



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 10:41 AM UTC

PDB ID : 9P1U / pdb_00009p1u
EMDB ID : EMD-71134
Title : beta-barrel assembly machine from Escherichia coli in an late state of LptD assembly
Authors : Thomson, B.D.; Marquez, M.D.; Kahne, D.
Deposited on : 2025-06-10
Resolution : 4.10 Å (reported)
Based on initial models : ., 5LJ0

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:

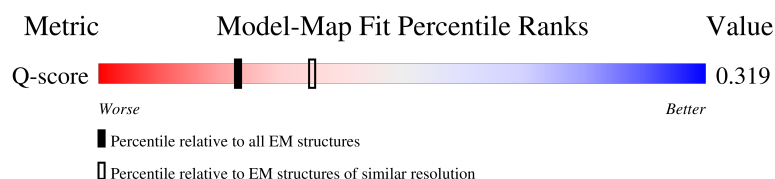
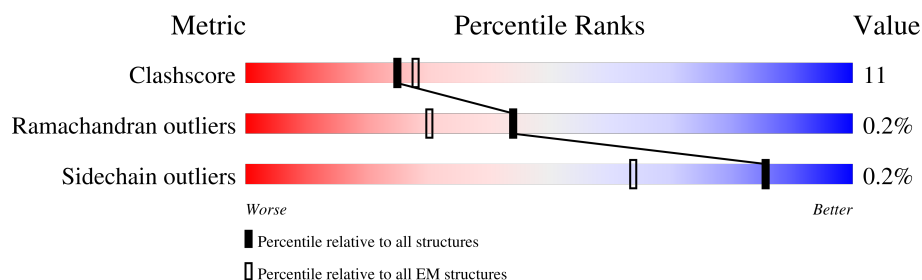
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	C	344	 12% 84%
2	D	245	 64% 22% 14%
3	E	113	 71% 6% 23%
4	G	193	 59% 19% 23%

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Mol	Chain	Length	Quality of chain
5	F	819	<p>42% 14% 44%</p>
6	B	392	<p>5% 64% 24%</p>
7	A	818	<p>20% 78% 16% 5%</p>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 30798 atoms, of which 14946 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 BamC.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	54	Total	C	H	N	O	S	0	0
			751	239	374	62	75	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	211	Total	C	H	N	O	S	0	0
			3362	1076	1654	301	324	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	87	Total	C	H	N	O	S	0	0
			1352	432	667	119	132	2		

- Molecule 4 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	149	Total	C	H	N	O	S	0	0
			2370	731	1200	211	220	8		

- Molecule 5 is a protein called LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	459	Total	C	H	N	O	S	0	0
			7266	2360	3512	642	741	11		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	TRP	-	expression tag	UNP P31554
F	-6	SER	-	expression tag	UNP P31554
F	-5	HIS	-	expression tag	UNP P31554

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	PRO	-	expression tag	UNP P31554
F	-3	GLN	-	expression tag	UNP P31554
F	-2	PHE	-	expression tag	UNP P31554
F	-1	GLU	-	expression tag	UNP P31554
F	0	LYS	-	expression tag	UNP P31554
F	1	GLY	-	expression tag	UNP P31554
F	2	GLY	-	expression tag	UNP P31554
F	3	GLY	-	expression tag	UNP P31554
F	4	SER	-	expression tag	UNP P31554
F	5	GLY	-	expression tag	UNP P31554
F	6	GLY	-	expression tag	UNP P31554
F	7	GLY	-	expression tag	UNP P31554
F	8	SER	-	expression tag	UNP P31554
F	9	GLY	-	expression tag	UNP P31554
F	10	GLY	-	expression tag	UNP P31554
F	11	SER	-	expression tag	UNP P31554
F	12	ALA	-	expression tag	UNP P31554
F	13	TRP	-	expression tag	UNP P31554
F	14	SER	-	expression tag	UNP P31554
F	15	HIS	-	expression tag	UNP P31554
F	16	PRO	-	expression tag	UNP P31554
F	17	GLN	-	expression tag	UNP P31554
F	18	PHE	-	expression tag	UNP P31554
F	19	GLU	-	expression tag	UNP P31554
F	20	LYS	-	expression tag	UNP P31554
F	21	GLY	-	expression tag	UNP P31554
F	22	SER	-	expression tag	UNP P31554
F	23	GLY	-	expression tag	UNP P31554
F	24	SER	-	expression tag	UNP P31554
F	25	GLY	-	expression tag	UNP P31554
F	26	GLY	-	expression tag	UNP P31554
F	27	SER	-	expression tag	UNP P31554
F	28	ALA	-	expression tag	UNP P31554
F	259	CYS	ILE	engineered mutation	UNP P31554
F	?	-	ASP	deletion	UNP P31554

- Molecule 6 is a protein called Outer membrane protein assembly factor BamB.

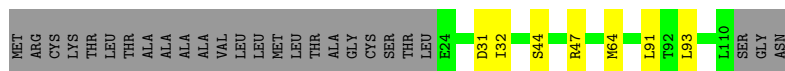
Mol	Chain	Residues	Atoms						AltConf	Trace
6	B	343	Total	C	H	N	O	S	0	0
			5102	1616	2532	440	508	6		

- Molecule 7 is a protein called Outer membrane protein assembly factor BamA.

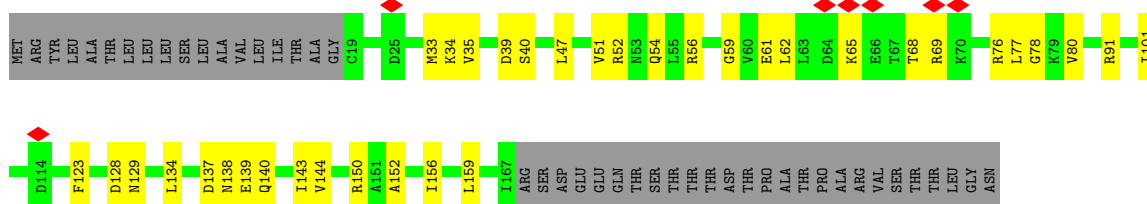
Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	777	Total	C	H	N	O	S	0	0
			10595	3453	5007	987	1133	15		

There are 9 discrepancies between the modelled and reference sequences:

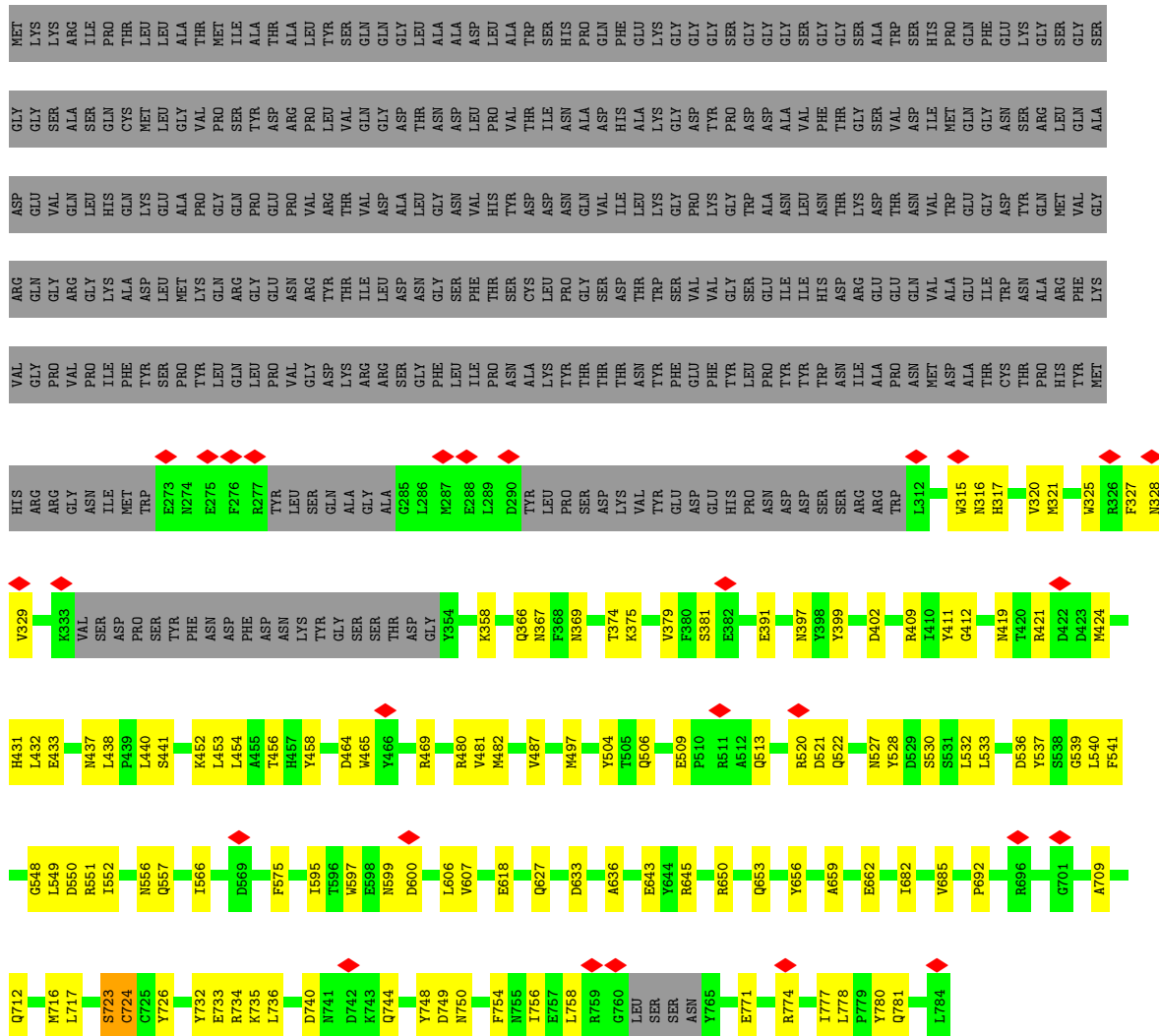
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	HIS	-	expression tag	UNP P0A940
A	17	HIS	-	expression tag	UNP P0A940
A	18	HIS	-	expression tag	UNP P0A940
A	19	HIS	-	expression tag	UNP P0A940
A	20	HIS	-	expression tag	UNP P0A940
A	21	HIS	-	expression tag	UNP P0A940
A	22	HIS	-	expression tag	UNP P0A940
A	23	HIS	-	expression tag	UNP P0A940
A	512	CYS	ASP	engineered mutation	UNP P0A940



• Molecule 4: LPS-assembly lipoprotein LptE

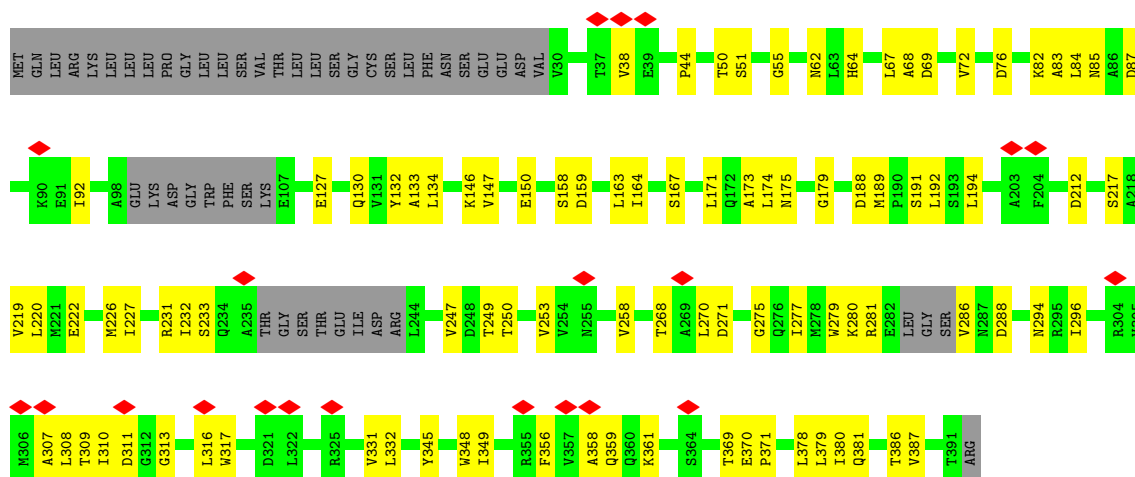


• Molecule 5: LPS-assembly protein LptD




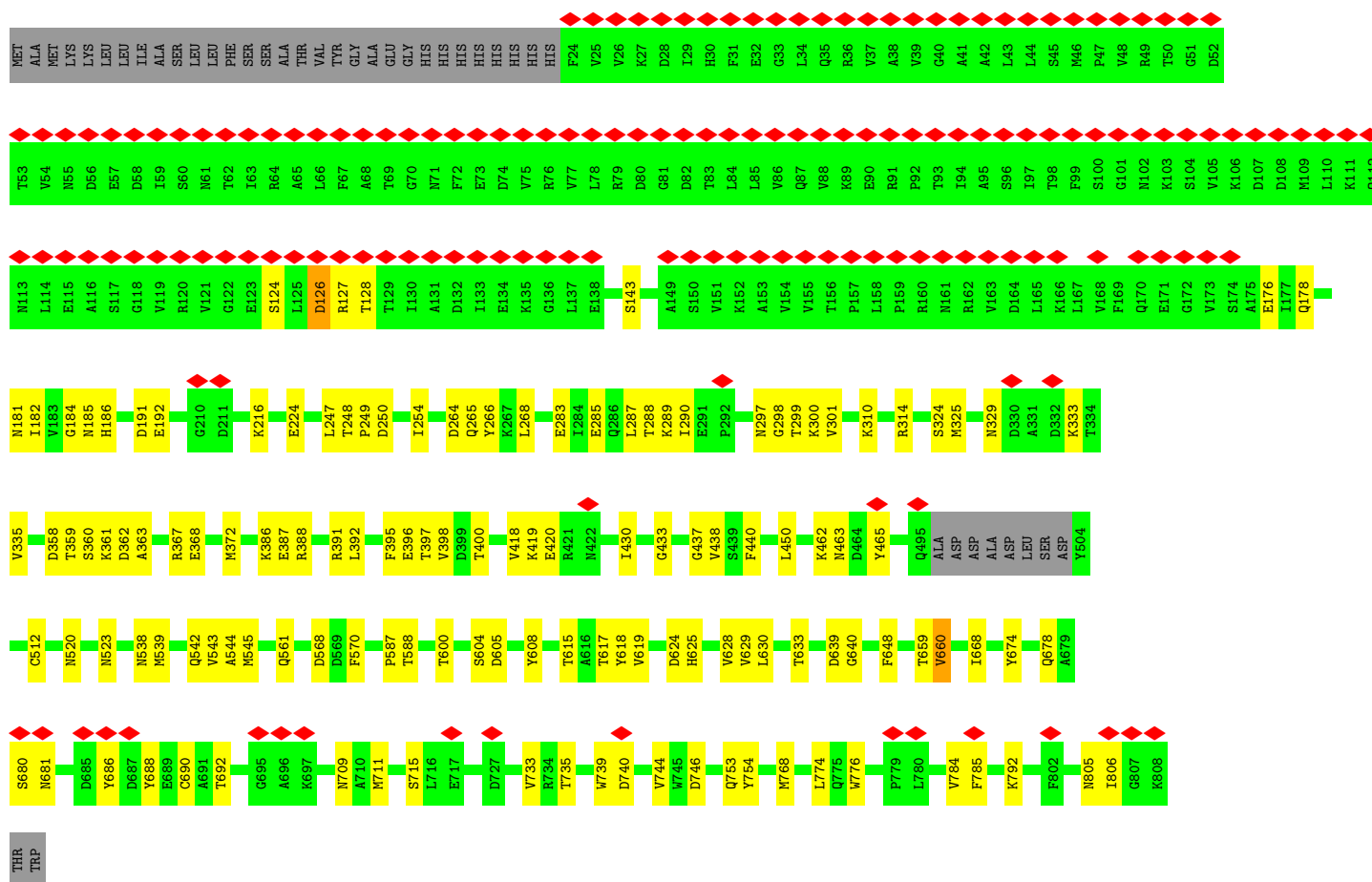
• Molecule 6: Outer membrane protein assembly factor BamB

Chain B: 



• Molecule 7: Outer membrane protein assembly factor BamA

Chain A: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79819	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 ($e^-/\text{\AA}^2$)	49.55	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	34.349	Depositor
Minimum map value	-19.043	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	6.1	Depositor
Map size (\AA)	323.84, 323.84, 323.84	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.736, 0.736, 0.736	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	C	0.15	0/386	0.36	0/531
2	D	0.20	0/1745	0.41	0/2367
3	E	0.17	0/700	0.32	0/955
4	G	0.19	0/1187	0.42	0/1603
5	F	0.22	0/3843	0.51	0/5220
6	B	0.13	0/2614	0.34	0/3565
7	A	0.17	0/5715	0.39	0/7689
All	All	0.18	0/16190	0.42	0/21930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	377	374	373	10	0
2	D	1708	1654	1653	45	0
3	E	685	667	666	4	0
4	G	1170	1200	1199	28	0
5	F	3754	3512	3506	99	0
6	B	2570	2532	2528	61	0
7	A	5588	5007	4865	92	0
All	All	15852	14946	14790	322	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 322 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)
5:F:774:ARG:NH2	5:F:780:TYR:O	1.93	1.00
7:A:715:SER:OG	7:A:740:ASP:OD1	1.90	0.88
6:B:188:ASP:O	6:B:189:MET:HE2	1.85	0.77
7:A:678:GLN:NE2	7:A:692:THR:OG1	2.17	0.77
7:A:387:GLU:OE2	7:A:391:ARG:NH2	2.18	0.76

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	C	52/344 (15%)	50 (96%)	2 (4%)	0	100	100
2	D	209/245 (85%)	201 (96%)	8 (4%)	0	100	100
3	E	85/113 (75%)	83 (98%)	2 (2%)	0	100	100
4	G	147/193 (76%)	145 (99%)	2 (1%)	0	100	100
5	F	449/819 (55%)	431 (96%)	18 (4%)	0	100	100
6	B	335/392 (86%)	323 (96%)	12 (4%)	0	100	100
7	A	773/818 (94%)	727 (94%)	42 (5%)	4 (0%)	24	61
All	All	2050/2924 (70%)	1960 (96%)	86 (4%)	4 (0%)	44	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	127	ARG
7	A	124	SER

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Mol	Chain	Res	Type
7	A	126	ASP
7	A	660	VAL

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	C	38/276 (14%)	38 (100%)	0	100	100
2	D	176/204 (86%)	176 (100%)	0	100	100
3	E	76/95 (80%)	76 (100%)	0	100	100
4	G	130/167 (78%)	130 (100%)	0	100	100
5	F	402/702 (57%)	400 (100%)	2 (0%)	81	82
6	B	277/321 (86%)	277 (100%)	0	100	100
7	A	533/696 (77%)	531 (100%)	2 (0%)	84	83
All	All	1632/2461 (66%)	1628 (100%)	4 (0%)	85	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	723	SER
5	F	724	CYS
7	A	178	GLN
7	A	512	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	542	GLN
7	A	678	GLN
6	B	135	ASN
6	B	144	GLN
6	B	170	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.

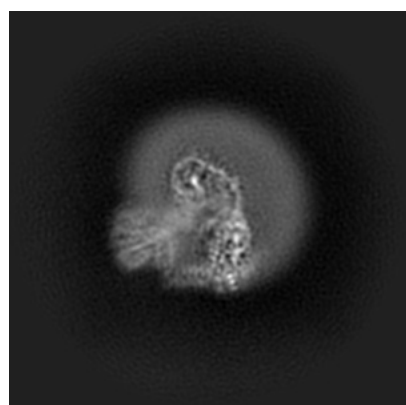
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71134. These allow visual inspection of the internal detail of the map and identification of artifacts.

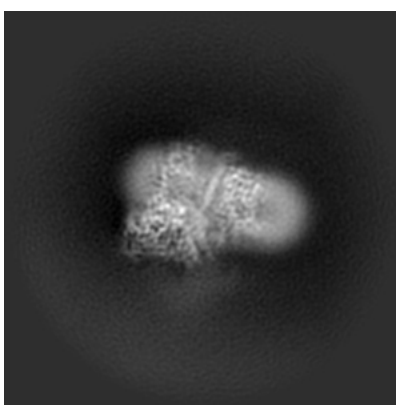
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

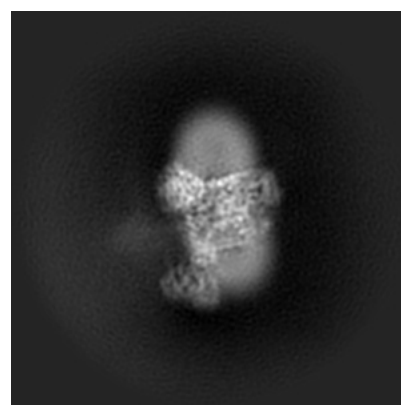
6.1.1 Primary map



X



Y

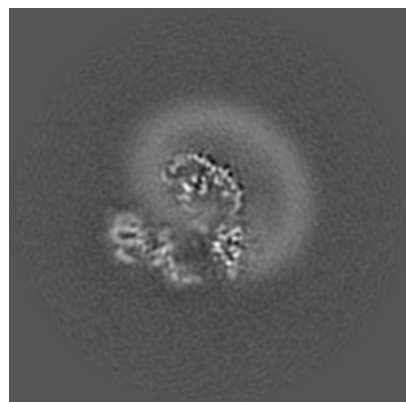


Z

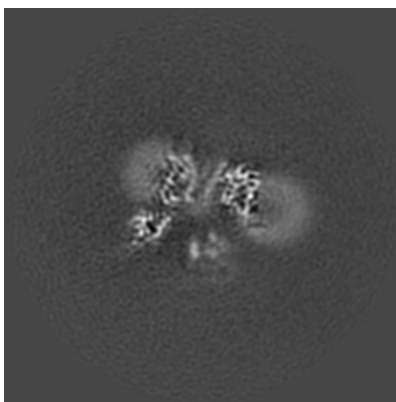
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

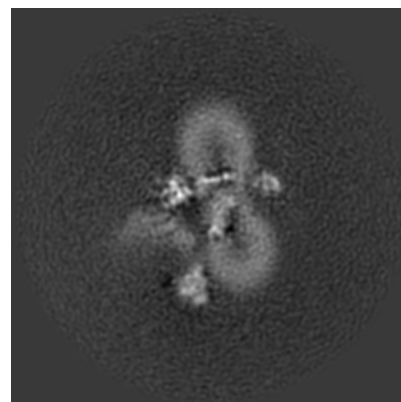
6.2.1 Primary map



X Index: 220



Y Index: 220

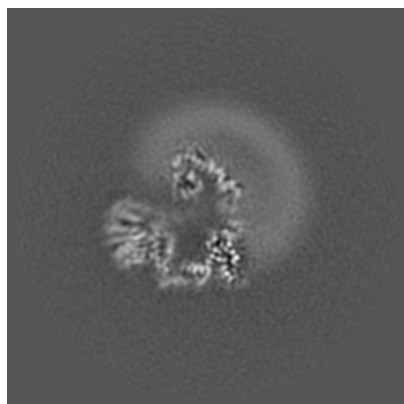


Z Index: 220

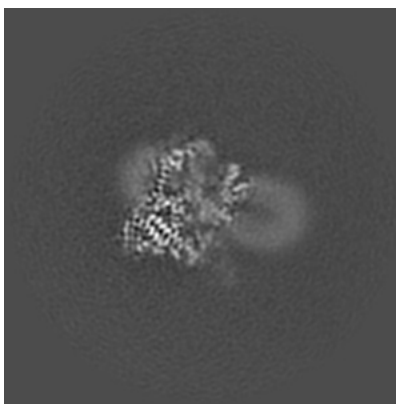
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

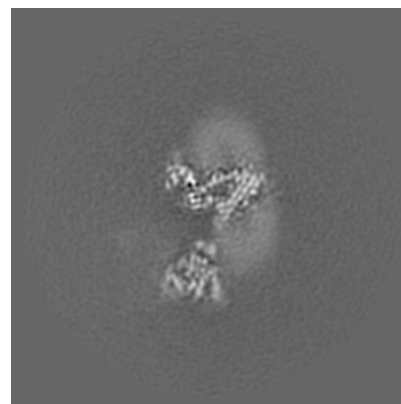
6.3.1 Primary map



X Index: 208



Y Index: 249

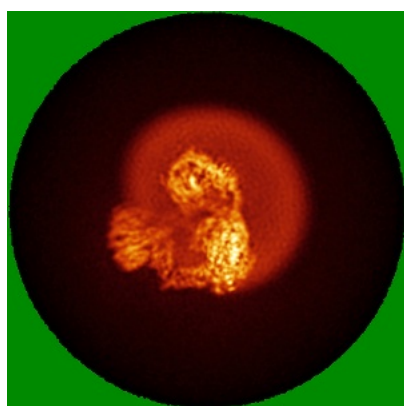


Z Index: 176

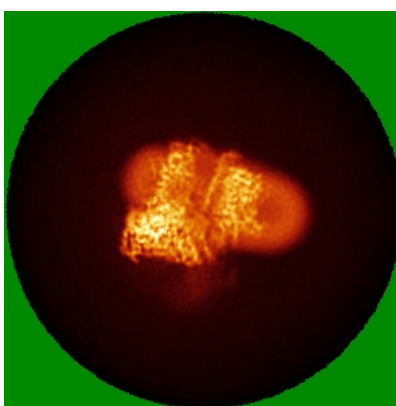
The images above show the largest variance slices of the map in three orthogonal directions.

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

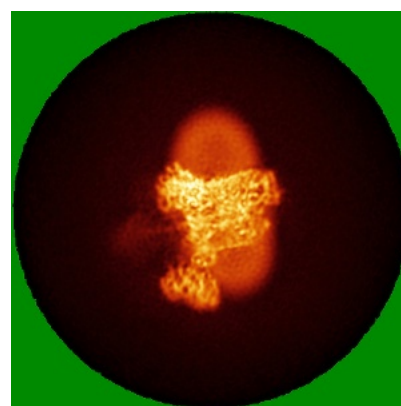
6.4.1 Primary map



X



Y



Z

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

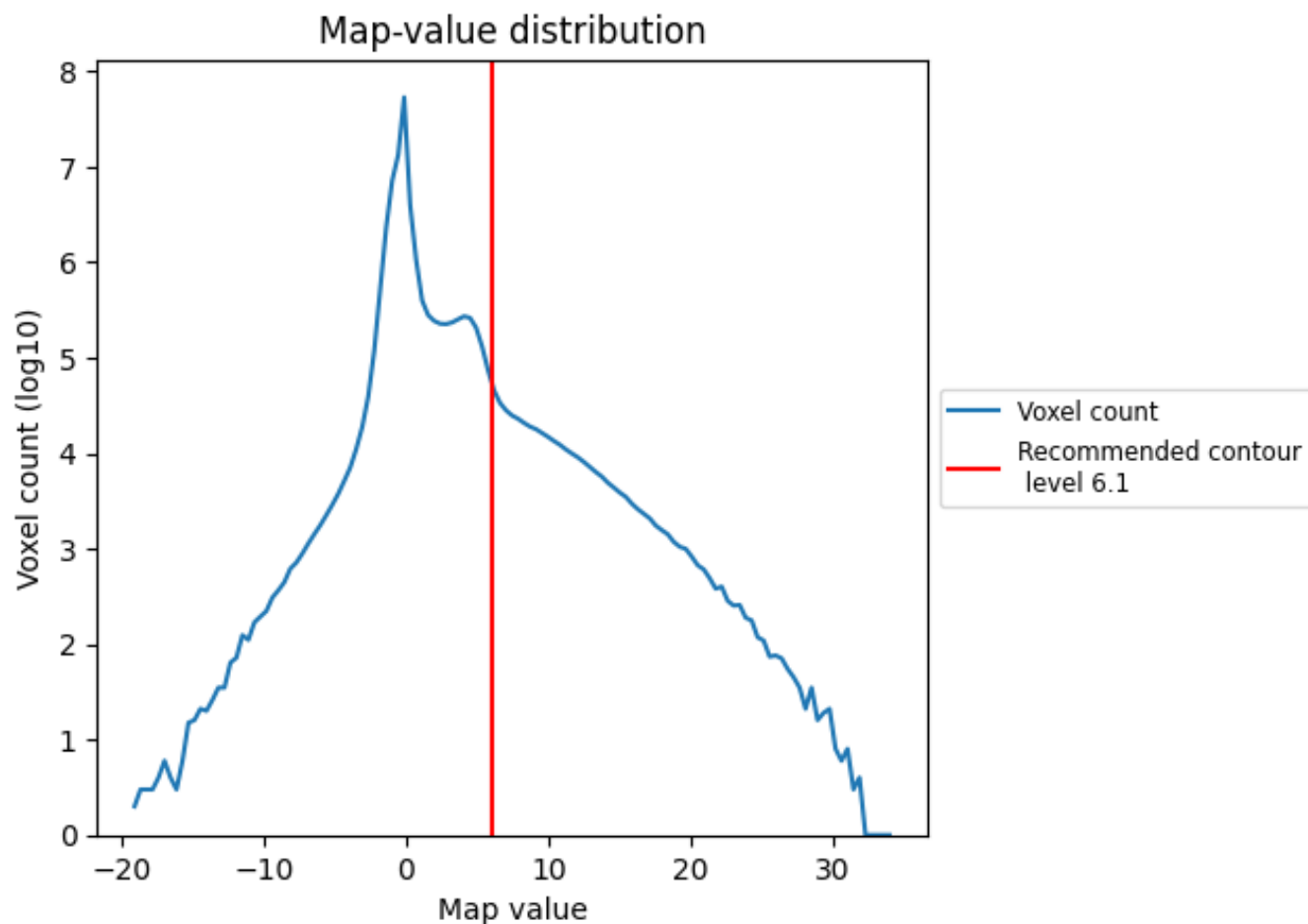
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

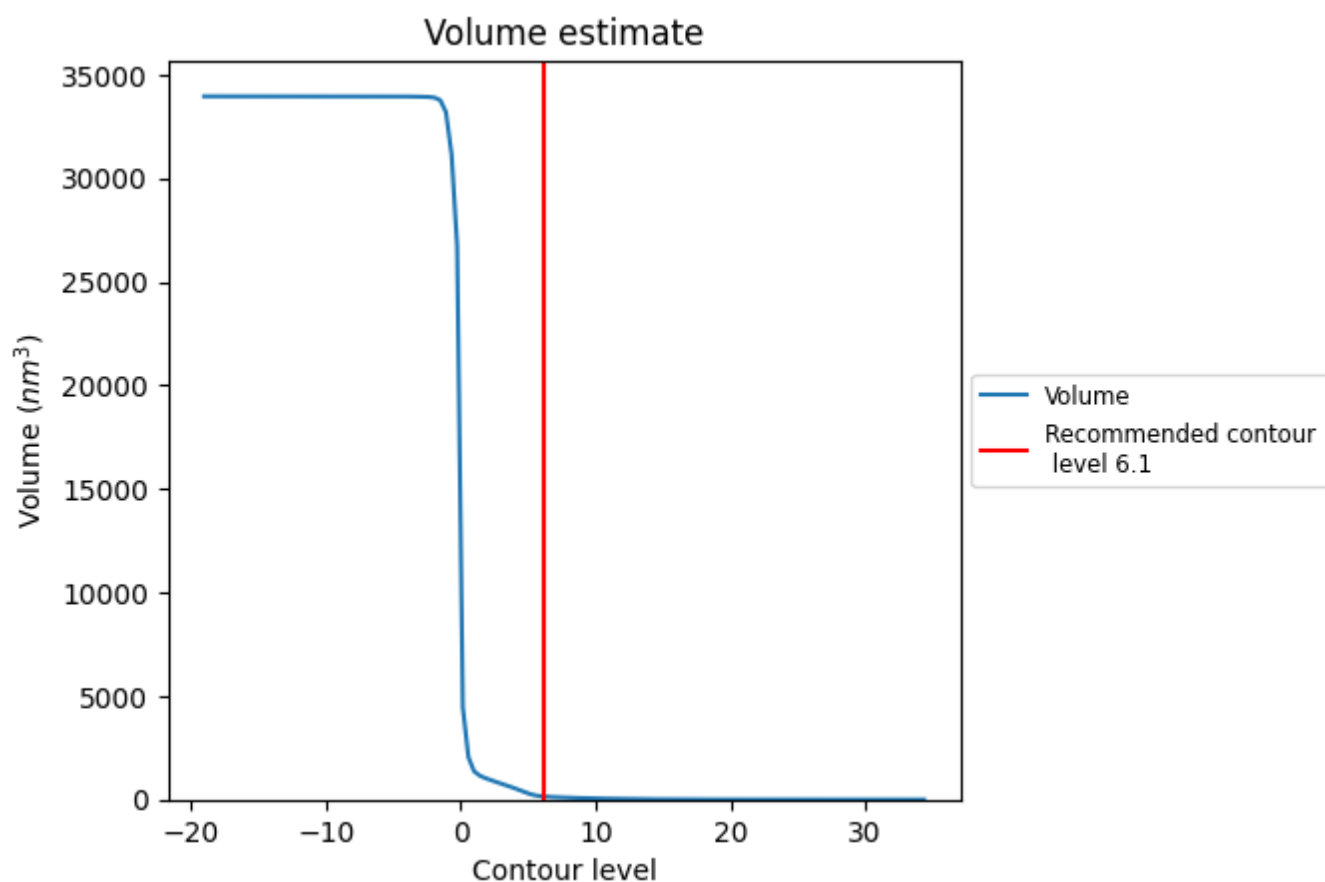
This section contains the results of statistical analysis of the map.

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.

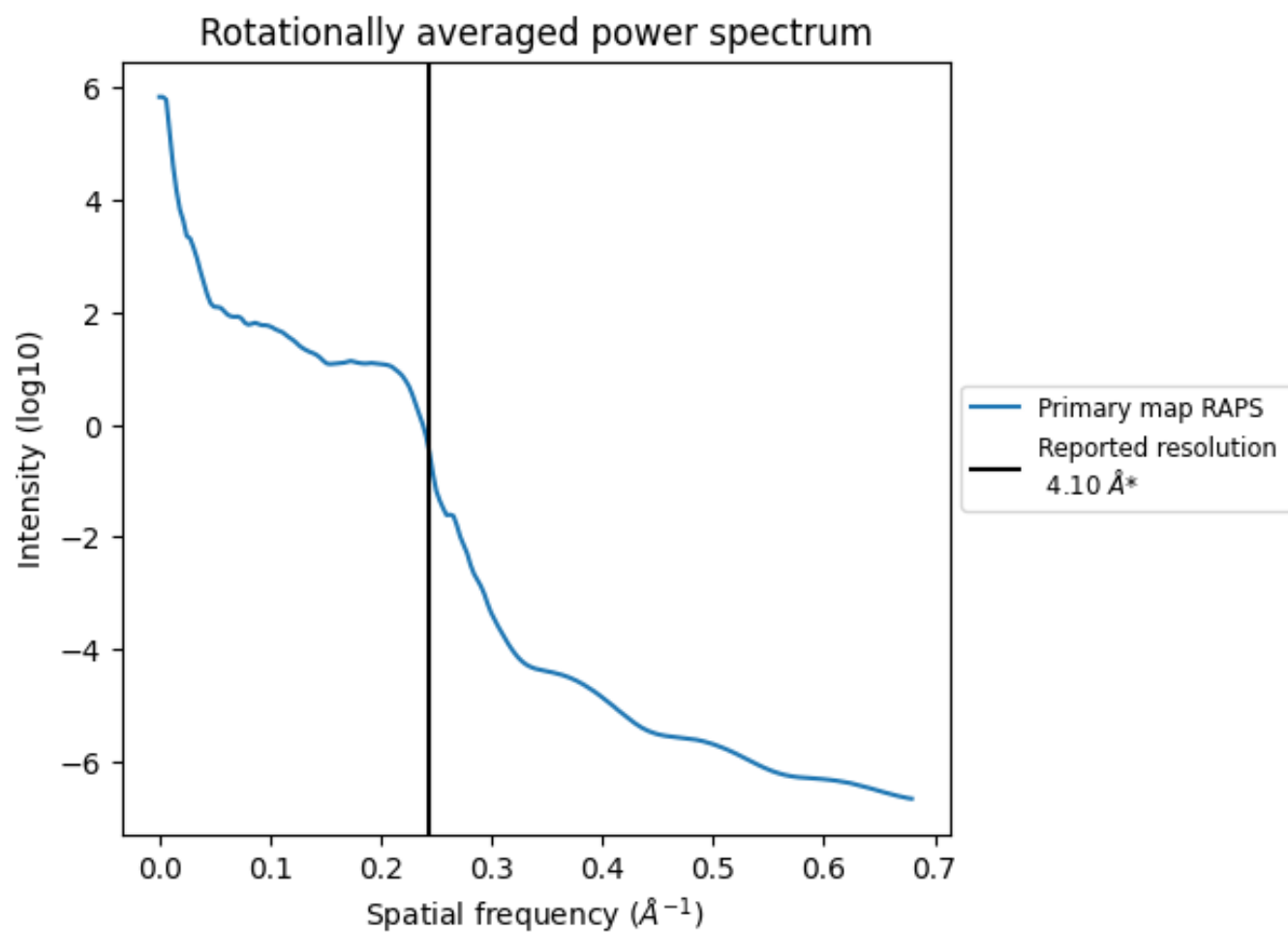
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 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 0.244 Å⁻¹

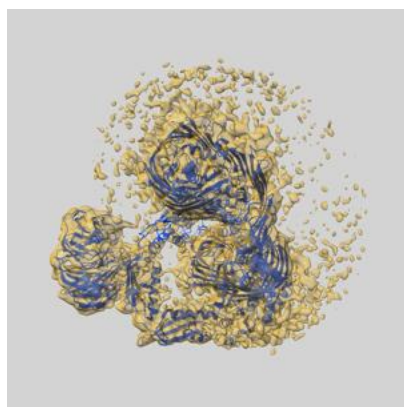
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

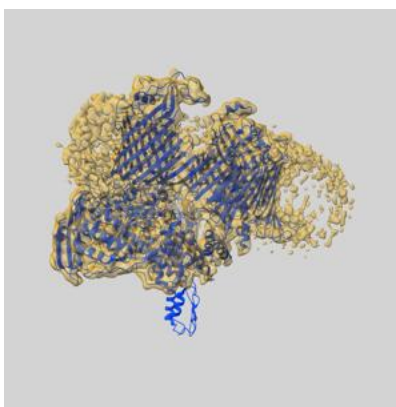
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71134 and PDB model 9P1U. Per-residue inclusion information can be found in section [3](#) on page [7](#).

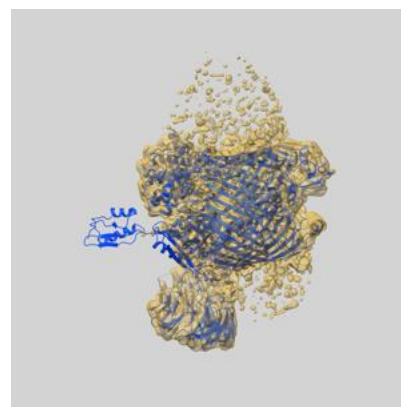
9.1 Map-model overlay [i](#)



X



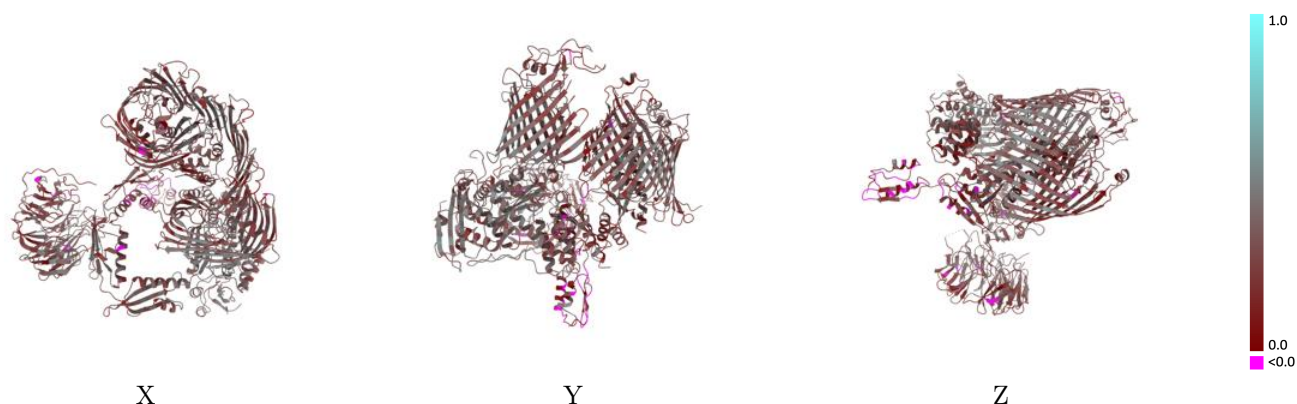
Y



Z

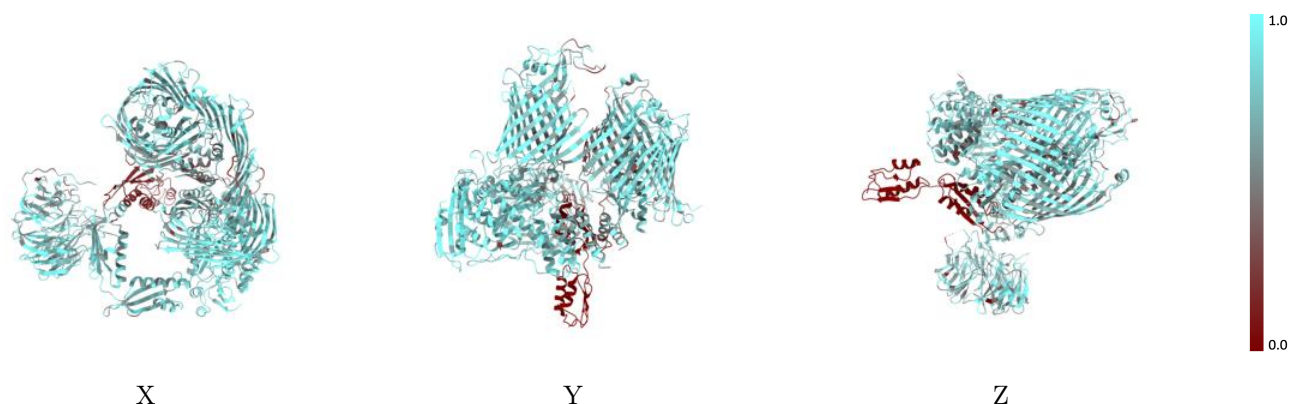
The images above show the 3D surface view of the map at the recommended contour level 6.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



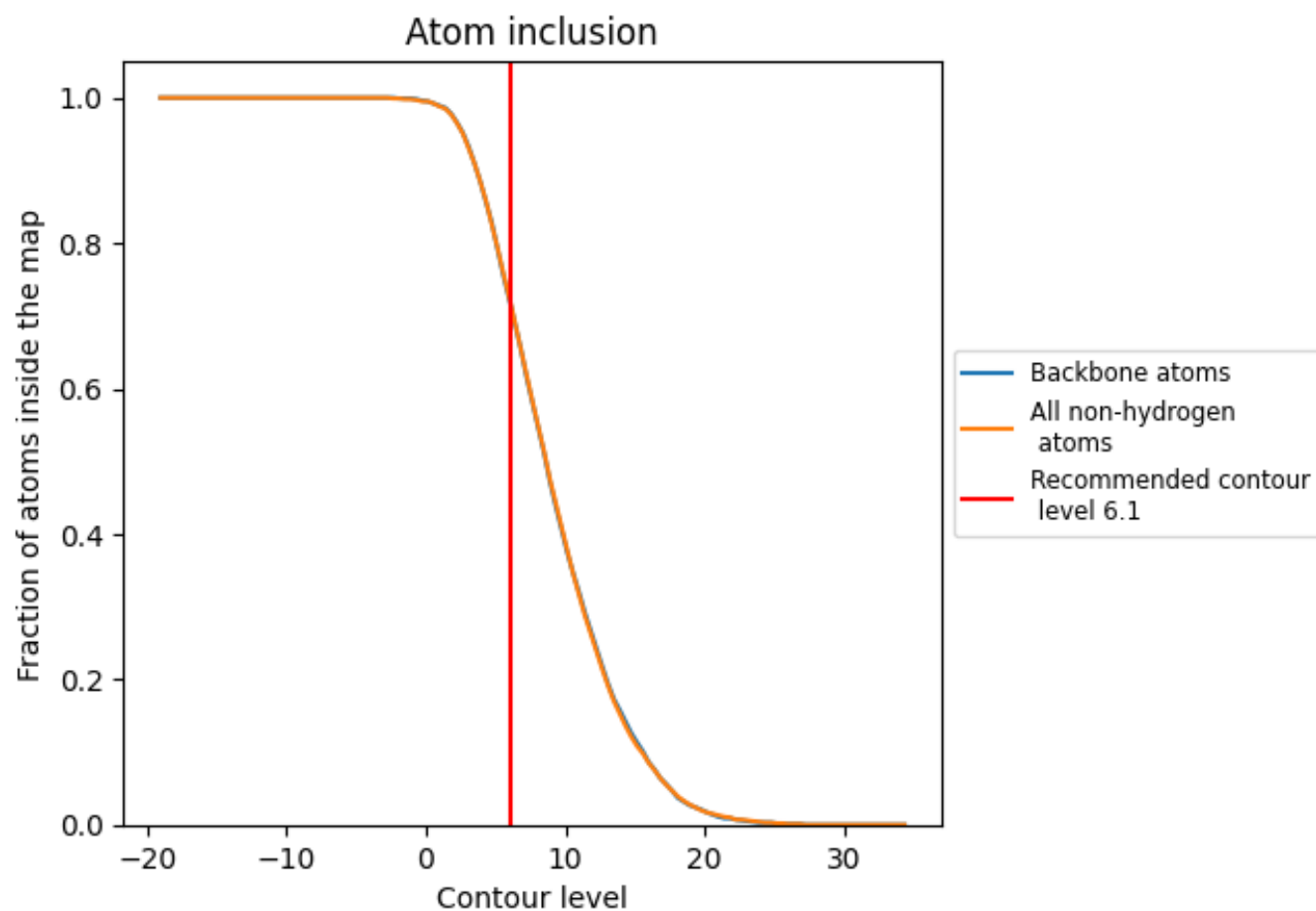
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 72% 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 (6.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7160	<div></div> 0.3190
A	<div></div> 0.6810	<div></div> 0.3220
B	<div></div> 0.7210	<div></div> 0.2920
C	<div></div> 0.7400	<div></div> 0.3620
D	<div></div> 0.7530	<div></div> 0.3320
E	<div></div> 0.8900	<div></div> 0.4070
F	<div></div> 0.7300	<div></div> 0.3030
G	<div></div> 0.7290	<div></div> 0.3330

1.0

0.0

<0.0