



## wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 09:13 PM EST

PDB ID : 6VKL  
EMDB ID : EMD-21226  
Title : Negative stain reconstruction of the yeast exocyst octameric complex.  
Authors : Frost, A.; Munson, M.  
Deposited on : 2020-01-21  
Resolution : 4.40 Å(reported)  
Based on initial model : 5YFP

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

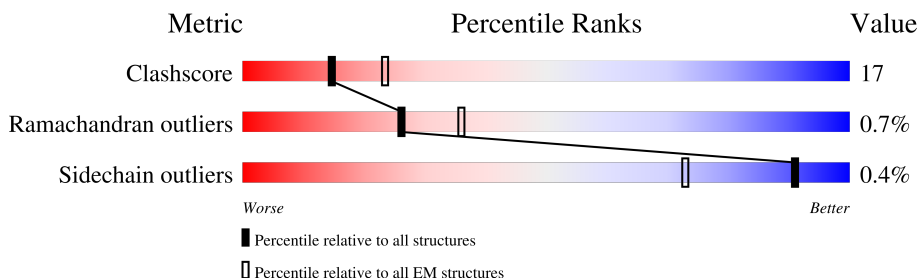
# 1 Overall quality at a glance

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  $\geq 3$ , 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		

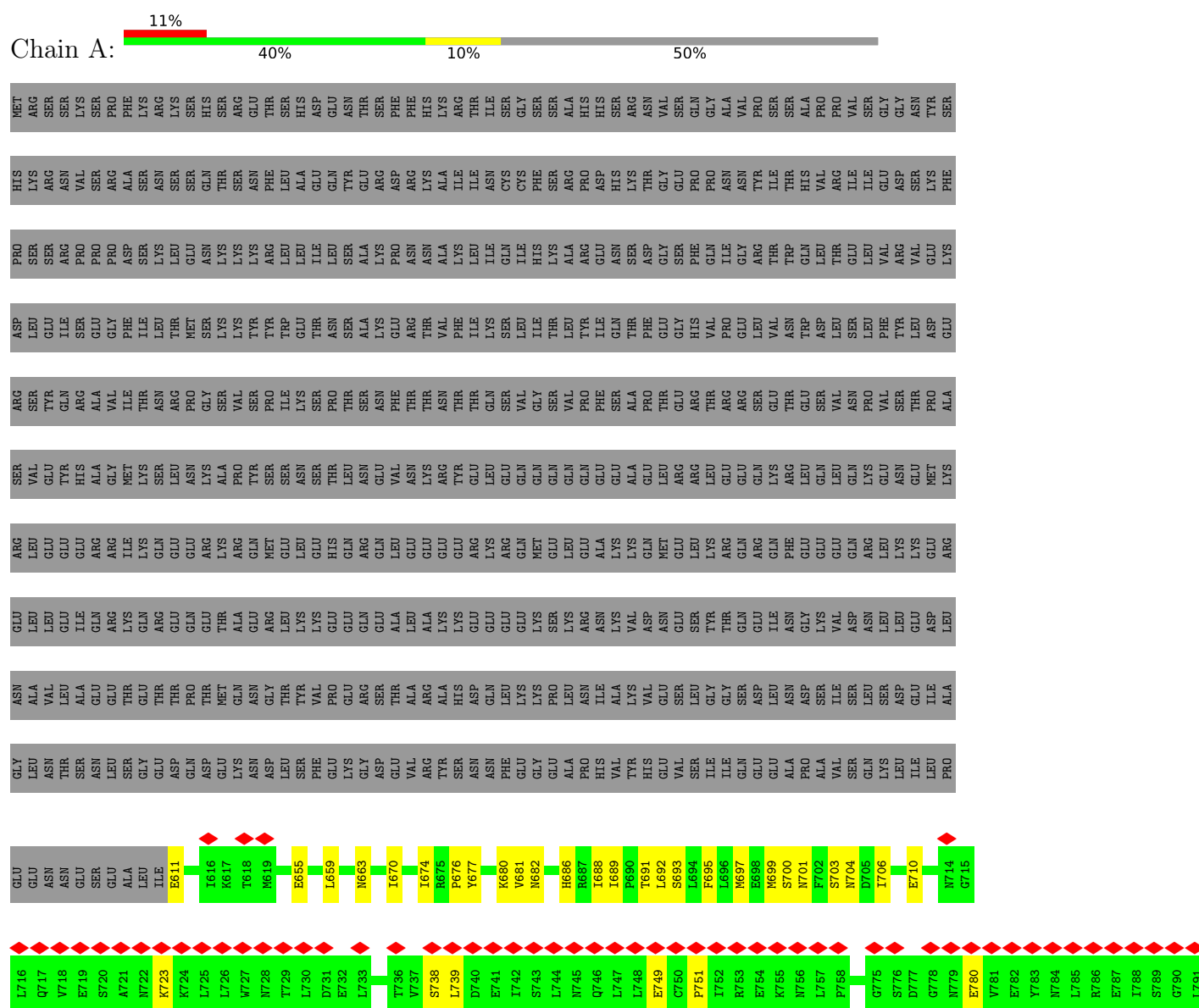
- Molecule 8 is a protein called Exocyst complex component EXO84.

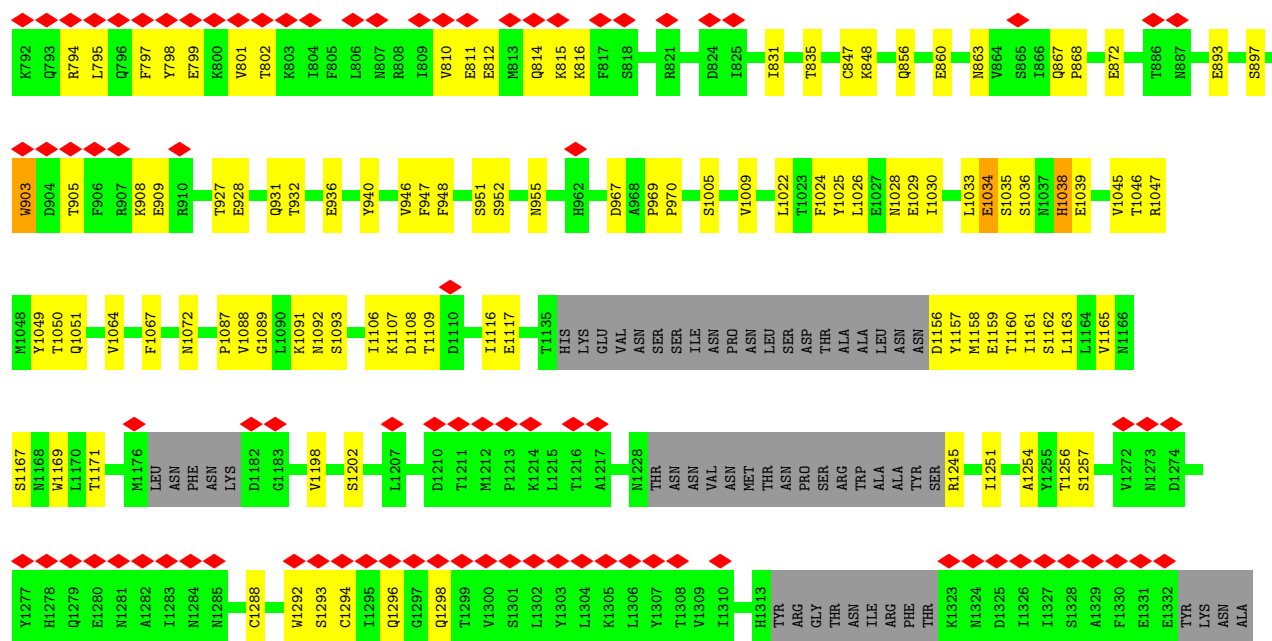
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	518	Total	C	N	O	S	0	0
			3240	2002	591	643	4		

### 3 Residue-property plots

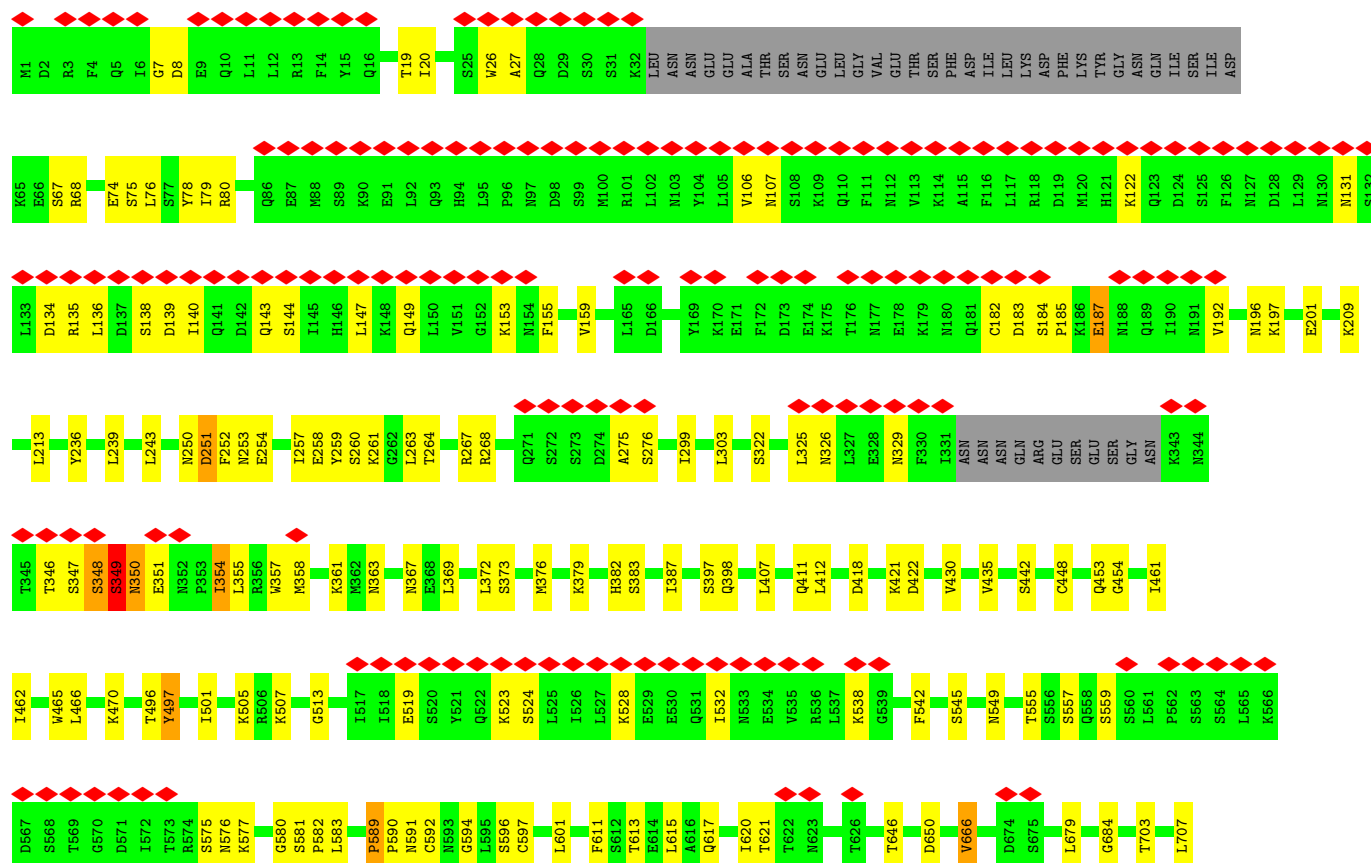
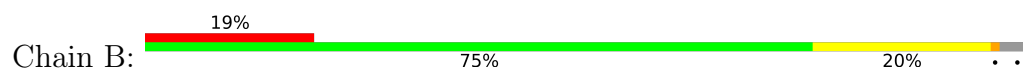
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

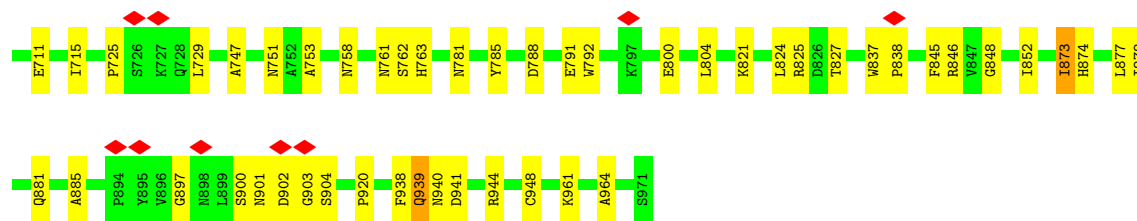
#### • Molecule 1: Exocyst complex component SEC3



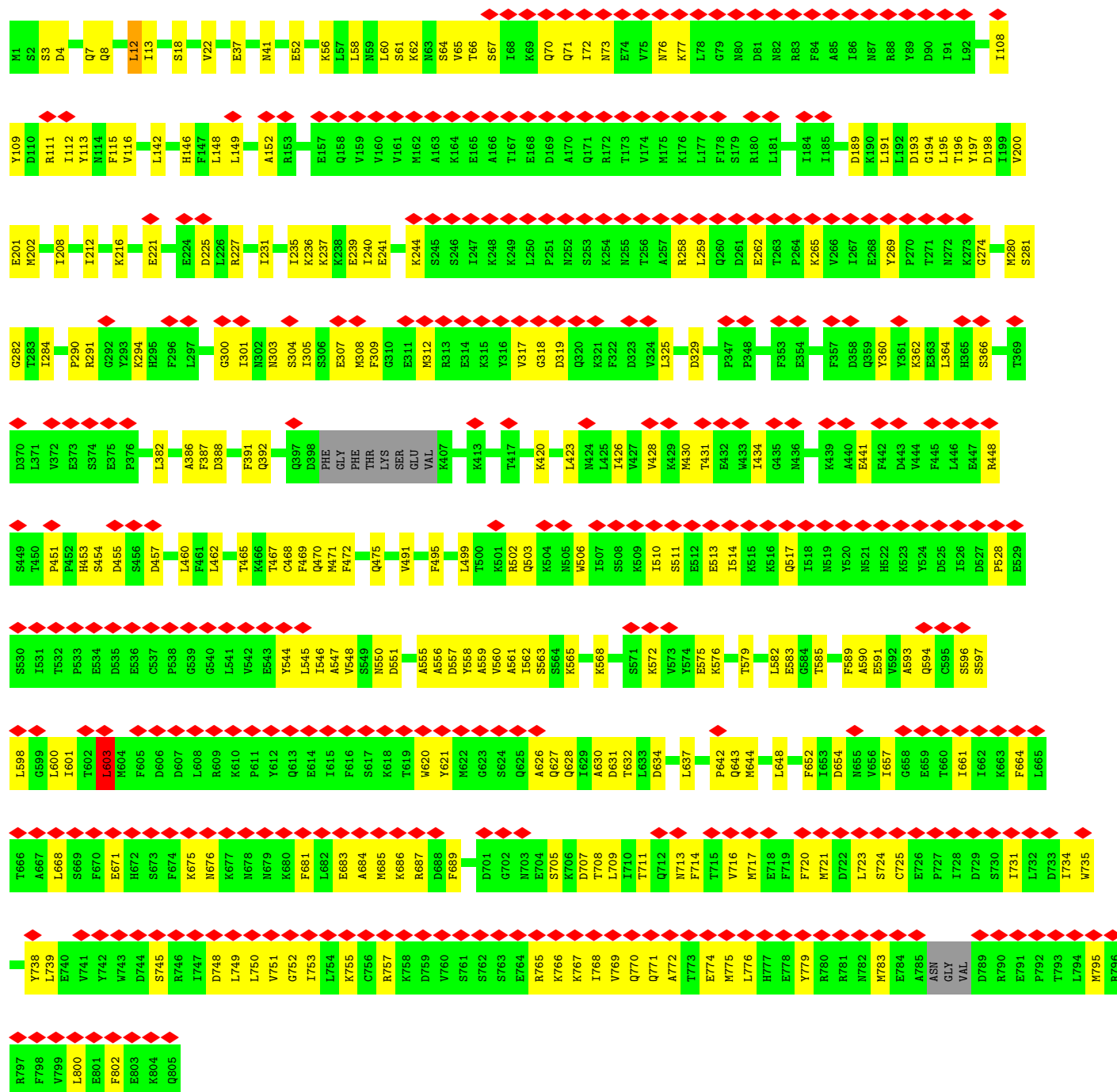
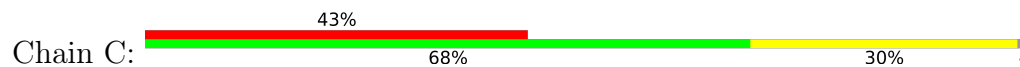


• Molecule 2: Exocyst complex component SEC5

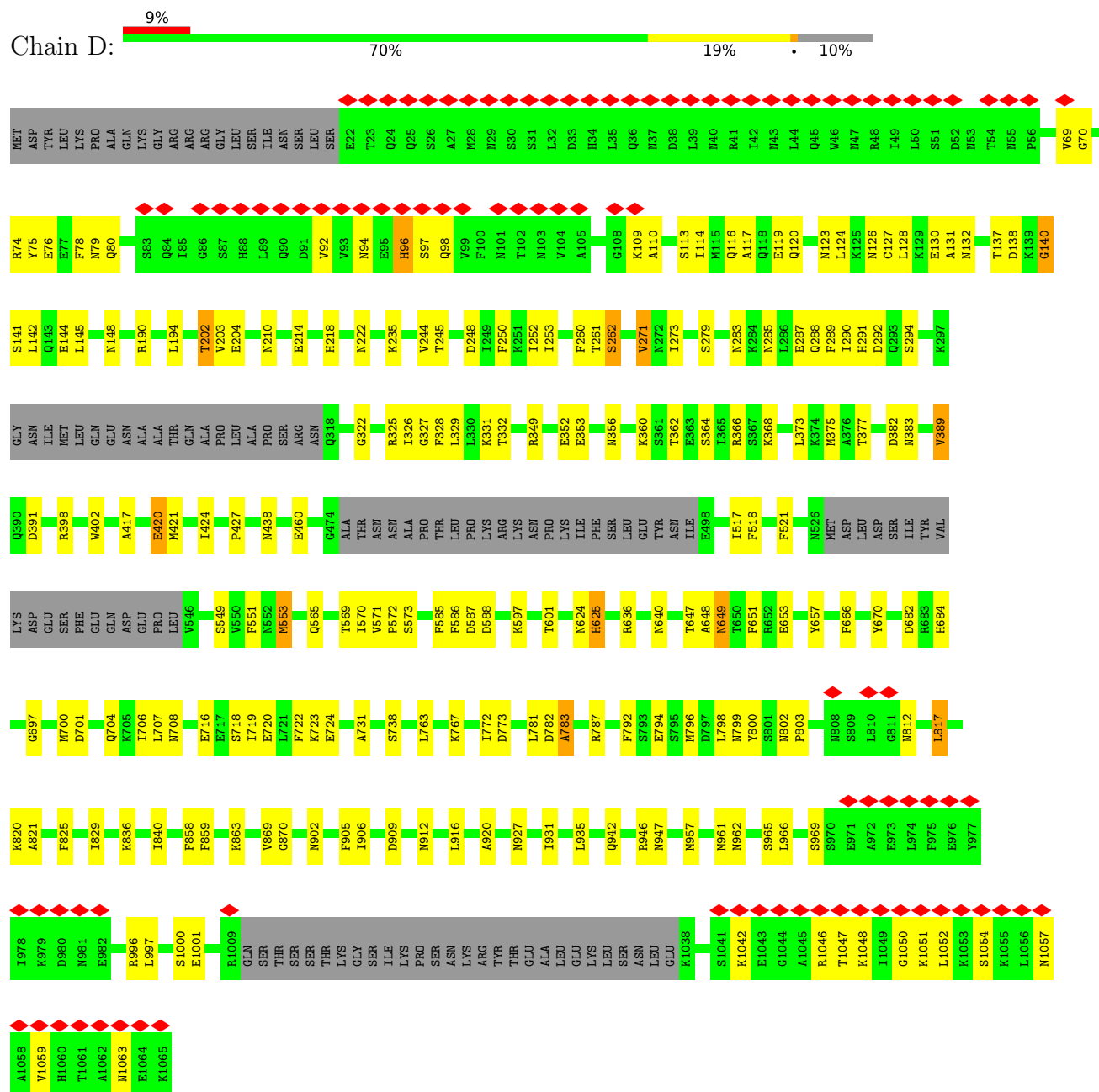




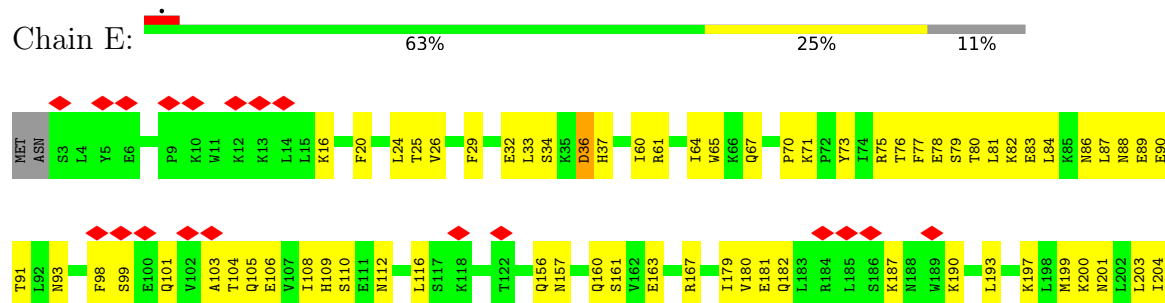
• Molecule 3: Exocyst complex component SEC6



- Molecule 4: Exocyst complex component SEC8

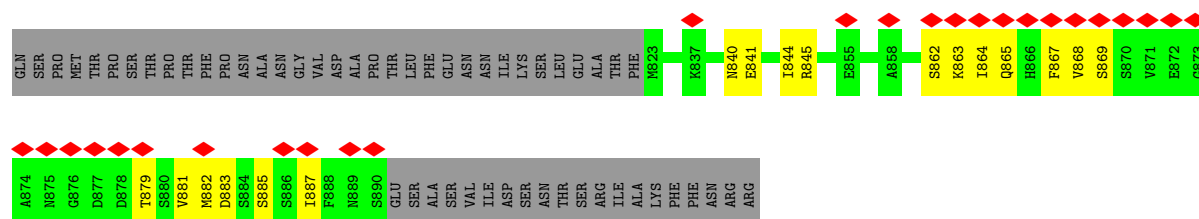


- Molecule 5: Exocyst complex component SEC10

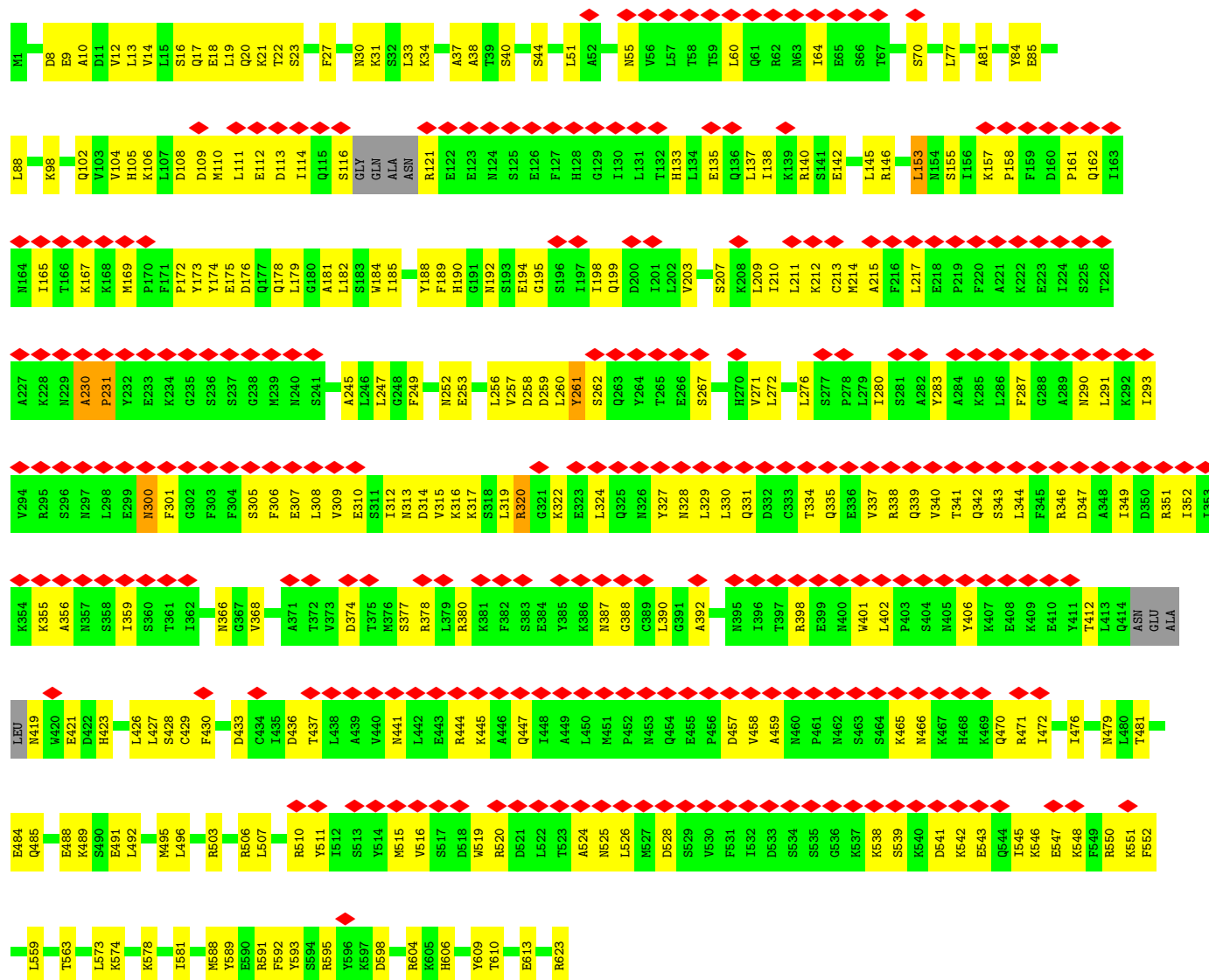
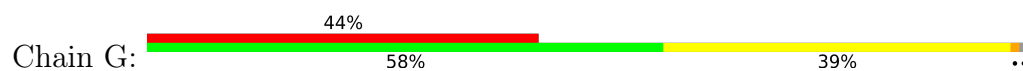








• Molecule 7: Exocyst complex component EXO70



• Molecule 8: Exocyst complex component EXO84



ALA	ARG	GLU	SER	ARG	SER	ARG	GLY	ARG	VAL	ALA	THR	SER	SER	MET	GLN	ARG	ARG	LEU	SER	THR	ALA	ASP	ILE	HIS	ASN	THR	THR	ALA	SER	PRO	PRO	THR	THR	LEU	ASP	LEU	LEU	ASP	MET	PRO	PRO	PRO	ASP	MET	ASN	ASN	ASN	MET	ILE	VAL	PRO	PRO	GLY	ASN	ASN	ASN	VAL	ASP	PHE	ASP	SER	SER	HIS	SER	ASN	ASN	SER	PHE	THR	THR	GLU	ASN	GLU
SER	VAL	SER	SER	LYS	GLY	PRO	VAL	SER	ASN	ASN	LEU	ASN	LEU	ASN	LEU	SER	THR	THR	ALA	ASP	LEU	SER	LEU	SER	LEU	SER	THR	ASN	ASN	SER	SER	PRO	THR	TYR	ASN	LYS	VAL	PRO	PRO	ALA	ALA	ARG	ASP	ASN	THR	THR	VAL	ASN	ASN	ASN	PRO	GLY	ASN	ASN	ASP	ASP	PRO	PHE	TSP	ASN	N169	S170	T171	S172	L173	R174	K175	M176	L177	A178	N179	P180	
H181	F182	N183	A184	K185	D186	F187	V188	H189	D190	K191	L192	G193	N194	A195	S196	A197	I198	L207	T208	S211	T212	Q213	V214	Q215	E216	E217	V218	K219	T222	N223	K224	S225	Y226	N227	E228	T229	N230	T231	V232	N233	N237	L243	R247	D252	L253	V256	L257	D258	Q259	I263																							
K266	Q269	L270	Q273	I274	Q275	D276	E277	R278	GLN	GLY	ASN	PHE	ASN	ASN	VAL	GLU	SER	HIS	SER	ASN	SER	PRO	ALA	LEU	PRO	PRO	LEU	LYS	ALA	GLY	GLN	ASN	GLY	ASN	LEU	H307	V314	L315	E318	W321	D322	L325	L328	N331	V332	A335	Q336	K337																									
F338	I339	L348	N349	N350	S351	M355	E356	L357	N358	K363	P364	M367	I370	F371	I372	L373	A380	S383	K384	Q387	V392	V403	T404	F415	K416	F417	S422	E432	C433	S434	R435	L436	L437	D438	V439	I440	A443	K444	D446	D447	C448	D449	I450																														
E454	E455	E456	R460	I461	S464	F465	S470	T471	Q472	P475	G476	P497	GLY	ARG	ASN	VAL	THR	GLY	ALA	MET	ASP	GLN	TYR	LEU	LEU	GLN	ASN	LEU	THR	LEU	SER	MET	HIS	SER	ARG	PRO	ARG	SER	D525	H526	S527	S528	T529	A530	Q531	R532	L533	K534	F535	L536	D537	Y540																					
I543	E546	L547	A555	V556	E557	L560	E563	E567	D568	L569	S570	GLU	ARG	ILE	SER	ASP	GLU	GLU	GLU	L578	H579	S585	I588	I595	L604	E608	T609	H611	L612	K613	S614	O615	T616	K621	L631	D642	L645	Q646	I647	GLY	SER	V650	D651	N652																													
L657	V662	Q666	E673	D677	L682	K685	S688	F702	K703	L704	I705	D706	K707	Q708	L709	L710	N711	ASP	GLU	MET	L715	Y739	K740	F744	I745	N748	S749	D750	K751	I752	R753																																										

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	67509, 67509	Depositor
Resolution determination method	FSC 0.5 CUT-OFF, FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.00	Depositor
Minimum defocus (nm)	2000.00	Depositor
Maximum defocus (nm)	3000.00	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.402	Depositor
Minimum map value	-2.171	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.405	Depositor
Recommended contour level	4.1	Depositor
Map size ( $\text{\AA}$ )	734.976, 734.976, 734.976	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.871, 2.871, 2.871	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	0.32	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	0.57	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	7.75	141.08	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	444	ILE	C-N-CA	7.21	139.72	121.70
7	G	153	LEU	CA-CB-CG	-6.69	99.91	115.30
4	D	649	ASN	C-N-CA	6.37	137.63	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	70	0
2	B	4610	0	1926	81	0
3	C	4994	0	3576	171	0
4	D	4739	0	2011	90	0
5	E	3860	0	1635	124	0
6	F	3612	0	1508	84	0
7	G	4696	0	4483	188	0
8	H	3240	0	2433	88	0
All	All	33096	0	18975	886	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 886 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	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:714:PHE:CD2	3:C:714:PHE:CZ	2.38	1.04
3:C:544:TYR:CG	3:C:544:TYR:CE2	2.40	1.02
3:C:558:TYR:O	3:C:562:ILE:HB	1.60	1.00
3:C:557:ASP:O	3:C:561:ALA:HB3	1.66	0.95

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%)	517 (78%)	144 (22%)	1 (0%)	47	81
2	B	922/971 (95%)	708 (77%)	201 (22%)	13 (1%)	11	47
3	C	788/805 (98%)	674 (86%)	113 (14%)	1 (0%)	51	85
4	D	944/1065 (89%)	717 (76%)	214 (23%)	13 (1%)	11	47
5	E	770/871 (88%)	639 (83%)	129 (17%)	2 (0%)	41	76
6	F	715/910 (79%)	577 (81%)	131 (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%)	4818 (81%)	1057 (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	297/740 (40%)	297 (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	979/2007 (49%)	975 (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 18 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	424	ASN
8	H	638	ASN
7	G	606	HIS
3	C	713	ASN
7	G	395	ASN

### 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-21226. These allow visual inspection of the internal detail of the map and identification of artifacts.

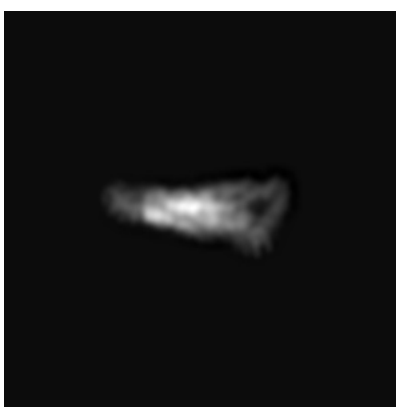
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

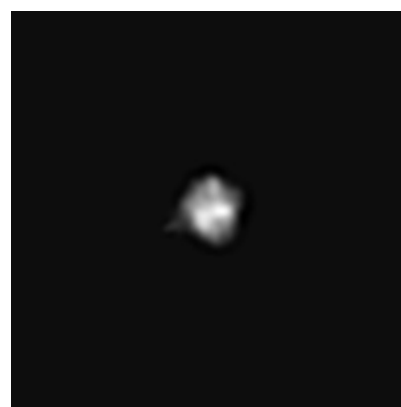
#### 6.1.1 Primary map



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: 128



Y Index: 128



Z Index: 128

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

## 6.3 Largest variance slices [i](#)

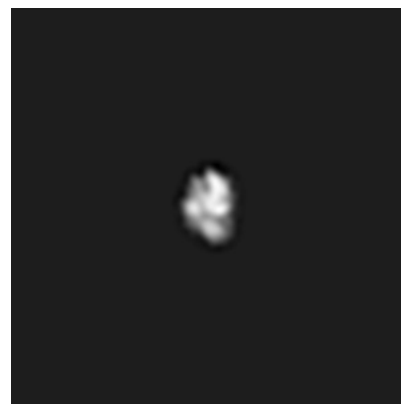
### 6.3.1 Primary map



X Index: 129



Y Index: 127



Z Index: 119

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

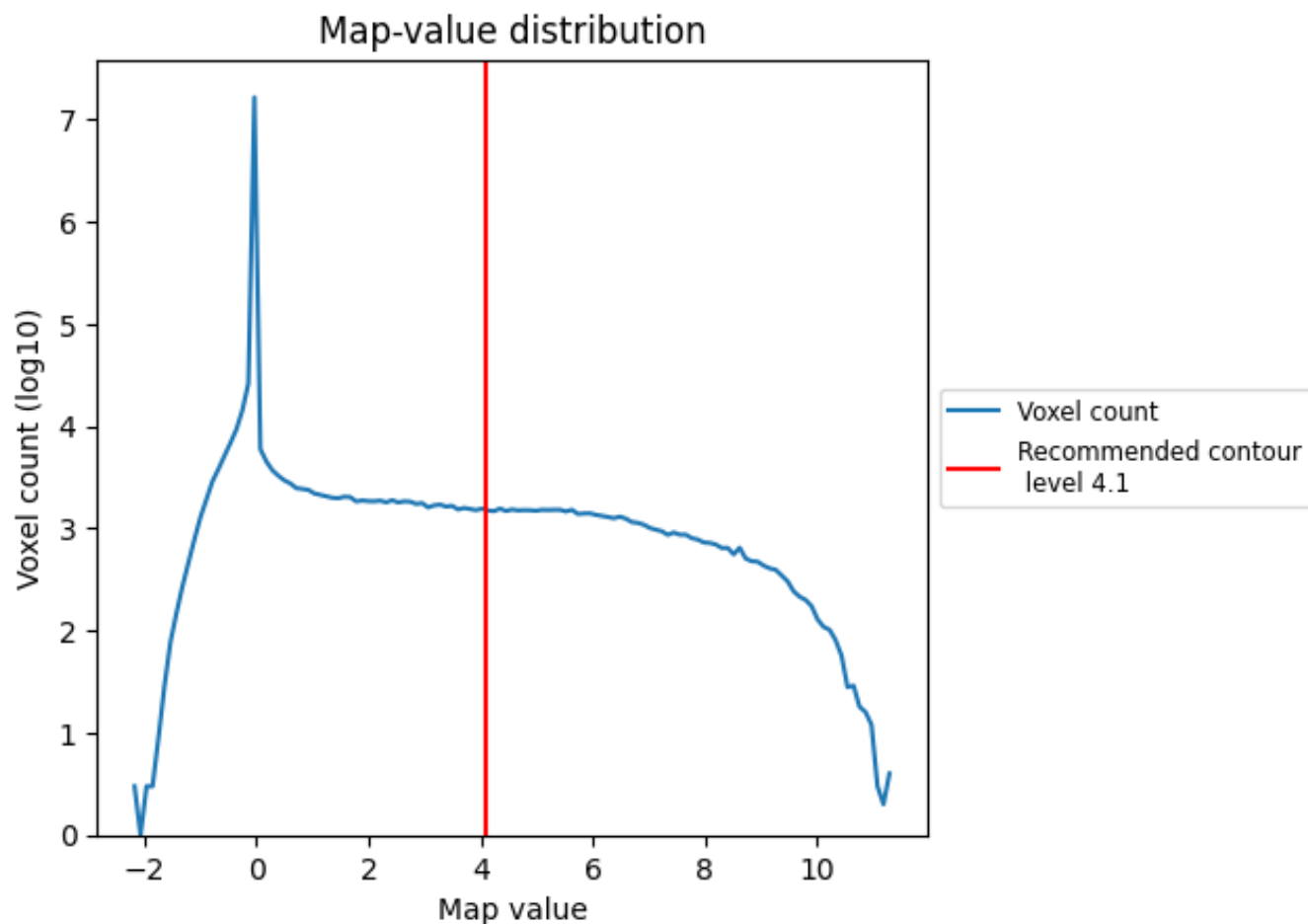
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

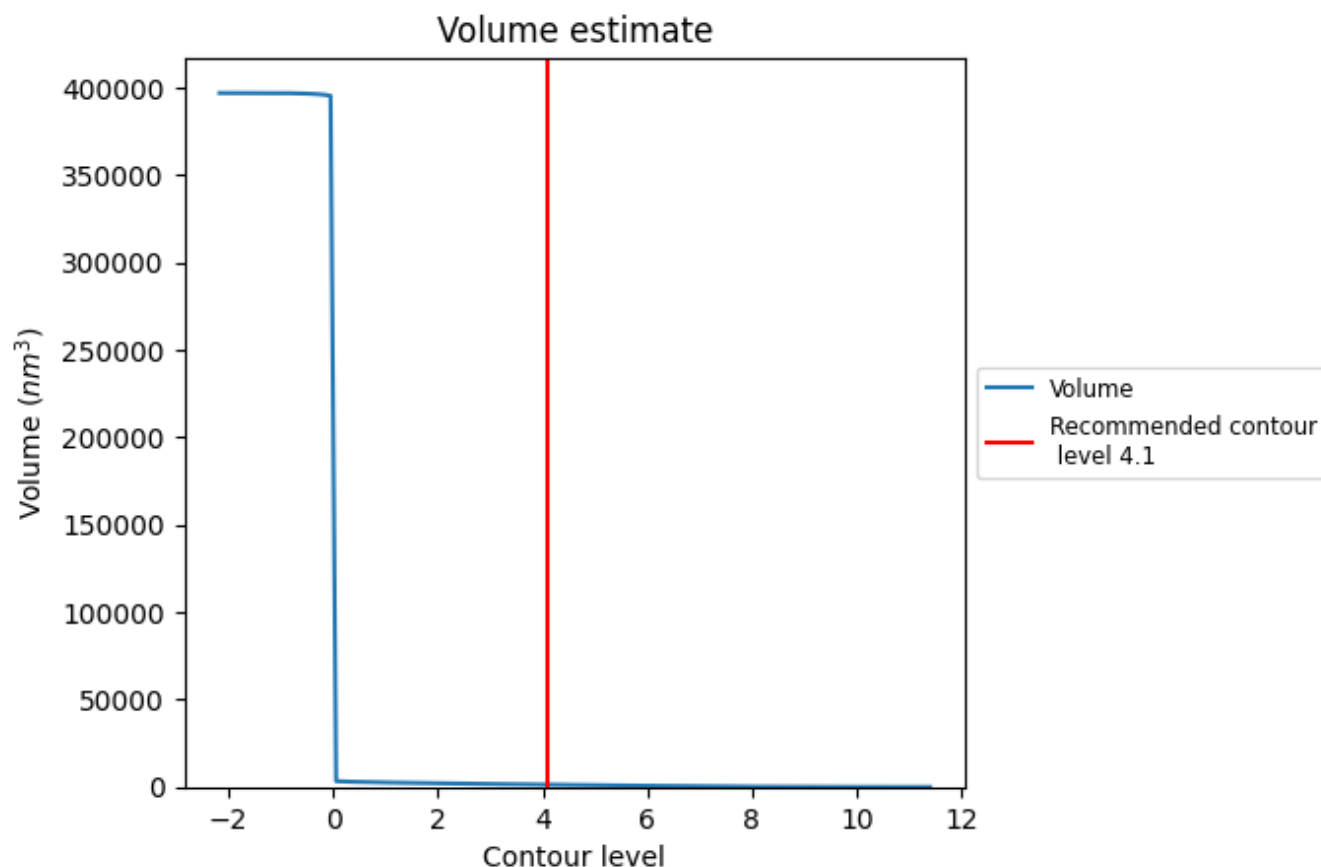
This section contains the results of statistical analysis of the map.

### 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.

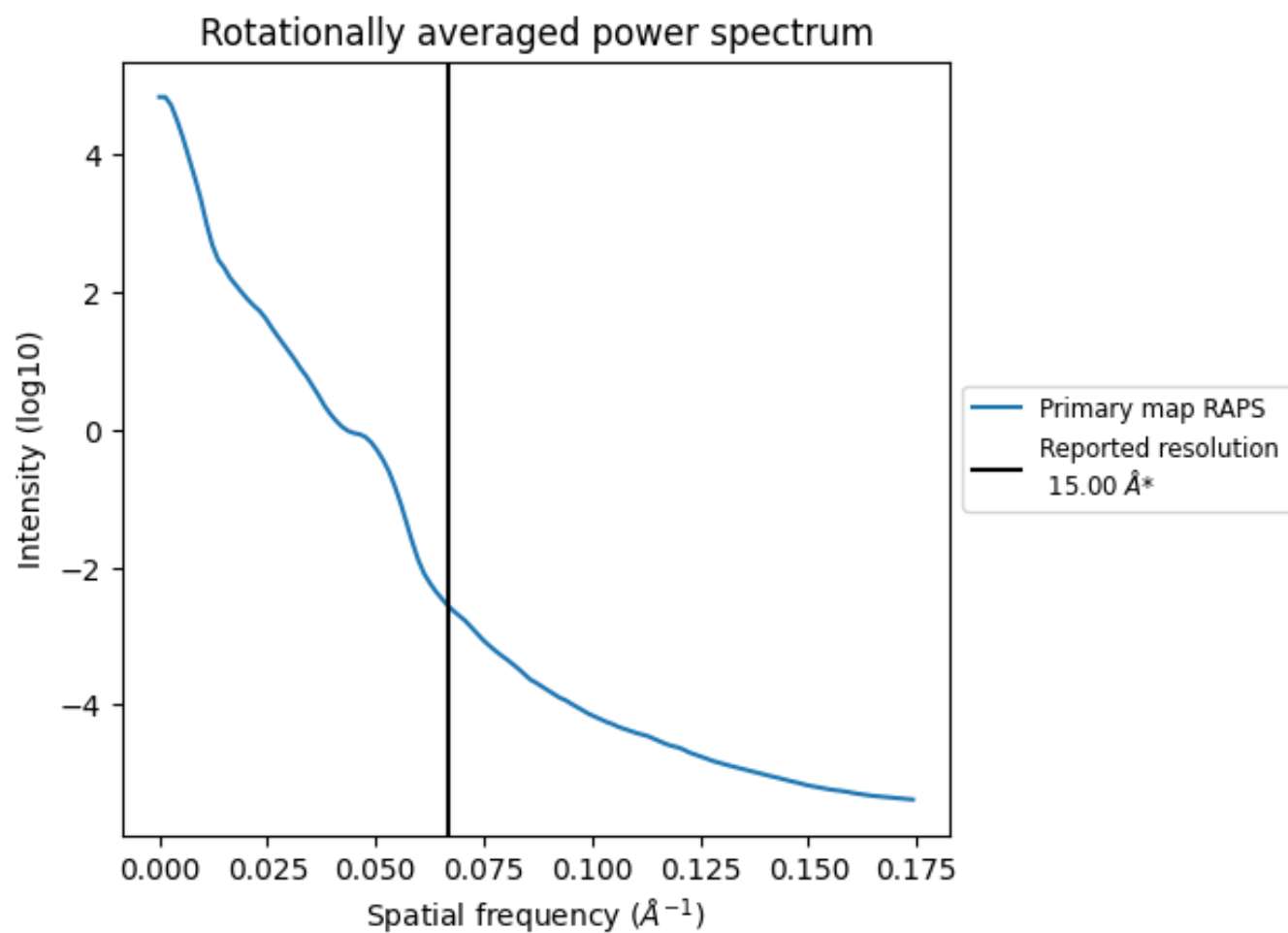
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1324  $\text{nm}^3$ ; this corresponds to an approximate mass of 1196 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 0.067 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

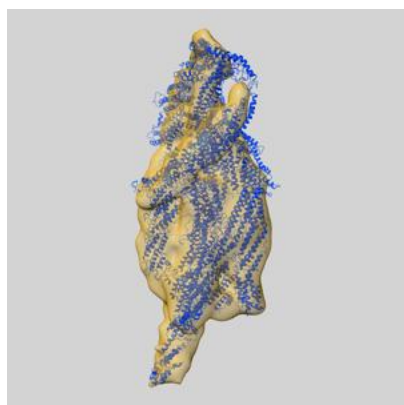
This section was not generated. No FSC curve or half-maps provided.



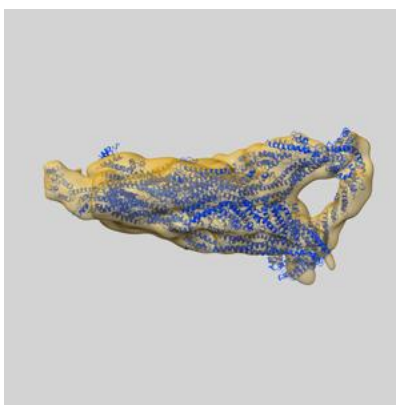
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21226 and PDB model 6VKL. Per-residue inclusion information can be found in section [3](#) on page [5](#).

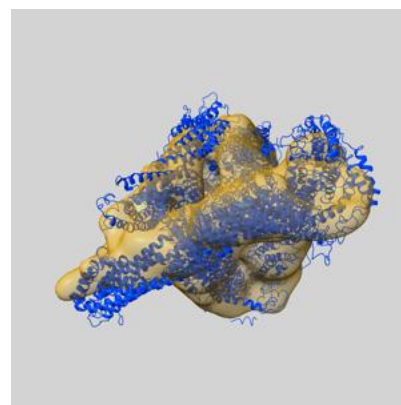
### 9.1 Map-model overlay [i](#)



X



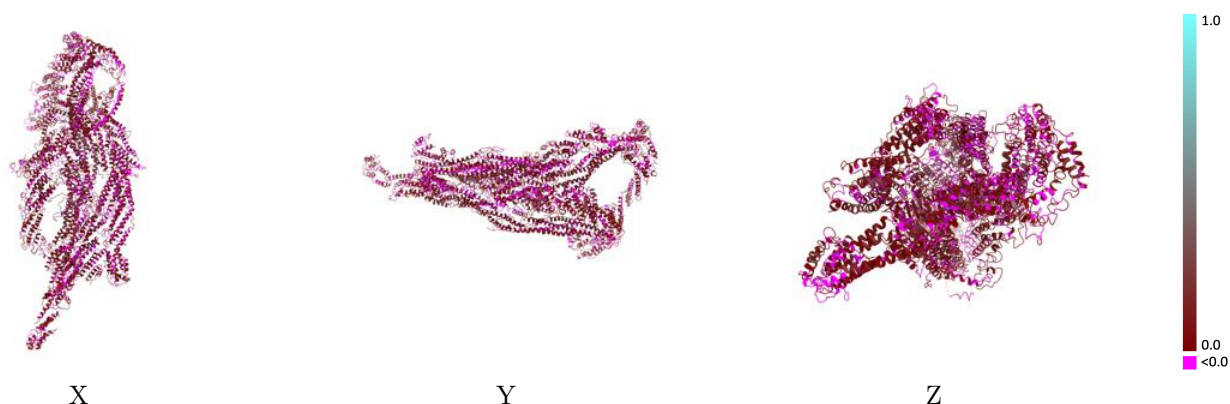
Y



Z

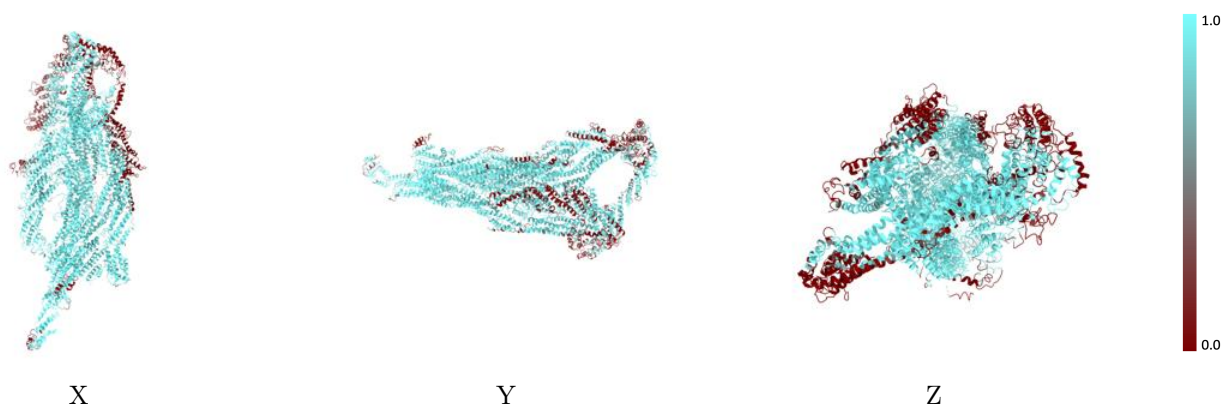
The images above show the 3D surface view of the map at the recommended contour level 4.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



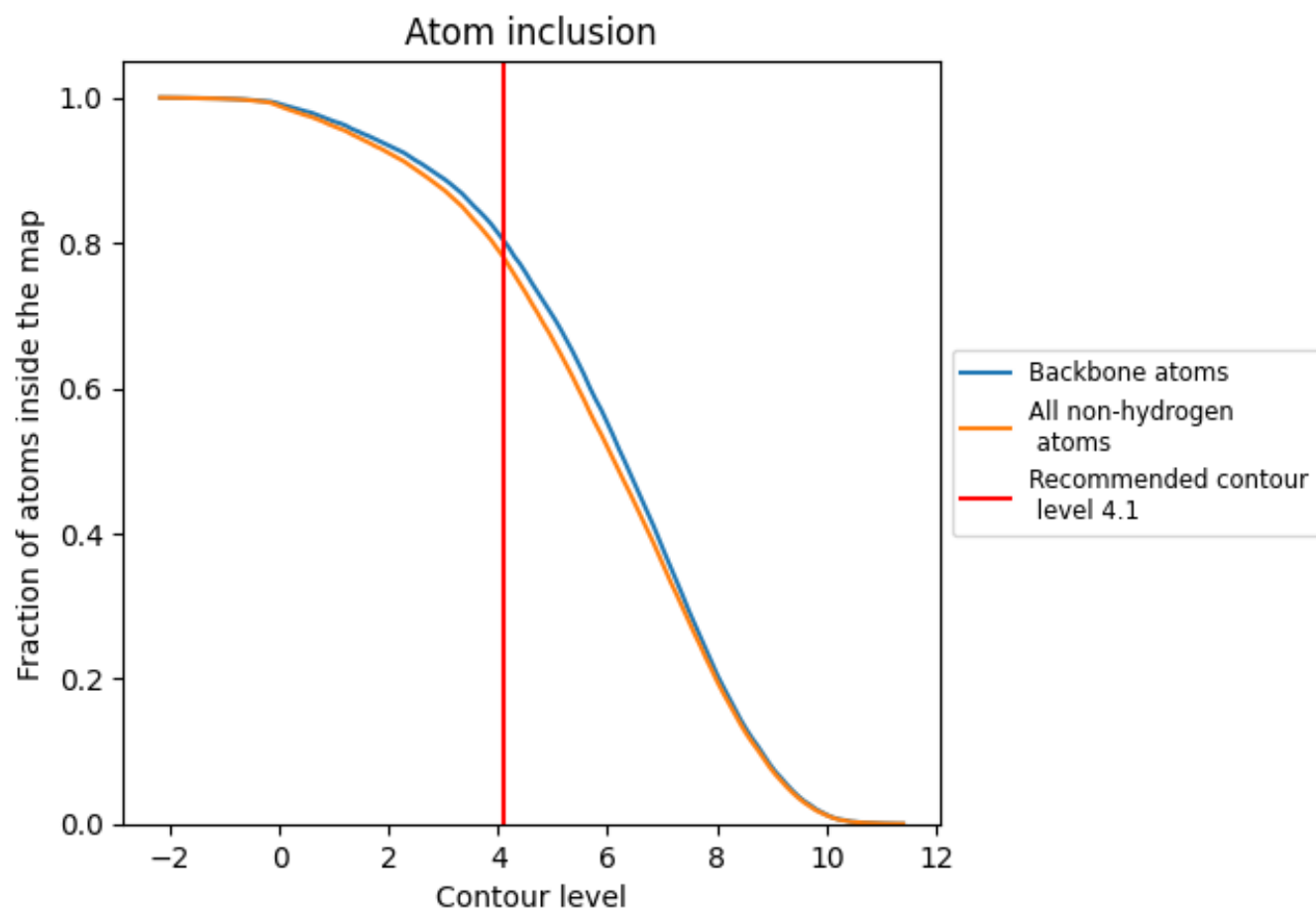
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (4.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7804	<div></div> 0.0530
A	<div></div> 0.7818	<div></div> 0.0630
B	<div></div> 0.8011	<div></div> 0.0490
C	<div></div> 0.5241	<div></div> 0.0400
D	<div></div> 0.8924	<div></div> 0.0530
E	<div></div> 0.9523	<div></div> 0.0710
F	<div></div> 0.9308	<div></div> 0.0620
G	<div></div> 0.5414	<div></div> 0.0330
H	<div></div> 0.9475	<div></div> 0.0670

