Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 03:13 am BST

PDB ID	:	7NG9
EMDB ID	:	EMD-12310
Title	:	Trimeric efflux pump Klebsiella TolC
Authors	:	Webby, M.N.; Housden, N.G.; Kleanthous, C.
Deposited on	:	2021-02-08
Resolution	:	3.30 Å(reported)
Based on initial model	:	1EK9

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 (i) 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 (i)) were used in the production of this report:

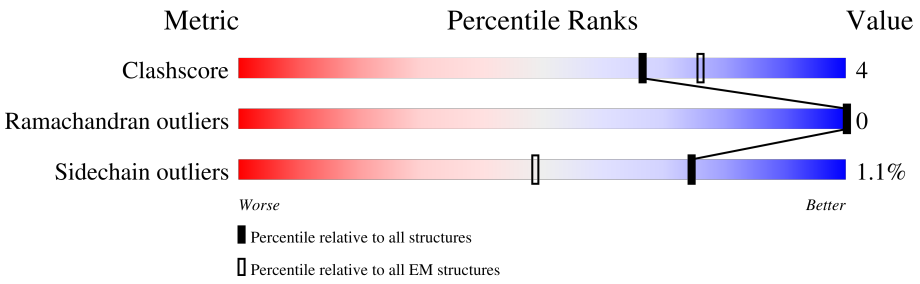
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	494	11% 76% 9% 15%
1	B	494	11% 76% 9% 15%
1	C	494	11% 76% 10% 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19368 atoms, of which 9615 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 channel protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	421	6456	2007	3205	576	665	3	0	0
1	B	421	6456	2007	3205	576	665	3	0	0
1	C	421	6456	2007	3205	576	665	3	0	0

There are 24 discrepancies between the modelled and reference sequences:

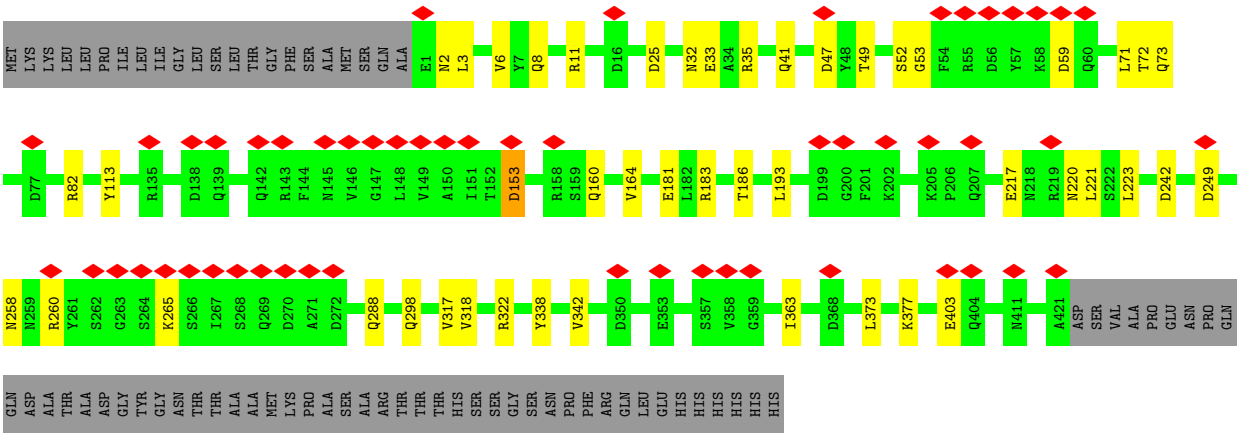
Chain	Residue	Modelled	Actual	Comment	Reference
A	465	LEU	-	expression tag	UNP A0A1C3Q001
A	466	GLU	-	expression tag	UNP A0A1C3Q001
A	467	HIS	-	expression tag	UNP A0A1C3Q001
A	468	HIS	-	expression tag	UNP A0A1C3Q001
A	469	HIS	-	expression tag	UNP A0A1C3Q001
A	470	HIS	-	expression tag	UNP A0A1C3Q001
A	471	HIS	-	expression tag	UNP A0A1C3Q001
A	472	HIS	-	expression tag	UNP A0A1C3Q001
B	465	LEU	-	expression tag	UNP A0A1C3Q001
B	466	GLU	-	expression tag	UNP A0A1C3Q001
B	467	HIS	-	expression tag	UNP A0A1C3Q001
B	468	HIS	-	expression tag	UNP A0A1C3Q001
B	469	HIS	-	expression tag	UNP A0A1C3Q001
B	470	HIS	-	expression tag	UNP A0A1C3Q001
B	471	HIS	-	expression tag	UNP A0A1C3Q001
B	472	HIS	-	expression tag	UNP A0A1C3Q001
C	465	LEU	-	expression tag	UNP A0A1C3Q001
C	466	GLU	-	expression tag	UNP A0A1C3Q001
C	467	HIS	-	expression tag	UNP A0A1C3Q001
C	468	HIS	-	expression tag	UNP A0A1C3Q001
C	469	HIS	-	expression tag	UNP A0A1C3Q001
C	470	HIS	-	expression tag	UNP A0A1C3Q001
C	471	HIS	-	expression tag	UNP A0A1C3Q001
C	472	HIS	-	expression tag	UNP A0A1C3Q001

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.

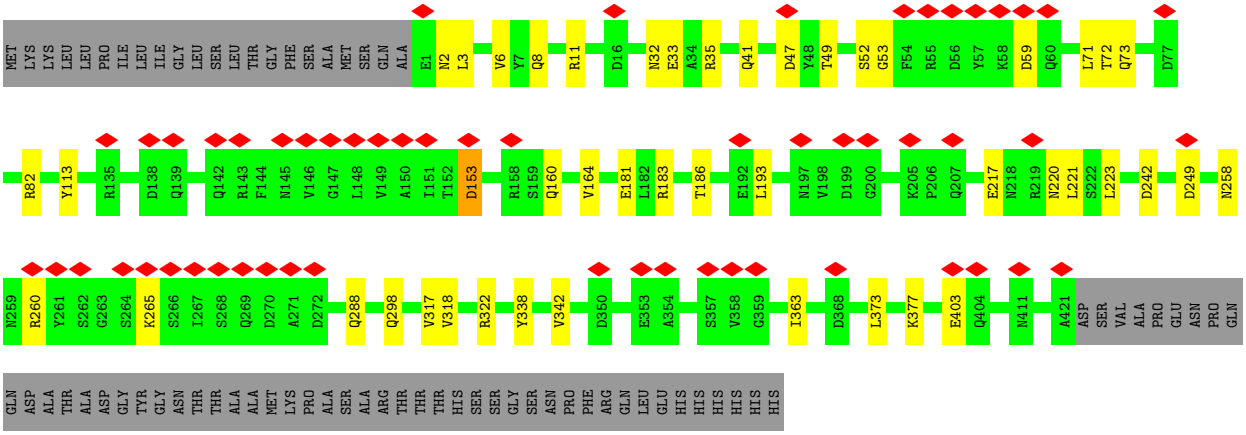
• Molecule 1: Outer membrane channel protein

Chain A:



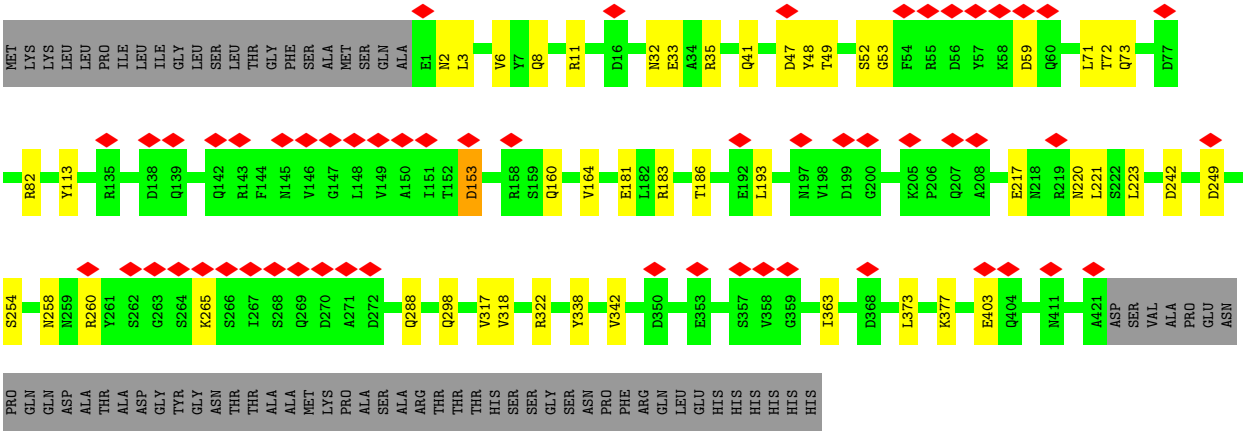
• Molecule 1: Outer membrane channel protein

Chain B:



• Molecule 1: Outer membrane channel protein

Chain C:


MET LYS LYS LEU LEU PRO ILE LEU ILE GLY LEU SER LEU THR GLY PHE SER ALA MET SER GLN ALA
E1 N2 L3 V6 Y7 Q8 R11 D16 N32 E33 A34 R35 Q41 D47 Y48 T49 S52 G53 F54 R55 D56 Y57 K58 D59 Q60 L71 T72 Q73 D77
R82 Y113 R135 D138 Q139 Q142 R143 F144 N145 V146 G147 L148 V149 A150 I151 T152 D153 R158 S159 Q160 V164 E181 L182 R183 T186 E192 L193 N197 V198 D199 G200 K205 P206 Q207 A208 E217 N218 R219 N220 L221 S222 L223 D242 D249
S254 N258 N259 R260 Y261 S262 G263 S264 K265 S266 I267 S268 Q269 D270 A271 D272 Q288 Q298 V317 V318 R322 Y338 V342 D350 E353 S357 V358 G359 I363 D368 L373 K377 E403 Q404 N411 A421
ASP SER VAL ALA PRO GLU ASN
PRO GLN GLN ASP ALA THR ALA ASP GLY TYR GLY ASN THR THR ALA ALA MET LYS PRO ALA SER ALA ARG THR THR THR HIS SER SER GLY SER ASN PRO PHE ARG GLN LEU GLU HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	188171	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 ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.467	Depositor
Minimum map value	-0.279	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0872	Depositor
Map size (Å)	177.552, 177.552, 177.552	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.34	0/3290	0.42	0/4467
1	B	0.34	0/3290	0.42	0/4467
1	C	0.34	0/3290	0.42	0/4467
All	All	0.34	0/9870	0.42	0/13401

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	A	3251	3205	3205	27	0
1	B	3251	3205	3205	27	0
1	C	3251	3205	3205	29	0
All	All	9753	9615	9615	77	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 (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLN:OE1	1:B:11:ARG:NH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:GLN:OE1	1:C:11:ARG:NH2	2.25	0.69
1:A:8:GLN:OE1	1:A:11:ARG:NH2	2.25	0.69
1:C:220:ASN:OD1	1:C:221:LEU:N	2.27	0.68
1:B:220:ASN:OD1	1:B:221:LEU:N	2.27	0.67
1:A:220:ASN:OD1	1:A:221:LEU:N	2.27	0.67
1:A:288:GLN:O	1:C:41:GLN:NE2	2.27	0.67
1:A:8:GLN:NE2	1:A:403:GLU:OE2	2.29	0.66
1:B:8:GLN:NE2	1:B:403:GLU:OE2	2.29	0.66
1:C:8:GLN:NE2	1:C:403:GLU:OE2	2.29	0.66
1:A:32:ASN:OD1	1:A:35:ARG:NH1	2.29	0.65
1:B:32:ASN:OD1	1:B:35:ARG:NH1	2.29	0.65
1:C:32:ASN:OD1	1:C:35:ARG:NH1	2.30	0.65
1:B:41:GLN:NE2	1:C:288:GLN:O	2.30	0.64
1:A:41:GLN:NE2	1:B:288:GLN:O	2.34	0.61
1:B:82:ARG:NH1	1:B:242:ASP:OD2	2.34	0.60
1:A:82:ARG:NH1	1:A:242:ASP:OD2	2.34	0.60
1:C:82:ARG:NH1	1:C:242:ASP:OD2	2.34	0.60
1:A:2:ASN:OD1	1:A:3:LEU:N	2.34	0.60
1:B:47:ASP:OD2	1:B:49:THR:HG23	2.03	0.58
1:B:2:ASN:OD1	1:B:3:LEU:N	2.34	0.58
1:C:160:GLN:O	1:C:164:VAL:HG23	2.04	0.58
1:A:47:ASP:OD2	1:A:49:THR:HG23	2.03	0.58
1:A:160:GLN:O	1:A:164:VAL:HG23	2.04	0.57
1:A:59:ASP:OD2	1:A:265:LYS:NZ	2.38	0.57
1:B:59:ASP:OD2	1:B:265:LYS:NZ	2.38	0.57
1:A:373:LEU:HD11	1:A:377:LYS:HE3	1.87	0.57
1:C:47:ASP:OD2	1:C:49:THR:HG23	2.03	0.57
1:C:2:ASN:OD1	1:C:3:LEU:N	2.34	0.56
1:B:160:GLN:O	1:B:164:VAL:HG23	2.04	0.56
1:A:298:GLN:NE2	1:C:33:GLU:OE1	2.36	0.56
1:C:59:ASP:OD2	1:C:265:LYS:NZ	2.38	0.56
1:A:2:ASN:O	1:A:6:VAL:HG23	2.06	0.56
1:B:373:LEU:HD11	1:B:377:LYS:HE3	1.87	0.56
1:B:2:ASN:O	1:B:6:VAL:HG23	2.06	0.56
1:C:373:LEU:HD11	1:C:377:LYS:HE3	1.87	0.55
1:C:2:ASN:O	1:C:6:VAL:HG23	2.06	0.55
1:C:338:TYR:O	1:C:342:VAL:HG23	2.07	0.55
1:B:338:TYR:O	1:B:342:VAL:HG23	2.07	0.54
1:A:338:TYR:O	1:A:342:VAL:HG23	2.07	0.53
1:A:71:LEU:HD23	1:A:72:THR:N	2.24	0.53
1:C:71:LEU:HD23	1:C:72:THR:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:TYR:CE2	1:C:193:LEU:HD22	2.44	0.53
1:A:113:TYR:CE2	1:A:193:LEU:HD22	2.44	0.53
1:B:113:TYR:CE2	1:B:193:LEU:HD22	2.44	0.53
1:B:71:LEU:HD23	1:B:72:THR:N	2.24	0.53
1:B:33:GLU:OE1	1:C:298:GLN:NE2	2.39	0.51
1:C:52:SER:OG	1:C:53:GLY:N	2.46	0.49
1:A:52:SER:OG	1:A:53:GLY:N	2.46	0.48
1:B:52:SER:OG	1:B:53:GLY:N	2.46	0.48
1:B:220:ASN:ND2	1:B:317:VAL:HG22	2.30	0.47
1:C:220:ASN:ND2	1:C:317:VAL:HG22	2.30	0.46
1:A:220:ASN:ND2	1:A:317:VAL:HG22	2.30	0.46
1:A:217:GLU:HA	1:A:223:LEU:HD23	1.98	0.46
1:C:217:GLU:HA	1:C:223:LEU:HD23	1.98	0.45
1:B:217:GLU:HA	1:B:223:LEU:HD23	1.98	0.45
1:A:33:GLU:OE1	1:B:298:GLN:NE2	2.43	0.45
1:C:153:ASP:HB3	1:C:363:ILE:HG21	2.01	0.43
1:A:72:THR:HG22	1:A:73:GLN:N	2.34	0.43
1:B:6:VAL:HG13	1:B:186:THR:HG21	2.00	0.43
1:A:6:VAL:HG13	1:A:186:THR:HG21	2.00	0.43
1:C:72:THR:HG22	1:C:73:GLN:N	2.34	0.43
1:B:153:ASP:HB3	1:B:363:ILE:HG21	2.00	0.42
1:A:153:ASP:HB3	1:A:363:ILE:HG21	2.01	0.42
1:C:6:VAL:HG13	1:C:186:THR:HG21	2.00	0.42
1:B:72:THR:HG22	1:B:73:GLN:N	2.34	0.42
1:A:318:VAL:O	1:A:322:ARG:HG2	2.20	0.41
1:B:318:VAL:O	1:B:322:ARG:HG2	2.20	0.41
1:C:318:VAL:O	1:C:322:ARG:HG2	2.20	0.41
1:B:258:ASN:OD1	1:B:260:ARG:NH2	2.54	0.41
1:C:258:ASN:OD1	1:C:260:ARG:NH2	2.53	0.41
1:A:258:ASN:OD1	1:A:260:ARG:NH2	2.54	0.41
1:C:254:SER:O	1:C:254:SER:OG	2.34	0.41
1:B:153:ASP:OD1	1:B:153:ASP:N	2.54	0.41
1:C:47:ASP:OD2	1:C:48:TYR:N	2.55	0.40
1:C:153:ASP:OD1	1:C:153:ASP:N	2.54	0.40
1:A:25:ASP:N	1:A:25:ASP:OD1	2.55	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	419/494 (85%)	404 (96%)	15 (4%)	0	100	100
1	B	419/494 (85%)	404 (96%)	15 (4%)	0	100	100
1	C	419/494 (85%)	404 (96%)	15 (4%)	0	100	100
All	All	1257/1482 (85%)	1212 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	354/414 (86%)	350 (99%)	4 (1%)	73	85
1	B	354/414 (86%)	350 (99%)	4 (1%)	73	85
1	C	354/414 (86%)	350 (99%)	4 (1%)	73	85
All	All	1062/1242 (86%)	1050 (99%)	12 (1%)	74	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASP
1	A	181	GLU
1	A	183	ARG
1	A	249	ASP
1	B	153	ASP

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Mol	Chain	Res	Type
1	B	181	GLU
1	B	183	ARG
1	B	249	ASP
1	C	153	ASP
1	C	181	GLU
1	C	183	ARG
1	C	249	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	B	139	GLN
1	B	340	GLN
1	C	139	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 monosaccharides 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.

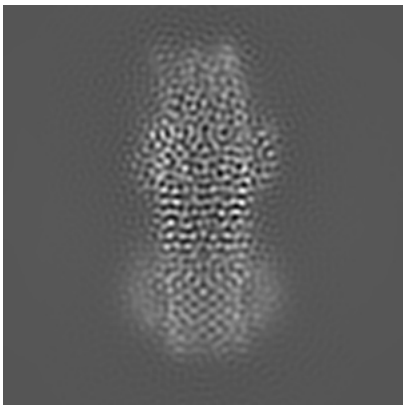
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12310. These allow visual inspection of the internal detail of the map and identification of artifacts.

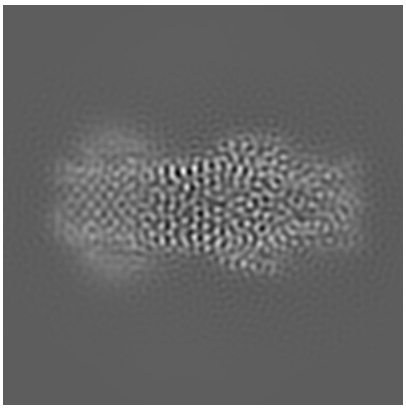
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

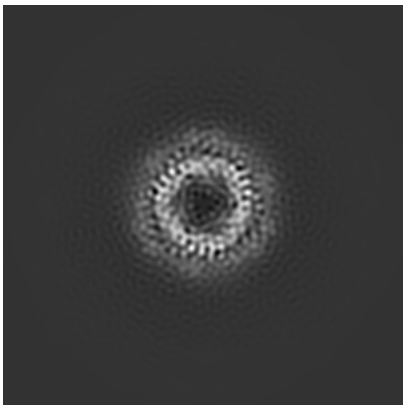
6.1.1 Primary map



X

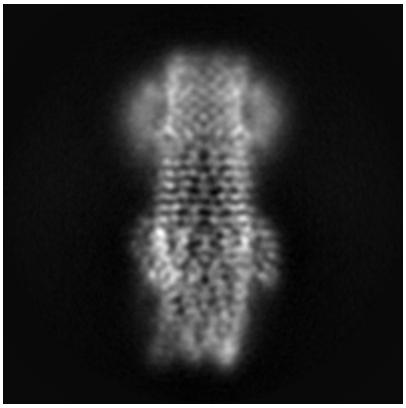


Y

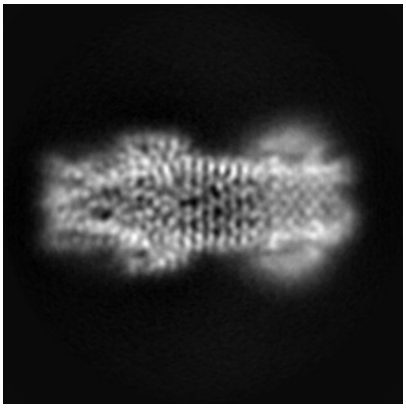


Z

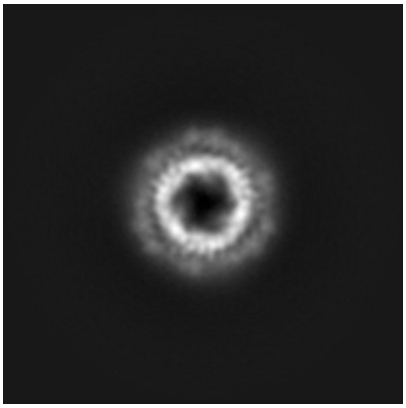
6.1.2 Raw map



X



Y

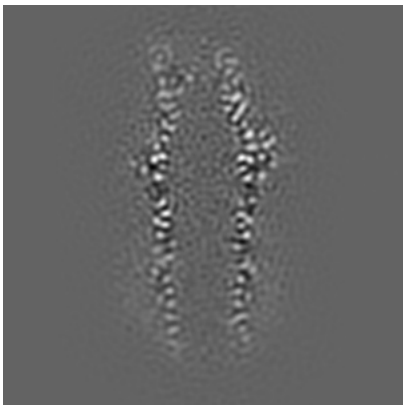


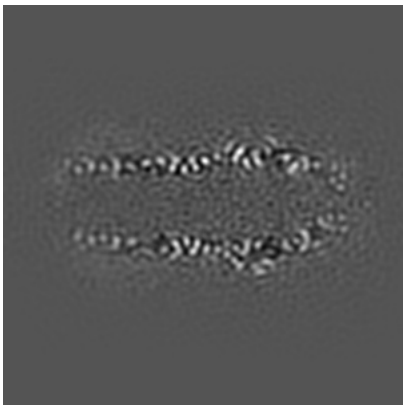
Z

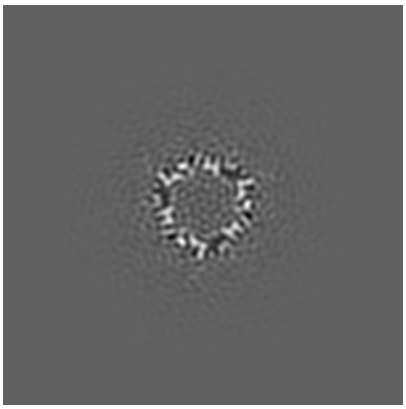
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

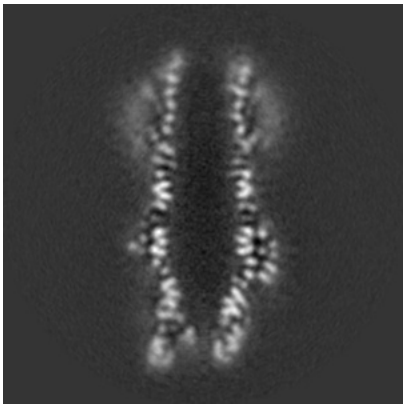
6.2.1 Primary map

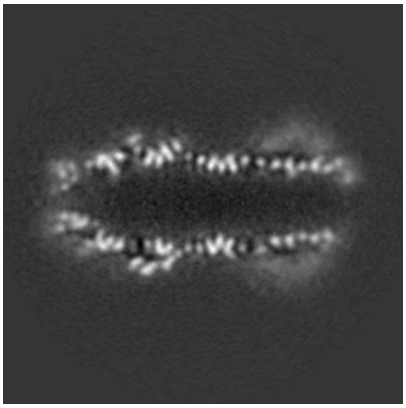

X Index: 108

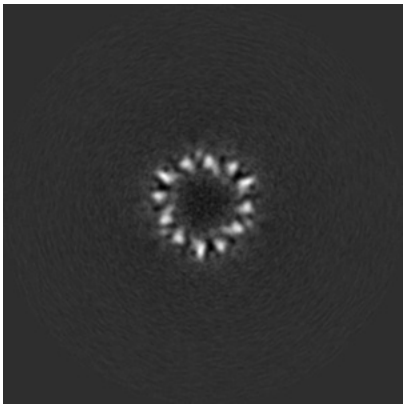

Y Index: 108


Z Index: 108

6.2.2 Raw map


X Index: 108

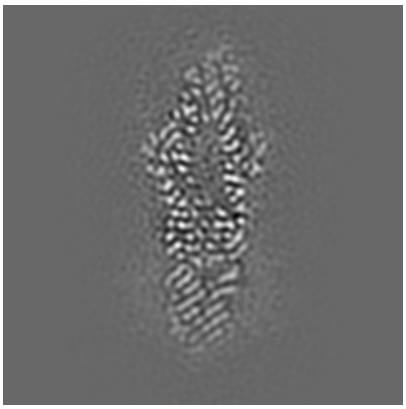

Y Index: 108

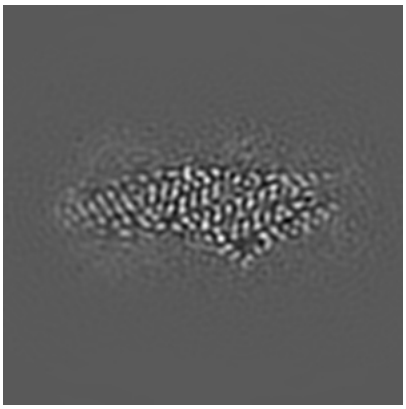

Z Index: 108

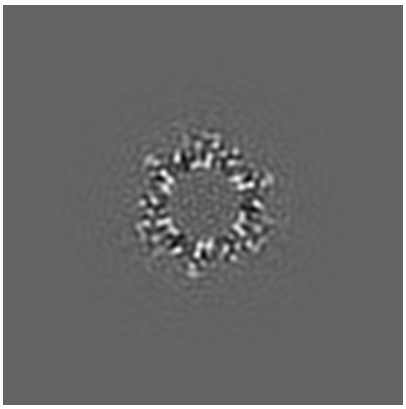
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

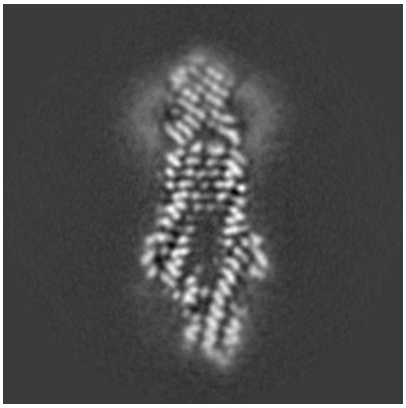
6.3.1 Primary map

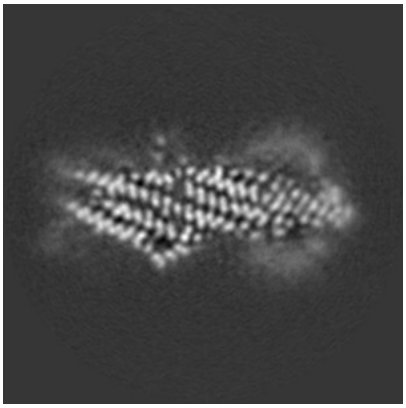

X Index: 125

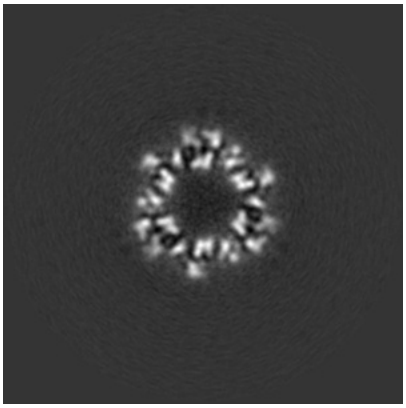

Y Index: 128


Z Index: 128

6.3.2 Raw map


X Index: 125

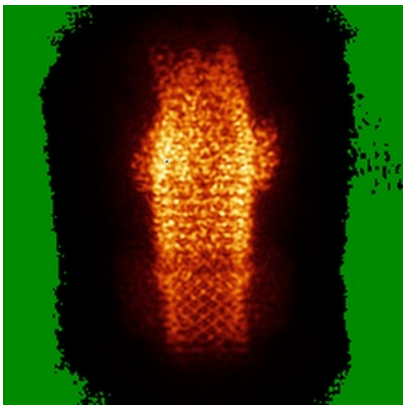

Y Index: 128

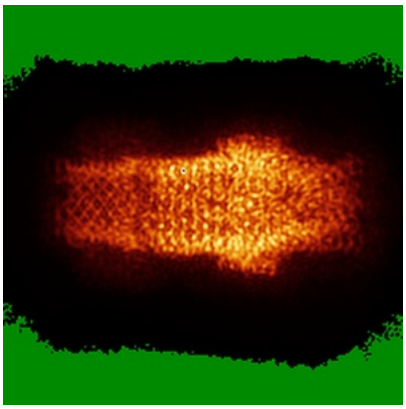

Z Index: 87

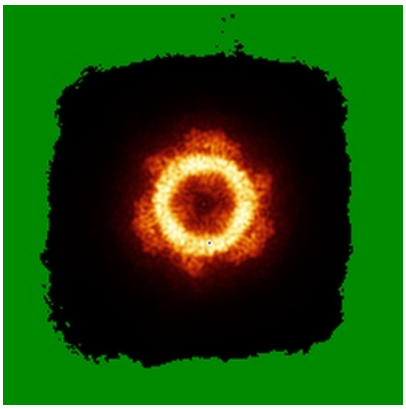
The images above show the largest variance slices of the map in three orthogonal directions.

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

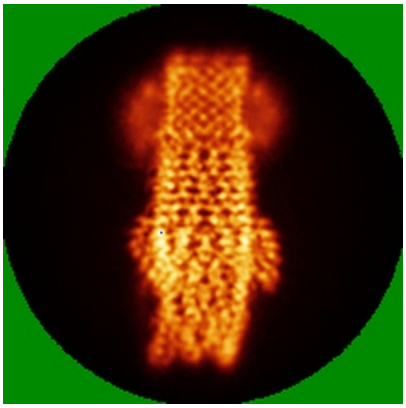
6.4.1 Primary map

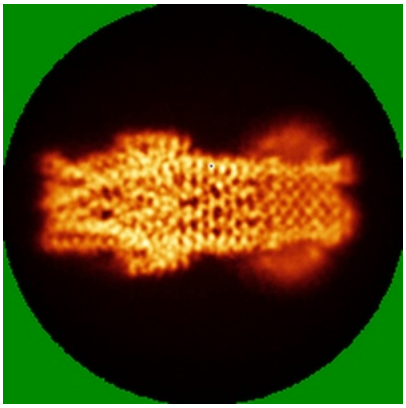

X

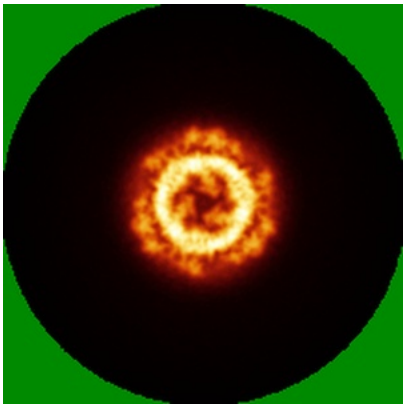

Y


Z

6.4.2 Raw map


X

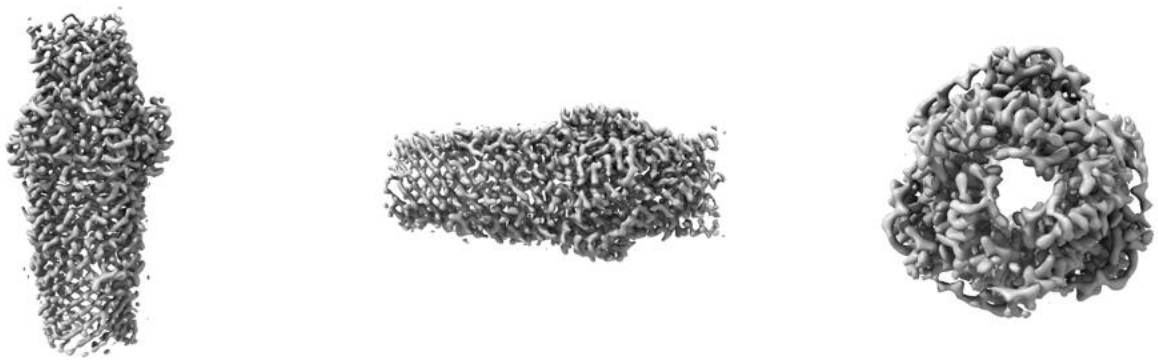

Y


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)

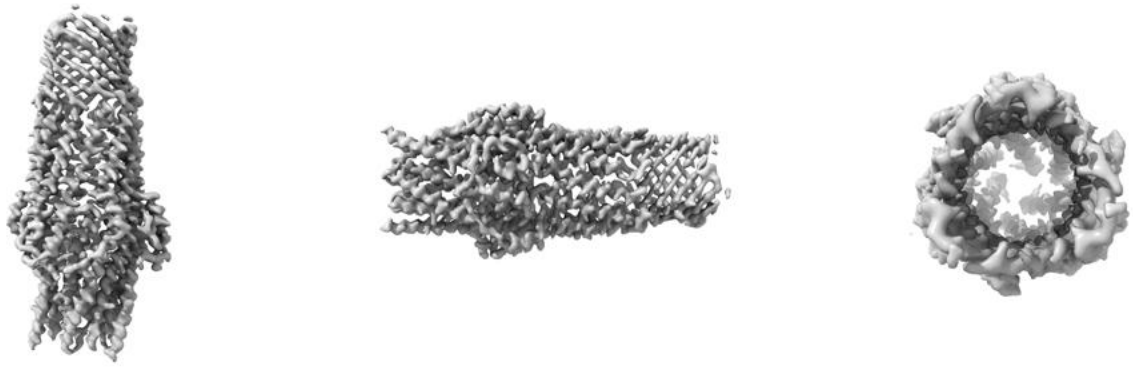
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0872. 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.

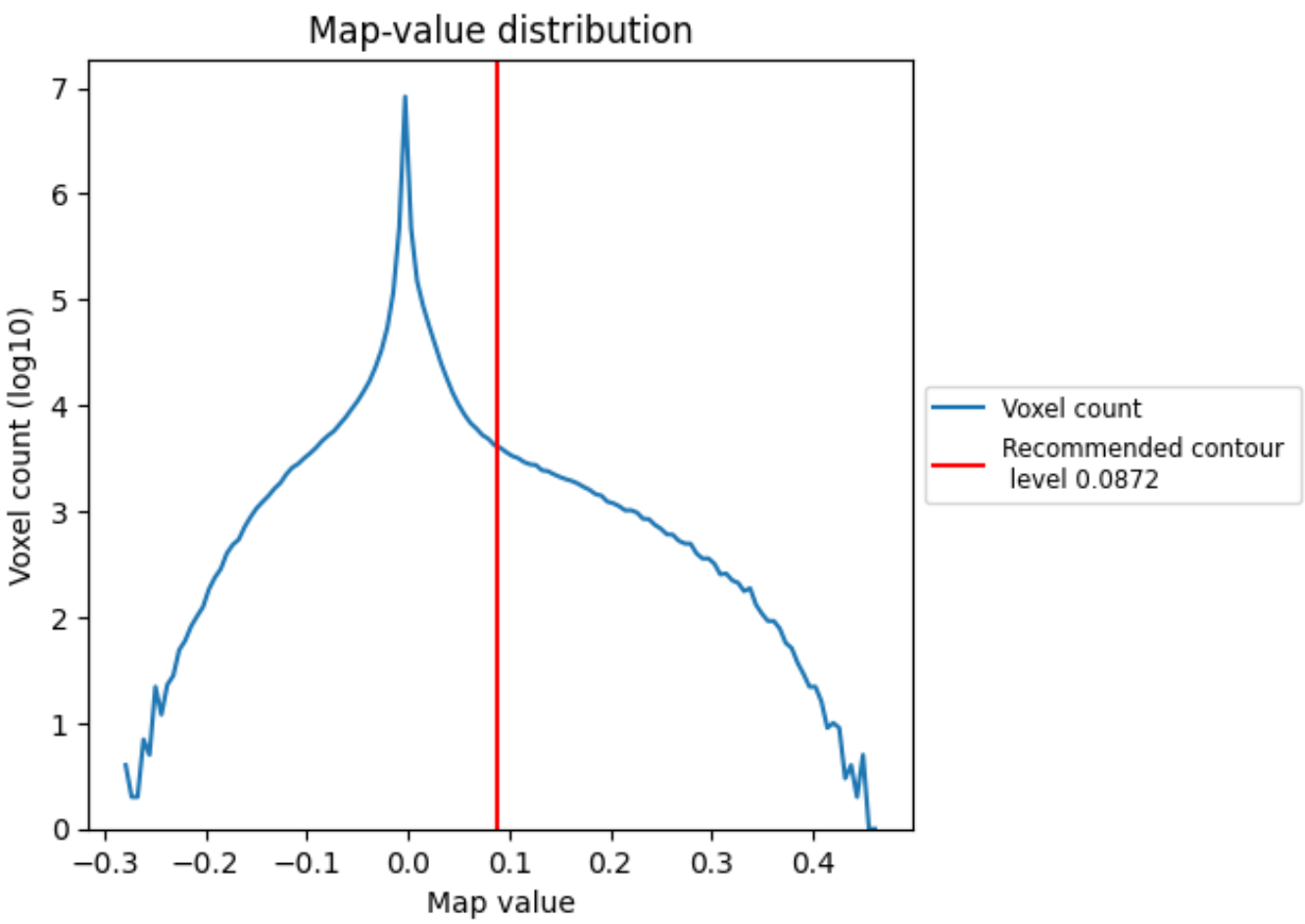
6.6 Mask visualisation (i)

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

7 Map analysis (i)

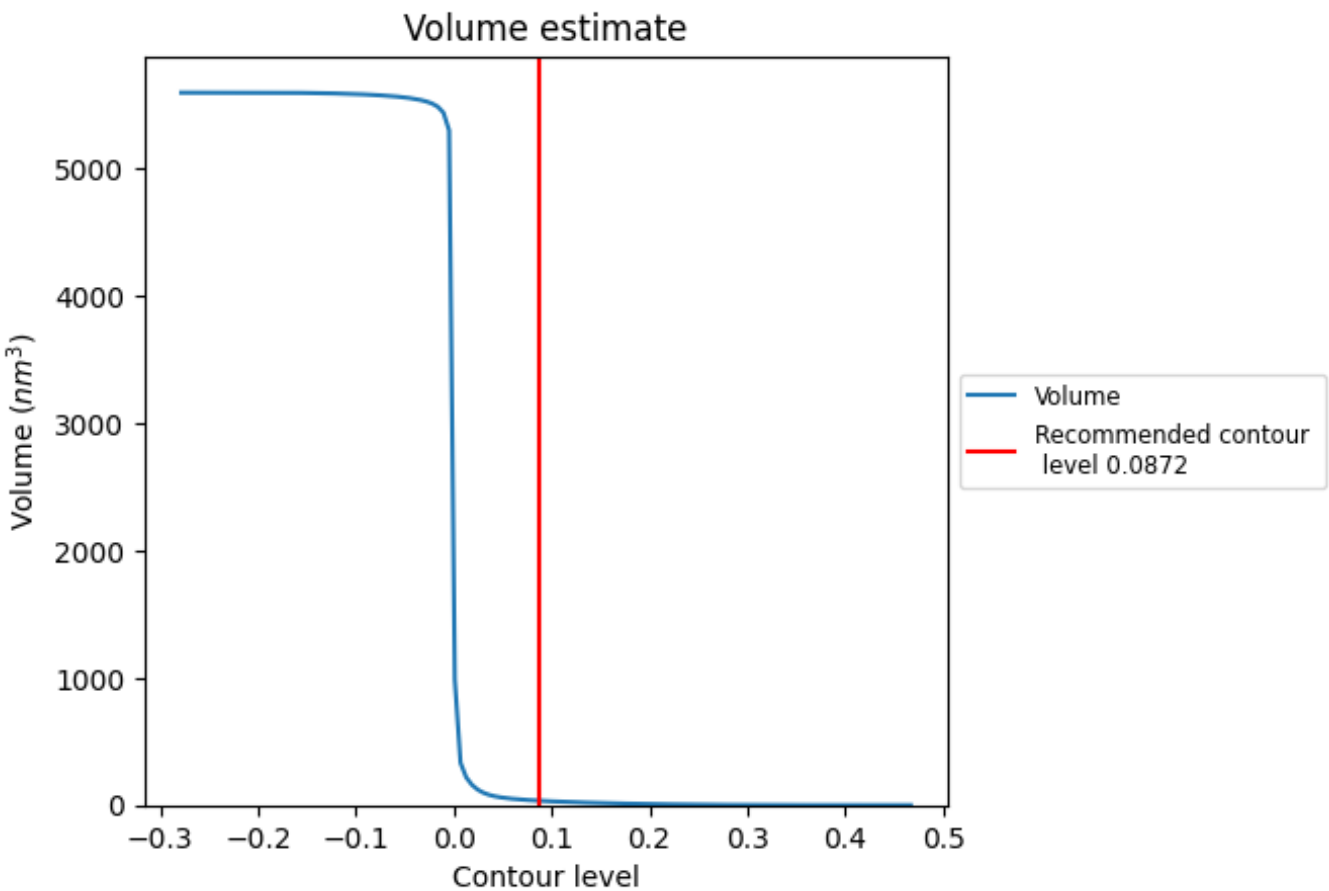
This section contains the results of statistical analysis of the map.

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.

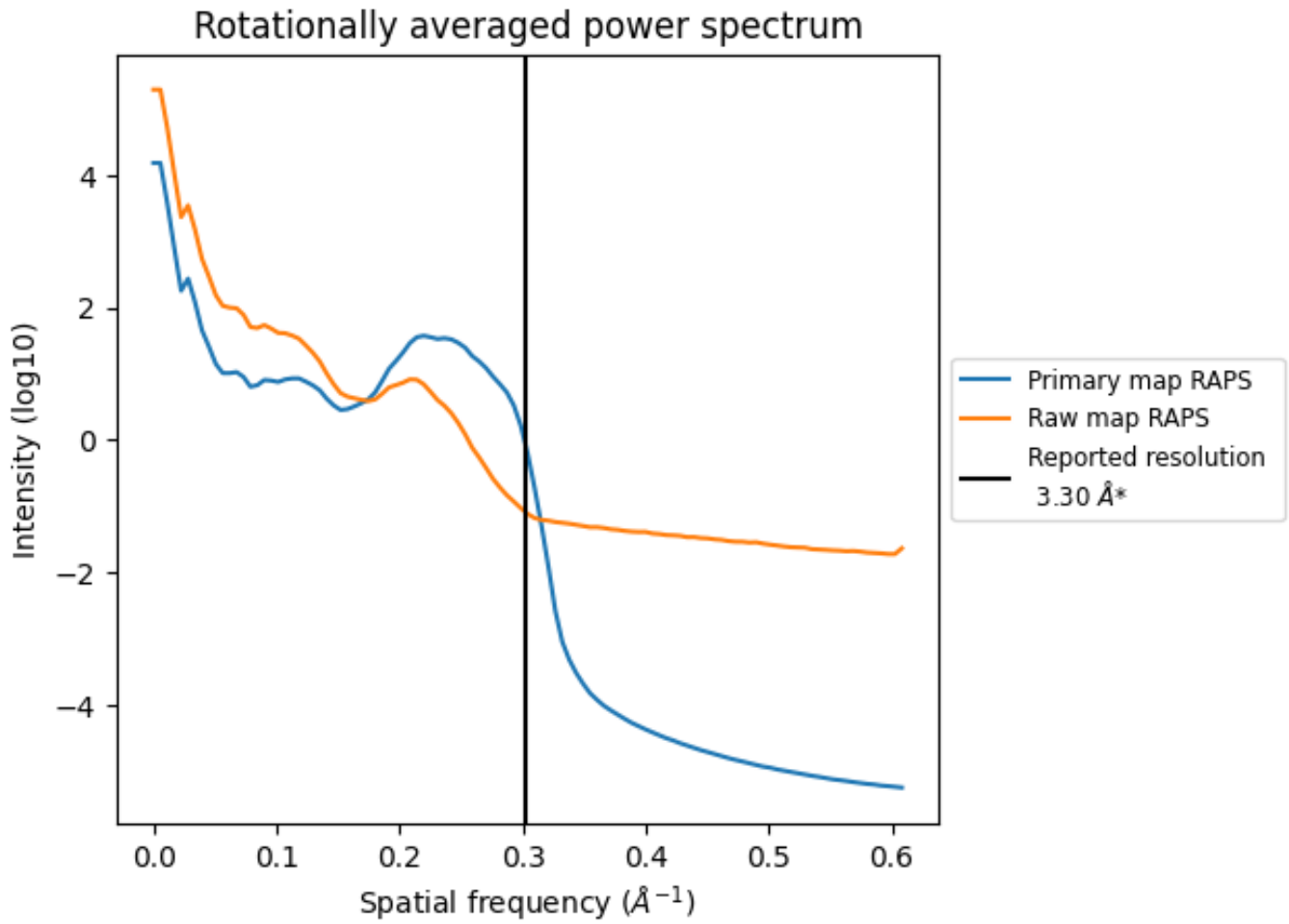
7.2 Volume estimate (i)



The volume at the recommended contour level is 35 nm^3; this corresponds to an approximate mass of 31 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)

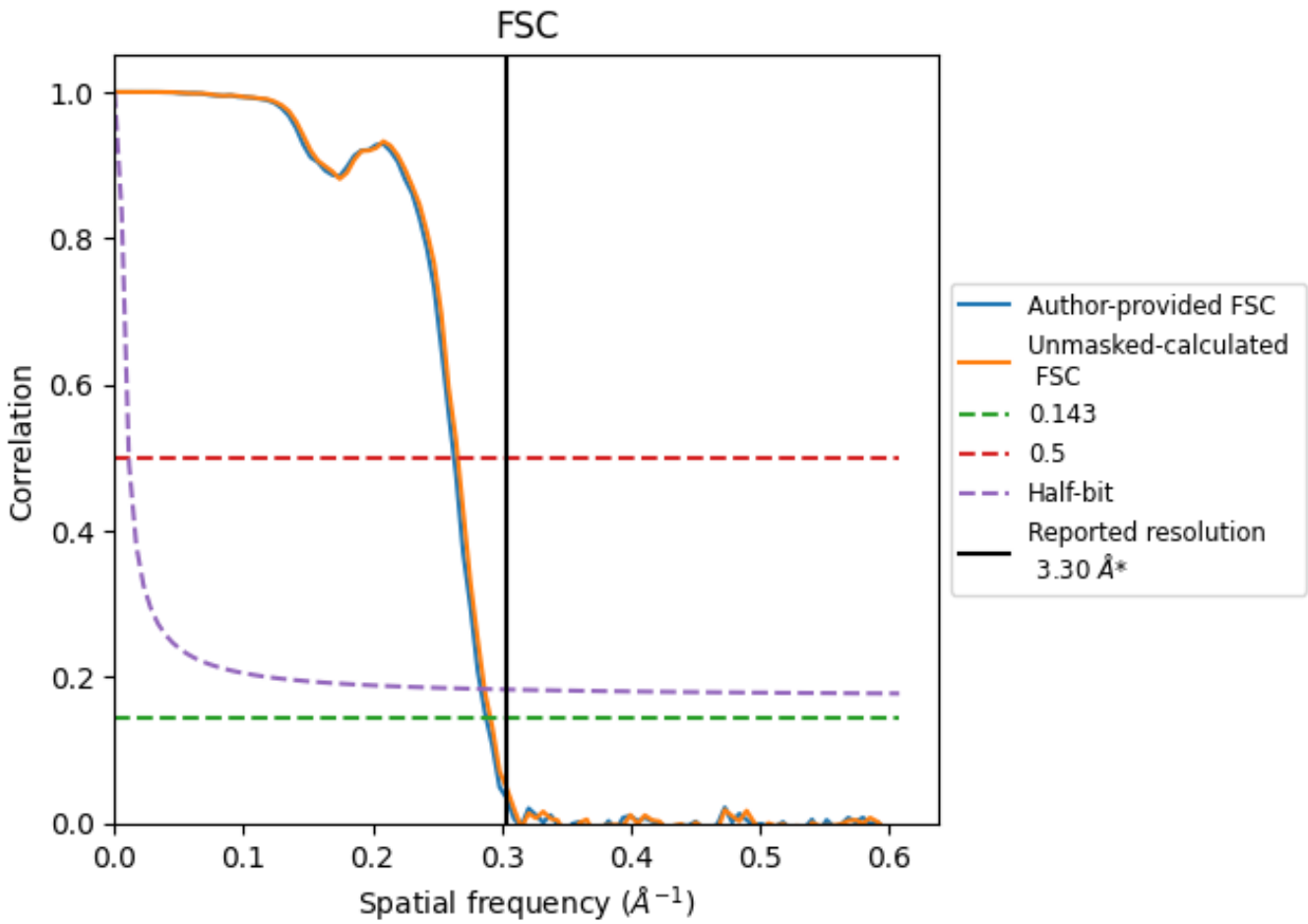


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

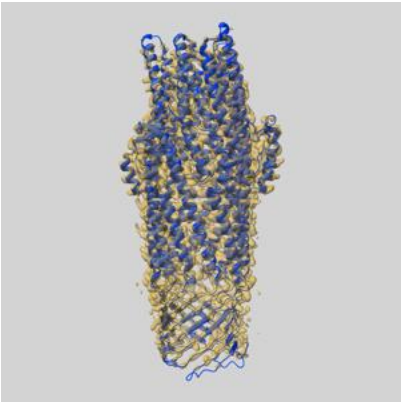
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.47	3.80	3.52
Unmasked-calculated*	3.43	3.76	3.49

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

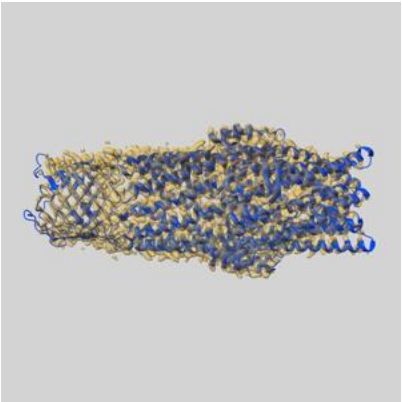
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12310 and PDB model 7NG9. Per-residue inclusion information can be found in section 3 on page 4.

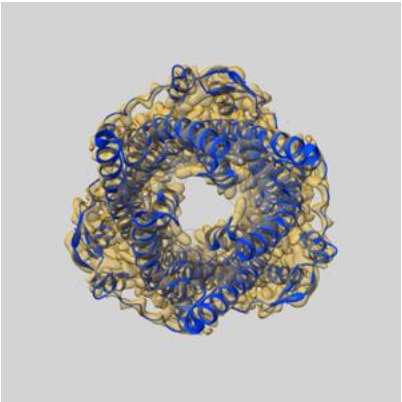
9.1 Map-model overlay (i)



X



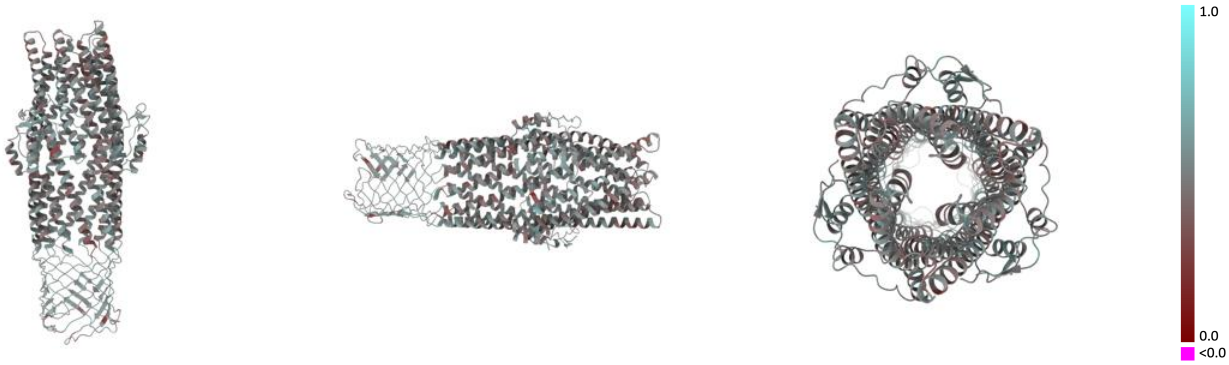
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0872 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.

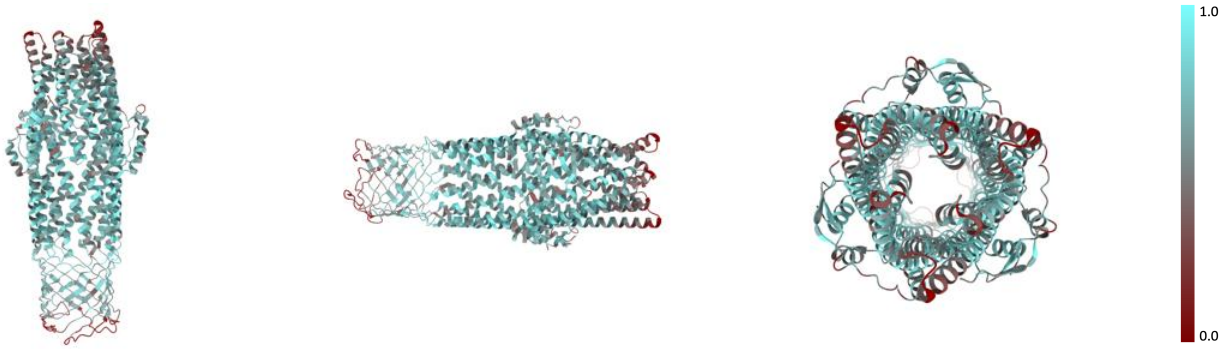
9.2 Q-score mapped to coordinate model (i)



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.

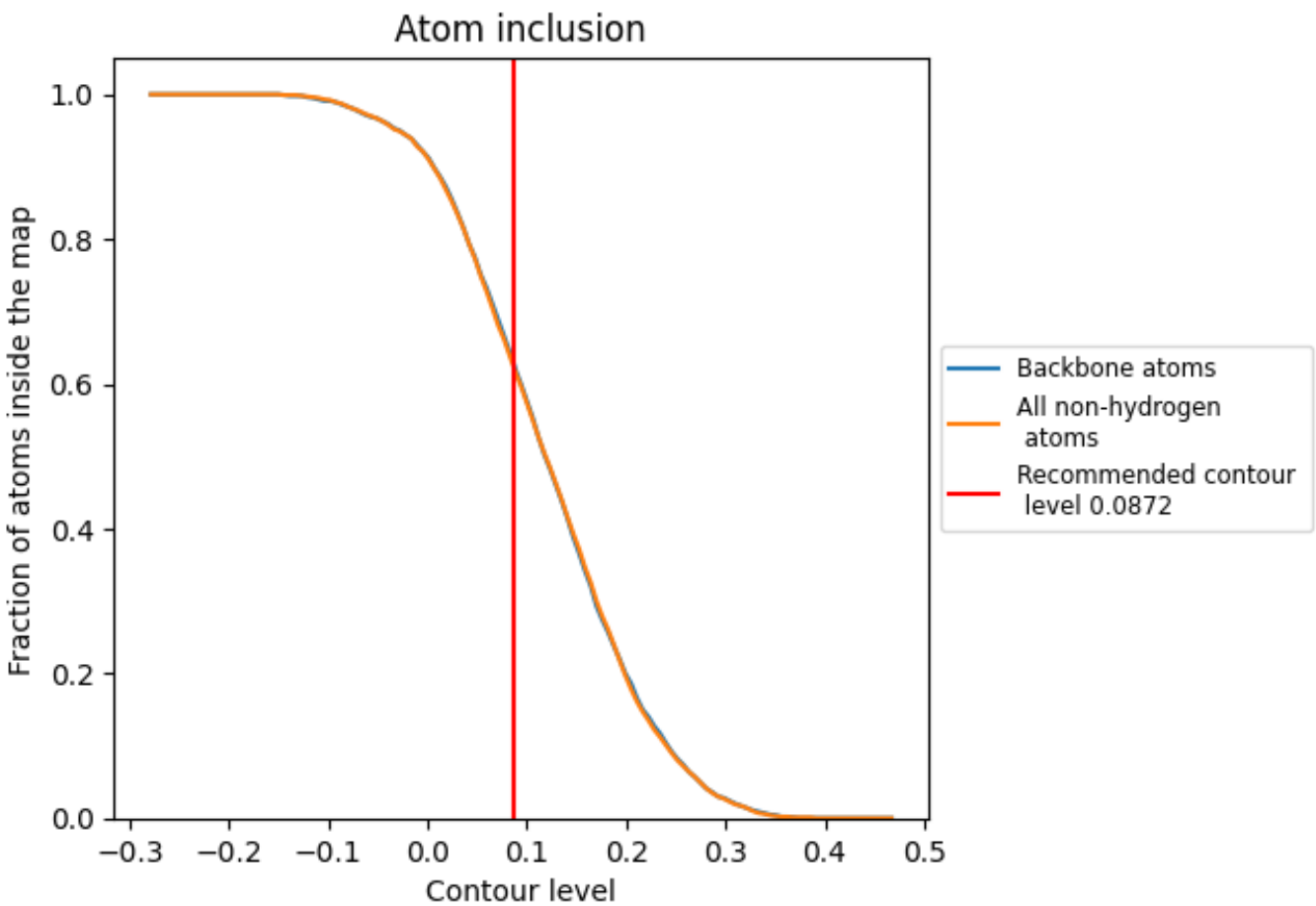
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0872).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 62% 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 (0.0872) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6210	0.4850
A	0.6330	0.4860
B	0.6310	0.4850
C	0.6310	0.4840