wwPDB EM Validation Summary Report

Oct 26, 2026 – 12:26 PM EDT

PDB ID	:	38FH / pdb_000038fh
EMDB ID	:	EMD-78773
Title	:	Bacteroides SusCD Unliganded - Closed w/o Plug
Authors	:	Cadigan, M.C.; Koropatkin, N.M.
Deposited on	:	2026-08-23
Resolution	:	3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

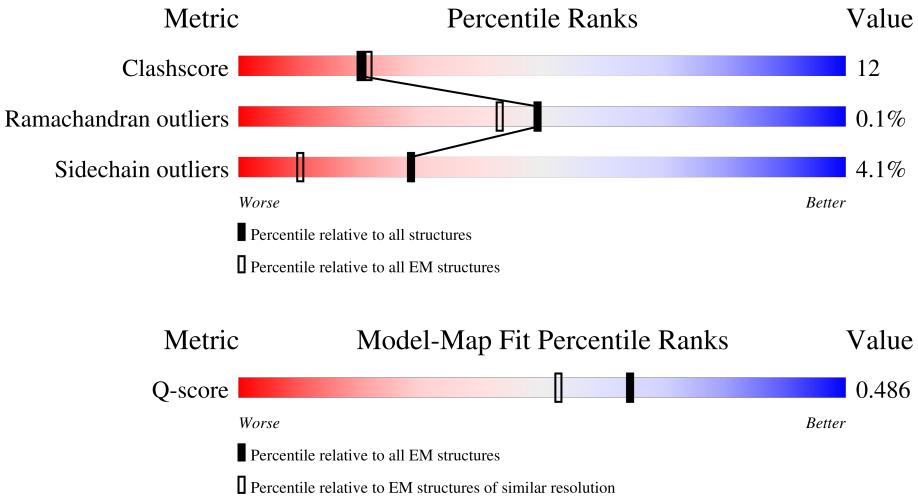
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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 <=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	899	63% 20% 16%
2	B	536	60% 37%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10252 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 TonB-dependent receptor SusC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	755	Total	C	N	O	S	0	0
			6046	3849	1015	1171	11		

- Molecule 2 is a protein called Starch-binding protein SusD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			4204	2642	720	823	19		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	552	ALA	-	expression tag	UNP Q8A1G2
B	553	ALA	-	expression tag	UNP Q8A1G2
B	554	ALA	-	expression tag	UNP Q8A1G2
B	555	HIS	-	expression tag	UNP Q8A1G2
B	556	HIS	-	expression tag	UNP Q8A1G2
B	557	HIS	-	expression tag	UNP Q8A1G2
B	558	HIS	-	expression tag	UNP Q8A1G2
B	559	HIS	-	expression tag	UNP Q8A1G2
B	560	HIS	-	expression tag	UNP Q8A1G2

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mn	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Ca	0
			1	1	

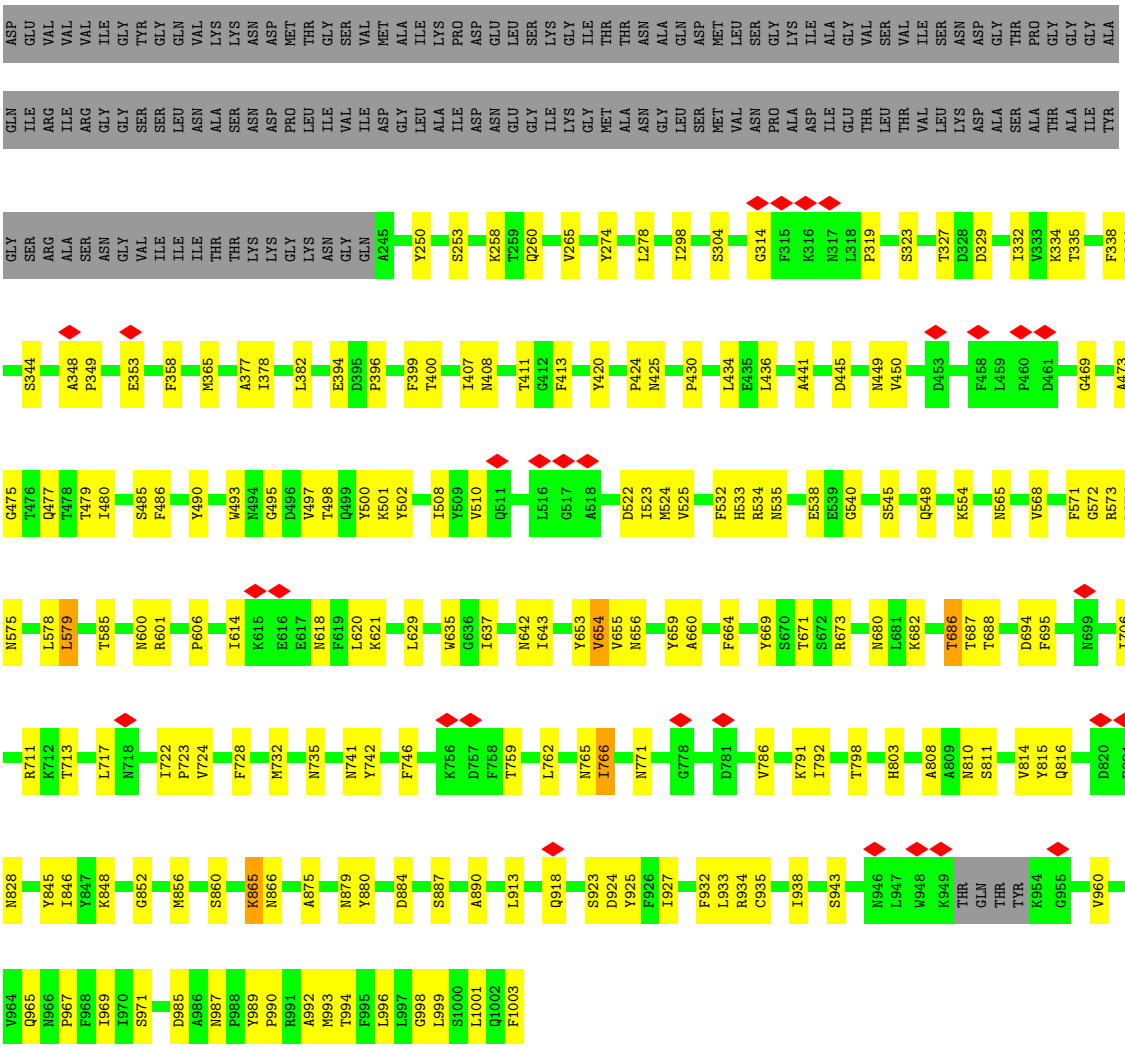
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TonB-dependent receptor SusC

Chain A:

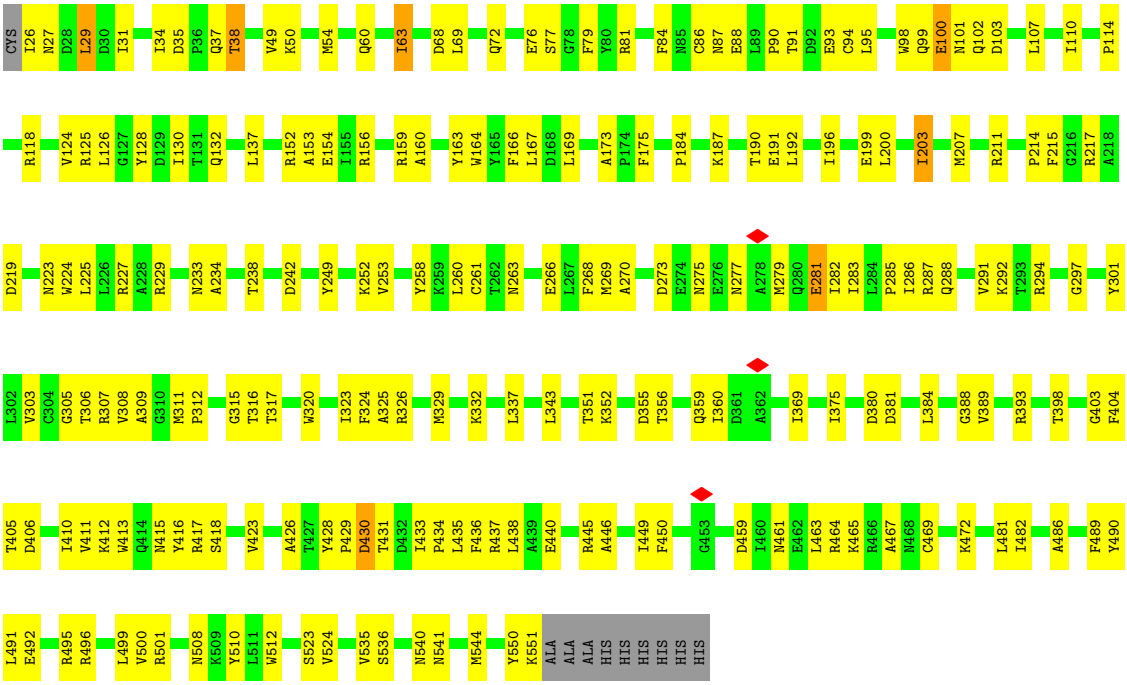




• Molecule 2: Starch-binding protein SusD

Chain B:




CYS I26 N27 D28 L29 D30 I31 I34 D35 P36 Q37 T38 V49 K50 M54 Q60 I63 D68 L69 Q72 E76 S77 G78 F79 Y80 R81 F84 N85 C86 N87 E88 L89 P90 T91 D92 E93 C94 L95 W98 Q99 E100 N101 Q102 D103 L107 I110 P114
R118 V124 R125 L126 G127 Y128 D129 I130 T131 Q132 L137 R152 A153 E154 I155 R156 R159 A160 Y163 W164 Y165 F166 L167 D168 L169 A173 P174 F175 P184 K187 T190 E191 L192 I196 E199 L200 I203 M207 R211 P214 F215 G216 R217 A218
D219 N223 W224 L225 L226 R227 A228 R229 N233 A234 T238 D242 Y249 K252 V253 Y258 K259 L260 C261 T262 N263 E266 L267 F268 M269 A270 D273 E274 N275 E276 N277 A278 M279 Q280 E281 I282 I283 L284 P285 I286 R287 Q288 V291 K292 T293 R294 G297 Y301
L302 V303 C304 G305 T306 R307 V308 A309 G310 M311 P312 G315 T316 T317 W320 I323 F324 A325 R326 M329 K332 L337 L343 T351 K352 D355 T356 Q359 I360 D361 A362 I369 I375 D380 D381 L384 G388 V389 R393 T398 G403 F404
T405 D406 I410 V411 K412 W413 Q414 N415 Y416 R417 S418 V423 A426 T427 Y428 P429 D430 T431 D432 I433 P434 L435 F436 R437 L438 A439 E440 R445 A446 I449 F450 G453 D459 I460 N461 E462 L463 R464 K465 R466 A467 N468 C469 K472 L481 I482 A486 F489 Y490
L491 E492 R495 R496 L499 V500 R501 N508 K509 Y510 L511 W512 S523 V524 V535 S536 N540 N541 M544 Y550 K551 ALA ALA ALA HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF estimation used for curation, no correction done	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.511	Depositor
Minimum map value	-1.677	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.226	Depositor
Map size (Å)	384.192, 384.192, 384.192	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0672, 1.0672, 1.0672	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.18	0/6211	0.38	0/8429
2	B	0.24	0/4300	0.45	2/5825 (0.0%)
All	All	0.21	0/10511	0.41	2/14254 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	100	GLU	N-CA-C	-7.09	98.73	109.79
2	B	102	GLN	N-CA-C	6.24	118.84	110.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	152	ARG	Sidechain

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	6046	0	5687	116	0
2	B	4204	0	4000	145	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	10252	0	9687	245	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 245 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:153:ALA:HA	2:B:203:ILE:HG13	1.53	0.88
1:A:524:MET:HE3	1:A:571:PHE:HE2	1.49	0.77
1:A:394:GLU:HG2	1:A:396:PRO:HD2	1.66	0.77
1:A:473:ALA:HB3	1:A:501:LYS:HB2	1.66	0.77
2:B:541:ASN:HD22	2:B:544:MET:HG2	1.52	0.75

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	751/899 (84%)	708 (94%)	43 (6%)	0	100	100
2	B	524/536 (98%)	499 (95%)	24 (5%)	1 (0%)	43	73
All	All	1275/1435 (89%)	1207 (95%)	67 (5%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	101	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	642/754 (85%)	613 (96%)	29 (4%)	24	56
2	B	441/448 (98%)	426 (97%)	15 (3%)	32	63
All	All	1083/1202 (90%)	1039 (96%)	44 (4%)	28	59

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	963	THR
2	B	154	GLU
2	B	29	LEU
2	B	37	GLN
2	B	203	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	945	GLN
1	A	987	ASN
2	B	547	ASN
2	B	151	GLN
2	B	331	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

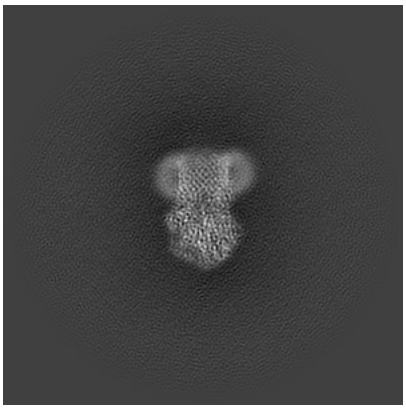
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-78773. These allow visual inspection of the internal detail of the map and identification of artifacts.

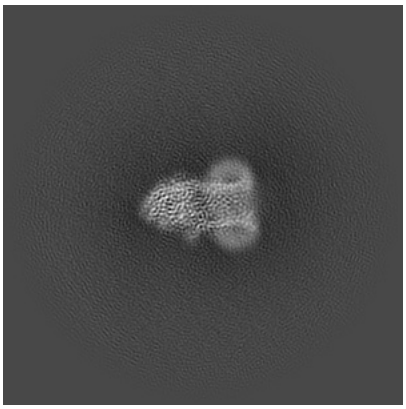
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

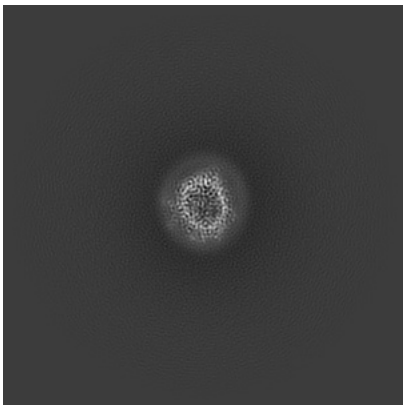
6.1.1 Primary map



X

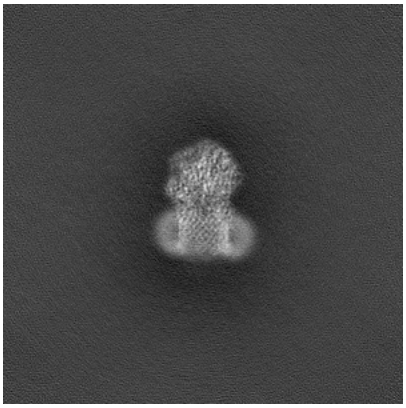


Y

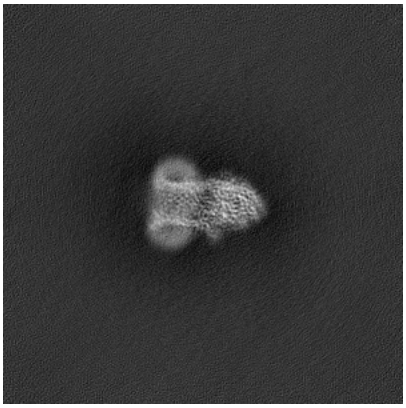


Z

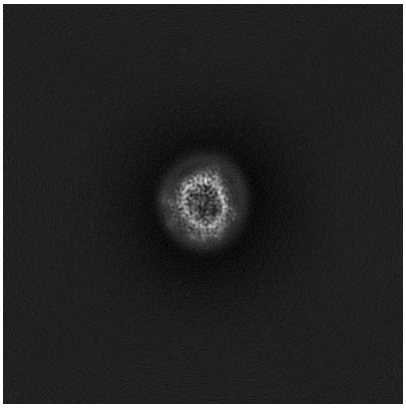
6.1.2 Raw map



X



Y

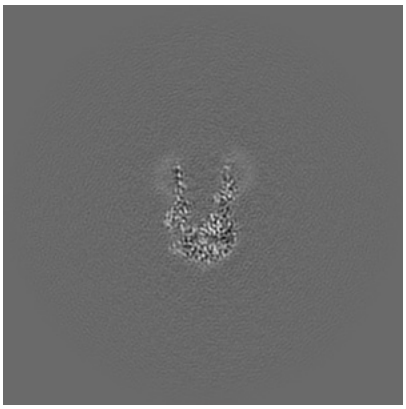


Z

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

6.2 Central slices (i)

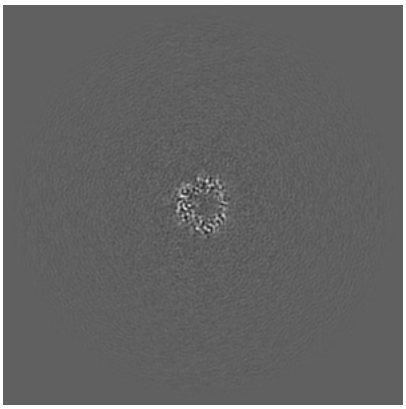
6.2.1 Primary map



X Index: 180

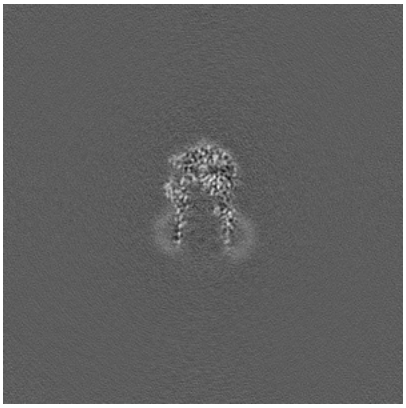


Y Index: 180

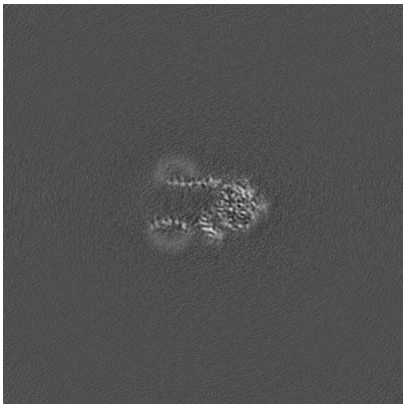


Z Index: 180

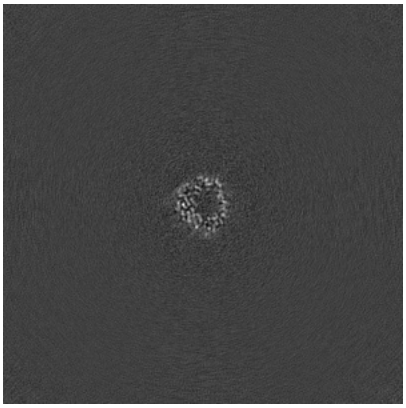
6.2.2 Raw map



X Index: 180



Y Index: 180

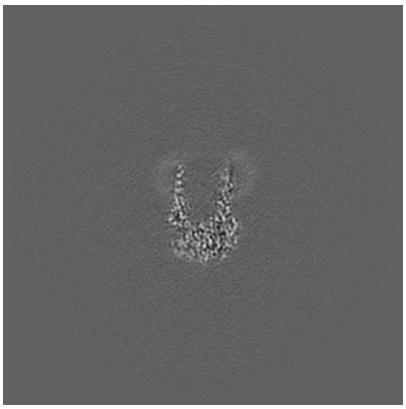


Z Index: 180

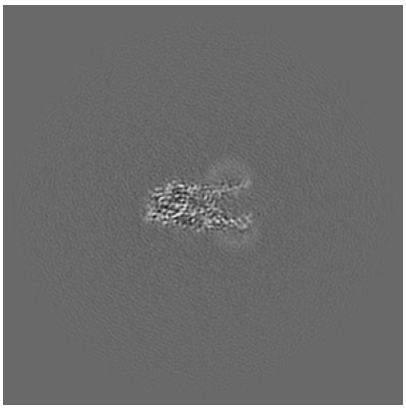
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

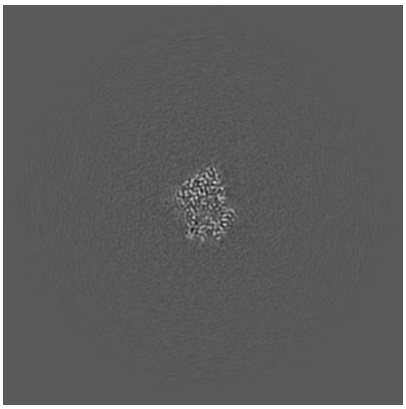
6.3.1 Primary map



X Index: 186

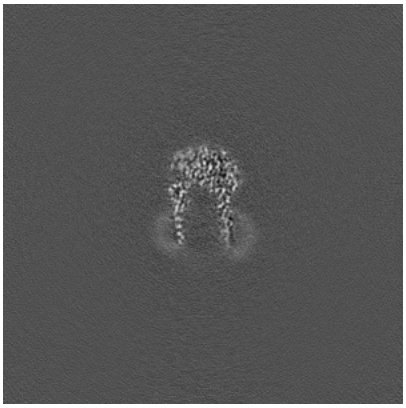


Y Index: 194

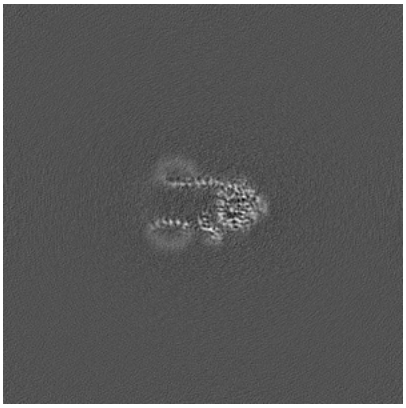


Z Index: 161

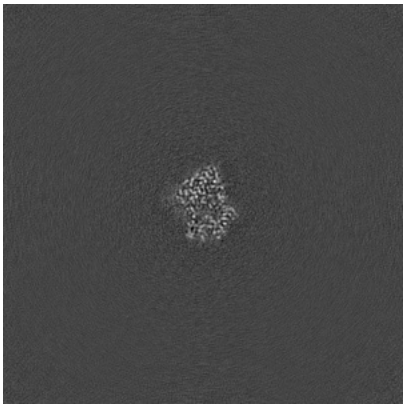
6.3.2 Raw map



X Index: 186



Y Index: 181

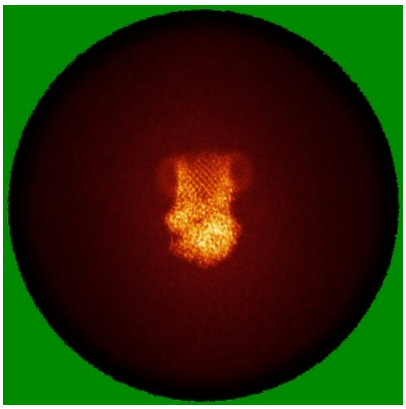


Z Index: 198

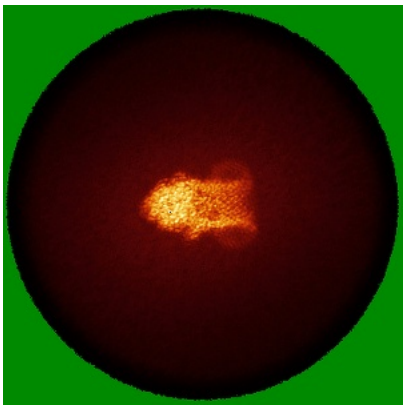
The images above show the largest variance slices of the map in three orthogonal directions.

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

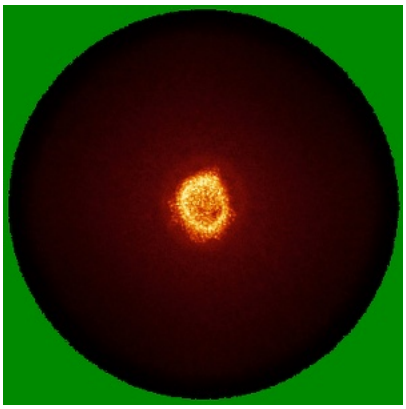
6.4.1 Primary map



X

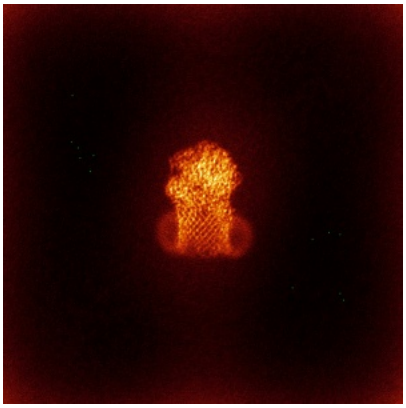


Y

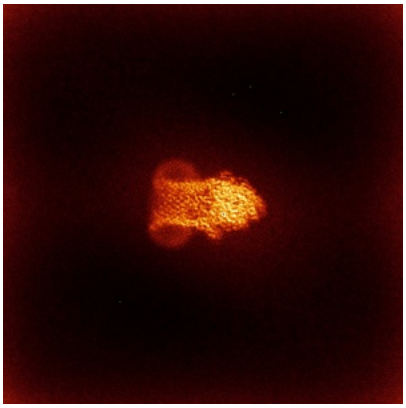


Z

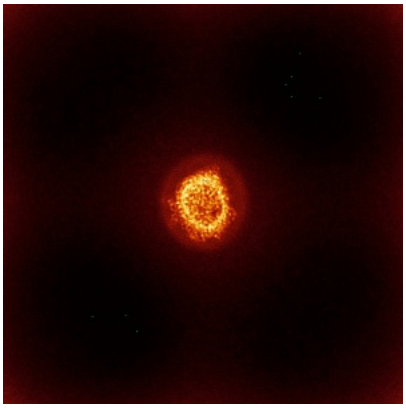
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.226. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

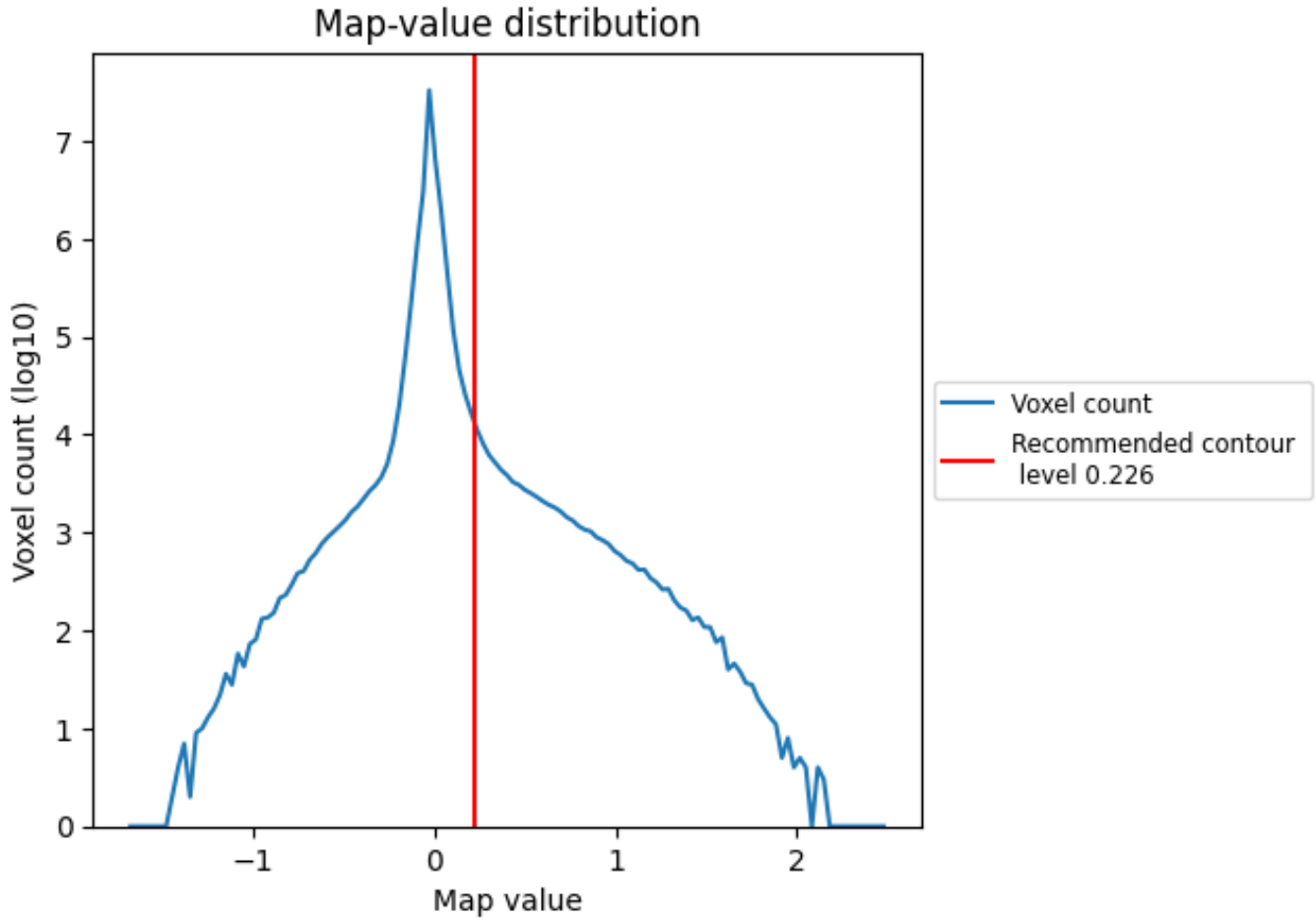
6.6 Mask visualisation (i)

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

7 Map analysis

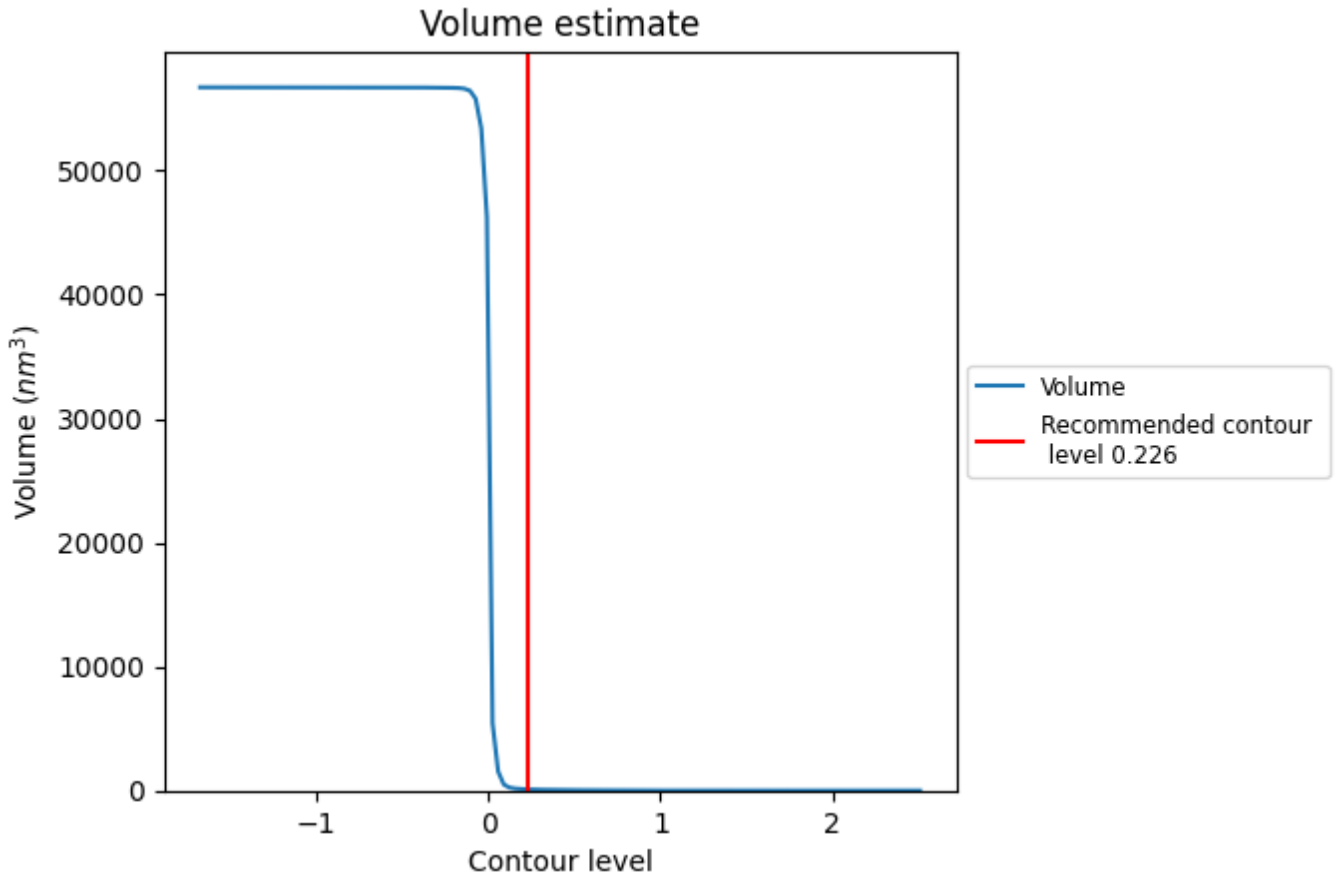
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

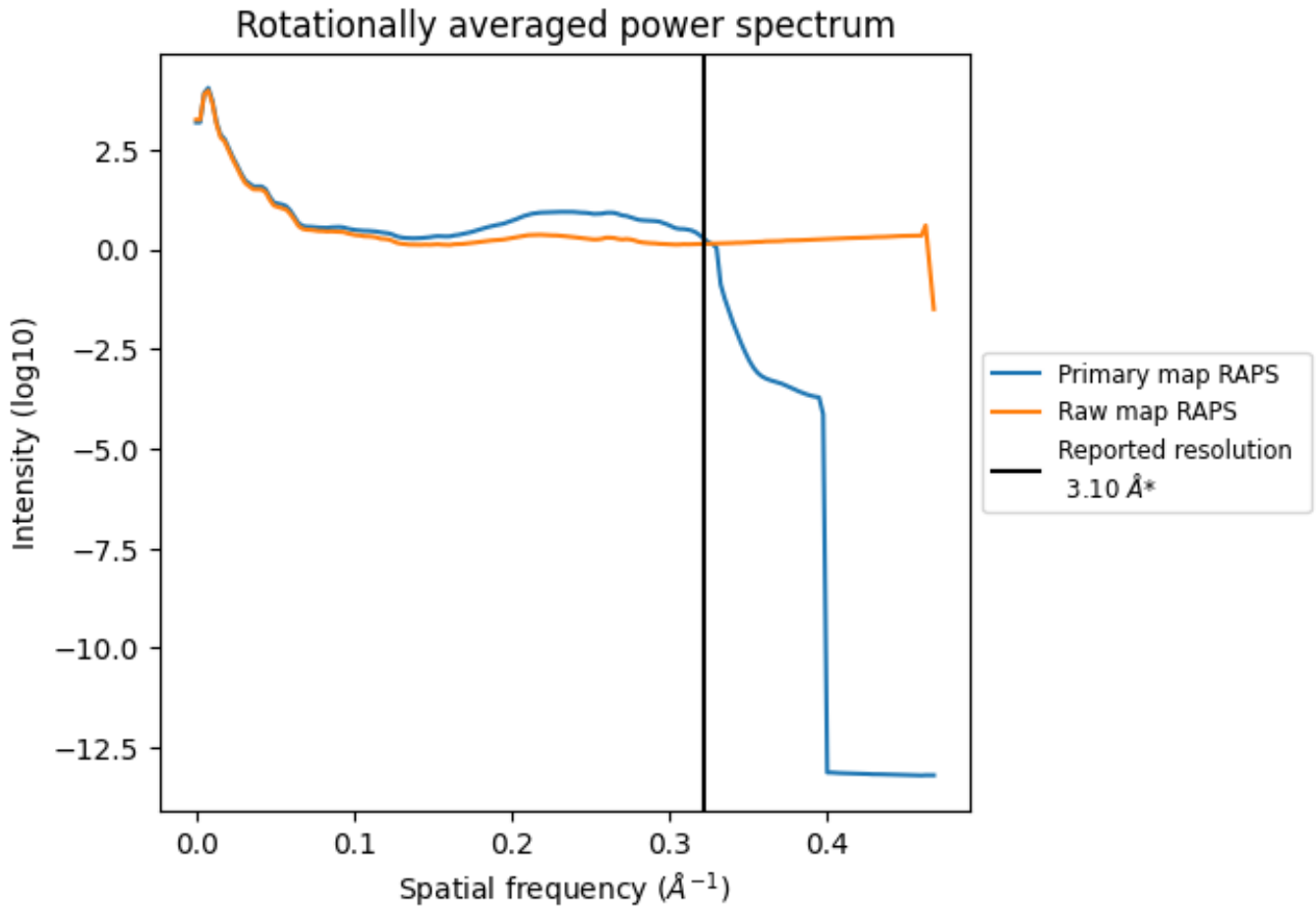
7.2 Volume estimate (i)



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

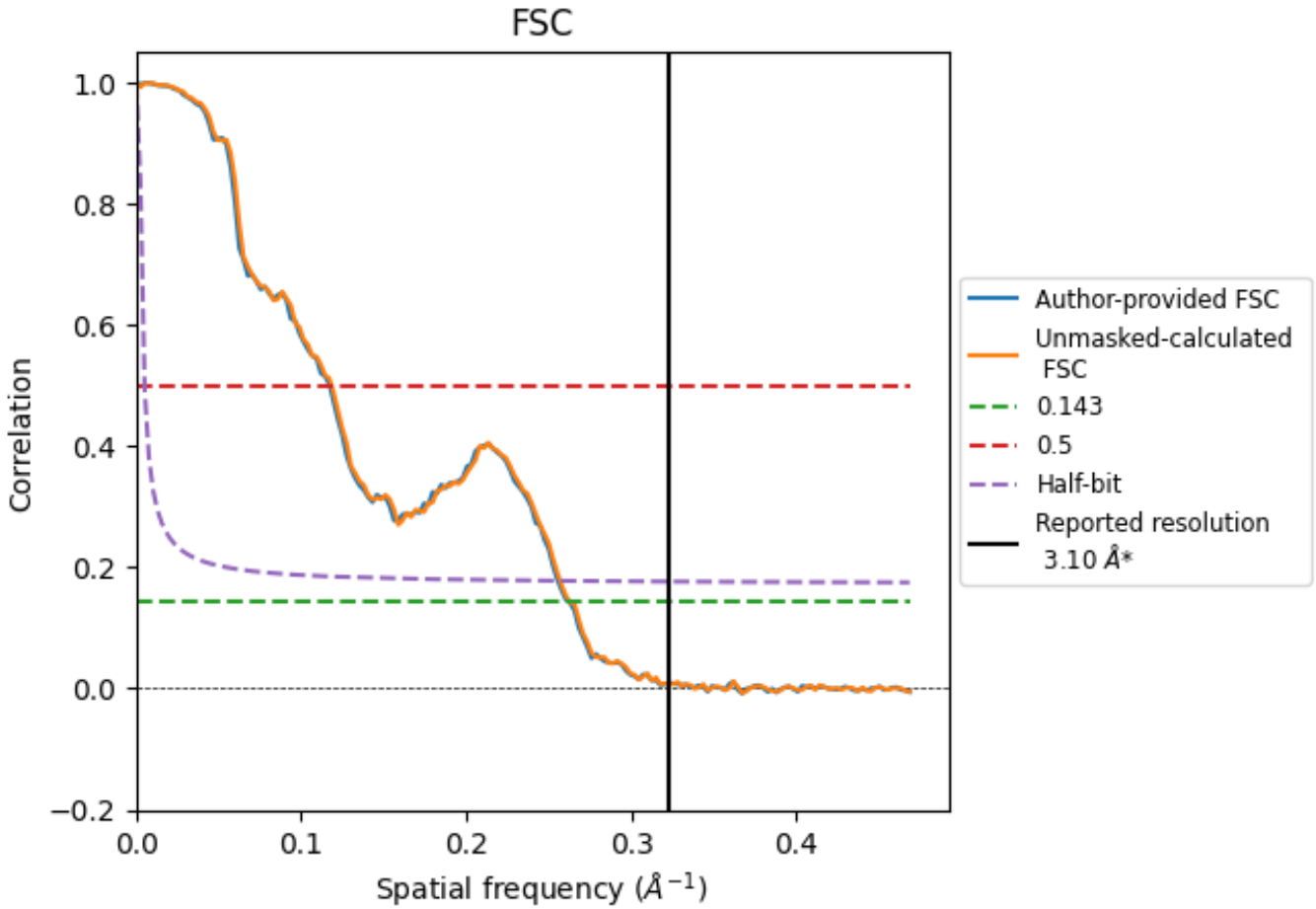


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.82	8.53	3.92
Unmasked-calculated*	3.81	8.45	3.89

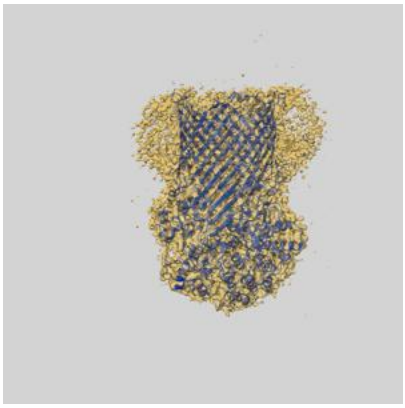
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.81 differs from the reported value 3.1 by more than 10 %

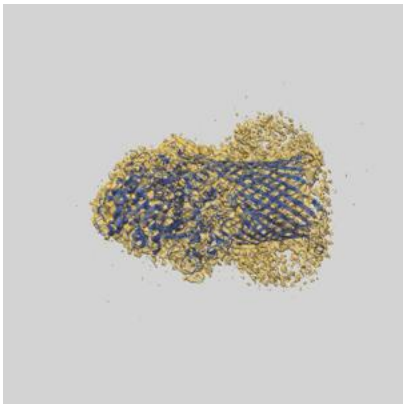
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-78773 and PDB model 38FH. Per-residue inclusion information can be found in section 3 on page 4.

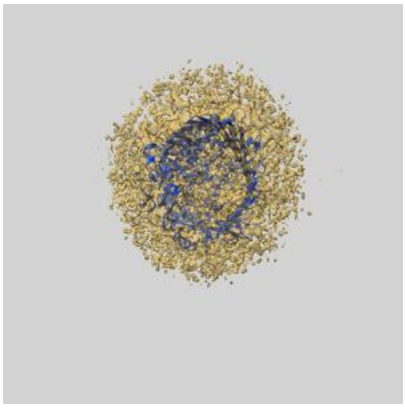
9.1 Map-model overlay



X



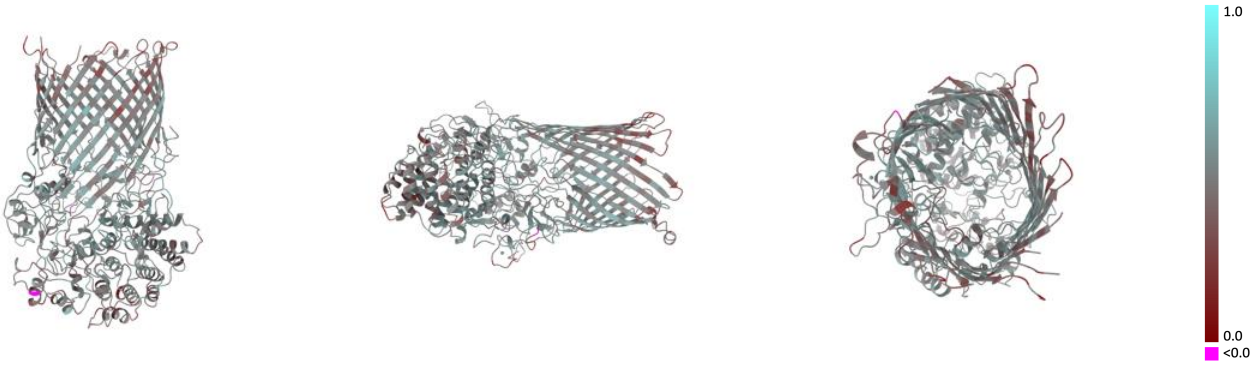
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.226 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.

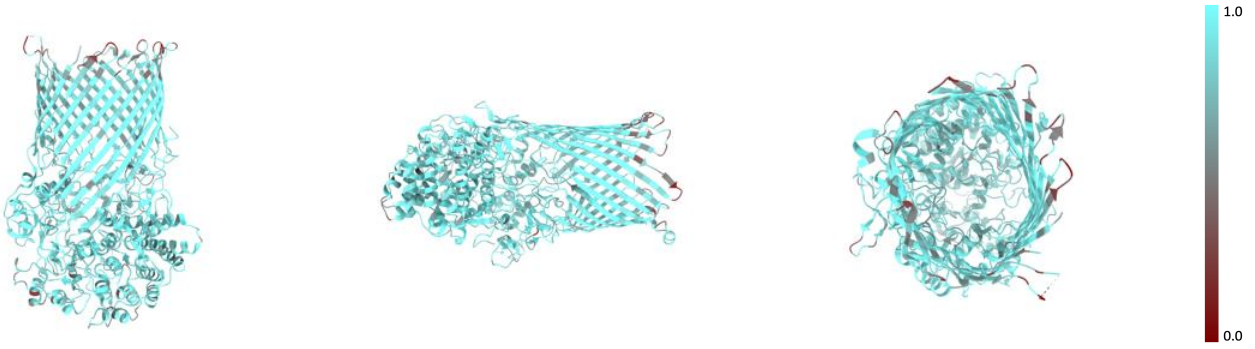
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

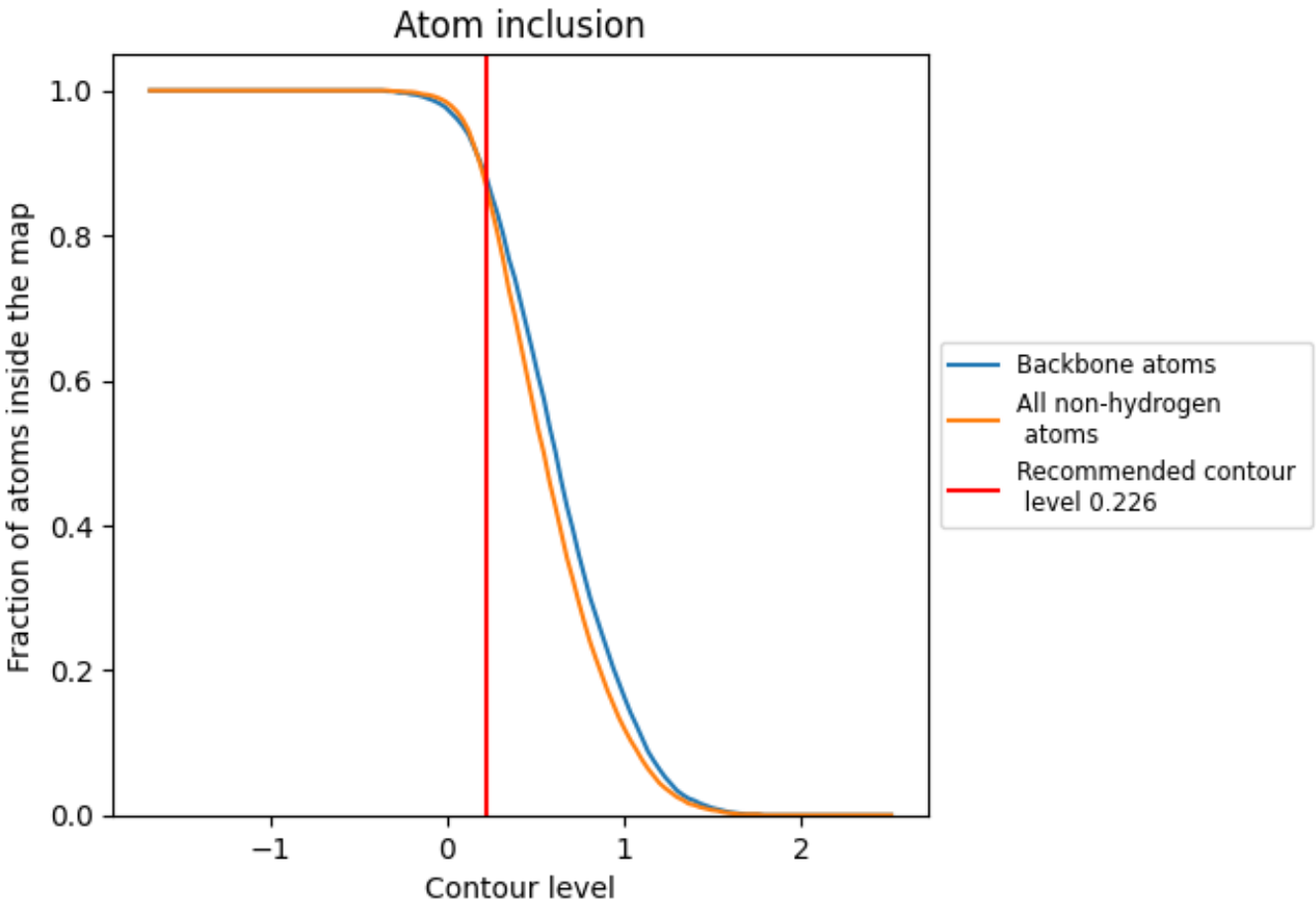
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.226).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.226) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8650	0.4860
A	0.8500	0.4840
B	0.8860	0.4880