



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 10:39 PM EDT

PDB ID : 9MDR / pdb_00009mdr
EMDB ID : EMD-48178
Title : Clostridioides difficile Transferase B Component Symmetric Heptamer
Authors : Sheedlo, M.J.; Mullard, R.M.
Deposited on : 2024-12-05
Resolution : 3.33 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

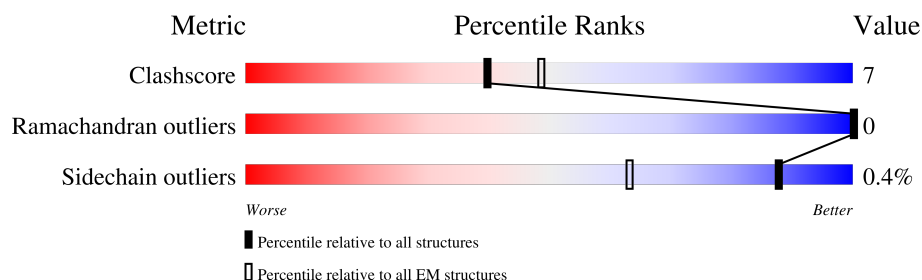
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	876	 32% 7% 62%
1	B	876	 32% 7% 62%
1	C	876	 32% 7% 62%
1	D	876	 32% 7% 62%
1	E	876	 32% 6% 62%
1	F	876	 32% 7% 62%
1	G	876	 32% 7% 62%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18389 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.

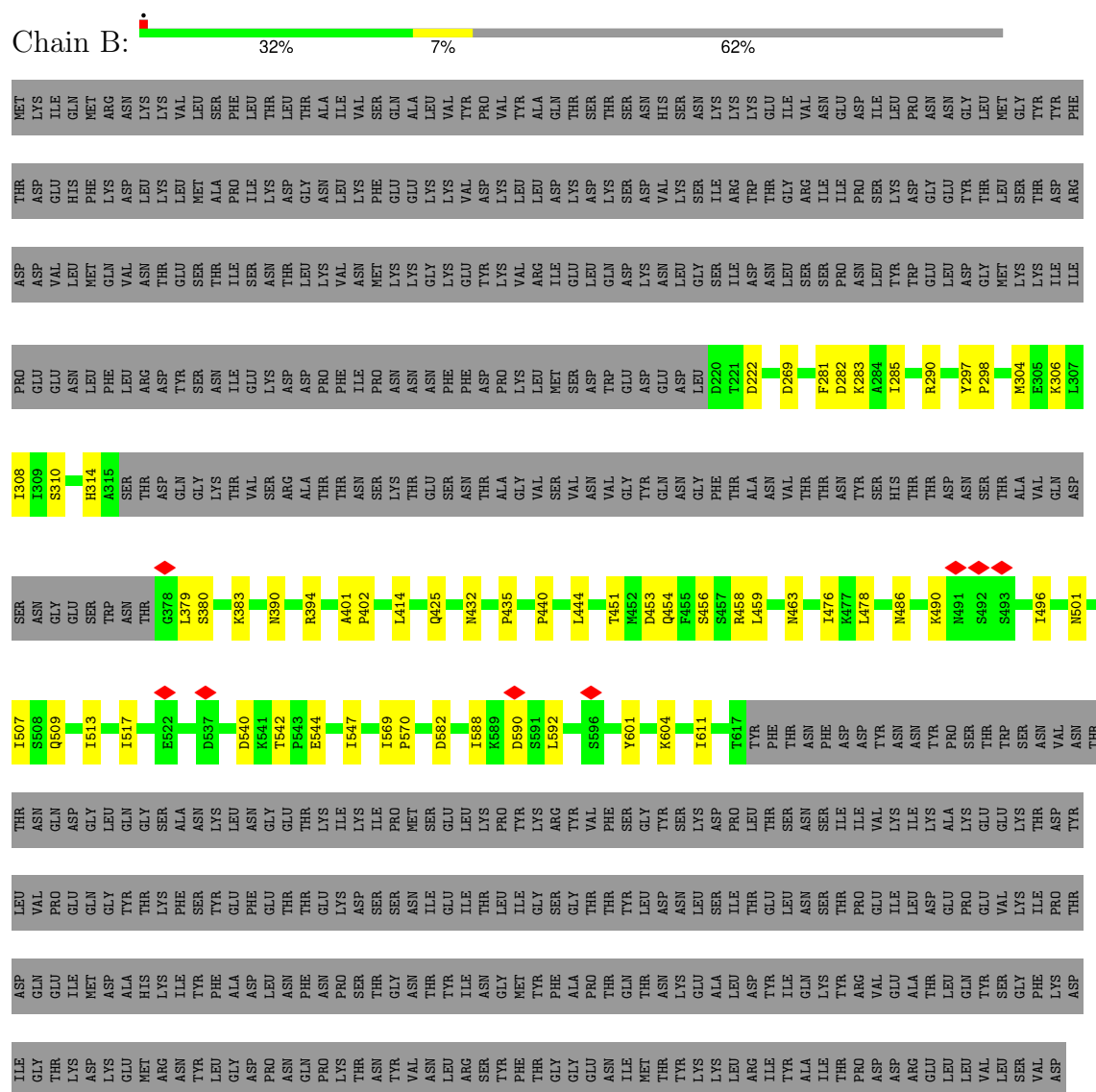
- Molecule 1 is a protein called Adp-ribosyltransferase binding component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2625	1647	427	546	5		
1	B	336	Total	C	N	O	S	1	0
			2625	1647	427	546	5		
1	C	336	Total	C	N	O	S	1	0
			2625	1647	427	546	5		
1	D	336	Total	C	N	O	S	1	0
			2625	1647	427	546	5		
1	E	336	Total	C	N	O	S	1	0
			2625	1647	427	546	5		
1	F	336	Total	C	N	O	S	1	0
			2625	1647	427	546	5		
1	G	336	Total	C	N	O	S	1	0
			2625	1647	427	546	5		

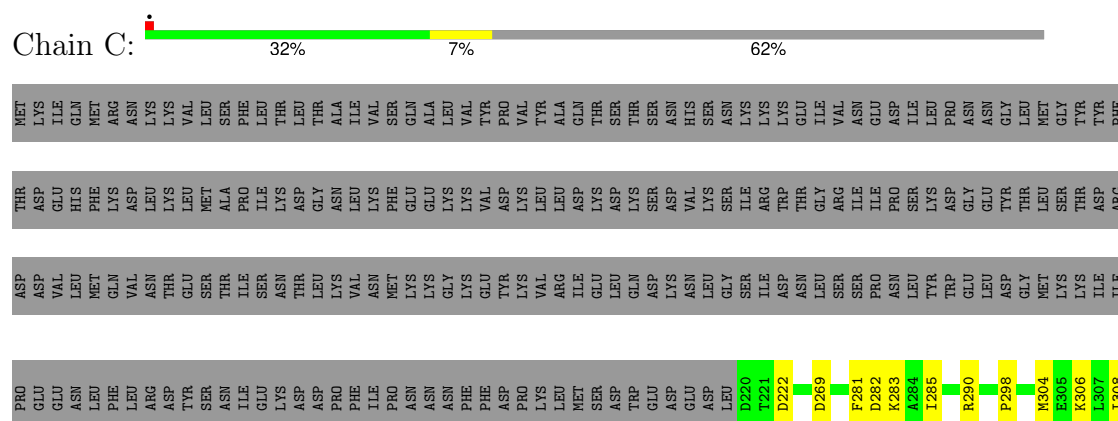
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Ca	0
			2	2	
2	B	2	Total	Ca	0
			2	2	
2	C	2	Total	Ca	0
			2	2	
2	D	2	Total	Ca	0
			2	2	
2	E	2	Total	Ca	0
			2	2	
2	F	2	Total	Ca	0
			2	2	
2	G	2	Total	Ca	0
			2	2	

- Molecule 1: Adp-ribosyltransferase binding component



- Molecule 1: Adp-ribosyltransferase binding component



ASP	ILE	GLY	THR	LYS	ASP	LYS	GLU	MET	ARG	ASN	TYR	LEU	GLY	ASP	PRO	ASN	GLN	PRO	LYS	THR	ASN	TYR	VAL	ASN	LEU	ARG	SER	PHE	THR	GLY	GLY	GLU	GLU	ASN	ILE	MET	THR	TYR	LYS	LYS	LEU	ARG	ILE	THR	ALA	ILE	THR	PRO	ASP	ASP	ARG	GLU	LEU	LEU	VAL	LEU	SER	LEU	VAL	ASP
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- Molecule 1: Adp-ribosyltransferase binding component



THR	ASP	GLU	HIS	PHE	LYS	ASP	LEU	LEU	LEU	LEU	MET	ALA	PRO	ILE	LYS	ASP	ASN	LEU	LYS	PHE	GLU	GLU	LYS	LYS	VAL	ASP	LYS	LYS	ASP	SER	ASP	VAL	LYS	SER	ILE	ILE	ILE	TRP	THR	GLY	ARG	ILE	ILE	PRO	PRO	SER	LYS	ASP	GLY	GLY	TYR	THR	LEU	LEU	SER	THR	THR	ASP	ARG
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PRO	GLU	GLU	ASN	LEU	PHE	LEU	ARG	ASP	TYR	SER	ASN	ILE	GLY	GLU	ASP	ASP	PRO	PHE	ILE	PRO	PRO	ASN	ASN	PHE	PHE	ASP	ASP	LYS	LEU	MET	ASP	ASP	TRP	TRP	GLU	ASP	GLU	ASP	ASP	LEU	D220	D221	D222	D269	F261	D262	K263	A264	I285	R290	Y297	P298	M304	S305	K306	E307
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[illegible][illegible]

3508	Q509	1513	1517	E522	D537	D540	K541	P543	E544	1547	1569	P570	D582	1588	K589	D590	S591	L592	S596	Y601	K604	1611	1617	TYR	PHE	THR	ASN	ASN	PHE	ASP	ASP	TYR	ASN	ASN	TYR	PRO	SER	THR	TRP	SER	ASN	ASN	VAL	ASN	THR	THR
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ASN GLN ASP ASP GLY GLN GLY SER SER ASN ASN LYS LEU LYS ASN ASN GLY GLU GLU THR LYS LYS ILE ILE ILE PRO MET MET SER SER GLU GLU LEU LYS PRO PRO TYR TYR LYS ARG TYR VAL PHE SER SER GLY TYR SER LYS ASP ASP PRO PRO LEU THR SER ASN SER SER ILE ILE VAL LYS ILE LYS ALA ALA LYS LYS GLU GLU GLU THR ASP TYR LEU

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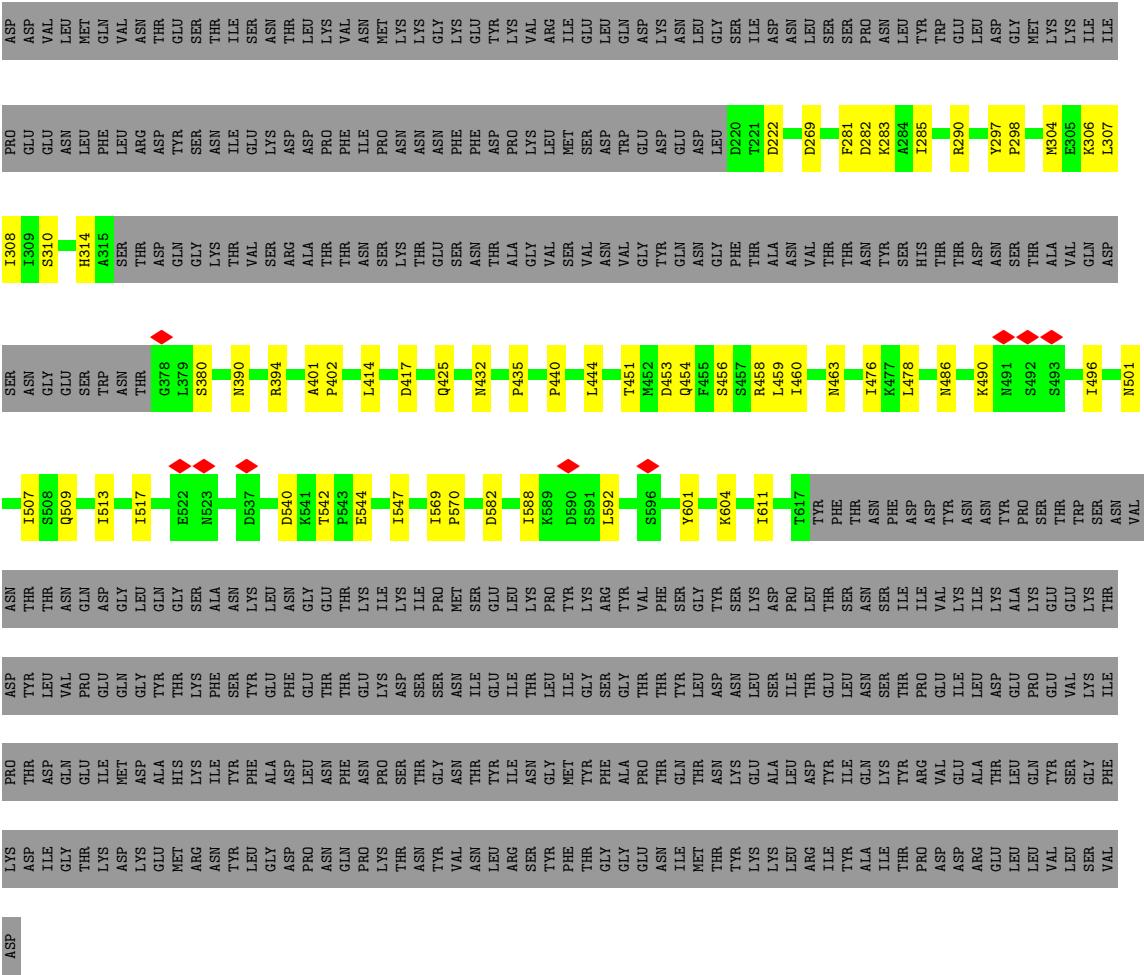
GLY THR LYS ASP LYS GLU MET ARG ASN TYR LEU GLY PRO ASP ASN GLN GLN LYS THR ASN TYR PHE GLY GLY VAL ASN LEU ARG SER TYR THR THR GLY GLU ASN ILE MET TYR LYS TYR LYS LEU ARG ILE ALA TYR ILE THR THR ASP ASP ARG ARG ILE TYR LEU VAL LEU SER ASP

- Molecule 1: Adp-ribosyltransferase binding component

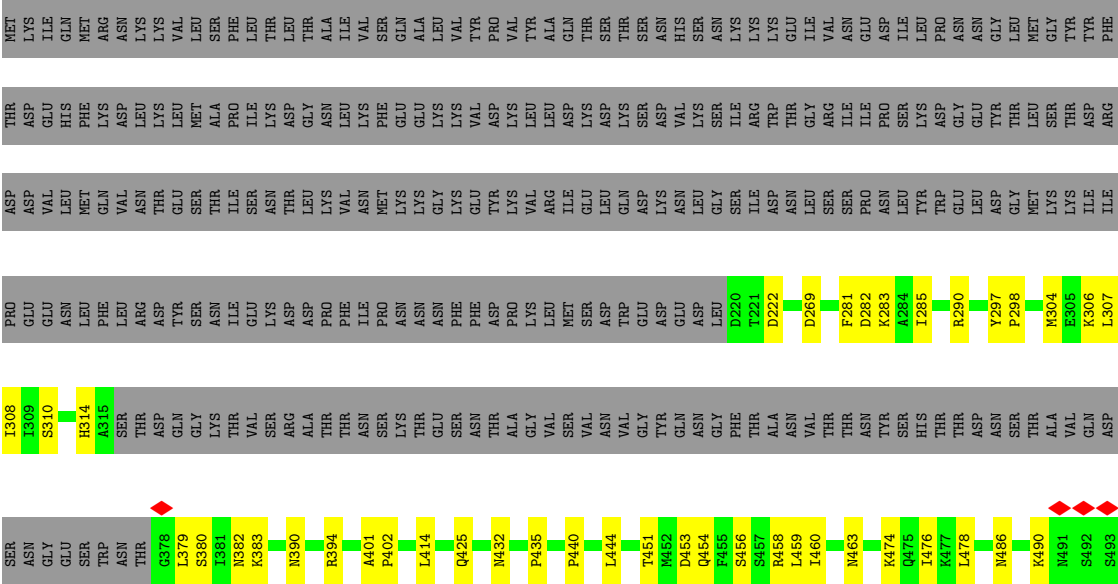


MET	LYS	ILE	GLN	MET	ARG	ASN	LYS	LYS	VAL	LEU	SER	PHE	LEU	THR	LEU	LEU	THR	THR	ALA	VAL	SER	GLN	LEU	VAL	TYR	PRO	TYR	THR	VAL	TYR	ALA	GLN	THR	SER	SER	ASN	ASN	HIS	SER	ASN	LYS	LYS	LYS	GLU	ILE	VAL	ASN	GLU	ASP	ILE	LEU	PRO	PRO	MET	GLY	TYR	THR	PHE
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THR	ASP	GLU	ASP	GLY	HIS	PHE	LYS	LYS	ASP	LEU	LEU	LEU	MET	ALA	PRO	PRO	ILE	LYS	GLY	ASP	ASN	LEU	LYS	PHE	GLU	GLU	LYS	LYS	VAL	ASP	ASP	LYS	LYS	LEU	LEU	ASP	LYS	VAL	VAL	SER	SER	LYS	LYS	ARG	ARG	TRP	THR	GLY	ARG	ILE	ILE	ILE	PRO	PRO	LYS	ASP	ASP	GLY	GLY	TYR	THR	SER	SER	LEU	LEU	THR	THR	ASP	ASP	ARG
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● Molecule 1: Adp-ribosyltransferase binding component





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39547	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.769	Depositor
Minimum map value	-1.980	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	292.4, 292.4, 292.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85999995, 0.85999995, 0.85999995	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0/2671	0.37	0/3619
1	B	0.13	0/2671	0.37	0/3619
1	C	0.13	0/2671	0.37	0/3619
1	D	0.13	0/2671	0.37	0/3619
1	E	0.13	0/2671	0.37	0/3619
1	F	0.13	0/2671	0.37	0/3619
1	G	0.13	0/2671	0.37	0/3619
All	All	0.13	0/18697	0.37	0/25333

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	2625	0	2583	42	0
1	B	2625	0	2583	41	0
1	C	2625	0	2583	42	0
1	D	2625	0	2583	42	0
1	E	2625	0	2583	40	0
1	F	2625	0	2583	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2625	0	2583	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
All	All	18389	0	18081	250	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 7.

The worst 5 of 250 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:B:509:GLN:HG3	1:C:283:LYS:HB2	1.81	0.63
1:C:509:GLN:HG3	1:D:283:LYS:HB2	1.81	0.62
1:A:509:GLN:HG3	1:B:283:LYS:HB2	1.82	0.62
1:A:283:LYS:HB2	1:G:509:GLN:HG3	1.82	0.62
1:F:509:GLN:HG3	1:G:283:LYS:HB2	1.81	0.62

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	333/876 (38%)	316 (95%)	17 (5%)	0	100	100
1	B	333/876 (38%)	316 (95%)	17 (5%)	0	100	100
1	C	333/876 (38%)	316 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	333/876 (38%)	315 (95%)	18 (5%)	0	100	100
1	E	333/876 (38%)	315 (95%)	18 (5%)	0	100	100
1	F	333/876 (38%)	316 (95%)	17 (5%)	0	100	100
1	G	333/876 (38%)	316 (95%)	17 (5%)	0	100	100
All	All	2331/6132 (38%)	2210 (95%)	121 (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	294/790 (37%)	292 (99%)	2 (1%)	81	88
1	B	294/790 (37%)	292 (99%)	2 (1%)	81	88
1	C	294/790 (37%)	293 (100%)	1 (0%)	91	94
1	D	294/790 (37%)	292 (99%)	2 (1%)	81	88
1	E	294/790 (37%)	294 (100%)	0	100	100
1	F	294/790 (37%)	294 (100%)	0	100	100
1	G	294/790 (37%)	293 (100%)	1 (0%)	91	94
All	All	2058/5530 (37%)	2050 (100%)	8 (0%)	88	93

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	379	LEU
1	D	590	ASP
1	C	590	ASP
1	B	590	ASP
1	D	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	501	ASN
1	E	501	ASN
1	G	432	ASN
1	E	425	GLN
1	E	509	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](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

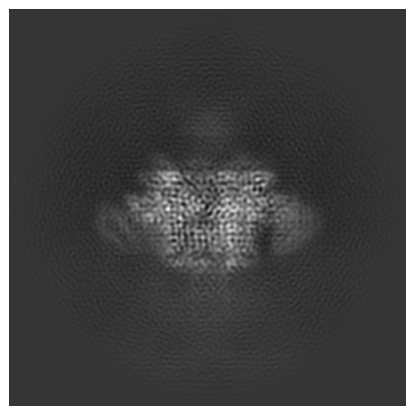
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48178. These allow visual inspection of the internal detail of the map and identification of artifacts.

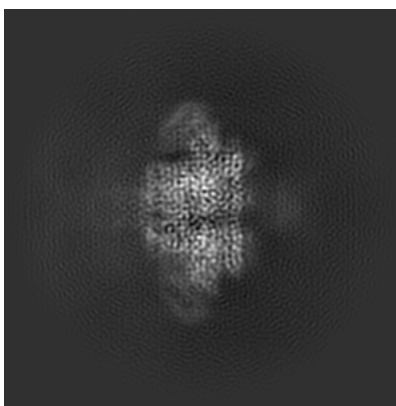
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

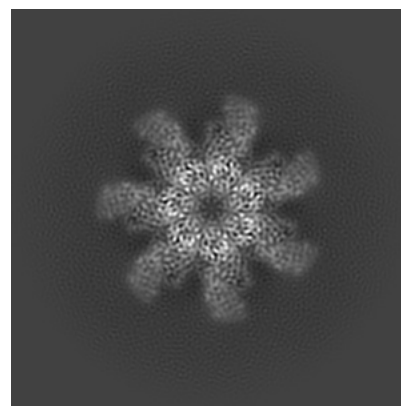
6.1.1 Primary map



X

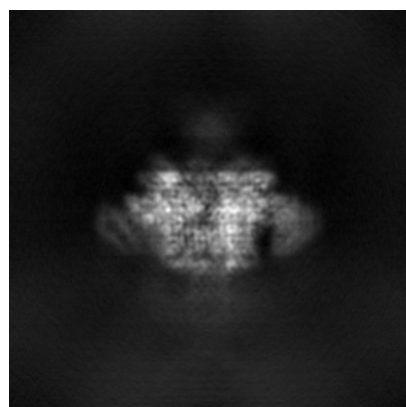


Y

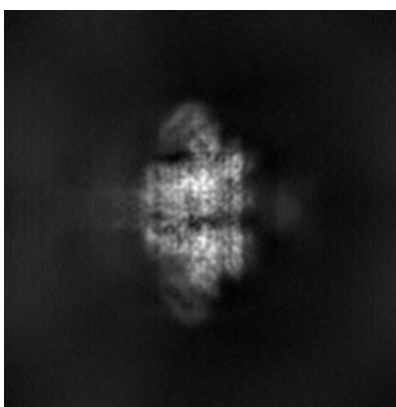


Z

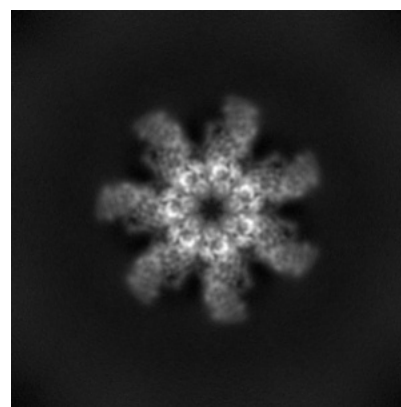
6.1.2 Raw map



X



Y

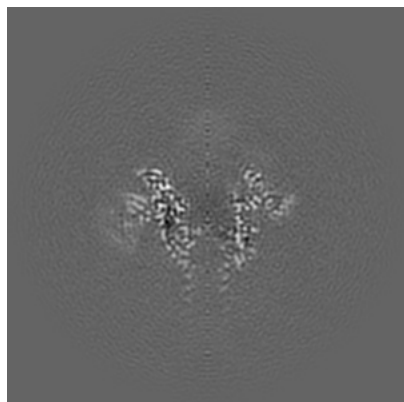


Z

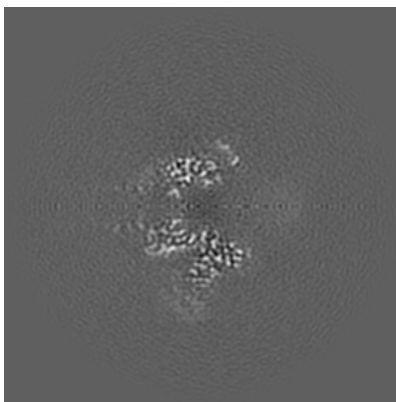
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

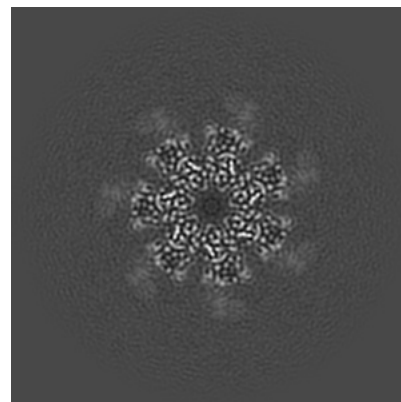
6.2.1 Primary map



X Index: 170

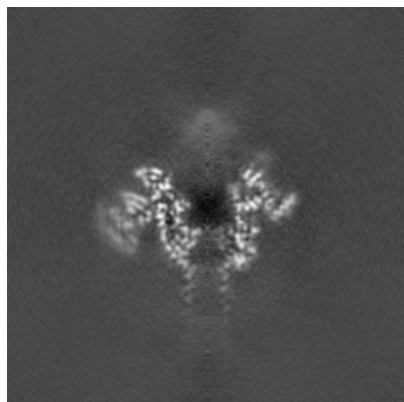


Y Index: 170

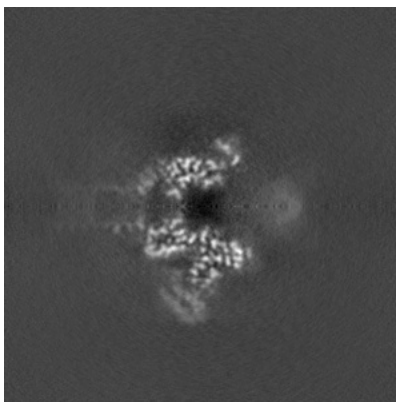


Z Index: 170

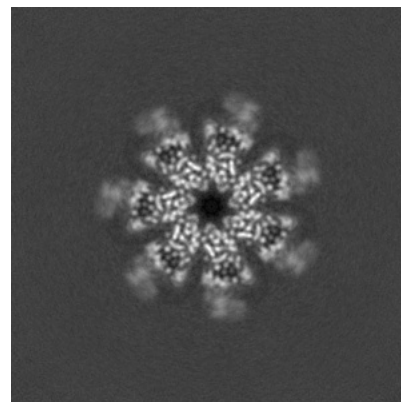
6.2.2 Raw map



X Index: 170



Y Index: 170

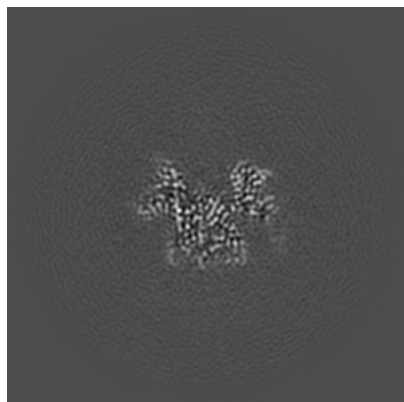


Z Index: 170

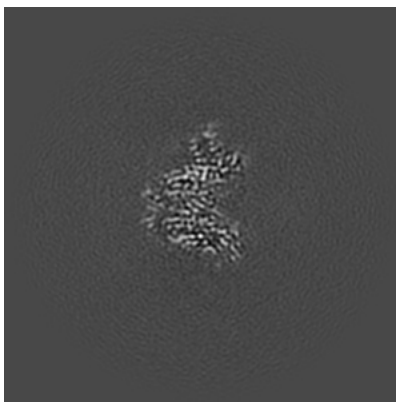
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

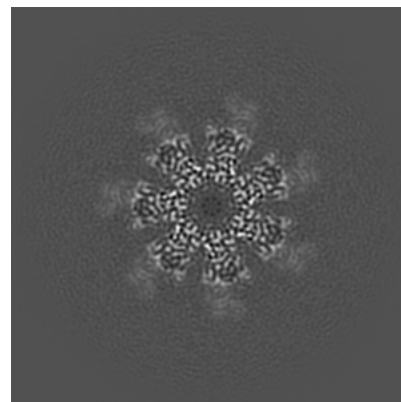
6.3.1 Primary map



X Index: 145

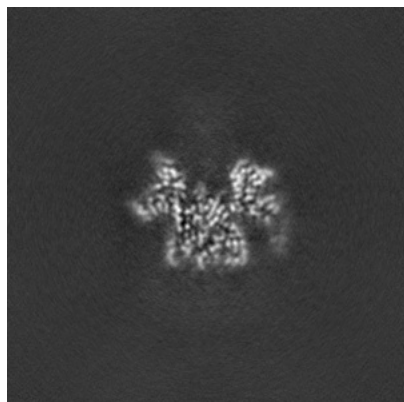


Y Index: 146

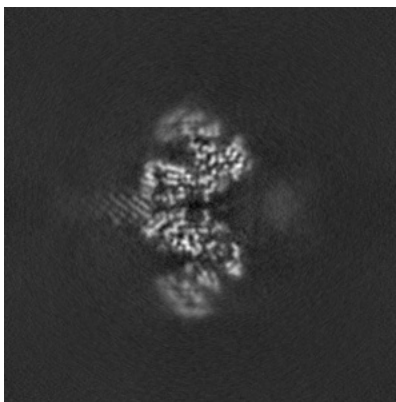


Z Index: 169

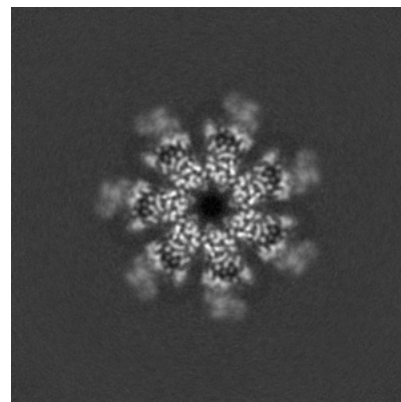
6.3.2 Raw map



X Index: 145



Y Index: 186

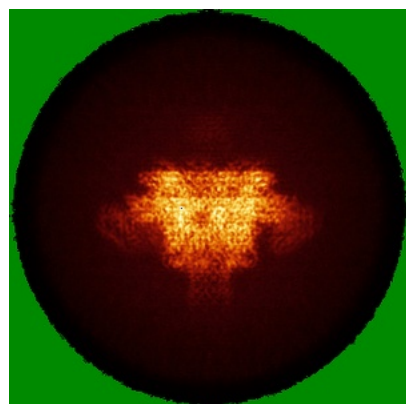


Z Index: 169

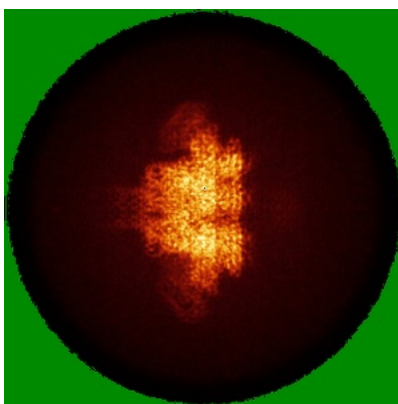
The images above show the largest variance slices of the map in three orthogonal directions.

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

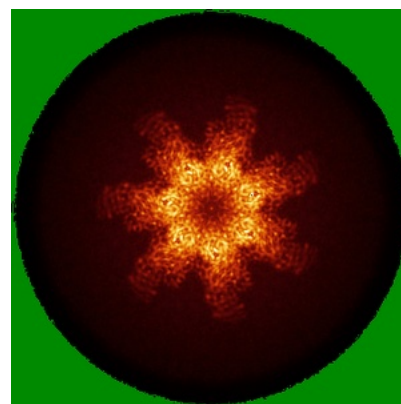
6.4.1 Primary map



X

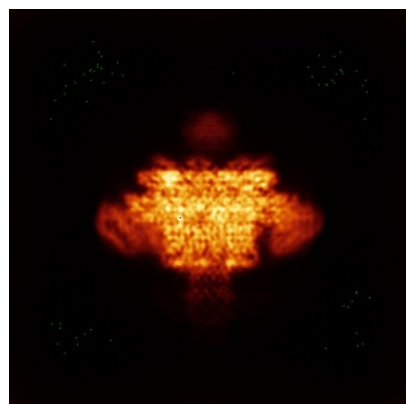


Y

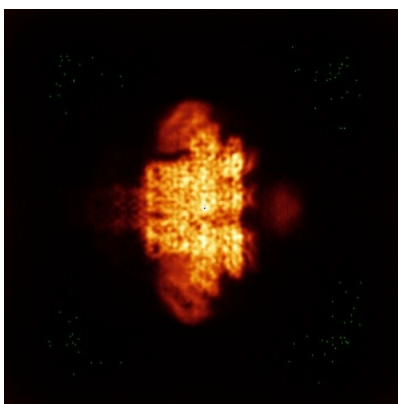


Z

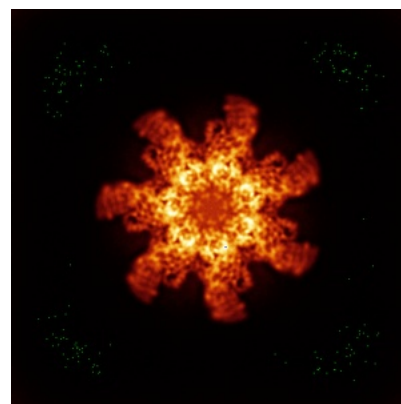
6.4.2 Raw map



X



Y

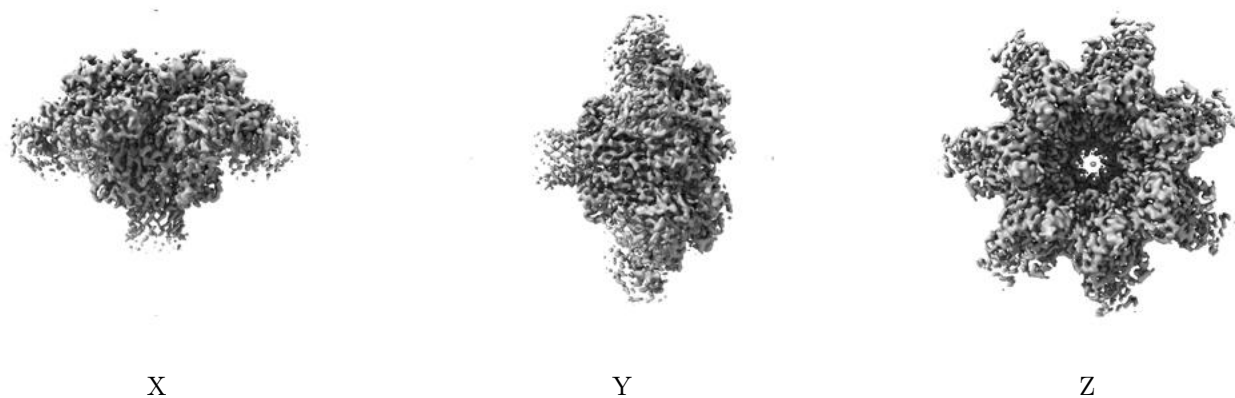


Z

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.

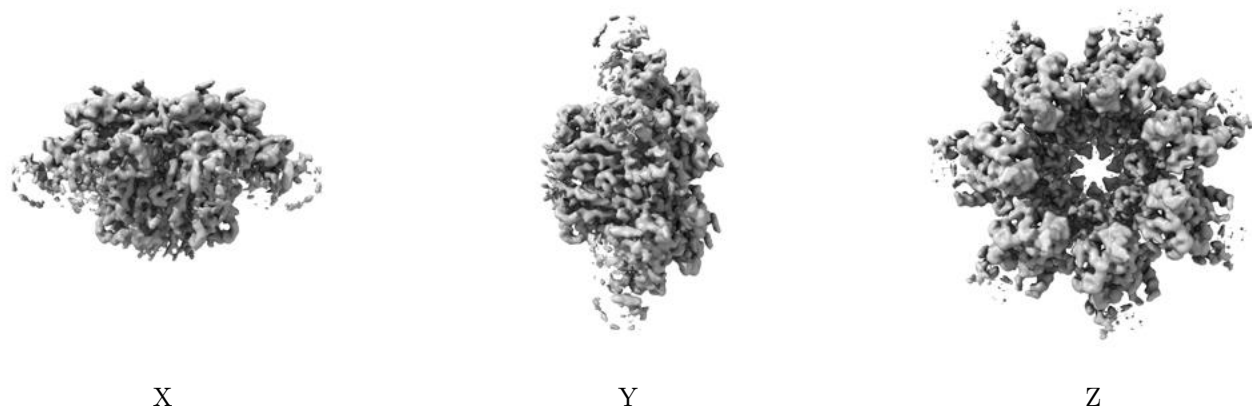
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

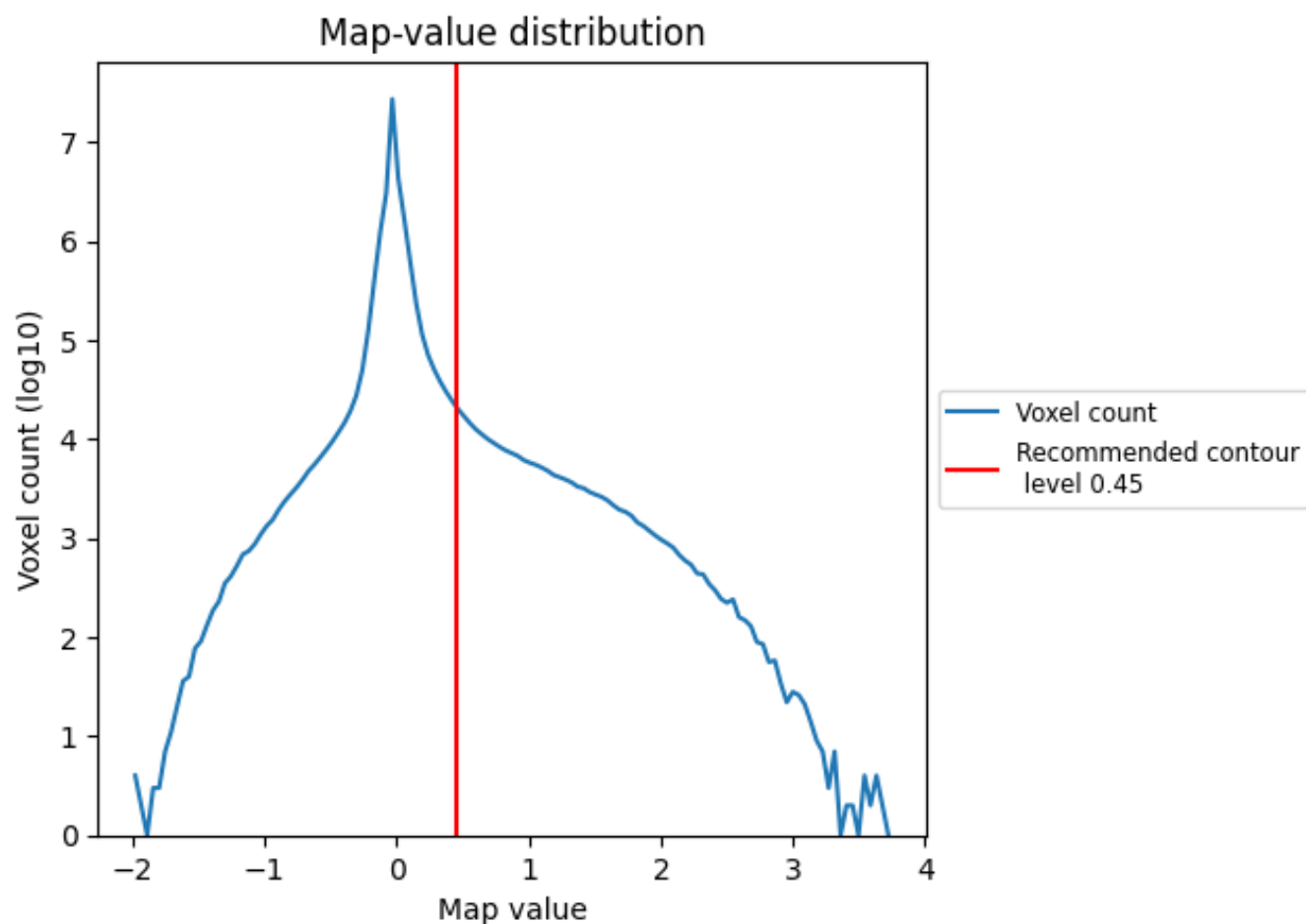
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

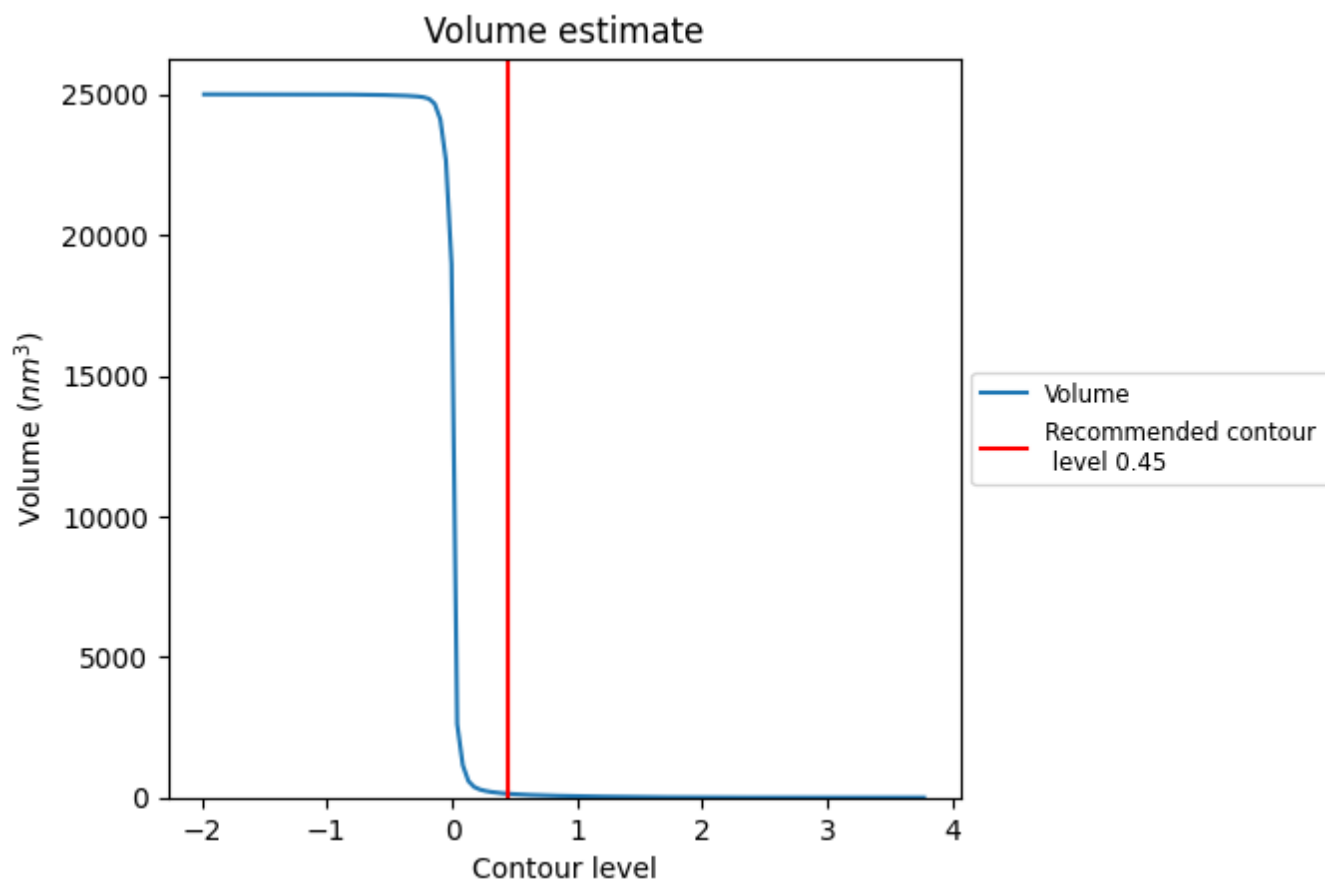
This section contains the results of statistical analysis of the map.

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.

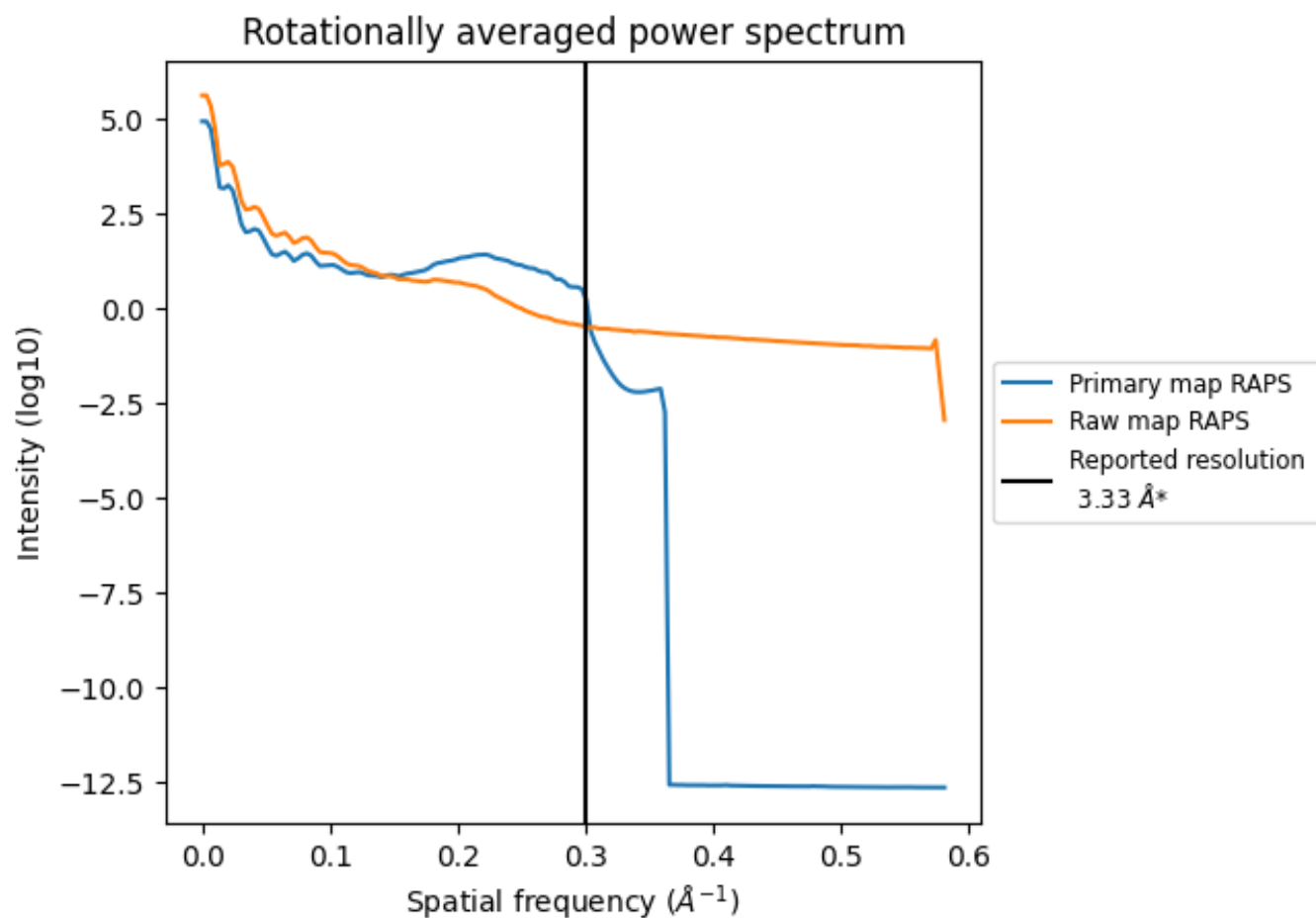
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 ⓘ

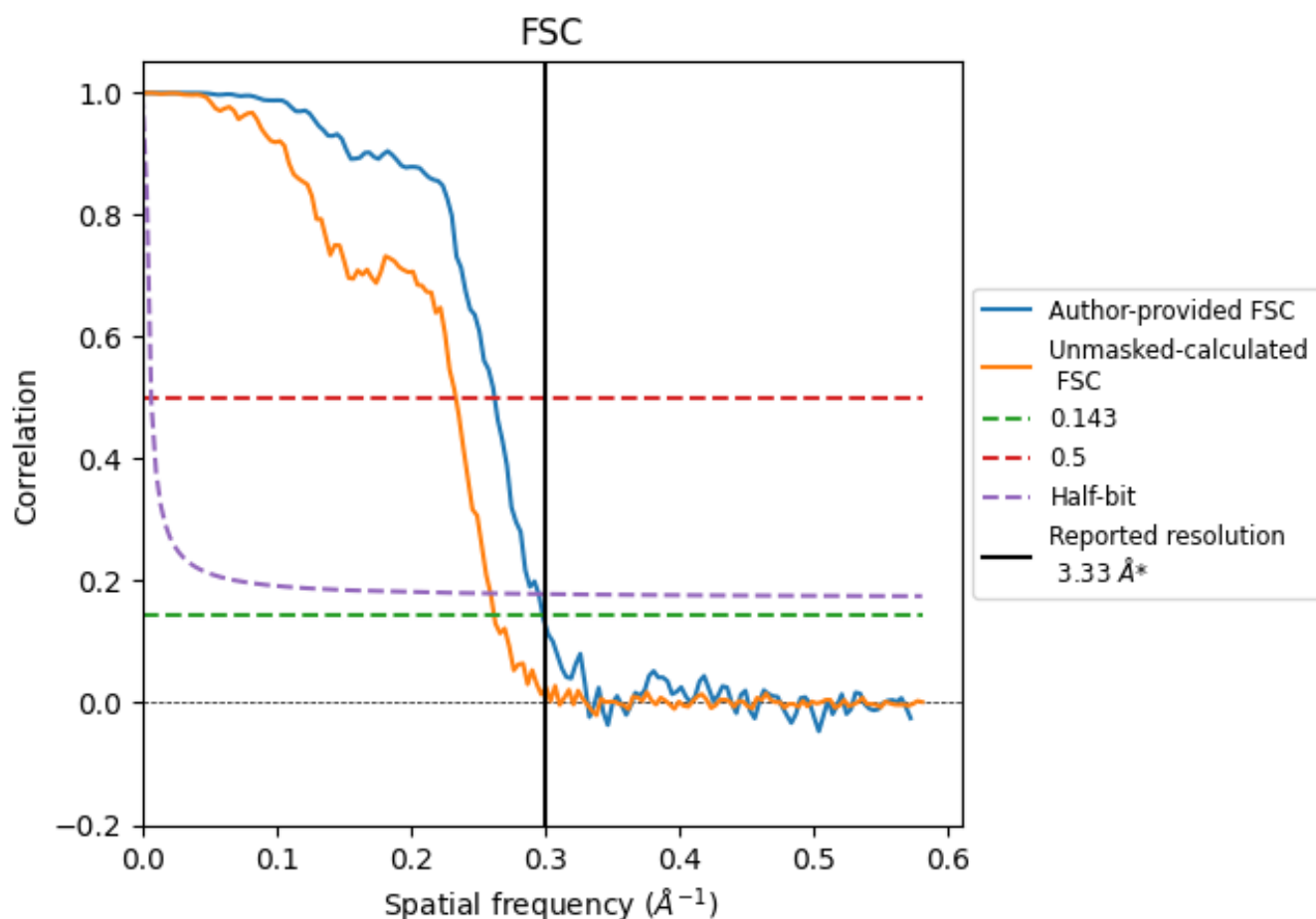


*Reported resolution corresponds to spatial frequency of 0.300 \AA^{-1}

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 0.300 \AA^{-1}

8.2 Resolution estimates [i](#)

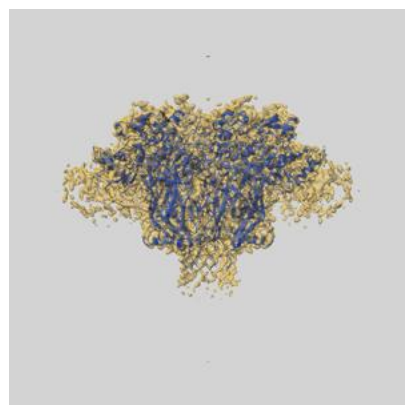
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.35	3.81	3.38
Unmasked-calculated*	3.81	4.28	3.85

*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 3.81 differs from the reported value 3.33 by more than 10 %

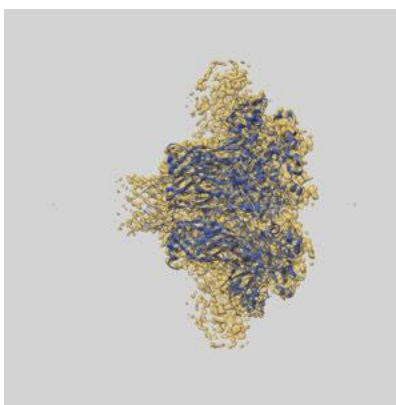
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48178 and PDB model 9MDR. Per-residue inclusion information can be found in section [3](#) on page [4](#).

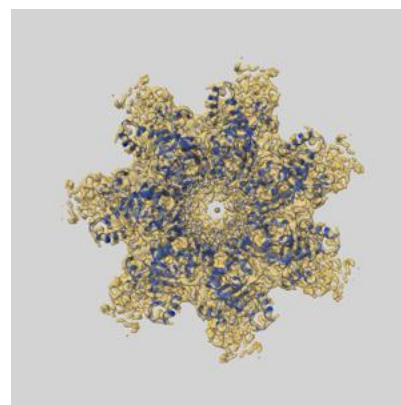
9.1 Map-model overlay [i](#)



X



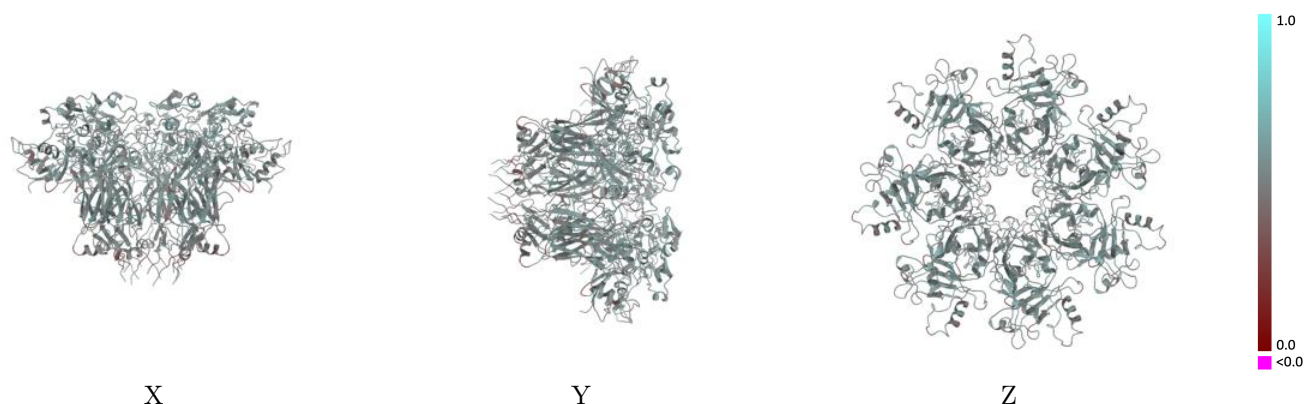
Y



Z

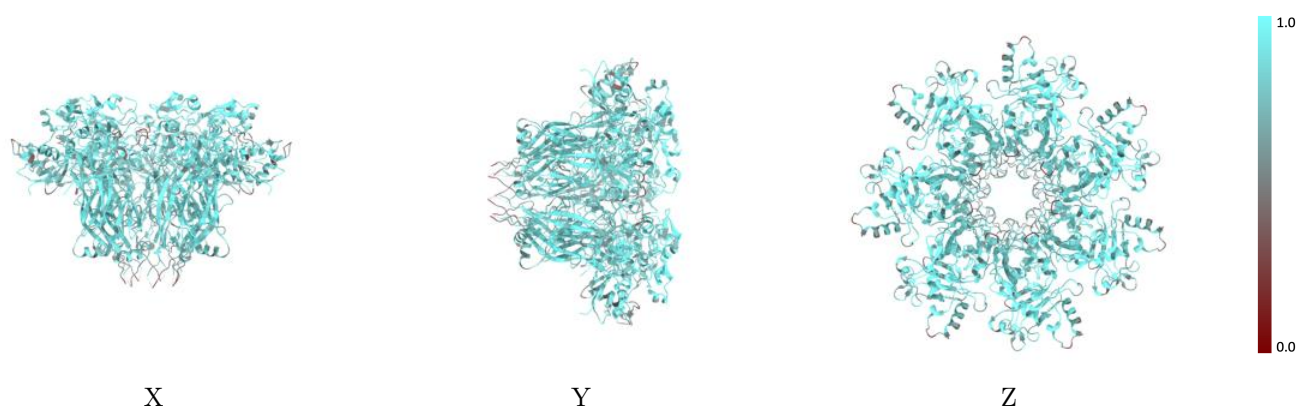
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



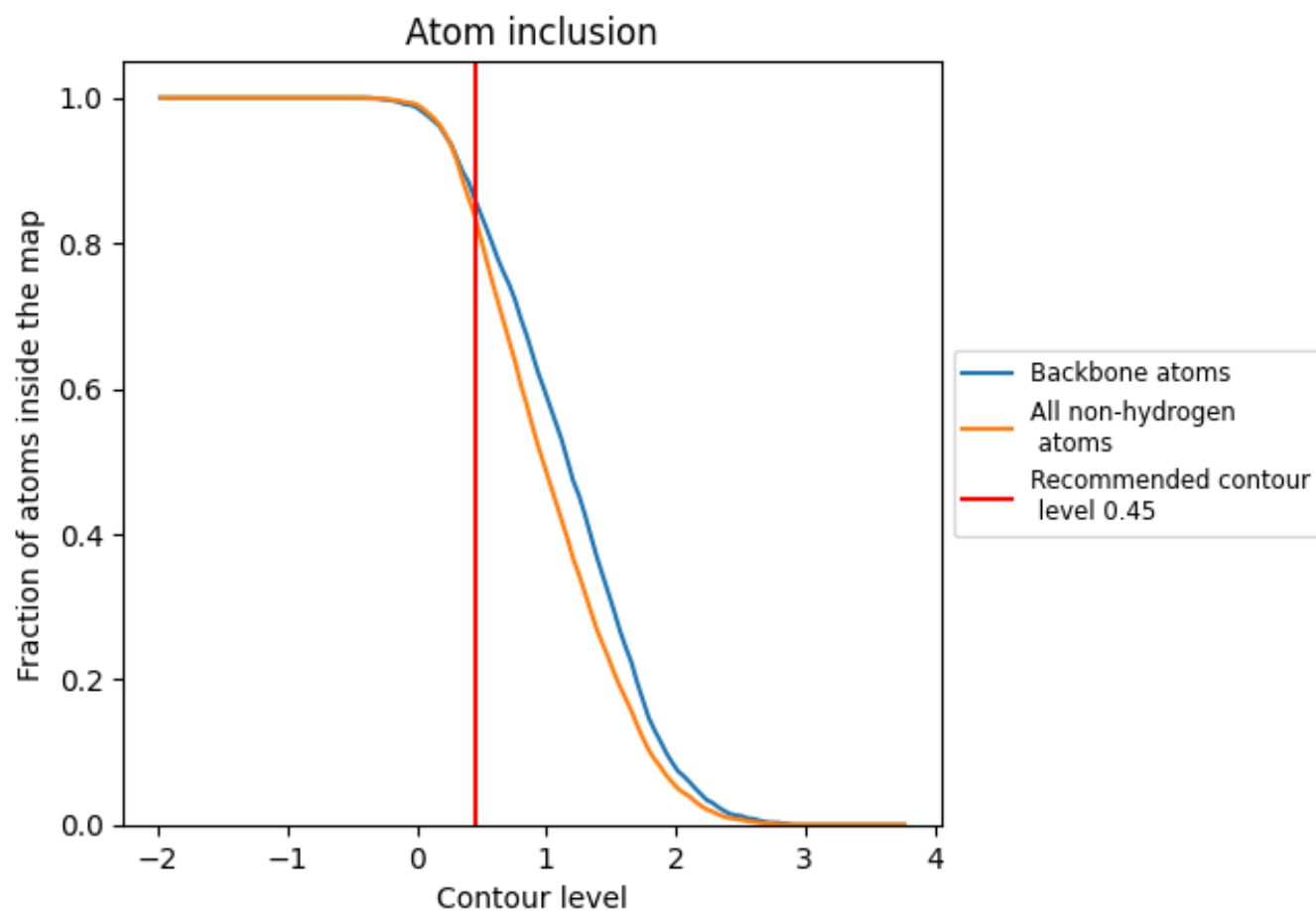
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8370	<div><div></div></div> 0.5210
A	<div><div></div></div> 0.8370	<div><div></div></div> 0.5210
B	<div><div></div></div> 0.8360	<div><div></div></div> 0.5210
C	<div><div></div></div> 0.8370	<div><div></div></div> 0.5210
D	<div><div></div></div> 0.8380	<div><div></div></div> 0.5210
E	<div><div></div></div> 0.8390	<div><div></div></div> 0.5200
F	<div><div></div></div> 0.8360	<div><div></div></div> 0.5200
G	<div><div></div></div> 0.8370	<div><div></div></div> 0.5220

1.0

0.0

<0.0