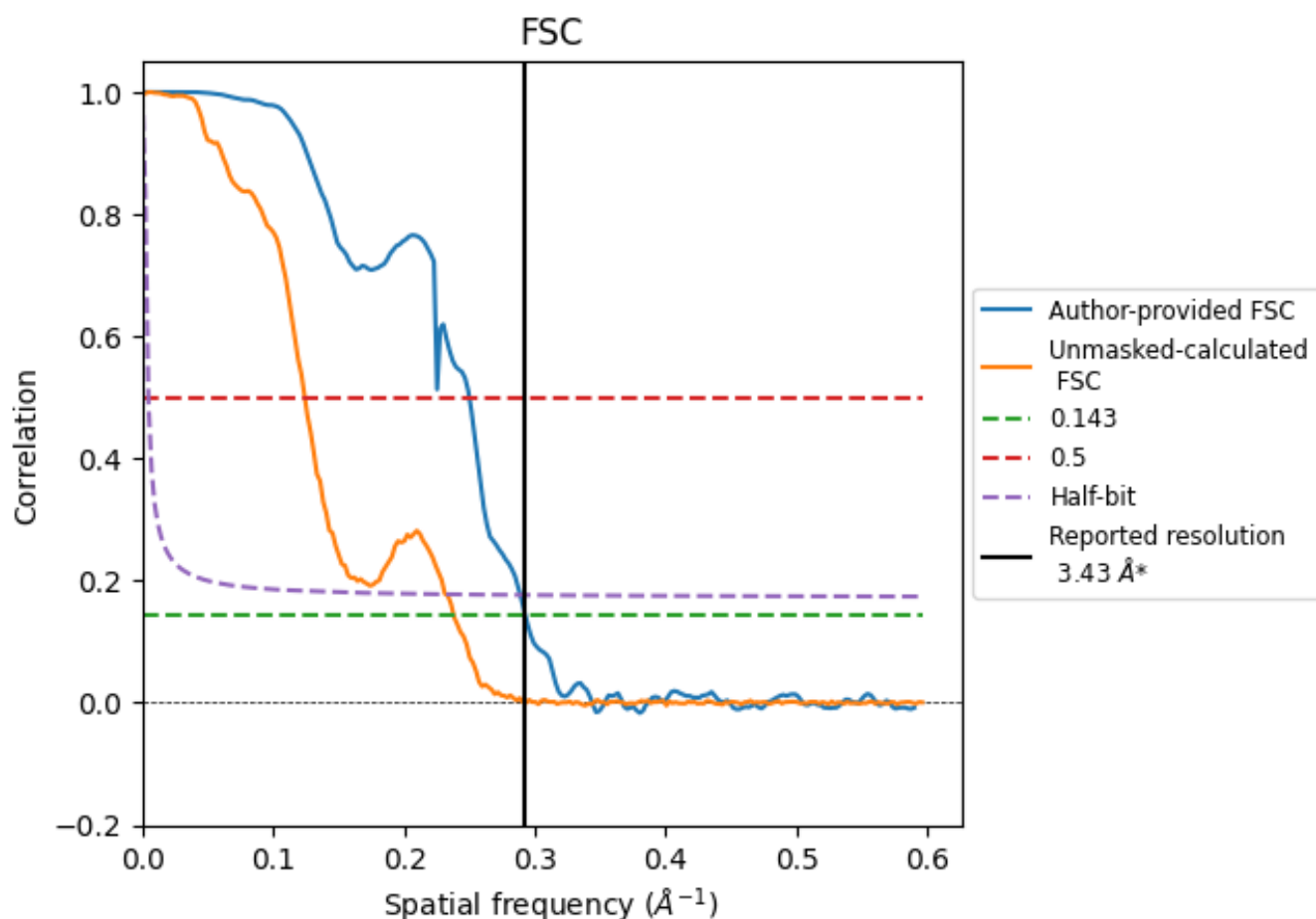


*Reported resolution corresponds to spatial frequency of $0.292 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

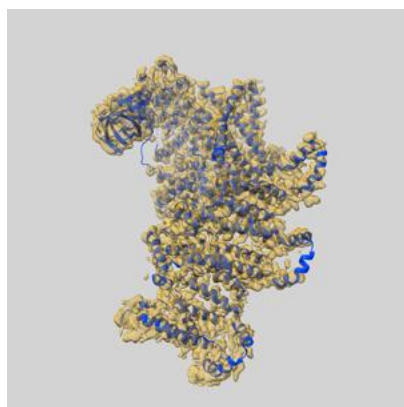
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	3.42	4.00	3.46
Unmasked-calculated*	4.20	8.05	4.31

*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 4.20 differs from the reported value 3.43 by more than 10 %

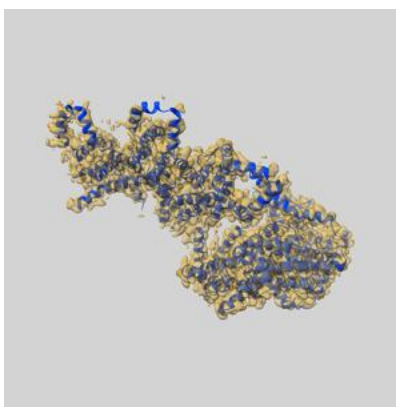
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50571 and PDB model 9FMV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

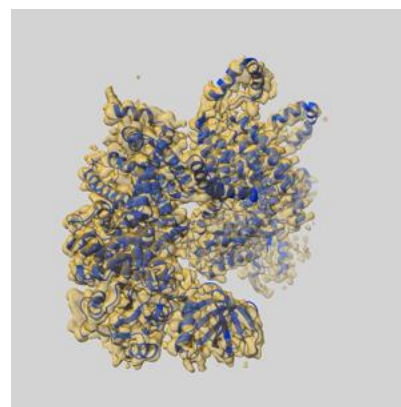
9.1 Map-model overlay [i](#)



X



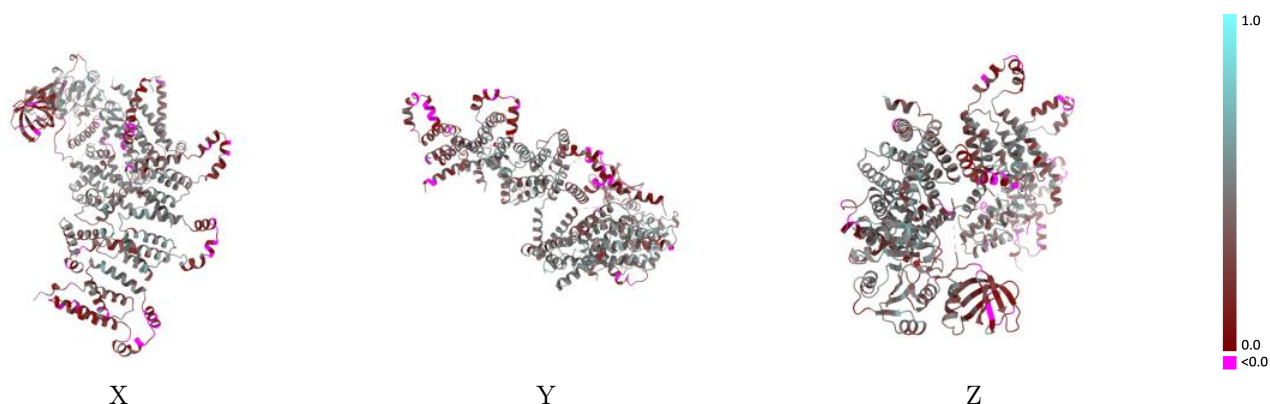
Y



Z

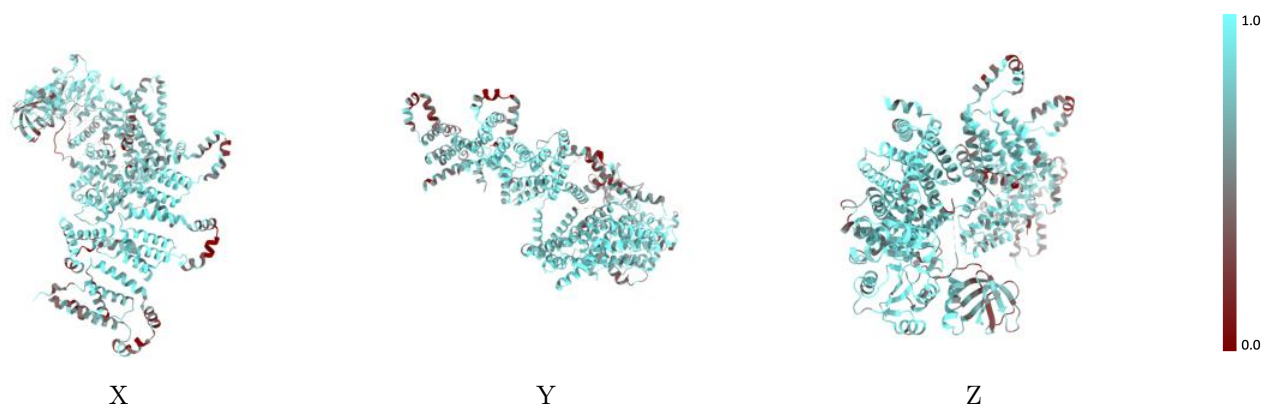
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



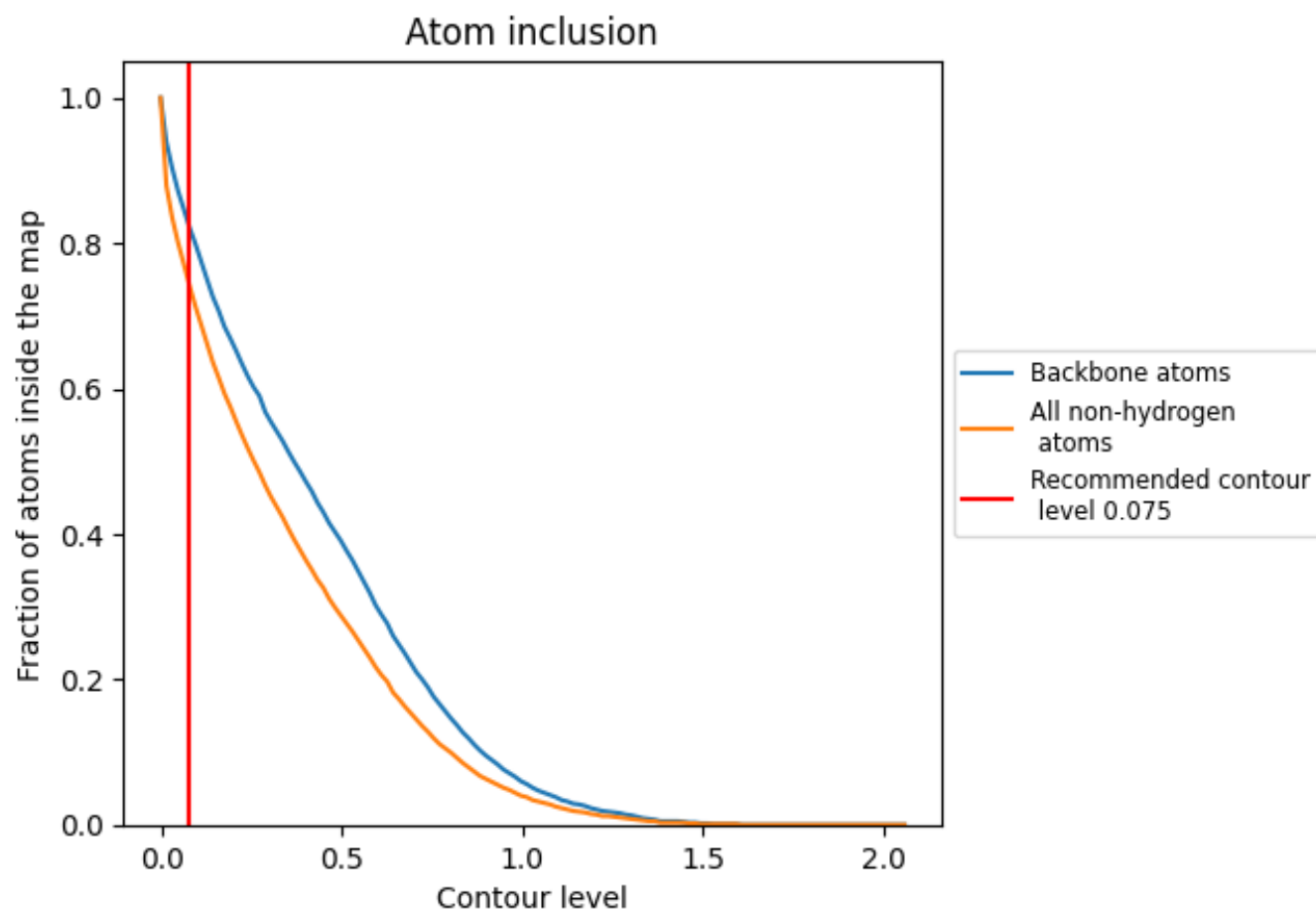
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.3620
A	0.7630	0.3800
B	0.6210	0.2330
C	0.7650	0.3790
D	0.7490	0.3600
E	0.8340	0.4220

