wwPDB EM Validation Summary Report

Nov 7, 2026 – 12:05 pm GMT

PDB ID	:	28KO / pdb_000028ko
EMDB ID	:	EMD-56579
Title	:	Cryo-EM structure of B. bacteriovorus Bd1152 2C mutant (I112C, L238C) residues 155-276
Authors	:	Ratkeviciute, G.; Cooper, B.F.; Gragera, M.; Knowles, T.J.
Deposited on	:	2026-02-04
Resolution	:	3.40 Å(reported)

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:

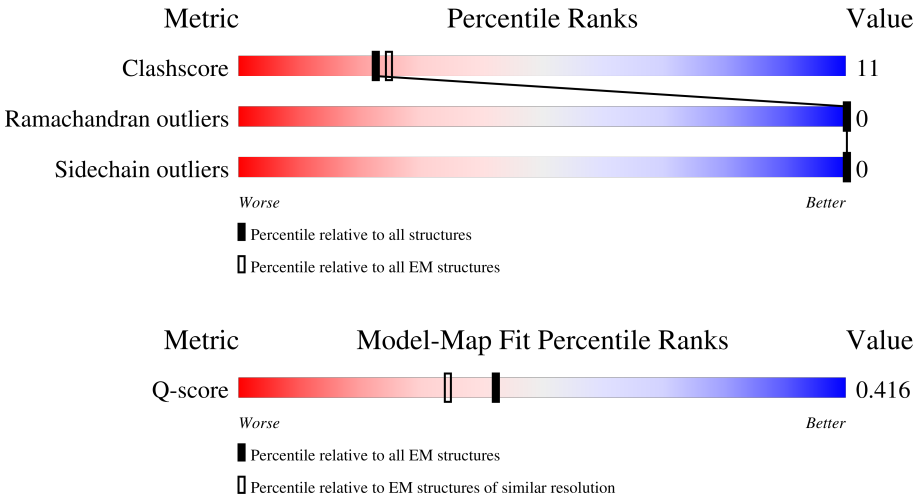
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



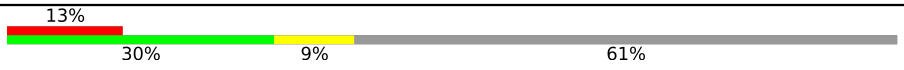
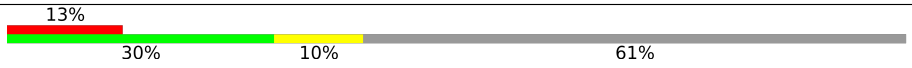
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 <=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	247	13% 28% 11% 61%
1	B	247	13% 29% 11% 61%
1	C	247	12% 29% 10% 61%
1	D	247	12% 29% 10% 61%

Continued on next page...

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Mol	Chain	Length	Quality of chain
1	E	247	
1	F	247	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4566 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 PqiB protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			761	480	136	144	1		
1	B	97	Total	C	N	O	S	0	0
			761	480	136	144	1		
1	C	97	Total	C	N	O	S	0	0
			761	480	136	144	1		
1	D	97	Total	C	N	O	S	0	0
			761	480	136	144	1		
1	E	97	Total	C	N	O	S	0	0
			761	480	136	144	1		
1	F	97	Total	C	N	O	S	0	0
			761	480	136	144	1		

There are 12 discrepancies between the modelled and reference sequences:

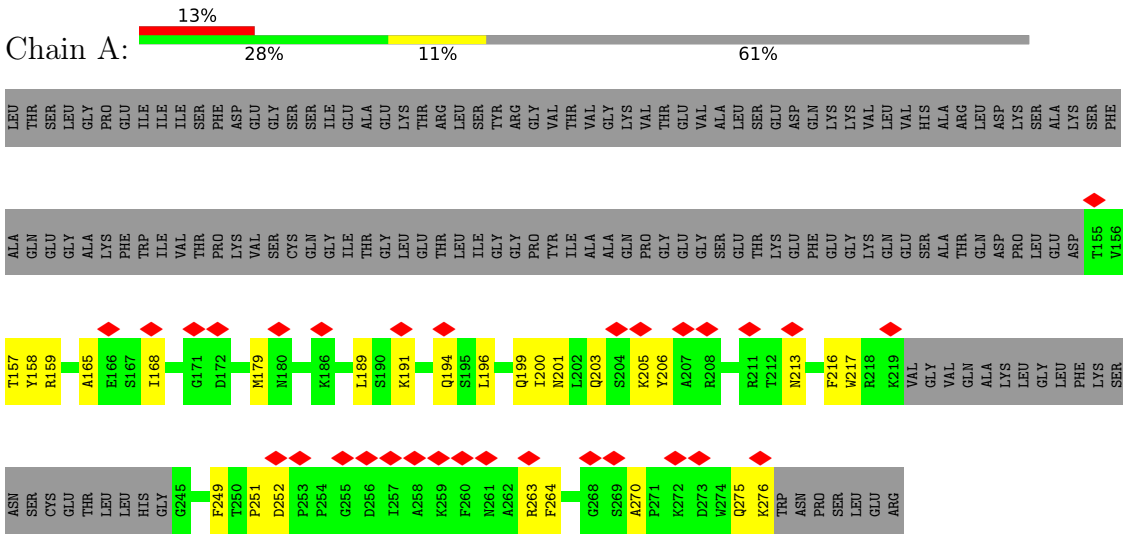
Chain	Residue	Modelled	Actual	Comment	Reference
A	112	CYS	ILE	engineered mutation	UNP Q6MNT4
A	238	CYS	LEU	engineered mutation	UNP Q6MNT4
B	112	CYS	ILE	engineered mutation	UNP Q6MNT4
B	238	CYS	LEU	engineered mutation	UNP Q6MNT4
C	112	CYS	ILE	engineered mutation	UNP Q6MNT4
C	238	CYS	LEU	engineered mutation	UNP Q6MNT4
D	112	CYS	ILE	engineered mutation	UNP Q6MNT4
D	238	CYS	LEU	engineered mutation	UNP Q6MNT4
E	112	CYS	ILE	engineered mutation	UNP Q6MNT4
E	238	CYS	LEU	engineered mutation	UNP Q6MNT4
F	112	CYS	ILE	engineered mutation	UNP Q6MNT4
F	238	CYS	LEU	engineered mutation	UNP Q6MNT4

3 Residue-property plots (i)

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.

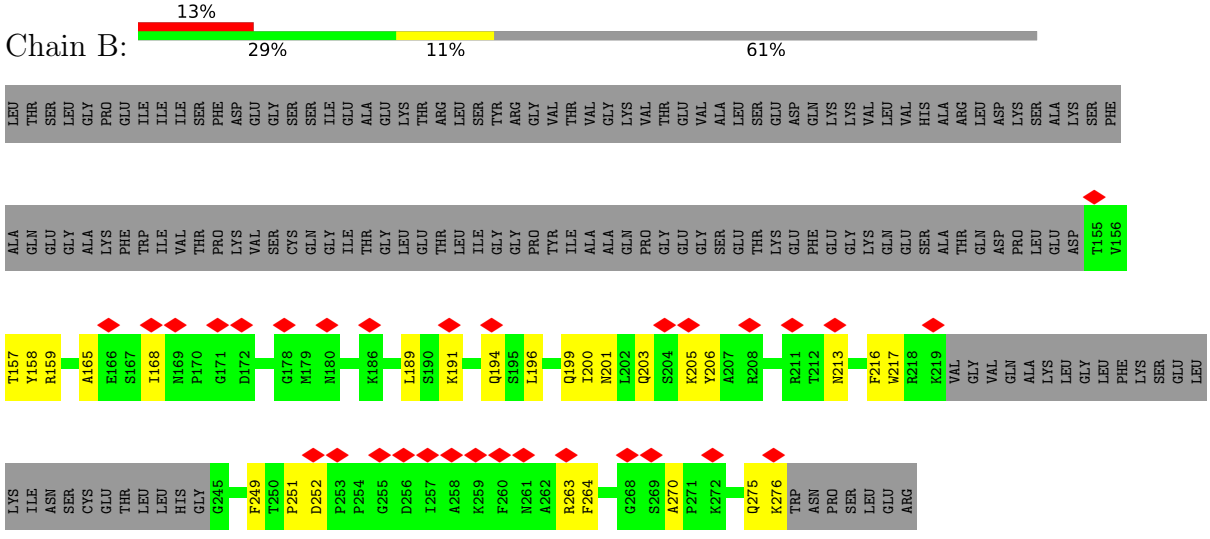
- Molecule 1: PqiB protein

Chain A:



- Molecule 1: PqiB protein

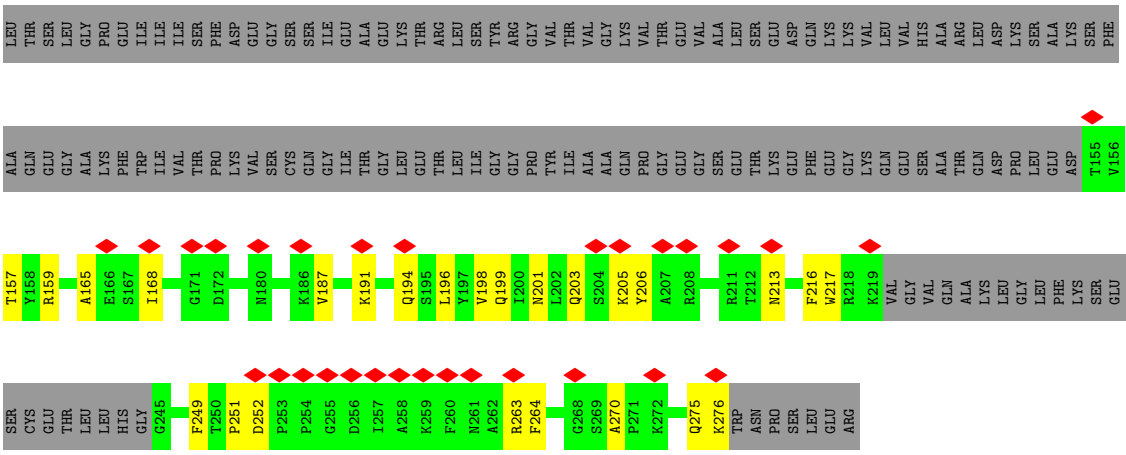
Chain B:



- Molecule 1: PqiB protein

Chain C:

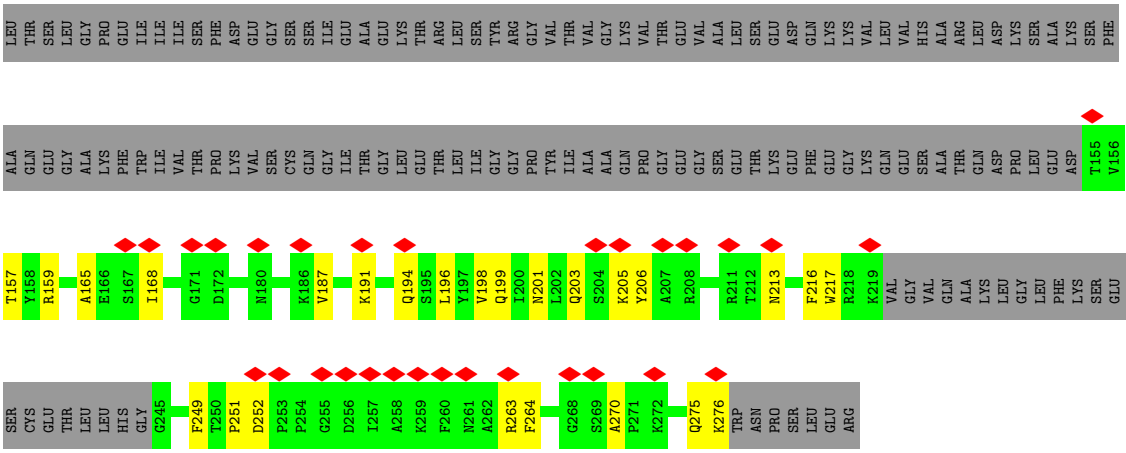




• Molecule 1: PqiB protein

Chain D:

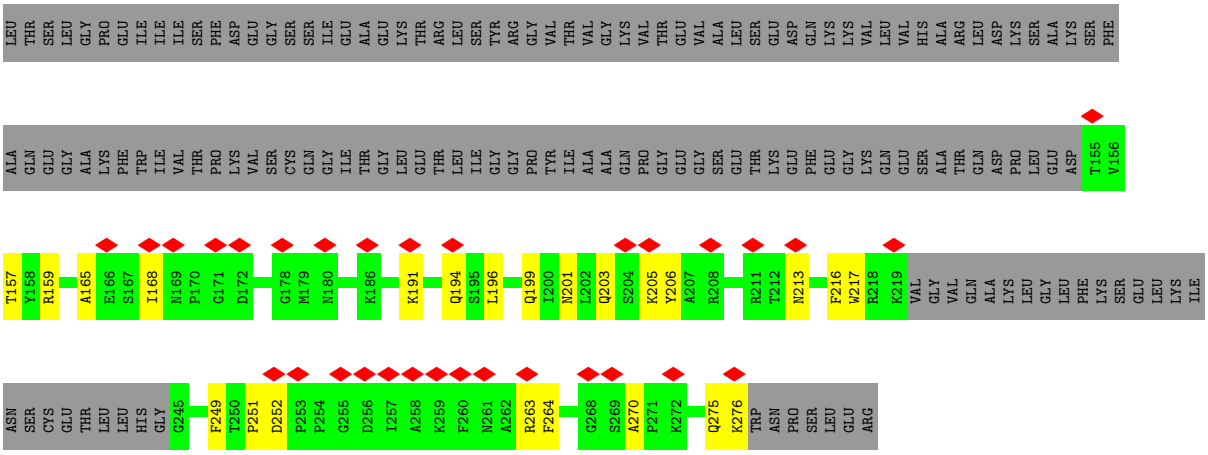




• Molecule 1: PqiB protein

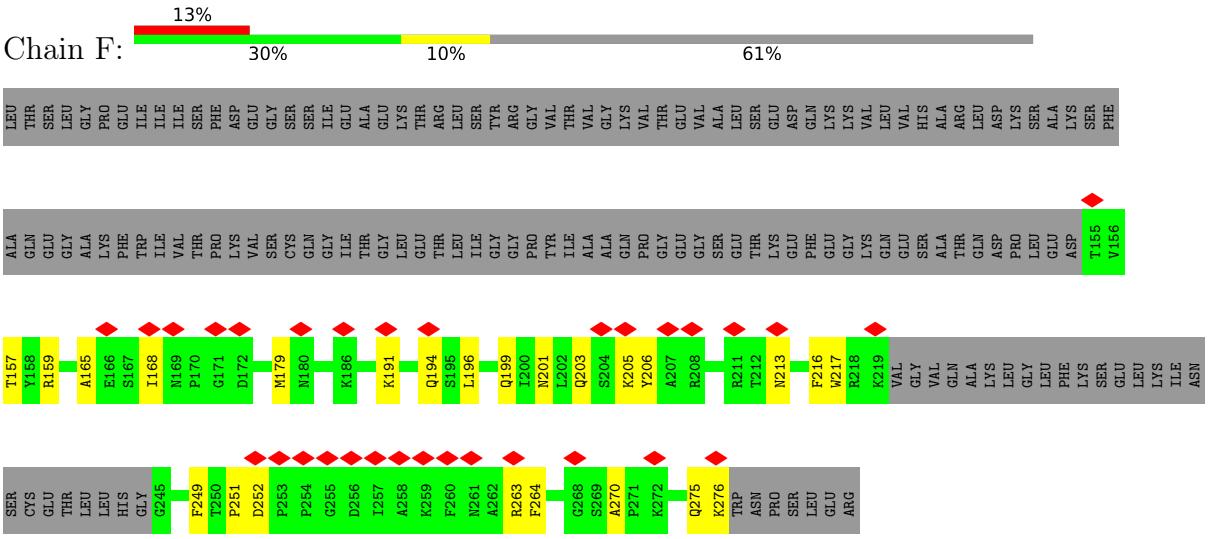
Chain E:





• Molecule 1: PqiB protein

Chain F:


13%
30%
10%
61%
LEU THR SER LEU GLY PRO GLU ILE ILE ILE SER PHE ASP GLU GLY SER SER ILE GLU ALA GLU LYS THR ARG LEU SER TYR ARG GLY VAL THR VAL GLY LYS VAL THR GLU VAL ALA LEU SER GLU ASP GLN LYS LYS VAL LEU VAL HIS ALA ARG LEU ASP LYS SER ALA LYS SER PHE
ALA GLN GLU GLY ALA LYS PHE TRP ILE VAL THR PRO LYS VAL SER CYS GLN GLY ILE THR GLY LEU GLU THR LEU ILE GLY GLY PRO TYR ILE ALA ALA GLN PRO GLY GLU GLY SER GLU THR LYS GLU PHE GLU GLY LYS GLN GLU SER ALA THR GLN ASP PRO LEU GLU ASP T155 V156
T157 Y158 R159 A165 E166 S167 I168 N169 P170 G171 D172 M179 N180 K186 K191 Q194 S195 L196 Q199 I200 N201 L202 Q203 S204 K205 Y206 A207 R208 R211 T212 N213 F216 W217 R218 K219 VAL GLY VAL GLN ALA LYS LEU GLY LEU PHE LYS SER GLU LEU LYS ILE ASN
SER CYS GLU THR LEU LEU HIS GLY G245 F249 T250 P251 D252 P253 P254 G255 D256 I257 A258 K259 F260 N261 A262 R263 F264 G268 S269 A270 P271 K272 Q275 K276 TRP ASN PRO SER LEU GLU ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	43319	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.368	Depositor
Minimum map value	-0.539	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.683	Depositor
Map size (Å)	300.6, 300.6, 300.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2525, 1.2525, 1.2525	Depositor

5 Model quality

5.1 Standard geometry

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	0.16	0/776	0.42	0/1051
1	B	0.16	0/776	0.42	0/1051
1	C	0.16	0/776	0.42	0/1051
1	D	0.16	0/776	0.42	0/1051
1	E	0.16	0/776	0.42	0/1051
1	F	0.16	0/776	0.42	0/1051
All	All	0.16	0/4656	0.42	0/6306

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

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	761	0	749	20	0
1	B	761	0	749	19	0
1	C	761	0	749	18	0
1	D	761	0	749	18	0
1	E	761	0	749	17	0
1	F	761	0	749	18	0
All	All	4566	0	4494	102	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 11.

The worst 5 of 102 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:194:GLN:HE22	1:F:276:LYS:HE2	1.65	0.61
1:E:276:LYS:HE2	1:F:194:GLN:HE22	1.66	0.61
1:D:276:LYS:HE2	1:E:194:GLN:HE22	1.66	0.60
1:B:276:LYS:HE2	1:C:194:GLN:HE22	1.66	0.60
1:C:276:LYS:HE2	1:D:194:GLN:HE22	1.66	0.60

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	93/247 (38%)	89 (96%)	4 (4%)	0	100	100
1	B	93/247 (38%)	89 (96%)	4 (4%)	0	100	100
1	C	93/247 (38%)	89 (96%)	4 (4%)	0	100	100
1	D	93/247 (38%)	89 (96%)	4 (4%)	0	100	100
1	E	93/247 (38%)	89 (96%)	4 (4%)	0	100	100
1	F	93/247 (38%)	89 (96%)	4 (4%)	0	100	100
All	All	558/1482 (38%)	534 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	83/210 (40%)	83 (100%)	0	100	100
1	B	83/210 (40%)	83 (100%)	0	100	100
1	C	83/210 (40%)	83 (100%)	0	100	100
1	D	83/210 (40%)	83 (100%)	0	100	100
1	E	83/210 (40%)	83 (100%)	0	100	100
1	F	83/210 (40%)	83 (100%)	0	100	100
All	All	498/1260 (40%)	498 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	194	GLN
1	E	203	GLN
1	F	194	GLN
1	B	203	GLN
1	C	194	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 (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56579. These allow visual inspection of the internal detail of the map and identification of artifacts.

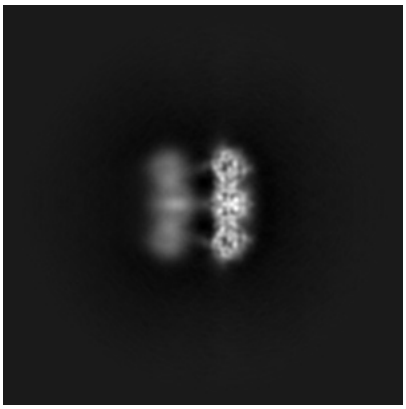
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

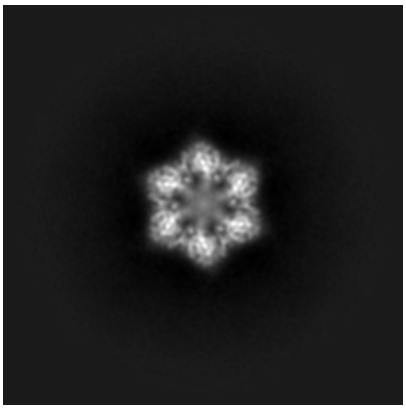
6.1.1 Primary map



X

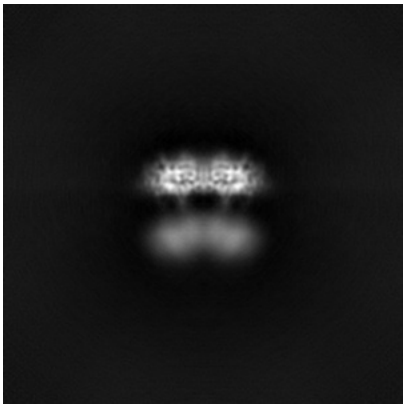


Y

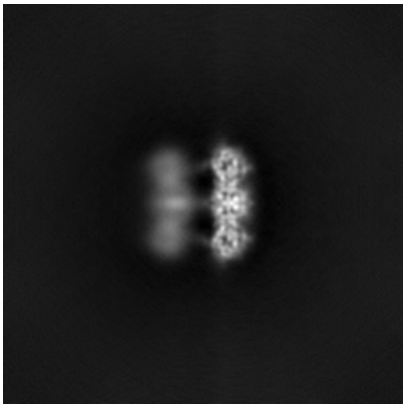


Z

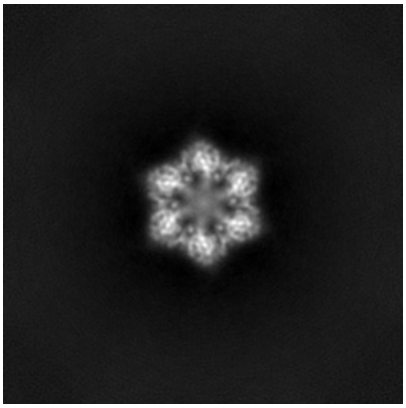
6.1.2 Raw map



X



Y

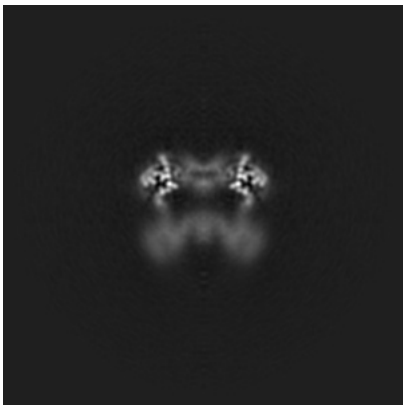


Z

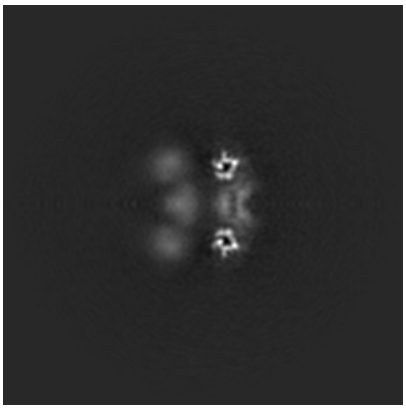
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

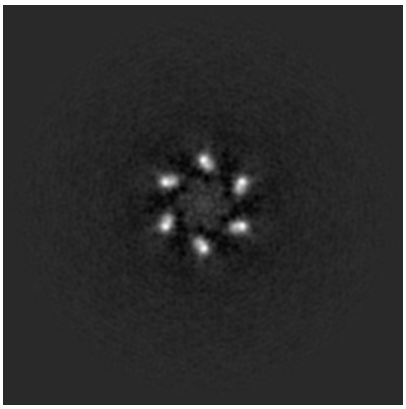
6.2.1 Primary map



X Index: 120

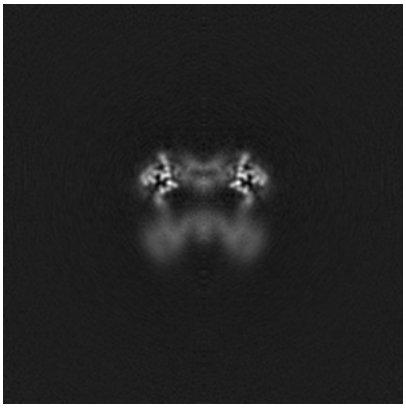


Y Index: 120

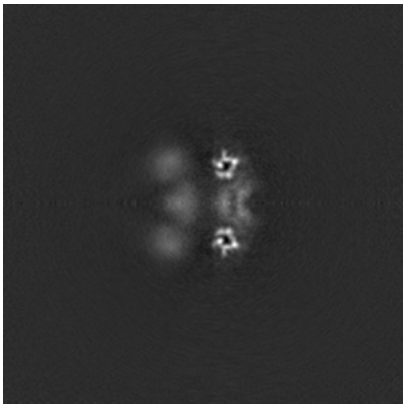


Z Index: 120

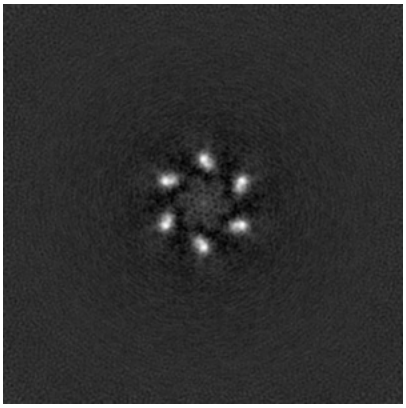
6.2.2 Raw map



X Index: 120



Y Index: 120

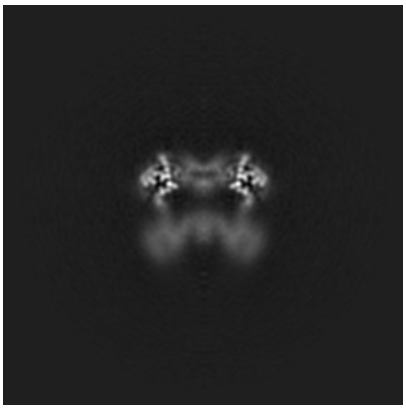


Z Index: 120

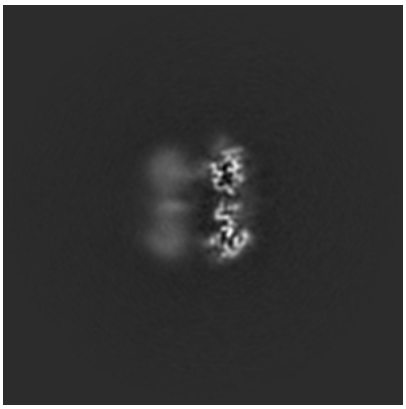
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

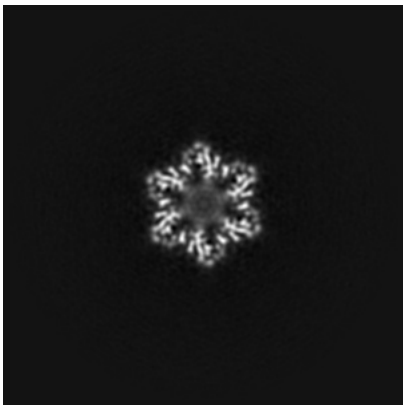
6.3.1 Primary map



X Index: 120

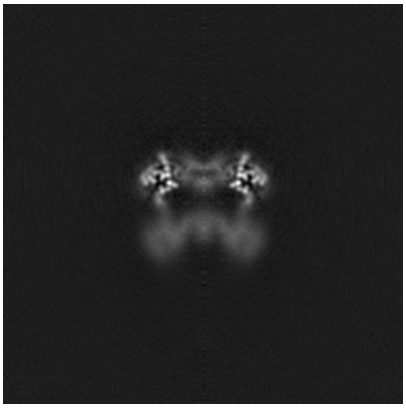


Y Index: 104

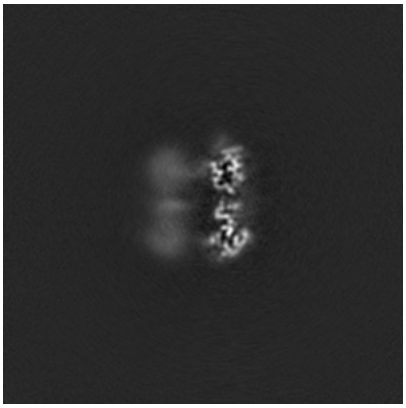


Z Index: 139

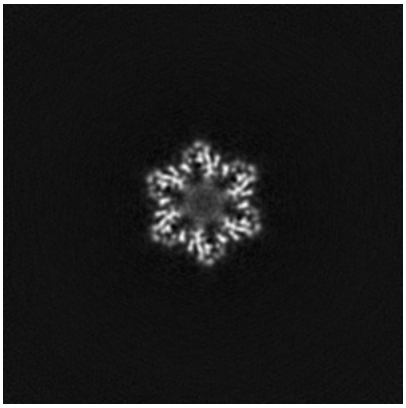
6.3.2 Raw map



X Index: 120



Y Index: 104

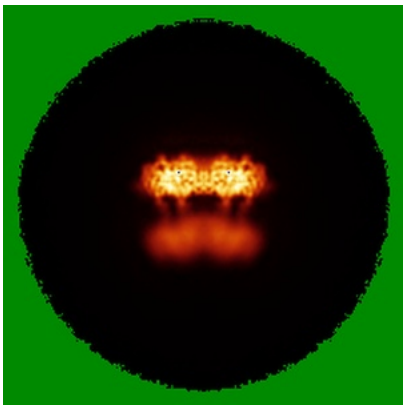


Z Index: 139

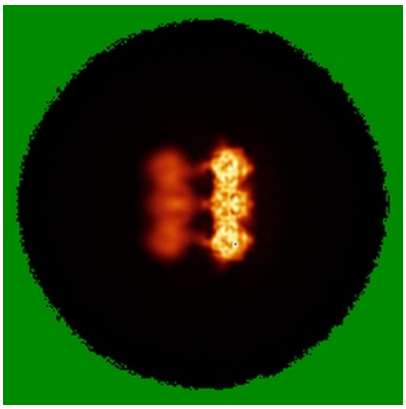
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

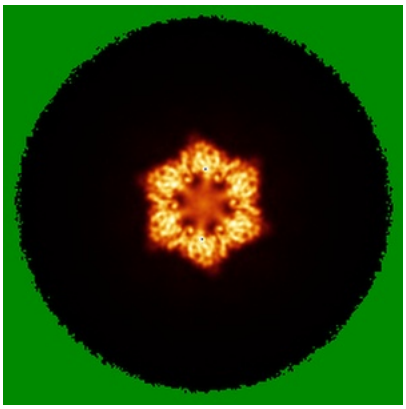
6.4.1 Primary map



X

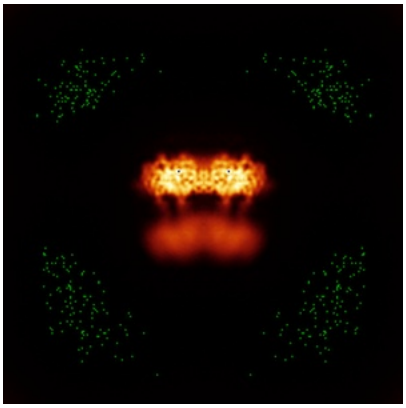


Y

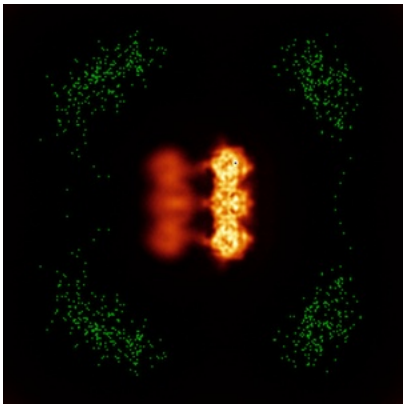


Z

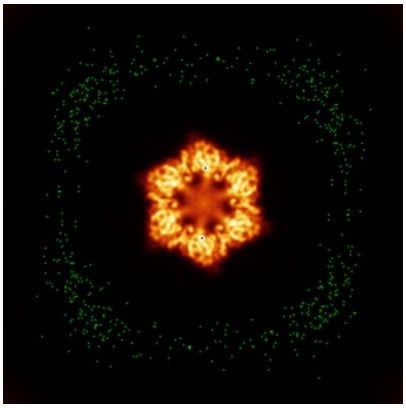
6.4.2 Raw map



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 0.683. 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.

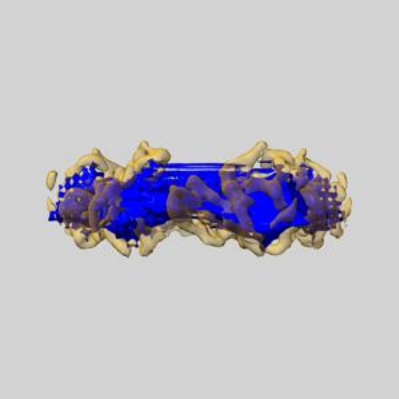
6.6 Mask visualisation

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

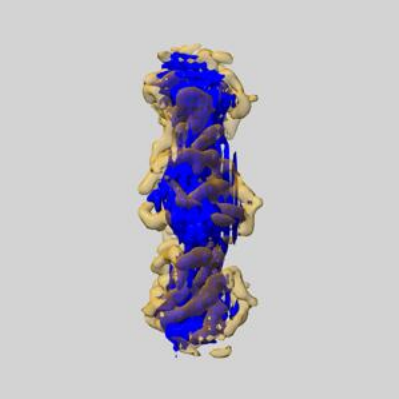
A mask typically either:

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

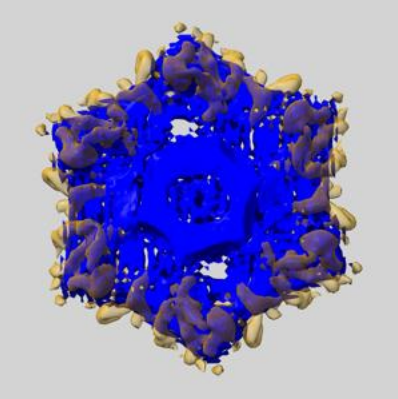
6.6.1 emd_56579_msk_1.map



X



Y

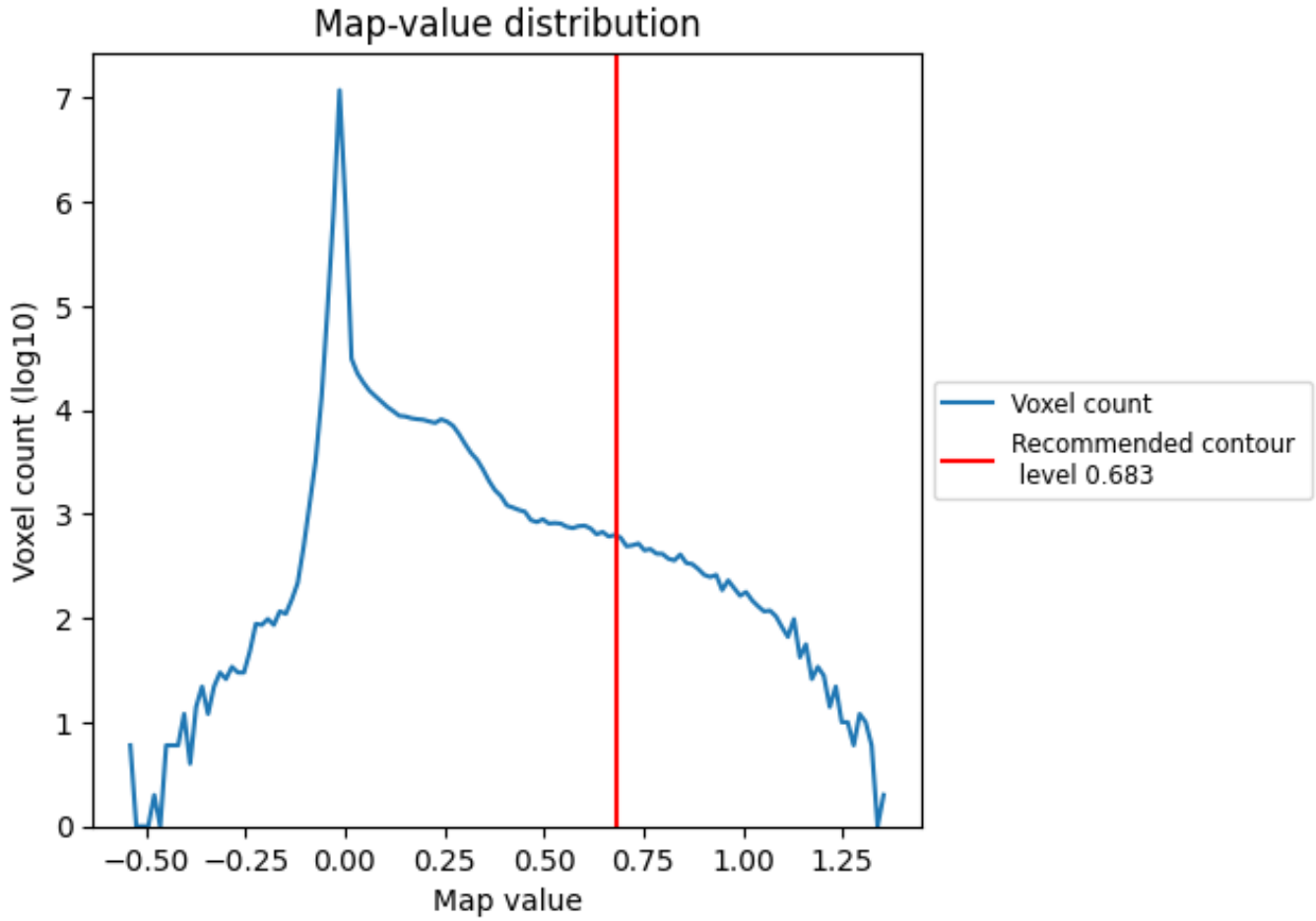


Z

7 Map analysis

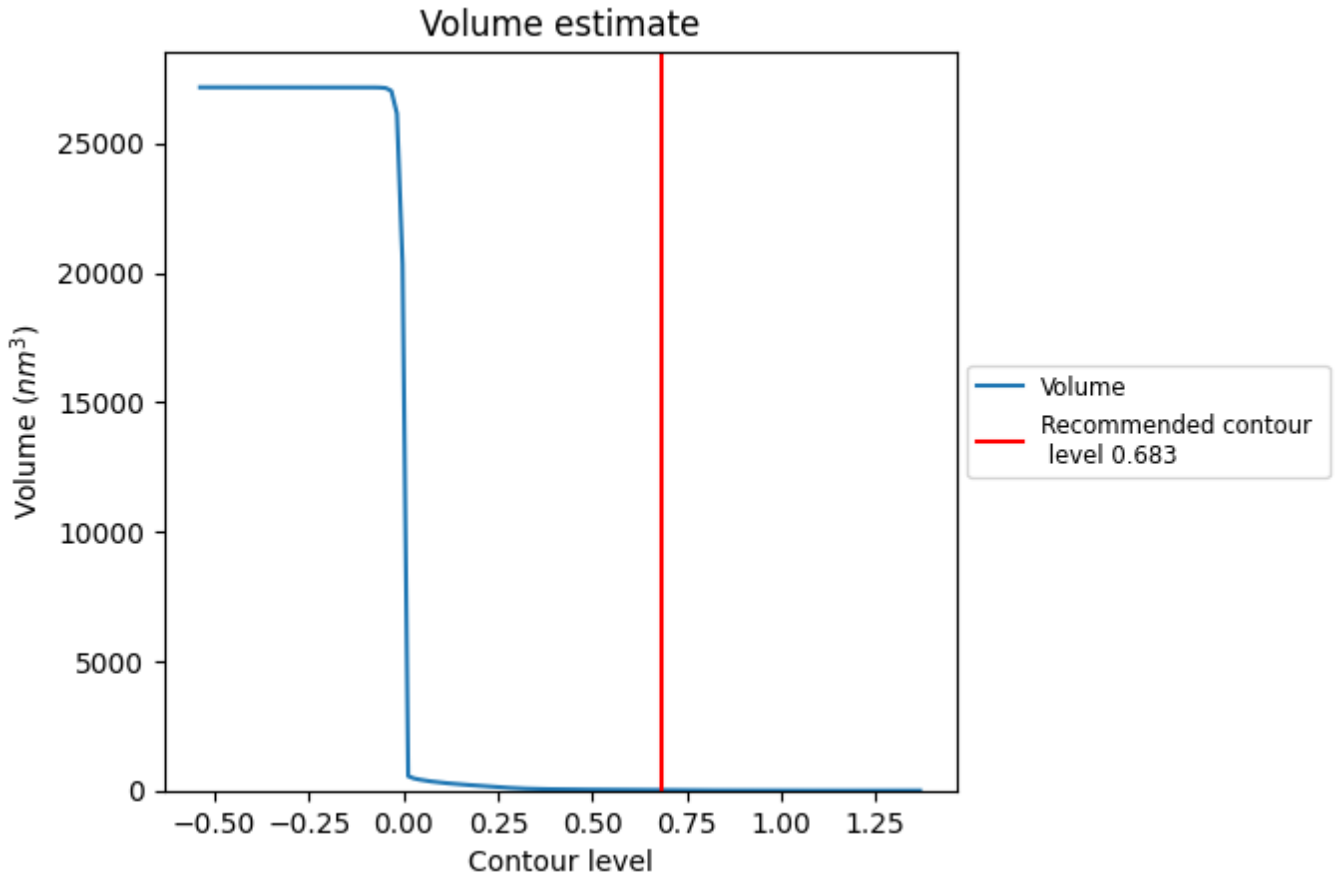
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

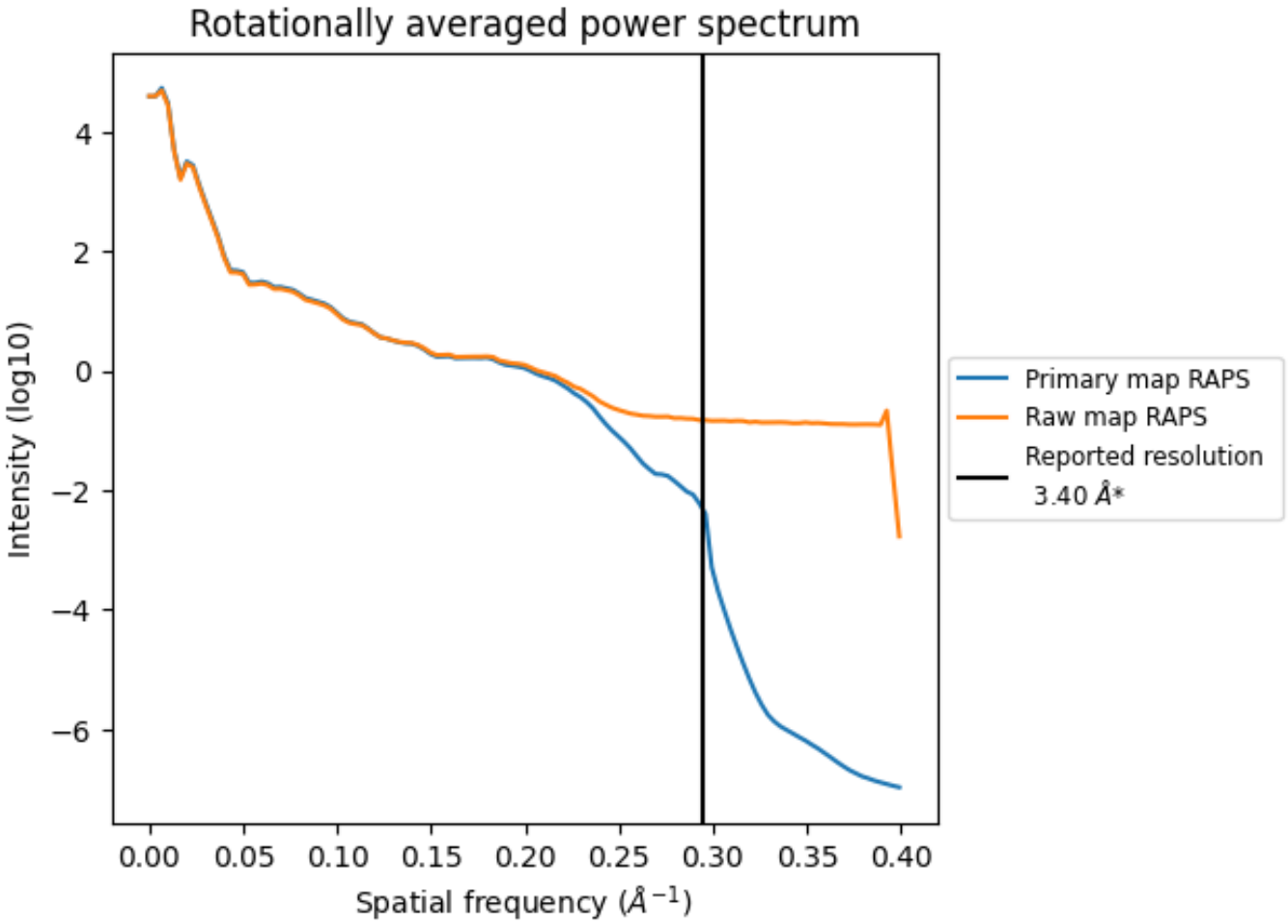
7.2 Volume estimate



The volume at the recommended contour level is 18 nm^3; this corresponds to an approximate mass of 16 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 (i)

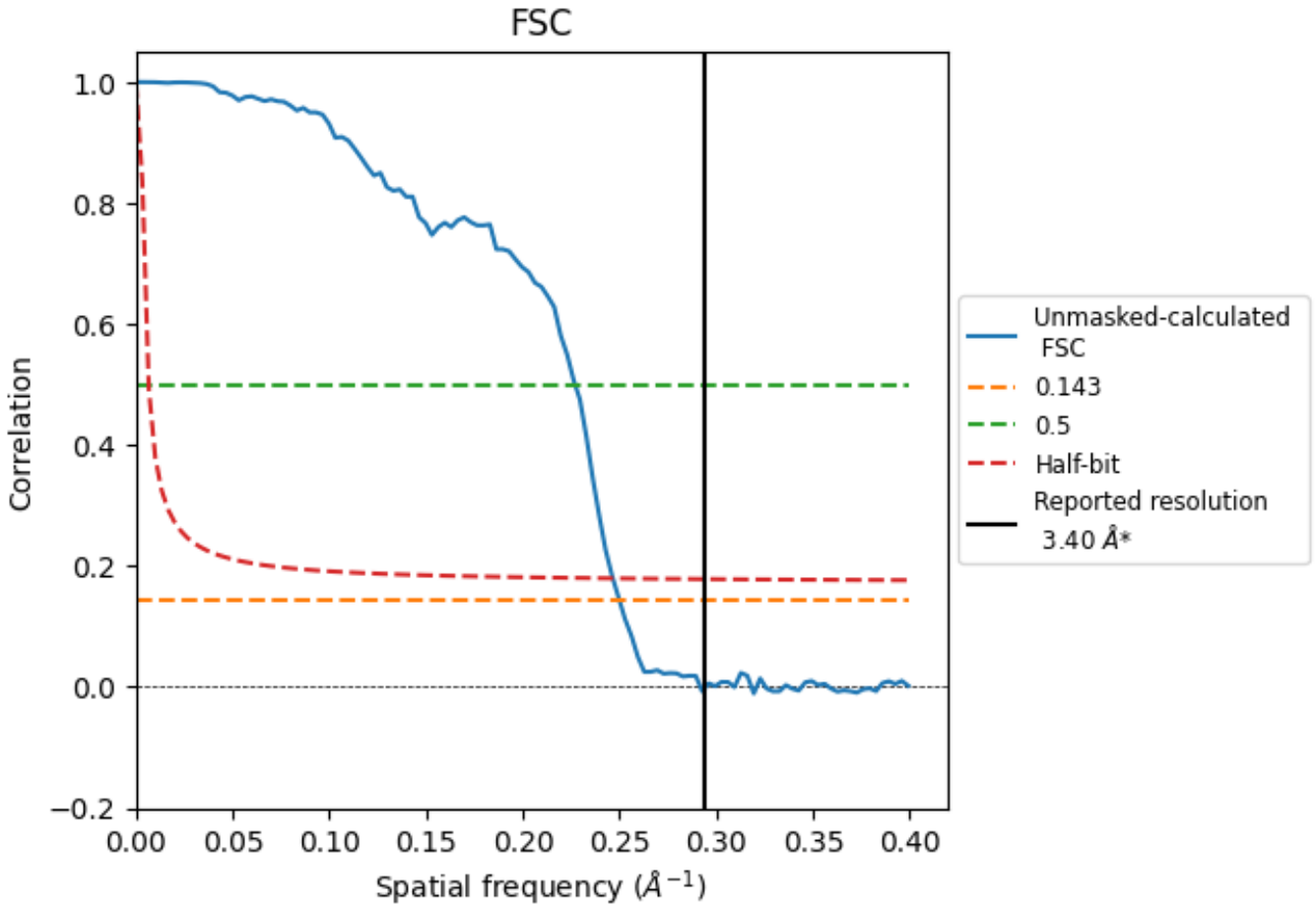


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

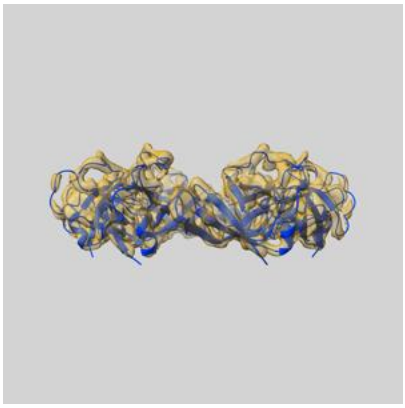
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	4.41	4.06

*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 4.00 differs from the reported value 3.4 by more than 10 %

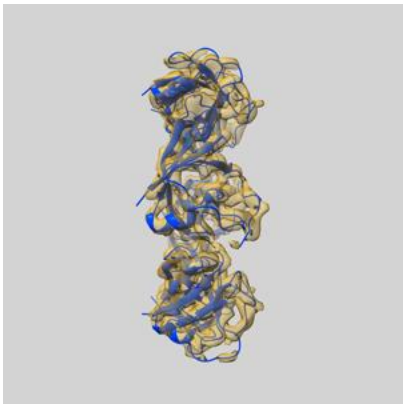
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56579 and PDB model 28KO. Per-residue inclusion information can be found in section 3 on page 5.

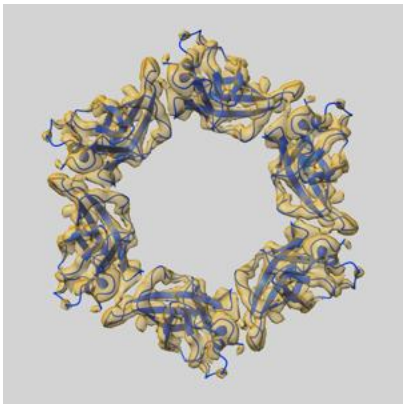
9.1 Map-model overlay



X



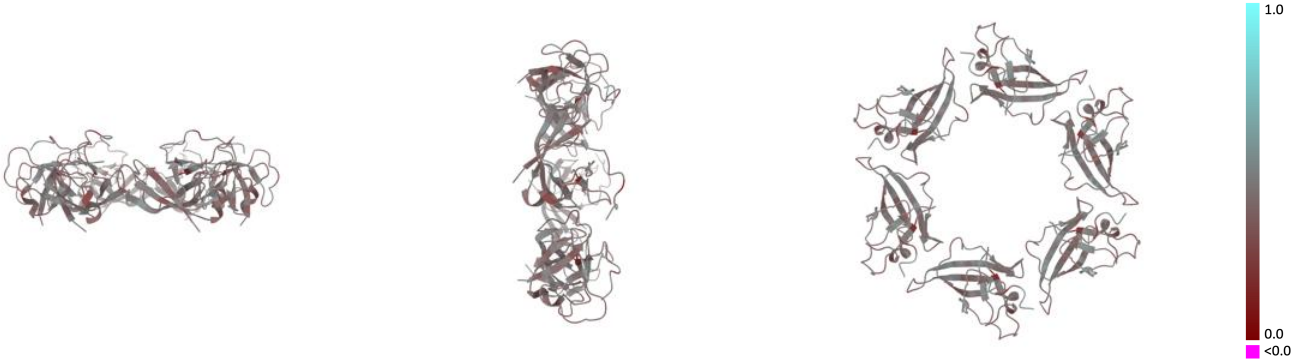
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.683 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.

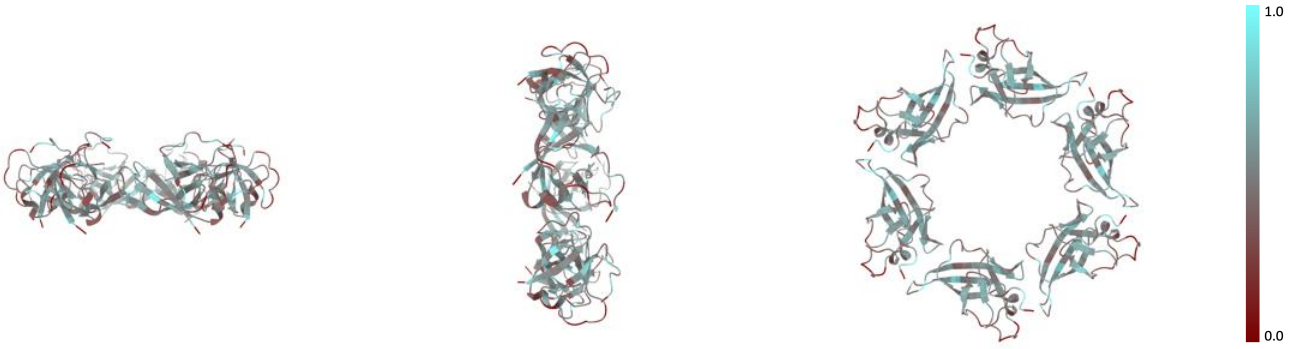
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

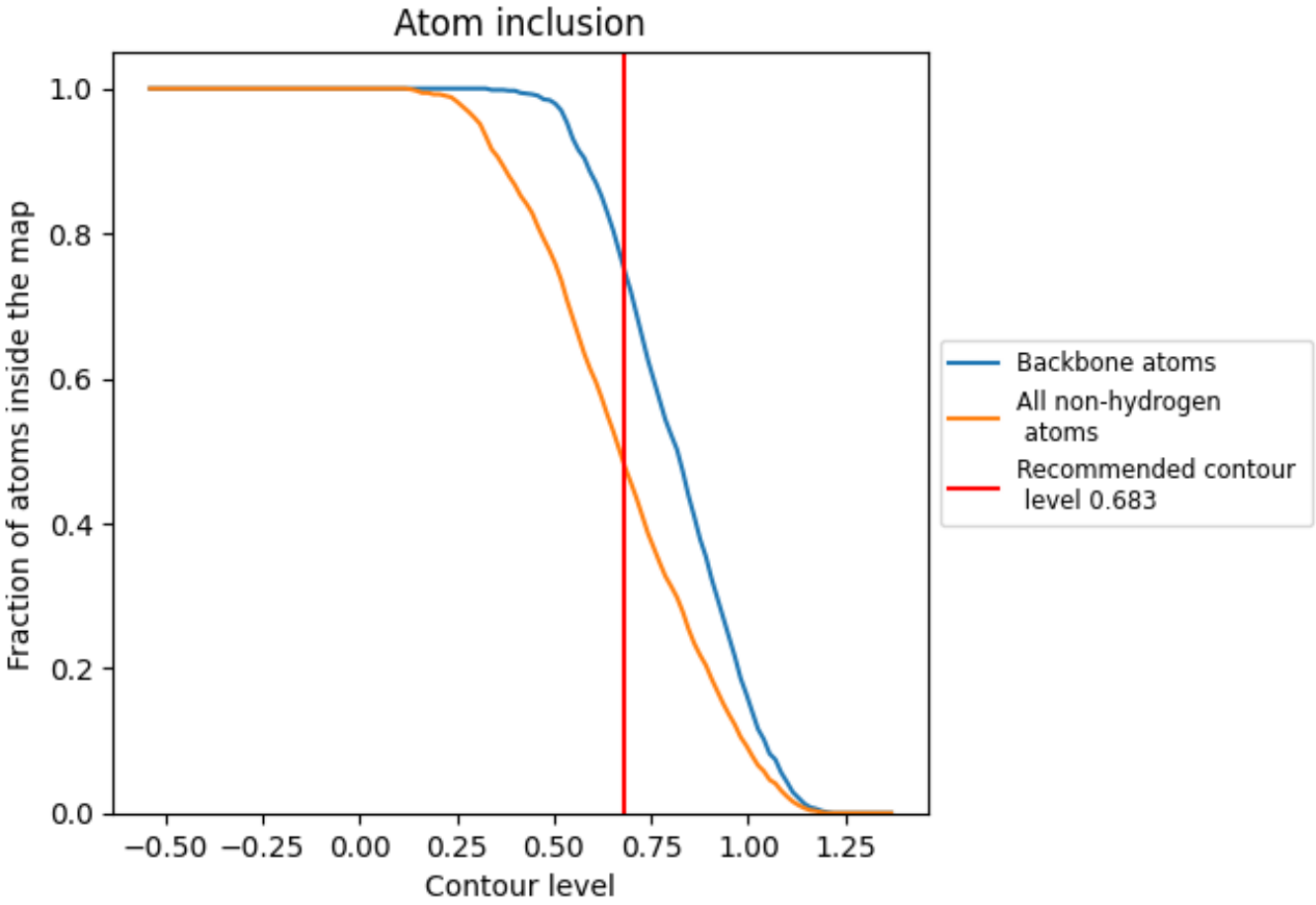
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.683).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 48% 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 (0.683) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4780	0.4160
A	0.4780	0.4160
B	0.4780	0.4160
C	0.4830	0.4150
D	0.4740	0.4180
E	0.4760	0.4160
F	0.4800	0.4160

