



Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 12:35 AM EDT

PDB ID : 7LBY
EMDB ID : EMD-23267
Title : Bacterial cellulose synthase BcsB with polyalanine BcsA model
Authors : Acheson, J.F.; Zimmer, J.
Deposited on : 2021-01-09
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation 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.dev113
MolProbity : 4.02b-467
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) : 2.39

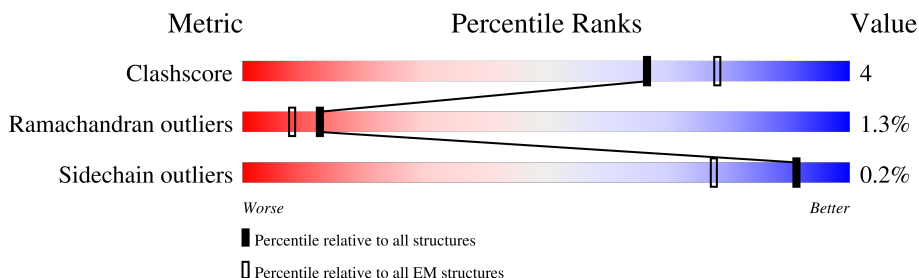
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	886	
2	B	779	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cellulose synthase catalytic subunit [UDP-forming].

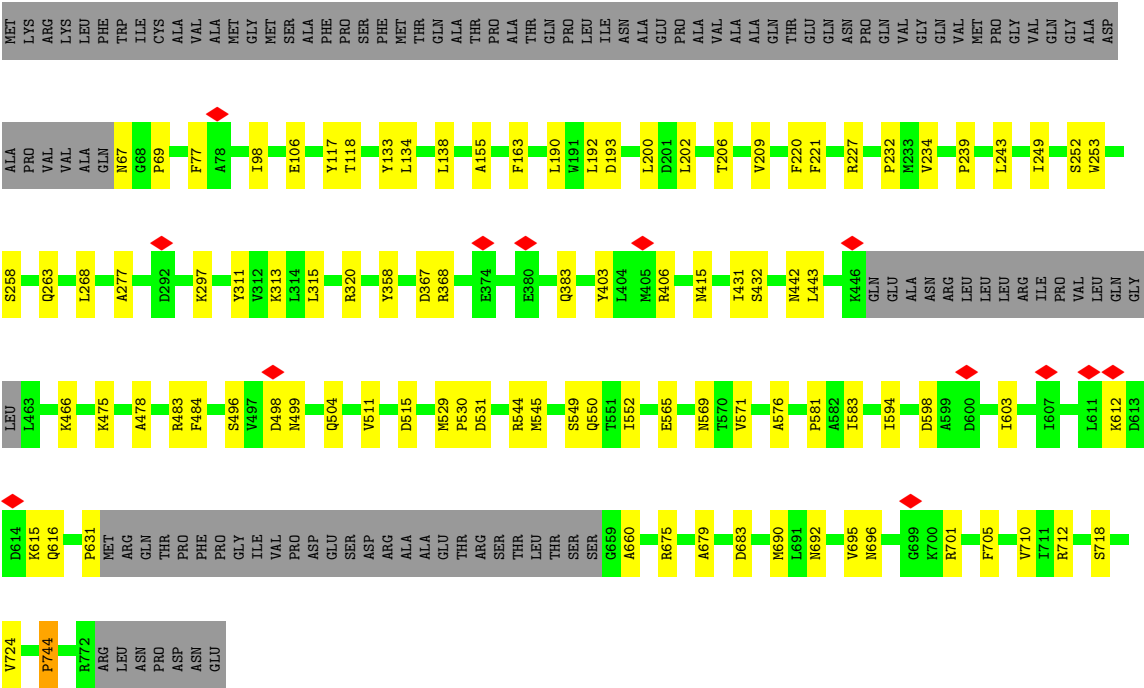
Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	755	Total	C	N	O	0	0
			3724	2214	755	755		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	expression tag	UNP P37653
A	956	PRO	ARG	conflict	UNP P37653
A	975	HIS	-	expression tag	UNP P37653
A	976	HIS	-	expression tag	UNP P37653
A	977	HIS	-	expression tag	UNP P37653
A	978	HIS	-	expression tag	UNP P37653
A	979	HIS	-	expression tag	UNP P37653
A	980	HIS	-	expression tag	UNP P37653
A	981	LEU	-	expression tag	UNP P37653
A	982	GLU	-	expression tag	UNP P37653
A	983	HIS	-	expression tag	UNP P37653
A	984	HIS	-	expression tag	UNP P37653
A	985	HIS	-	expression tag	UNP P37653
A	986	HIS	-	expression tag	UNP P37653
A	987	HIS	-	expression tag	UNP P37653
A	988	HIS	-	expression tag	UNP P37653

- Molecule 2 is a protein called Cyclic di-GMP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	663	Total	C	N	O	S	0	0
			5076	3227	869	957	23		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193152	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.841	Depositor
Minimum map value	-1.783	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.235	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/3721	0.68	40/5174 (0.8%)
2	B	0.25	0/5193	0.46	2/7074 (0.0%)
All	All	0.27	0/8914	0.57	42/12248 (0.3%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	706	PRO	N-CA-CB	7.56	112.37	103.30
1	A	147	PRO	N-CA-CB	7.06	111.77	103.30
1	A	475	PRO	N-CA-CB	6.86	111.53	103.30
1	A	342	PRO	N-CA-CB	6.77	111.42	103.30
1	A	360	PRO	N-CA-CB	6.69	111.33	103.30
1	A	763	PRO	N-CA-CB	6.66	111.30	103.30
1	A	557	PRO	N-CA-CB	6.62	111.24	103.30
1	A	477	PRO	N-CA-CB	6.54	111.15	103.30
1	A	764	PRO	N-CA-CB	6.38	110.96	103.30
1	A	445	PRO	N-CA-CB	6.11	110.63	103.30
1	A	337	PRO	N-CA-CB	6.10	110.62	103.30
1	A	714	PRO	N-CA-CB	6.09	110.60	103.30
2	B	631	PRO	N-CA-CB	5.89	110.38	103.30
1	A	705	PRO	N-CA-CB	5.85	110.32	103.30
1	A	740	PRO	N-CA-CB	5.85	110.32	103.30
1	A	489	PRO	N-CA-CB	5.83	110.29	103.30
1	A	274	PRO	N-CA-CB	5.82	110.29	103.30
1	A	590	PRO	N-CA-CB	5.77	110.22	103.30
1	A	469	PRO	N-CA-CB	5.75	110.20	103.30
1	A	181	PRO	N-CA-CB	5.72	110.16	103.30
1	A	353	PRO	N-CA-CB	5.70	110.14	103.30
1	A	346	PRO	N-CA-CB	5.70	110.14	103.30
2	B	744	PRO	N-CA-CB	5.69	110.13	103.30
1	A	670	PRO	N-CA-CB	5.69	110.13	103.30
1	A	861	PRO	N-CA-CB	5.69	110.13	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	PRO	N-CA-CB	5.69	110.13	103.30
1	A	204	PRO	N-CA-CB	5.69	110.13	103.30
1	A	133	PRO	N-CA-CB	5.69	110.12	103.30
1	A	253	PRO	N-CA-CB	5.69	110.12	103.30
1	A	154	PRO	N-CA-CB	5.68	110.12	103.30
1	A	159	PRO	N-CA-CB	5.67	110.11	103.30
1	A	250	PRO	N-CA-CB	5.67	110.11	103.30
1	A	638	PRO	N-CA-CB	5.67	110.11	103.30
1	A	808	PRO	N-CA-CB	5.66	110.10	103.30
1	A	156	PRO	N-CA-CB	5.66	110.09	103.30
1	A	522	PRO	N-CA-CB	5.65	110.08	103.30
1	A	382	PRO	N-CA-CB	5.65	110.08	103.30
1	A	646	PRO	N-CA-CB	5.64	110.07	103.30
1	A	307	PRO	N-CA-CB	5.64	110.07	103.30
1	A	660	PRO	N-CA-CB	5.60	110.02	103.30
1	A	179	PRO	N-CA-CB	5.59	110.01	103.30
1	A	344	PRO	N-CA-CB	5.57	109.98	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3724	0	1686	3	0
2	B	5076	0	4927	54	0
All	All	8800	0	6613	57	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 4.

All (57) 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)
2:B:569:ASN:ND2	2:B:692:ASN:OD1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:VAL:HG12	2:B:268:LEU:HB2	1.73	0.69
2:B:695:VAL:O	2:B:701:ARG:NH2	2.30	0.65
2:B:705:PHE:O	2:B:718:SER:OG	2.15	0.64
2:B:475:LYS:HG2	2:B:478:ALA:HB3	1.81	0.62
2:B:403:TYR:O	2:B:406:ARG:NH1	2.32	0.62
2:B:598:ASP:OD1	2:B:675:ARG:NH1	2.32	0.61
2:B:367:ASP:OD2	2:B:368:ARG:N	2.36	0.58
2:B:263:GLN:HE22	2:B:576:ALA:HB2	1.71	0.56
2:B:358:TYR:OH	2:B:544:ARG:NH1	2.39	0.56
2:B:569:ASN:ND2	2:B:696:ASN:OD1	2.36	0.55
2:B:297:LYS:O	2:B:320:ARG:NH2	2.40	0.55
2:B:545:MET:HG2	2:B:550:GLN:HE22	1.71	0.55
2:B:118:THR:OG1	2:B:193:ASP:OD1	2.27	0.52
2:B:660:ALA:HB3	2:B:690:MET:HE1	1.94	0.50
2:B:415:ASN:HD21	2:B:515:ASP:HB3	1.77	0.49
2:B:612:LYS:O	2:B:616:GLN:NE2	2.46	0.49
2:B:565:GLU:OE1	2:B:692:ASN:ND2	2.46	0.48
2:B:232:PRO:HG2	2:B:277:ALA:HB2	1.94	0.48
2:B:239:PRO:HB3	2:B:243:LEU:HD23	1.95	0.48
2:B:683:ASP:N	2:B:683:ASP:OD1	2.45	0.48
2:B:530:PRO:HG2	2:B:724:VAL:HA	1.95	0.47
1:A:416:HIS:O	1:A:420:LYS:N	2.40	0.47
2:B:383:GLN:HB3	2:B:511:VAL:HG23	1.96	0.47
2:B:498:ASP:OD1	2:B:499:ASN:N	2.48	0.47
2:B:77:PHE:HA	2:B:98:ILE:HG12	1.97	0.46
2:B:252:SER:HB2	2:B:571:VAL:HG22	1.96	0.46
2:B:69:PRO:HG2	2:B:206:THR:HG21	1.96	0.46
2:B:249:ILE:HG12	2:B:583:ILE:HA	1.97	0.46
2:B:106:GLU:OE2	2:B:206:THR:HA	2.16	0.45
2:B:552:ILE:HG21	2:B:594:ILE:HG22	1.99	0.45
2:B:415:ASN:HB3	2:B:466:LYS:NZ	2.33	0.44
2:B:695:VAL:HA	2:B:701:ARG:HG3	2.00	0.44
2:B:603:ILE:HB	2:B:679:ALA:HA	1.98	0.44
2:B:710:VAL:HG11	2:B:712:ARG:HH11	1.83	0.44
2:B:545:MET:HG3	2:B:549:SER:OG	2.18	0.44
2:B:496:SER:OG	2:B:499:ASN:O	2.36	0.43
2:B:134:LEU:HD23	2:B:163:PHE:HB2	2.01	0.43
1:A:465:MET:O	1:A:469:PRO:N	2.52	0.43
2:B:432:SER:OG	2:B:483:ARG:O	2.23	0.43
2:B:253:TRP:HA	2:B:581:PRO:HB3	2.01	0.43
2:B:202:LEU:H	2:B:202:LEU:HD23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LEU:O	1:A:716:LYS:CB	2.67	0.43
2:B:117:TYR:HE1	2:B:155:ALA:HB2	1.85	0.42
2:B:67:ASN:O	2:B:311:TYR:OH	2.29	0.42
2:B:529:MET:O	2:B:531:ASP:N	2.51	0.42
2:B:190:LEU:H	2:B:190:LEU:HD23	1.85	0.42
2:B:133:TYR:HE2	2:B:138:LEU:HB3	1.85	0.42
2:B:192:LEU:HD12	2:B:192:LEU:HA	1.89	0.42
2:B:220:PHE:CZ	2:B:315:LEU:HB2	2.55	0.41
2:B:221:PHE:CZ	2:B:258:SER:HA	2.55	0.41
2:B:442:ASN:OD1	2:B:443:LEU:N	2.52	0.41
2:B:504:GLN:H	2:B:504:GLN:CD	2.24	0.41
2:B:615:LYS:HD3	2:B:615:LYS:HA	1.69	0.41
2:B:431:ILE:HA	2:B:484:PHE:HB3	2.03	0.40
2:B:98:ILE:HG21	2:B:200:LEU:HD13	2.04	0.40
2:B:209:VAL:HB	2:B:313:LYS:HE3	2.03	0.40

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	749/886 (84%)	684 (91%)	48 (6%)	17 (2%)	5	31
2	B	657/779 (84%)	617 (94%)	39 (6%)	1 (0%)	44	77
All	All	1406/1665 (84%)	1301 (92%)	87 (6%)	18 (1%)	13	42

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	342	PRO
1	A	475	PRO

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Mol	Chain	Res	Type
1	A	489	PRO
1	A	557	PRO
1	A	589	ASN
1	A	706	PRO
1	A	763	PRO
1	A	360	PRO
1	A	477	PRO
1	A	750	VAL
1	A	790	VAL
1	A	273	MET
1	A	659	ALA
1	A	714	PRO
2	B	744	PRO
1	A	444	VAL
1	A	335	VAL

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	
2	B	542/669 (81%)	541 (100%)	1 (0%)	92	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	305	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	45:ILE	C	123:LEU	N	30.07
1	A	611:PHE	C	634:LEU	N	17.28

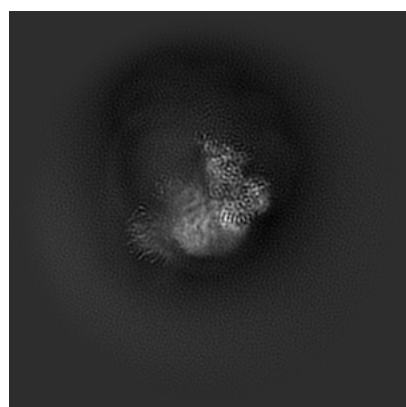
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23267. These allow visual inspection of the internal detail of the map and identification of artifacts.

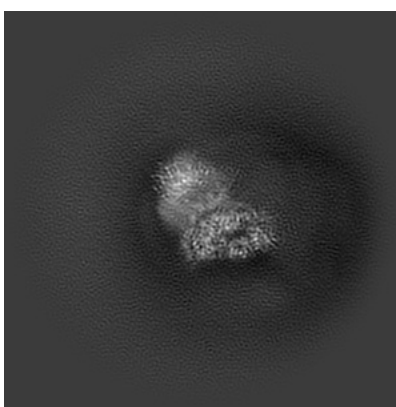
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

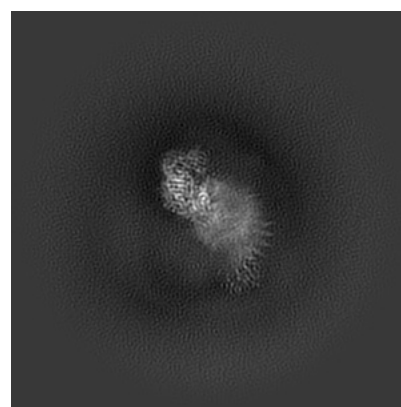
6.1.1 Primary map



X



Y

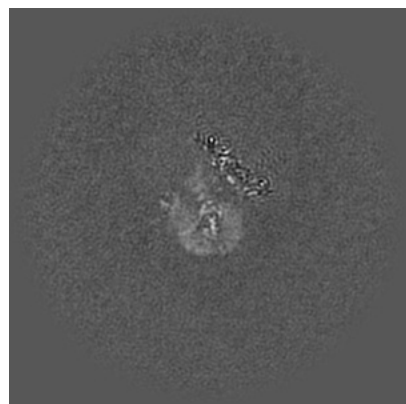


Z

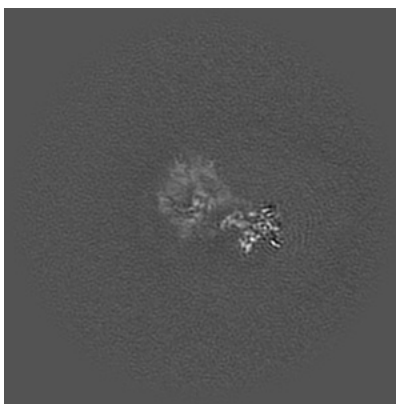
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

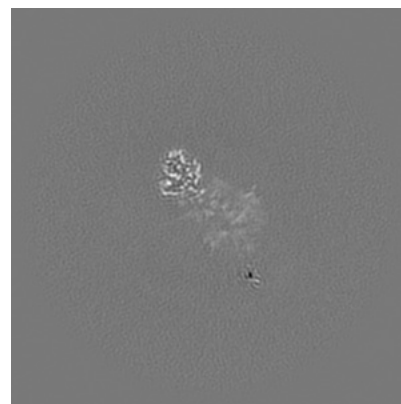
6.2.1 Primary map



X Index: 200



Y Index: 200

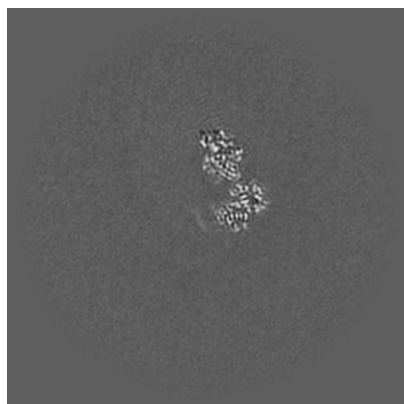


Z Index: 200

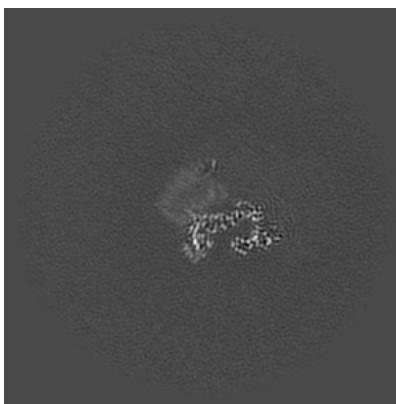
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

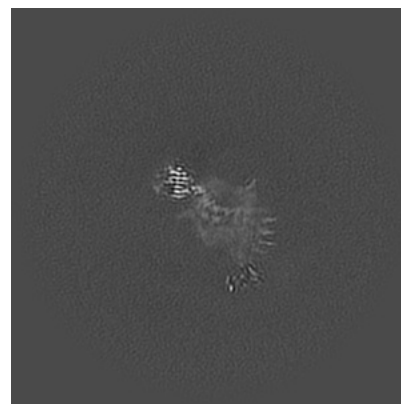
6.3.1 Primary map



X Index: 169



Y Index: 216

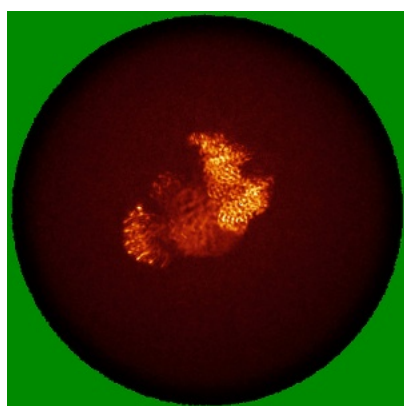


Z Index: 190

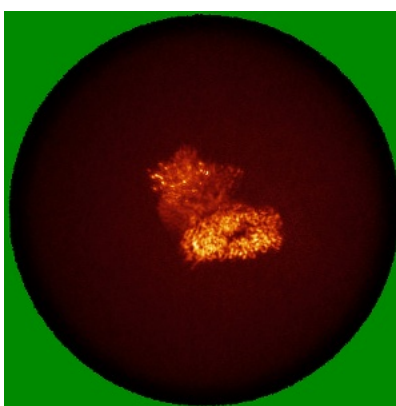
The images above show the largest variance slices of the map in three orthogonal directions.

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

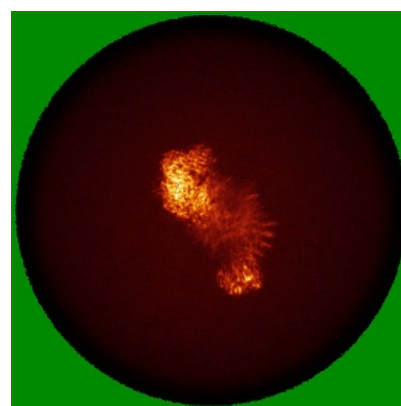
6.4.1 Primary map



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

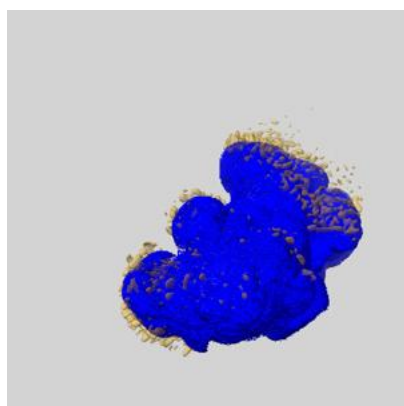
6.6 Mask visualisation [i](#)

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

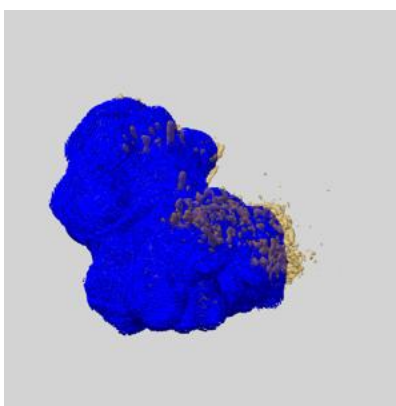
A mask typically either:

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

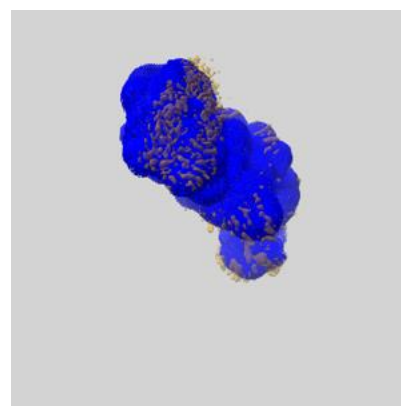
6.6.1 emd_23267_msk_1.map [i](#)



X



Y

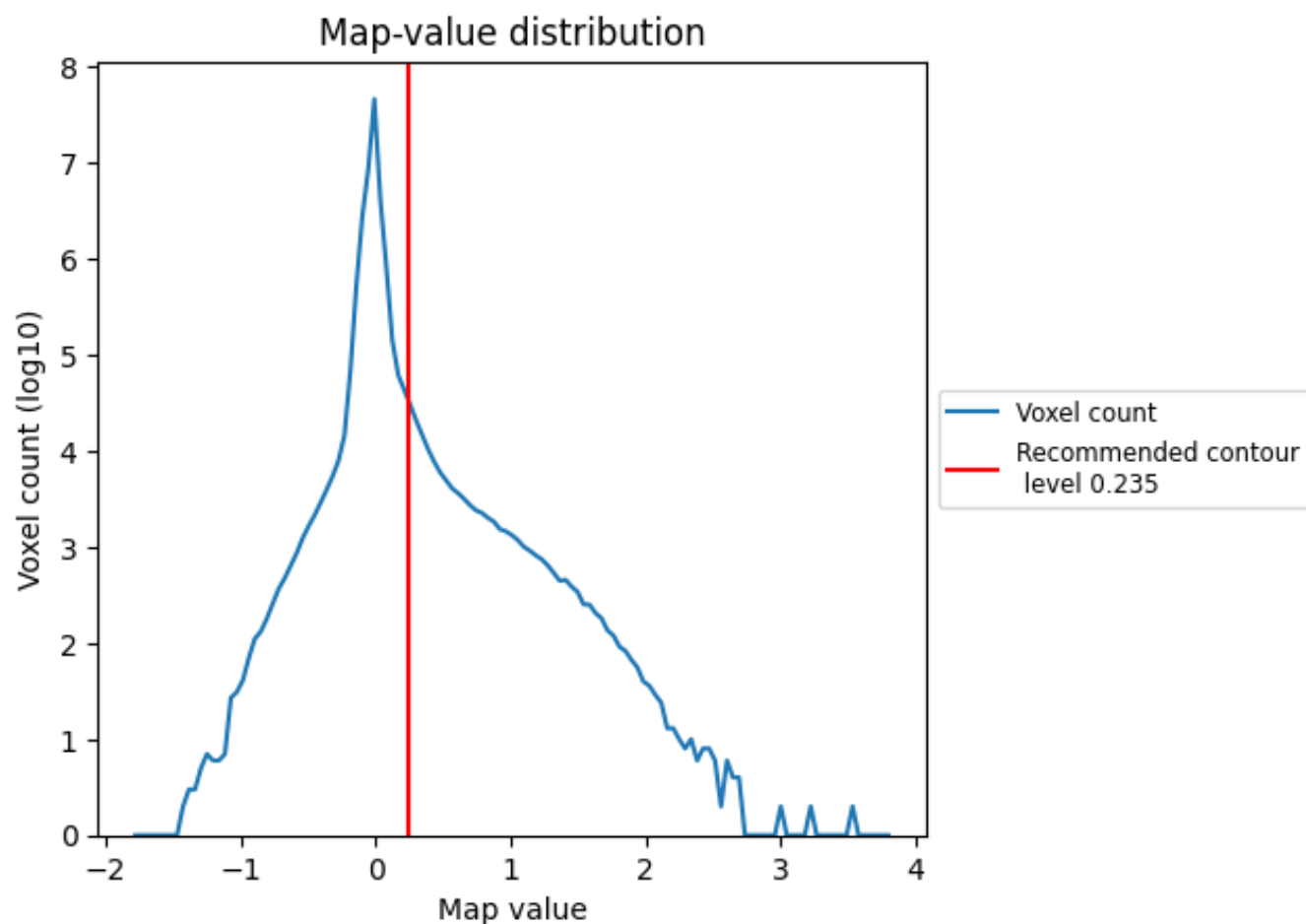


Z

7 Map analysis [i](#)

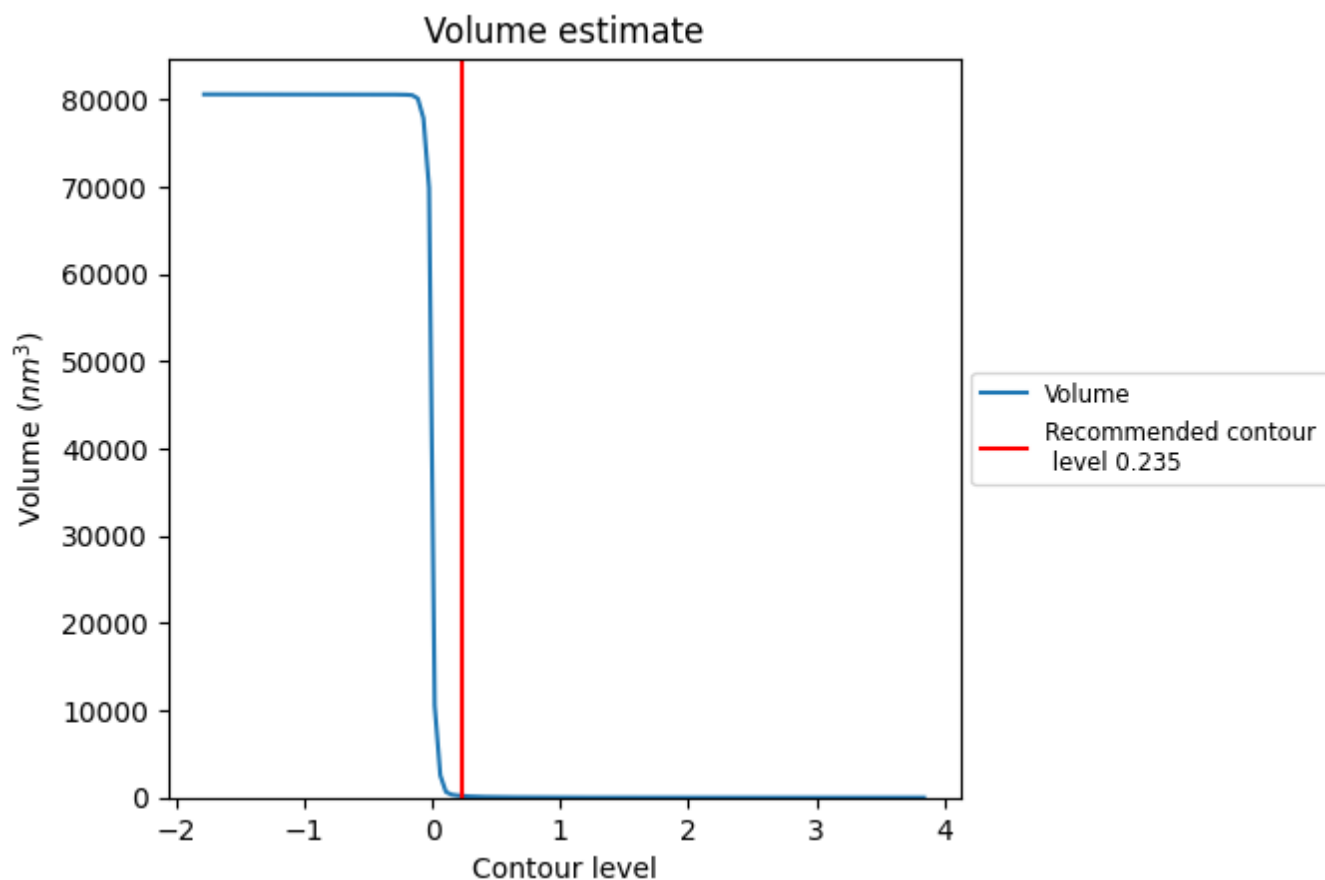
This section contains the results of statistical analysis of the map.

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.

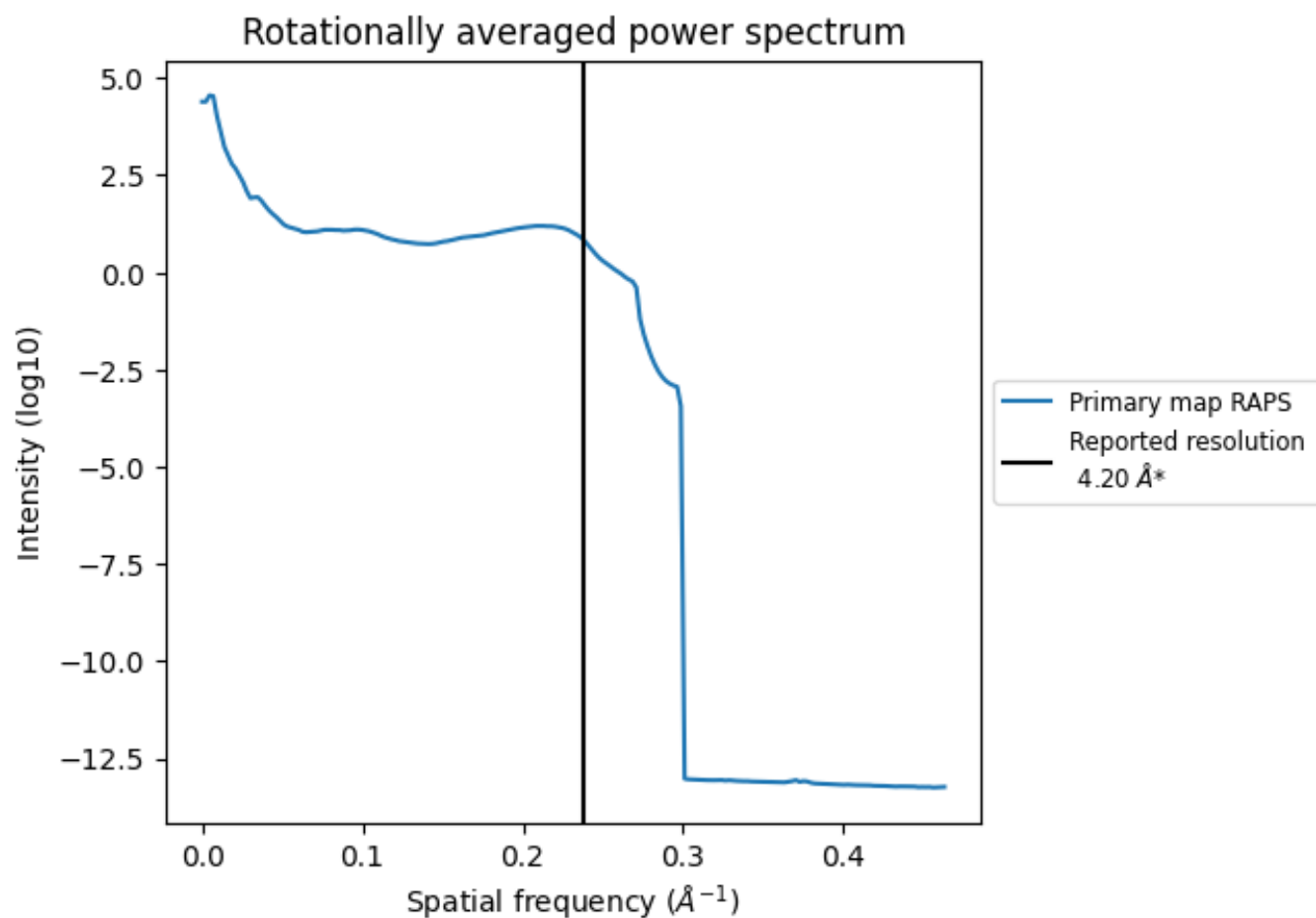
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm^3 ; this corresponds to an approximate mass of 168 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 ⓘ

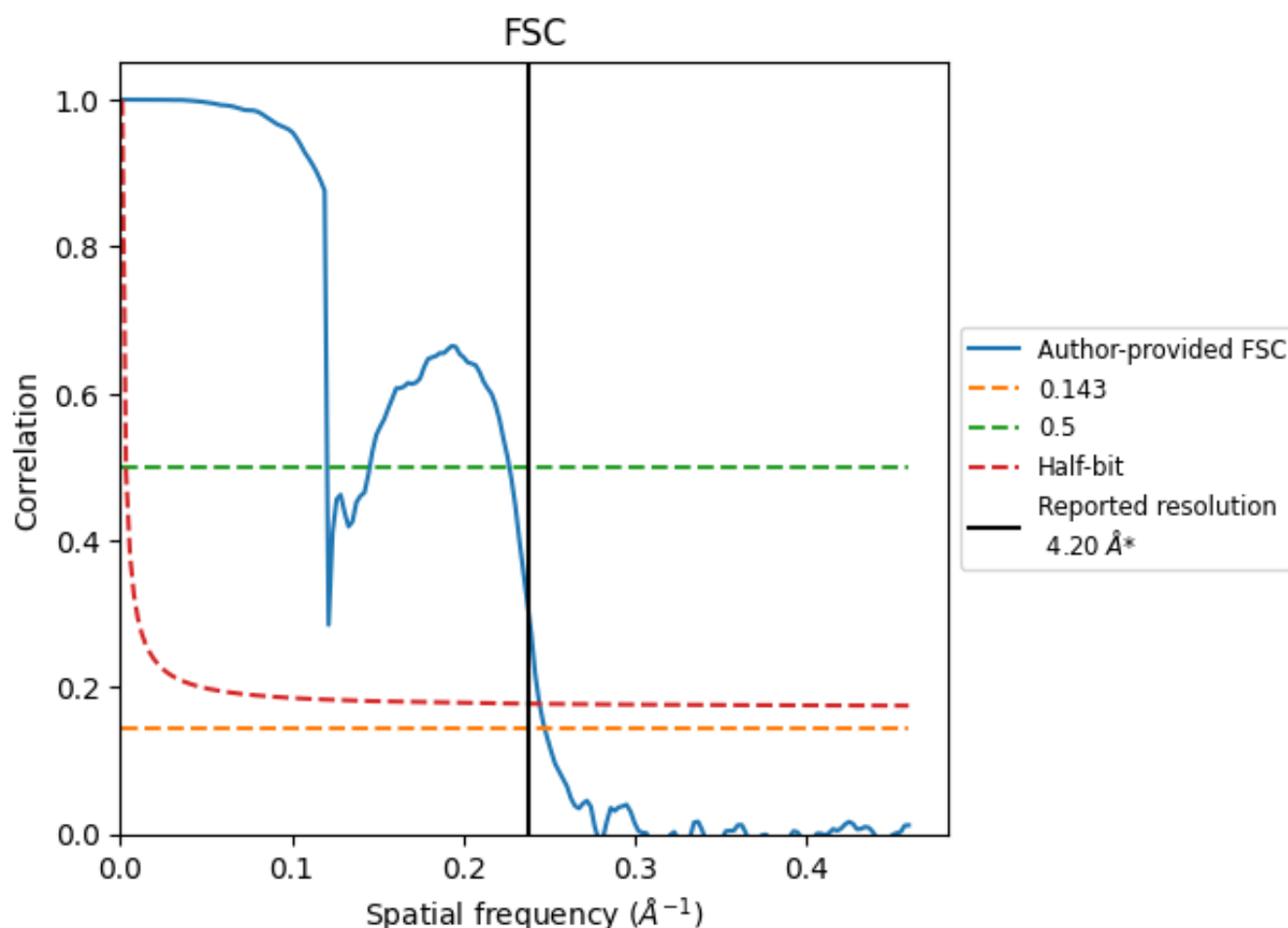


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

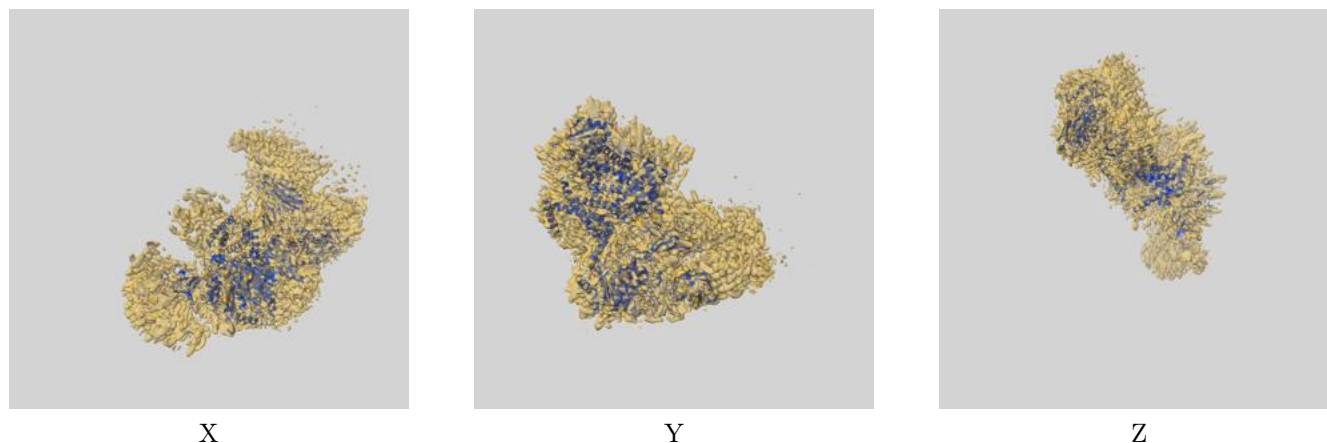
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.04	8.29	4.09
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

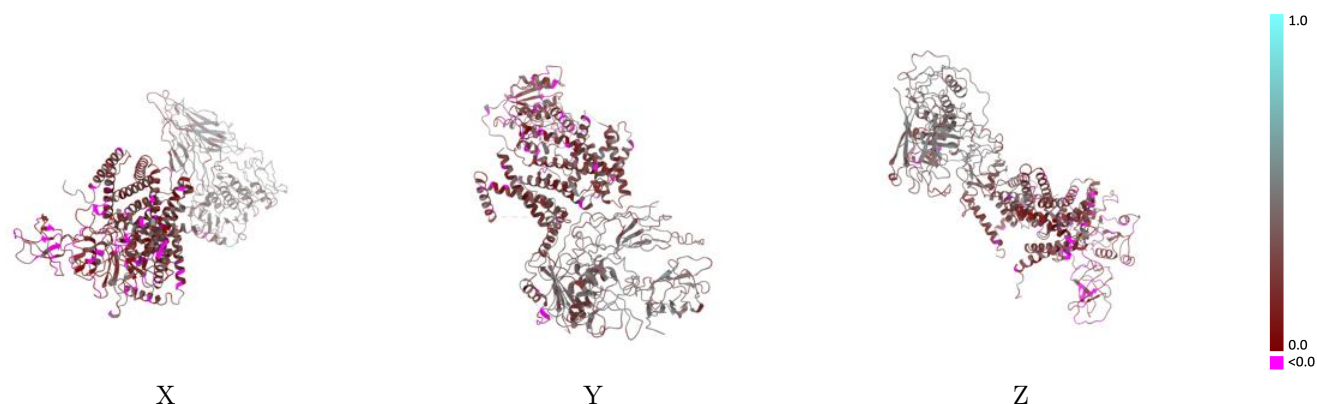
This section contains information regarding the fit between EMDB map EMD-23267 and PDB model 7LBY. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



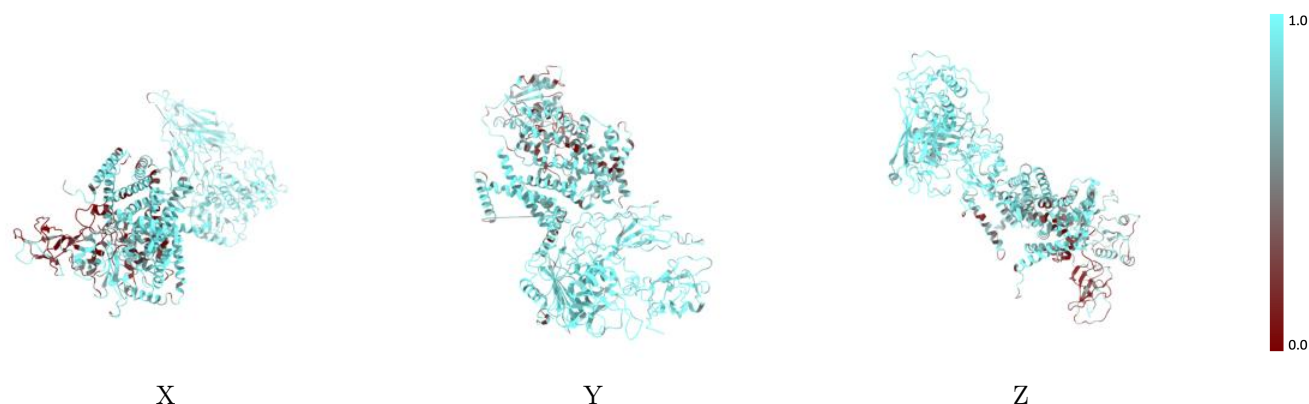
The images above show the 3D surface view of the map at the recommended contour level 0.235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



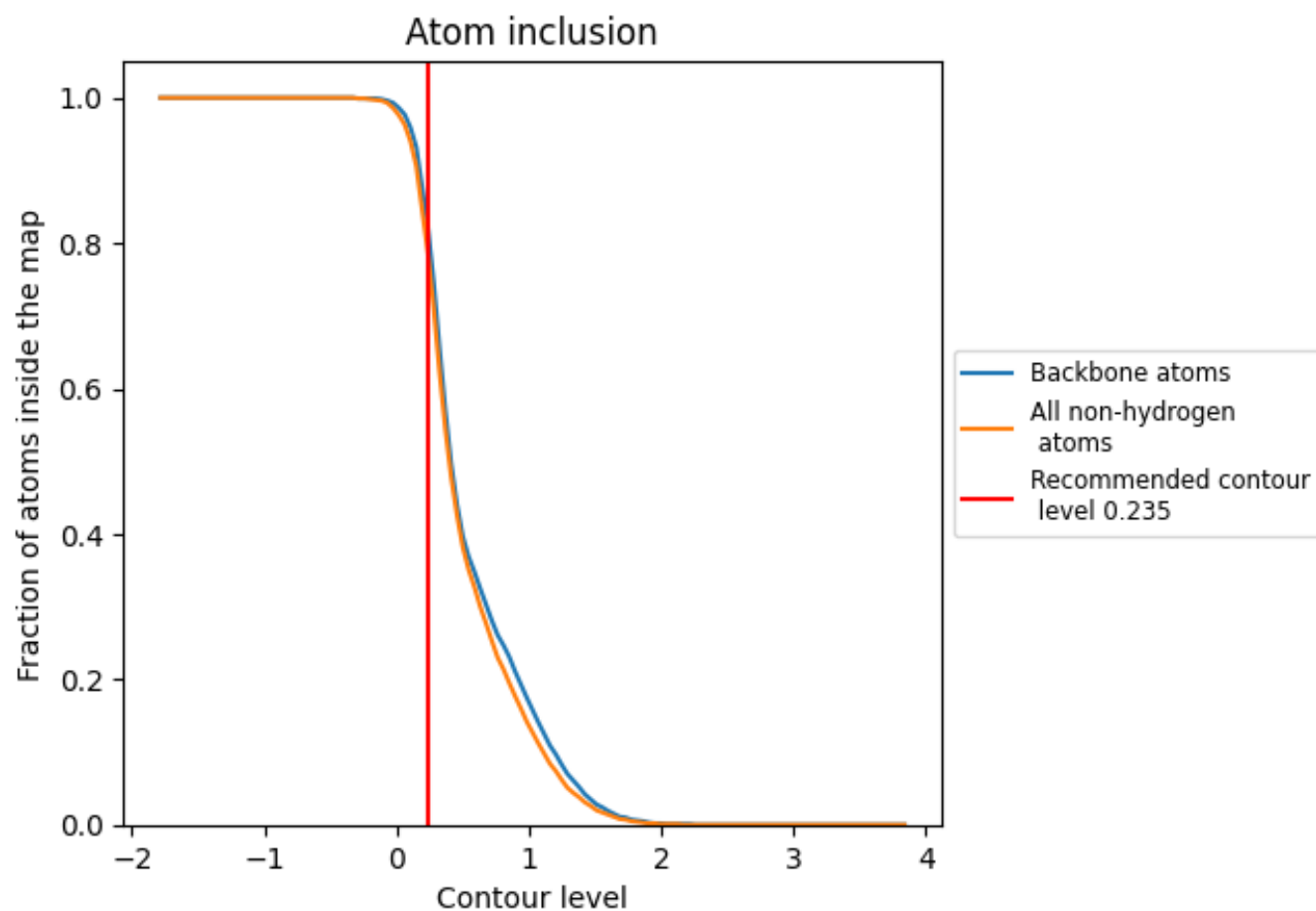
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.235).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7900	<div></div> 0.3080
A	<div></div> 0.6720	<div></div> 0.2030
B	<div></div> 0.8790	<div></div> 0.3850

