wwPDB EM Validation Summary Report (i)

Feb 12, 2024 – 09:33 pm GMT

PDB ID	:	8QOX
EMDB ID	:	EMD-18127
Title	:	Two-component assembly of SlaA and SlaB S-layer proteins of Sulfolobus acidocaldarius
Authors	:	Gambelli, L.; McLaren, M.; Isupov, M.; Conners, R.; Daum, B.
Deposited on	:	2023-09-29
Resolution	:	11.20 Å(reported)
Based on initial models	:	7ZCX, .

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:

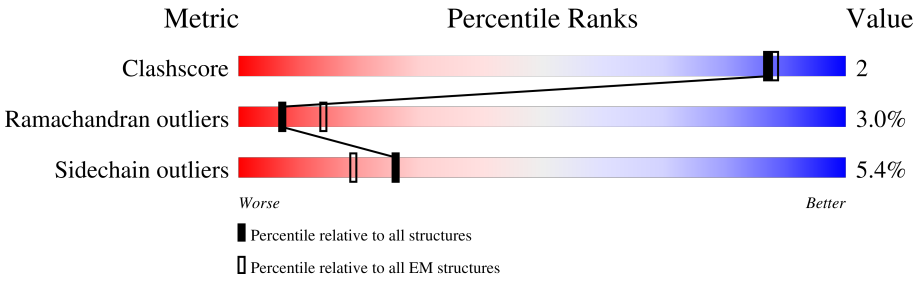
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 11.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	1424	69% 23% 5%
1	V	1424	5% 72% 21%
1	W	1424	29% 69% 24%
1	Z	1424	71% 23%
2	B	475	33% 72% 19% 5%
2	C	475	36% 75% 19% 5%
2	X	475	39% 72% 21% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 51848 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 S-layer protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	V	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	W	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		
1	Z	1395	Total	C	N	O	S	0	0
			10478	6781	1616	2065	16		

- Molecule 2 is a protein called Conserved membrane protein.

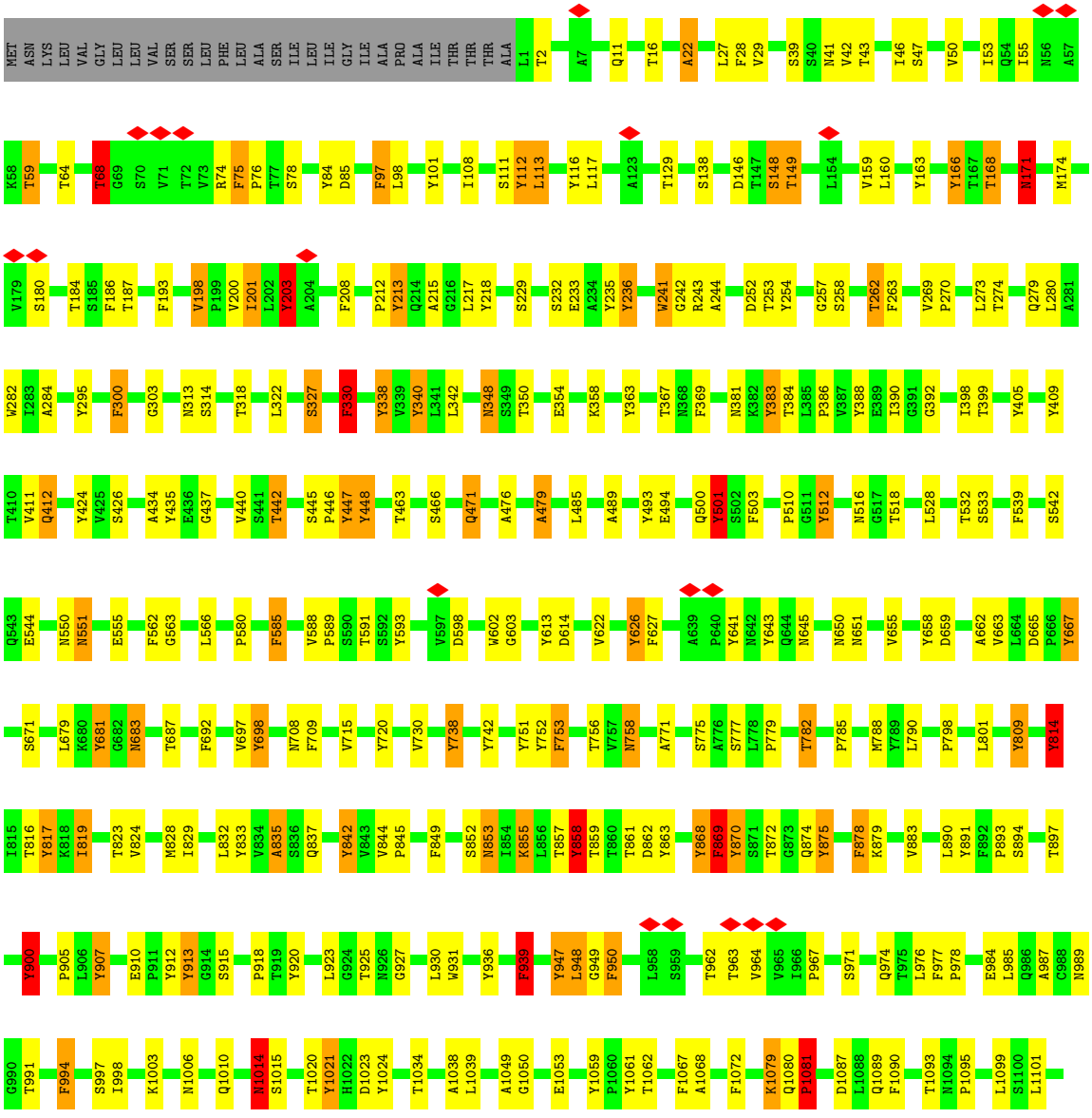
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		
2	C	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		
2	X	451	Total	C	N	O	S	0	0
			3312	2091	541	676	4		

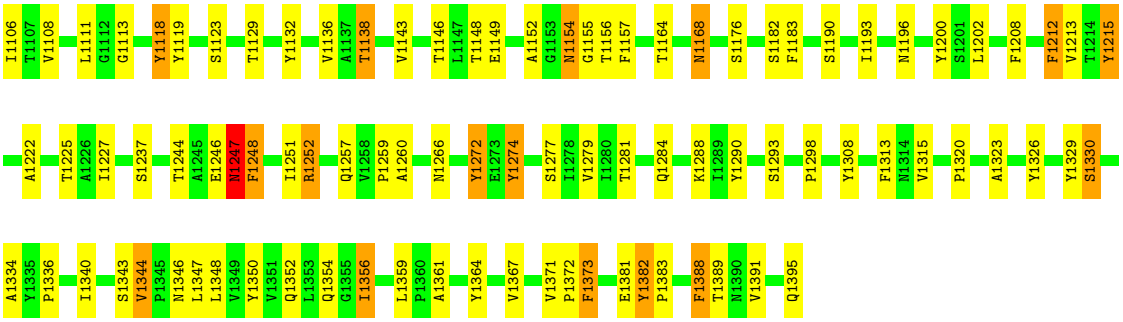
3 Residue-property plots (i)

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: S-layer protein A

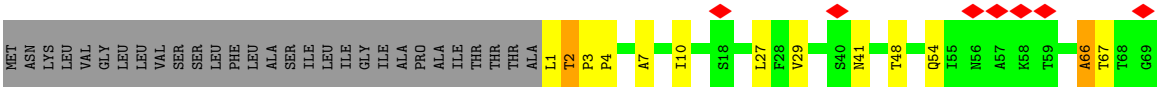
Chain A:

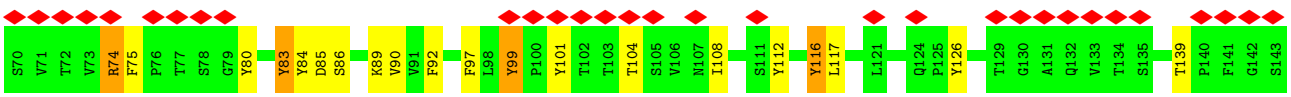


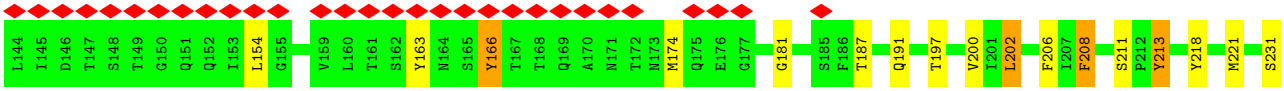


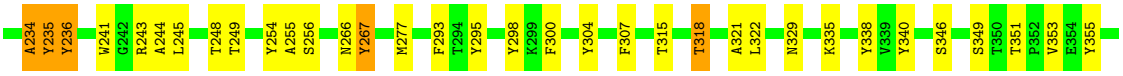
• Molecule 1: S-layer protein A

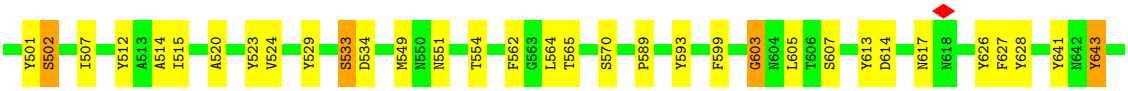
Chain V:

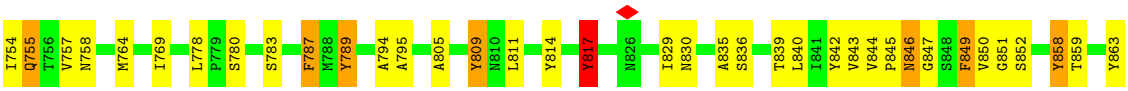


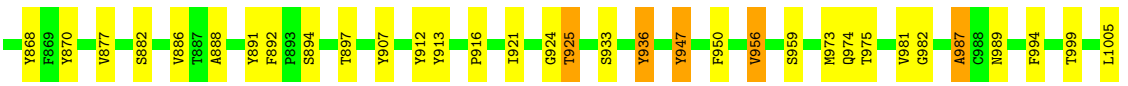


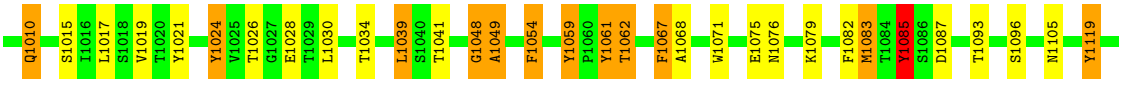






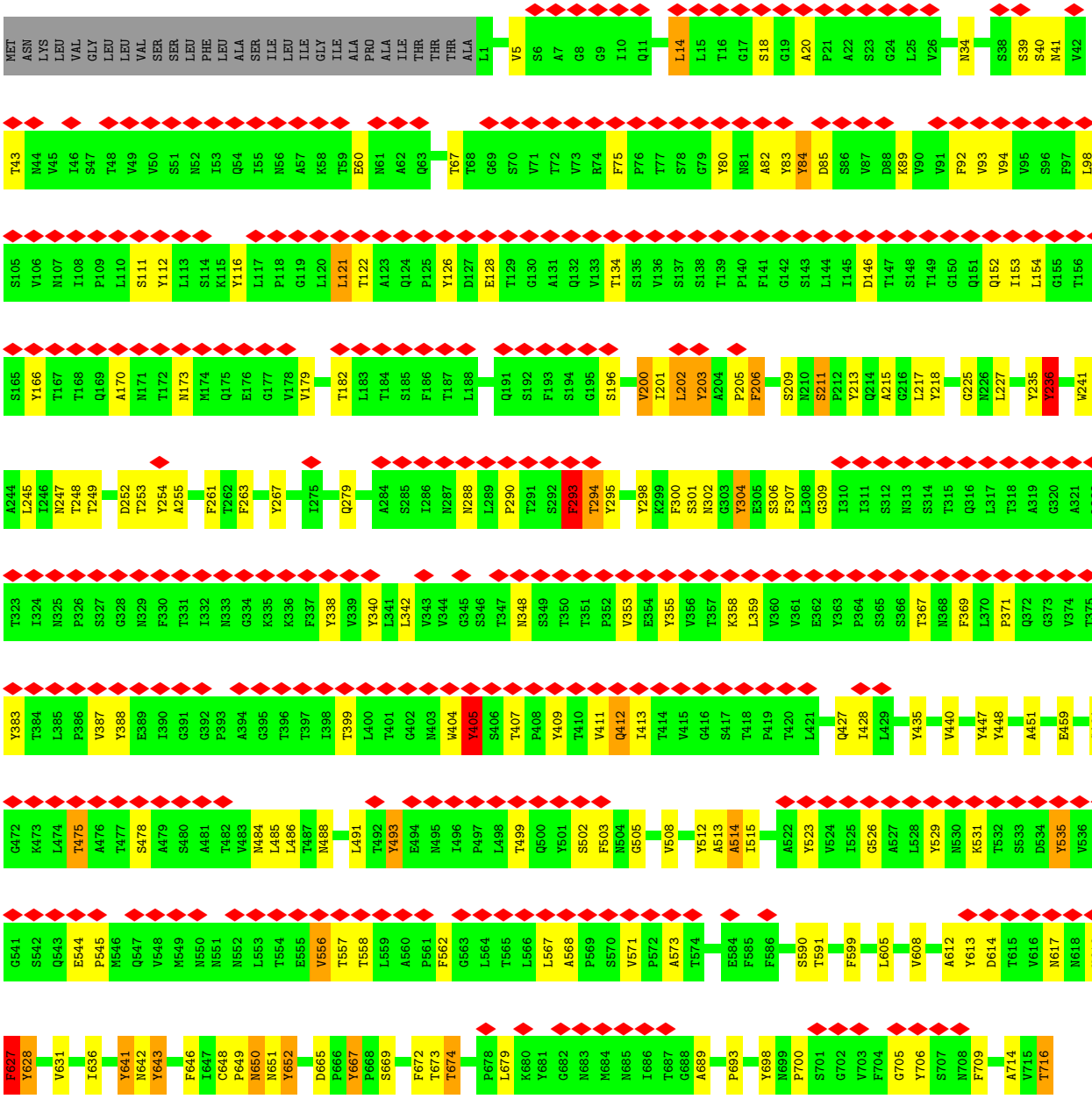


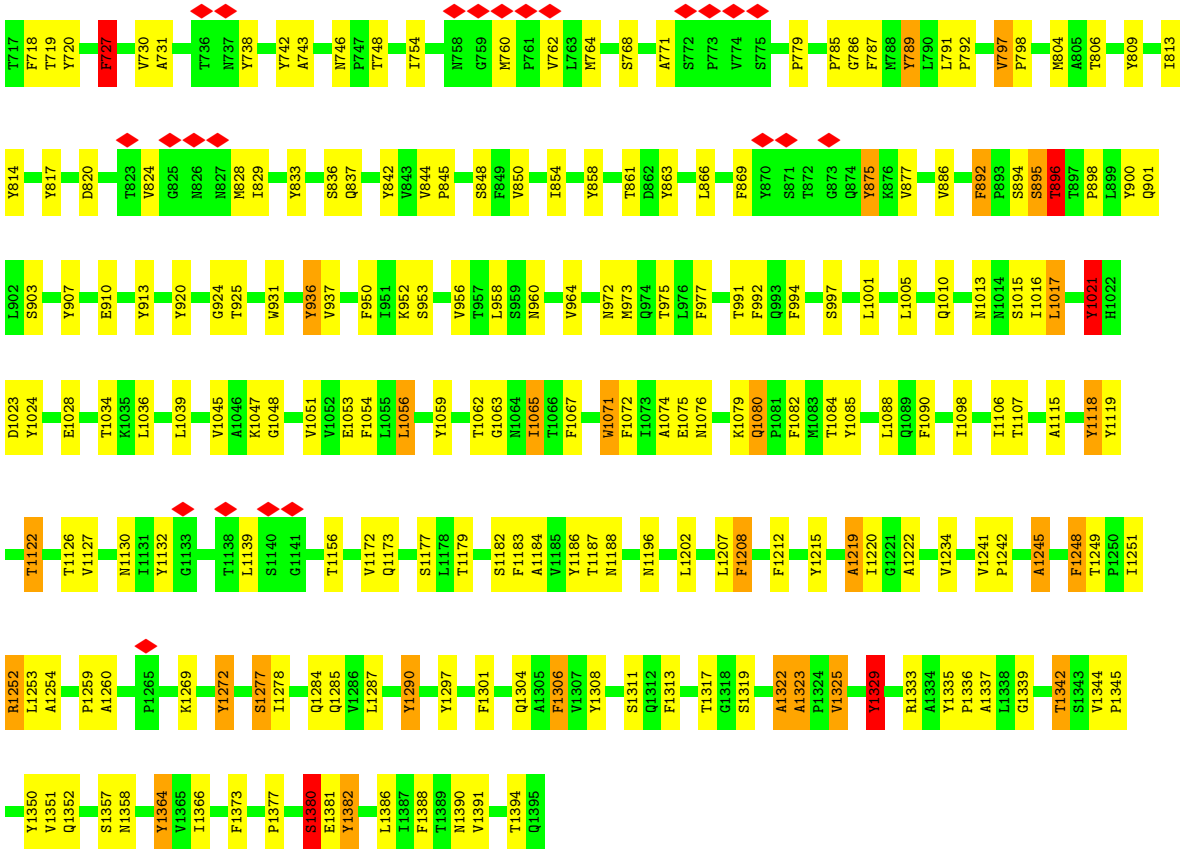




• Molecule 1: S-layer protein A

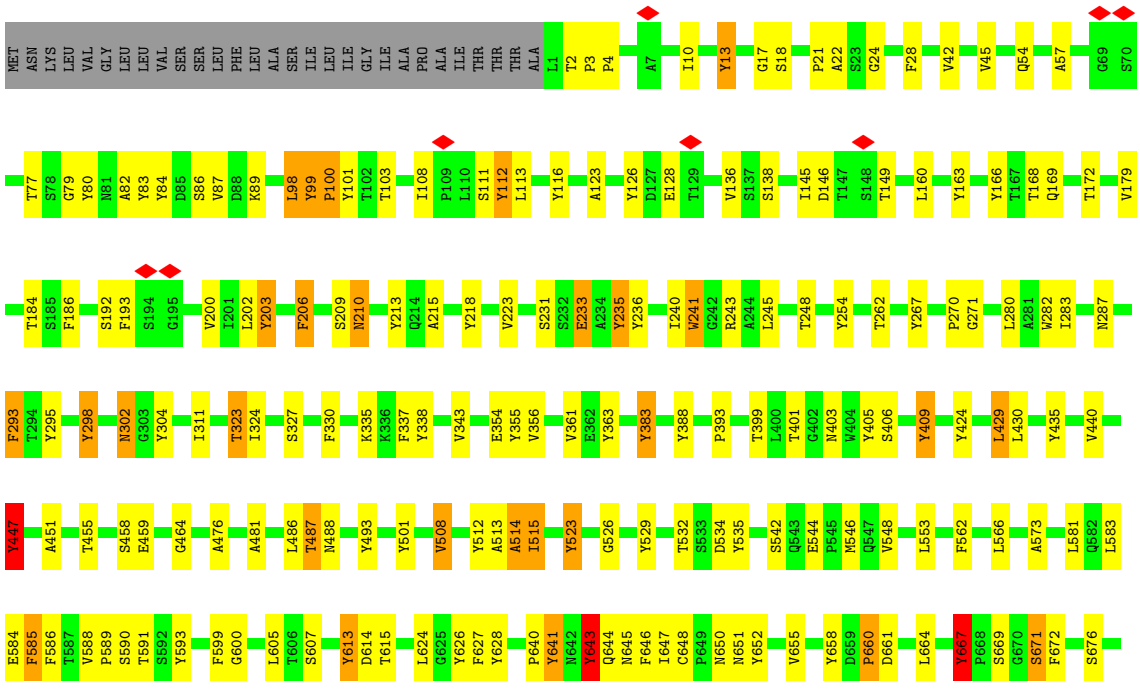
Chain W:

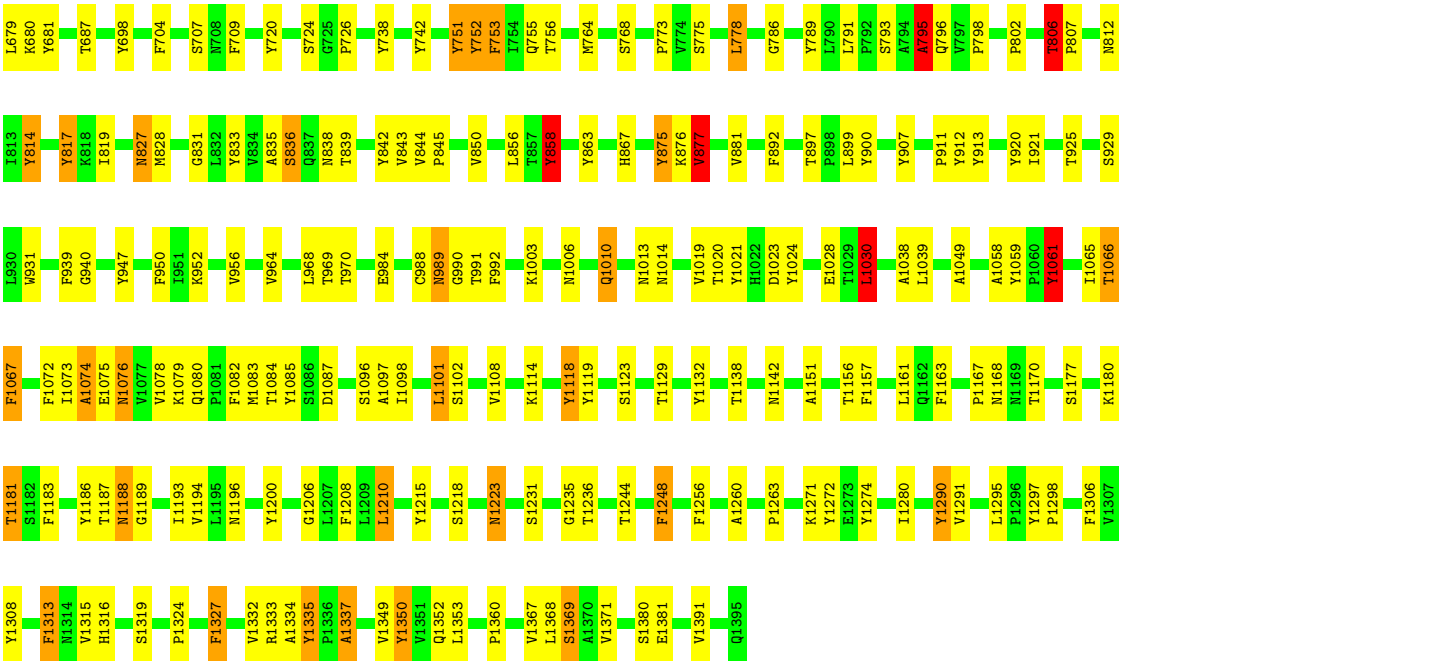




• Molecule 1: S-layer protein A

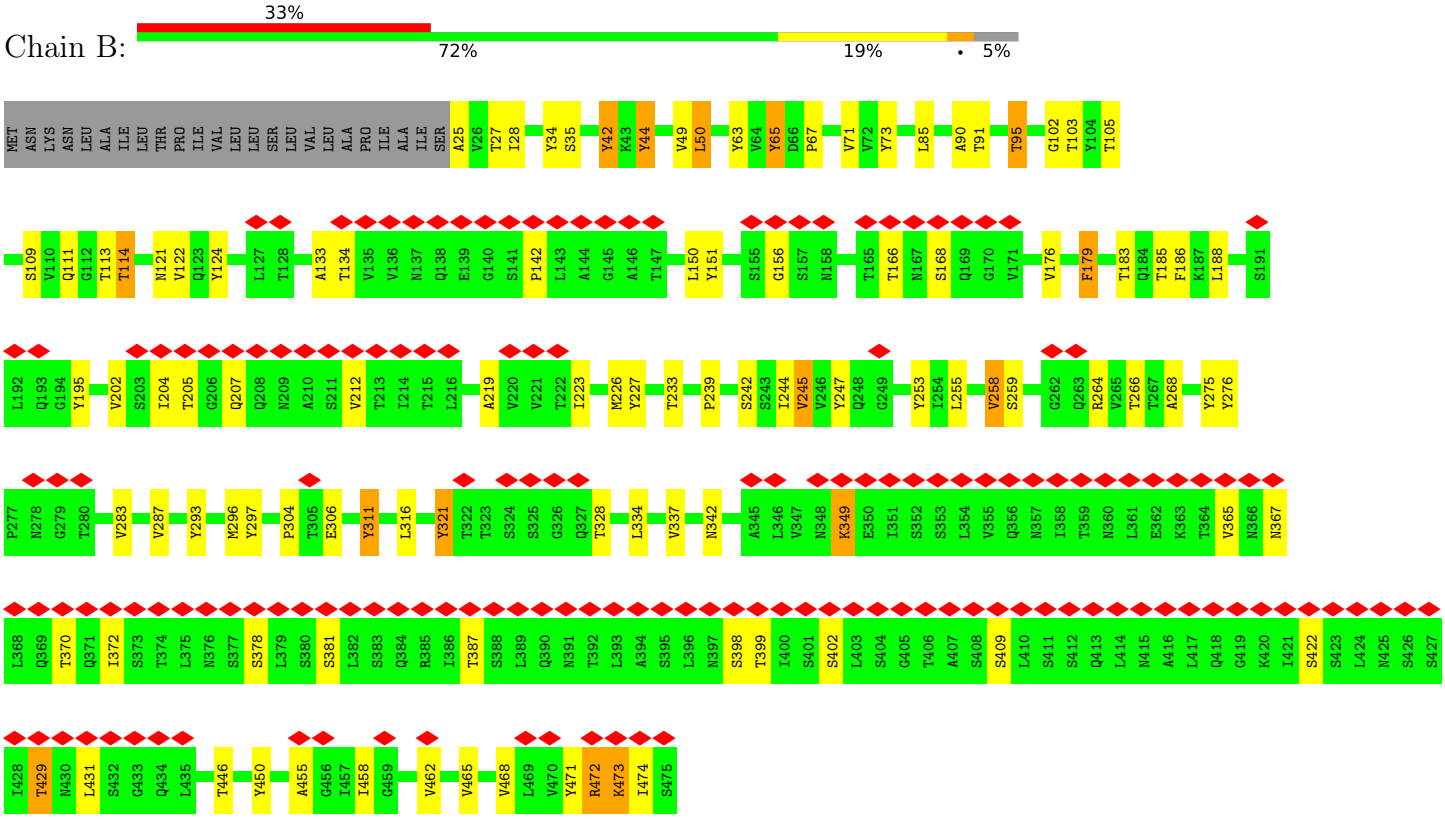
Chain Z:





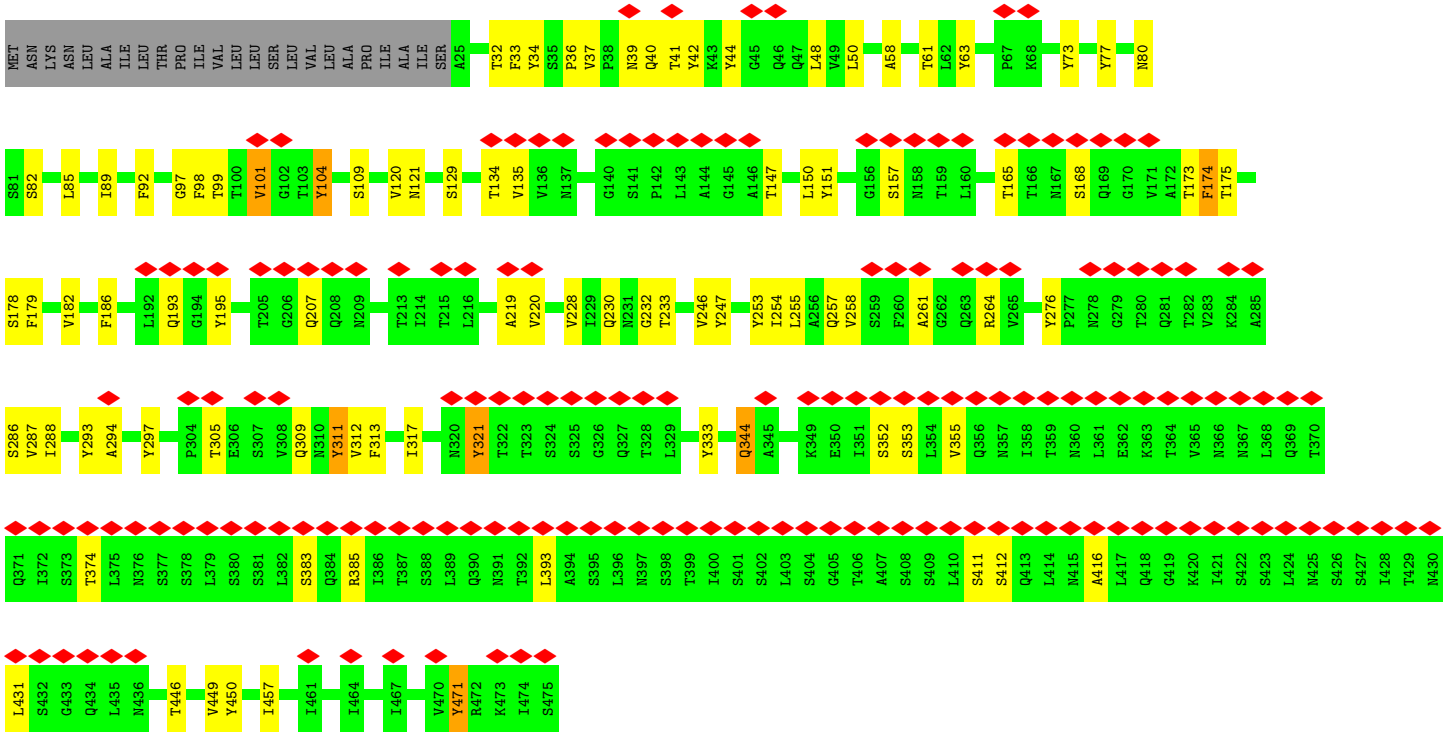
• Molecule 2: Conserved membrane protein

Chain B:



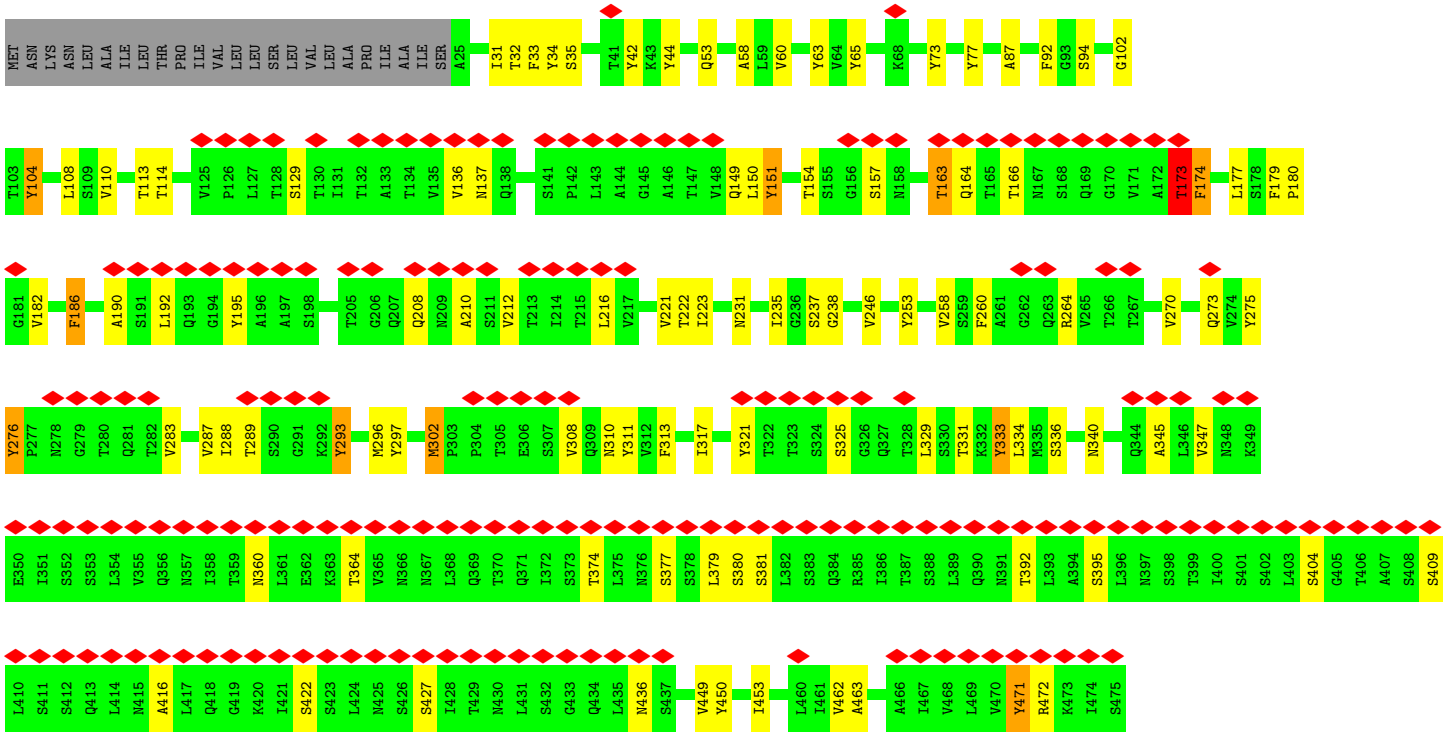
• Molecule 2: Conserved membrane protein

Chain C:



• Molecule 2: Conserved membrane protein

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	2771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, TFS TALOS	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ($e^-/Å^2$)	83, 83	Depositor
Minimum defocus (nm)	4000, 4000	Depositor
Maximum defocus (nm)	6000, 6000	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	TFS FALCON 4i (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00509	Depositor
Map size (Å)	700.0, 700.0, 700.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.5, 3.5, 3.5	Depositor

5 Model quality

5.1 Standard geometry

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	1.71	74/10749 (0.7%)	1.97	257/14803 (1.7%)
1	V	1.73	79/10749 (0.7%)	1.93	260/14803 (1.8%)
1	W	1.72	90/10749 (0.8%)	1.96	274/14803 (1.9%)
1	Z	1.69	78/10749 (0.7%)	1.91	229/14803 (1.5%)
2	B	1.68	25/3359 (0.7%)	1.86	66/4606 (1.4%)
2	C	1.66	19/3359 (0.6%)	1.81	62/4606 (1.3%)
2	X	1.69	32/3359 (1.0%)	1.89	68/4606 (1.5%)
All	All	1.71	397/53073 (0.7%)	1.93	1216/73030 (1.7%)

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	A	0	60
1	V	0	40
1	W	0	47
1	Z	0	53
2	B	0	11
2	C	0	8
2	X	0	7
All	All	0	226

The worst 5 of 397 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	1326	TYR	CE2-CZ	9.60	1.51	1.38
1	Z	1119	TYR	CG-CD1	9.42	1.51	1.39
1	W	464	GLY	CA-C	-9.24	1.37	1.51
1	A	39	SER	CA-CB	9.04	1.66	1.52
1	V	1096	SER	CA-CB	8.38	1.65	1.52

The worst 5 of 1216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	1252	ARG	NE-CZ-NH2	-20.21	110.19	120.30
1	A	1364	TYR	CB-CG-CD1	-17.88	110.28	121.00
1	Z	512	TYR	CB-CG-CD2	-16.12	111.33	121.00
1	V	1024	TYR	CB-CG-CD2	-16.02	111.39	121.00
1	V	789	TYR	CB-CG-CD2	-15.91	111.46	121.00

There are no chirality outliers.

5 of 226 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	TYR	Sidechain
1	A	55	ILE	Peptide
1	A	75	PHE	Sidechain
1	A	84	TYR	Sidechain
1	A	97	PHE	Sidechain

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	10478	0	10402	48	0
1	V	10478	0	10402	31	0
1	W	10478	0	10402	40	0
1	Z	10478	0	10402	49	0
2	B	3312	0	3388	9	0
2	C	3312	0	3388	15	0
2	X	3312	0	3388	17	0
All	All	51848	0	51772	203	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 2.

The worst 5 of 203 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:V:255:ALA:HB2	1:V:617:ASN:HD21	1.59	0.66
2:C:344:GLN:H	2:C:344:GLN:HE21	1.43	0.65
1:V:1215:TYR:CD1	1:V:1371:VAL:HG13	2.33	0.64
2:X:288:ILE:HD12	2:X:296:MET:HB2	1.80	0.63
1:V:1010:GLN:HE22	1:V:1039:LEU:HD23	1.62	0.63

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	1393/1424 (98%)	1150 (83%)	177 (13%)	66 (5%)	2 21
1	V	1393/1424 (98%)	1218 (87%)	137 (10%)	38 (3%)	5 31
1	W	1393/1424 (98%)	1209 (87%)	135 (10%)	49 (4%)	3 25
1	Z	1393/1424 (98%)	1187 (85%)	158 (11%)	48 (3%)	3 26
2	B	449/475 (94%)	424 (94%)	24 (5%)	1 (0%)	47 81
2	C	449/475 (94%)	420 (94%)	24 (5%)	5 (1%)	14 52
2	X	449/475 (94%)	414 (92%)	32 (7%)	3 (1%)	22 63
All	All	6919/7121 (97%)	6022 (87%)	687 (10%)	210 (3%)	7 28

5 of 210 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	THR
1	A	166	TYR
1	A	171	ASN
1	A	200	VAL
1	A	203	TYR

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	1189/1212 (98%)	1116 (94%)	73 (6%)	18	44
1	V	1189/1212 (98%)	1128 (95%)	61 (5%)	24	48
1	W	1189/1212 (98%)	1120 (94%)	69 (6%)	20	45
1	Z	1189/1212 (98%)	1123 (94%)	66 (6%)	21	46
2	B	386/407 (95%)	361 (94%)	25 (6%)	17	42
2	C	386/407 (95%)	371 (96%)	15 (4%)	32	56
2	X	386/407 (95%)	376 (97%)	10 (3%)	46	66
All	All	5914/6069 (97%)	5595 (95%)	319 (5%)	26	47

5 of 319 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	1084	THR
1	Z	764	MET
1	W	1287	LEU
1	Z	241	TRP
1	Z	1020	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	74	ASN
2	X	310	ASN
1	Z	737	ASN
2	C	207	GLN
2	C	78	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.

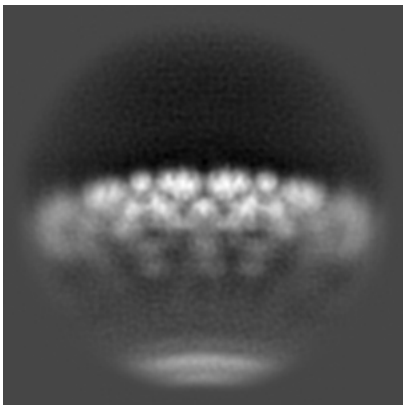
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18127. These allow visual inspection of the internal detail of the map and identification of artifacts.

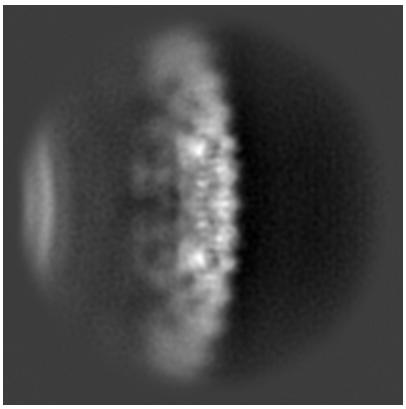
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

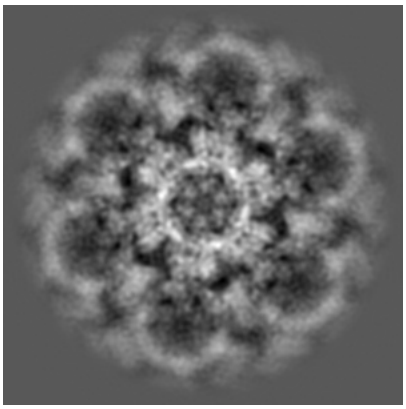
6.1.1 Primary map



X

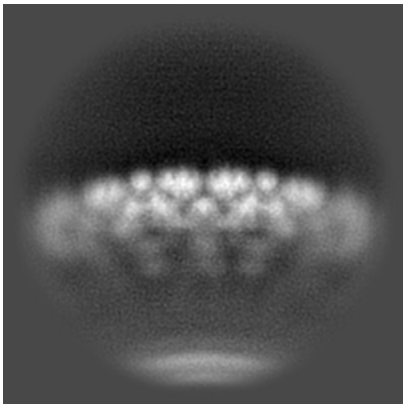


Y

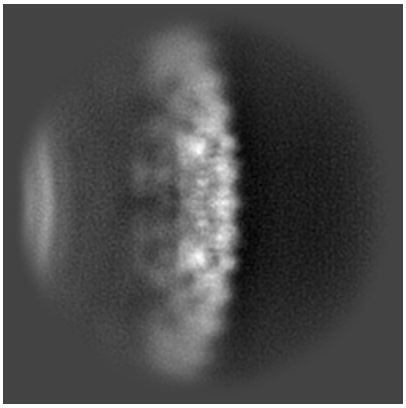


Z

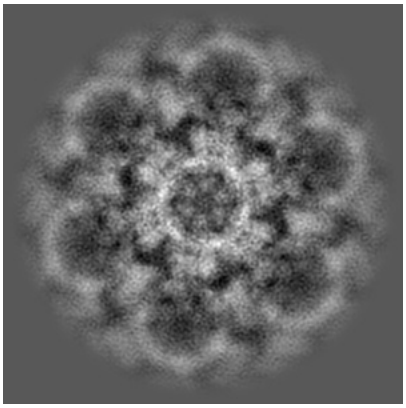
6.1.2 Raw map



X



Y

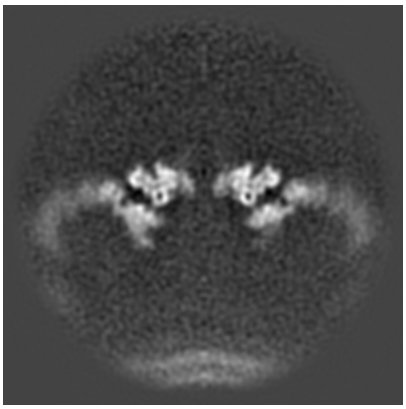


Z

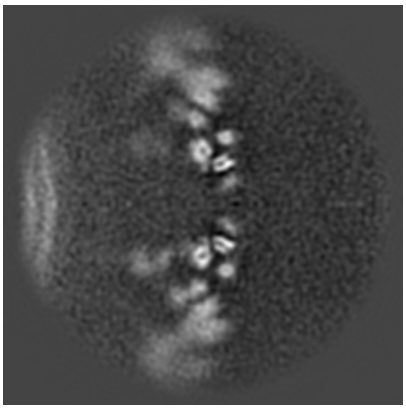
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

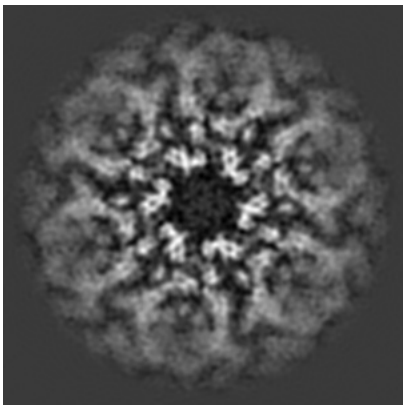
6.2.1 Primary map



X Index: 100

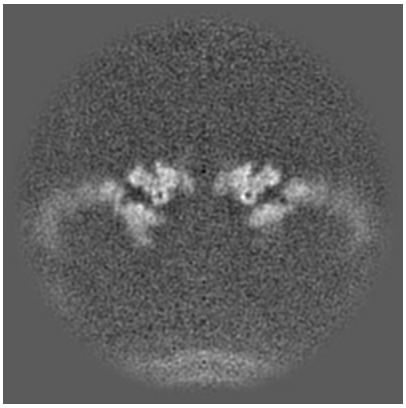


Y Index: 100

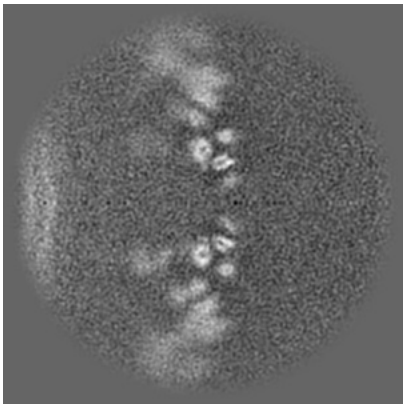


Z Index: 100

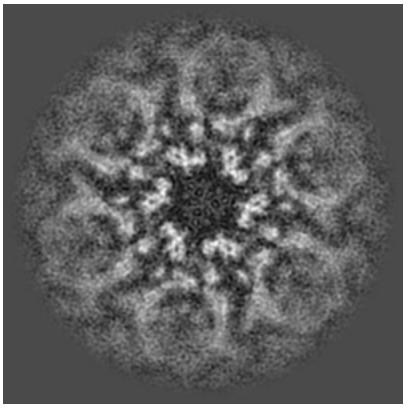
6.2.2 Raw map



X Index: 100



Y Index: 100

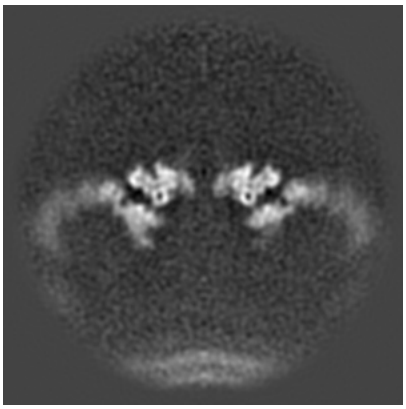


Z Index: 100

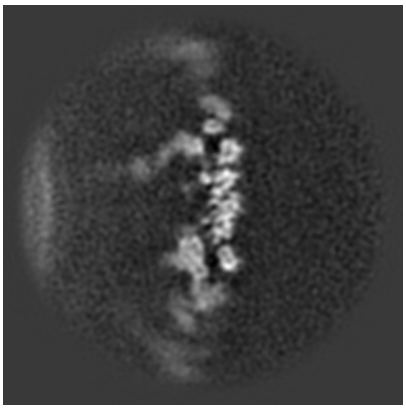
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

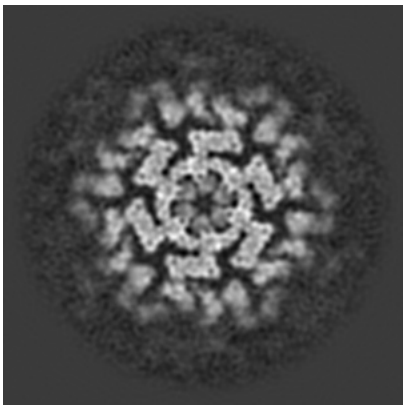
6.3.1 Primary map



X Index: 100

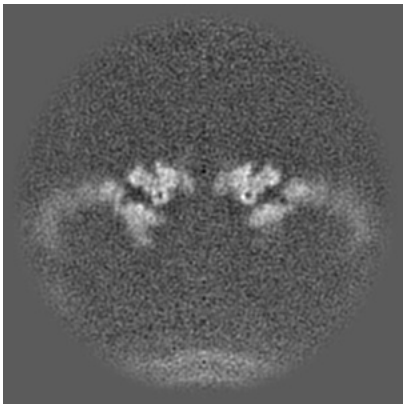


Y Index: 117

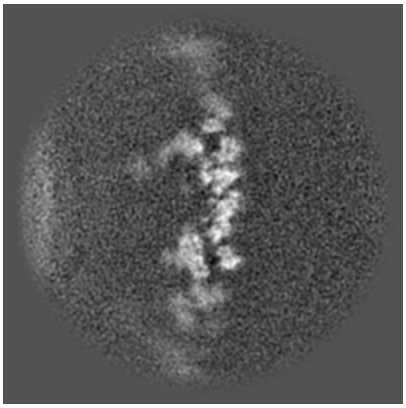


Z Index: 110

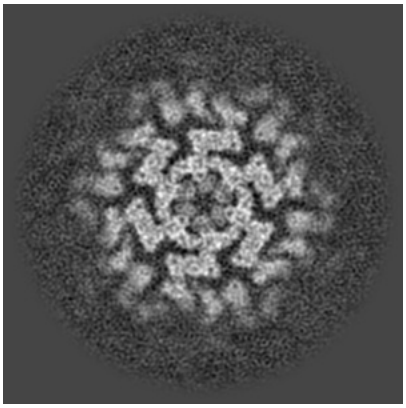
6.3.2 Raw map



X Index: 100



Y Index: 116

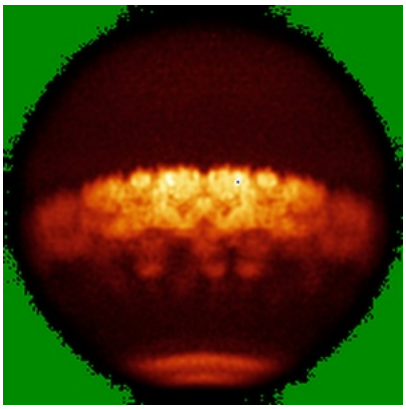


Z Index: 110

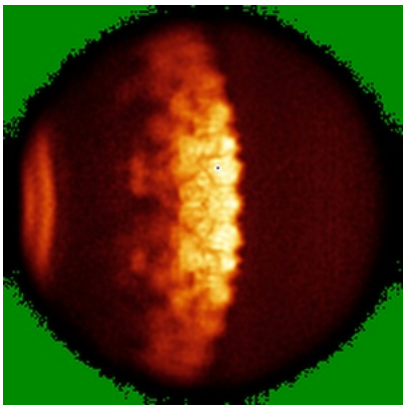
The images above show the largest variance slices of the map in three orthogonal directions.

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

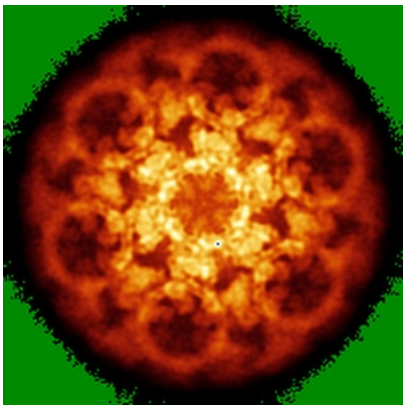
6.4.1 Primary map



X

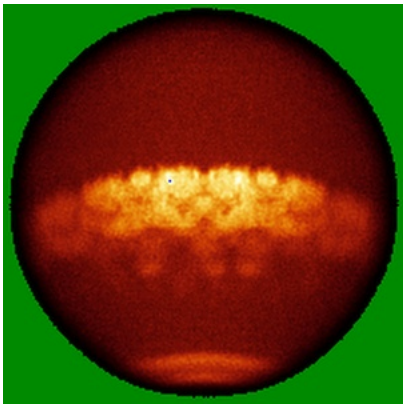


Y

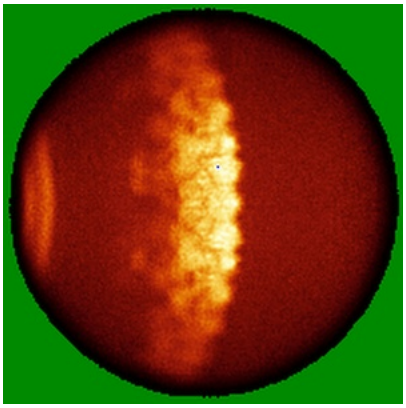


Z

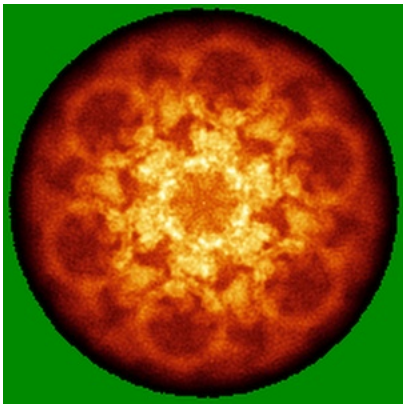
6.4.2 Raw map



X



Y

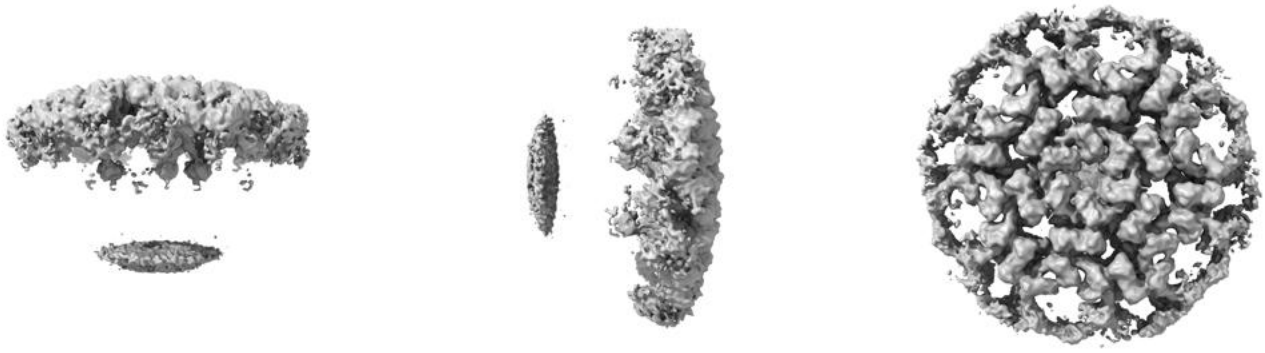


Z

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)

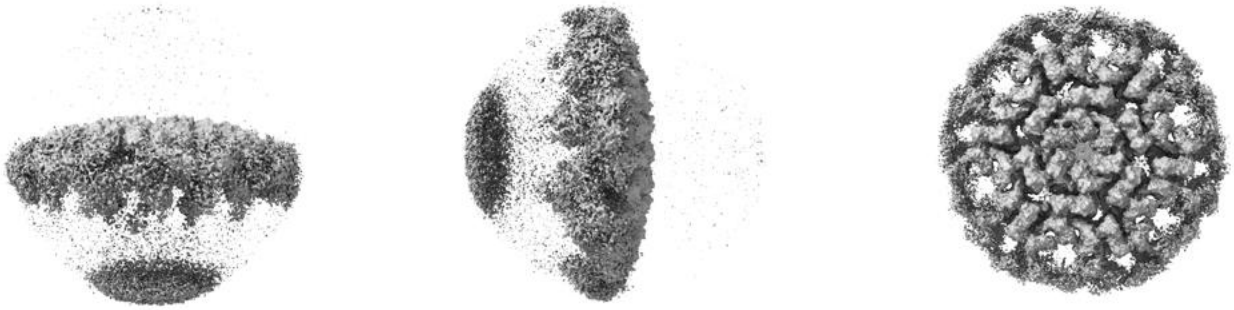
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00509. 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.

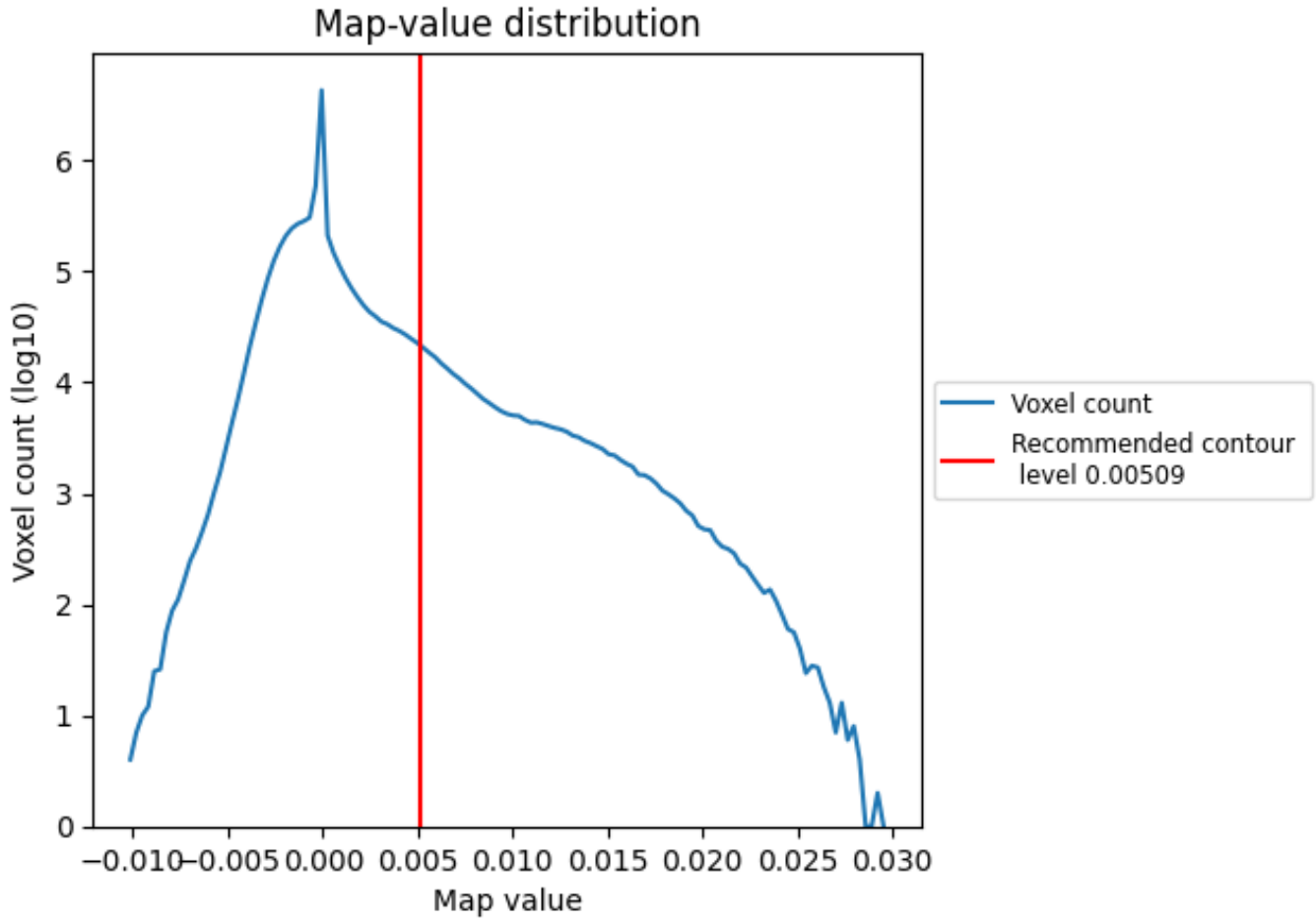
6.6 Mask visualisation (i)

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

7 Map analysis

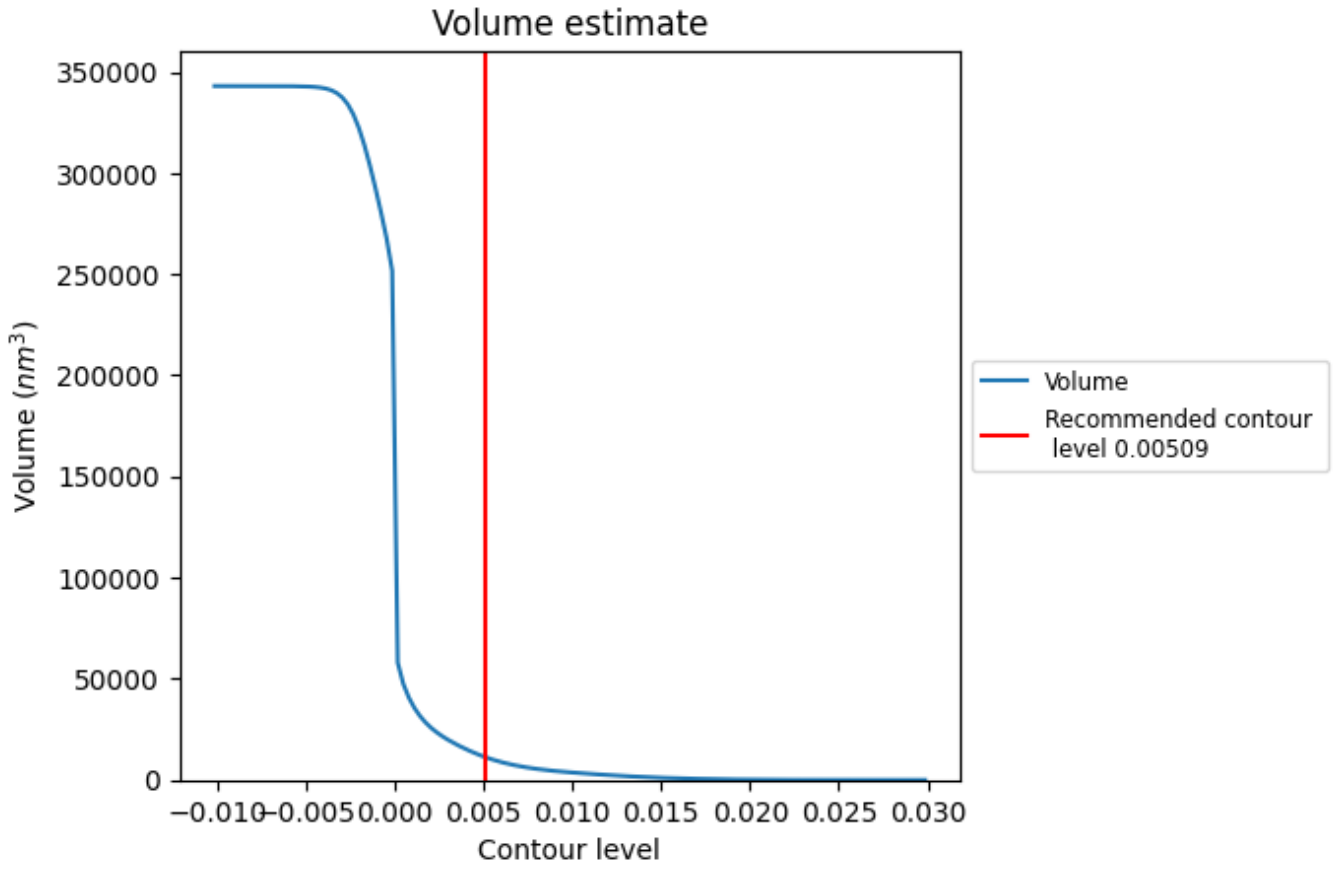
This section contains the results of statistical analysis of the map.

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.

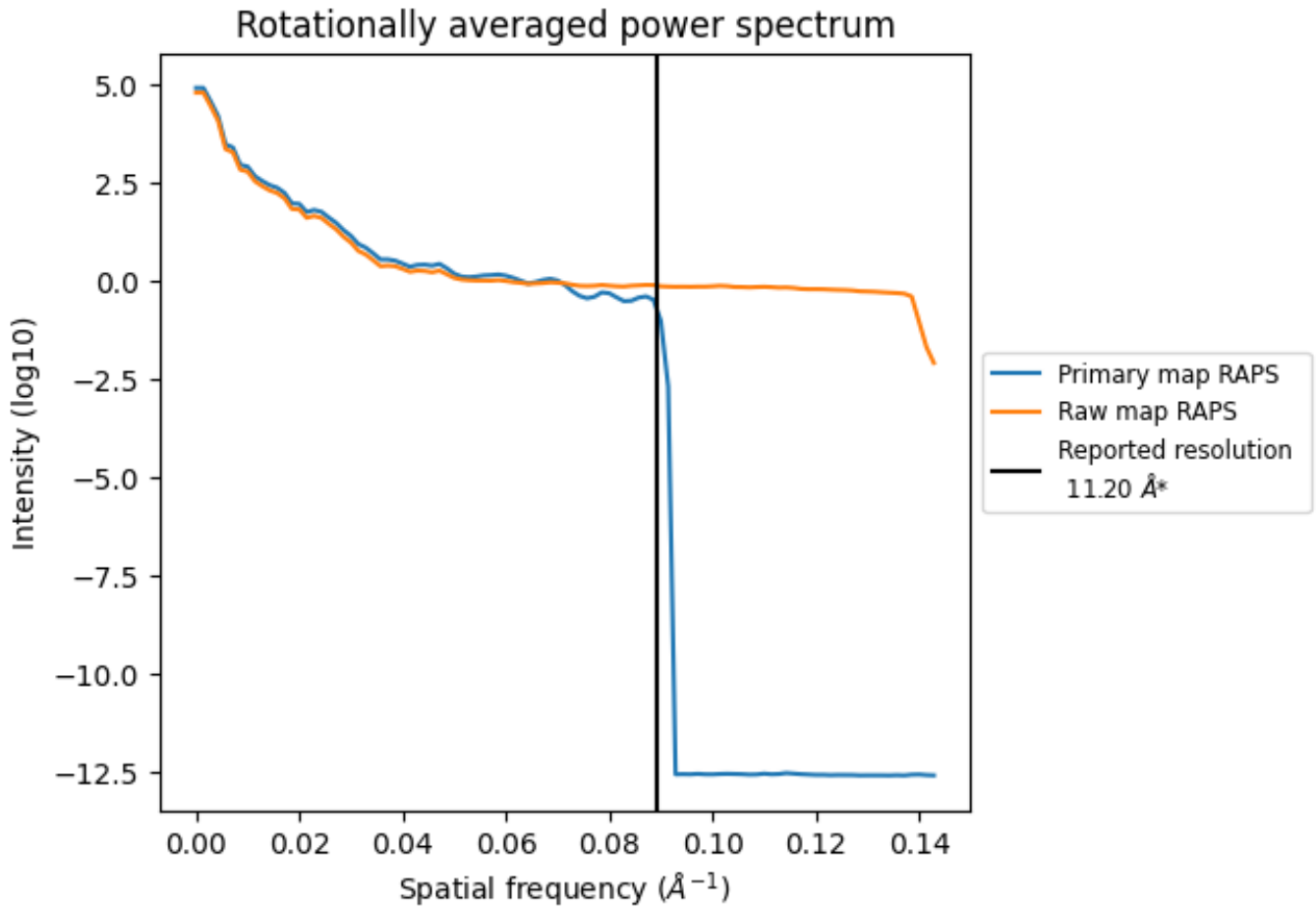
7.2 Volume estimate (i)



The volume at the recommended contour level is 11315 nm^3; this corresponds to an approximate mass of 10221 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)

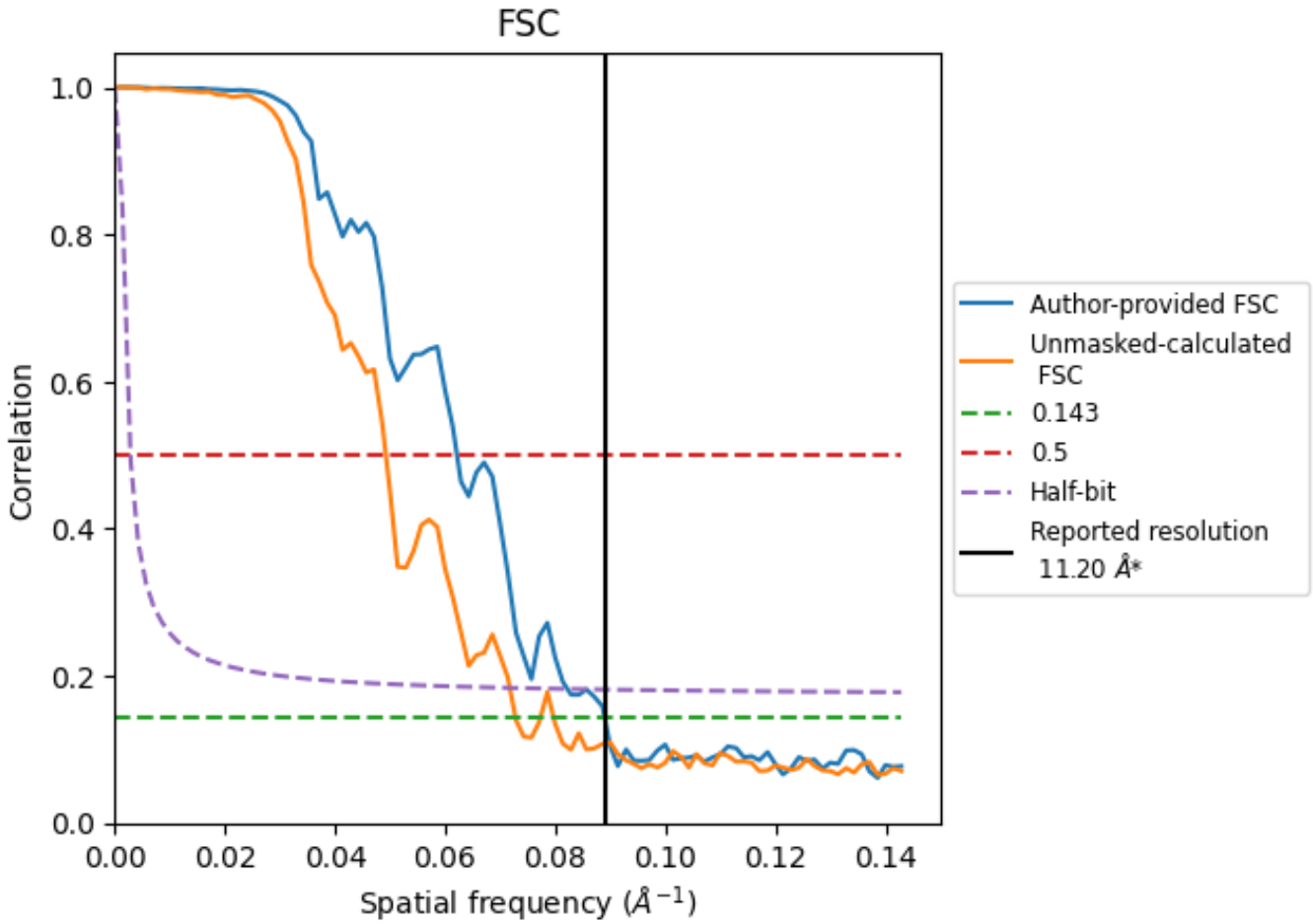


*Reported resolution corresponds to spatial frequency of 0.089 $Å^{-1}$

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 0.089 Å^{-1}

8.2 Resolution estimates (i)

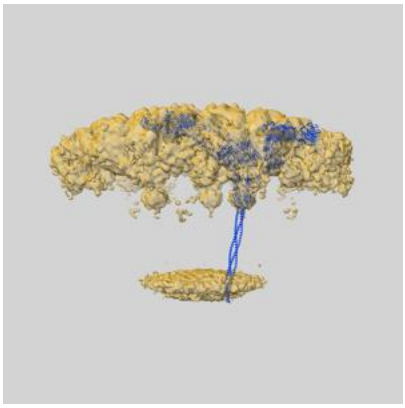
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.20	-	-
Author-provided FSC curve	11.24	16.08	12.17
Unmasked-calculated*	13.74	20.33	13.93

*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 13.74 differs from the reported value 11.2 by more than 10 %

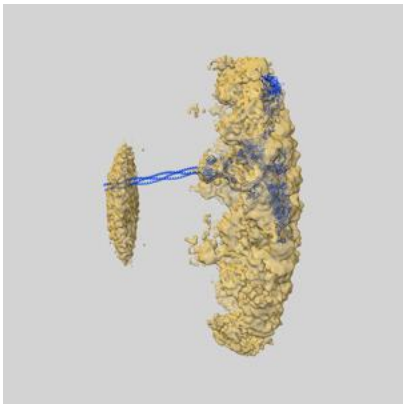
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18127 and PDB model 8QOX. Per-residue inclusion information can be found in section 3 on page 4.

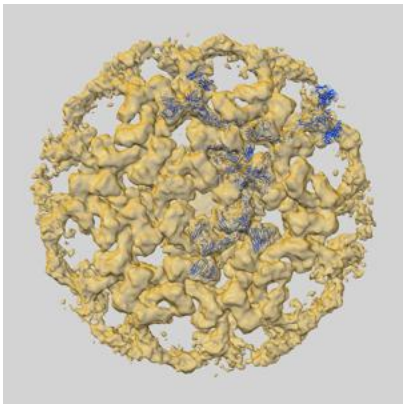
9.1 Map-model overlay



X



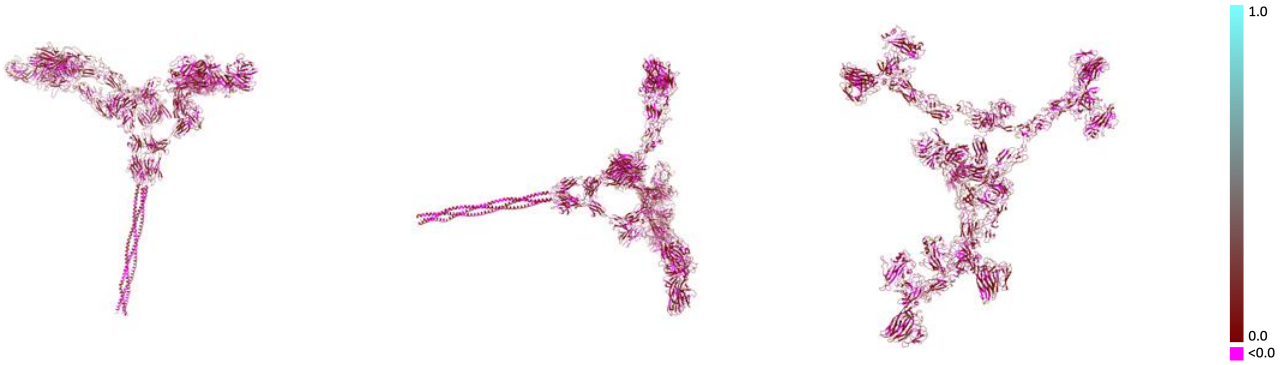
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00509 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.

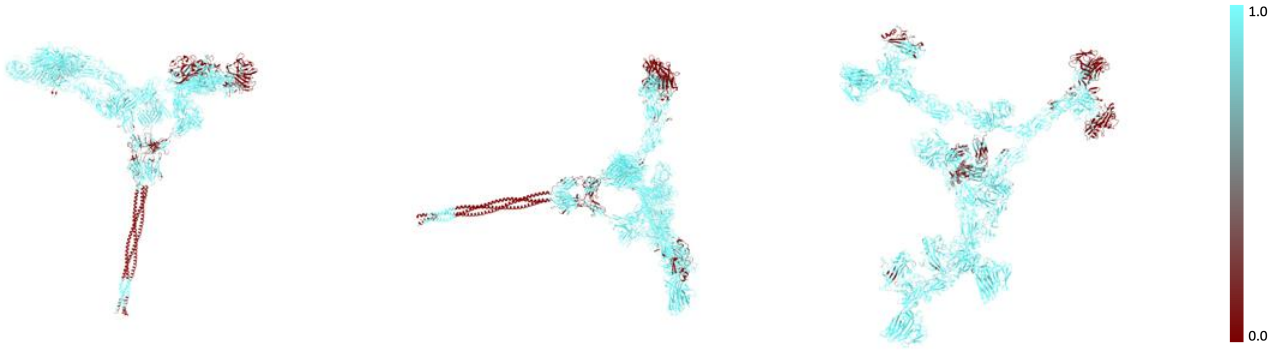
9.2 Q-score mapped to coordinate model (i)



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.

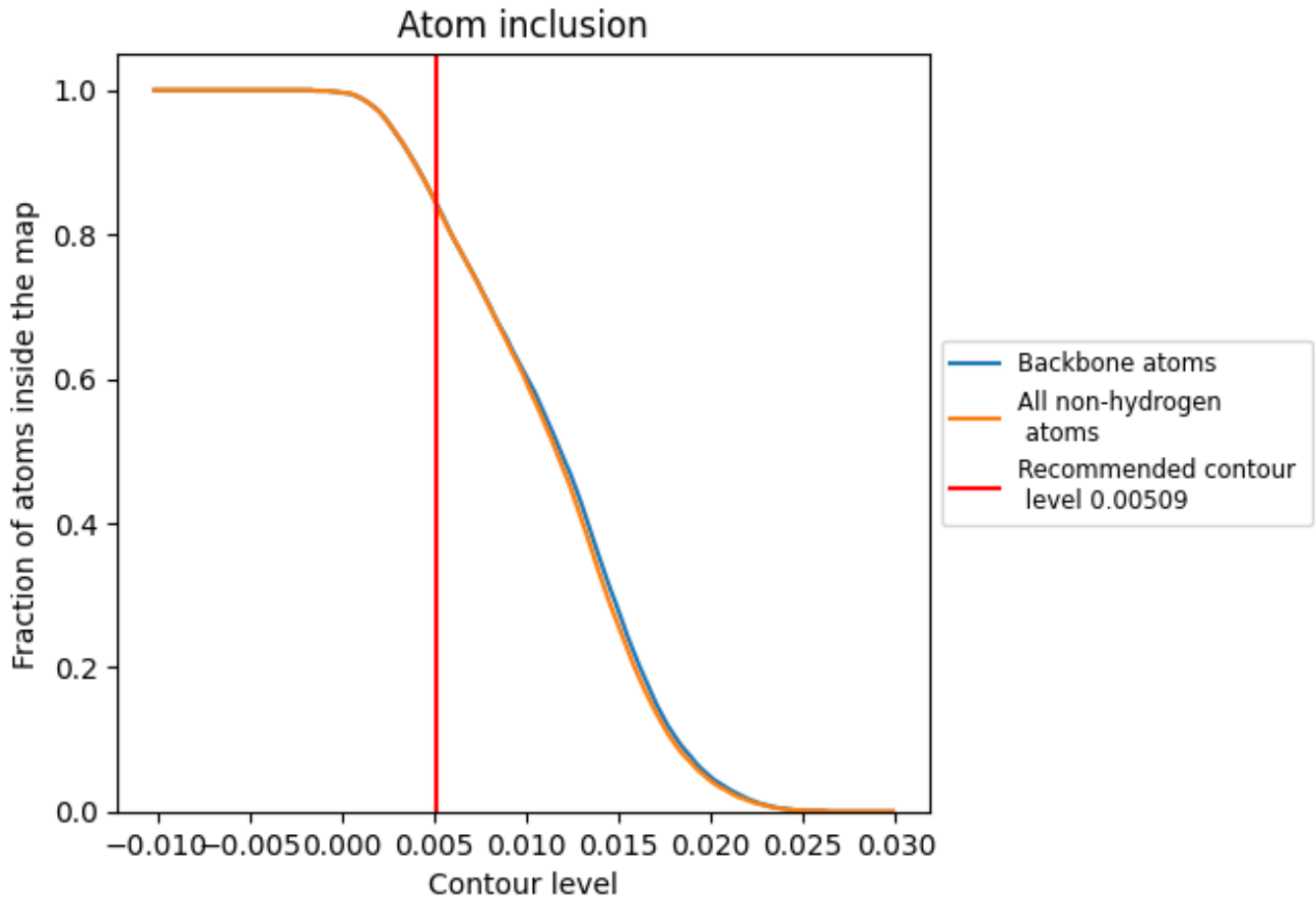
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00509).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00509) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.0660
A	0.9780	0.0790
B	0.6270	0.0550
C	0.6100	0.0560
V	0.9390	0.0660
W	0.6970	0.0510
X	0.5710	0.0460
Z	0.9890	0.0810