



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 01:58 AM UTC

PDB ID : 8PZV / pdb_00008pzv
EMDB ID : EMD-18046
Title : Wait Complex: BAM bound Darobactin-B and Extended SurA
Authors : Fenn, K.L.; Ranson, N.A.
Deposited on : 2023-07-27
Resolution : 2.90 Å(reported)
Based on initial models : 7P1C, 8PZ2, 7NRI

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:

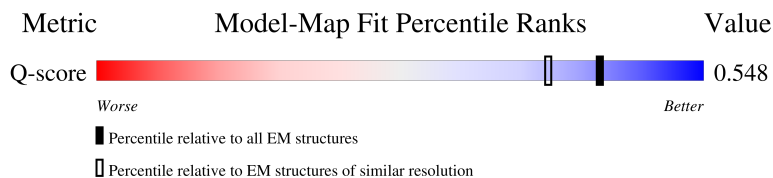
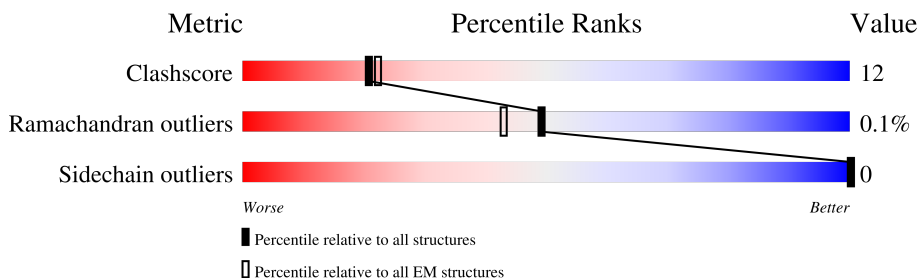
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 2.90 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	13054 (2.40 - 3.40)

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	790	15% 79% 20% .
2	B	373	9% 64% 35% .
3	C	320	12% 6% 82% .
4	D	226	8% 79% 18% .

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Mol	Chain	Length	Quality of chain
5	E	104	
6	F	450	
7	I	7	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26040 atoms, of which 12738 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	785	Total	C	H	N	O	S	0	0
			12115	3912	5913	1043	1230	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	CYS	ARG	engineered mutation	UNP C3TPJ2

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	369	Total	C	H	N	O	S	0	0
			5375	1739	2600	476	554	6		

- Molecule 3 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	58	Total	C	H	N	O	S	0	0
			804	263	388	71	81	1		

- Molecule 4 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	219	Total	C	H	N	O	S	0	0
			3485	1117	1713	311	337	7		

- Molecule 5 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	84	Total	C	H	N	O	S	0	0
			1291	414	634	113	128	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP P0A937
E	115	GLY	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937
E	120	HIS	-	expression tag	UNP P0A937
E	121	HIS	-	expression tag	UNP P0A937
E	122	HIS	-	expression tag	UNP P0A937
E	123	HIS	-	expression tag	UNP P0A937

- Molecule 6 is a protein called Chaperone SurA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	175	Total	C	H	N	O	S	0	0
			2828	861	1427	262	266	12		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	GLY	-	expression tag	UNP C3TR42
F	-20	SER	-	expression tag	UNP C3TR42
F	-19	SER	-	expression tag	UNP C3TR42
F	-18	ALA	-	expression tag	UNP C3TR42
F	-17	TRP	-	expression tag	UNP C3TR42
F	-16	SER	-	expression tag	UNP C3TR42
F	-15	HIS	-	expression tag	UNP C3TR42
F	-14	PRO	-	expression tag	UNP C3TR42
F	-13	GLN	-	expression tag	UNP C3TR42
F	-12	PHE	-	expression tag	UNP C3TR42
F	-11	GLU	-	expression tag	UNP C3TR42
F	-10	LYS	-	expression tag	UNP C3TR42
F	-9	GLY	-	expression tag	UNP C3TR42
F	-8	GLY	-	expression tag	UNP C3TR42
F	-7	GLY	-	expression tag	UNP C3TR42
F	-6	SER	-	expression tag	UNP C3TR42
F	-5	GLY	-	expression tag	UNP C3TR42
F	-4	GLY	-	expression tag	UNP C3TR42
F	-3	GLY	-	expression tag	UNP C3TR42
F	-2	SER	-	expression tag	UNP C3TR42
F	-1	GLY	-	expression tag	UNP C3TR42
F	0	GLY	-	expression tag	UNP C3TR42
F	1	SER	-	expression tag	UNP C3TR42

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2	ALA	-	expression tag	UNP C3TR42
F	3	TRP	-	expression tag	UNP C3TR42
F	4	SER	-	expression tag	UNP C3TR42
F	5	HIS	-	expression tag	UNP C3TR42
F	6	PRO	-	expression tag	UNP C3TR42
F	7	GLN	-	expression tag	UNP C3TR42
F	8	PHE	-	expression tag	UNP C3TR42
F	9	GLU	-	expression tag	UNP C3TR42
F	10	LYS	-	expression tag	UNP C3TR42
F	11	SER	-	expression tag	UNP C3TR42
F	12	SER	-	expression tag	UNP C3TR42
F	13	GLY	-	expression tag	UNP C3TR42
F	14	GLU	-	expression tag	UNP C3TR42
F	15	ASN	-	expression tag	UNP C3TR42
F	16	LEU	-	expression tag	UNP C3TR42
F	17	TYR	-	expression tag	UNP C3TR42
F	18	PHE	-	expression tag	UNP C3TR42
F	19	GLN	-	expression tag	UNP C3TR42
F	20	GLY	-	expression tag	UNP C3TR42
F	27	CYS	LYS	engineered mutation	UNP C3TR42

- Molecule 7 is a protein called Darobactin-B.

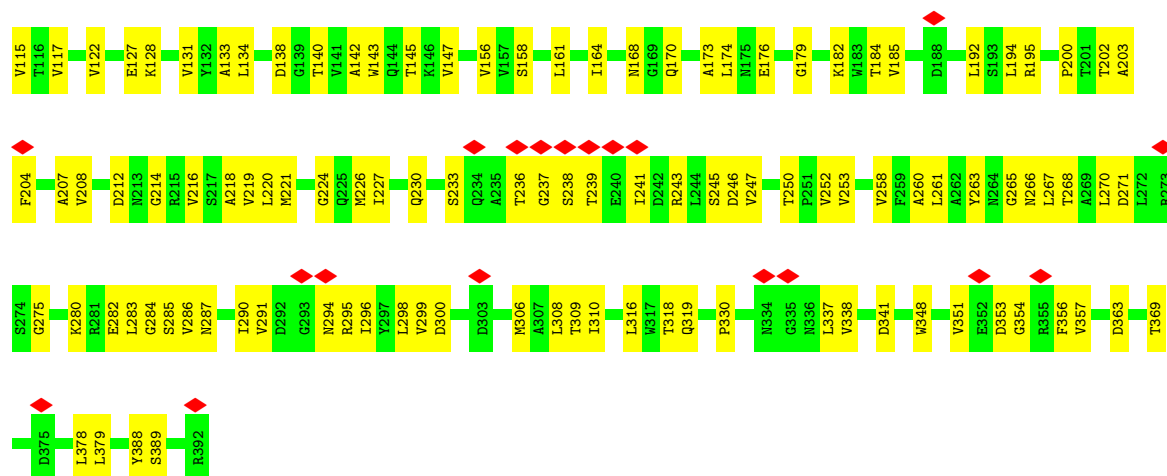
Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	7	Total	C	H	N	O	0	0
			139	51	63	14	11		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

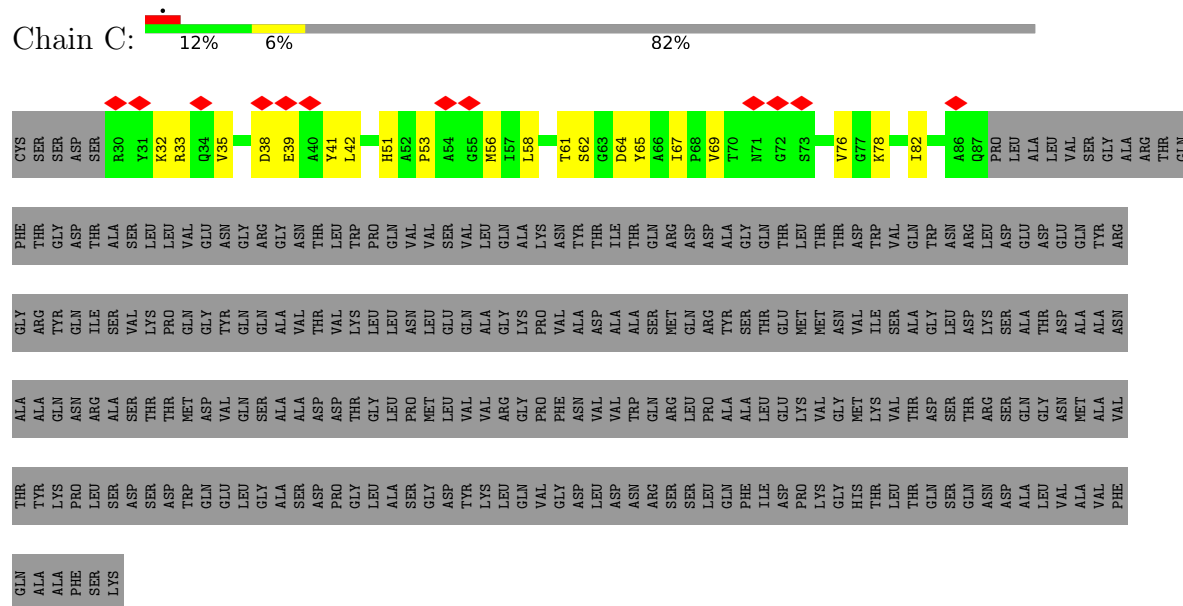
Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	

- Molecule 9 is water.

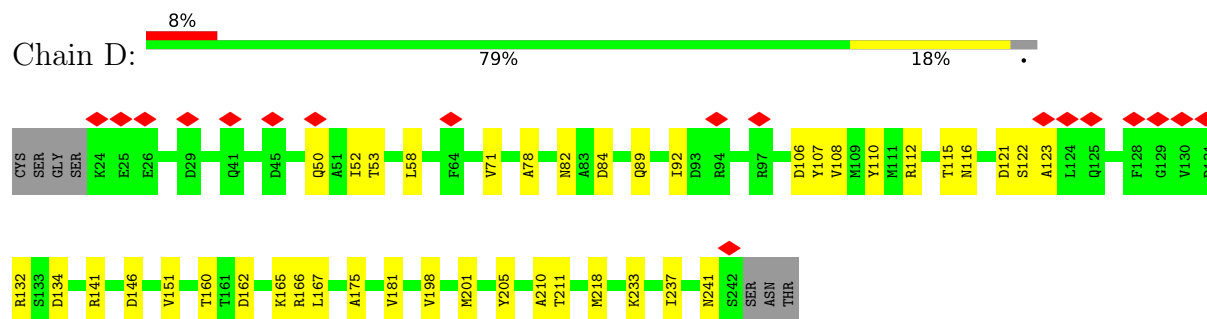
Mol	Chain	Residues	Atoms		AltConf
9	B	2	Total	O	0
			2	2	



• Molecule 3: Outer membrane protein assembly factor BamC



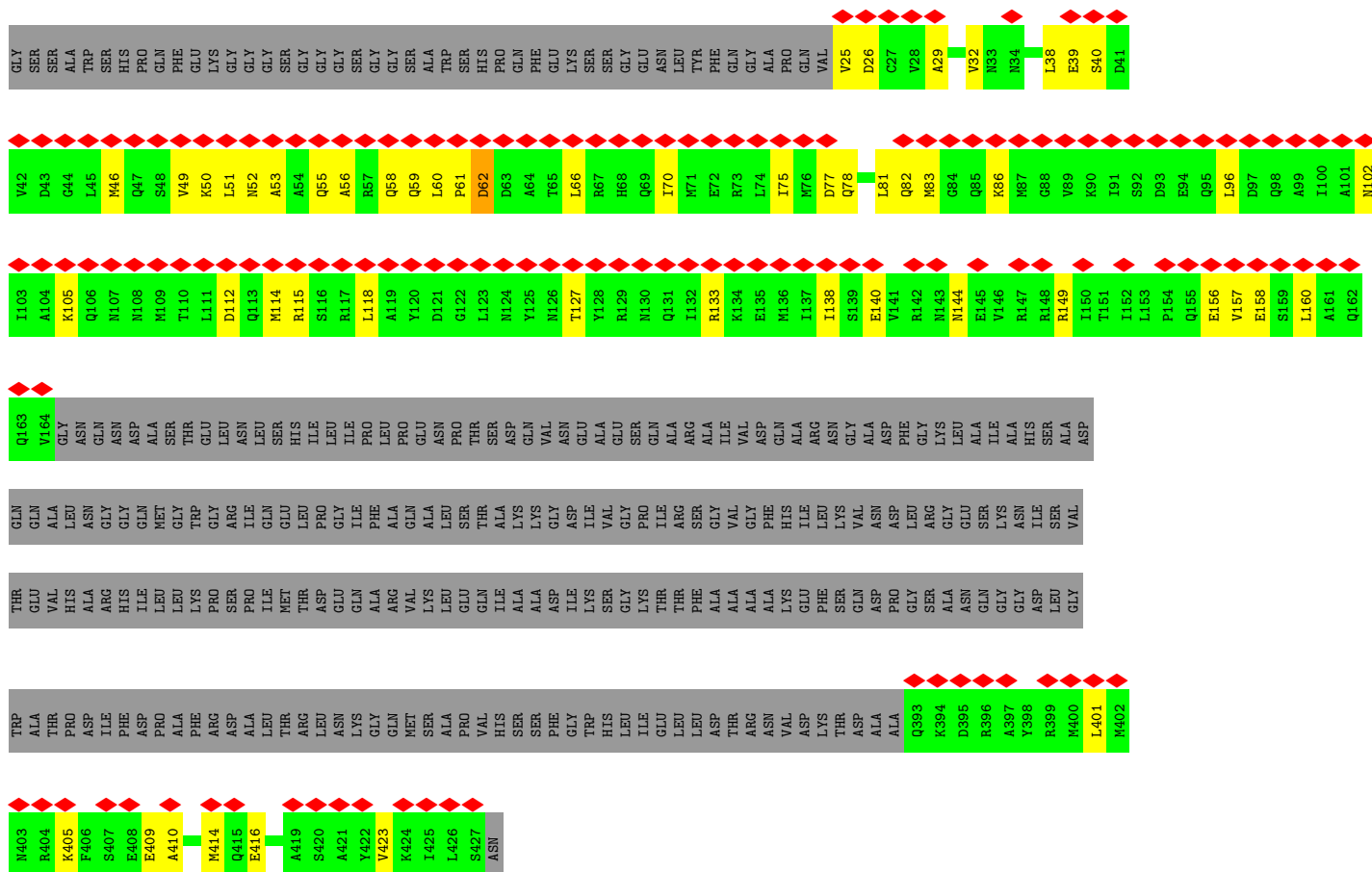
• Molecule 4: Outer membrane protein assembly factor BamD



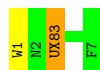
• Molecule 5: Outer membrane protein assembly factor BamE



- Molecule 6: Chaperone SurA



- Molecule 7: Darobactin-B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	164058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.8	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0153	Depositor
Map size ($\text{\AA}$)	273.0, 273.0, 273.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.91, 0.91, 0.91	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UX8

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	0.22	0/6345	0.31	0/8608
2	B	0.21	0/2825	0.34	0/3852
3	C	0.18	0/425	0.43	0/581
4	D	0.21	0/1812	0.29	0/2460
5	E	0.21	0/672	0.31	0/917
6	F	0.14	0/1410	0.32	0/1892
7	I	0.18	0/62	0.25	0/79
All	All	0.21	0/13551	0.32	0/18389

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	6202	5913	5913	119	0
2	B	2775	2600	2718	109	0
3	C	416	388	411	27	0
4	D	1772	1713	1713	42	0
5	E	657	634	634	17	0
6	F	1401	1427	1427	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	76	63	60	2	0
8	B	1	0	0	0	0
9	B	2	0	0	0	0
All	All	13302	12738	12876	315	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 12.

The worst 5 of 315 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)
6:F:149:ARG:NE	6:F:409:GLU:OE2	2.04	0.90
3:C:56:MET:HE2	4:D:237:ILE:HD11	1.56	0.88
2:B:194:LEU:N	2:B:246:ASP:OD2	2.07	0.87
5:E:51:THR:OG1	5:E:54:GLN:OE1	1.91	0.87
1:A:470:GLU:OE2	1:A:472:SER:OG	1.96	0.84

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	783/790 (99%)	739 (94%)	44 (6%)	0	100	100
2	B	367/373 (98%)	332 (90%)	35 (10%)	0	100	100
3	C	56/320 (18%)	47 (84%)	9 (16%)	0	100	100
4	D	217/226 (96%)	208 (96%)	9 (4%)	0	100	100
5	E	82/104 (79%)	78 (95%)	4 (5%)	0	100	100
6	F	171/450 (38%)	157 (92%)	13 (8%)	1 (1%)	21	51
7	I	4/7 (57%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1680/2270 (74%)	1565 (93%)	114 (7%)	1 (0%)	49 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	62	ASP

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	669/672 (100%)	669 (100%)	0	100	100
2	B	300/304 (99%)	300 (100%)	0	100	100
3	C	41/258 (16%)	41 (100%)	0	100	100
4	D	184/190 (97%)	184 (100%)	0	100	100
5	E	73/90 (81%)	73 (100%)	0	100	100
6	F	154/367 (42%)	154 (100%)	0	100	100
7	I	6/6 (100%)	6 (100%)	0	100	100
All	All	1427/1887 (76%)	1427 (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 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	336	ASN
4	D	72	GLN
7	I	2	ASN
6	F	107	ASN
6	F	130	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	UX8	I	3	7	13,16,17	3.56	9 (69%)	17,22,24	5.23	10 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	UX8	I	3	7	-	0/9/10/12	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	3	UX8	CD2-CG	6.70	1.57	1.44
7	I	3	UX8	O9-CB	-5.46	1.31	1.42
7	I	3	UX8	CD2-CE2	5.09	1.47	1.41
7	I	3	UX8	CA-N	-4.85	1.33	1.47
7	I	3	UX8	CZ3-CE3	3.39	1.44	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	3	UX8	CE2-NE1-CD1	12.24	119.97	109.08
7	I	3	UX8	CG-CD1-NE1	-9.66	102.47	110.31
7	I	3	UX8	CD2-CG-CD1	7.66	112.10	106.25
7	I	3	UX8	O-C-CA	6.87	142.44	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	3	UX8	CE2-CD2-CG	-6.14	101.26	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	3	UX8	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

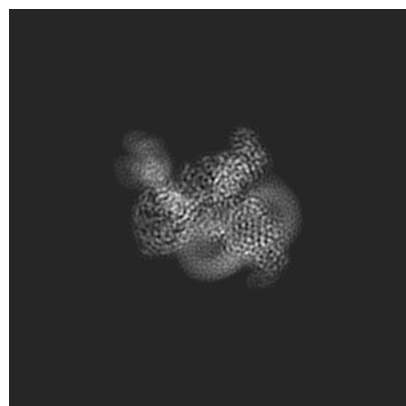
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18046. These allow visual inspection of the internal detail of the map and identification of artifacts.

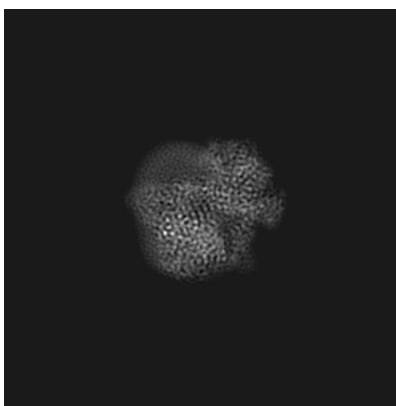
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

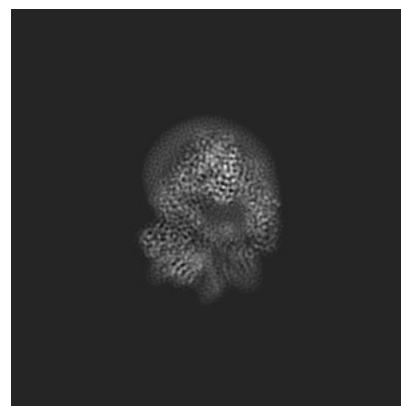
6.1.1 Primary map



X

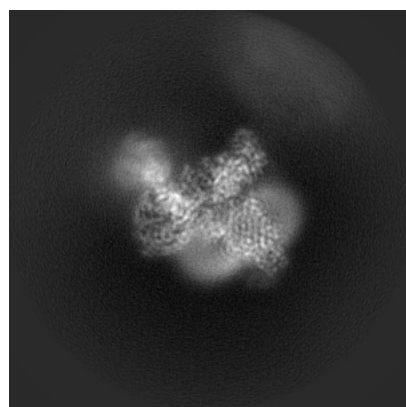


Y

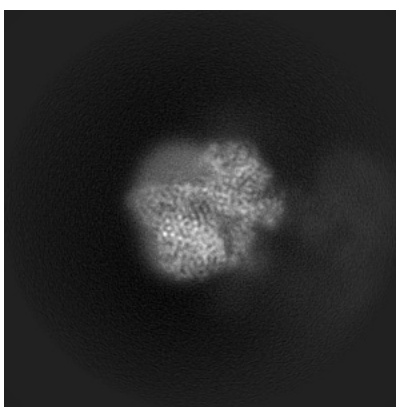


Z

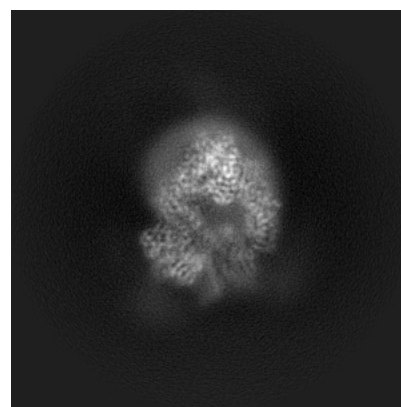
6.1.2 Raw map



X



Y

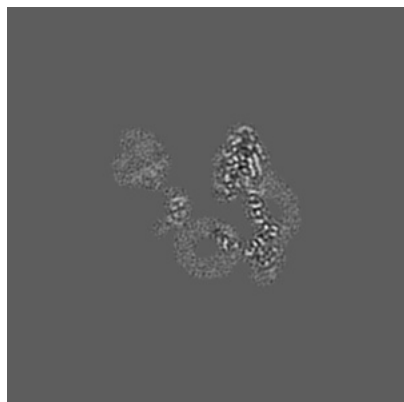


Z

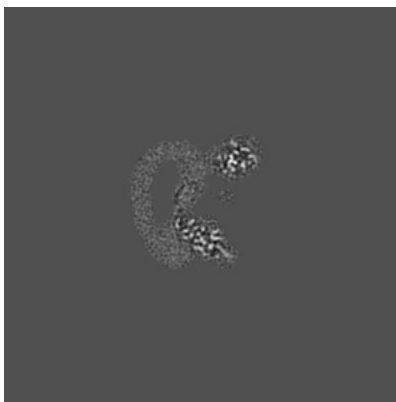
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

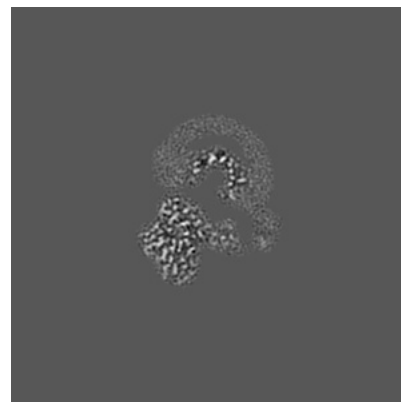
6.2.1 Primary map



X Index: 150



Y Index: 150

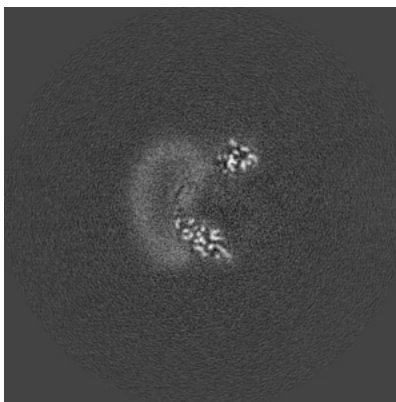


Z Index: 150

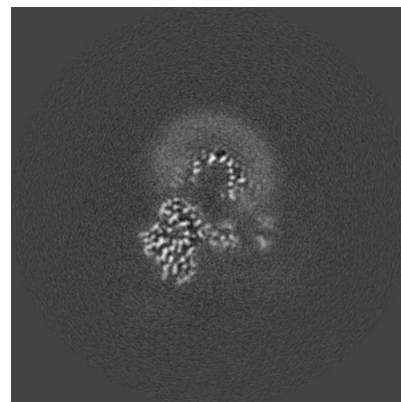
6.2.2 Raw map



X Index: 150



Y Index: 150

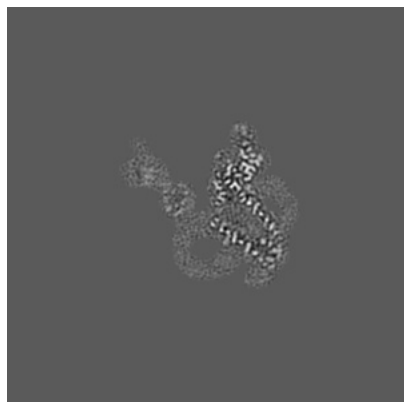


Z Index: 150

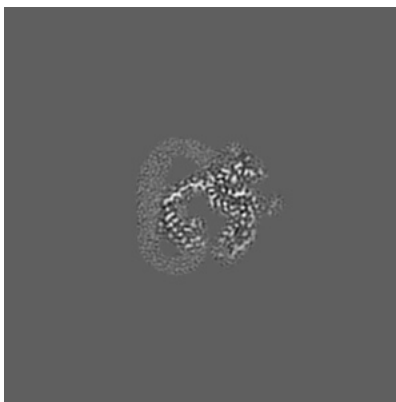
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

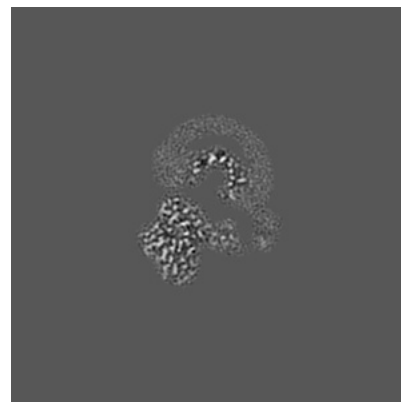
6.3.1 Primary map



X Index: 160

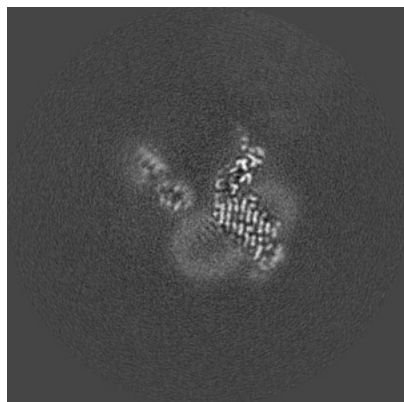


Y Index: 166

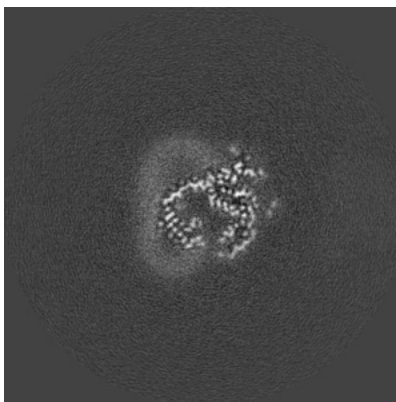


Z Index: 150

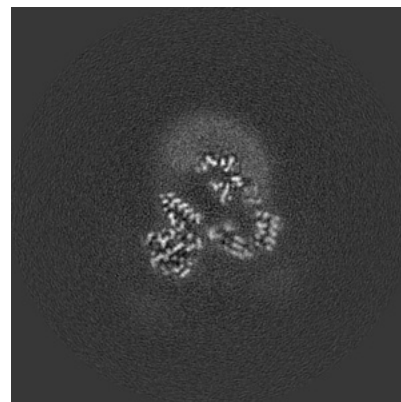
6.3.2 Raw map



X Index: 165



Y Index: 166

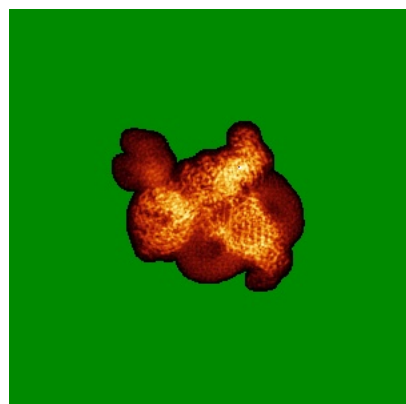


Z Index: 156

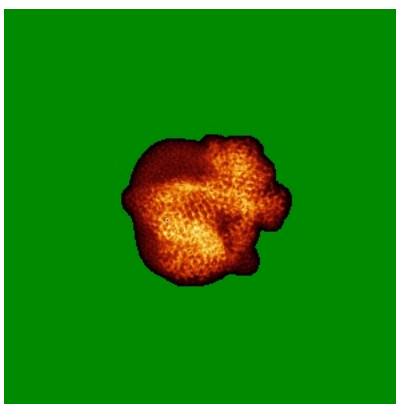
The images above show the largest variance slices of the map in three orthogonal directions.

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

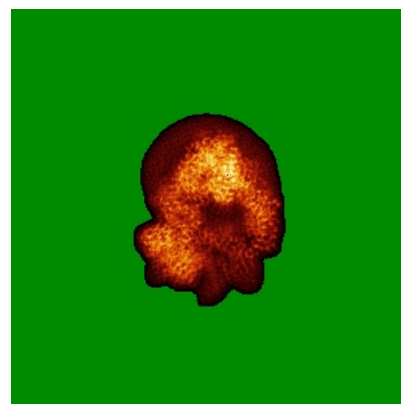
6.4.1 Primary map



X

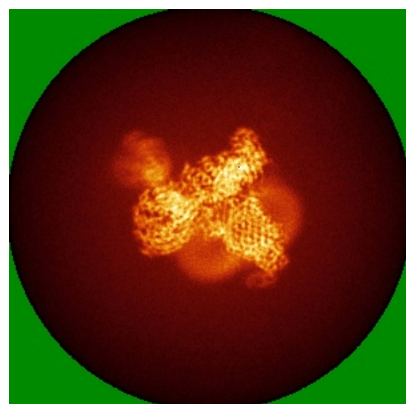


Y

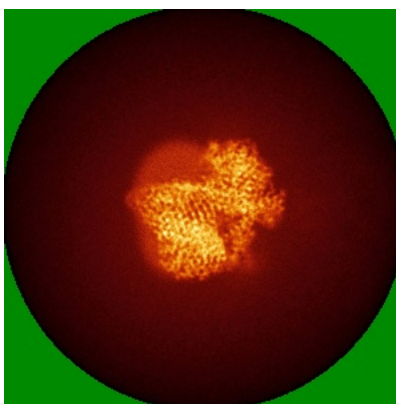


Z

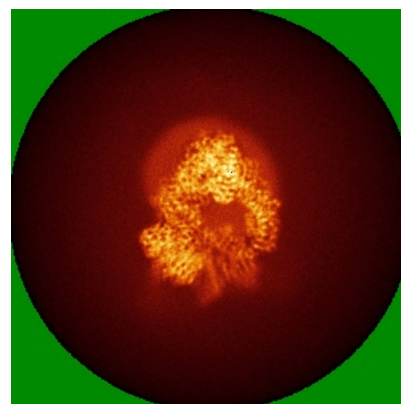
6.4.2 Raw map



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 0.0153. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

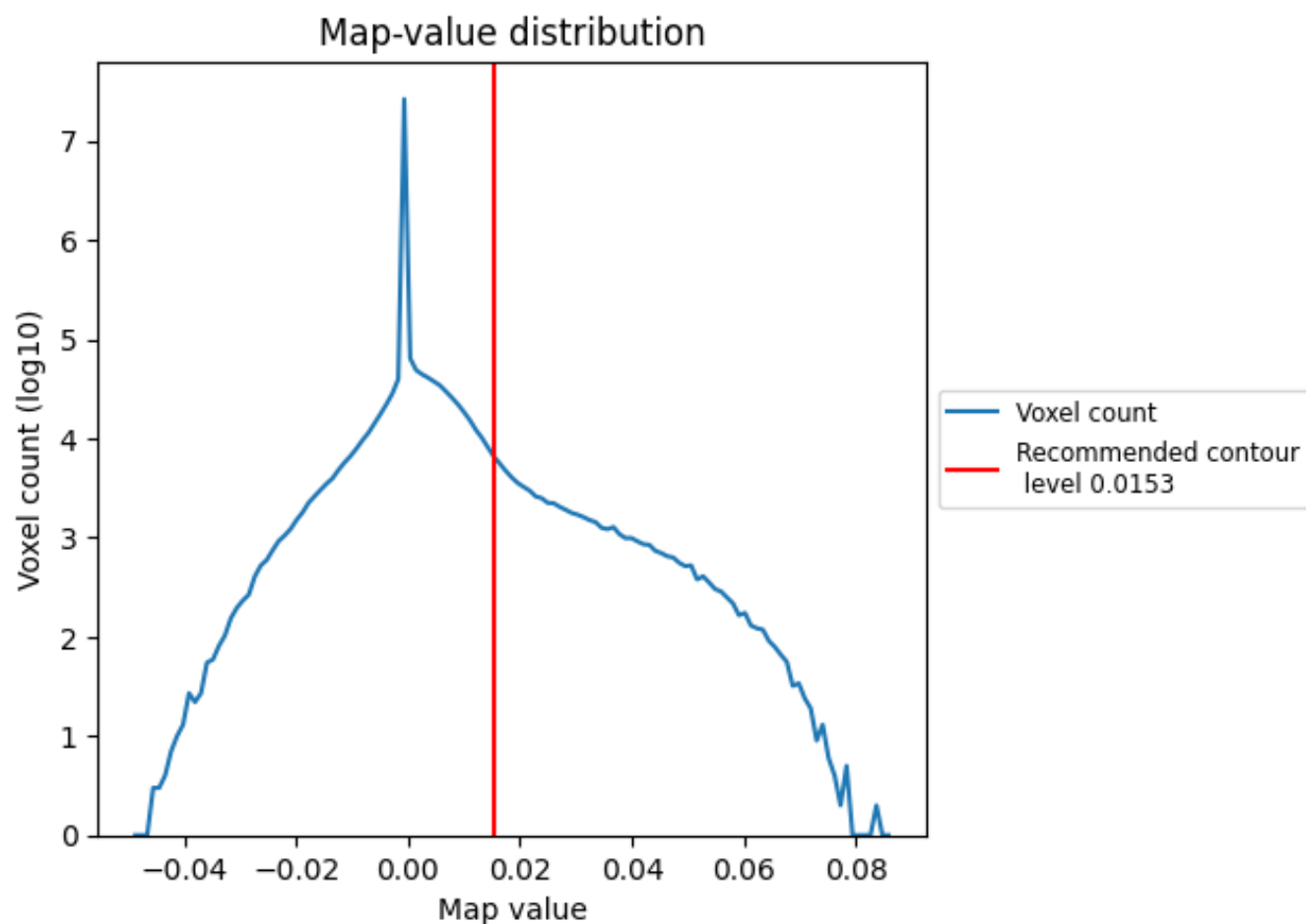
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

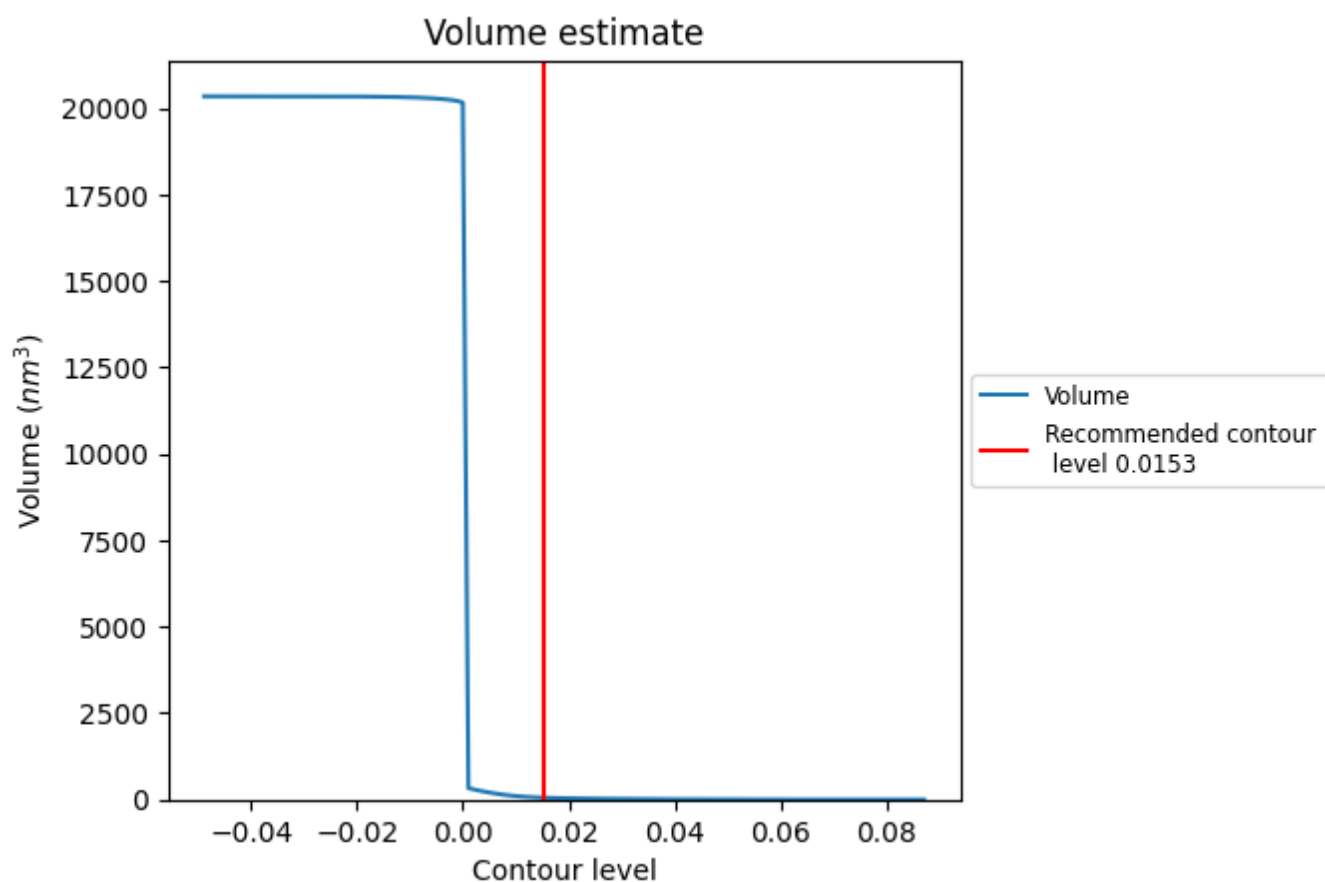
This section contains the results of statistical analysis of the map.

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.

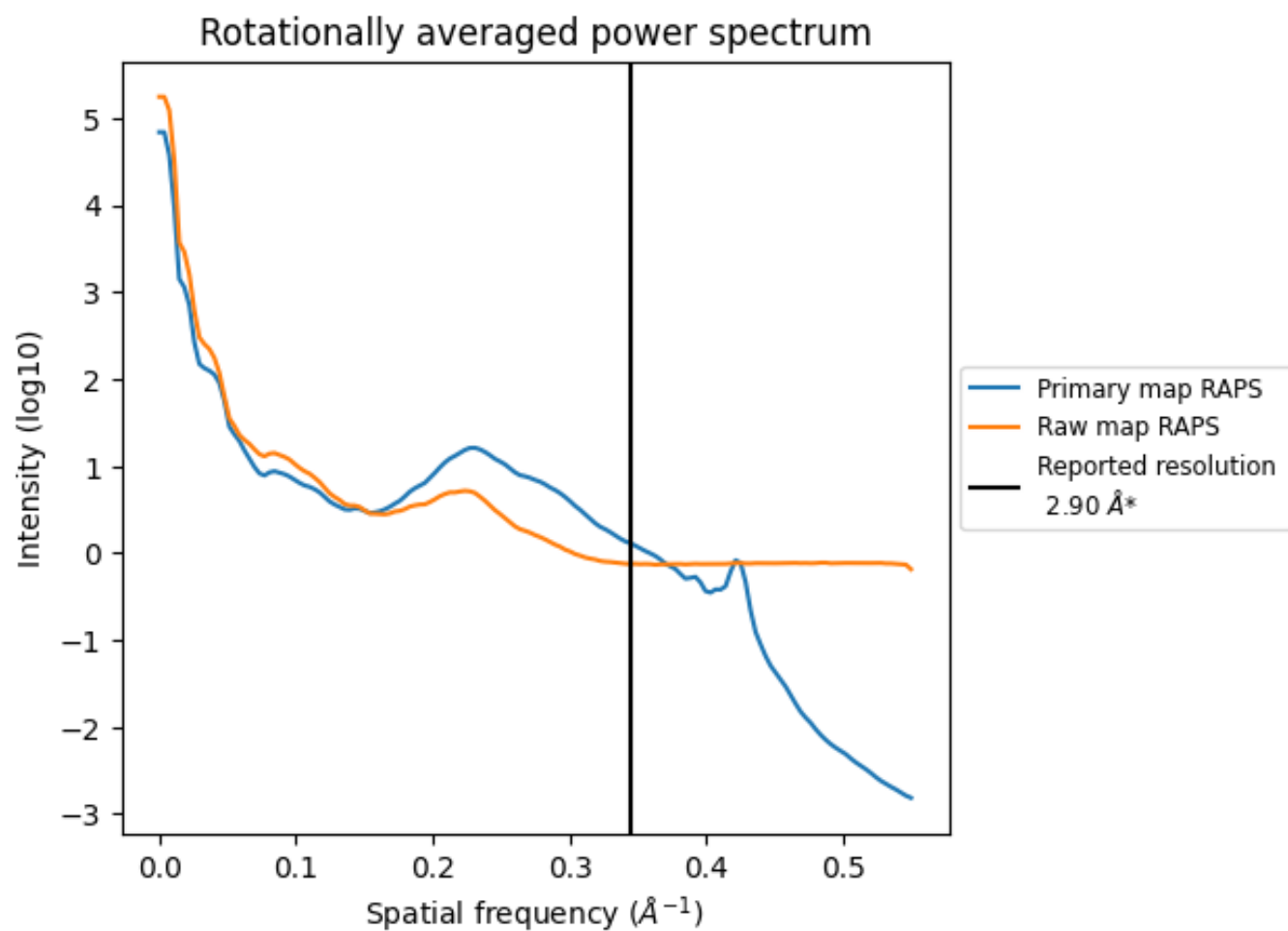
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm^3 ; this corresponds to an approximate mass of 47 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 ⓘ

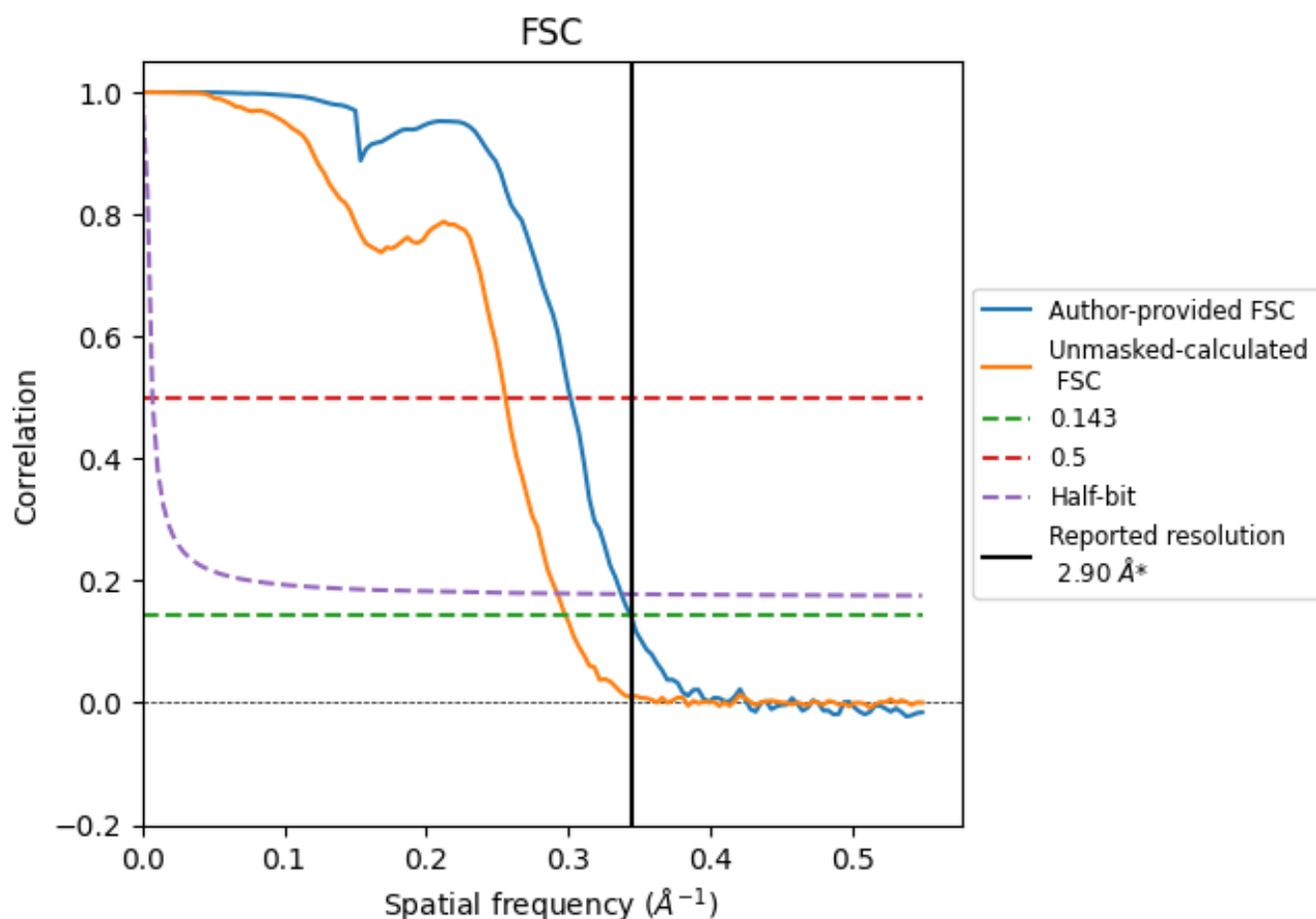


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

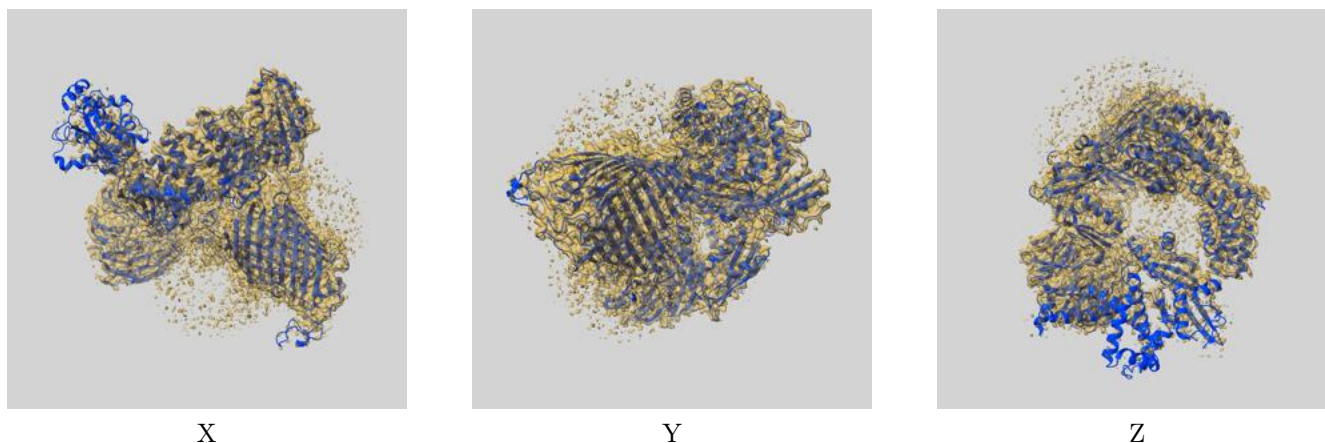
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.31	2.96
Unmasked-calculated*	3.35	3.91	3.42

*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 3.35 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

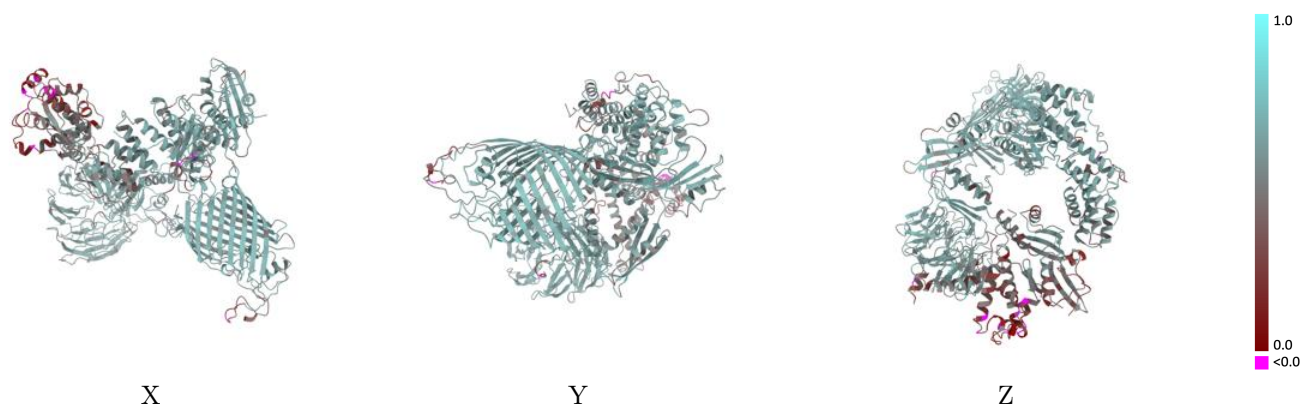
This section contains information regarding the fit between EMDB map EMD-18046 and PDB model 8PZV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0153 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](#)

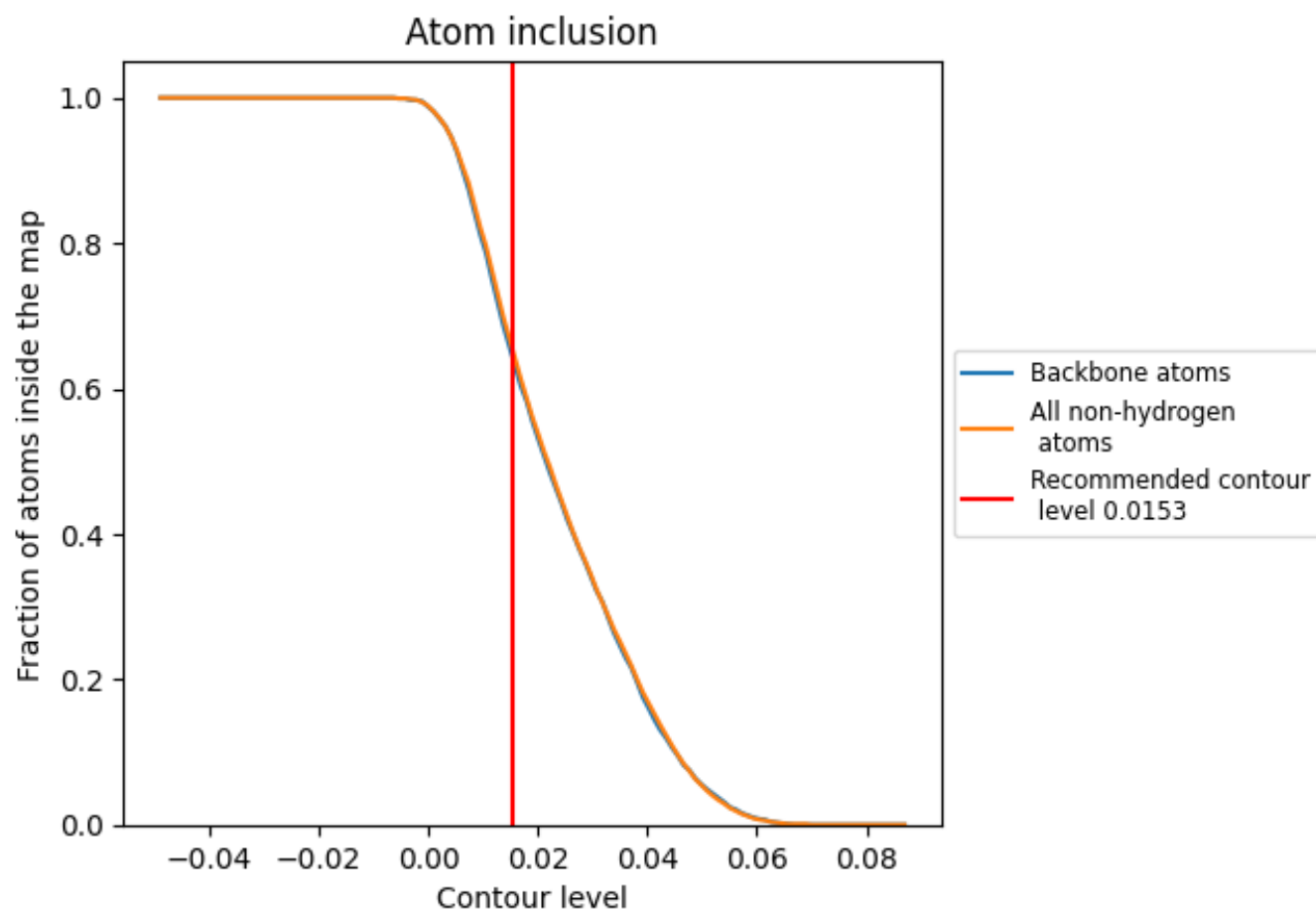


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 66% 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 (0.0153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.5480
A	0.7120	0.5740
B	0.7370	0.5790
C	0.5670	0.4880
D	0.7390	0.5770
E	0.7570	0.5760
F	0.1950	0.3330
I	0.8190	0.5920

1.0

0.0

<0.0