



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 06:22 AM JST

PDB ID : 5YFP
EMDB ID : EMD-6827
Title : Cryo-EM Structure of the Exocyst Complex
Authors : Mei, K.; Li, Y.; Wang, S.; Shao, G.; Wang, J.; Ding, Y.; Luo, G.; Yue, P.; Liu, J.J.; Wang, X.; Dong, M.Q.; Guo, W.; Wang, H.W.
Deposited on : 2017-09-21
Resolution : 4.40 Å (reported)
Based on initial models : 2D2S, ?, 2FJI, 1ZC4, 5H11, 2B1E, 2A2F

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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) : 2.31.2

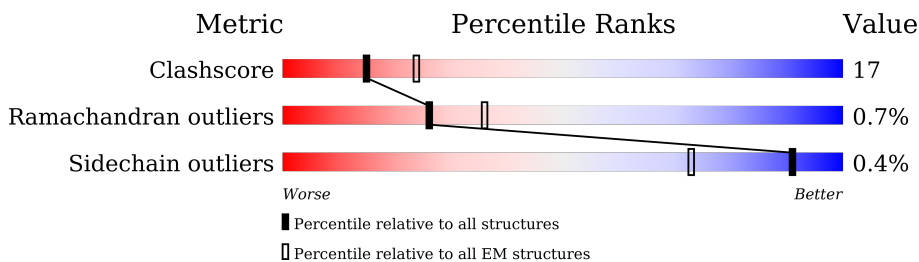
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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 $\leq 5\%$. 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	1336	
2	B	971	
3	C	805	
4	D	1065	
5	E	871	
6	F	910	
7	G	623	
8	H	753	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33096 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 Exocyst complex component SEC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	672	Total	C	N	O	0	0
			3345	2001	672	672		

- Molecule 2 is a protein called Exocyst complex component SEC5.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	928	Total	C	N	O	0	0
			4610	2755	927	928		

- Molecule 3 is a protein called Exocyst complex component SEC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	794	Total	C	N	O	S	0	0
			4994	3097	892	989	16		

- Molecule 4 is a protein called Exocyst complex component SEC8.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	954	Total	C	N	O	0	0
			4739	2831	954	954		

- Molecule 5 is a protein called Exocyst complex component SEC10.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	776	Total	C	N	O	0	0
			3860	2308	776	776		

- Molecule 6 is a protein called Exocyst complex component SEC15.

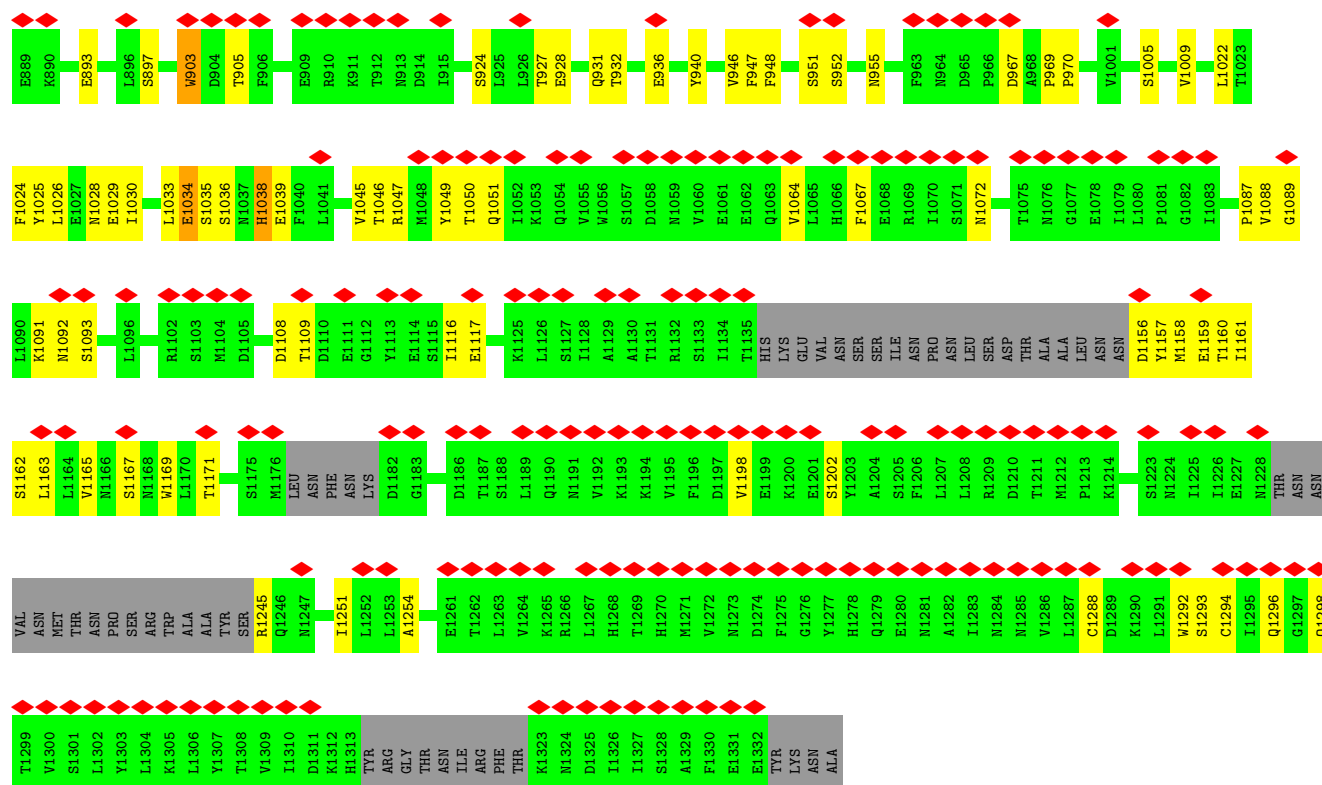
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	725	Total	C	N	O	0	0
			3612	2162	725	725		

- Molecule 7 is a protein called Exocyst complex component EXO70.

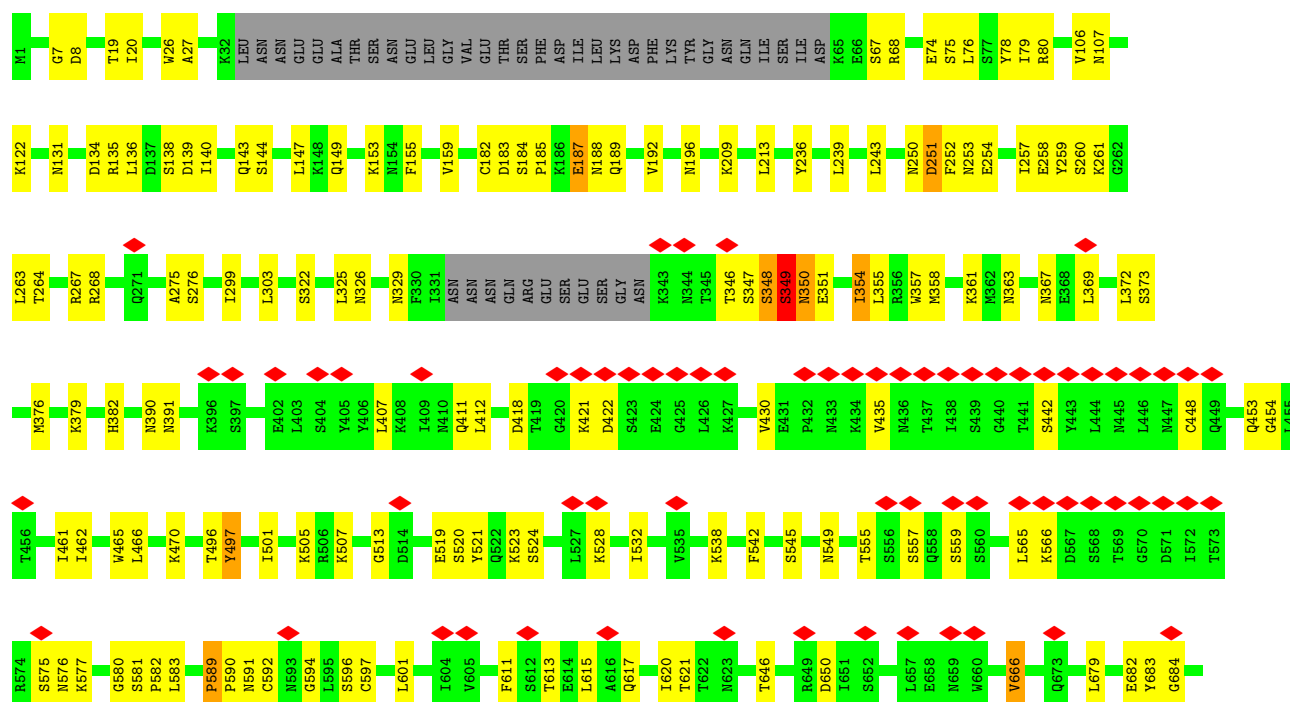
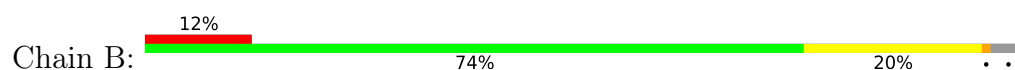
Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	615	Total	C	N	O	S	0	0
			4696	2968	809	902	17		

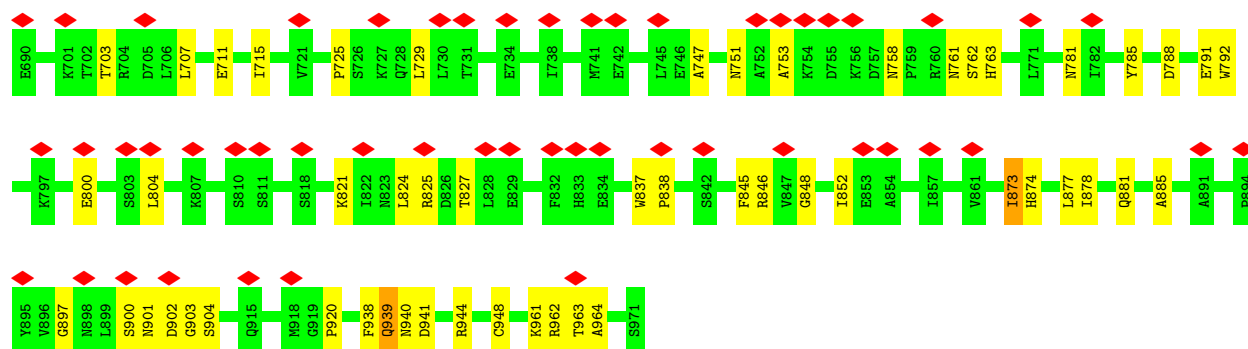
- Molecule 8 is a protein called Exocyst complex component EXO84.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	518	Total	C	N	O	S	0	0
			3240	2002	591	643	4		

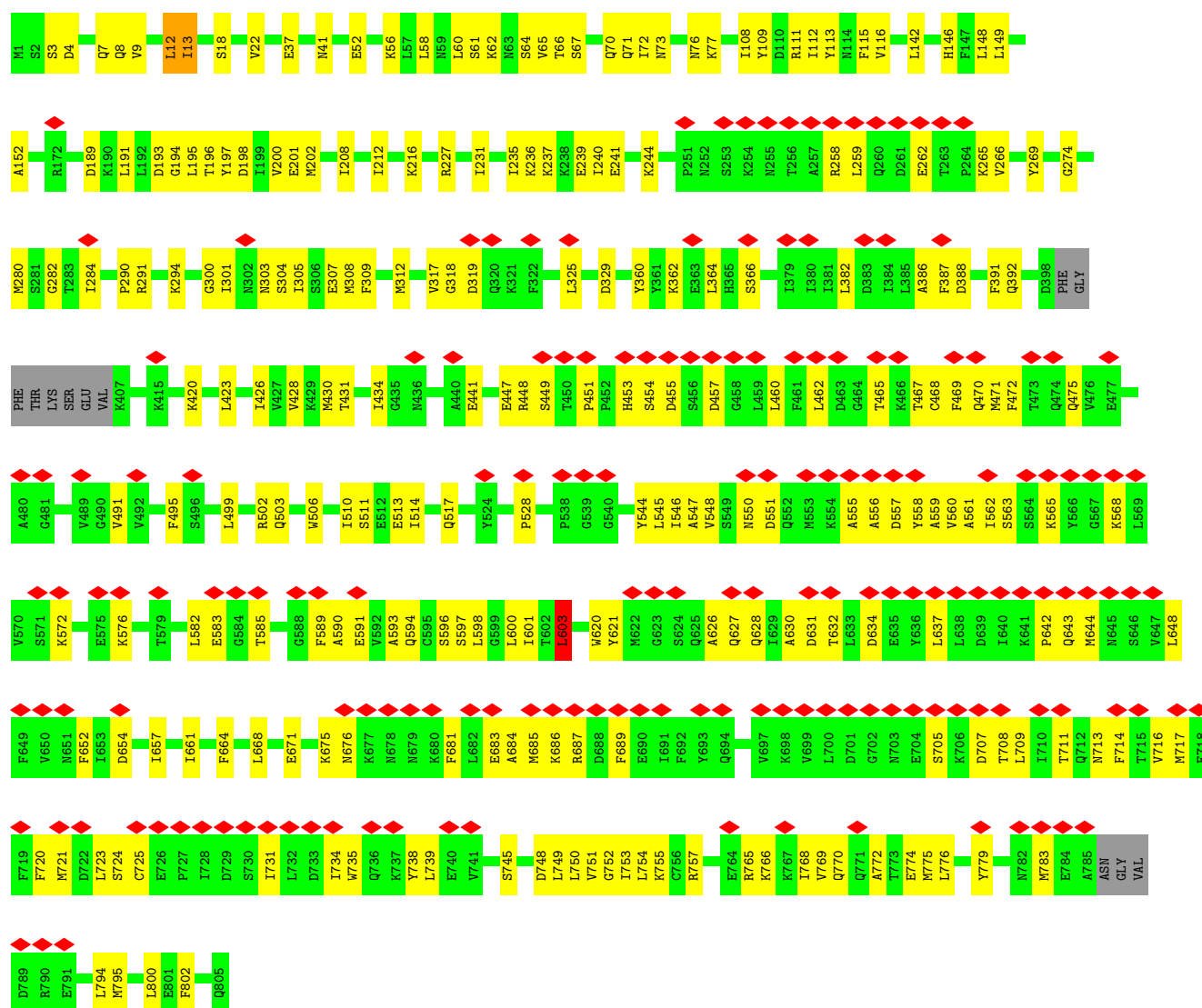


• Molecule 2: Exocyst complex component SEC5



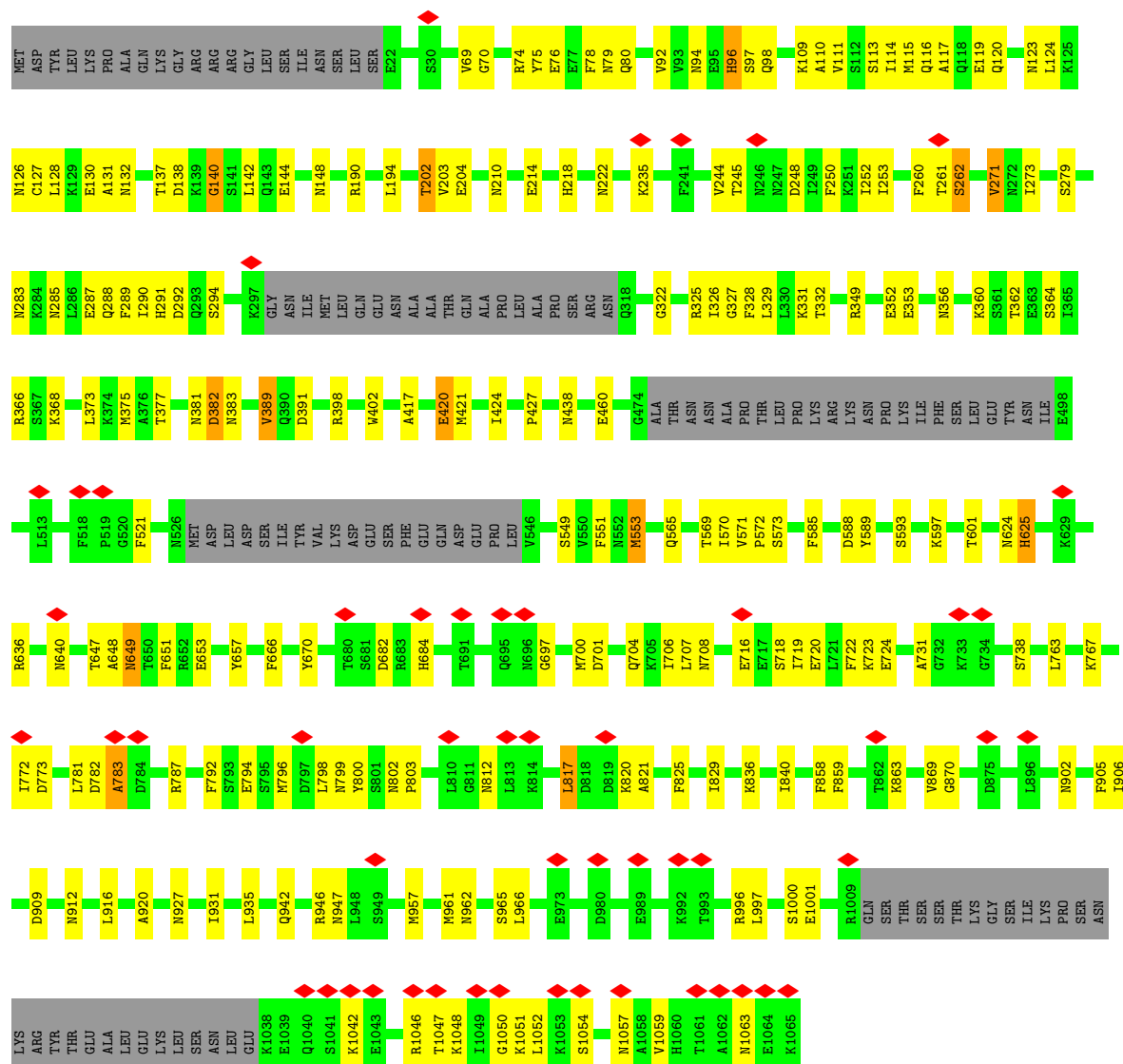


• Molecule 3: Exocyst complex component SEC6

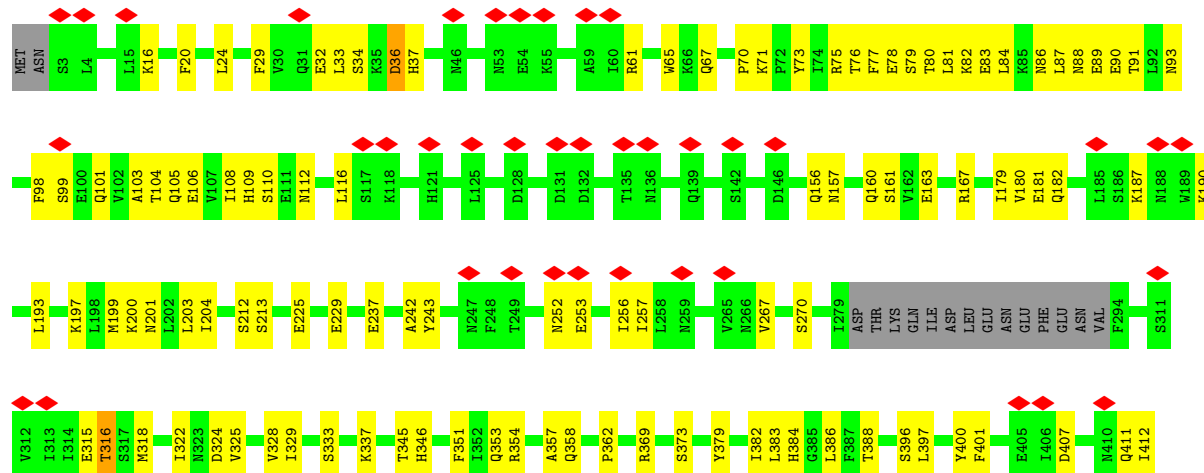


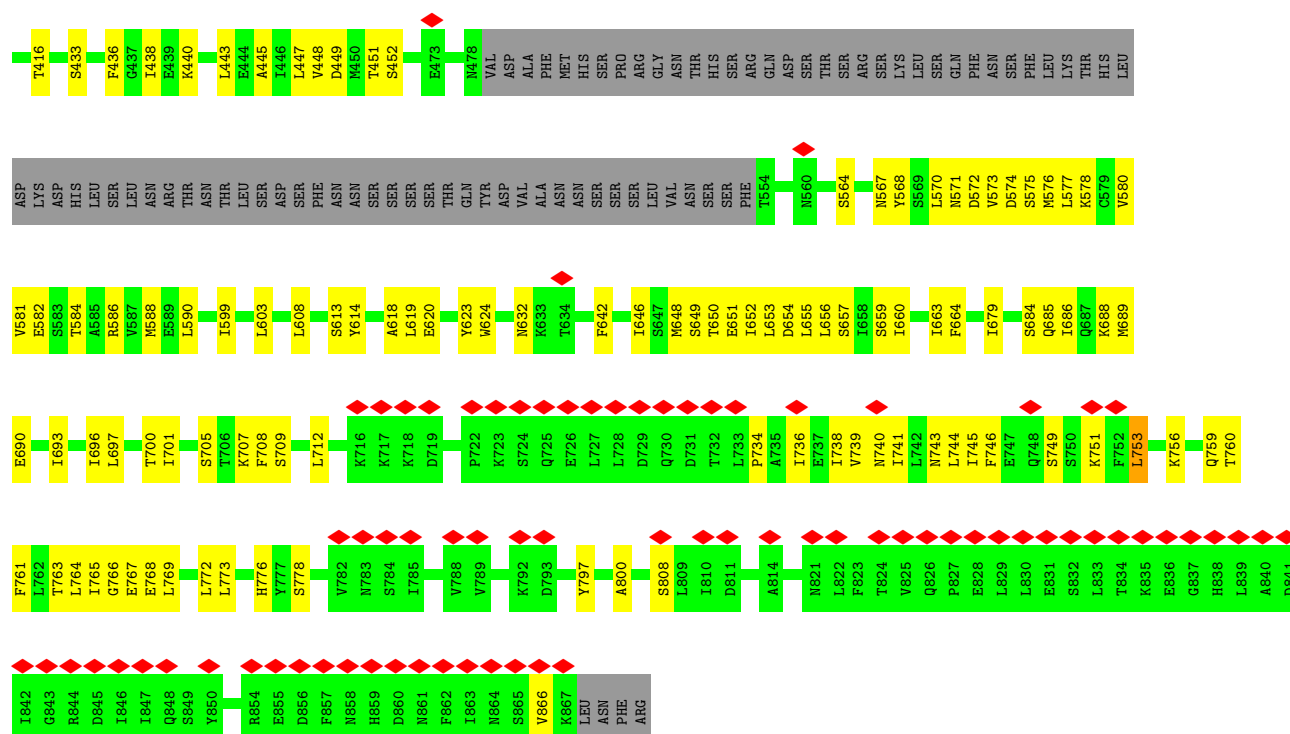
• Molecule 4: Exocyst complex component SEC8



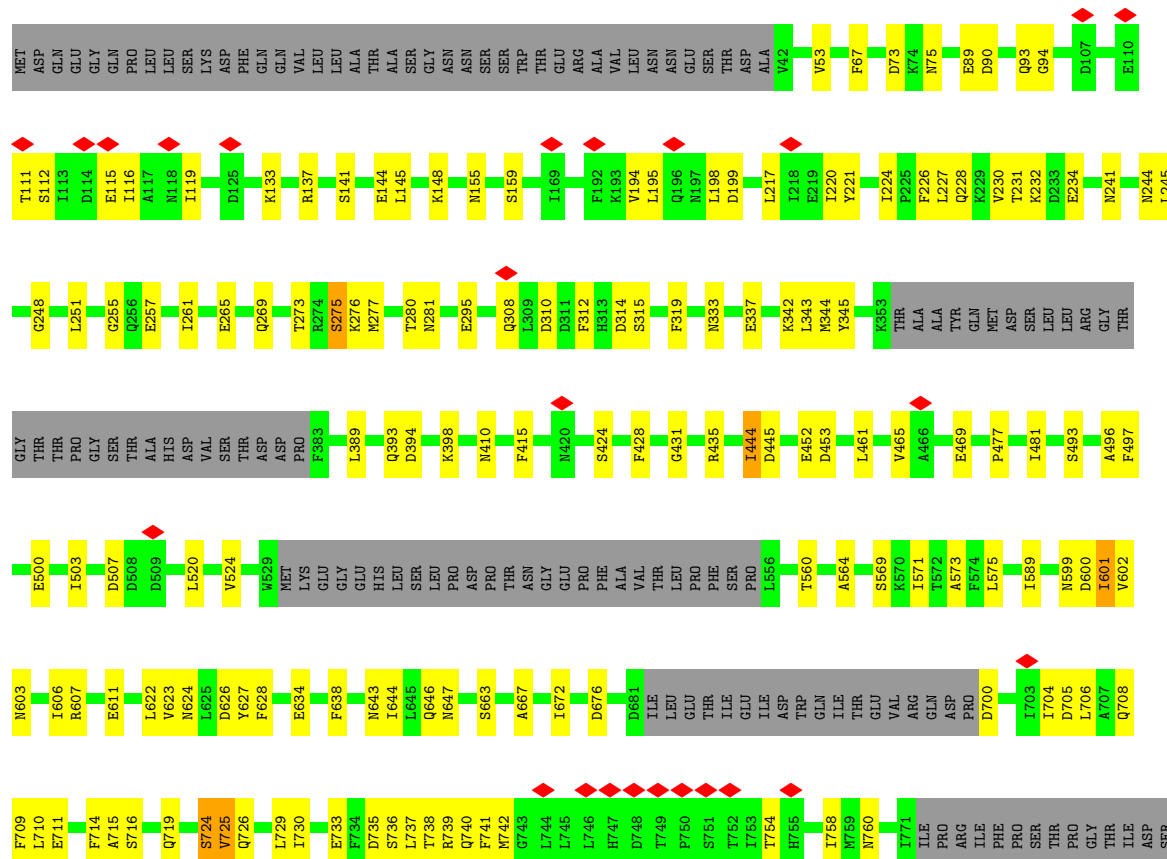


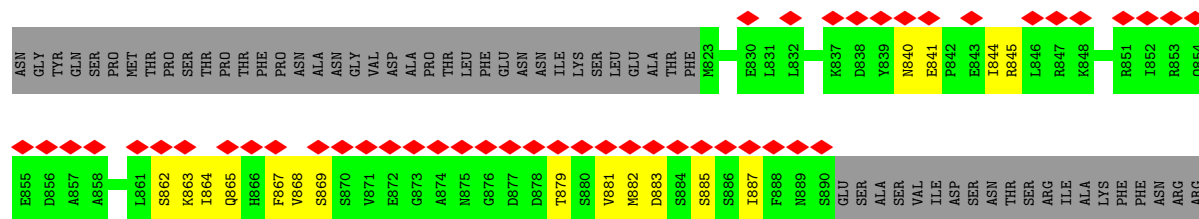
• Molecule 5: Exocyst complex component SEC10



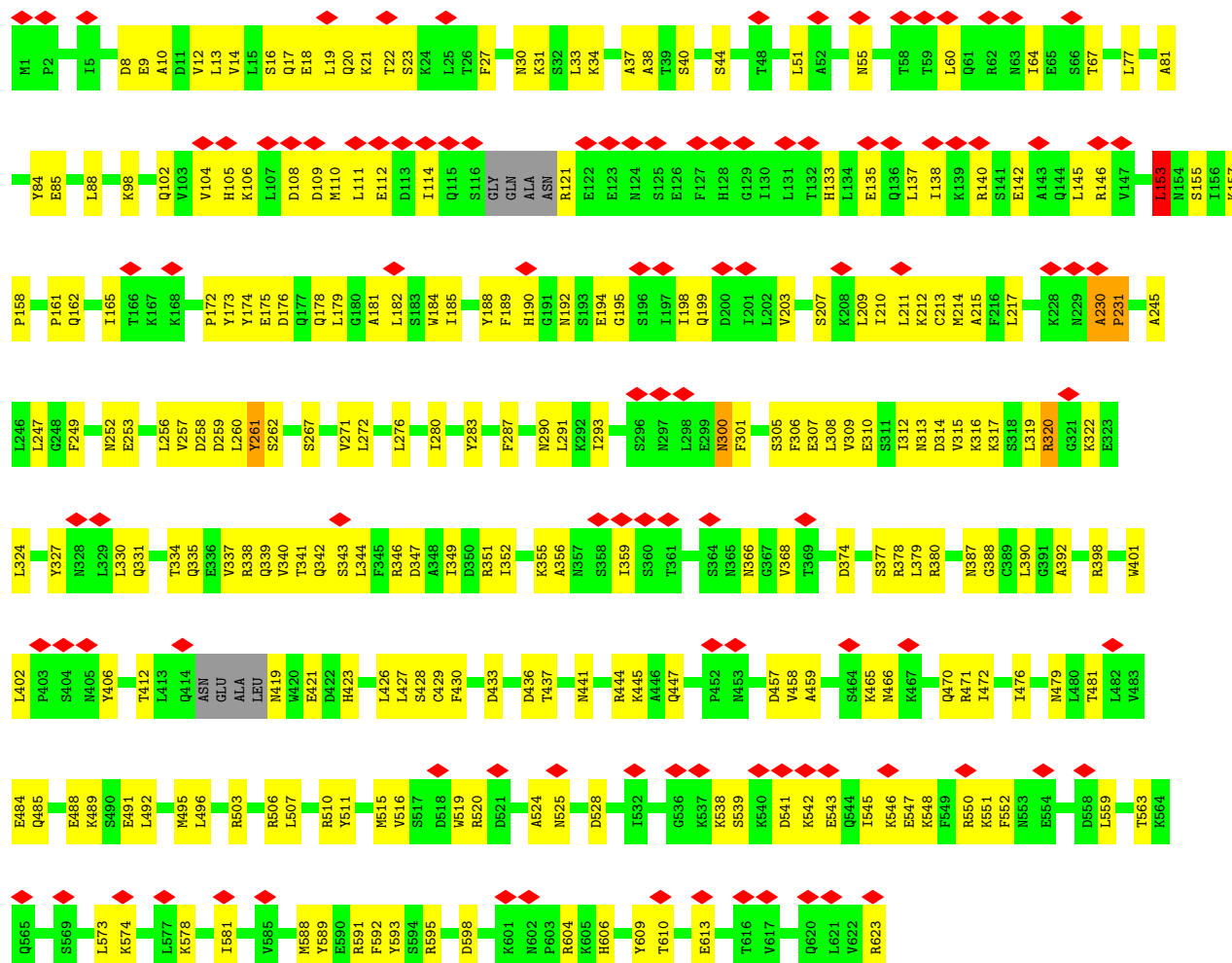


• Molecule 6: Exocyst complex component SEC15

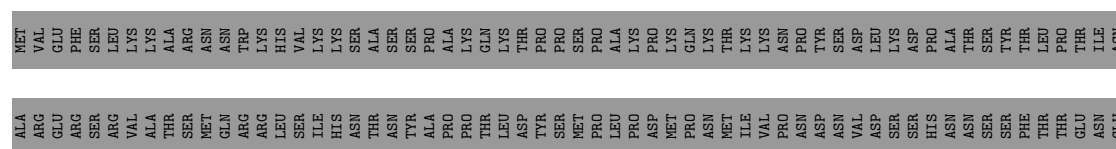


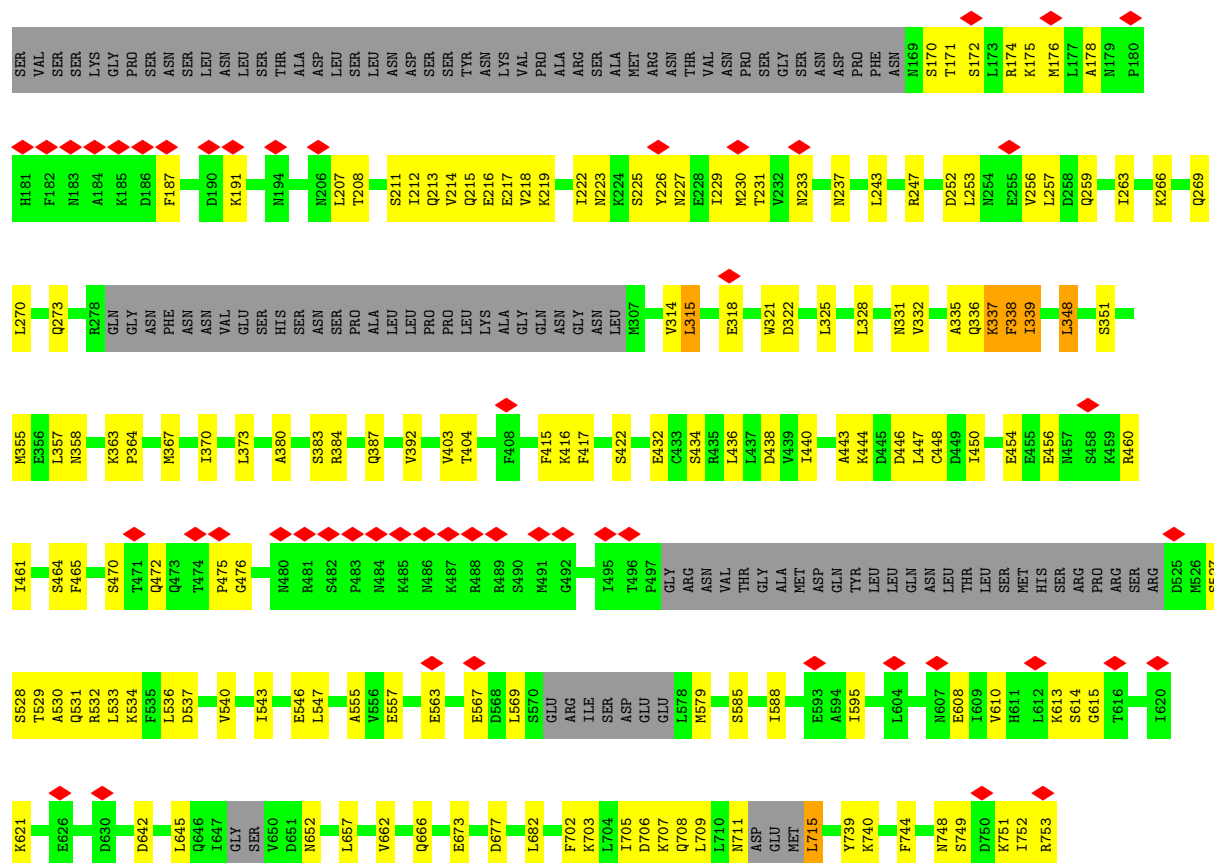


• Molecule 7: Exocyst complex component EXO70



• Molecule 8: Exocyst complex component EXO84





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	343342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The defocus value of each image was determined by CTFFIND3.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0203	Depositor
Map size (\AA)	470.3544, 470.3544, 470.3544	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.30654, 1.30654, 1.30654	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	0.28	0/3340	0.63	4/4659 (0.1%)
2	B	0.33	0/4607	0.71	13/6427 (0.2%)
3	C	0.31	0/5043	0.61	1/6885 (0.0%)
4	D	0.33	0/4734	0.75	7/6601 (0.1%)
5	E	0.27	0/3857	0.56	2/5383 (0.0%)
6	F	0.29	0/3607	0.61	5/5034 (0.1%)
7	G	0.37	0/4768	0.63	3/6443 (0.0%)
8	H	0.41	0/3253	0.65	2/4443 (0.0%)
All	All	0.33	0/33209	0.65	37/45875 (0.1%)

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	11
2	B	0	41
3	C	0	8
4	D	0	43
5	E	0	6
6	F	0	13
7	G	0	9
8	H	0	12
All	All	0	143

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	758	ASN	C-N-CA	7.96	155.41	122.00
1	A	1116	ILE	C-N-CA	7.77	141.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	444	ILE	C-N-CA	7.20	139.70	121.70
7	G	153	LEU	CA-CB-CG	-6.69	99.91	115.30
4	D	649	ASN	C-N-CA	6.38	137.65	121.70

There are no chirality outliers.

5 of 143 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	749	GLU	Peptide
1	A	780	GLU	Peptide
1	A	946	VAL	Peptide
1	A	947	PHE	Peptide
1	A	948	PHE	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	A	3345	0	1403	67	0
2	B	4610	0	1926	83	0
3	C	4994	0	3576	172	0
4	D	4739	0	2011	90	0
5	E	3860	0	1635	120	0
6	F	3612	0	1508	83	0
7	G	4696	0	4483	186	0
8	H	3240	0	2433	84	0
All	All	33096	0	18975	874	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 17.

The worst 5 of 874 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)
3:C:506:TRP:O	3:C:510:ILE:HB	1.54	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:558:TYR:O	3:C:562:ILE:HB	1.60	1.00
3:C:714:PHE:CD2	3:C:714:PHE:CZ	2.38	0.99
3:C:544:TYR:CG	3:C:544:TYR:CE2	2.40	0.97
3:C:557:ASP:O	3:C:561:ALA:HB3	1.66	0.96

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	662/1336 (50%)	518 (78%)	143 (22%)	1 (0%)	47	81
2	B	922/971 (95%)	707 (77%)	202 (22%)	13 (1%)	11	47
3	C	788/805 (98%)	673 (85%)	114 (14%)	1 (0%)	51	85
4	D	944/1065 (89%)	718 (76%)	213 (23%)	13 (1%)	11	47
5	E	770/871 (88%)	641 (83%)	127 (16%)	2 (0%)	41	76
6	F	715/910 (79%)	578 (81%)	130 (18%)	7 (1%)	15	54
7	G	609/623 (98%)	555 (91%)	52 (8%)	2 (0%)	41	76
8	H	506/753 (67%)	431 (85%)	73 (14%)	2 (0%)	34	72
All	All	5916/7334 (81%)	4821 (82%)	1054 (18%)	41 (1%)	26	62

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	349	SER
2	B	350	ASN
2	B	590	PRO
2	B	762	SER
4	D	97	SER

5.3.2 Protein sidechains ⓘ

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	
3	C	300/740 (40%)	300 (100%)	0	100	100
7	G	480/570 (84%)	478 (100%)	2 (0%)	91	94
8	H	202/697 (29%)	200 (99%)	2 (1%)	76	86
All	All	982/2007 (49%)	978 (100%)	4 (0%)	91	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	320	ARG
7	G	623	ARG
8	H	579	MET
8	H	753	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	470	GLN
8	H	638	ASN
3	C	694	GLN
7	G	105	HIS
7	G	190	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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-6827. These allow visual inspection of the internal detail of the map and identification of artifacts.

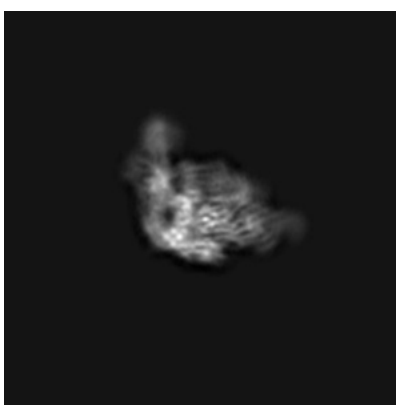
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

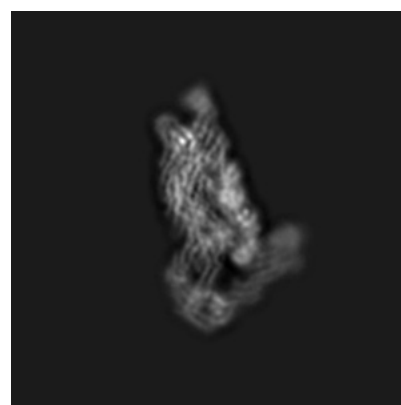
6.1.1 Primary map



X



Y

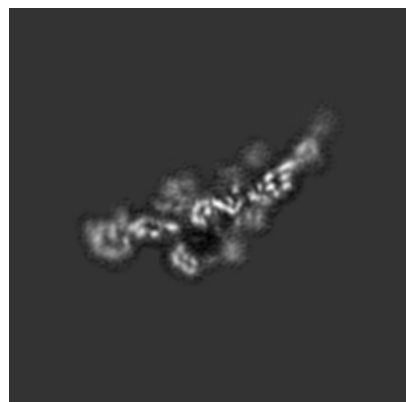


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180

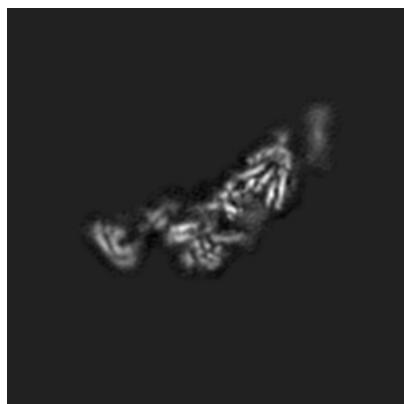


Z Index: 180

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 161



Y Index: 193

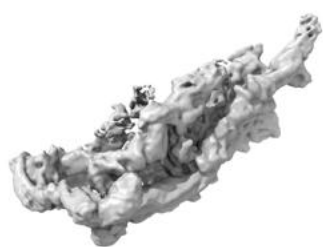


Z Index: 163

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 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

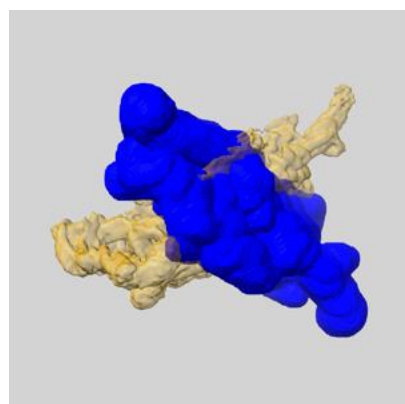
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

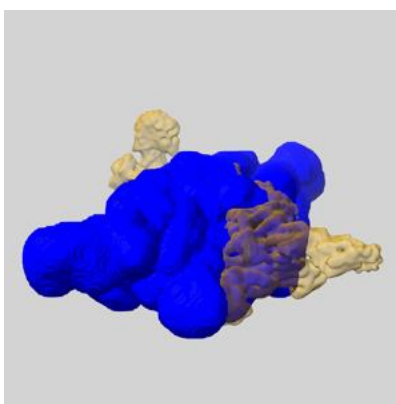
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

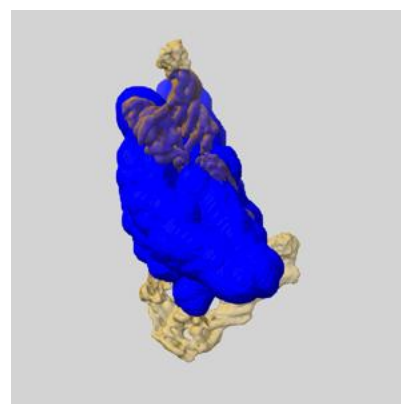
6.5.1 emd_6827_msk_5.map [i](#)



X

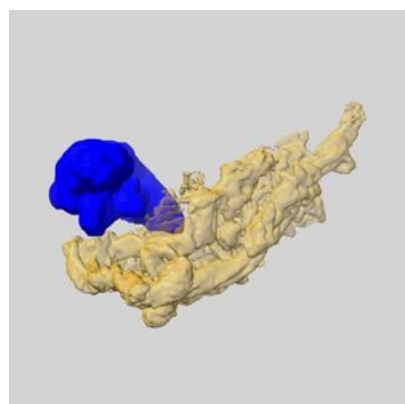


Y

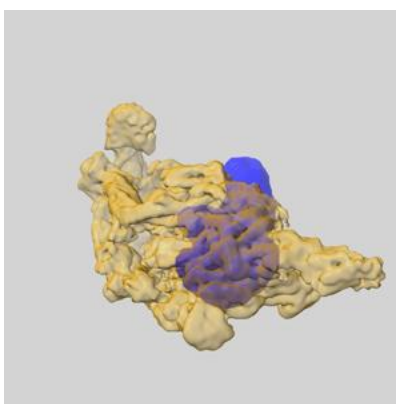


Z

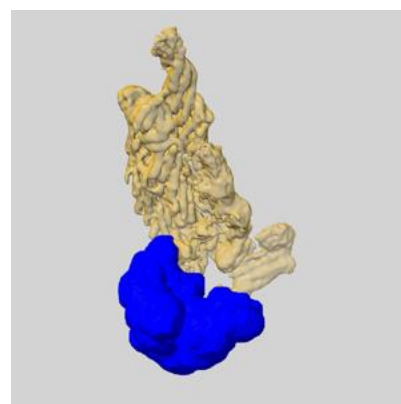
6.5.2 emd_6827_msk_4.map [i](#)



X

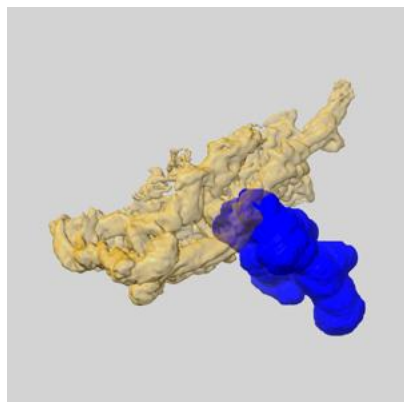


Y

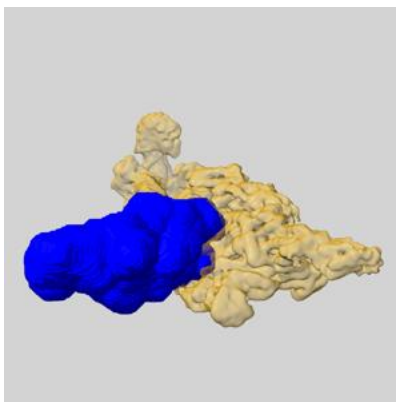


Z

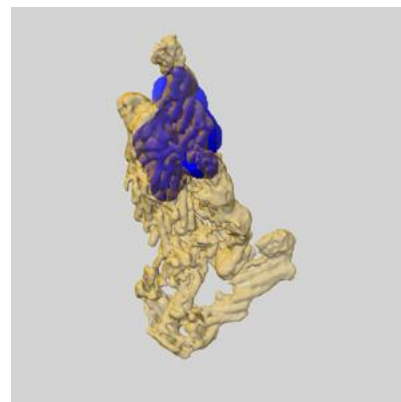
6.5.3 emd_6827_msk_3.map [i](#)



X

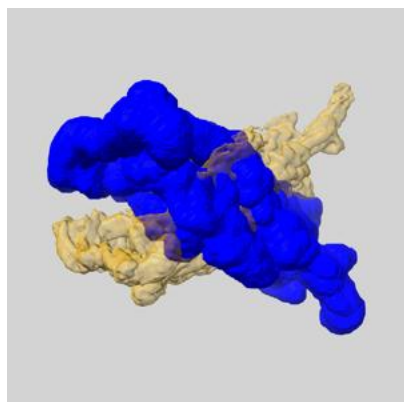


Y

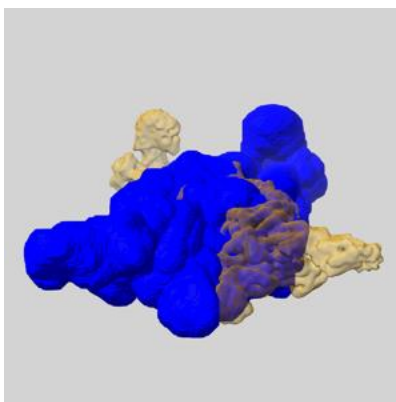


Z

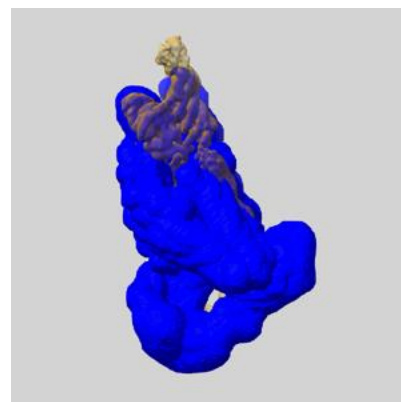
6.5.4 emd_6827_msk_2.map [i](#)



X

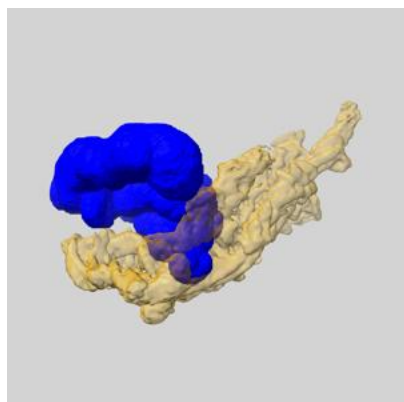


Y

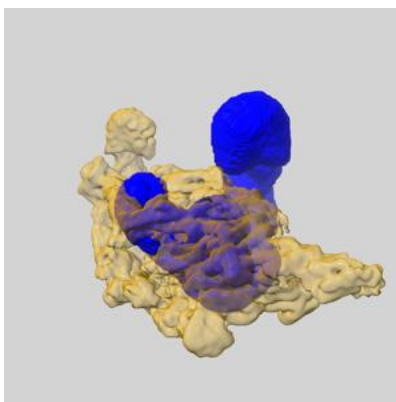


Z

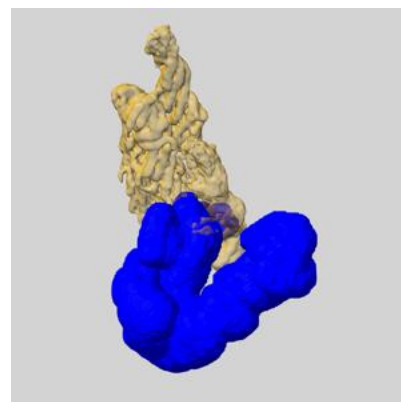
6.5.5 emd_6827_msk_1.map [i](#)



X



Y

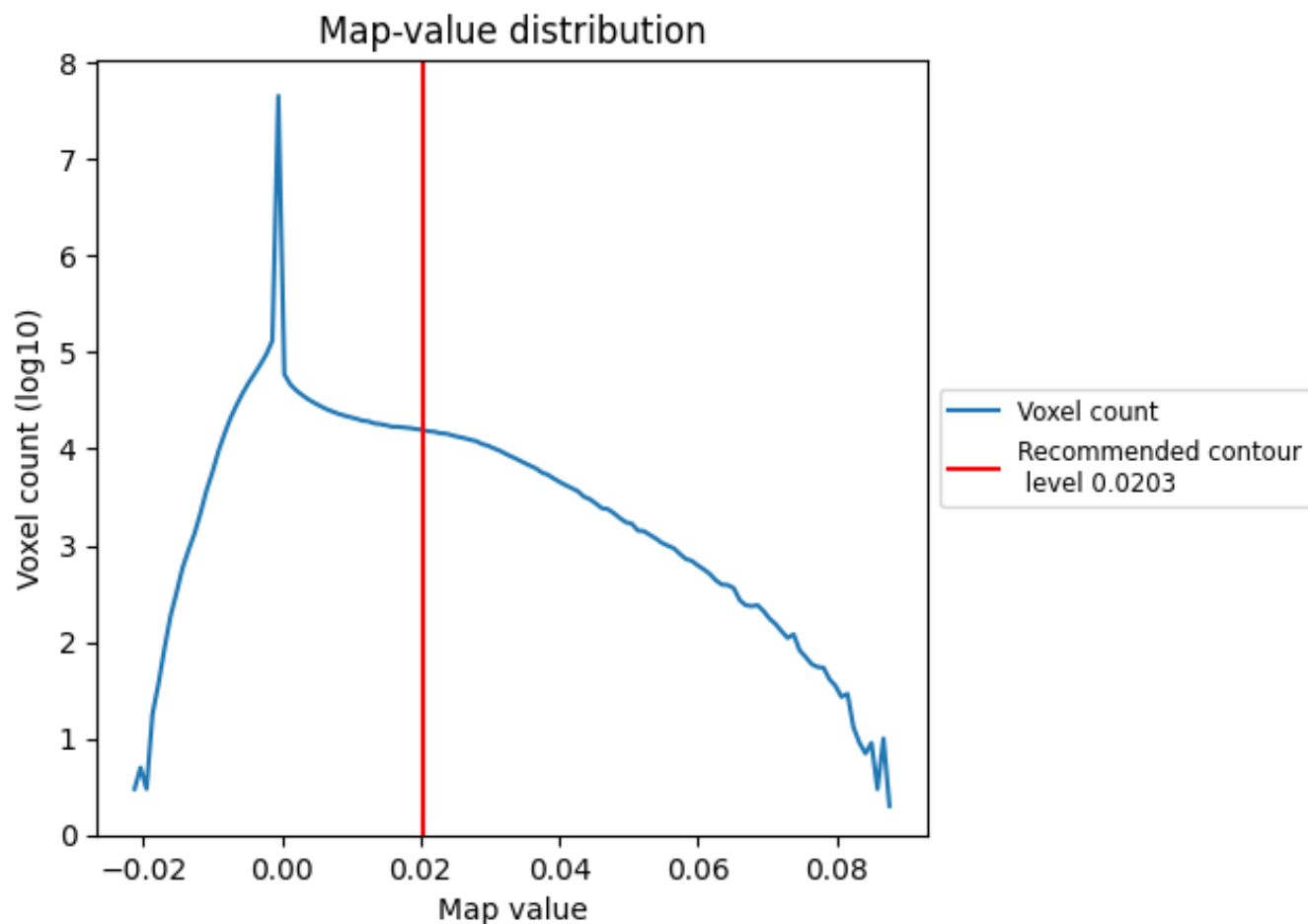


Z

7 Map analysis [i](#)

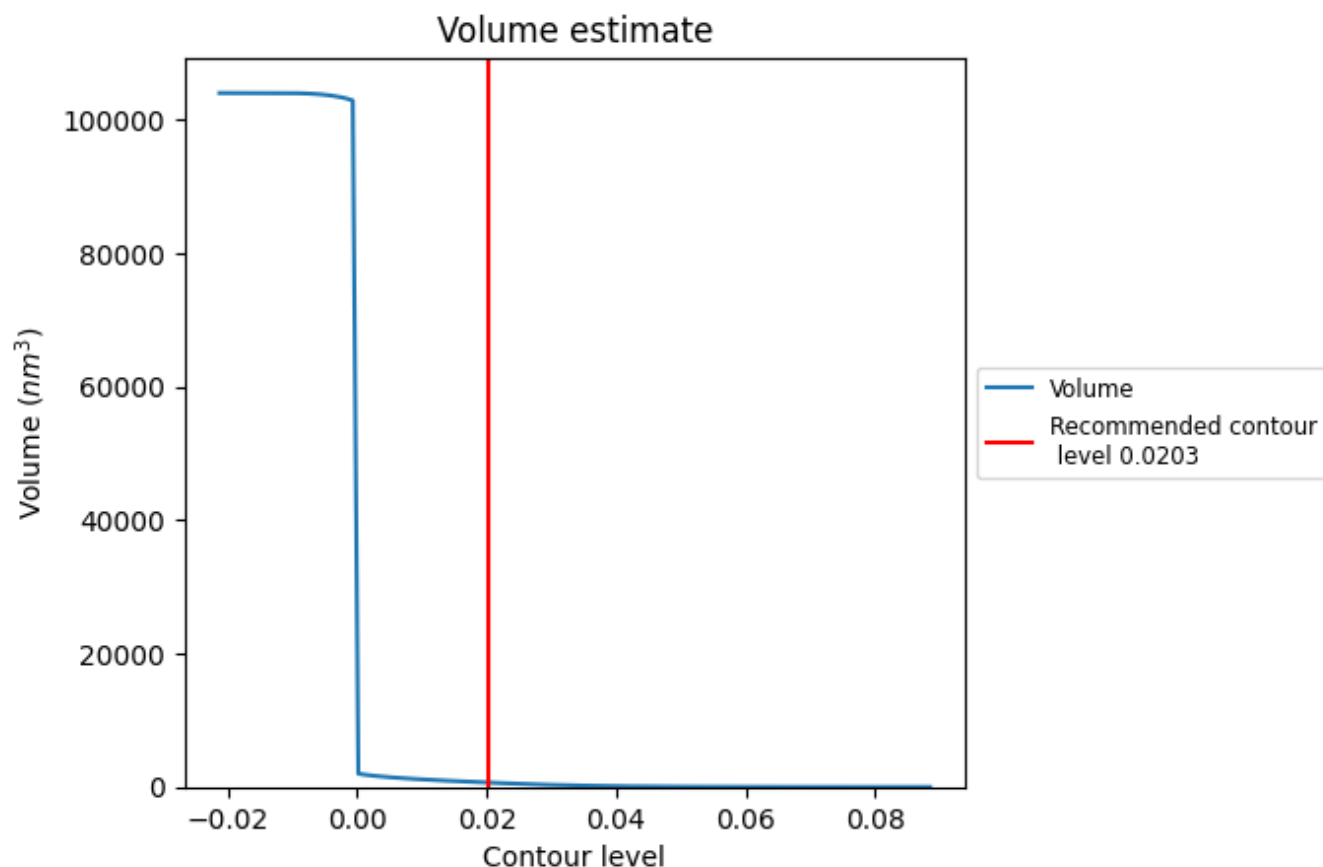
This section contains the results of statistical analysis of the map.

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.

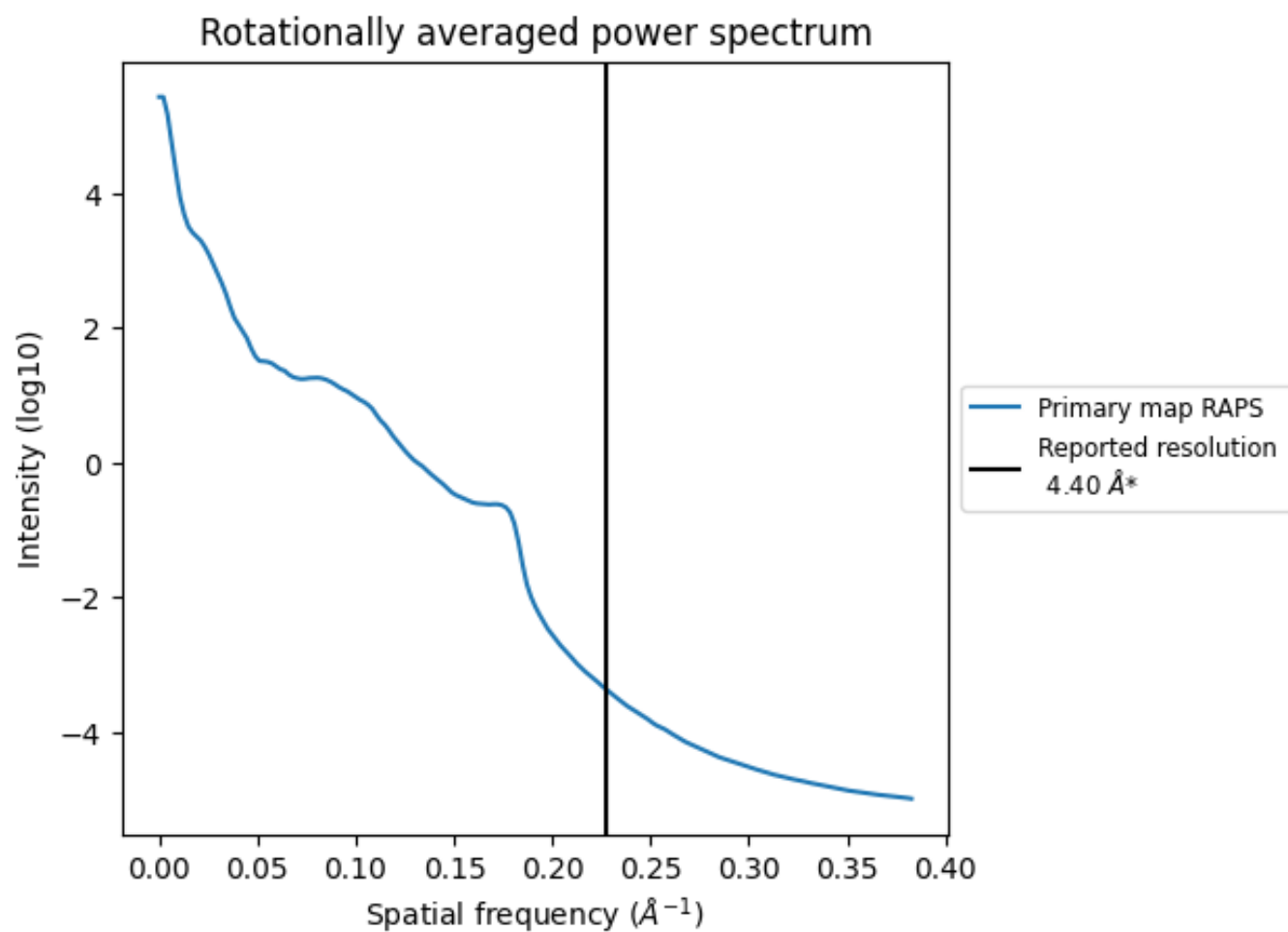
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 656 nm^3 ; this corresponds to an approximate mass of 593 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 ⓘ

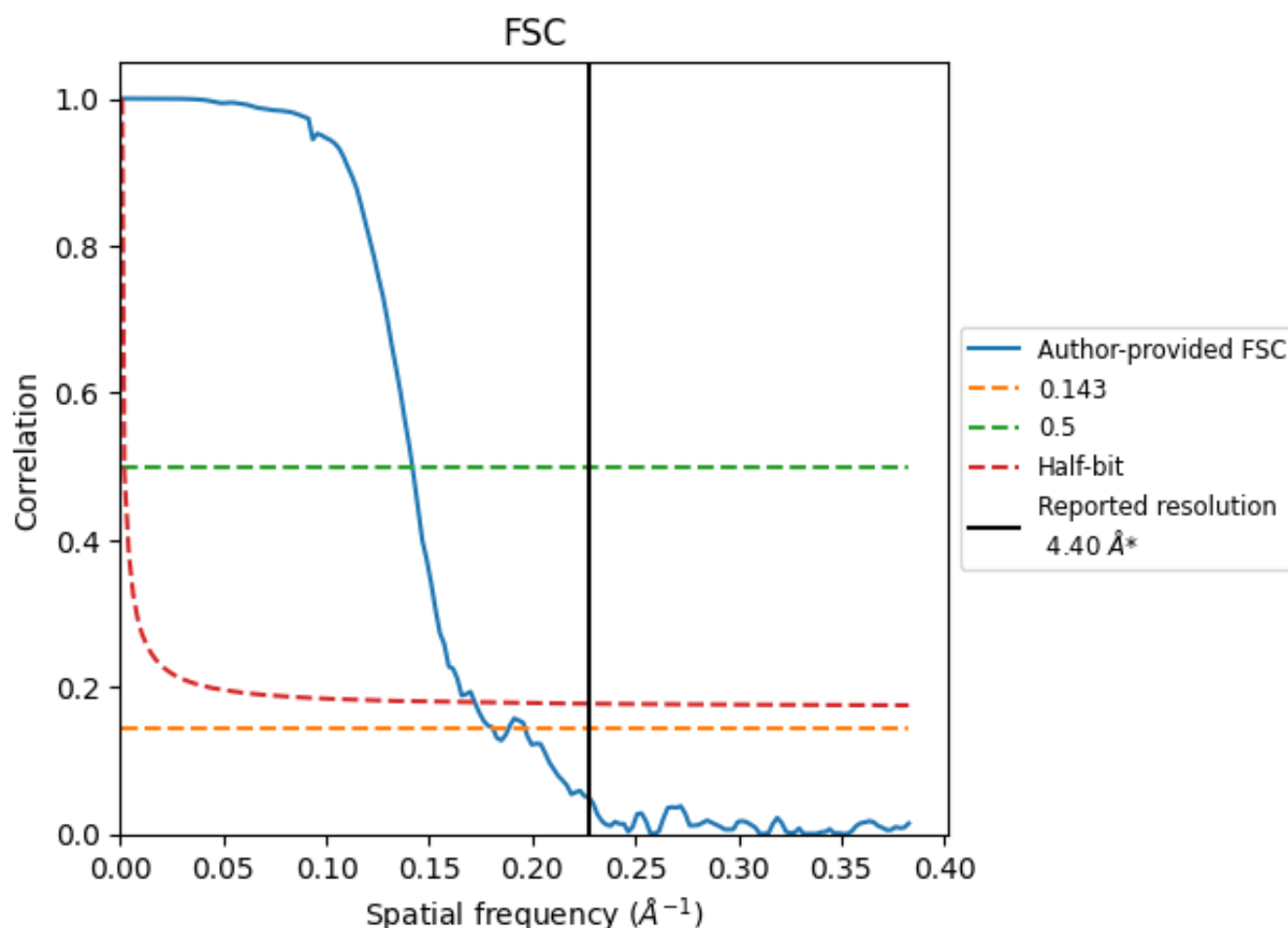


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

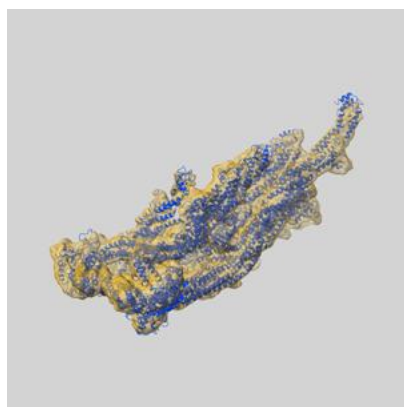
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	5.52	7.05	5.81
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 5.52 differs from the reported value 4.4 by more than 10 %

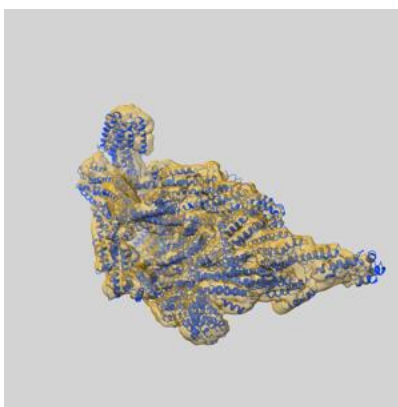
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6827 and PDB model 5YFP. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

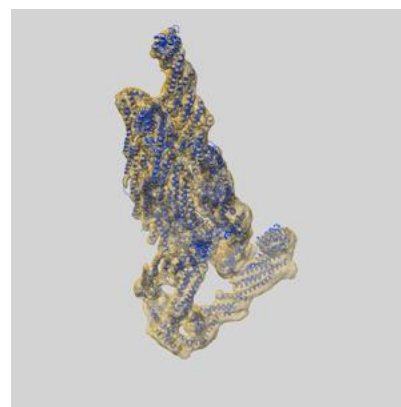
9.1 Map-model overlay [i](#)



X



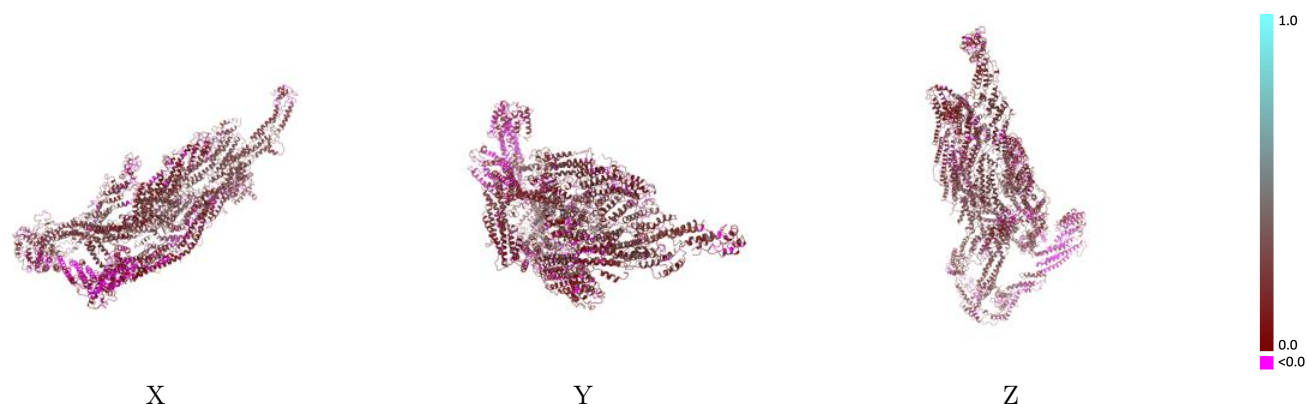
Y



Z

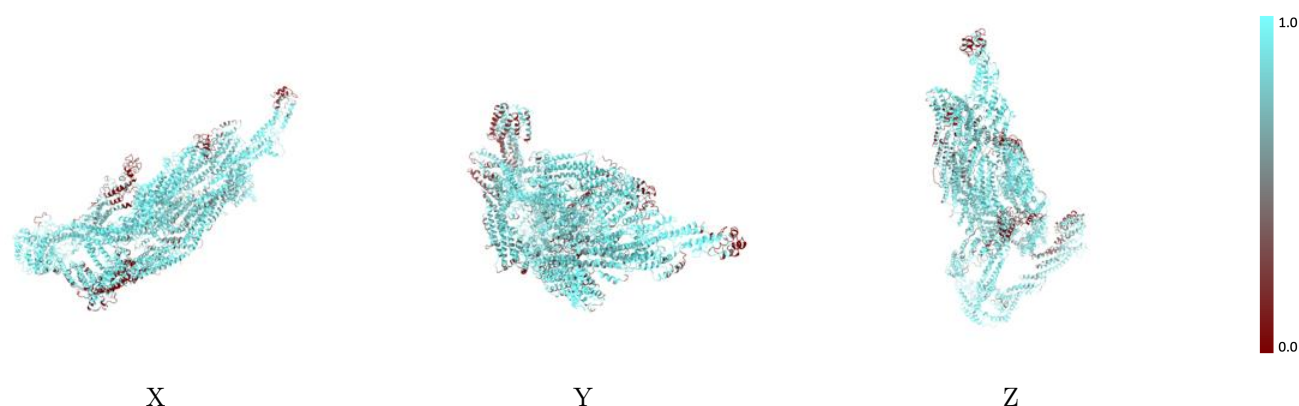
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



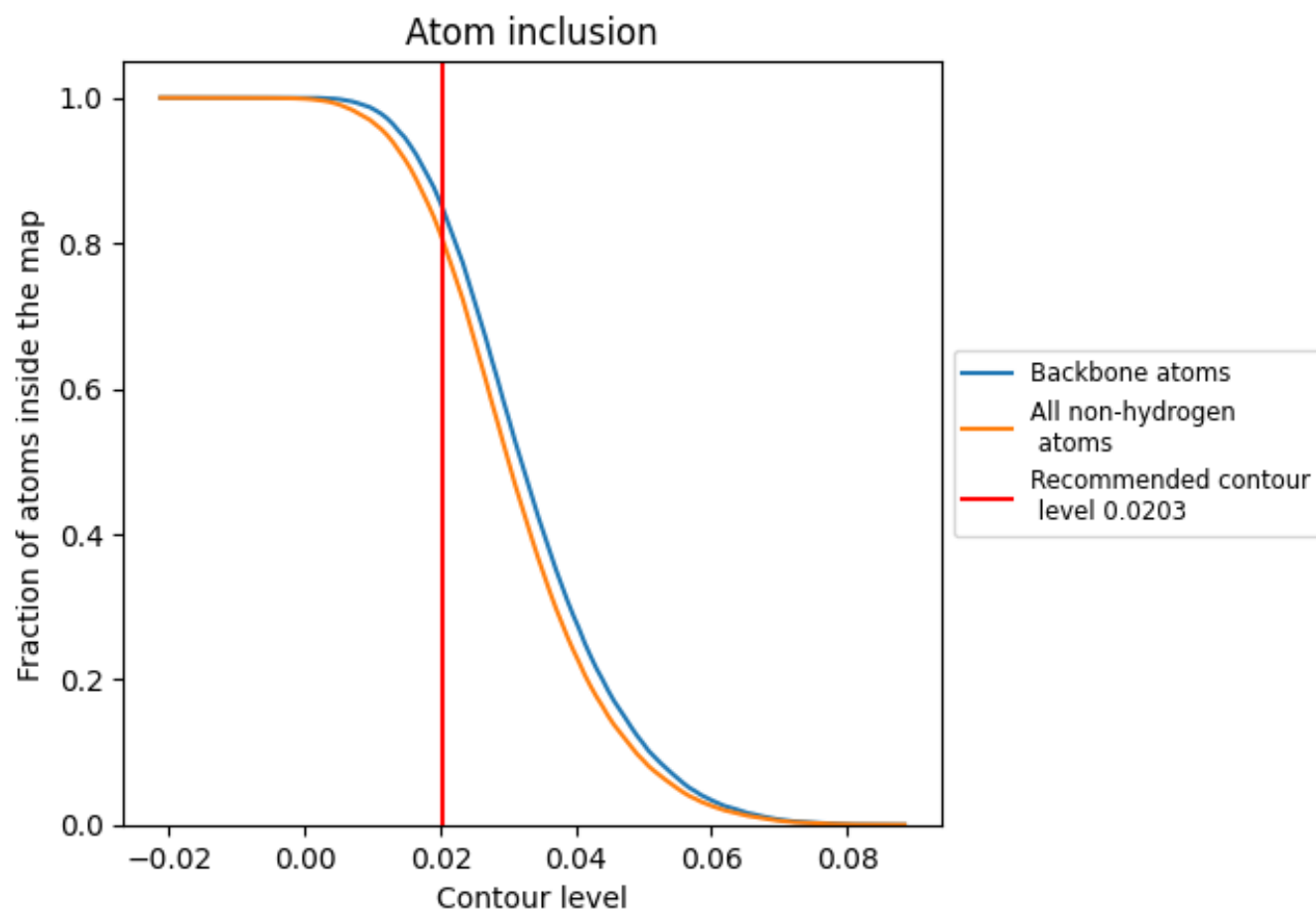
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0203).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8056</div>	<div><div></div>0.1550</div>
A	<div><div></div>0.6810</div>	<div><div></div>0.1830</div>
B	<div><div></div>0.8573</div>	<div><div></div>0.1700</div>
C	<div><div></div>0.7258</div>	<div><div></div>0.0710</div>
D	<div><div></div>0.9124</div>	<div><div></div>0.2150</div>
E	<div><div></div>0.8326</div>	<div><div></div>0.1590</div>
F	<div><div></div>0.8679</div>	<div><div></div>0.2050</div>
G	<div><div></div>0.7476</div>	<div><div></div>0.1070</div>
H	<div><div></div>0.8074</div>	<div><div></div>0.1530</div>

1.0

0.0

<0.0