wwPDB EM Validation Summary Report (i)

Mar 19, 2024 – 04:05 PM 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	:	2A2F, 2B1E, 2D2S, 1ZC4, 2FJI, ?, 5H11

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:

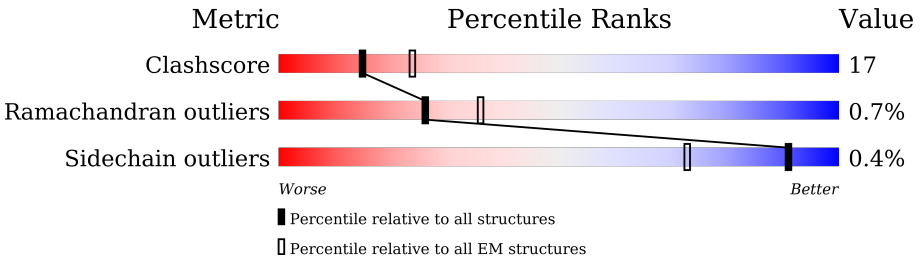
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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 <=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	15% 41% 10% 50%
2	B	971	12% 74% 20% • •
3	C	805	21% 68% 30% •
4	D	1065	5% 70% 18% • 10%
5	E	871	13% 64% 24% 11%
6	F	910	8% 61% 18% • 20%
7	G	623	17% 59% 38% ••
8	H	753	7% 48% 20% • 31%

2 Entry composition (i)

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
			Total	C	N	O		
1	A	672	3345	2001	672	672	0	0

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

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

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

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

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

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

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

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

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

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

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

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

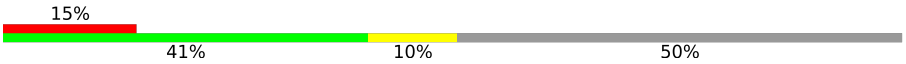
- Molecule 8 is a protein called Exocyst complex component EXO84.

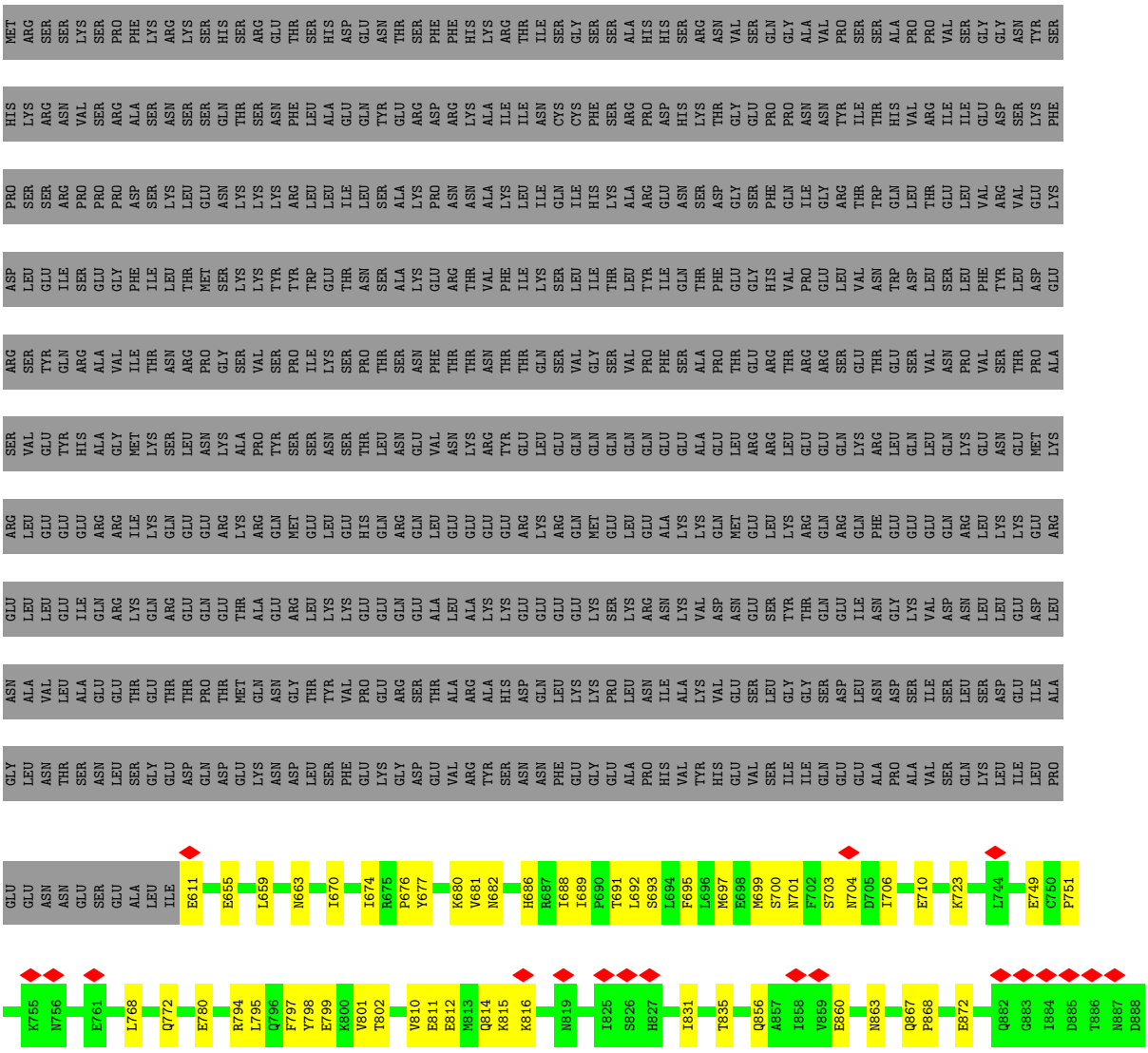
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	518	3240	2002	591	643	4	0	0

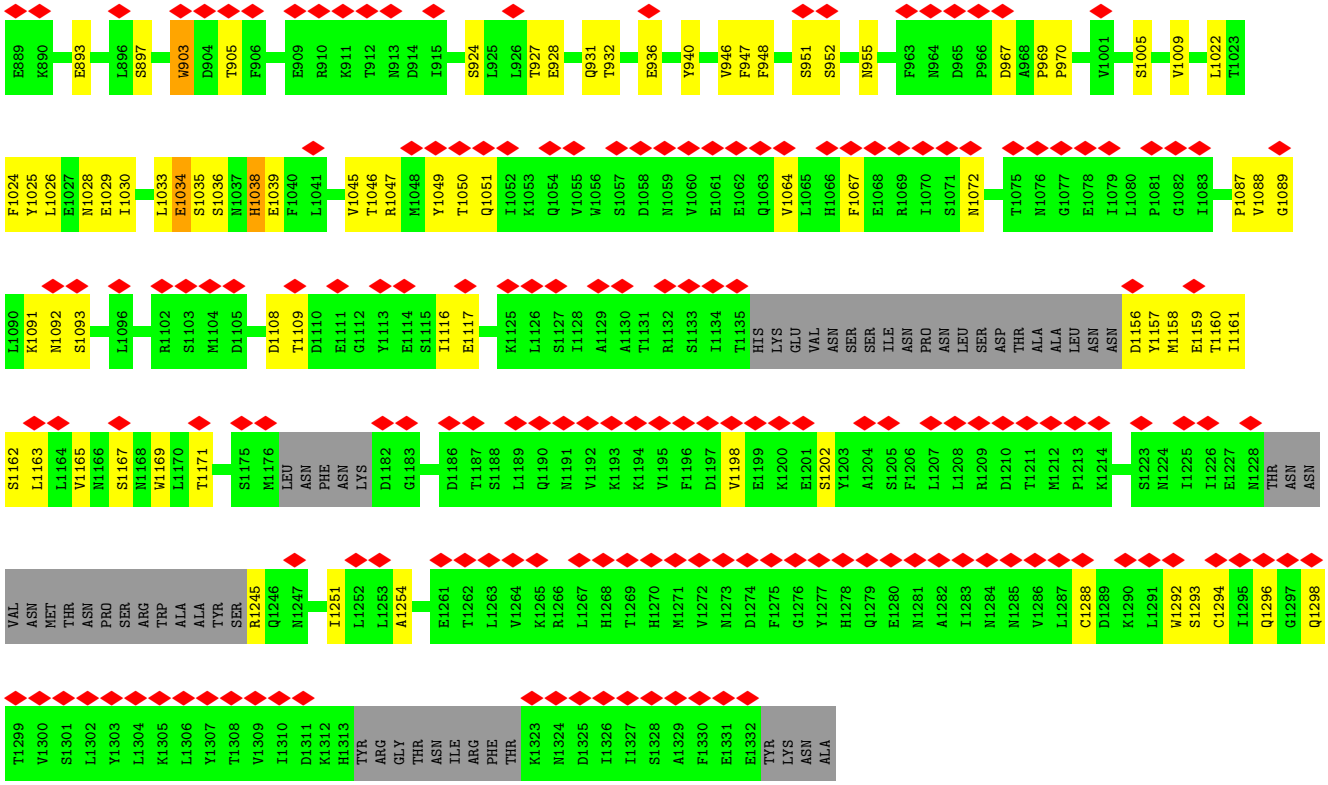
3 Residue-property plots (i)

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: Exocyst complex component SEC3

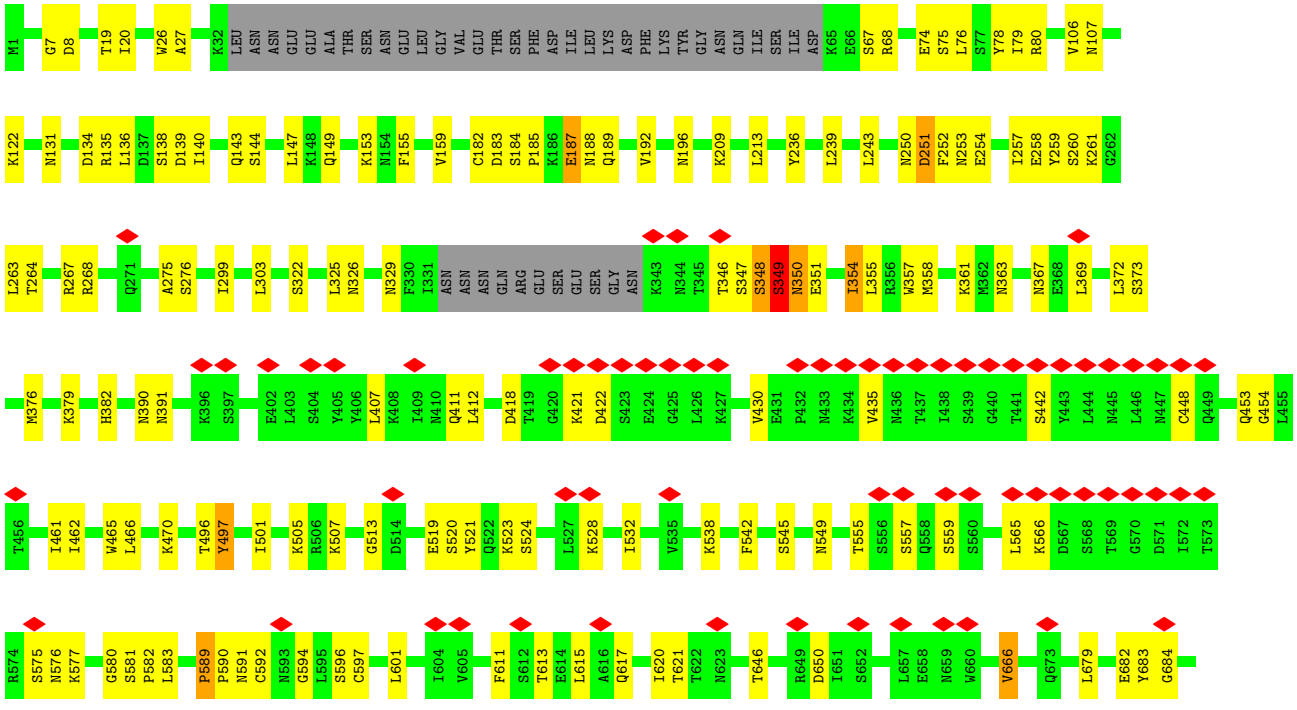
Chain A: 

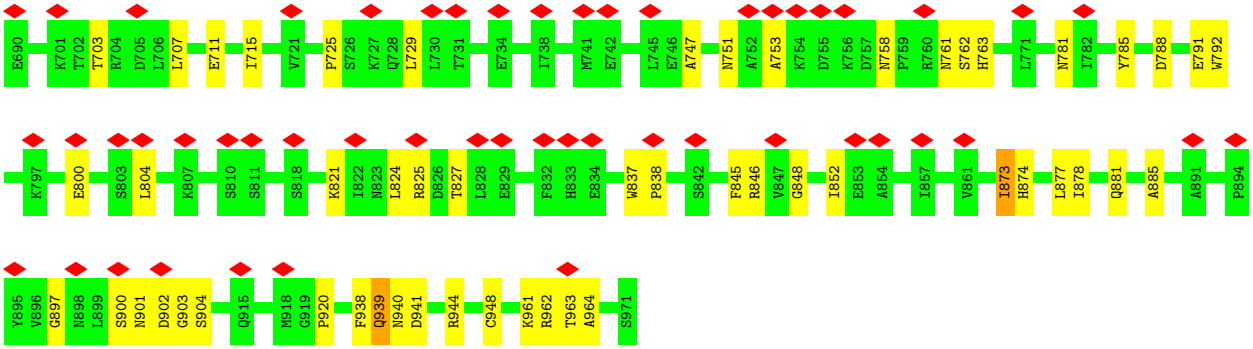




- Molecule 2: Exocyst complex component SEC5

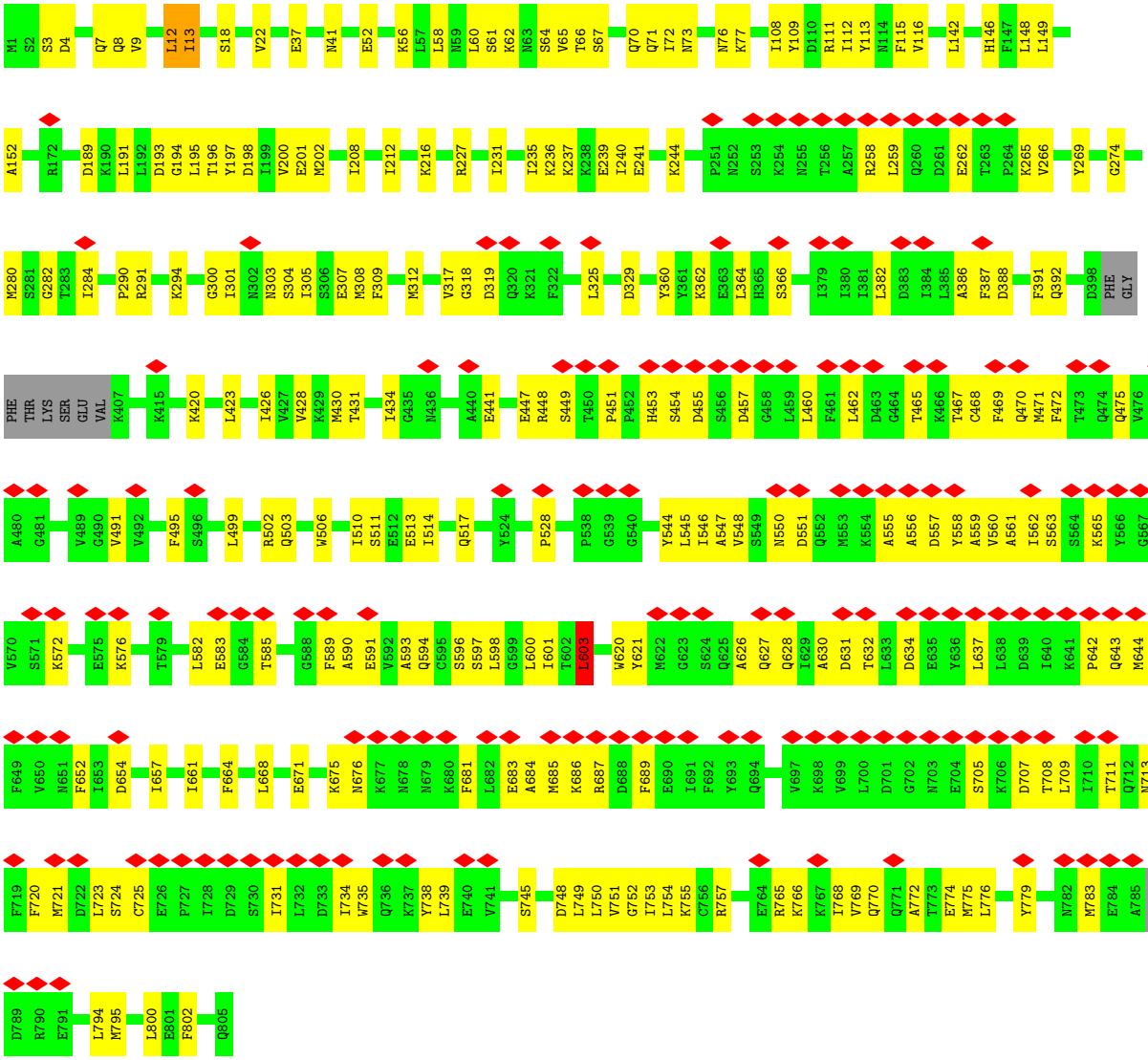
Chain B:





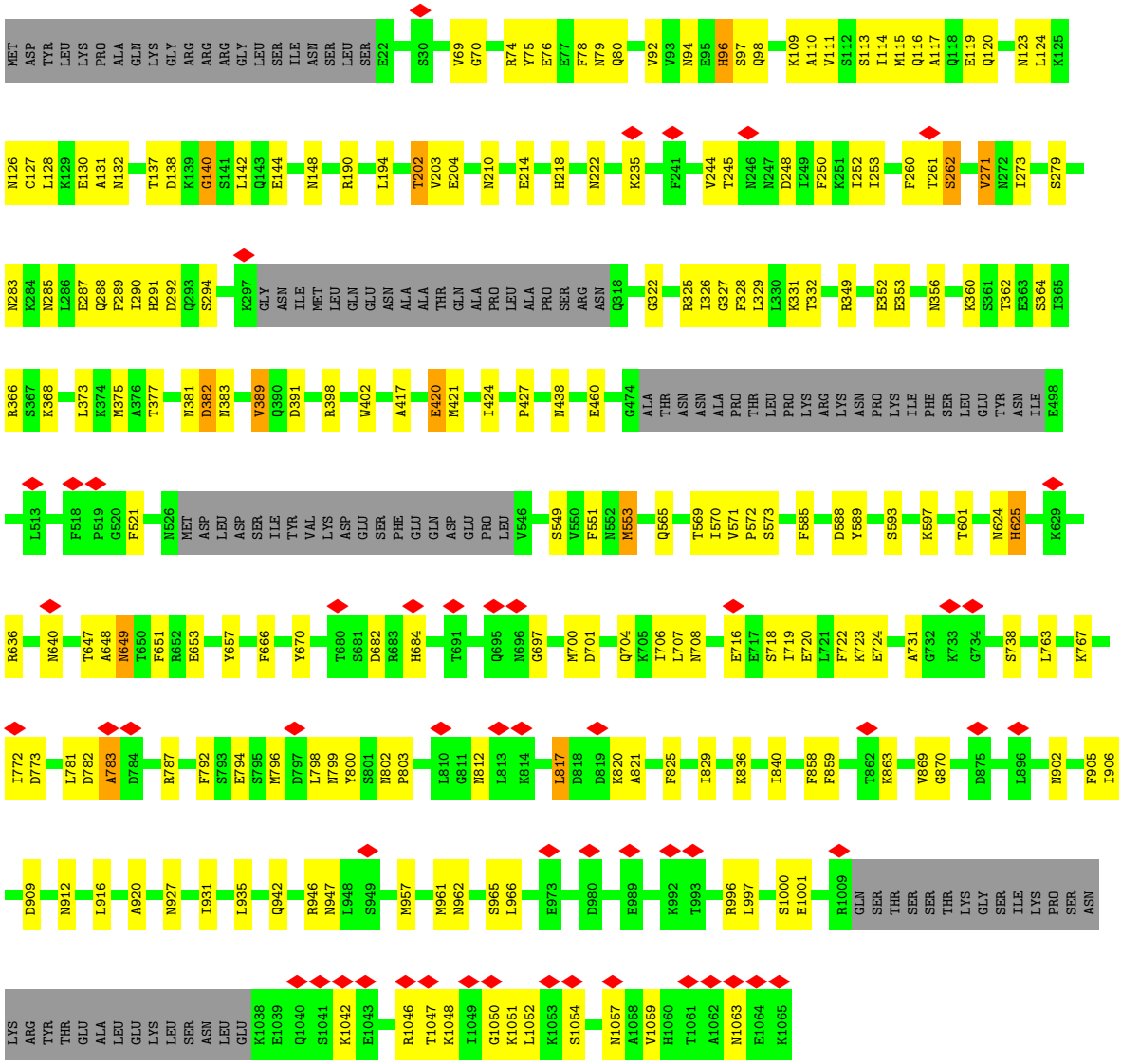
• Molecule 3: Exocyst complex component SEC6

Chain C:



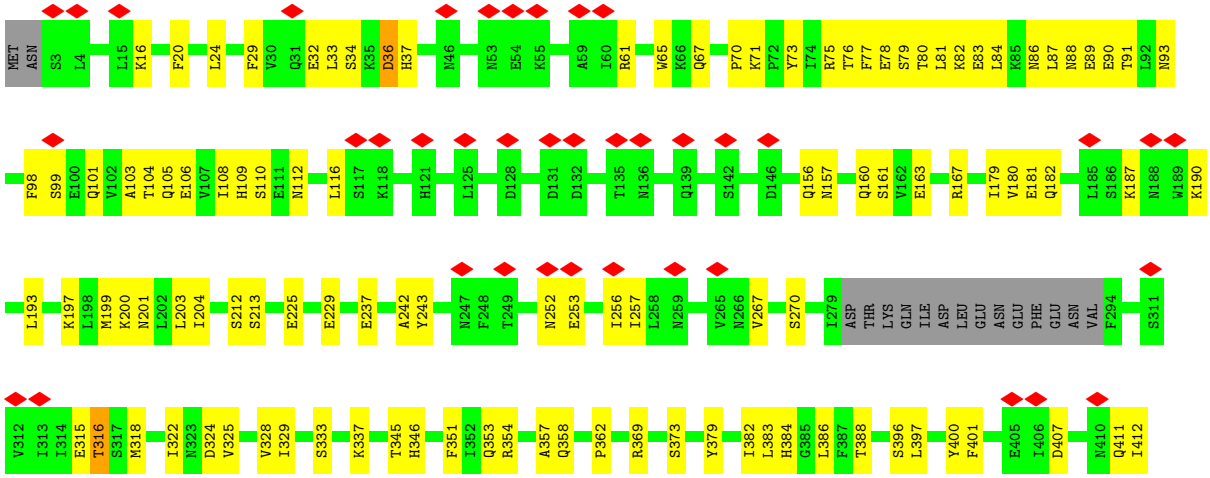
• Molecule 4: Exocyst complex component SEC8

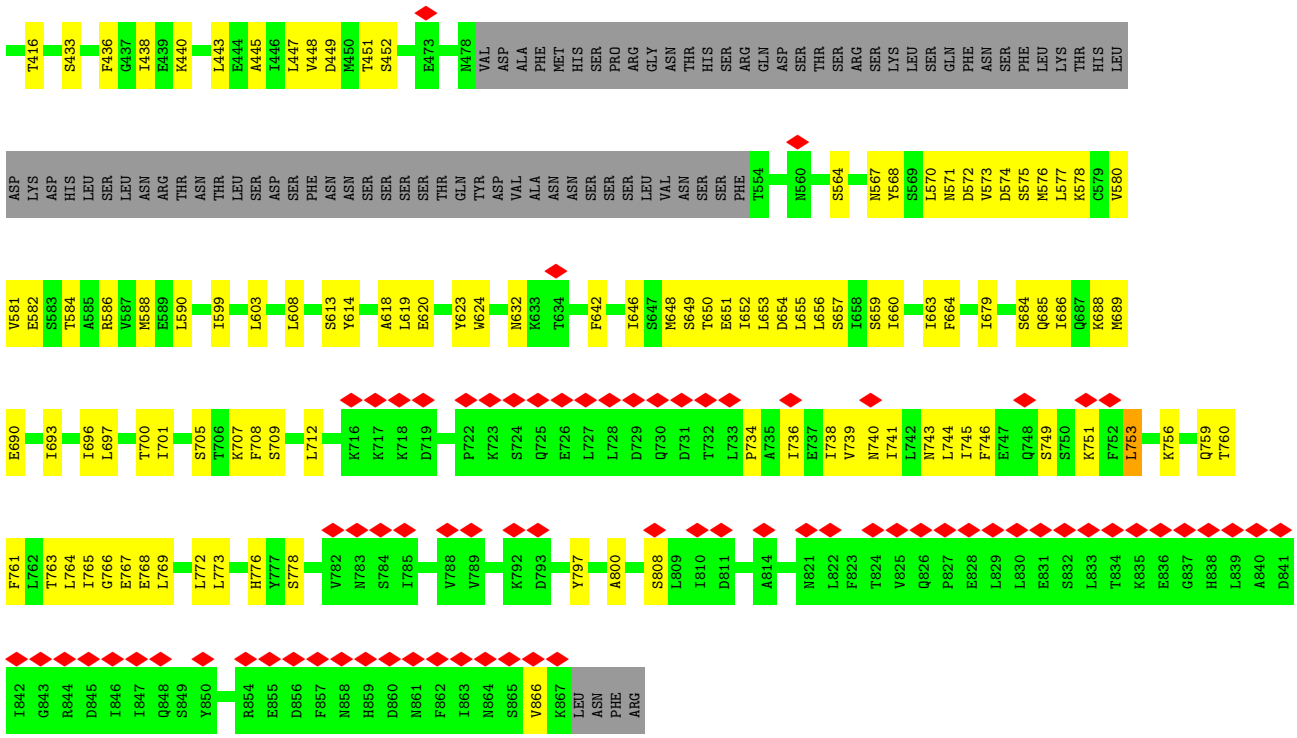
Chain D:



• Molecule 5: Exocyst complex component SEC10

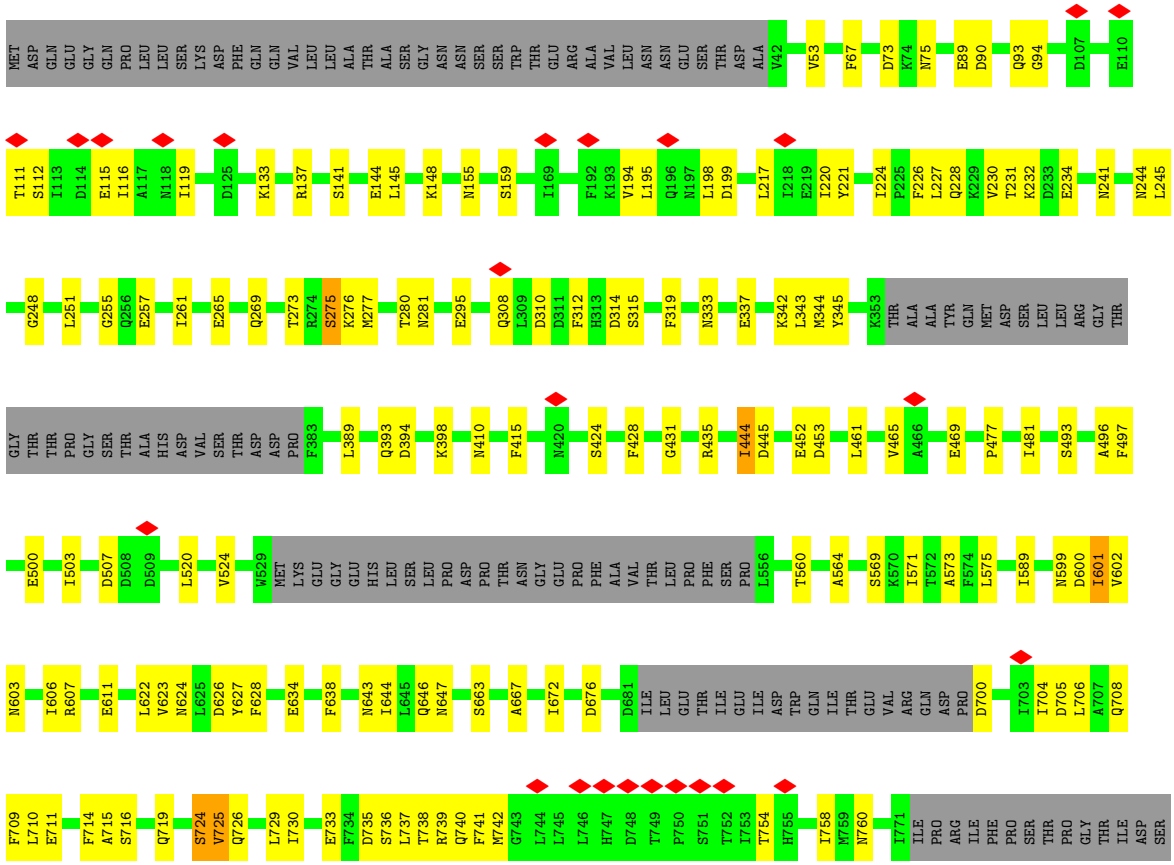
Chain E:

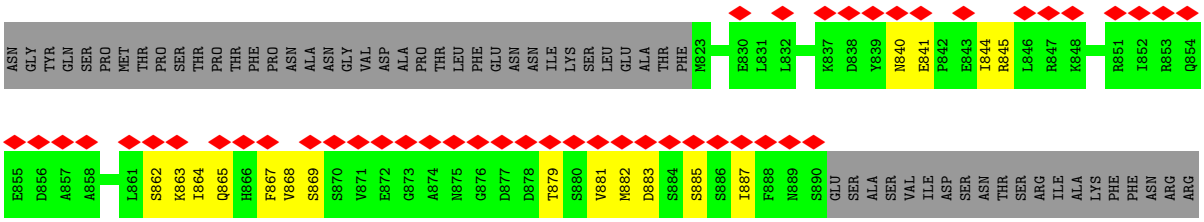




- Molecule 6: Exocyst complex component SEC15

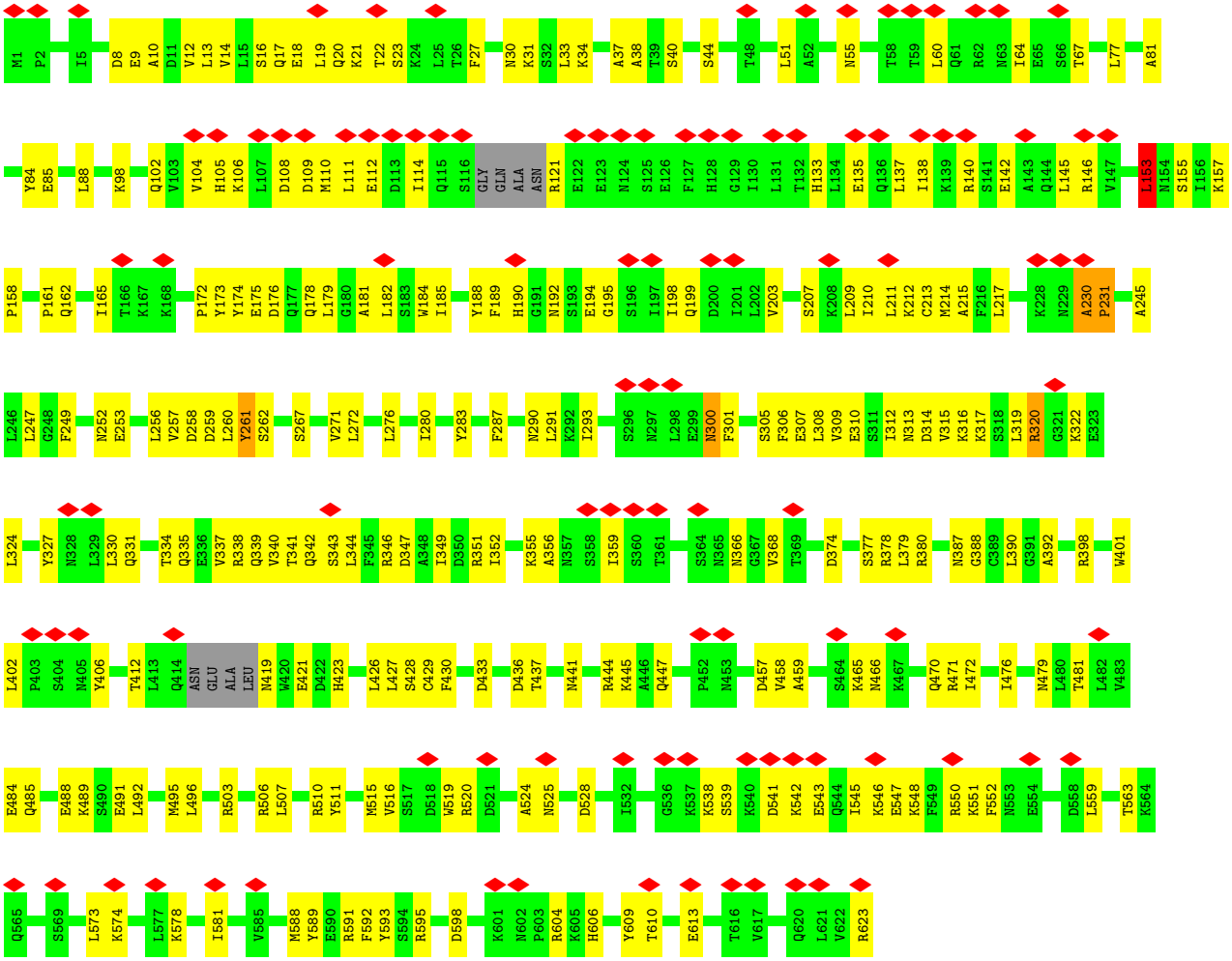
Chain F:





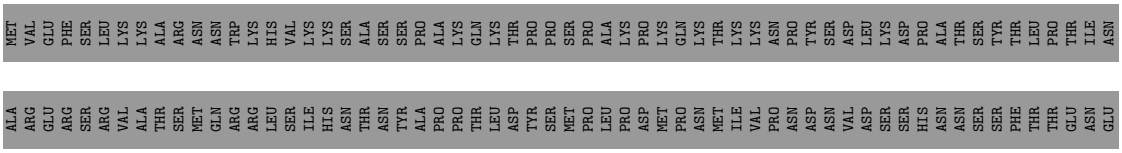
• Molecule 7: Exocyst complex component EXO70

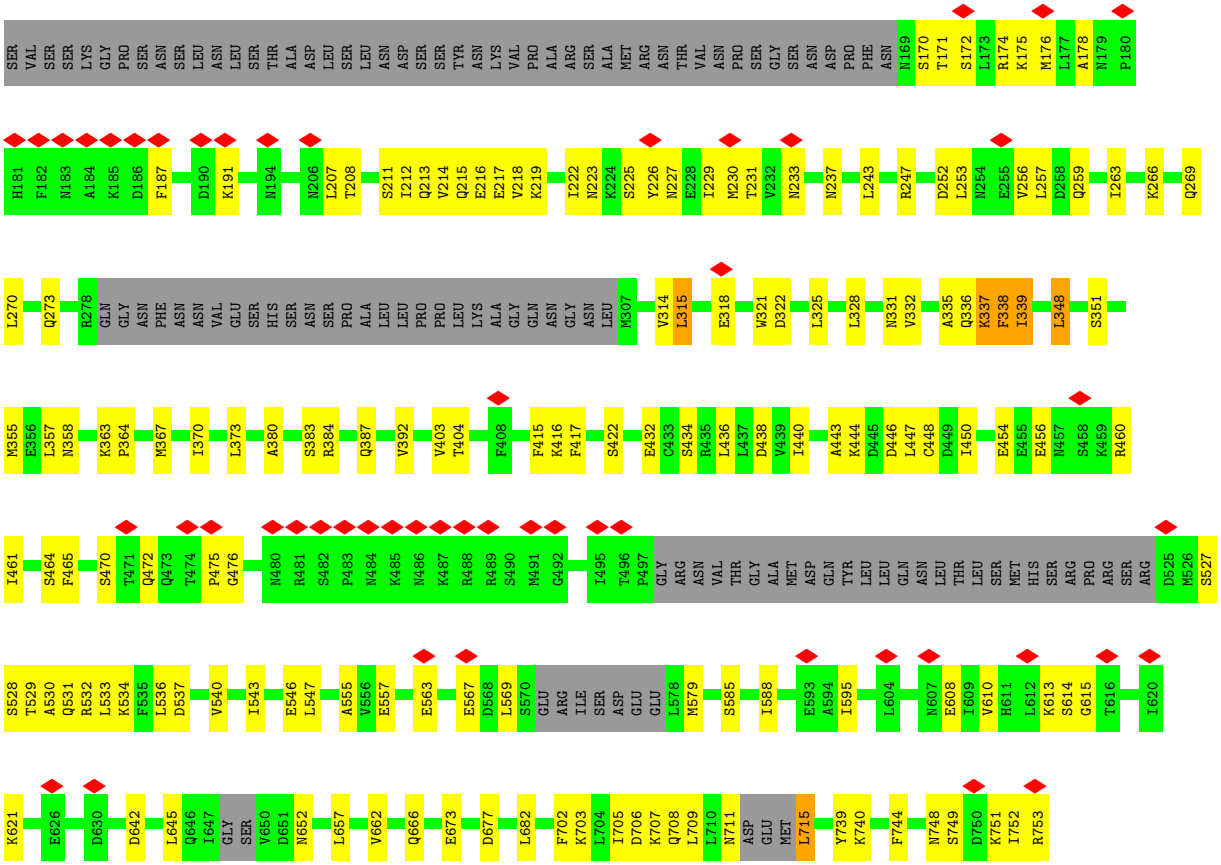
Chain G:



• Molecule 8: Exocyst complex component EXO84

Chain H:




SER VAL SER SER LYS GLY PRO SER ASN SER LEU ASN LEU SER THR ALA ASP LEU SER LEU ASN ASP SER SER TYR ASN LYS VAL PRO ALA ARG SER ALA MET ARG ASN THR VAL ASN PRO SER GLY SER ASN ASP PRO PHE ASN N169 S170 T171 S172 L173 R174 K175 M176 L177 A178 N179 P180
H181 F182 N183 A184 K185 D186 F187 D190 K191 N194 N206 L207 T208 S211 I212 Q213 V214 Q215 E216 E217 V218 K219 I222 N223 K224 S225 Y226 N227 E228 I229 M230 T231 V232 N233 N237 L243 R247 D252 L253 N254 E255 V256 L257 D258 Q259 I263 K266 Q269
L270 Q273 R278 GLN GLY ASN PHE ASN ASN VAL GLU SER HIS SER ASN SER PRO ALA LEU LEU PRO PRO LEU LYS ALA GLY GLN ASN GLY ASN LEU M307 V314 L315 E318 W321 D322 L325 L328 N331 V332 A335 Q336 K337 F338 I339 L348 S351
M355 E356 L357 N358 K363 P364 M367 I370 L373 A380 S383 R384 Q387 V392 V403 T404 F408 F415 K416 F417 S422 E432 C433 S434 R435 L436 L437 D438 V439 I440 A443 K444 D445 D446 L447 C448 D449 I450 E454 E455 E456 N457 S458 K459 R460
I461 S464 F465 S470 T471 Q472 Q473 T474 P475 G476 N480 R481 S482 P483 N484 K485 N486 K487 R488 R489 S490 M491 G492 I495 T496 P497 GLY ARG ASN VAL THR GLY ALA MET ASP GLN TYR LEU LEU LEU GLN ASN LEU THR LEU SER MET HIS SER ARG PRO ARG SER ARG D525 M526 S527
S528 T529 A530 Q531 R532 L533 K534 F535 L536 D537 V540 I543 E546 L547 A555 V556 E557 E563 E567 D568 L569 S570 GLU ARG ILE SER ASP GLU GLU L578 M579 S585 I588 E593 A594 I595 L604 N607 E608 I609 V610 H611 L612 K613 S614 G615 T616 I620
K621 E626 D630 D642 L645 Q646 I647 GLY SER V650 D651 N652 L657 V662 Q666 E673 D677 L682 F702 K703 L704 I705 D706 K707 Q708 L709 L710 N711 ASP GLU MET L715 Y739 K740 F744 N748 S749 D750 K751 I752 R753

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	470.3544, 470.3544, 470.3544	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.28	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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

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 (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	
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 (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)

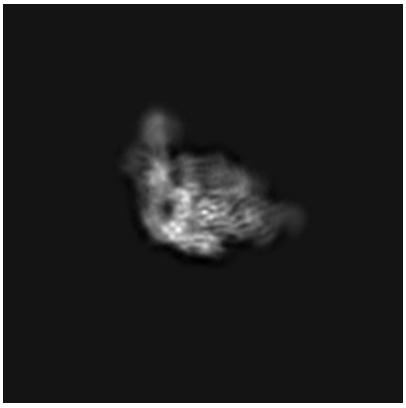
This section contains visualisations of the EMDB entry EMD-6827. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

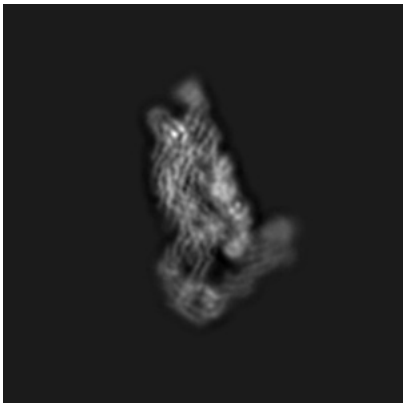
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y



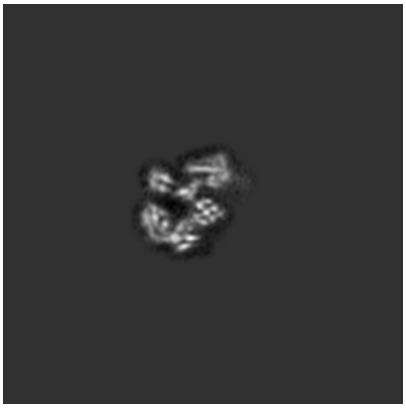
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 180



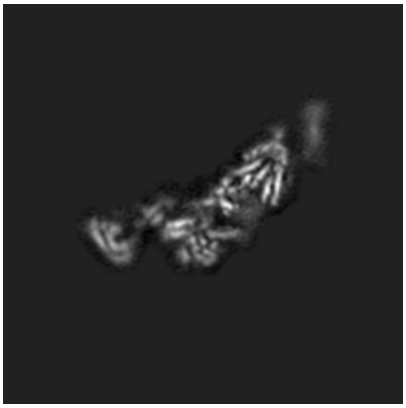
Y Index: 180

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

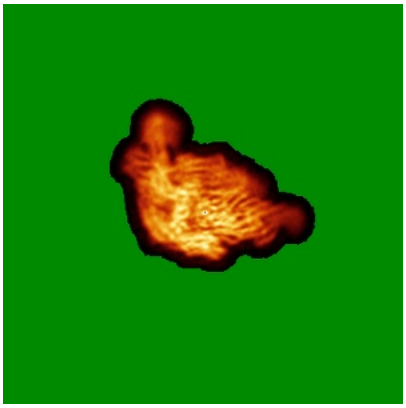
Z Index: 163

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

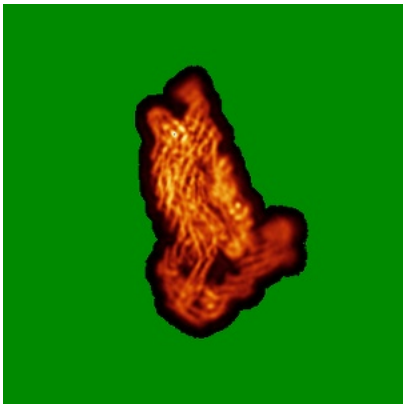
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

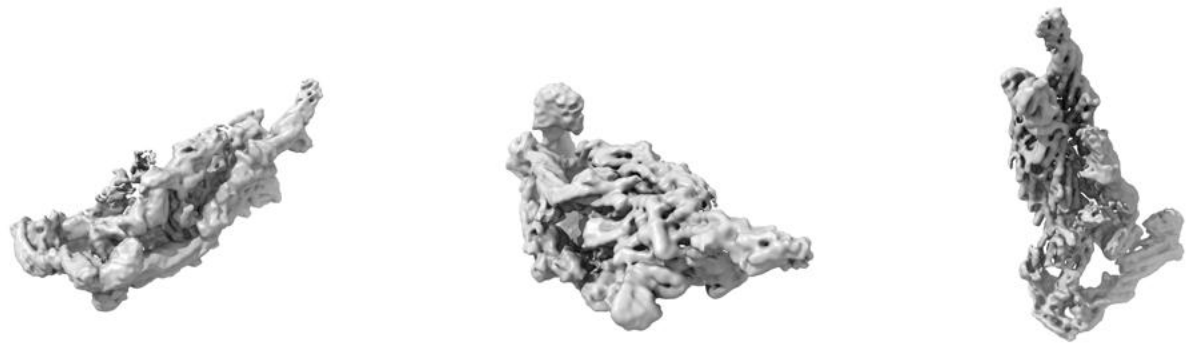


Z

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

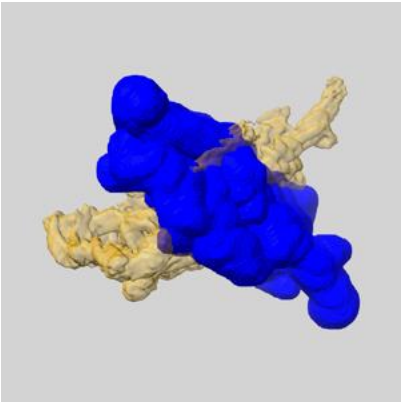
6.6 Mask visualisation (i)

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

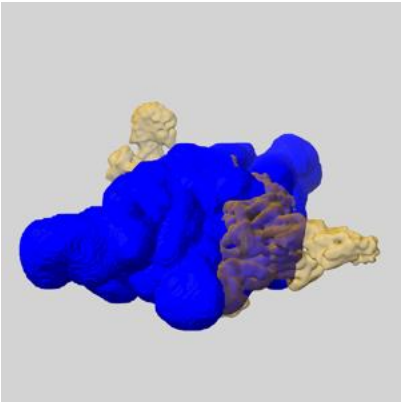
A mask typically either:

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

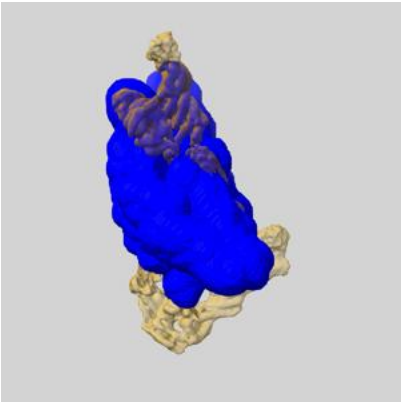
6.6.1 emd_6827_msk_5.map (i)



X

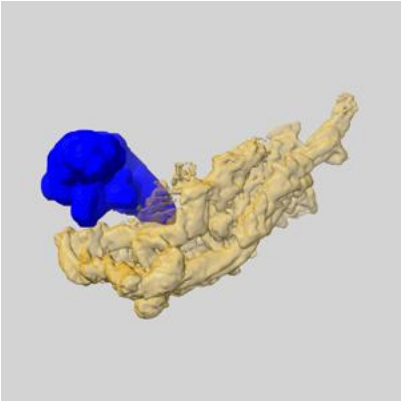


Y

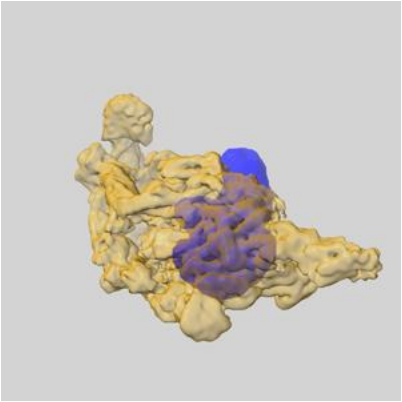


Z

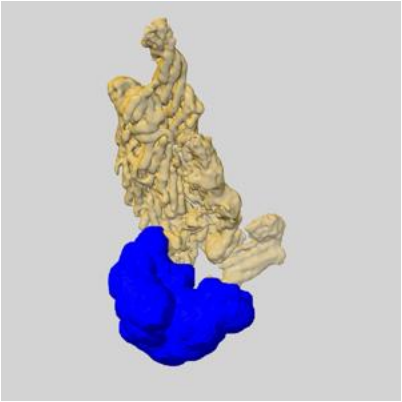
6.6.2 emd_6827_msk_4.map (i)



X

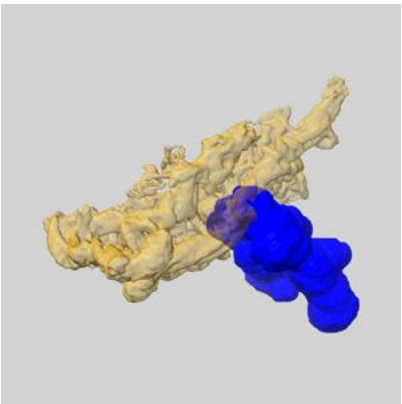


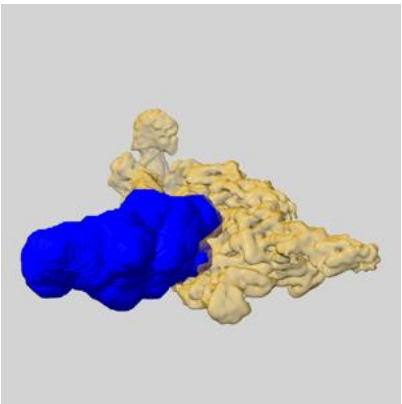
Y

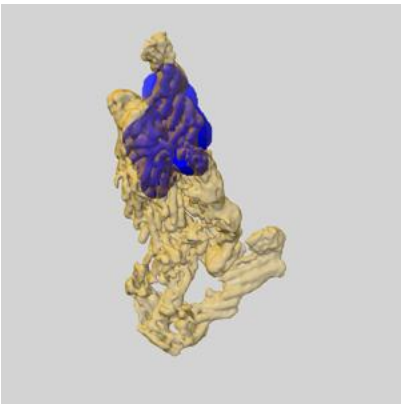


Z

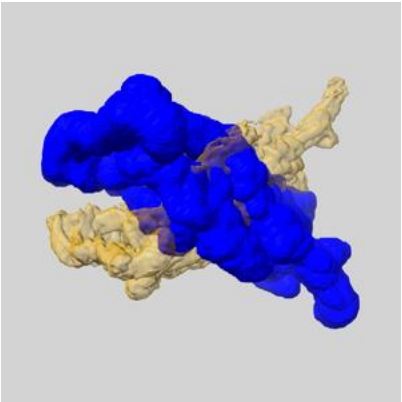
6.6.3 emd_6827_msk_3.map

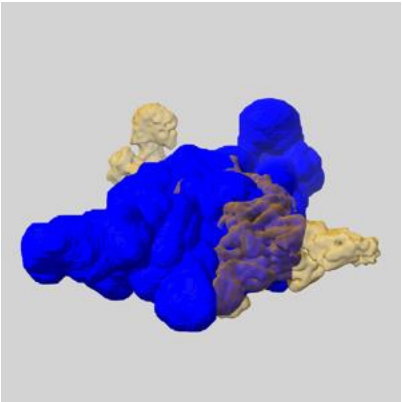

X

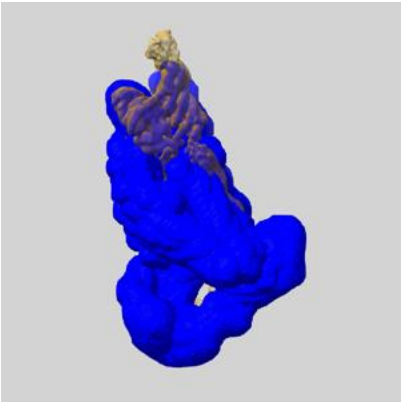

Y


Z

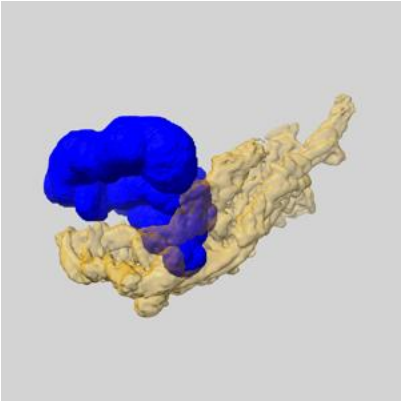
6.6.4 emd_6827_msk_2.map

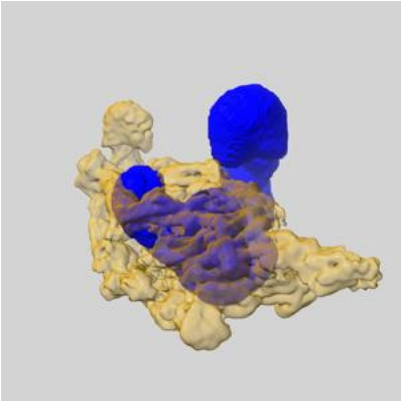

X

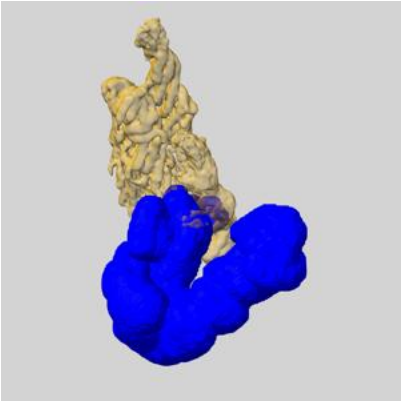

Y


Z

6.6.5 emd_6827_msk_1.map


X

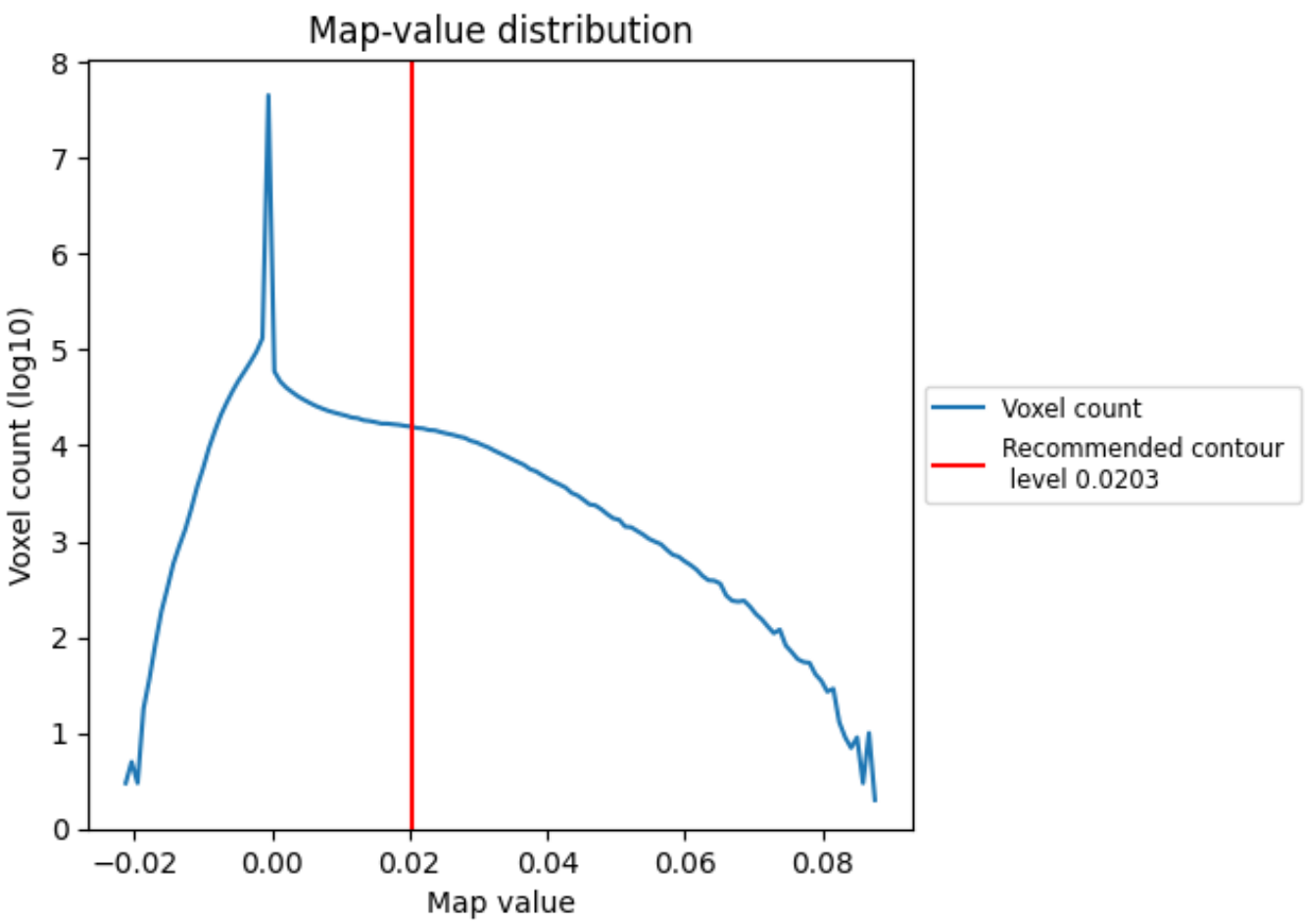

Y


Z

7 Map analysis (i)

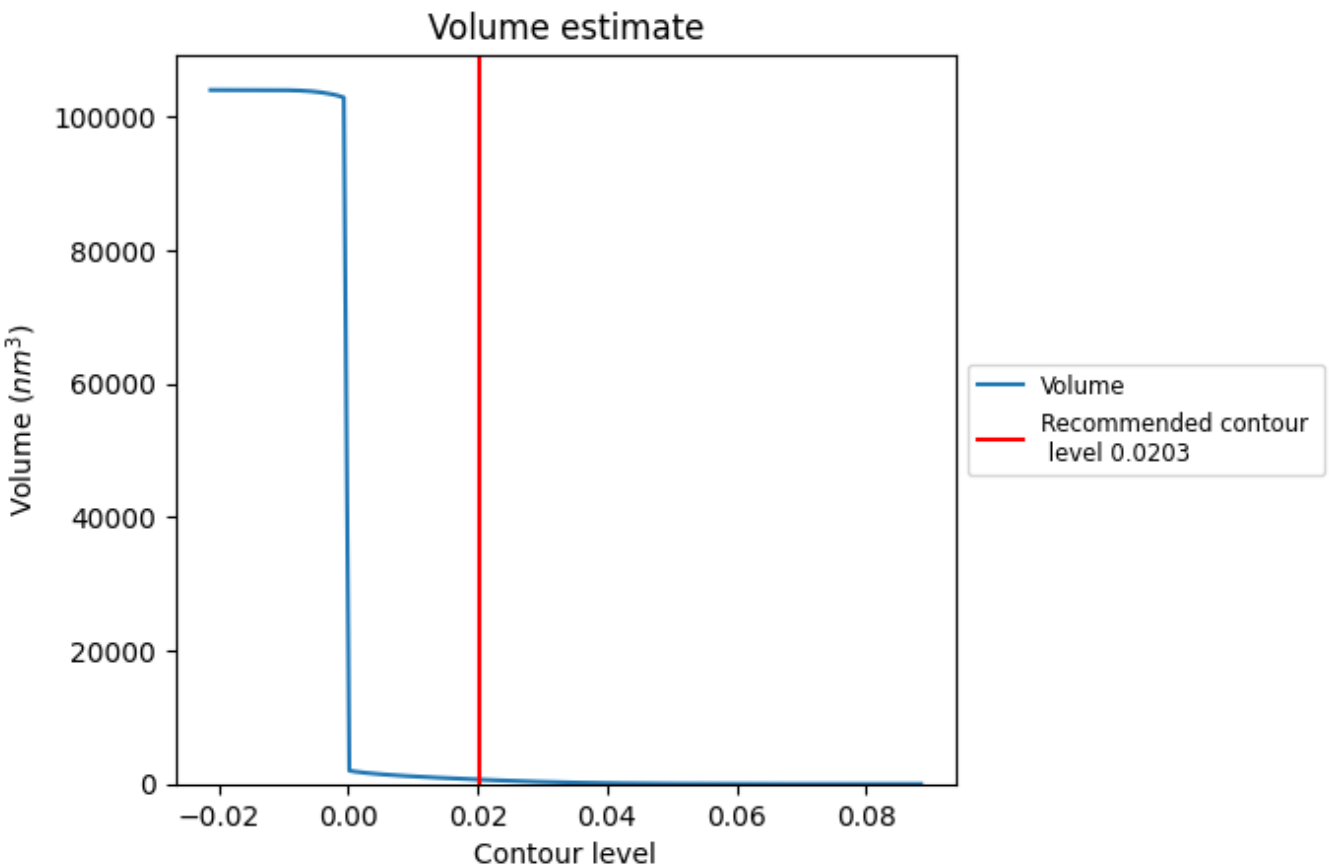
This section contains the results of statistical analysis of the map.

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.

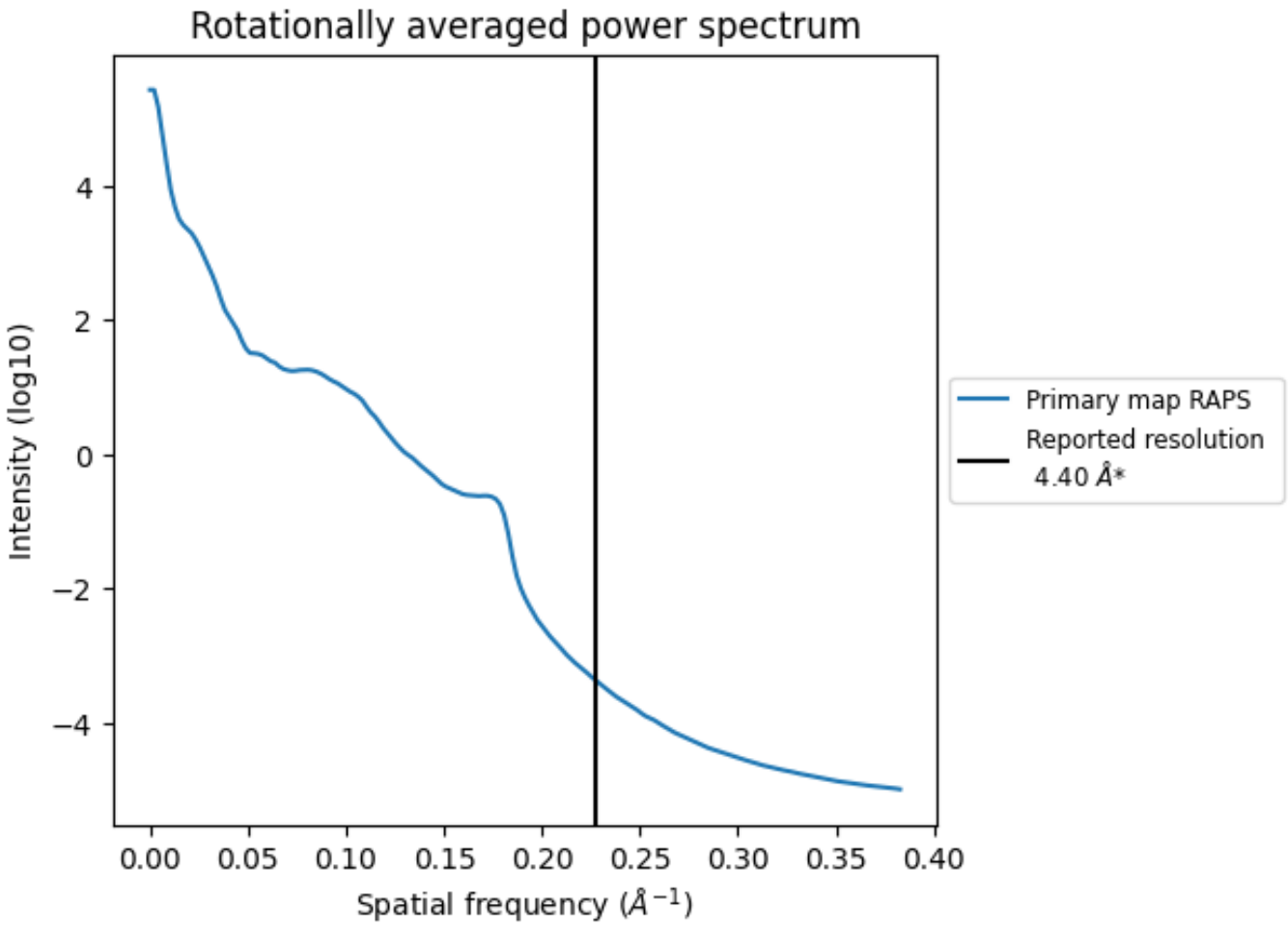
7.2 Volume estimate (i)



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 (i)

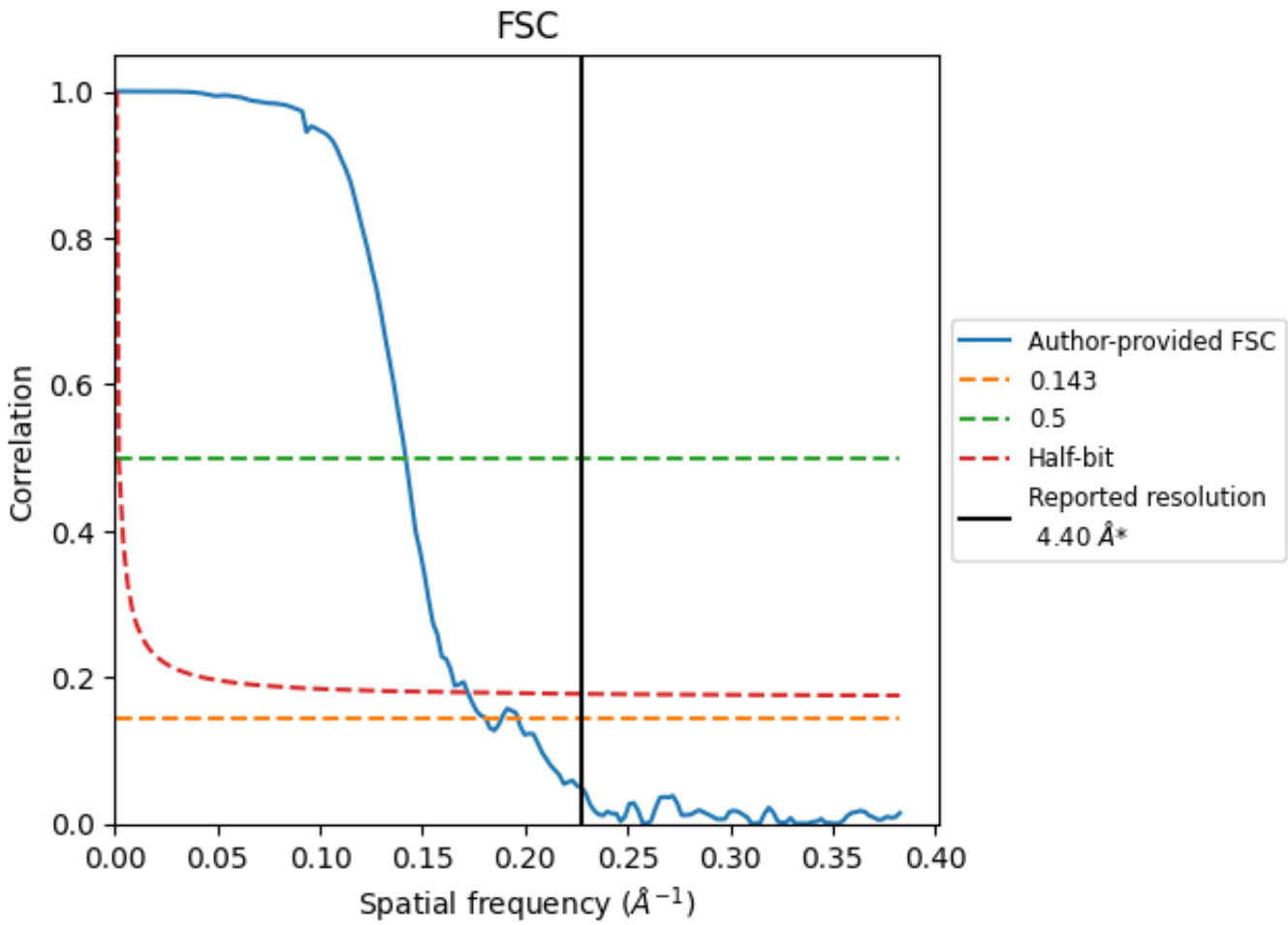


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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)

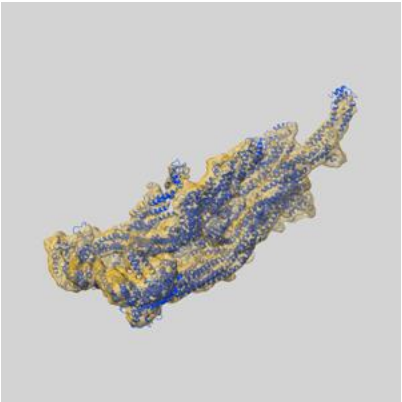
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	5.52	7.05	5.81
Unmasked-calculated*	-	-	-

*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 %

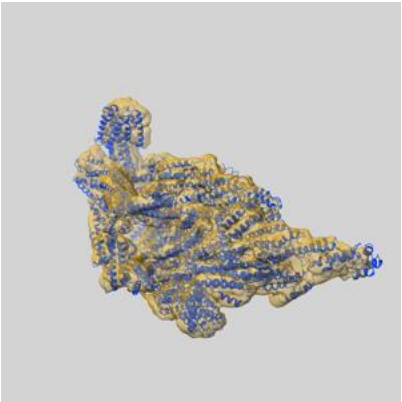
9 Map-model fit (i)

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.

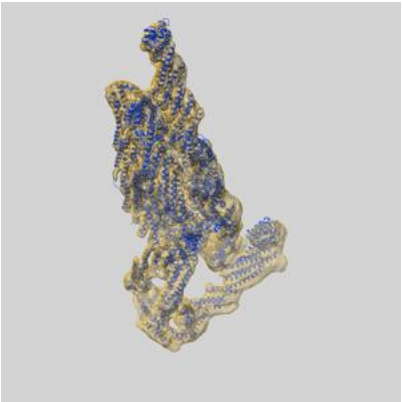
9.1 Map-model overlay (i)



X



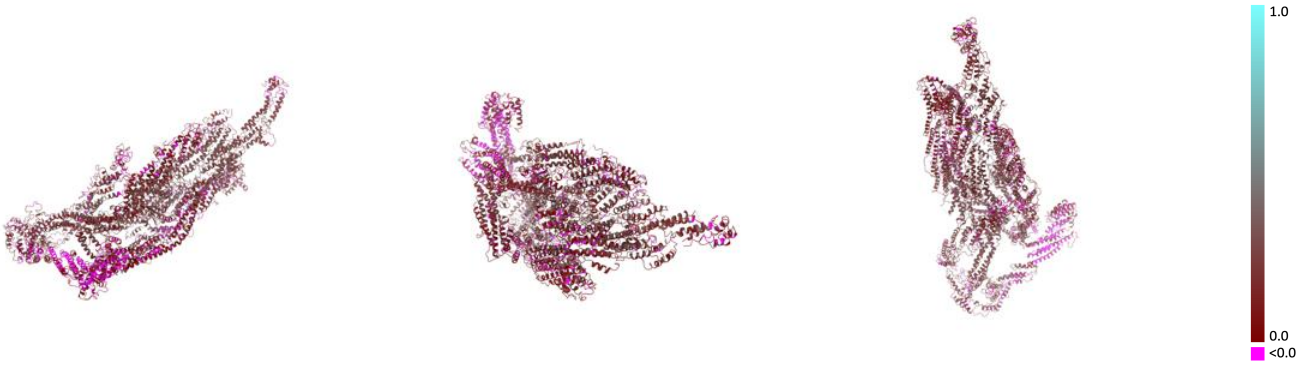
Y



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.

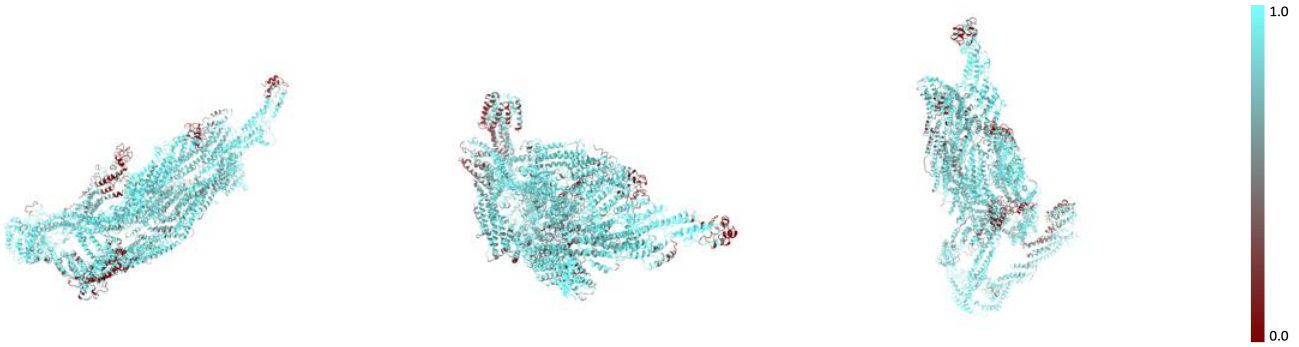
9.2 Q-score mapped to coordinate model (i)



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.

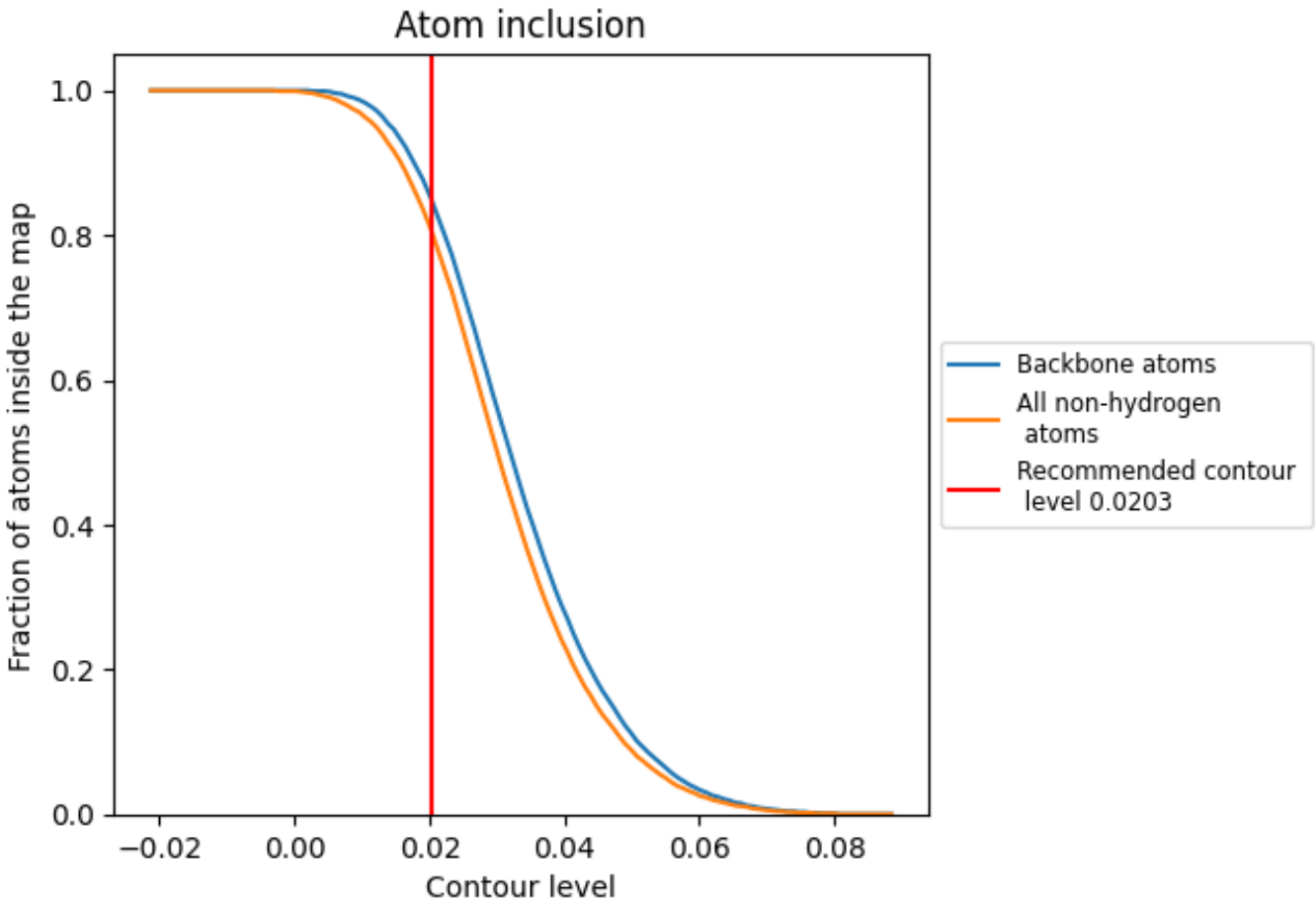
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0203).

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 (i)

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	0.8060	0.1550
A	0.6810	0.1830
B	0.8570	0.1700
C	0.7260	0.0710
D	0.9120	0.2150
E	0.8330	0.1590
F	0.8680	0.2050
G	0.7480	0.1070
H	0.8070	0.1530