wwPDB EM Validation Summary Report (i)

May 12, 2024 – 08:57 am BST

PDB ID	:	6TE9
EMDB ID	:	EMD-10477
Title	:	Neck of native GTA particle computed with C6 symmetry
Authors	:	Bardy, P.; Fuzik, T.; Hrebik, D.; Pantucek, R.; Beatty, J.T.; Plevka, P.
Deposited on	:	2019-11-11
Resolution	:	3.58 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 (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:

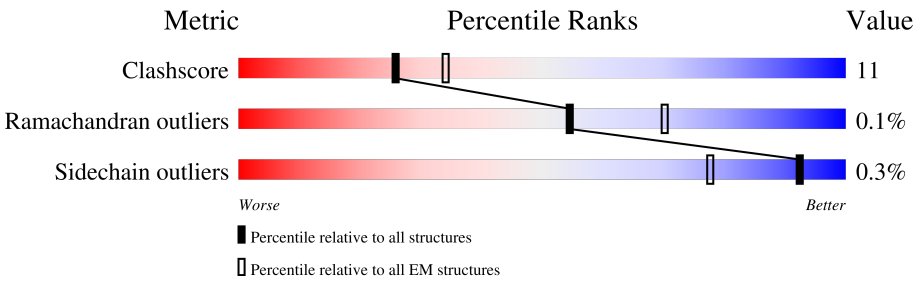
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.58 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	C	197	13% 75% 23% • •
1	D	197	7% 68% 30% • •
2	A	396	9% 76% 15% 9%
2	B	396	10% 75% 16% 9%
3	F	135	• 70% 27% • •
4	E	112	• 68% 30% •
5	G	137	15% 71% 23% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11151 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 Adaptor protein Rcc01688.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	194	1450	931	259	253	7	0	0
1	D	194	1456	936	259	253	8	0	0

- Molecule 2 is a protein called Phage portal protein, HK97 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	360	2723	1734	486	490	13	0	0
2	B	360	2723	1734	486	490	13	0	0

- Molecule 3 is a protein called Tail terminator protein Rcc01690.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	134	968	613	174	180	1	0	0

- Molecule 4 is a protein called Stopper protein Rcc01689.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	110	859	536	171	151	1	0	0

- Molecule 5 is a protein called Phage major tail protein, TP901-1 family.

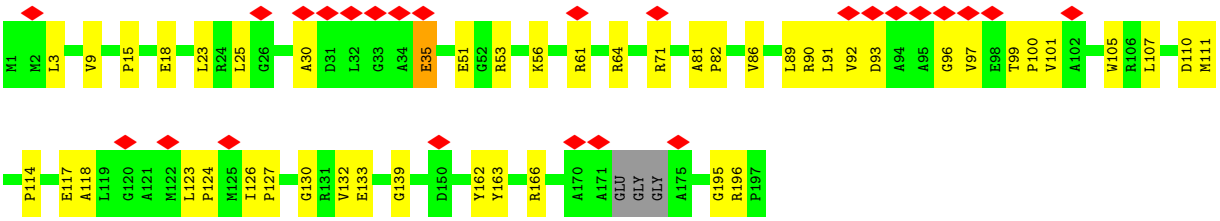
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	130	972	612	163	195	2	0	0

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.

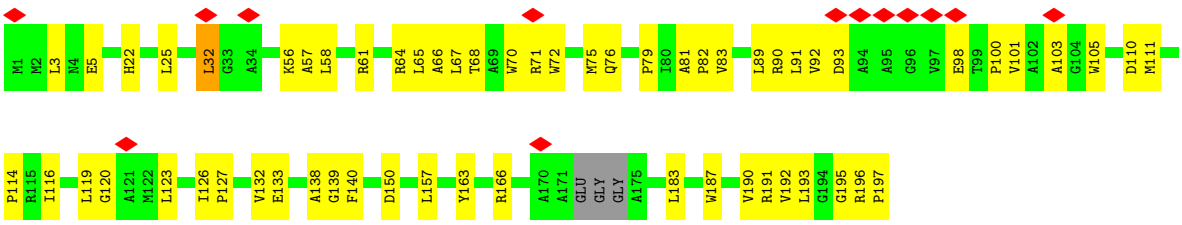
- Molecule 1: Adaptor protein Rcc01688

Chain C:



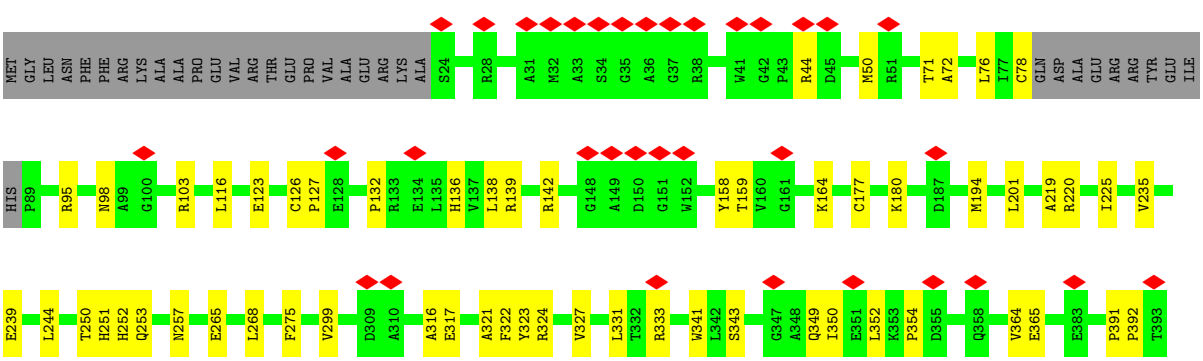
- Molecule 1: Adaptor protein Rcc01688

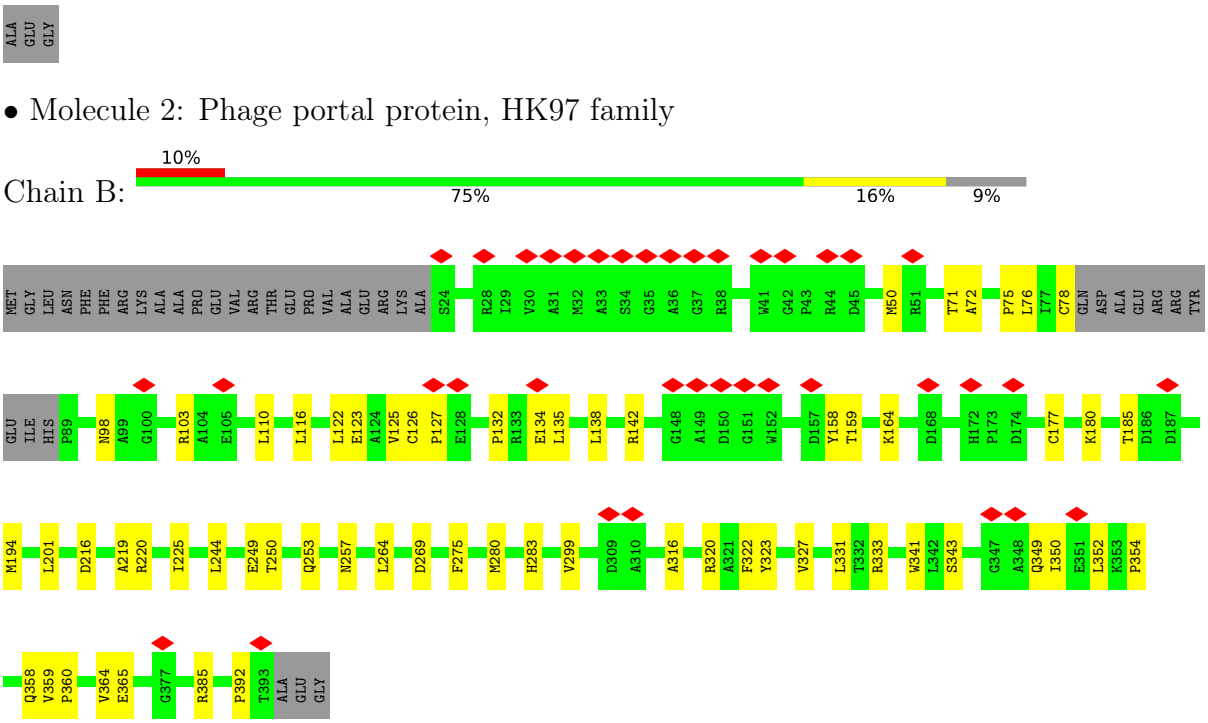
Chain D:

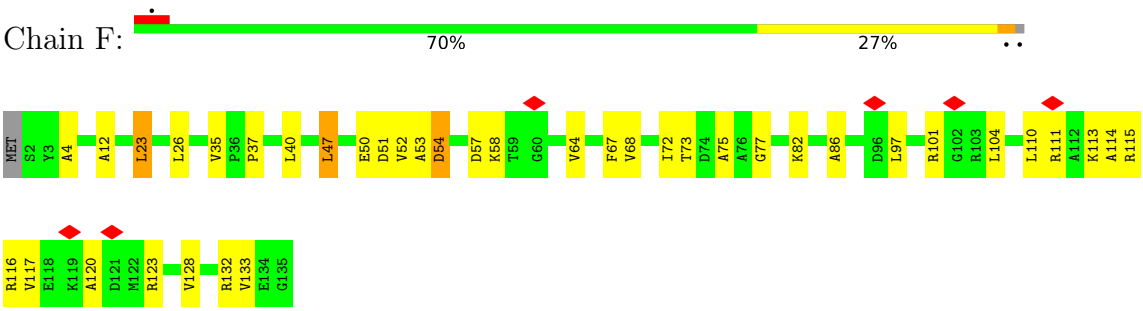


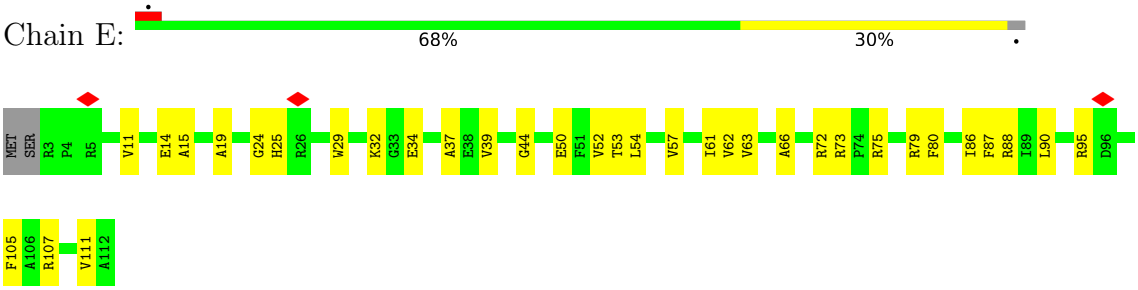
- Molecule 2: Phage portal protein, HK97 family

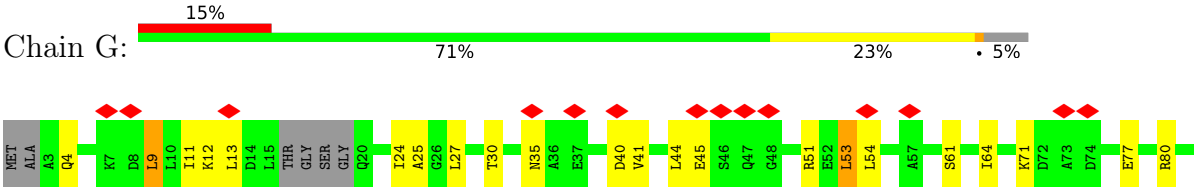
Chain A:

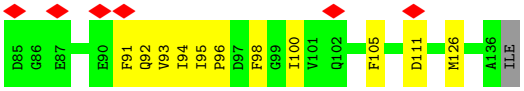



ALA GLU GLY
• Molecule 2: Phage portal protein, HK97 family
Chain B:
10%
75%
16%
9%
MET GLY LEU ASN PHE PHE ARG LYS ALA ALA PRO GLU VAL ARG THR GLU PRO VAL ALA GLU ARG LYS ALA S24 R28 I29 V30 A31 M32 A33 S34 G35 A36 G37 R38 W41 G42 P43 R44 D45 N50 R51 T71 A72 P75 L76 I77 C78 GLN ASP ALA GLU ARG ARG TYR
GLU ILE HIS P89 N98 A99 G100 R103 A104 E105 L110 L116 L122 E123 A124 V125 C126 P127 E128 P132 R133 E134 L135 L138 R142 G148 A149 D150 G151 W152 D157 Y158 T159 K164 D168 H172 P173 D174 C177 K180 T185 D186 D187
M194 L201 D216 A219 R220 I225 L244 E249 T250 Q253 N257 L264 D269 F275 M280 H283 V299 D309 A310 A316 R320 A321 F322 Y323 V327 L331 T332 R333 W341 L342 S343 G347 A348 Q349 I350 E351 L352 K353 P354
Q358 V359 P360 V364 E365 G377 R385 P392 T393 ALA GLU GLY


• Molecule 3: Tail terminator protein Rcc01690
Chain F:
70%
27%
MET S2 Y3 A4 A12 L23 L26 V35 P36 P37 L40 L47 E50 D51 V52 A53 D54 D57 K58 T59 G60 V64 F67 V68 I72 T73 D74 A75 A76 G77 K82 A86 D96 L97 R101 G102 R103 L104 L110 R111 A112 K113 A114 R115
R116 V117 E118 K119 A120 D121 M122 R123 V128 R132 V133 E134 G135


• Molecule 4: Stopper protein Rcc01689
Chain E:
68%
30%
MET SER R3 P4 R5 V11 E14 A15 A19 G24 H25 R26 W29 K32 G33 E34 A37 E38 V39 G44 E50 F51 V52 T53 L54 V57 I61 V62 V63 A66 R72 R73 P74 R75 R79 F80 I86 F87 R88 I89 L90 R95 D96
F105 A106 R107 V111 A112


• Molecule 5: Phage major tail protein, TP901-1 family
Chain G:
15%
71%
23%
5%
MET ALA A3 Q4 K7 D8 L9 L10 I11 K12 L13 D14 L15 THR GLY SER GLY Q20 I24 A25 G26 L27 T30 N35 A36 E37 D40 V41 L44 E45 S46 Q47 G48 R51 E52 L53 L54 A57 S61 I64 K71 D72 A73 D74 E77 R80


D85
G86
E87
E90
F91
Q92
V93
I94
I95
P96
D97
F98
G99
I100
V101
Q102
F105
D111
M126
A136
ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	41516	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 ($e^-/Å^2$)	42.75	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.516	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.088	Depositor
Map size (Å)	318.9, 318.9, 318.9	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	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	0.58	1/1482 (0.1%)	0.81	3/2021 (0.1%)
1	D	0.54	0/1488	0.74	1/2028 (0.0%)
2	A	0.50	0/2794	0.65	2/3804 (0.1%)
2	B	0.49	0/2794	0.66	2/3804 (0.1%)
3	F	0.52	0/982	0.76	3/1337 (0.2%)
4	E	0.57	0/875	0.69	0/1182
5	G	0.44	0/987	0.74	2/1332 (0.2%)
All	All	0.52	1/11402 (0.0%)	0.71	13/15508 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	PRO	N-CD	-6.00	1.39	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	219	ALA	C-N-CA	-6.61	105.18	121.70
5	G	53	LEU	CA-CB-CG	6.58	130.44	115.30
3	F	54	ASP	CB-CG-OD1	6.54	124.19	118.30
5	G	9	LEU	CA-CB-CG	6.38	129.99	115.30
2	A	219	ALA	C-N-CA	-6.28	106.00	121.70

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	1450	0	1474	42	0
1	D	1456	0	1490	59	0
2	A	2723	0	2706	37	0
2	B	2723	0	2706	35	0
3	F	968	0	987	36	0
4	E	859	0	861	29	0
5	G	972	0	938	38	0
All	All	11151	0	11162	253	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 253 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:D:5:GLU:CD	1:D:61:ARG:HE	1.71	0.92
4:E:52:VAL:HG13	4:E:111:VAL:HG23	1.52	0.88
1:C:91:LEU:HD13	1:C:132:VAL:HG23	1.54	0.86
1:C:89:LEU:HD23	1:C:89:LEU:O	1.77	0.84
4:E:52:VAL:CG1	4:E:111:VAL:HG23	2.07	0.82

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	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	29 67
1	D	190/197 (96%)	164 (86%)	26 (14%)	0	100 100
2	A	356/396 (90%)	328 (92%)	28 (8%)	0	100 100
2	B	356/396 (90%)	328 (92%)	28 (8%)	0	100 100
3	F	132/135 (98%)	118 (89%)	14 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
5	G	126/137 (92%)	115 (91%)	11 (9%)	0	100	100
All	All	1458/1570 (93%)	1312 (90%)	145 (10%)	1 (0%)	54	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	30	ALA

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	C	138/141 (98%)	136 (99%)	2 (1%)	67	85
1	D	140/141 (99%)	140 (100%)	0	100	100
2	A	274/302 (91%)	274 (100%)	0	100	100
2	B	274/302 (91%)	274 (100%)	0	100	100
3	F	91/92 (99%)	91 (100%)	0	100	100
4	E	83/85 (98%)	83 (100%)	0	100	100
5	G	99/103 (96%)	98 (99%)	1 (1%)	76	89
All	All	1099/1166 (94%)	1096 (100%)	3 (0%)	92	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	35	GLU
1	C	71	ARG
5	G	45	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	319	ASN
2	B	253	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.

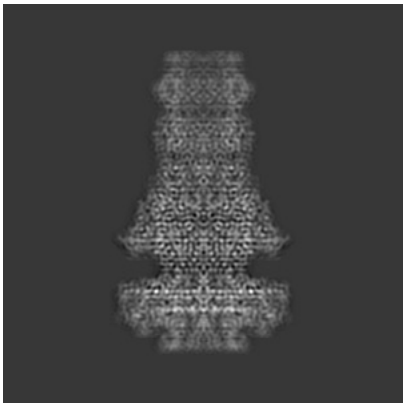
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10477. These allow visual inspection of the internal detail of the map and identification of artifacts.

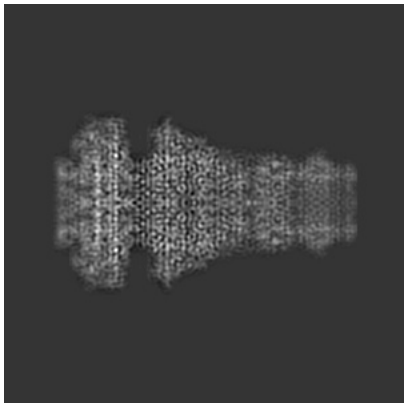
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

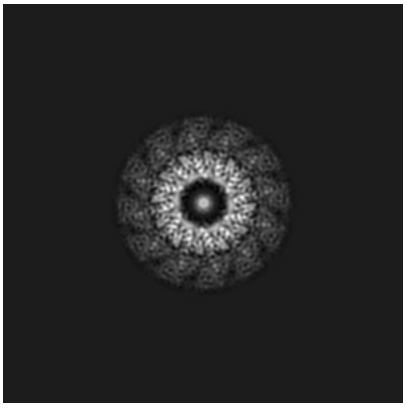
6.1.1 Primary map



X



Y

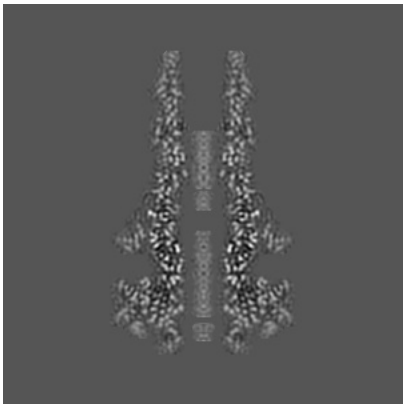


Z

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

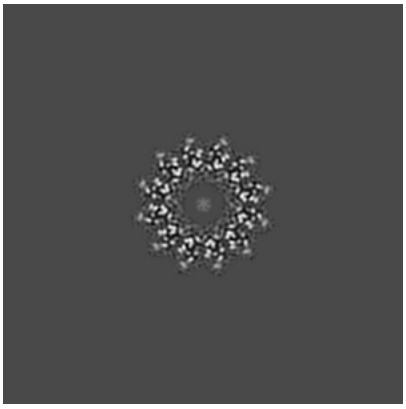
6.2 Central slices (i)

6.2.1 Primary map



X Index: 150

Y Index: 150

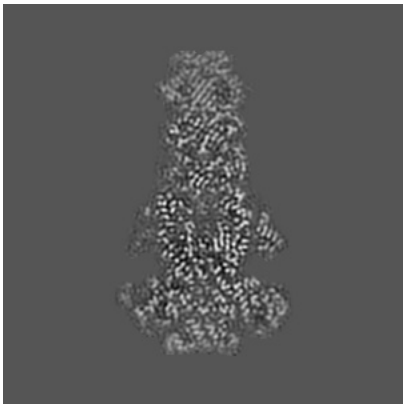


Z Index: 150

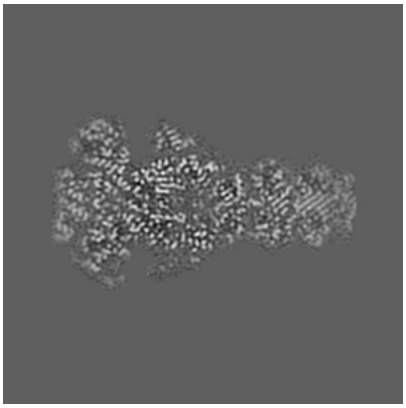
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

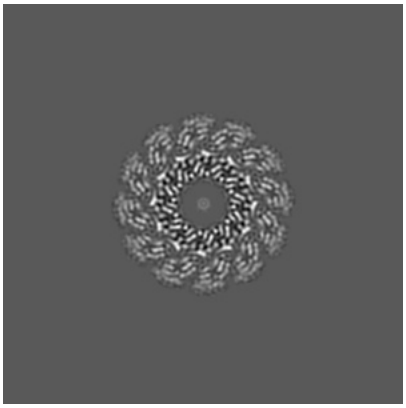
6.3.1 Primary map



X Index: 171



Y Index: 129

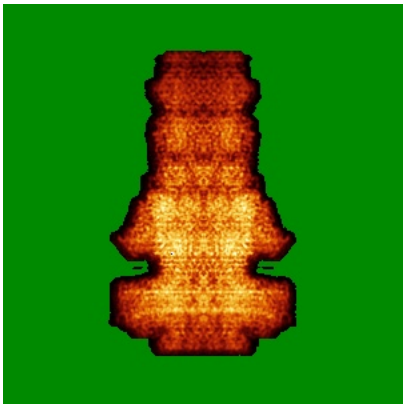


Z Index: 122

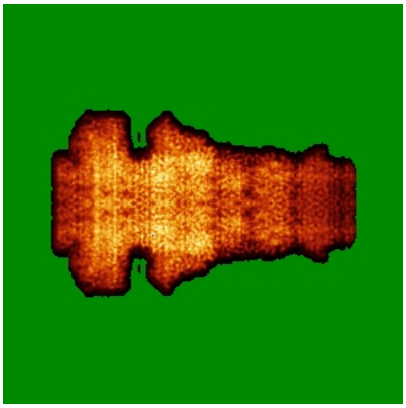
The images above show the largest variance slices of the map in three orthogonal directions.

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

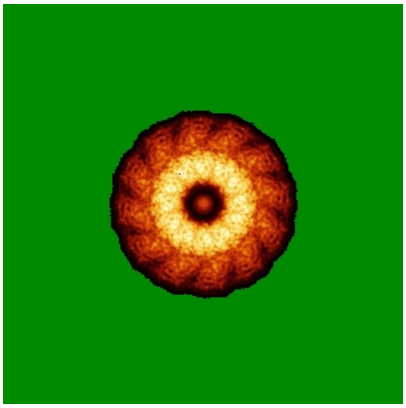
6.4.1 Primary map



X



Y

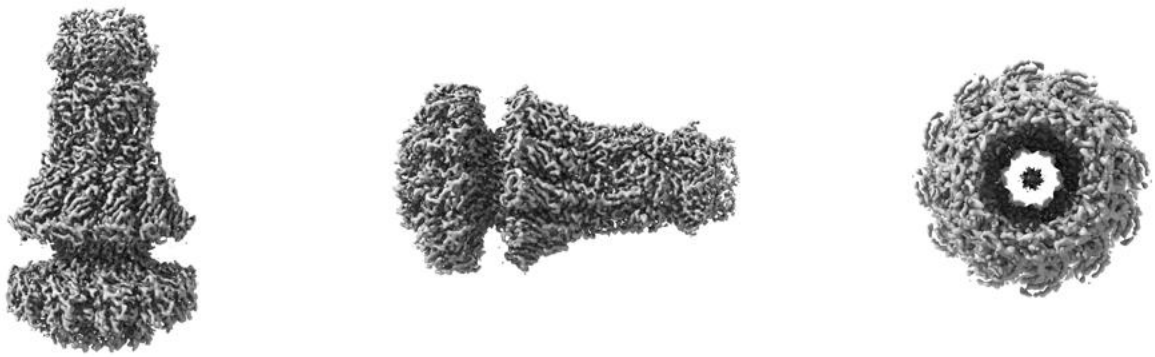


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

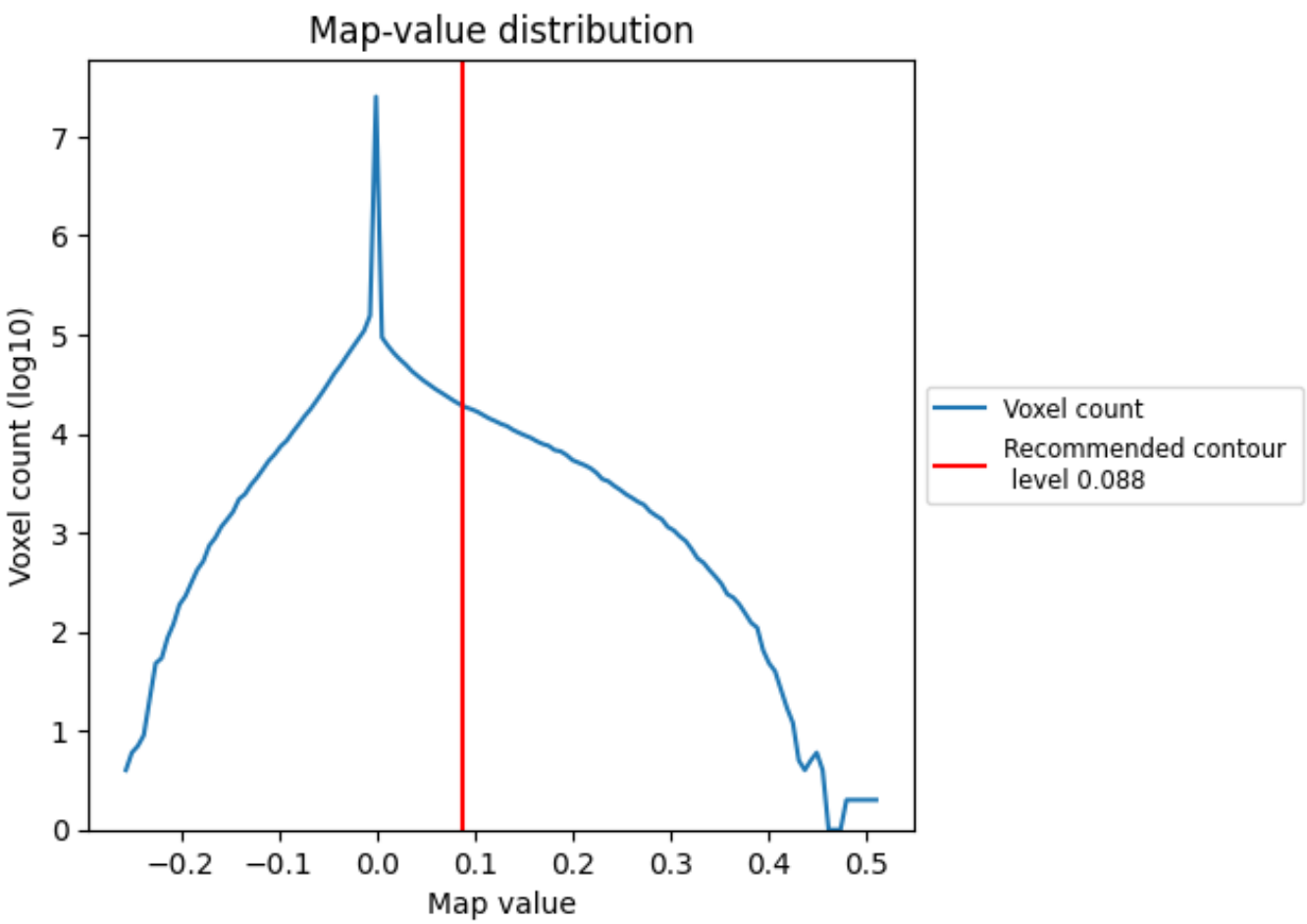
6.6 Mask visualisation (i)

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

7 Map analysis (i)

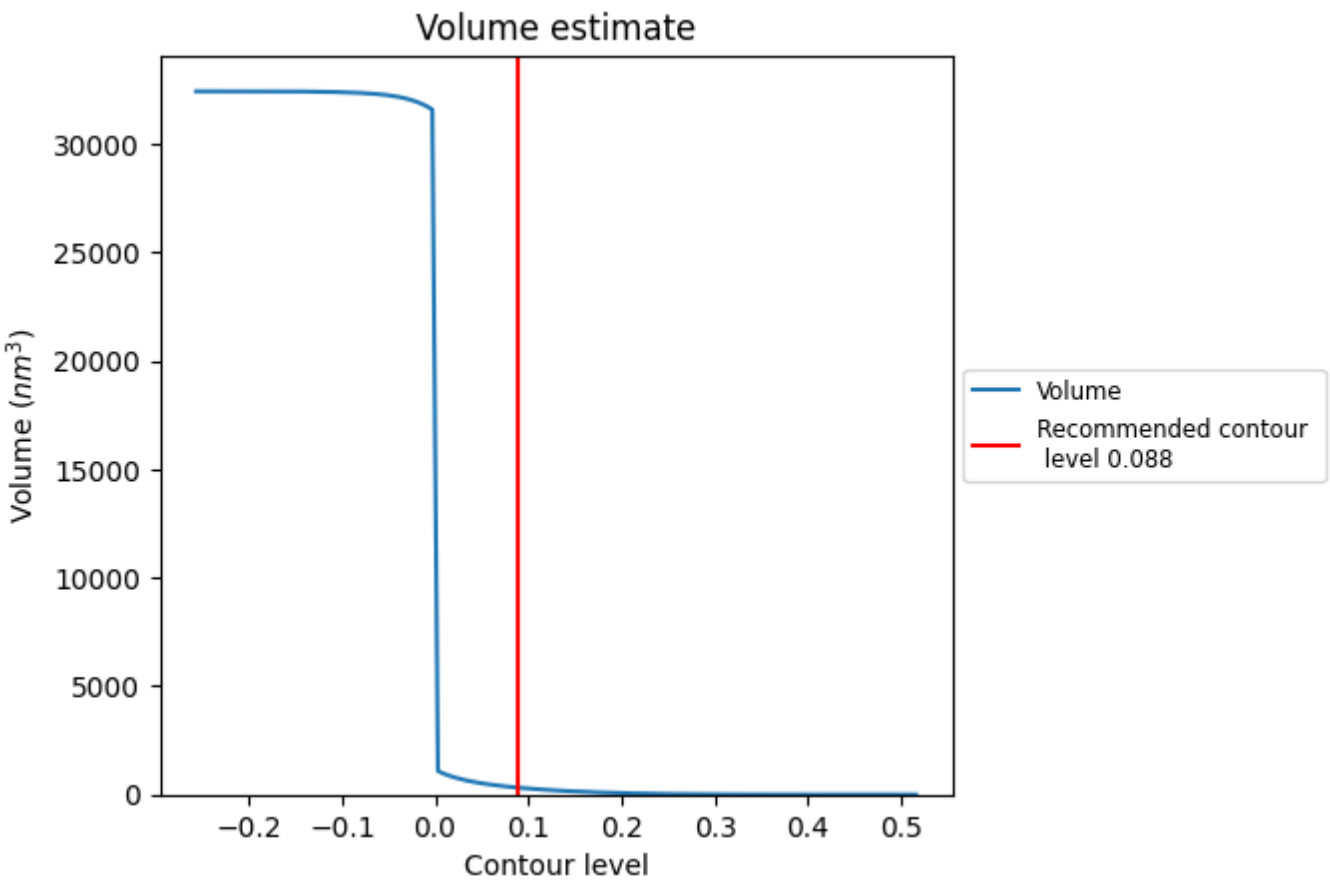
This section contains the results of statistical analysis of the map.

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.

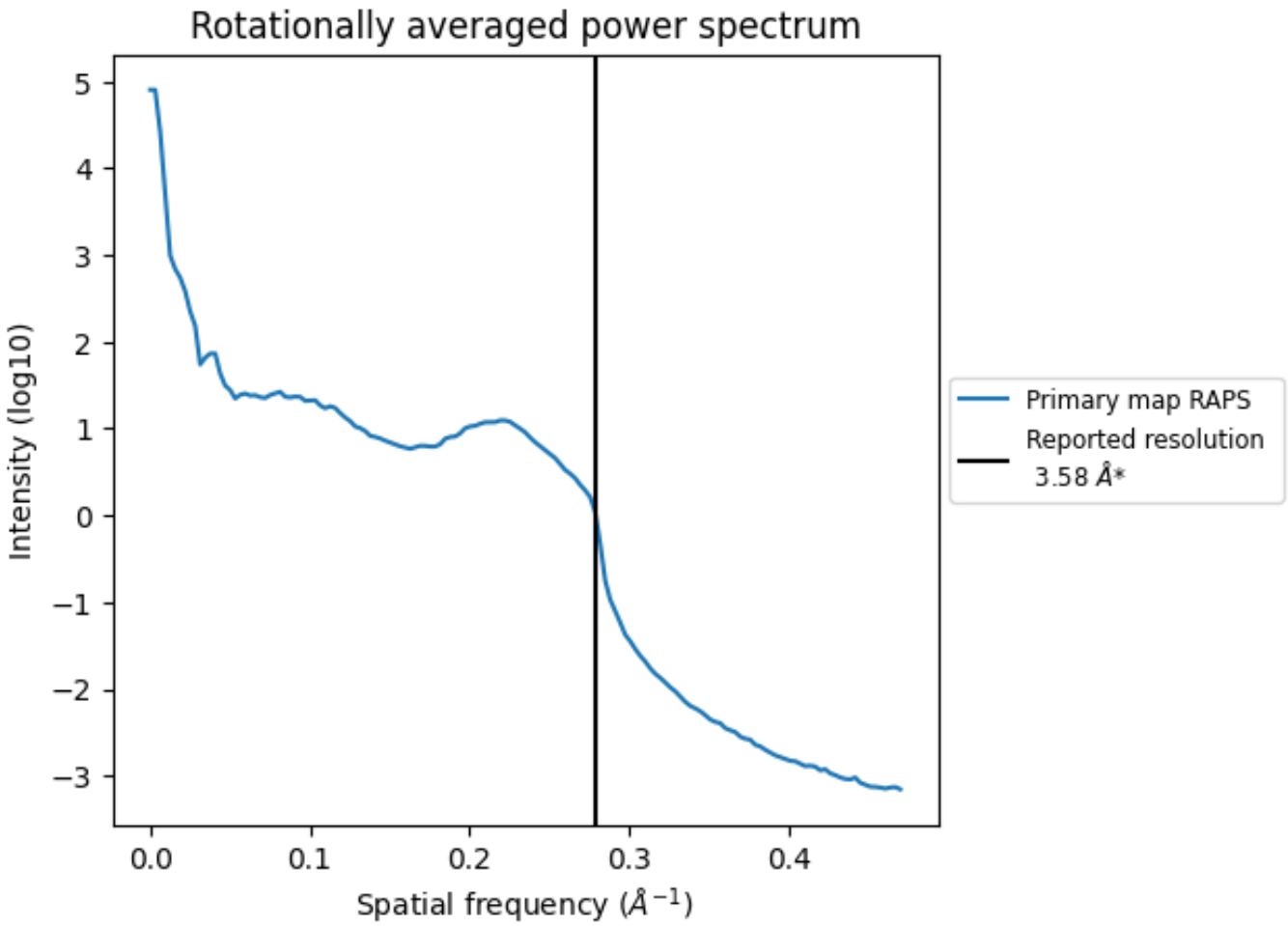
7.2 Volume estimate (i)



The volume at the recommended contour level is 323 nm^3; this corresponds to an approximate mass of 291 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)

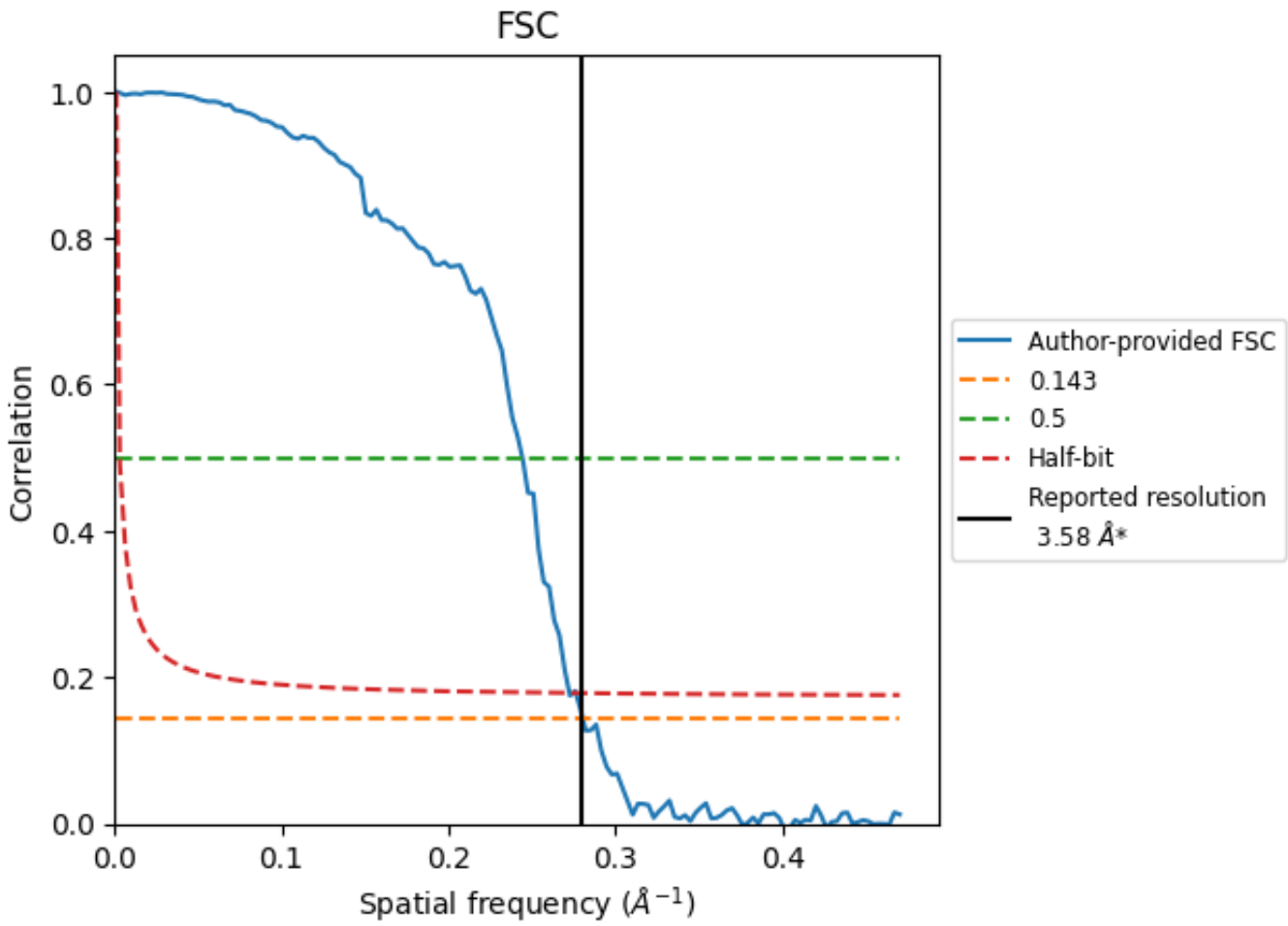


*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

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 0.279 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.57	4.10	3.67
Unmasked-calculated*	-	-	-

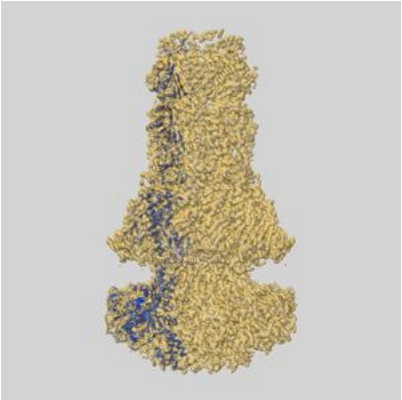
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

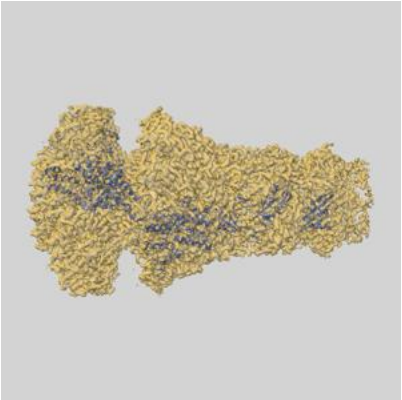
This section contains information regarding the fit between EMDB map EMD-10477 and PDB model 6TE9. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

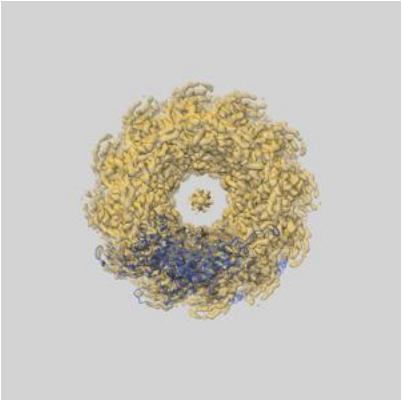
9.1.1 Map-model overlay (i)



X

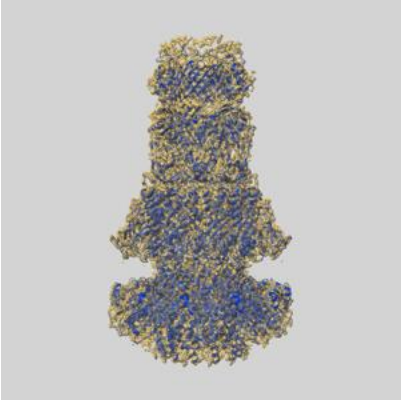


Y

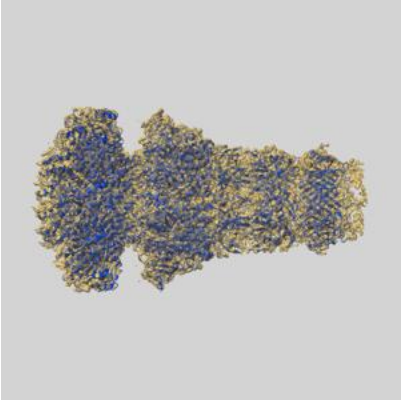


Z

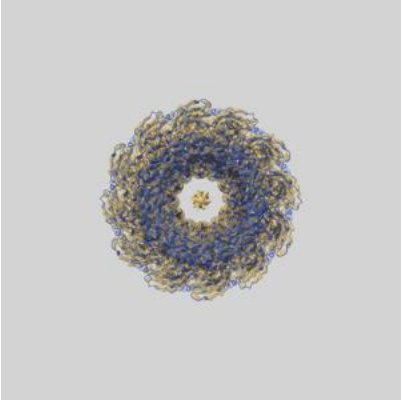
9.1.2 Map-model assembly overlay (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.088 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.

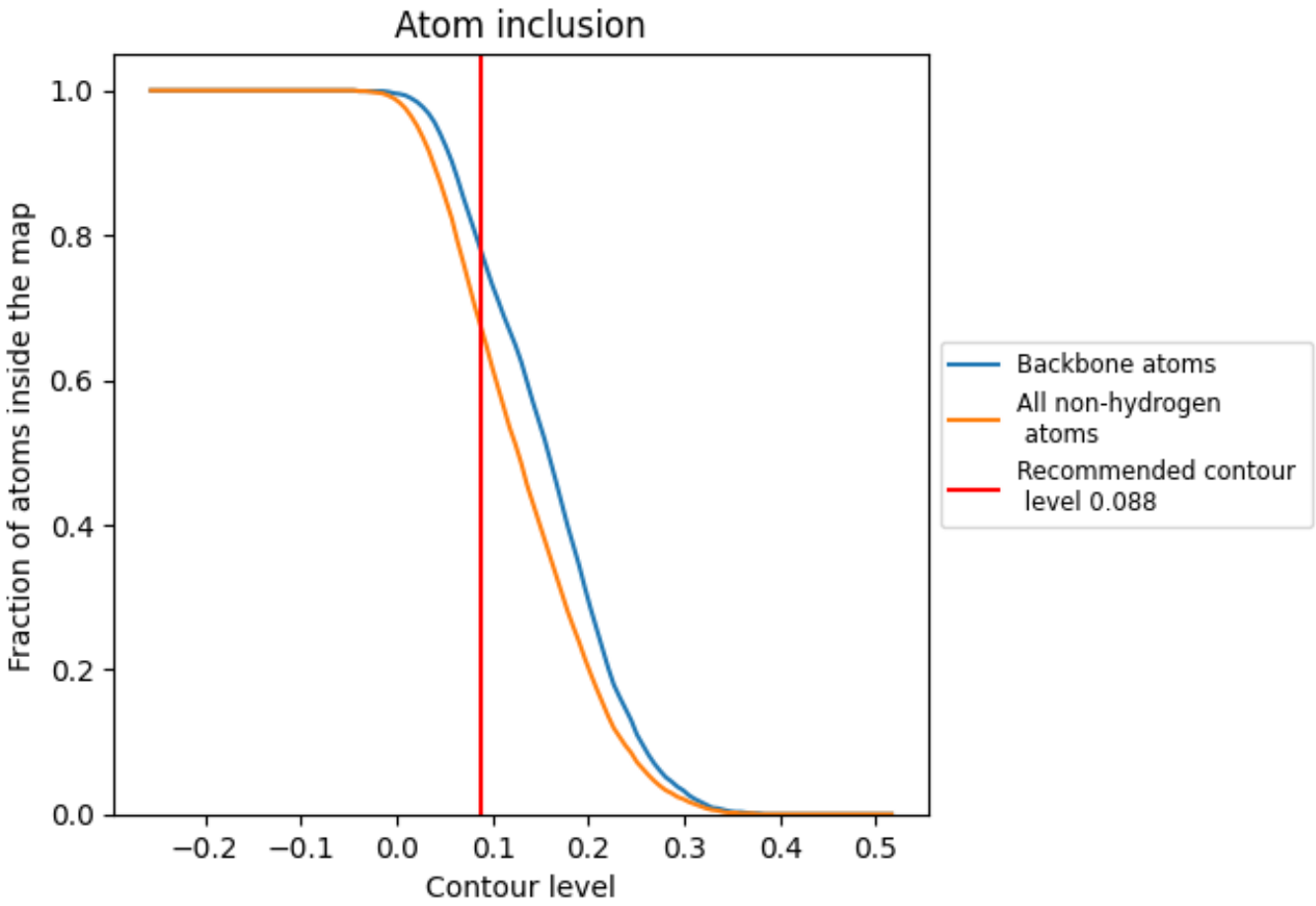
9.2 Q-score mapped to coordinate model (i)

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 (0.088).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.4900
A	0.6630	0.4890
B	0.6640	0.4890
C	0.6940	0.4970
D	0.7070	0.4980
E	0.7310	0.5160
F	0.7010	0.4860
G	0.5610	0.4530