wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 02:31 pm GMT

PDB ID	:	6SKI
EMDB ID	:	EMD-10225
Title	:	The Tle hydrolase bound to the TTR domain of the VgrG spike of the Type 6 secretion system
Authors	:	Rapisarda, C.; Fronzes, R.
Deposited on	:	2019-08-15
Resolution	:	2.60 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:

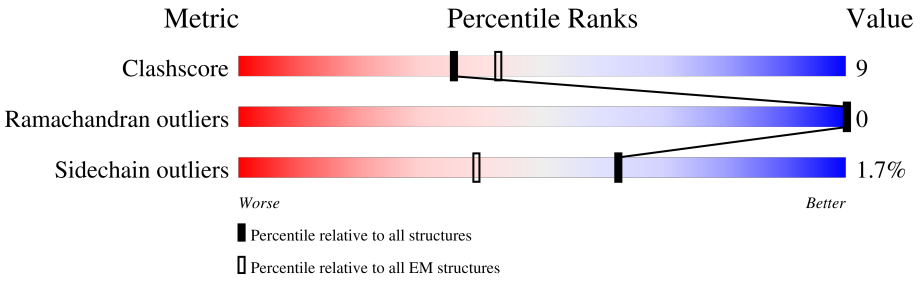
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.60 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	F	560	72% 19% • 7%
2	A	841	• • 94%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4434 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 Putative type VI secretion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	521	4092	2598	719	756	19	0	0

- Molecule 2 is a protein called Putative type VI secretion protein.

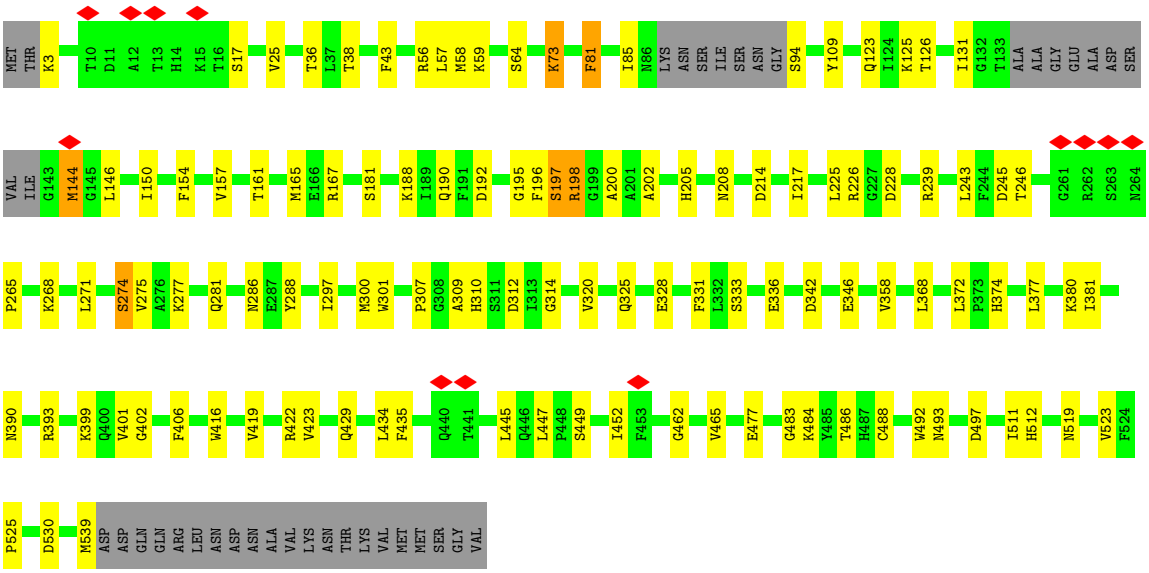
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	48	342	220	57	65	0	0

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.

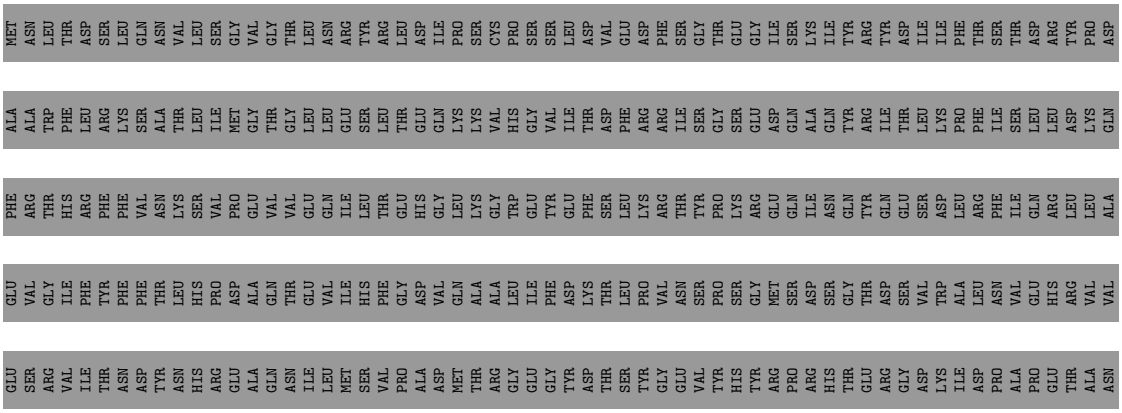
- Molecule 1: Putative type VI secretion protein

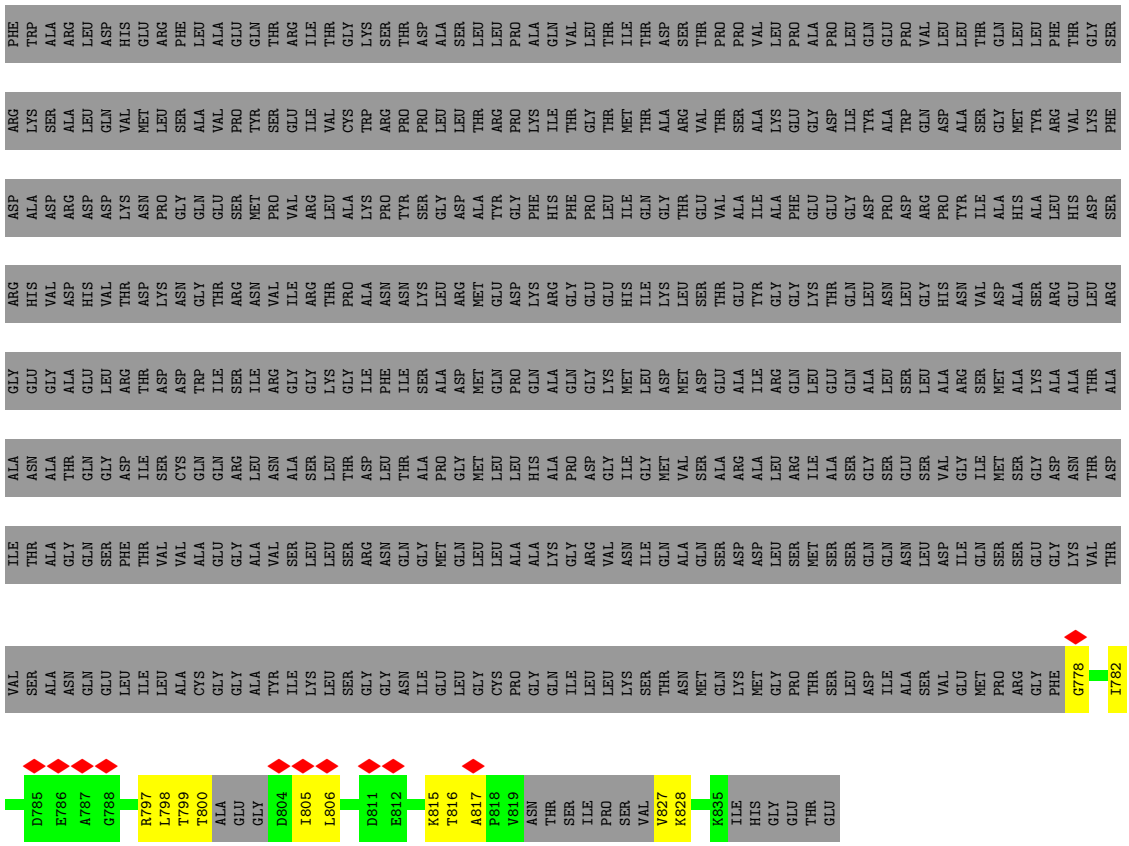
Chain F: 72% 19% 7%



- Molecule 2: Putative type VI secretion protein

Chain A: 94%




PHE TRP ALA ARG LEU ASP HIS GLU ARG PHE LEU ALA GLU GLN THR ARG ILE THR GLY LYS SER THR ASP ALA SER LEU LEU PRO ALA GLN VAL LEU THR ILE THR ASP SER THR PRO PRO VAL LEU PRO ALA PRO LEU GLN GLU PRO VAL LEU LEU THR GLN LEU LEU PHE THR GLY SER
ARG LYS SER ALA LEU GLN VAL MET LEU SER ALA VAL PRO TYR SER GLU ILE VAL CYS TRP ARG PRO PRO LEU LEU THR ARG PRO LYS ILE THR GLY THR MET THR ALA ARG VAL THR SER ALA LYS GLU GLY ASP ILE TYR ALA TRP GLN ASP ALA SER GLY MET HIS ALA LEU ASP PRO ASP ARG PRO TYR ILE ALA HIS ASP SER
ASP ALA ASP ARG ASP ASP LYS ASN PRO GLY GLN GLU SER MET PRO VAL ARG LEU ALA LYS PRO TYR SER GLY ASP ALA TYR GLY PHE HIS PHE PRO LEU ILE GLN GLY THR GLU VAL ALA ILE ALA PHE GLU GLU GLY GLN LEU ASN LEU ASP PRO ASP ARG PRO TYR ILE ALA HIS ALA LEU HIS ASP SER
ARG HIS VAL ASP HIS VAL THR ASP LYS ASN GLY THR ARG ASN VAL ILE ARG THR PRO ALA ASN ASN LYS LEU ARG MET GLU ASP LYS ARG GLY GLY LYS THR GLN LEU ASN LEU GLY GLY LYS LEU SER THR GLU TYR GLY GLY LYS THR GLN LEU ASN LEU GLY HIS ASN VAL ASP ALA HIS ALA SER ARG GLU LEU ARG
GLY GLU GLY ALA GLU LEU ARG THR ASP ASP TRP ILE SER ILE ARG GLY GLY LYS GLY ILE PHE ILE SER ALA ASP MET GLN PRO GLN ALA GLN GLY LYS MET ILE LEU ASP MET ASP GLU ALA ILE ARG GLN LEU GLU GLN ALA LEU SER LEU ALA ARG ALA LYS ALA ALA THR ALA
ALA ASN ALA THR GLN GLY ASP ILE SER CYS GLN GLN ARG LEU ASN ALA SER LEU THR ASP LEU THR ALA PRO GLY MET LEU LEU HIS ALA PRO ASP GLY ILE GLY MET VAL SER ALA ARG ALA LEU ARG ILE ALA SER GLY GLN GLN GLN ASN LEU ASP ILE GLN SER MET SER GLY ASP ASN THR ASP
ILE THR ALA GLY GLN SER PHE THR VAL VAL ALA GLU GLY ALA VAL SER LEU LEU SER ARG ASN GLN GLY MET GLN LEU LEU ALA ALA LYS GLY ARG VAL ASN ILE GLN ALA GLN SER ASP ASP LEU SER MET SER SER GLN GLN GLN SER SER GLU GLU GLY LYS VAL THR
VAL SER ALA ASN GLN GLU LEU ILE LEU ALA CYS GLY GLY ALA TYR ILE LYS LEU SER GLY GLY ASN ILE GLU LEU GLY CYS PRO GLY GLN ILE LEU LEU LYS SER THR ASN MET GLN LYS MET GLY PRO THR SER LEU ASP ILE ALA SER VAL GLU MET PRO ARG GLY PHE G778 I782
D785 E786 A787 G788 R797 L798 T799 T800 ALA GLU GLY D804 I805 L806 D811 E812 K815 T816 A817 P818 V819 ASN THR SER ILE PRO SER VAL V827 K828 K835 ILE HIS GLY GLU THR GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	468438	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 ($e^-/Å^2$)	1.28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	117.794	Depositor
Minimum map value	-57.759	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	10.0	Depositor
Map size (Å)	358.40002, 358.40002, 358.40002	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.024, 1.024, 1.024	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	F	0.31	0/4182	0.46	0/5652
2	A	0.27	0/346	0.51	0/467
All	All	0.31	0/4528	0.46	0/6119

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
1	F	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	197	SER	Mainchain
1	F	198	ARG	Peptide

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	F	4092	0	4025	71	0
2	A	342	0	338	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4434	0	4363	76	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 9.

The worst 5 of 76 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:F:123:GLN:HE22	1:F:434:LEU:H	1.28	0.81
1:F:205:HIS:HD2	1:F:268:LYS:H	1.34	0.75
1:F:422:ARG:NH2	1:F:445:LEU:O	2.21	0.72
1:F:342:ASP:HA	1:F:399:LYS:HD2	1.72	0.71
1:F:58:MET:HG3	1:F:150:ILE:HG23	1.80	0.64

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	F	515/560 (92%)	507 (98%)	8 (2%)	0	100	100
2	A	42/841 (5%)	41 (98%)	1 (2%)	0	100	100
All	All	557/1401 (40%)	548 (98%)	9 (2%)	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	F	431/467 (92%)	424 (98%)	7 (2%)	62	82
2	A	34/709 (5%)	33 (97%)	1 (3%)	42	68
All	All	465/1176 (40%)	457 (98%)	8 (2%)	62	81

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	828	LYS
1	F	530	ASP
1	F	144	MET
1	F	94	SER
1	F	274	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	493	ASN
1	F	487	HIS
1	F	281	GLN
1	F	387	ASN
1	F	213	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.

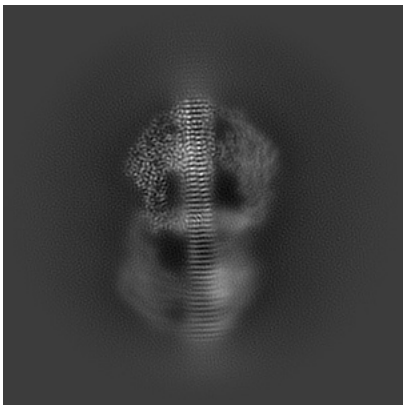
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10225. These allow visual inspection of the internal detail of the map and identification of artifacts.

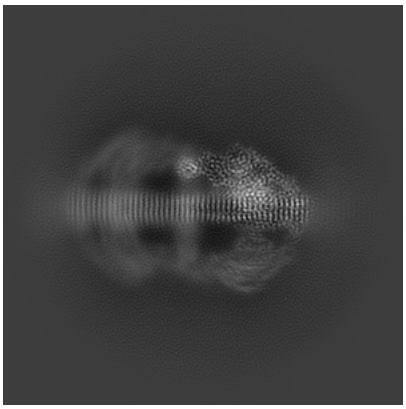
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

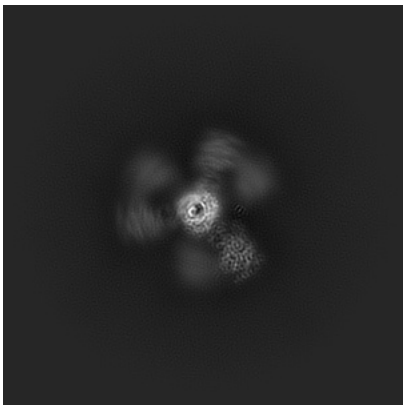
6.1.1 Primary map



X

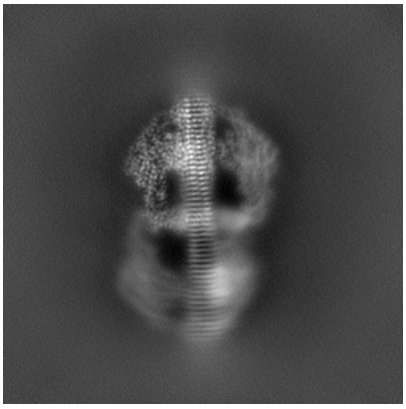


Y

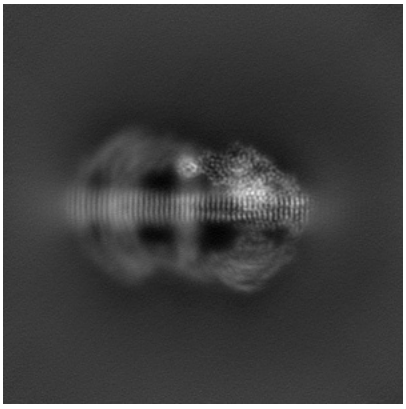


Z

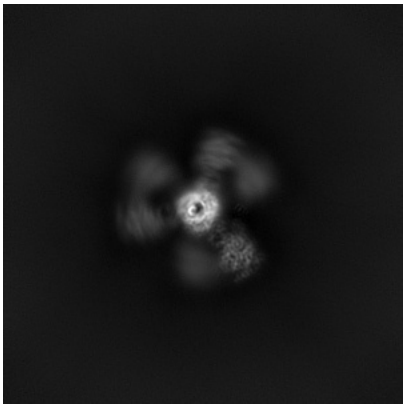
6.1.2 Raw map



X



Y



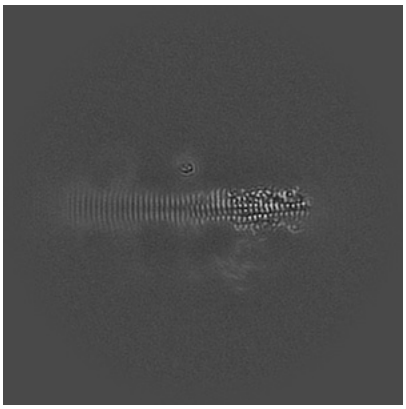
Z

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

6.2 Central slices (i)

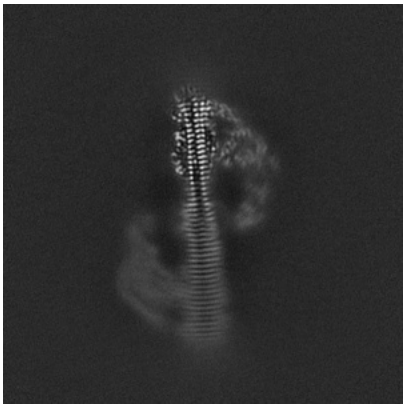
6.2.1 Primary map

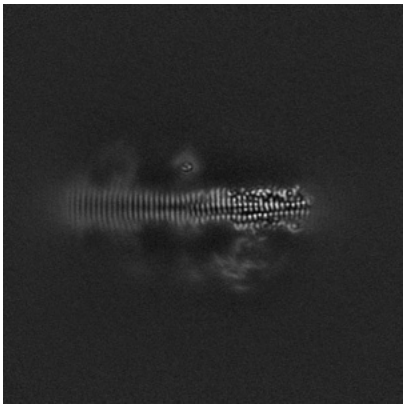
X Index: 175

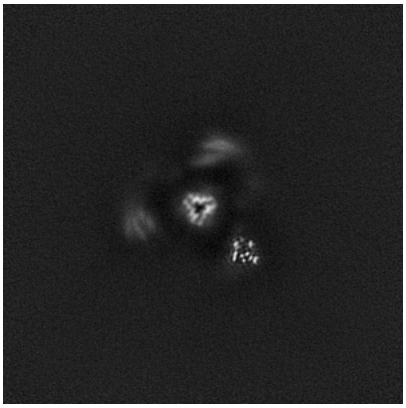

Y Index: 175

Z Index: 175

6.2.2 Raw map


X Index: 175

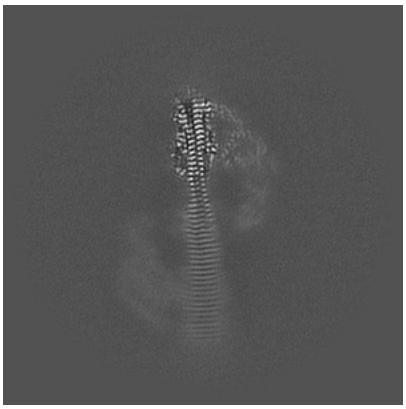

Y Index: 175


Z Index: 175

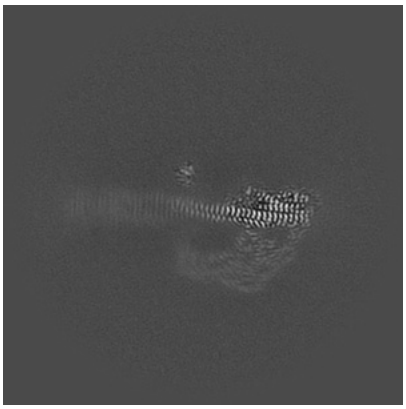
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

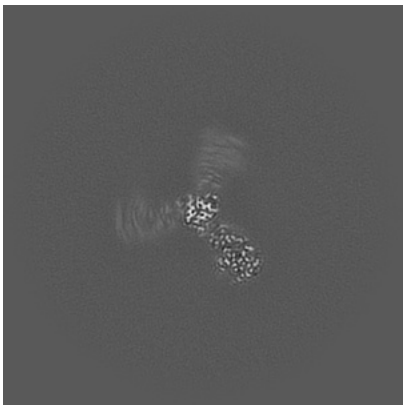
6.3.1 Primary map



X Index: 176

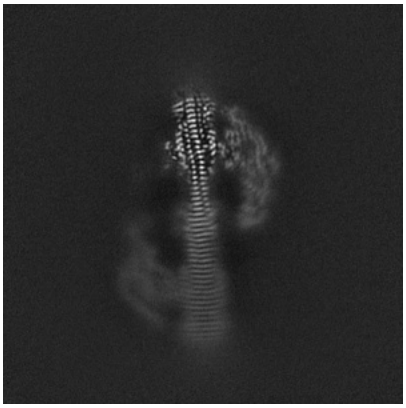


Y Index: 161

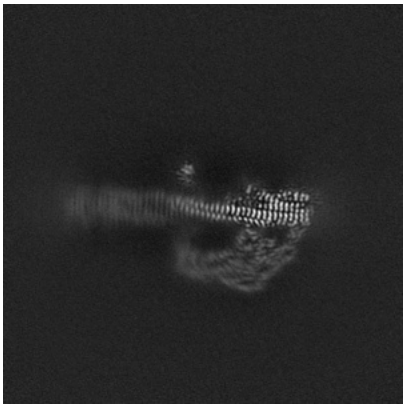


Z Index: 211

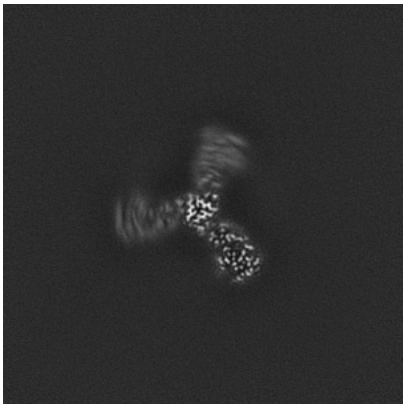
6.3.2 Raw map



X Index: 179



Y Index: 161



Z Index: 211

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

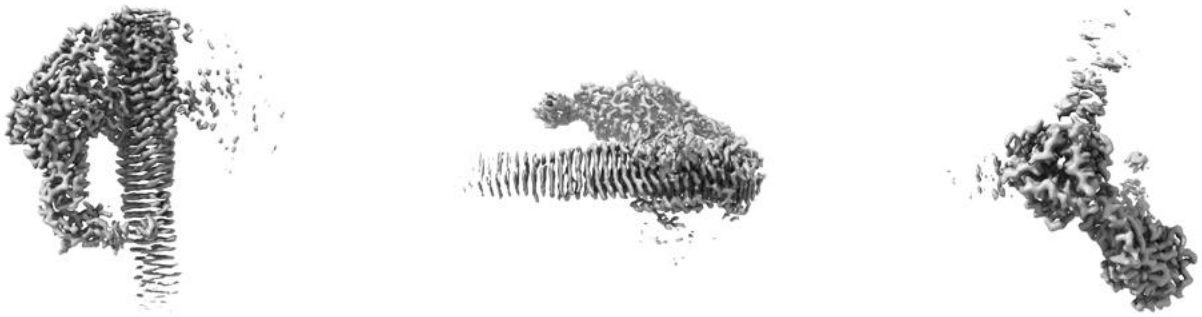
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

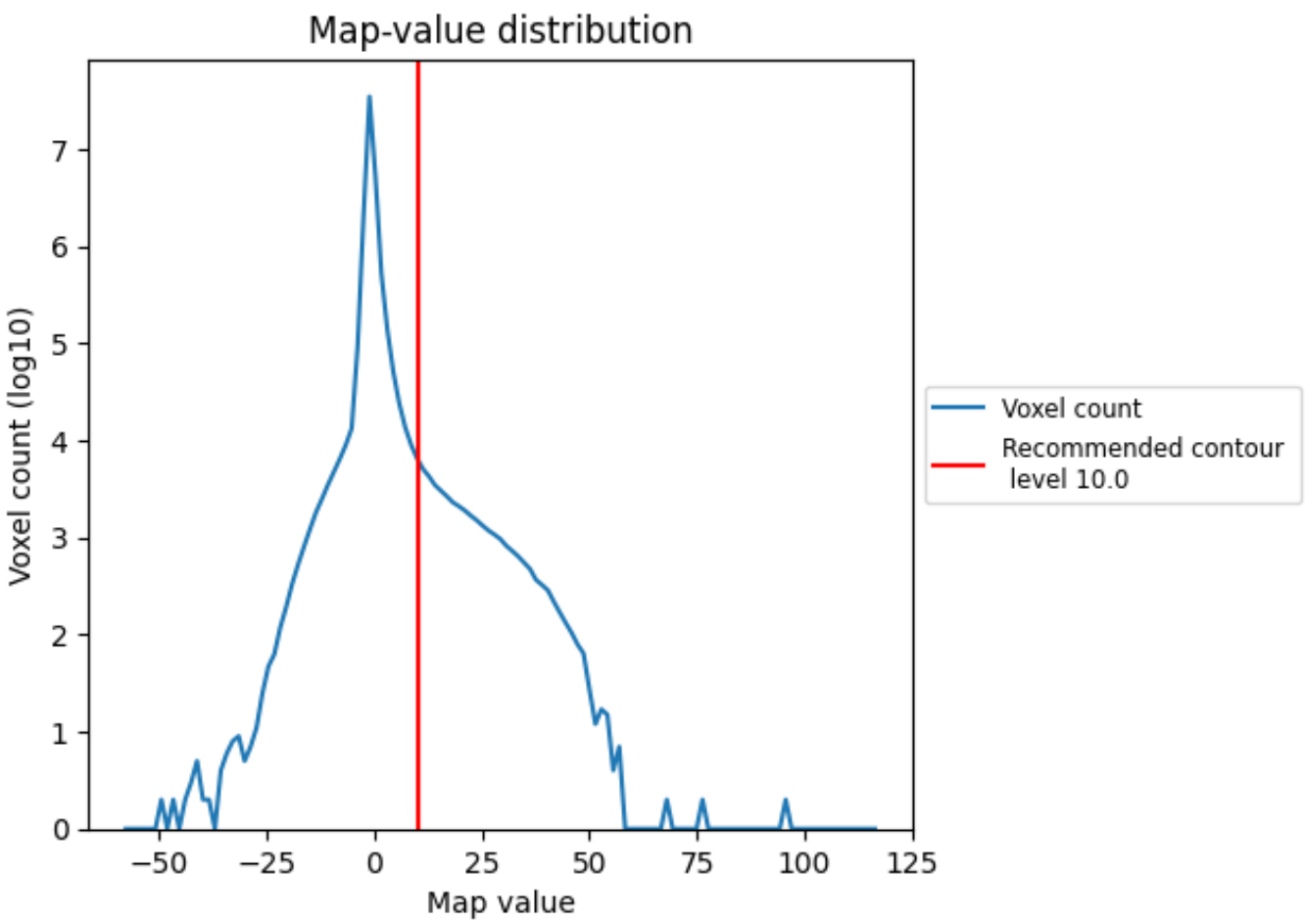
6.5 Mask visualisation (i)

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

7 Map analysis (i)

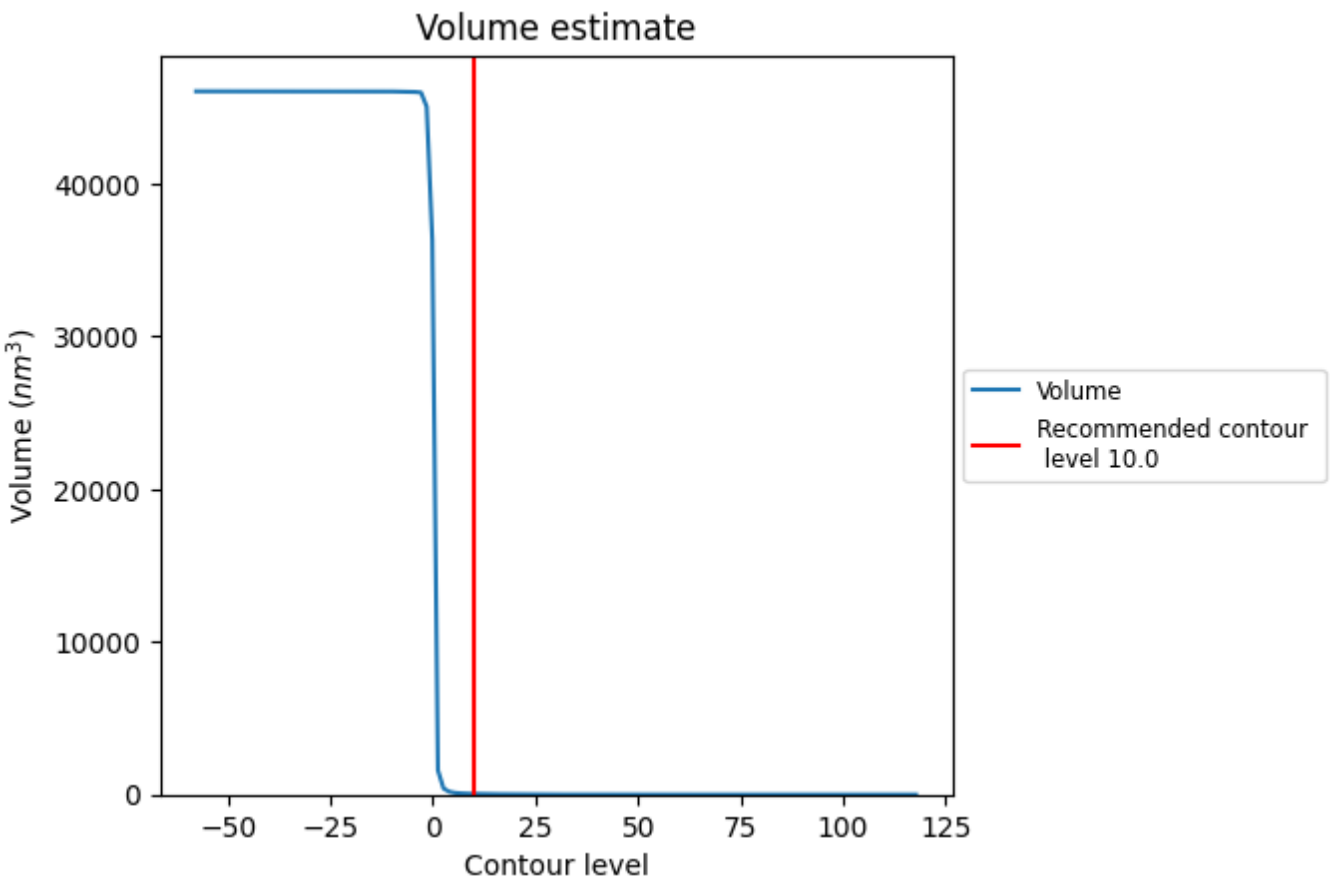
This section contains the results of statistical analysis of the map.

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.

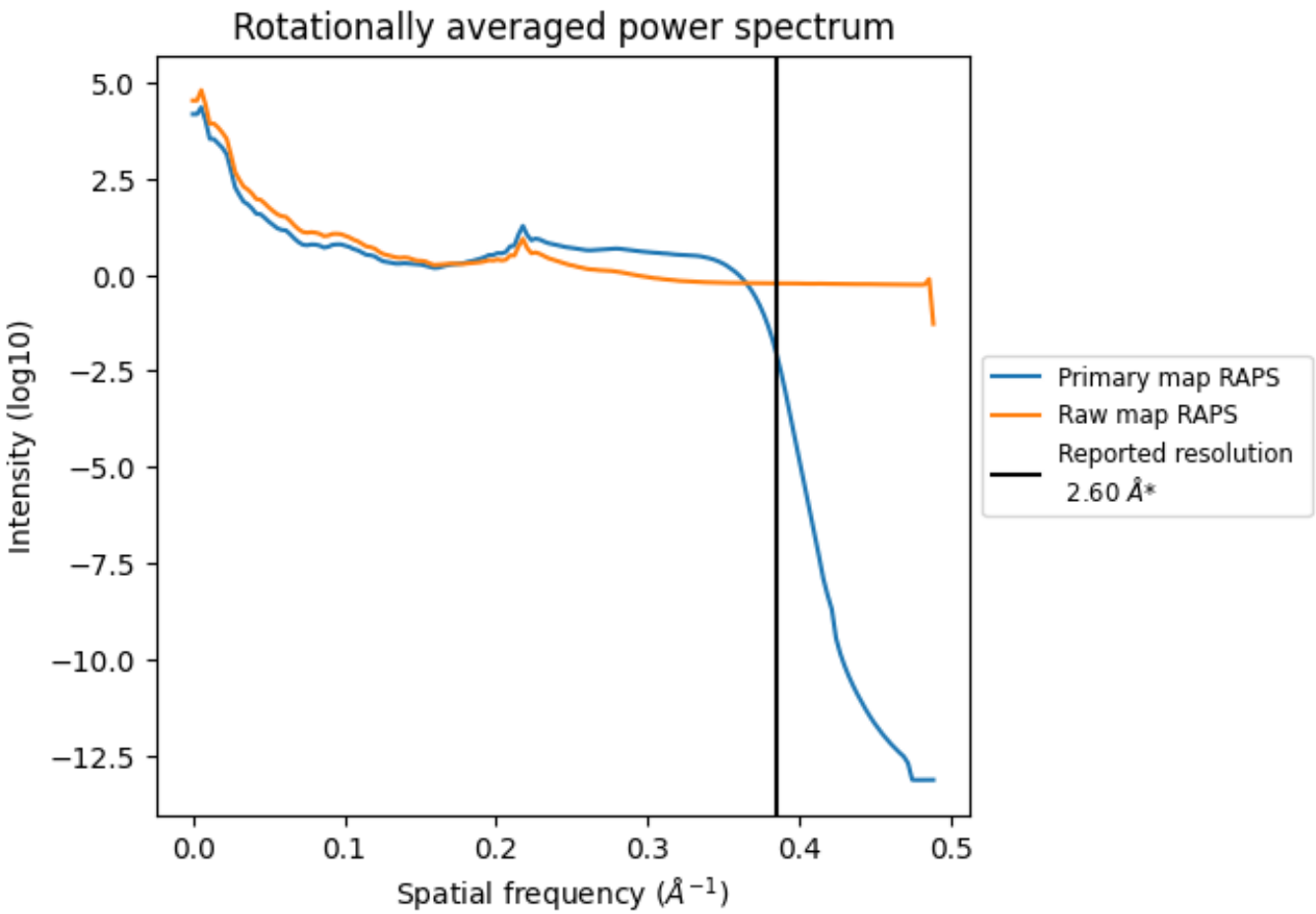
7.2 Volume estimate (i)



The volume at the recommended contour level is 47 nm^3; this corresponds to an approximate mass of 43 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)

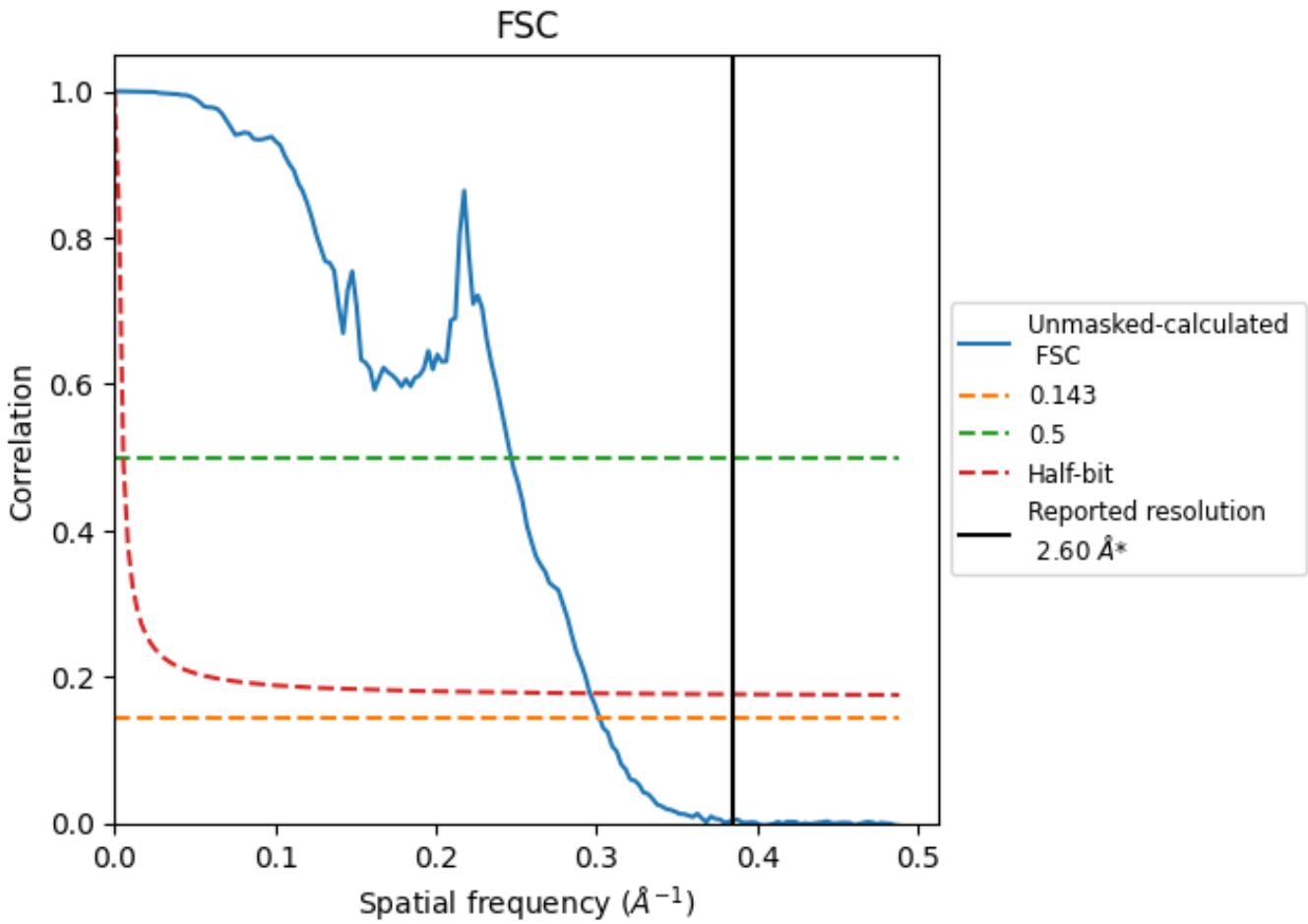


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.31	4.05	3.38

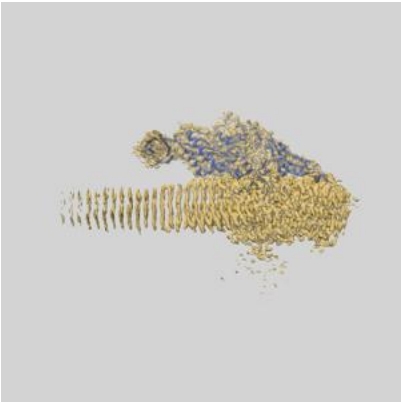
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.6 by more than 10 %

9 Map-model fit (i)

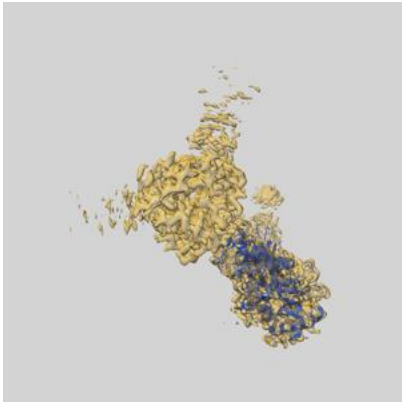
This section contains information regarding the fit between EMDB map EMD-10225 and PDB model 6SKI. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)

X



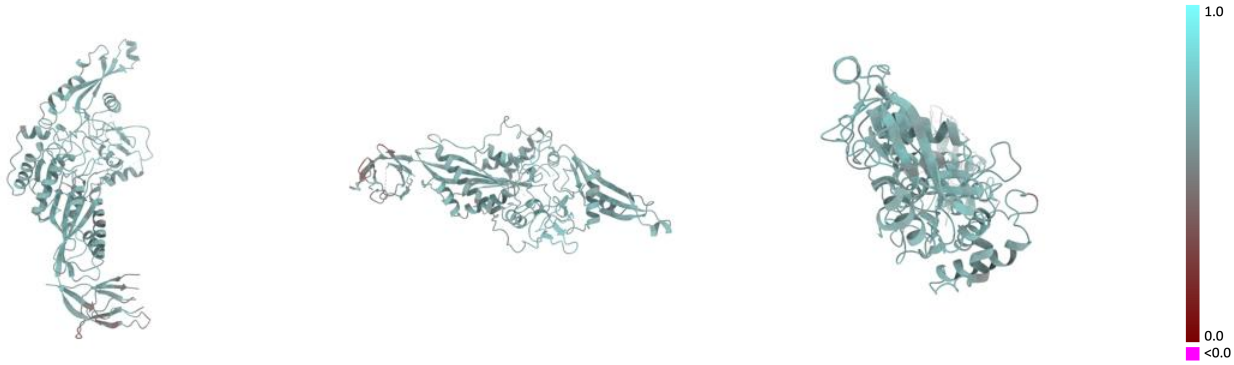
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 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.

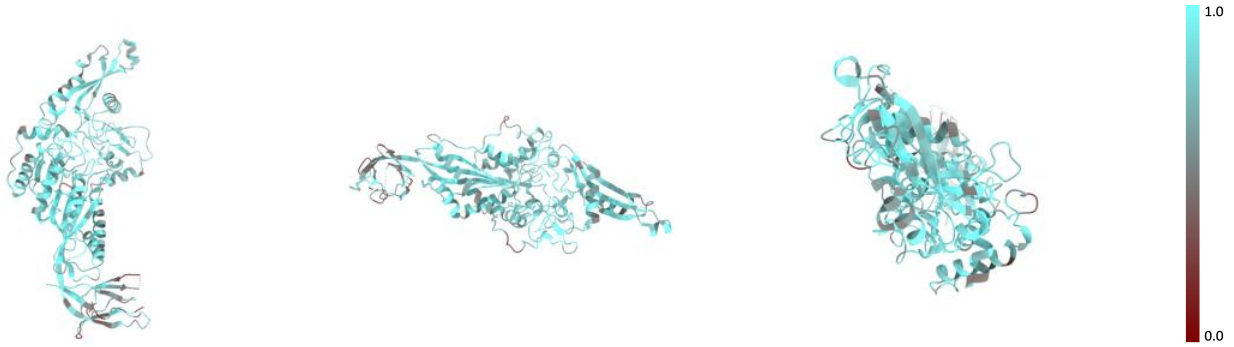
9.2 Q-score mapped to coordinate model (i)



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.

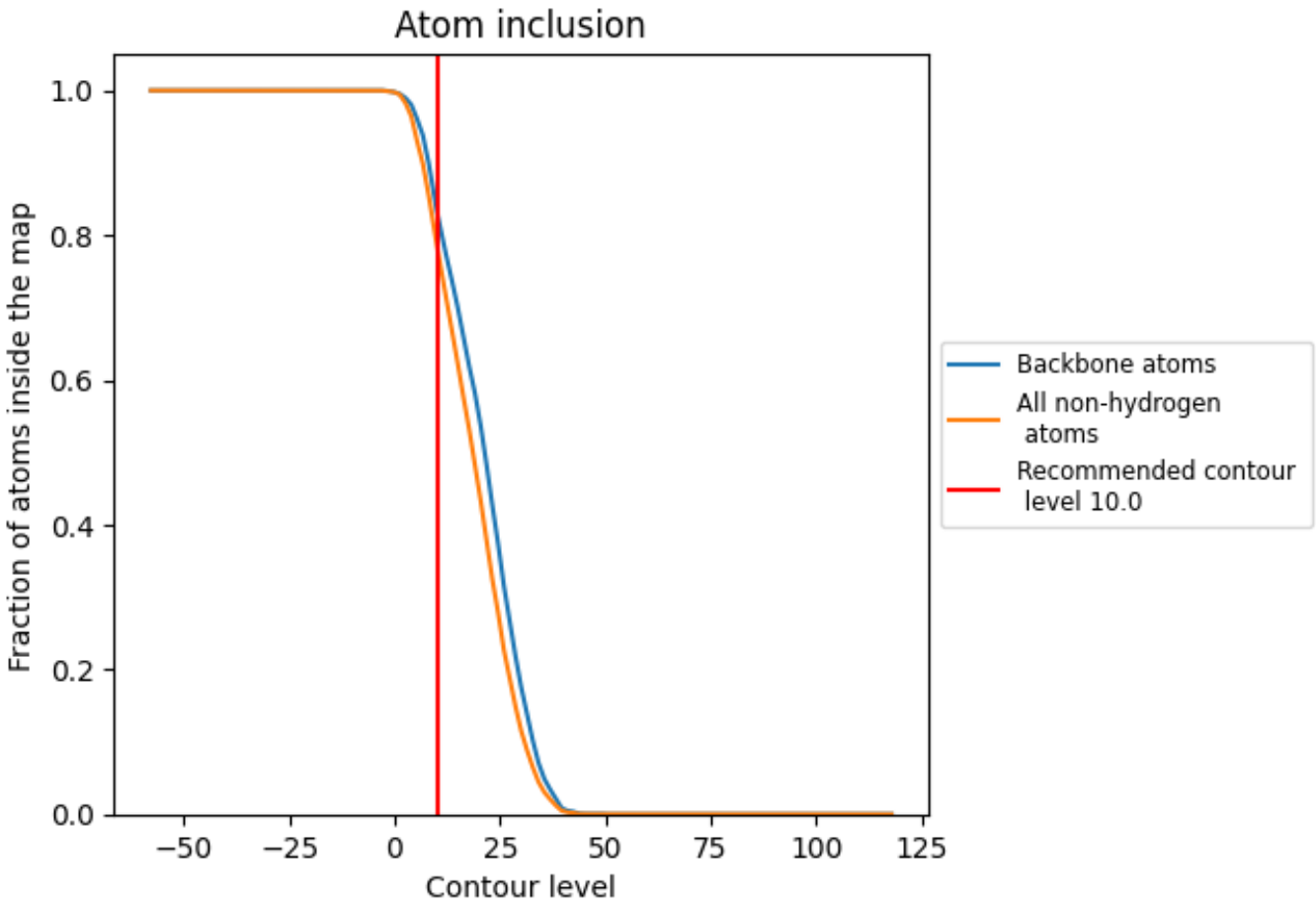
9.3 Atom inclusion mapped to coordinate model (i)



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 (10.0).

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 (i)

The table lists the average atom inclusion at the recommended contour level (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7864	0.6130
A	0.6136	0.5420
F	0.8010	0.6190