



Full wwPDB EM Validation Report ⓘ

Feb 24, 2024 – 08:57 am GMT

PDB ID : 8Q62
EMDB ID : EMD-18181
Title : Early closed conformation of the g-tubulin ring complex
Authors : Llorca, O.; Serna, M.; Fernandez-Leiro, R.
Deposited on : 2023-08-10
Resolution : 3.72 Å (reported)
Based on initial models : 7AS4, 6X0U

This is a Full wwPDB EM Validation 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:

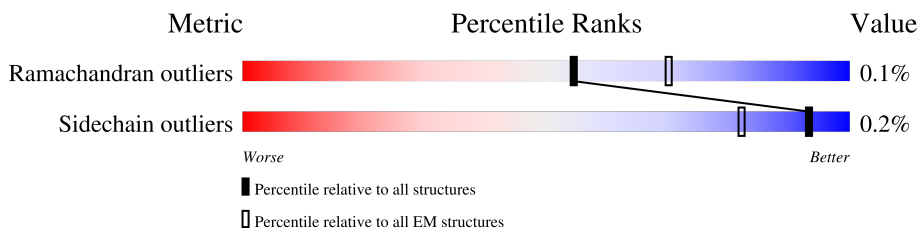
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.72 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)
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	451	41% 93% 7%
1	b	451	11% 93% 7%
1	c	451	93% 7%
1	d	451	93% 7%
1	e	451	93% 7%
1	f	451	93% 7%
1	g	451	93% 7%
1	h	451	93% 7%
1	i	451	93% 7%

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Mol	Chain	Length	Quality of chain
1	j	451	
1	k	451	
1	l	451	
1	m	451	
1	n	451	
2	J	1024	
3	I	667	
3	K	667	
4	B	907	
4	D	907	
4	F	907	
4	H	907	
4	N	907	
5	A	902	
5	C	902	
5	E	902	
5	G	902	
5	M	902	
6	L	1819	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 230788 atoms, of which 115024 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 Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	k	420	6707	2138	3327	587	640	15	2	0
1	a	420	6707	2138	3327	587	640	15	2	0
1	b	420	6707	2138	3327	587	640	15	2	0
1	c	420	6707	2138	3327	587	640	15	2	0
1	d	420	6707	2138	3327	587	640	15	2	0
1	e	420	6685	2138	3305	587	640	15	2	0
1	f	420	6690	2135	3316	584	640	15	2	0
1	g	420	6707	2138	3327	587	640	15	2	0
1	h	420	6679	2135	3305	584	640	15	2	0
1	i	420	6707	2138	3327	587	640	15	2	0
1	j	420	6707	2138	3327	587	640	15	2	0
1	l	420	6696	2138	3316	587	640	15	2	0
1	m	420	6696	2138	3316	587	640	15	2	0
1	n	420	6707	2138	3327	587	640	15	2	0

- Molecule 2 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	J	594	9558	3093	4769	807	863	26	0	0

- Molecule 3 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	K	553	Total	C	H	N	O	S	0	0
			9010	2918	4507	768	800	17		
3	I	521	Total	C	H	N	O	S	0	0
			8472	2734	4250	720	750	18		

- Molecule 4 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	B	610	Total	C	H	N	O	S	0	0
			9984	3195	4969	885	910	25		
4	D	581	Total	C	H	N	O	S	0	0
			9560	3061	4764	842	868	25		
4	F	599	Total	C	H	N	O	S	0	0
			9852	3146	4919	871	891	25		
4	H	586	Total	C	H	N	O	S	0	0
			9655	3087	4820	852	871	25		
4	N	594	Total	C	H	N	O	S	0	0
			9779	3125	4880	864	885	25		

- Molecule 5 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	C	620	Total	C	H	N	O	S	0	0
			10108	3254	5070	842	910	32		
5	E	638	Total	C	H	N	O	S	0	0
			10443	3354	5241	873	942	33		
5	G	636	Total	C	H	N	O	S	0	0
			10394	3342	5208	871	940	33		
5	M	636	Total	C	H	N	O	S	0	0
			10405	3342	5219	871	940	33		
5	A	609	Total	C	H	N	O	S	0	0
			9890	3181	4956	825	896	32		

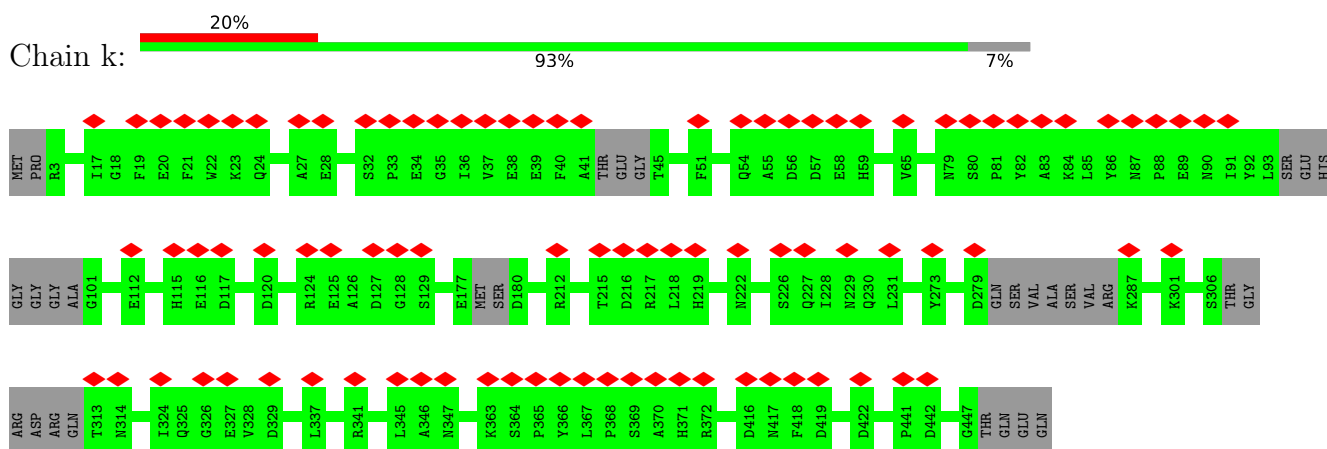
- Molecule 6 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	L	616	Total	C	H	N	O	S	0	0
			9869	3211	4951	826	855	26		

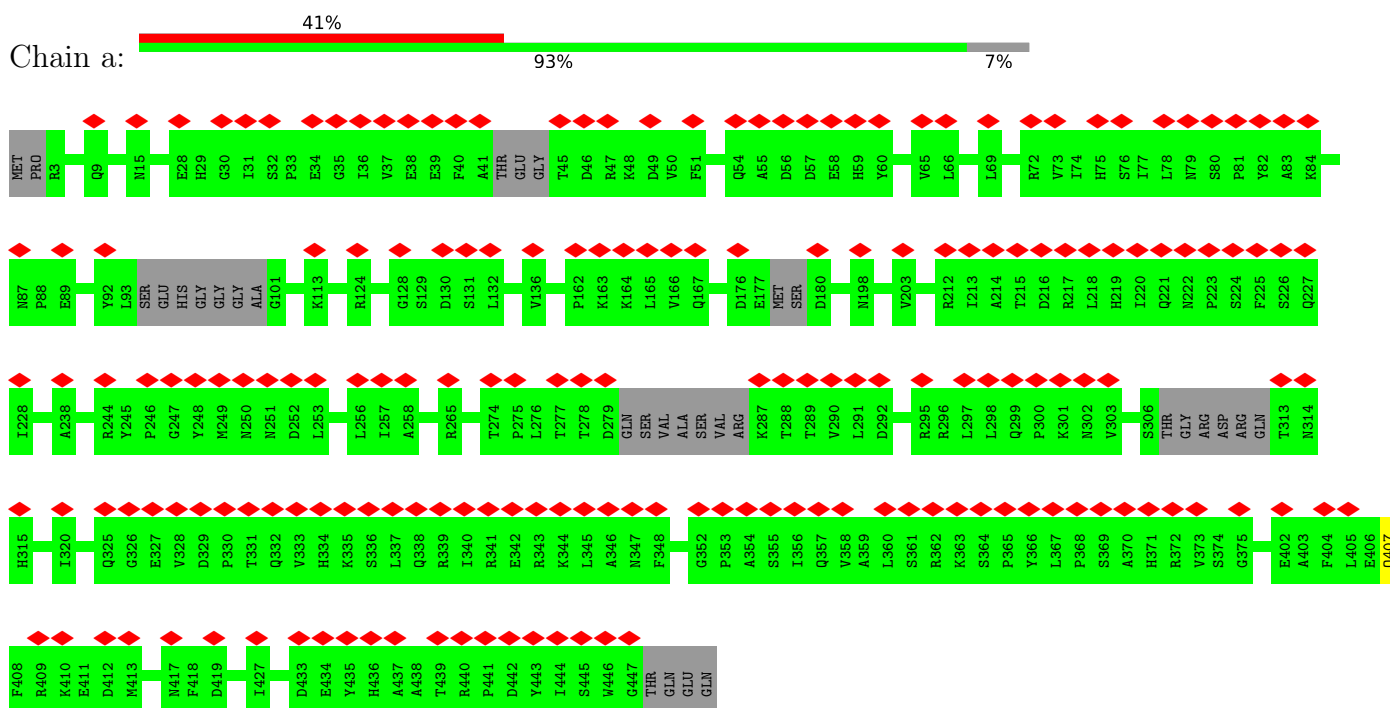
3 Residue-property plots [i](#)

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.

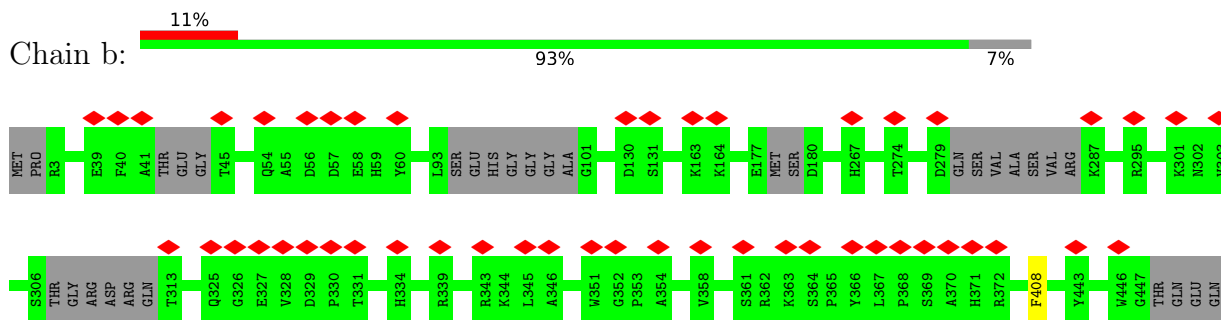
- Molecule 1: Tubulin gamma-1 chain



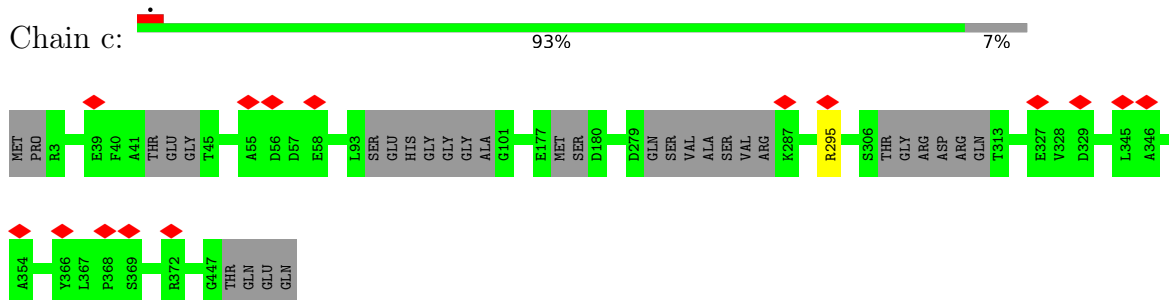
- Molecule 1: Tubulin gamma-1 chain



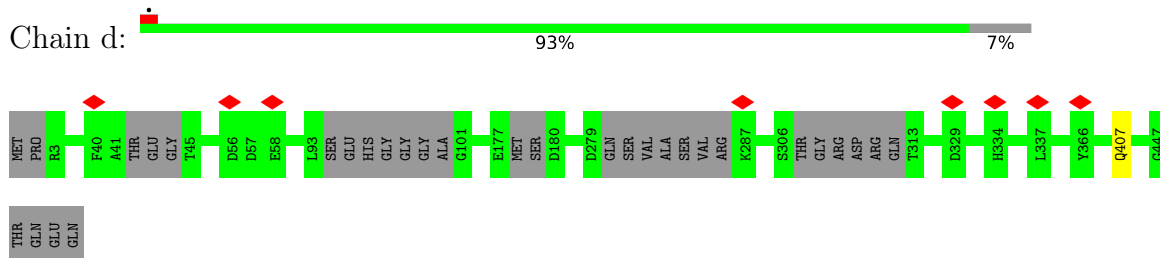
- Molecule 1: Tubulin gamma-1 chain



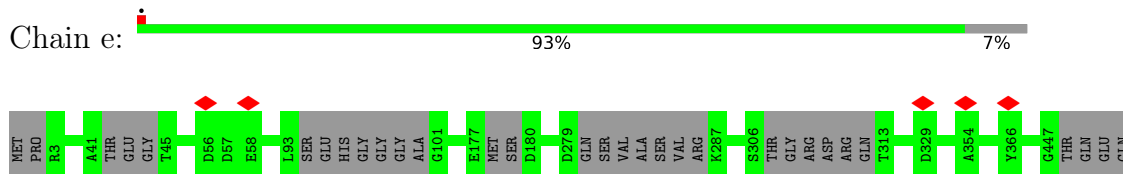
• Molecule 1: Tubulin gamma-1 chain



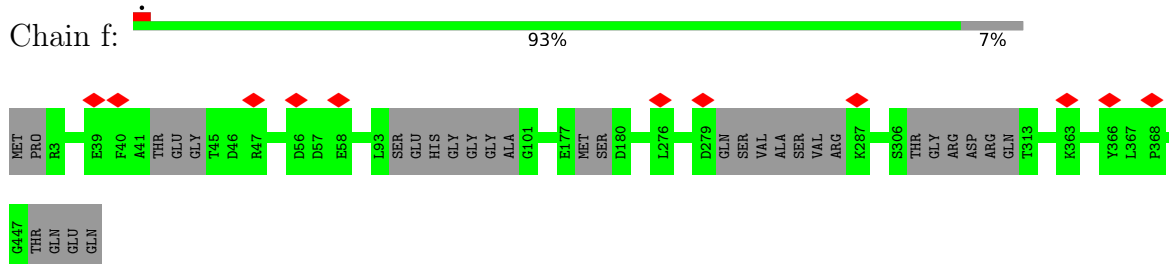
• Molecule 1: Tubulin gamma-1 chain




• Molecule 1: Tubulin gamma-1 chain

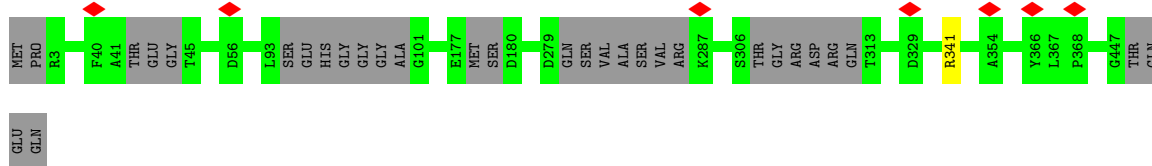


• Molecule 1: Tubulin gamma-1 chain



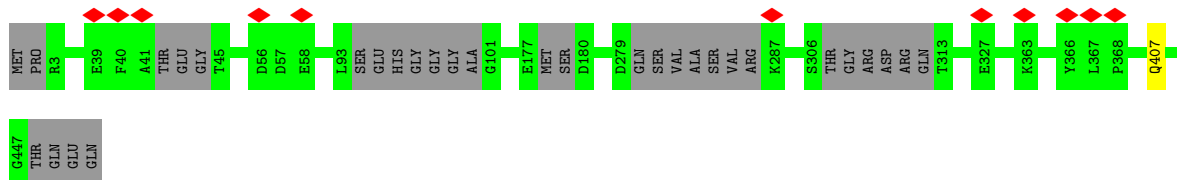
• Molecule 1: Tubulin gamma-1 chain

Chain g:  93% 7%



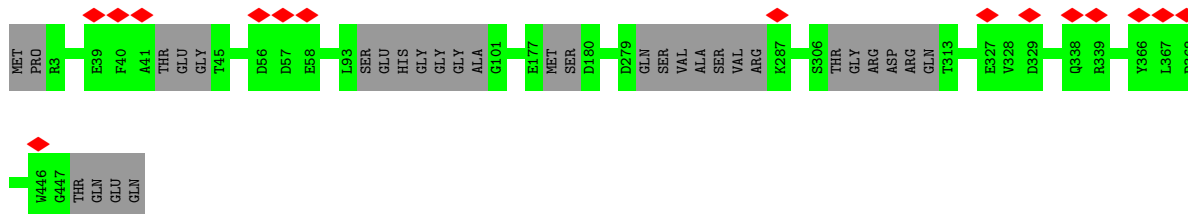
• Molecule 1: Tubulin gamma-1 chain

Chain h:  93% 7%




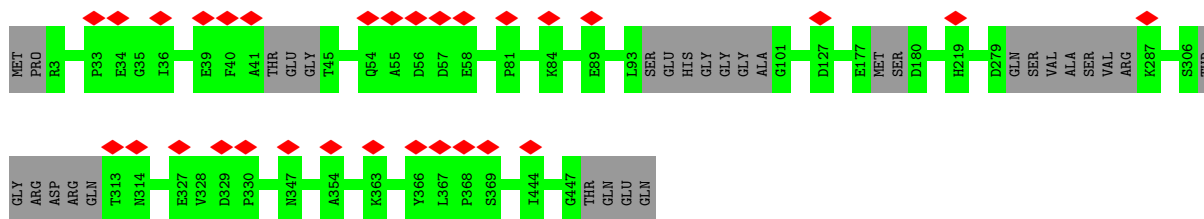
• Molecule 1: Tubulin gamma-1 chain

Chain i:  93% 7%



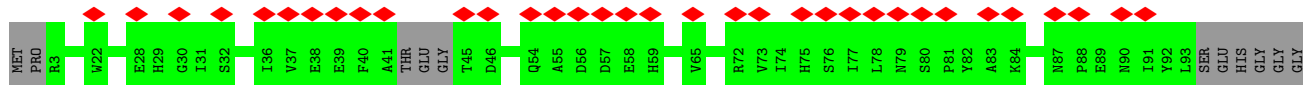
• Molecule 1: Tubulin gamma-1 chain

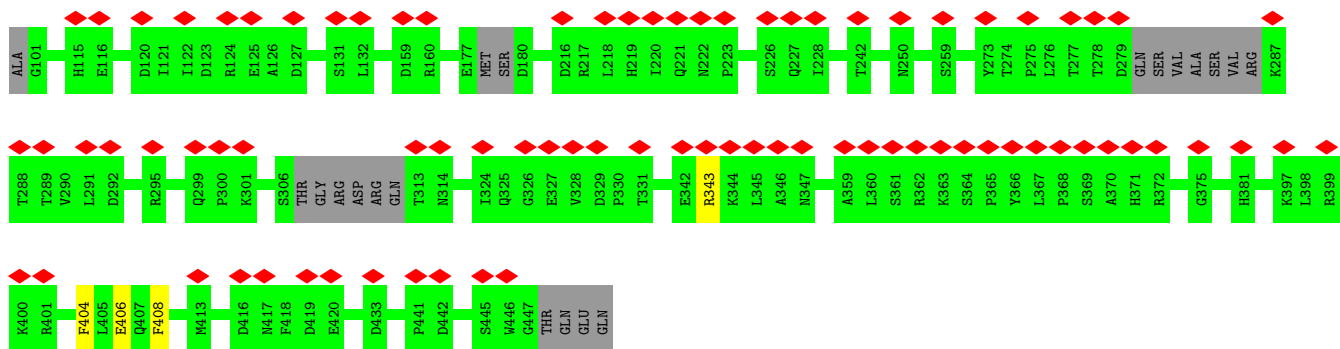
Chain j:  7% 93% 7%



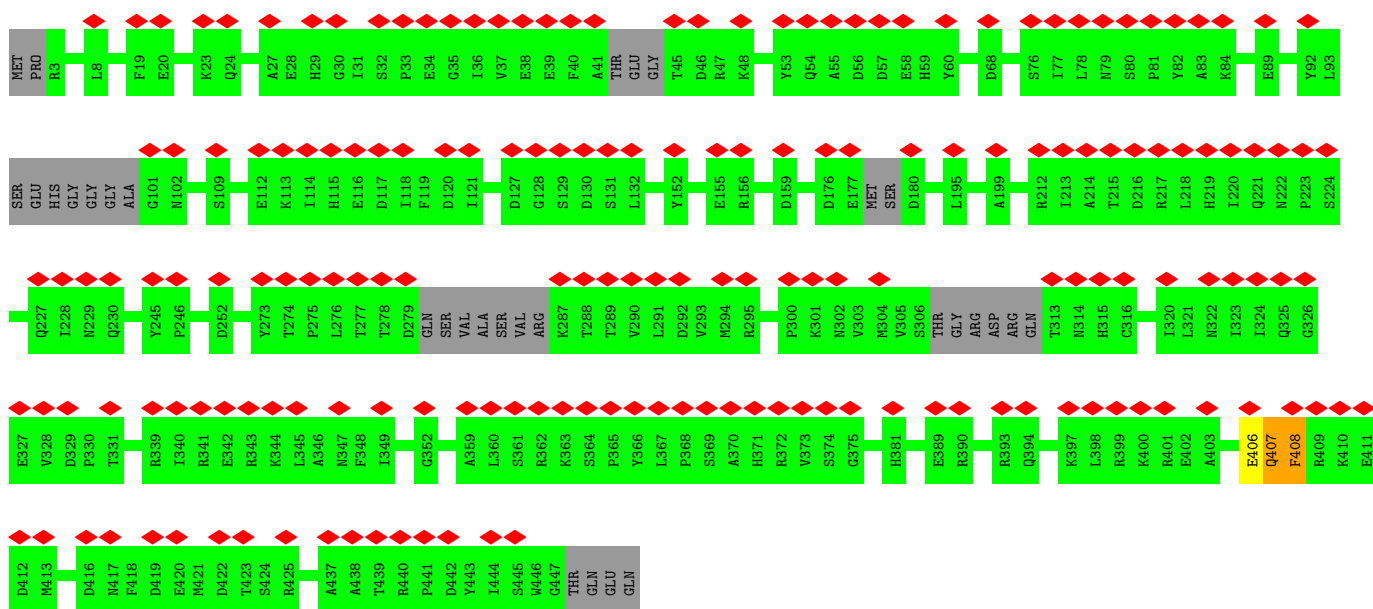
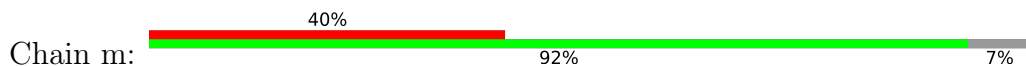
• Molecule 1: Tubulin gamma-1 chain

Chain l:  26% 92% 7%

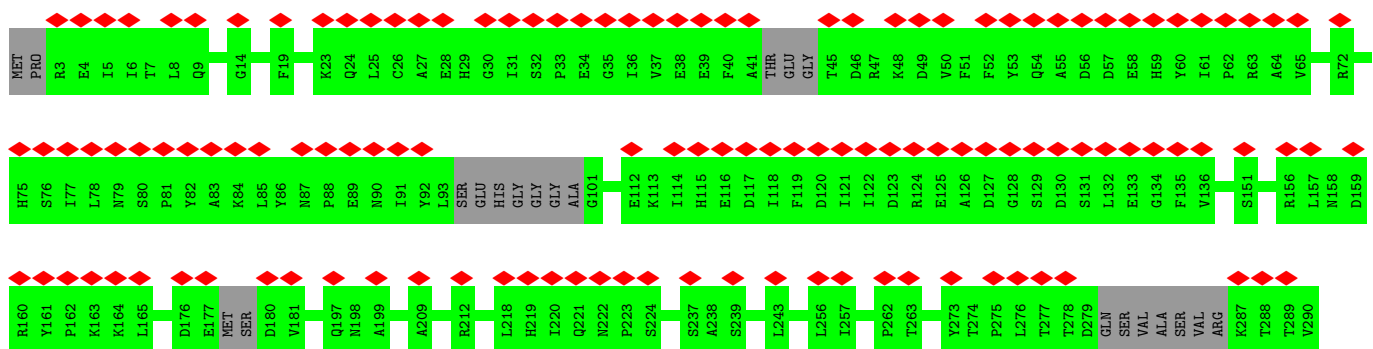
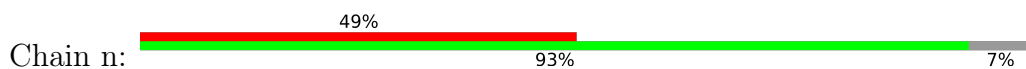


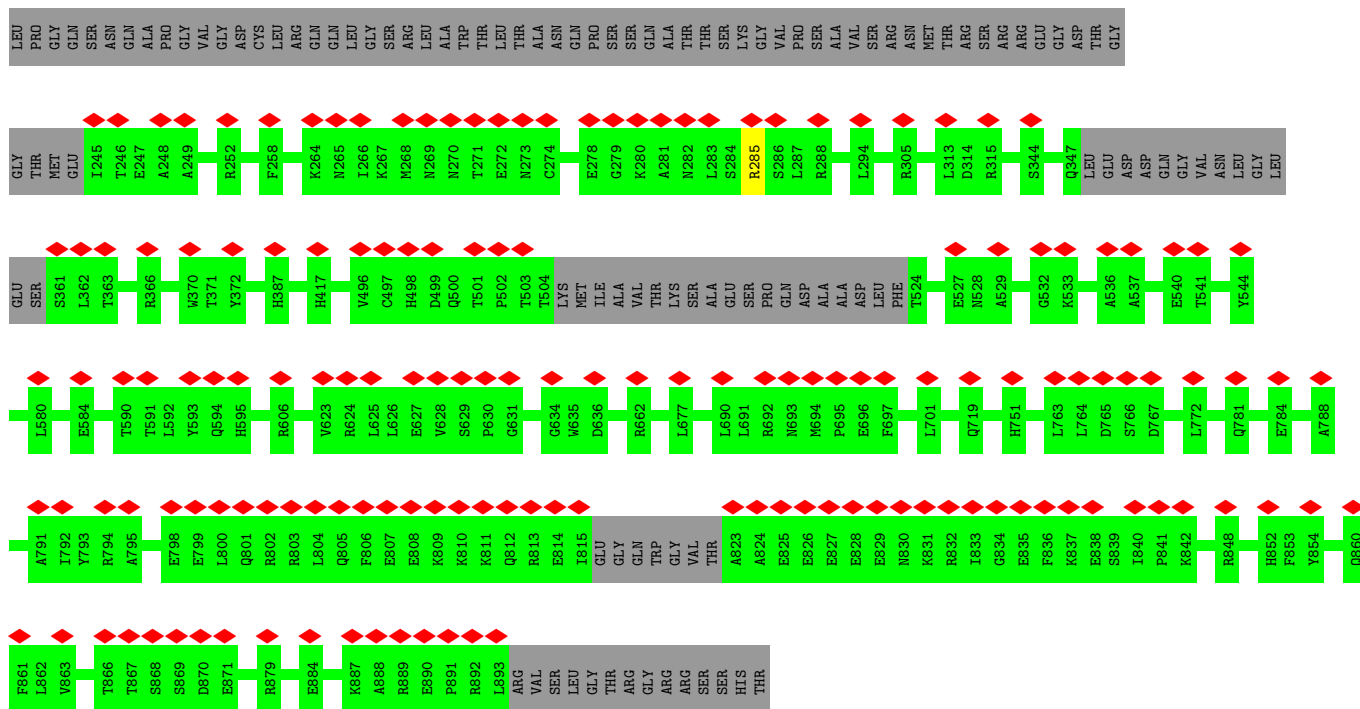


• Molecule 1: Tubulin gamma-1 chain

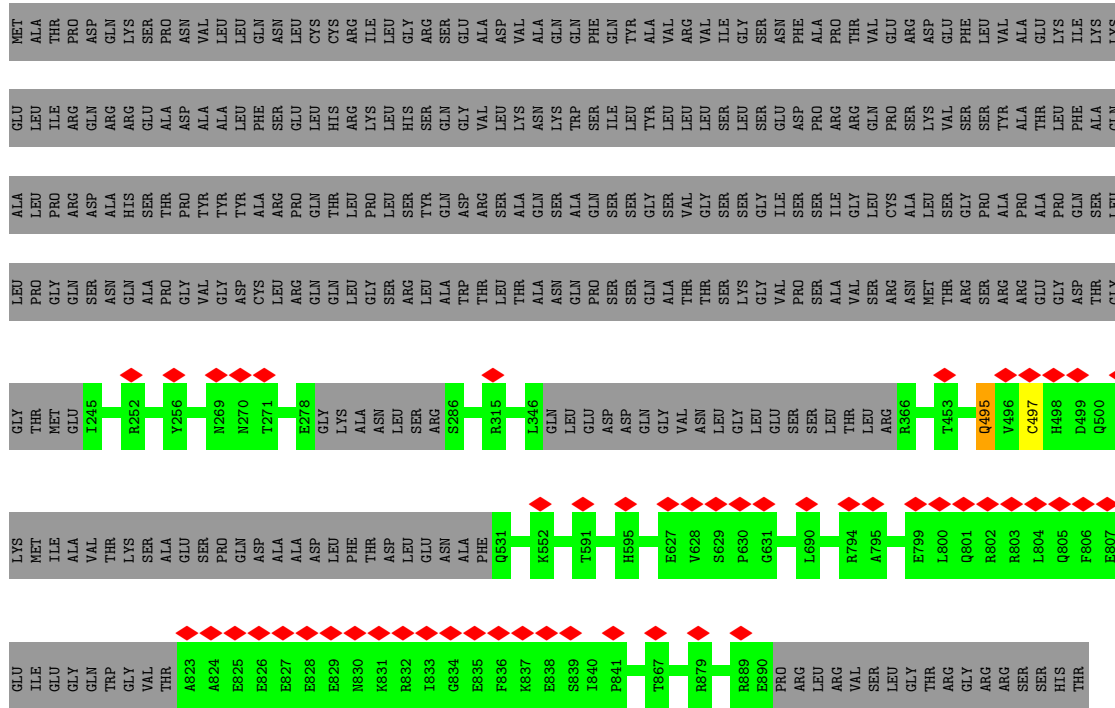


• Molecule 1: Tubulin gamma-1 chain



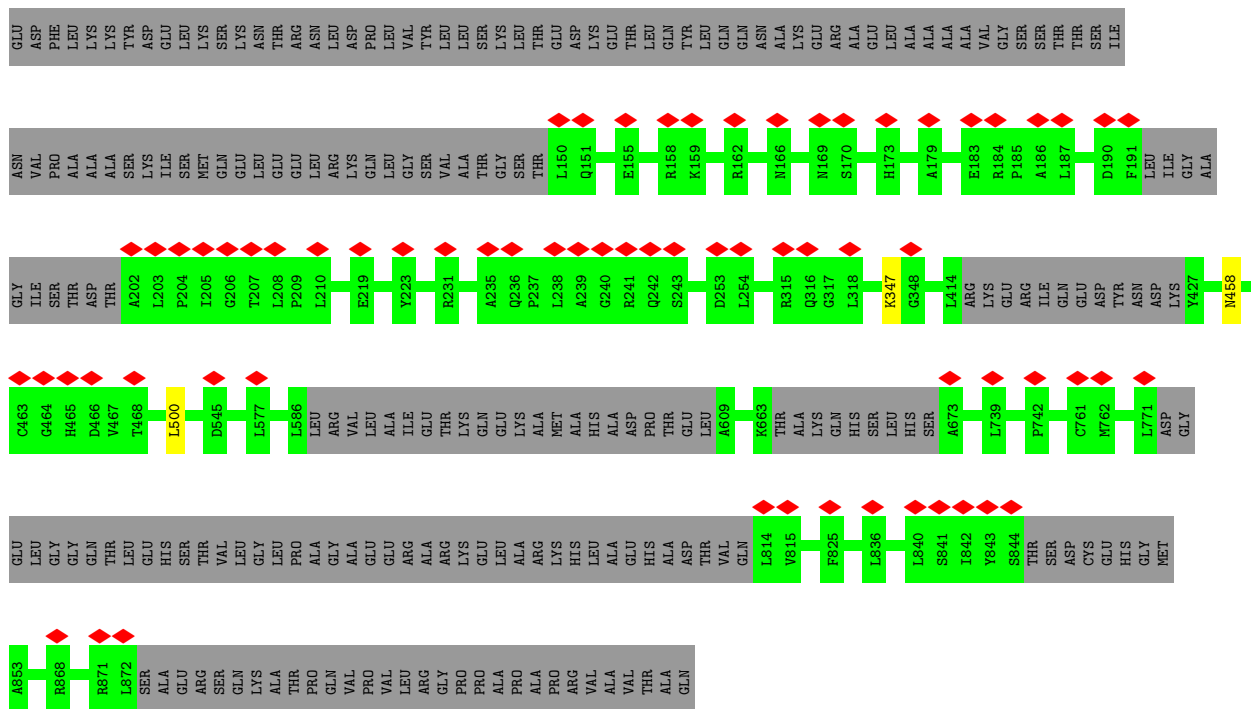


• Molecule 4: Gamma-tubulin complex component 3

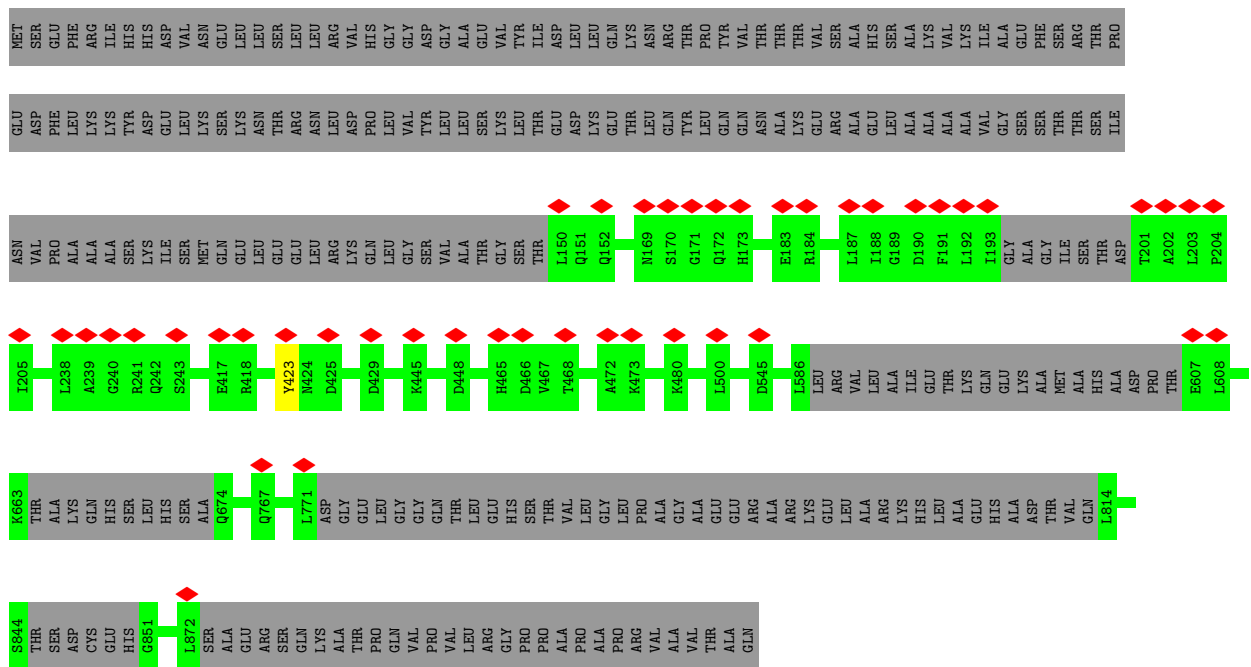


• Molecule 4: Gamma-tubulin complex component 3



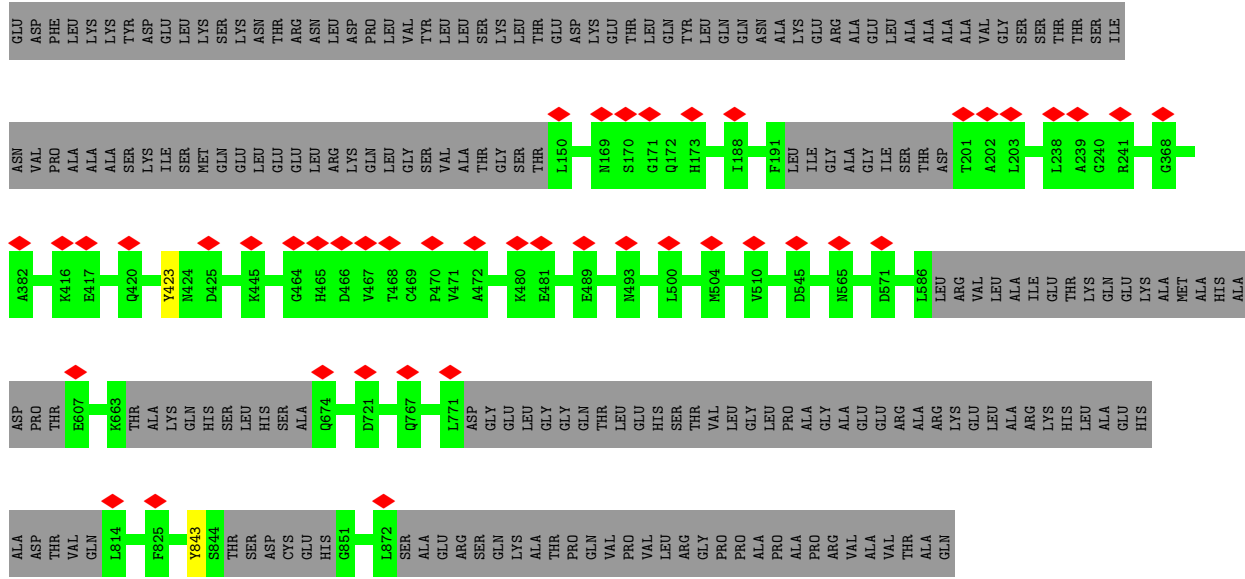


• Molecule 5: Gamma-tubulin complex component 2

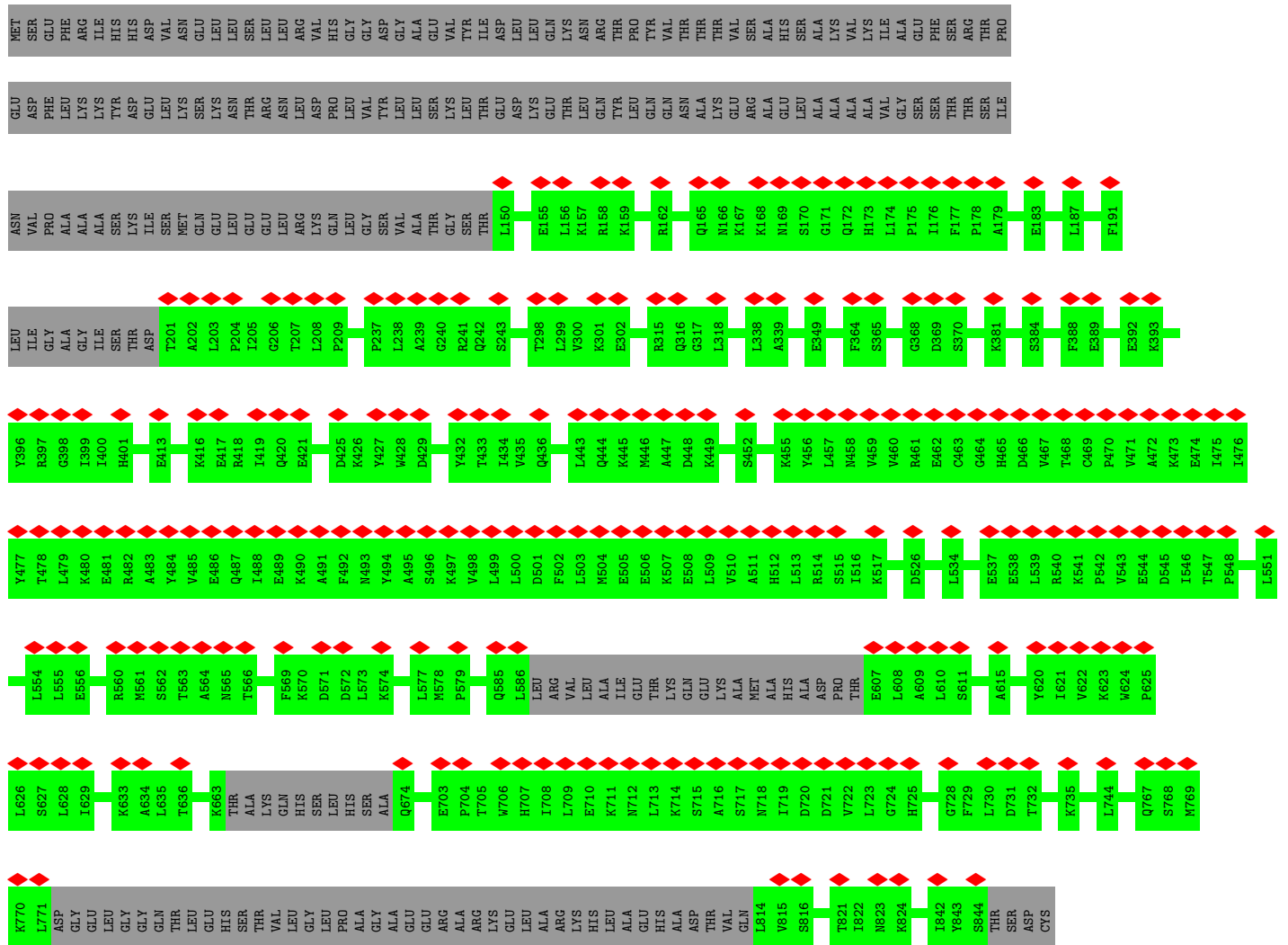


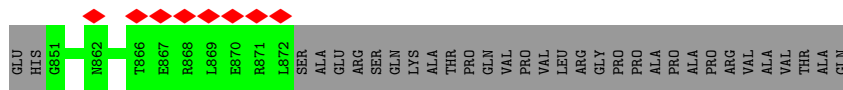
• Molecule 5: Gamma-tubulin complex component 2



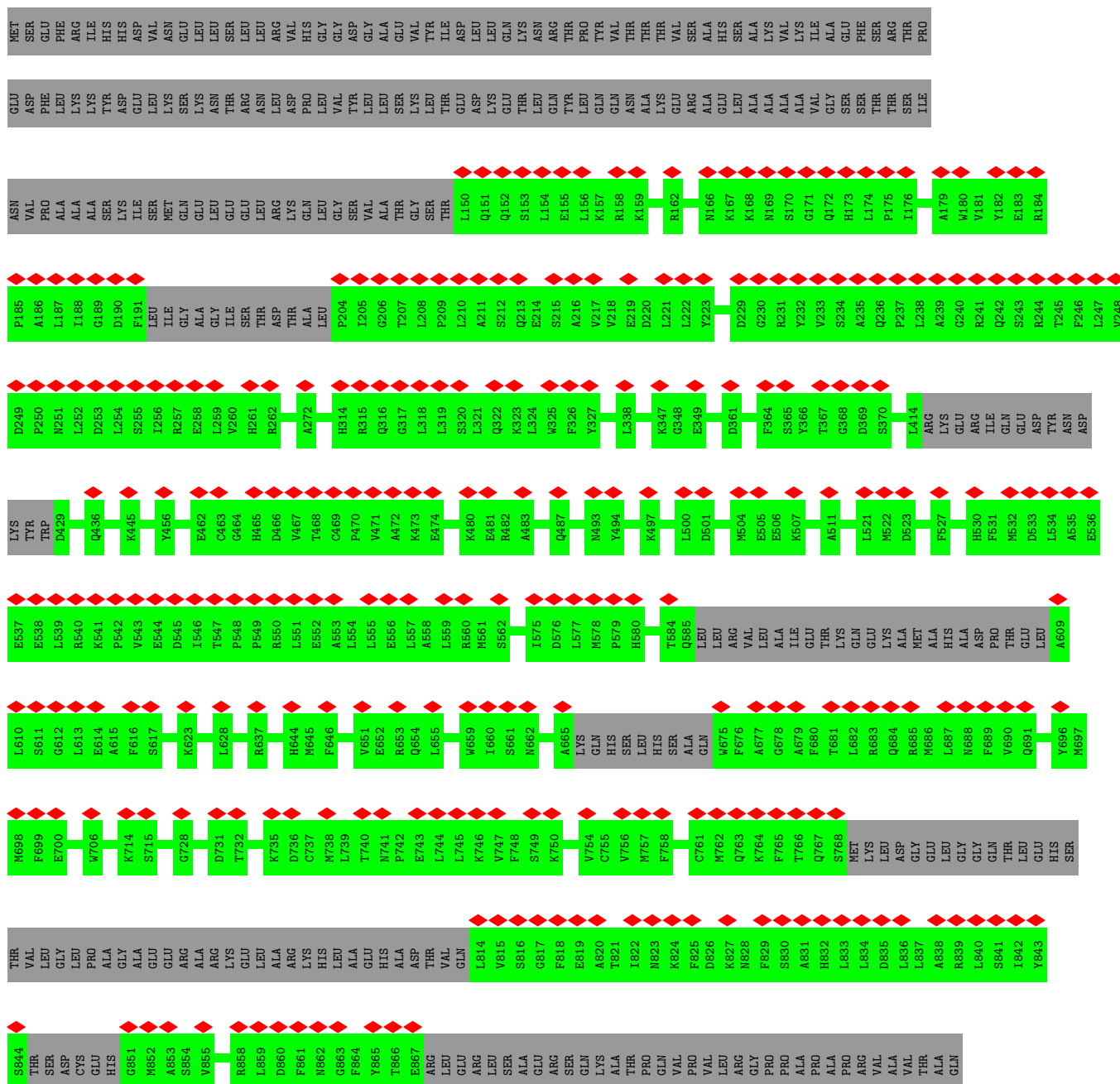


• Molecule 5: Gamma-tubulin complex component 2





• Molecule 5: Gamma-tubulin complex component 2



• Molecule 6: Gamma-tubulin complex component 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	357509	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.276	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	588.0422, 588.0422, 588.0422	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36754, 1.36754, 1.36754	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	0.33	0/3460	0.65	0/4686
1	b	0.32	0/3460	0.67	0/4686
1	c	0.33	0/3460	0.67	0/4686
1	d	0.34	0/3460	0.68	0/4686
1	e	0.35	0/3460	0.68	0/4686
1	f	0.35	0/3454	0.69	0/4679
1	g	0.34	0/3460	0.69	0/4686
1	h	0.35	0/3454	0.68	0/4679
1	i	0.33	0/3460	0.66	0/4686
1	j	0.32	0/3460	0.66	0/4686
1	k	0.32	0/3460	0.66	0/4686
1	l	0.33	0/3460	0.64	0/4686
1	m	0.32	0/3460	0.65	0/4686
1	n	0.33	0/3460	0.66	0/4686
2	J	0.34	0/4890	0.65	0/6625
3	I	0.35	0/4319	0.67	0/5849
3	K	0.35	0/4606	0.65	0/6234
4	B	0.34	0/5119	0.70	0/6912
4	D	0.39	0/4897	0.75	0/6610
4	F	0.36	0/5036	0.73	0/6798
4	H	0.37	0/4935	0.74	0/6659
4	N	0.34	0/5001	0.68	0/6750
5	A	0.35	0/5038	0.70	0/6801
5	C	0.37	0/5145	0.68	0/6948
5	E	0.40	0/5311	0.72	0/7169
5	G	0.39	0/5295	0.71	0/7147
5	M	0.34	0/5295	0.67	0/7147
6	L	0.36	0/5051	0.67	0/6860
All	All	0.35	0/118366	0.68	0/160099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
1	b	410/451 (91%)	397 (97%)	12 (3%)	1 (0%)	47	78
1	c	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
1	d	410/451 (91%)	395 (96%)	14 (3%)	1 (0%)	47	78
1	e	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
1	f	410/451 (91%)	393 (96%)	17 (4%)	0	100	100
1	g	410/451 (91%)	390 (95%)	20 (5%)	0	100	100
1	h	410/451 (91%)	396 (97%)	14 (3%)	0	100	100
1	i	410/451 (91%)	396 (97%)	14 (3%)	0	100	100
1	j	410/451 (91%)	391 (95%)	19 (5%)	0	100	100
1	k	410/451 (91%)	395 (96%)	15 (4%)	0	100	100
1	l	410/451 (91%)	397 (97%)	12 (3%)	1 (0%)	47	78
1	m	410/451 (91%)	394 (96%)	14 (3%)	2 (0%)	29	65
1	n	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
2	J	580/1024 (57%)	545 (94%)	35 (6%)	0	100	100
3	I	511/667 (77%)	488 (96%)	23 (4%)	0	100	100
3	K	539/667 (81%)	521 (97%)	18 (3%)	0	100	100
4	B	602/907 (66%)	573 (95%)	29 (5%)	0	100	100
4	D	571/907 (63%)	542 (95%)	27 (5%)	2 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	591/907 (65%)	554 (94%)	37 (6%)	0	100	100
4	H	576/907 (64%)	549 (95%)	27 (5%)	0	100	100
4	N	584/907 (64%)	562 (96%)	21 (4%)	1 (0%)	47	78
5	A	595/902 (66%)	570 (96%)	25 (4%)	0	100	100
5	C	606/902 (67%)	575 (95%)	30 (5%)	1 (0%)	47	78
5	E	626/902 (69%)	599 (96%)	27 (4%)	0	100	100
5	G	624/902 (69%)	593 (95%)	31 (5%)	0	100	100
5	M	624/902 (69%)	595 (95%)	29 (5%)	0	100	100
6	L	610/1819 (34%)	575 (94%)	34 (6%)	1 (0%)	47	78
All	All	13979/19536 (72%)	13361 (96%)	608 (4%)	10 (0%)	54	83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	500	LEU
4	D	495	GLN
4	N	542	SER
1	b	408	PHE
4	D	497	CYS
1	m	408	PHE
1	l	406	GLU
1	m	407	GLN
1	d	407	GLN
6	L	1688	ILE

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	377/400 (94%)	376 (100%)	1 (0%)	92	96
1	b	377/400 (94%)	377 (100%)	0	100	100
1	c	377/400 (94%)	376 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	377/400 (94%)	377 (100%)	0	100	100
1	e	377/400 (94%)	377 (100%)	0	100	100
1	f	376/400 (94%)	376 (100%)	0	100	100
1	g	377/400 (94%)	376 (100%)	1 (0%)	92	96
1	h	376/400 (94%)	375 (100%)	1 (0%)	92	96
1	i	377/400 (94%)	377 (100%)	0	100	100
1	j	377/400 (94%)	377 (100%)	0	100	100
1	k	377/400 (94%)	377 (100%)	0	100	100
1	l	377/400 (94%)	374 (99%)	3 (1%)	81	89
1	m	377/400 (94%)	374 (99%)	3 (1%)	81	89
1	n	377/400 (94%)	377 (100%)	0	100	100
2	J	525/933 (56%)	525 (100%)	0	100	100
3	I	471/594 (79%)	470 (100%)	1 (0%)	93	97
3	K	500/594 (84%)	499 (100%)	1 (0%)	93	97
4	B	547/798 (68%)	546 (100%)	1 (0%)	93	97
4	D	525/798 (66%)	524 (100%)	1 (0%)	93	97
4	F	539/798 (68%)	539 (100%)	0	100	100
4	H	528/798 (66%)	528 (100%)	0	100	100
4	N	536/798 (67%)	535 (100%)	1 (0%)	93	97
5	A	544/791 (69%)	544 (100%)	0	100	100
5	C	555/791 (70%)	553 (100%)	2 (0%)	91	95
5	E	574/791 (73%)	573 (100%)	1 (0%)	93	97
5	G	572/791 (72%)	570 (100%)	2 (0%)	92	96
5	M	572/791 (72%)	572 (100%)	0	100	100
6	L	539/1546 (35%)	539 (100%)	0	100	100
All	All	12803/17212 (74%)	12783 (100%)	20 (0%)	93	97

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	333	ARG
4	B	285	ARG
5	C	347	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	458	ASN
4	D	495	GLN
5	E	423	TYR
5	G	423	TYR
5	G	843	TYR
3	I	532	LEU
4	N	543	LYS
1	a	407	GLN
1	c	295	ARG
1	g	341	ARG
1	h	407	GLN
1	l	343	ARG
1	l	404	PHE
1	l	408	PHE
1	m	406	GLU
1	m	407	GLN
1	m	408	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	198	ASN
2	J	721	GLN
2	J	898	HIS
4	B	461	HIS
4	D	424	HIS
4	D	774	GLN
5	E	424	ASN
5	E	458	ASN
4	F	885	HIS
5	G	512	HIS
5	G	763	GLN
4	H	596	ASN
4	H	716	HIS
4	H	855	GLN
4	H	883	ASN
6	L	507	GLN
6	L	1522	HIS
5	A	412	HIS
5	A	465	HIS
1	a	198	ASN
1	b	332	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	198	ASN
1	d	16	GLN
1	d	198	ASN
1	d	357	GLN
1	e	139	HIS
1	e	198	ASN
1	e	299	GLN
1	e	371	HIS
1	f	198	ASN
1	f	371	HIS
1	g	198	ASN
1	g	347	ASN
1	h	29	HIS
1	h	198	ASN
1	h	357	GLN
1	h	407	GLN
1	j	198	ASN
1	l	198	ASN
1	m	198	ASN
1	m	407	GLN
1	n	198	ASN
1	n	221	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

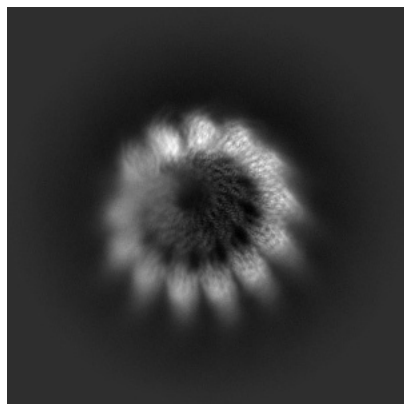
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18181. These allow visual inspection of the internal detail of the map and identification of artifacts.

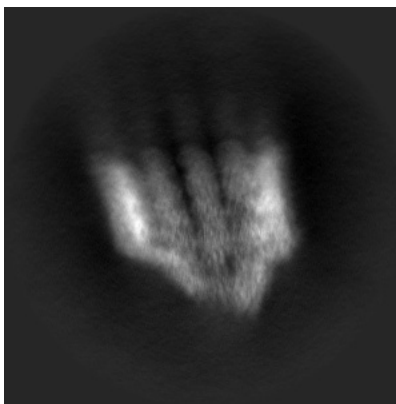
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

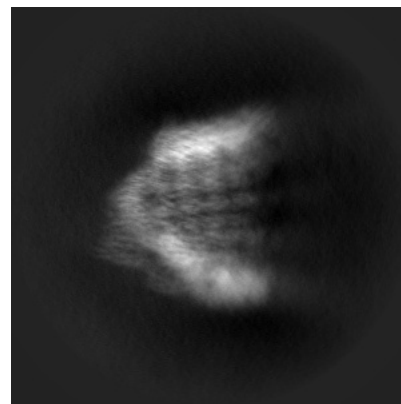
6.1.1 Primary map



X

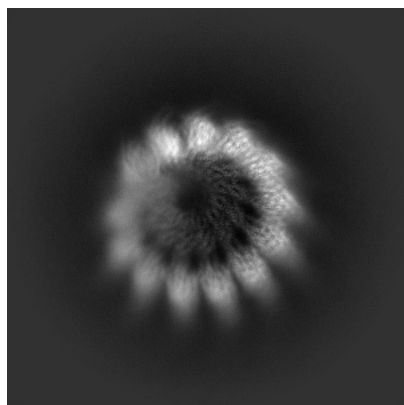


Y

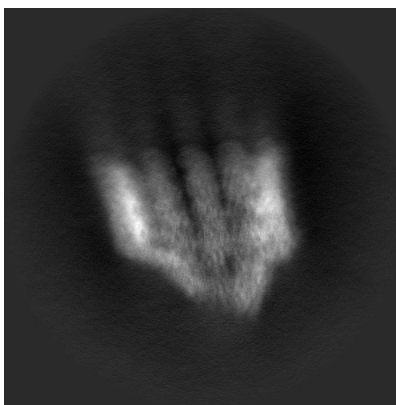


Z

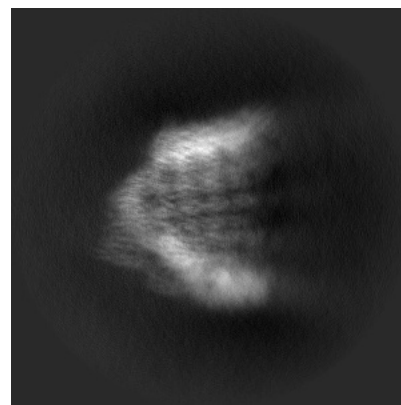
6.1.2 Raw map



X



Y

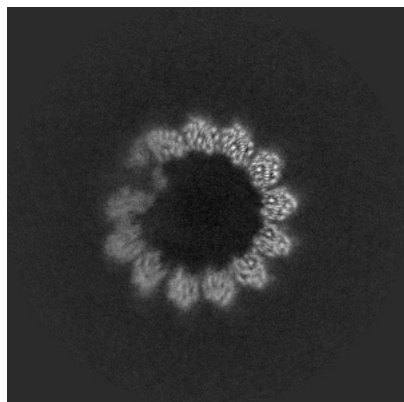


Z

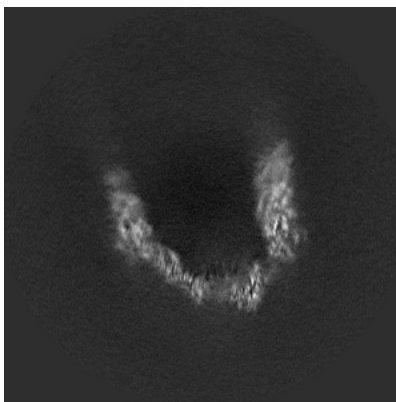
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

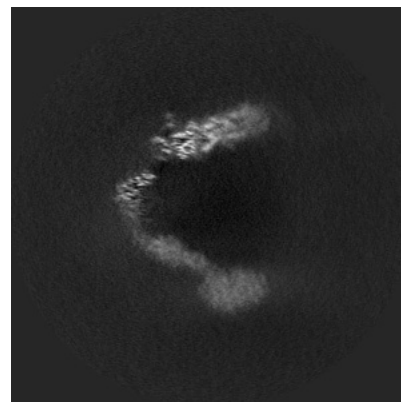
6.2.1 Primary map



X Index: 215

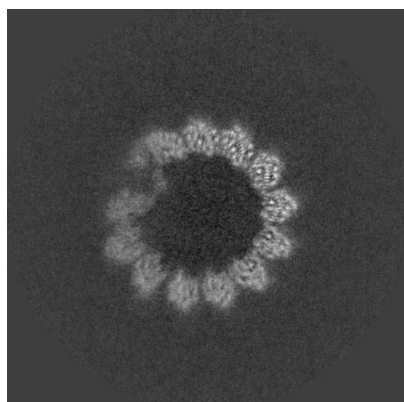


Y Index: 215

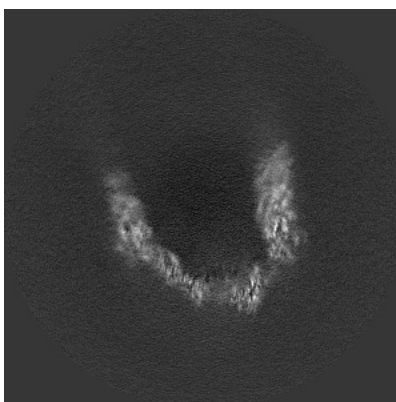


Z Index: 215

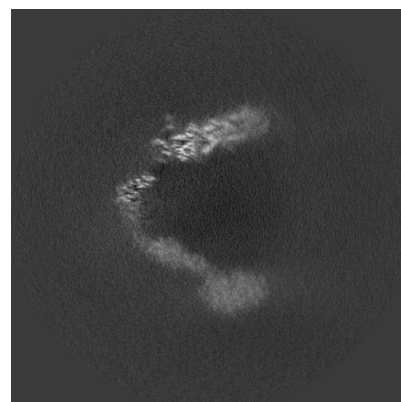
6.2.2 Raw map



X Index: 215



Y Index: 215

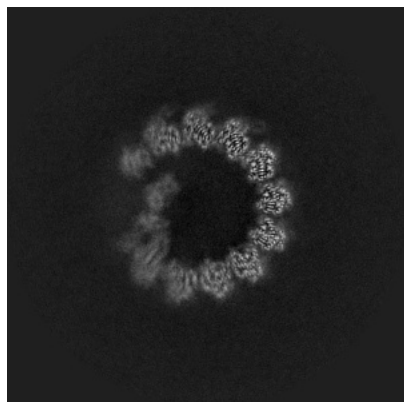


Z Index: 215

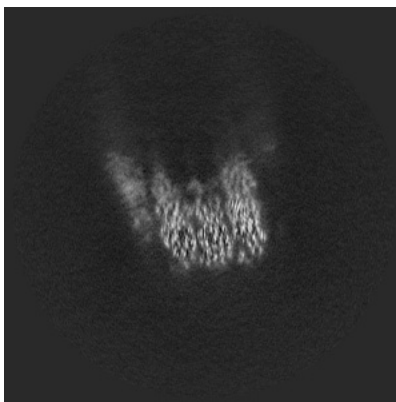
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

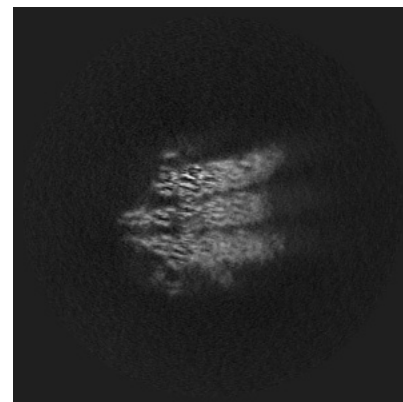
6.3.1 Primary map



X Index: 189

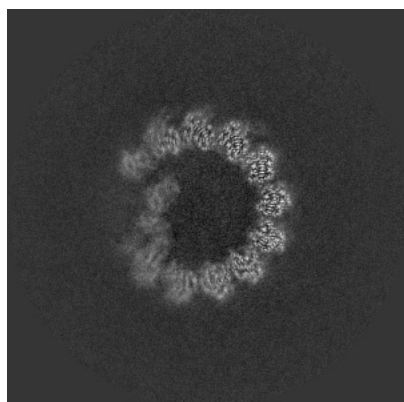


Y Index: 280

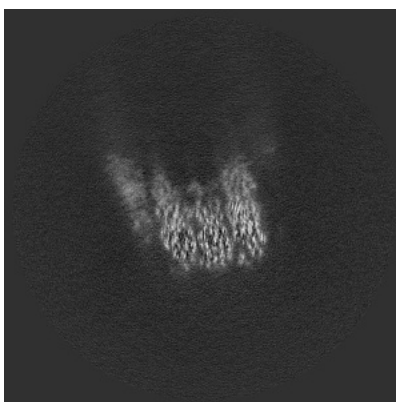


Z Index: 284

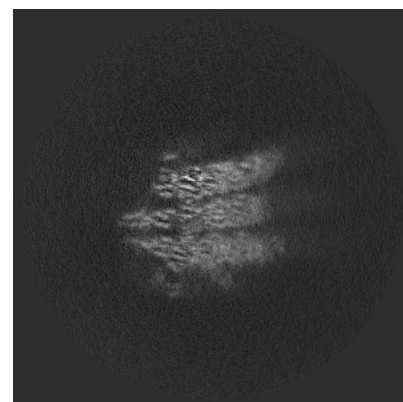
6.3.2 Raw map



X Index: 188



Y Index: 280

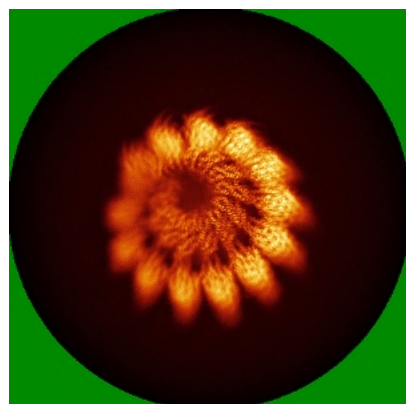


Z Index: 284

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

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

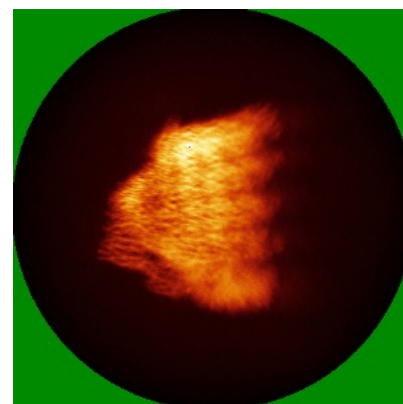
6.4.1 Primary map



X

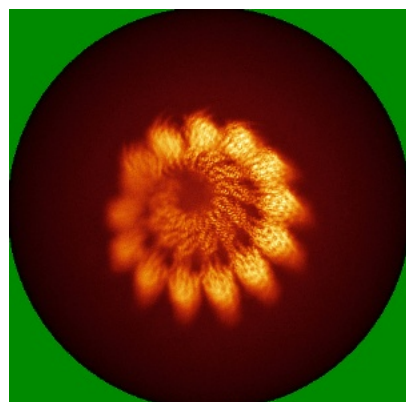


Y

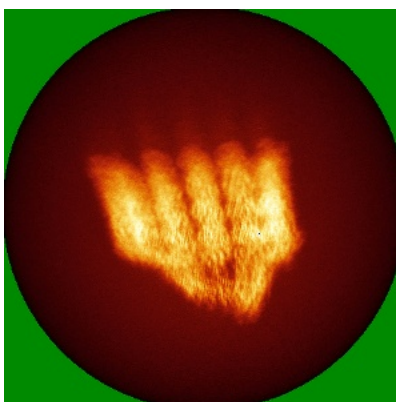


Z

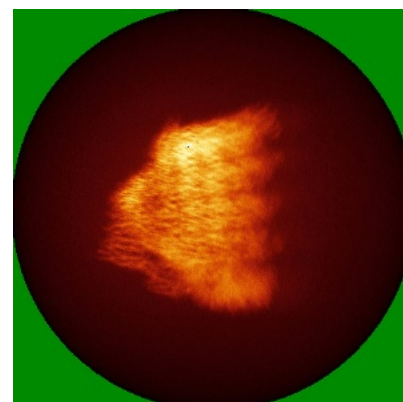
6.4.2 Raw map



X



Y

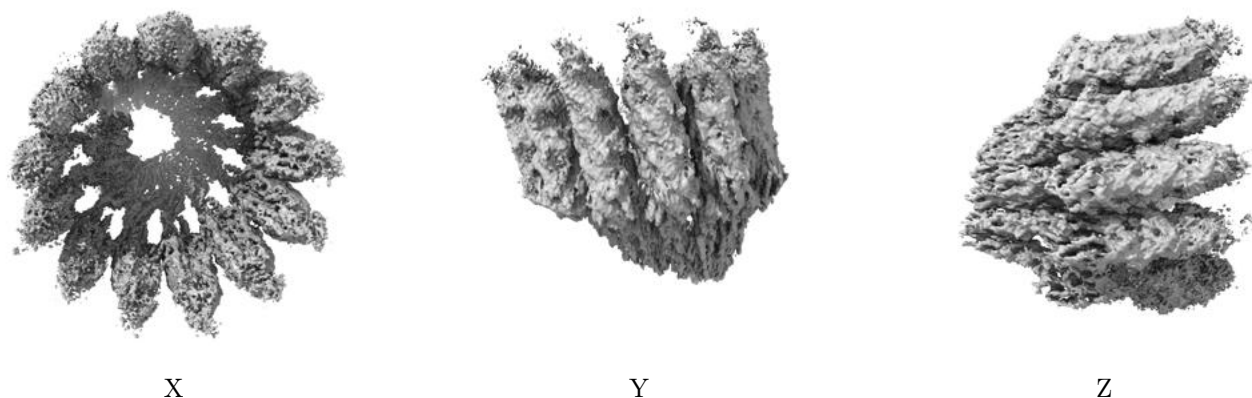


Z

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.

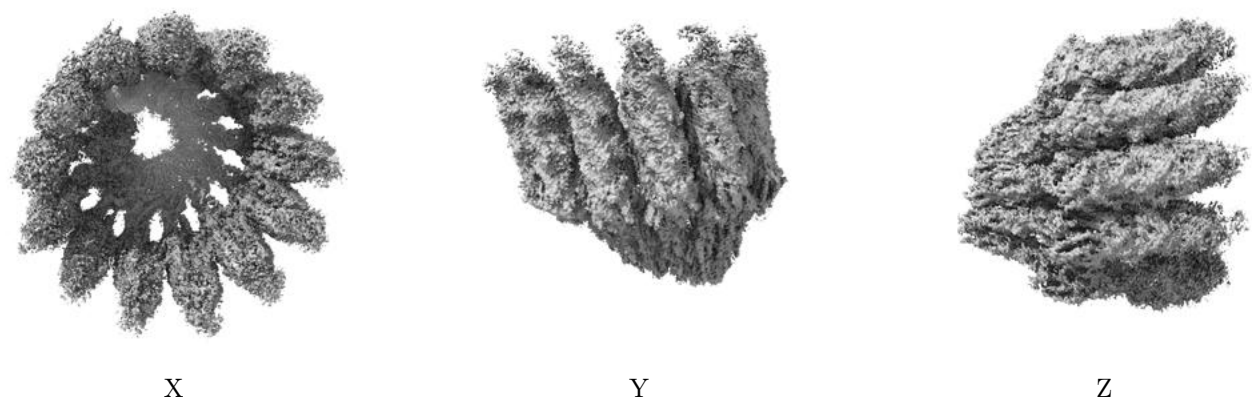
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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



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.

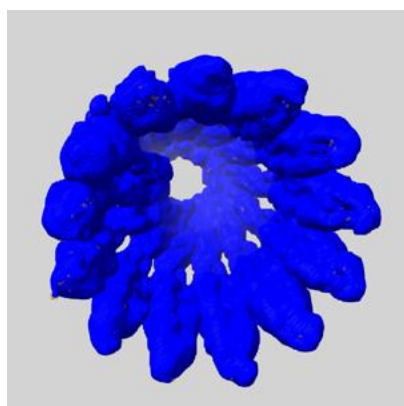
6.6 Mask visualisation [i](#)

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

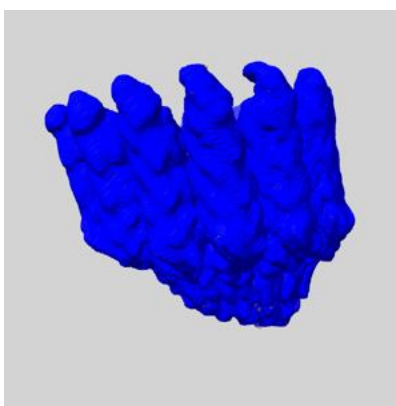
A mask typically either:

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

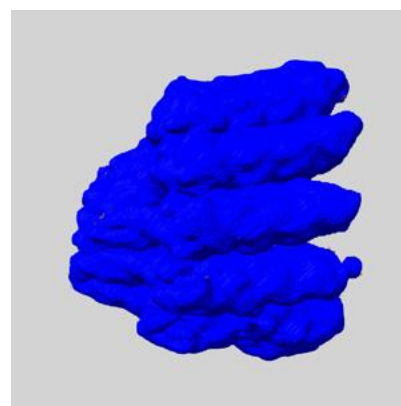
6.6.1 emd_18181_msk_1.map [i](#)



X



Y

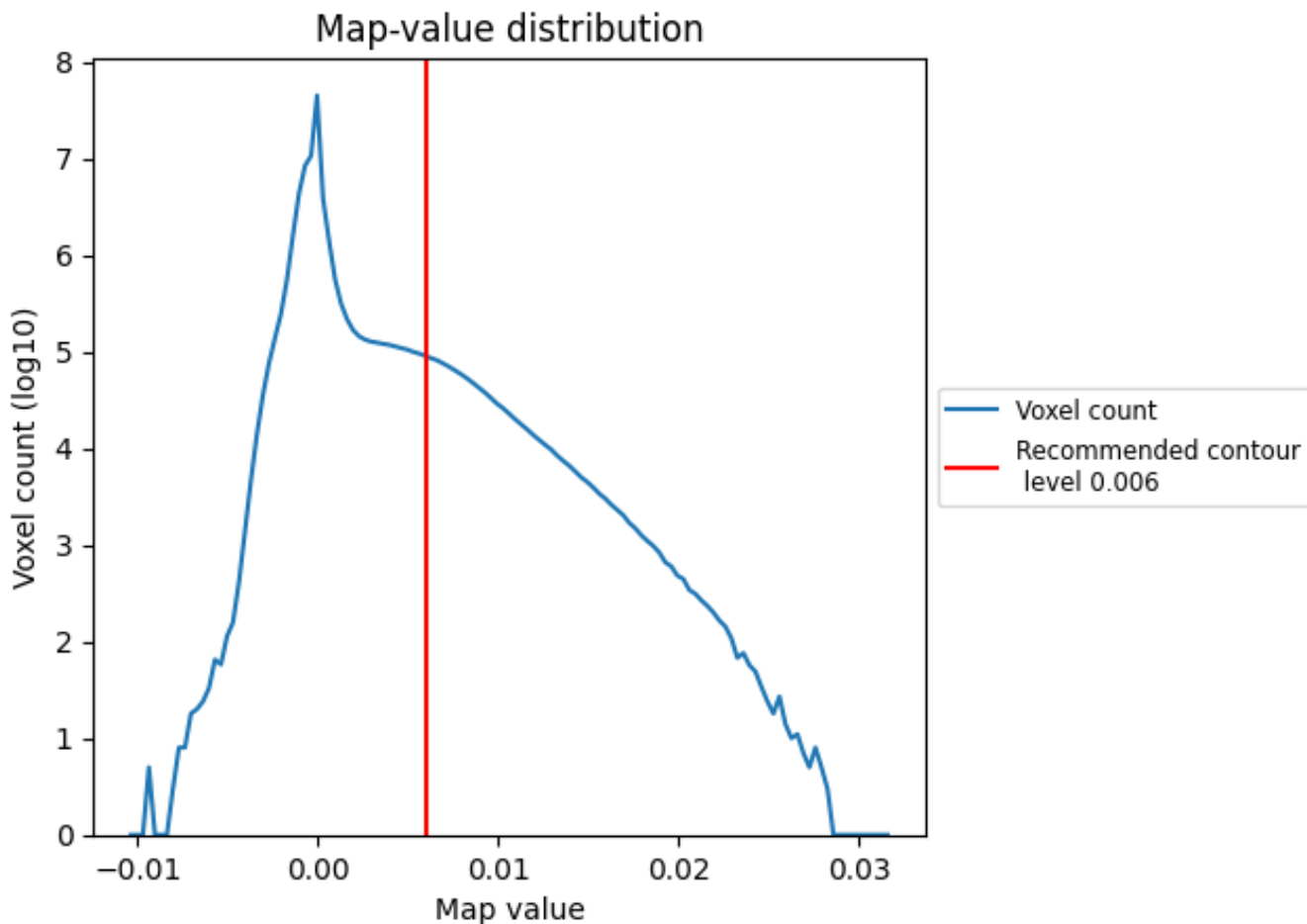


Z

7 Map analysis [i](#)

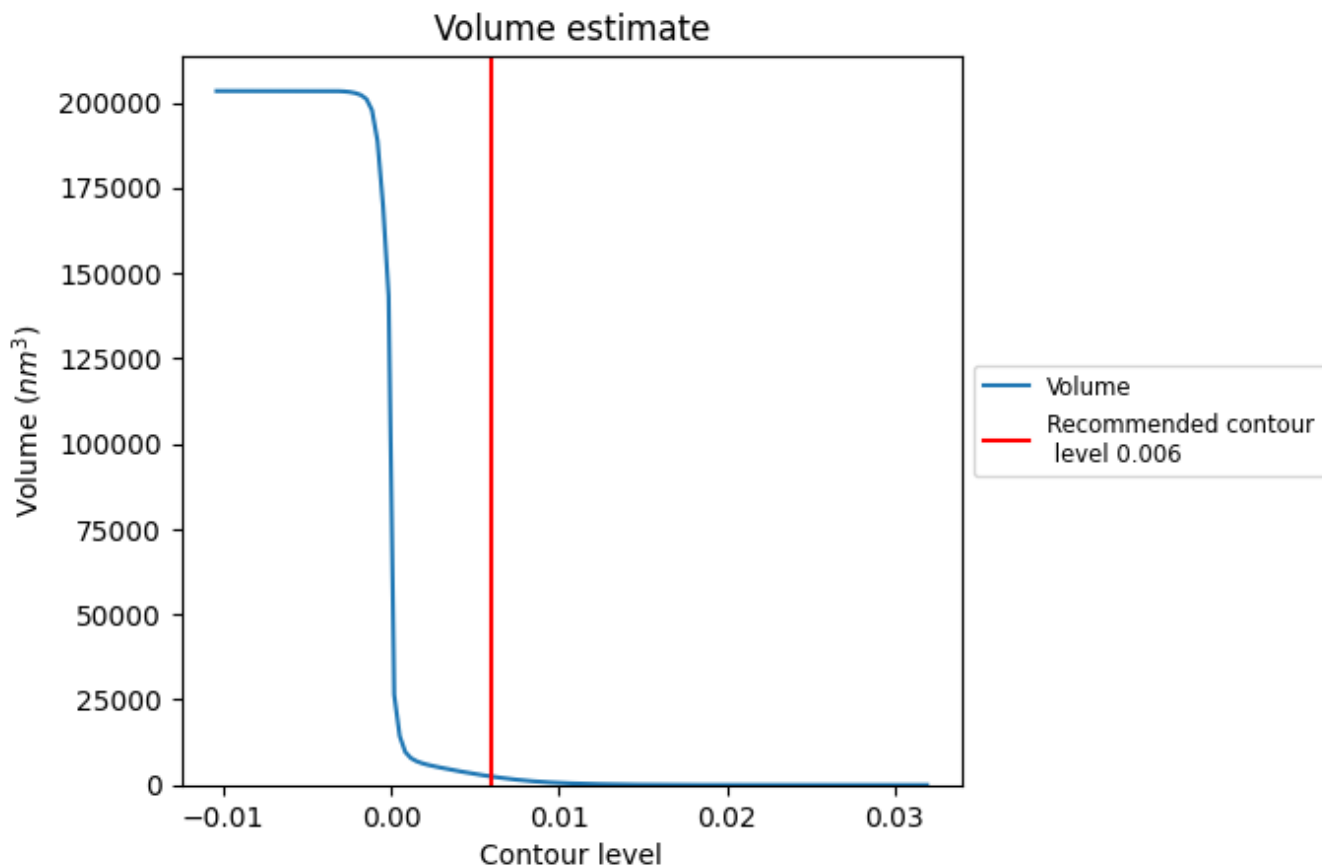
This section contains the results of statistical analysis of the map.

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.

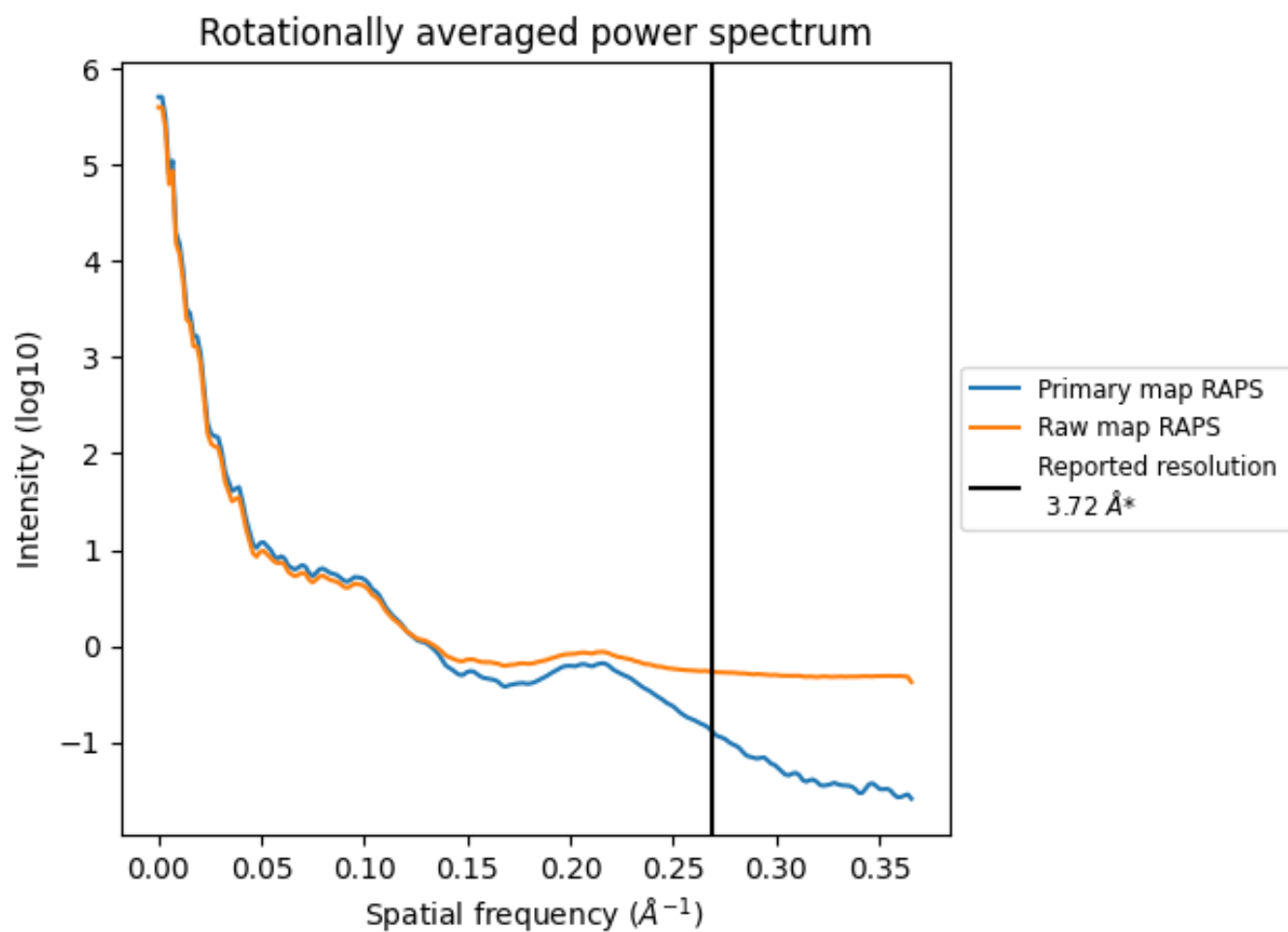
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2467 nm^3 ; this corresponds to an approximate mass of 2228 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

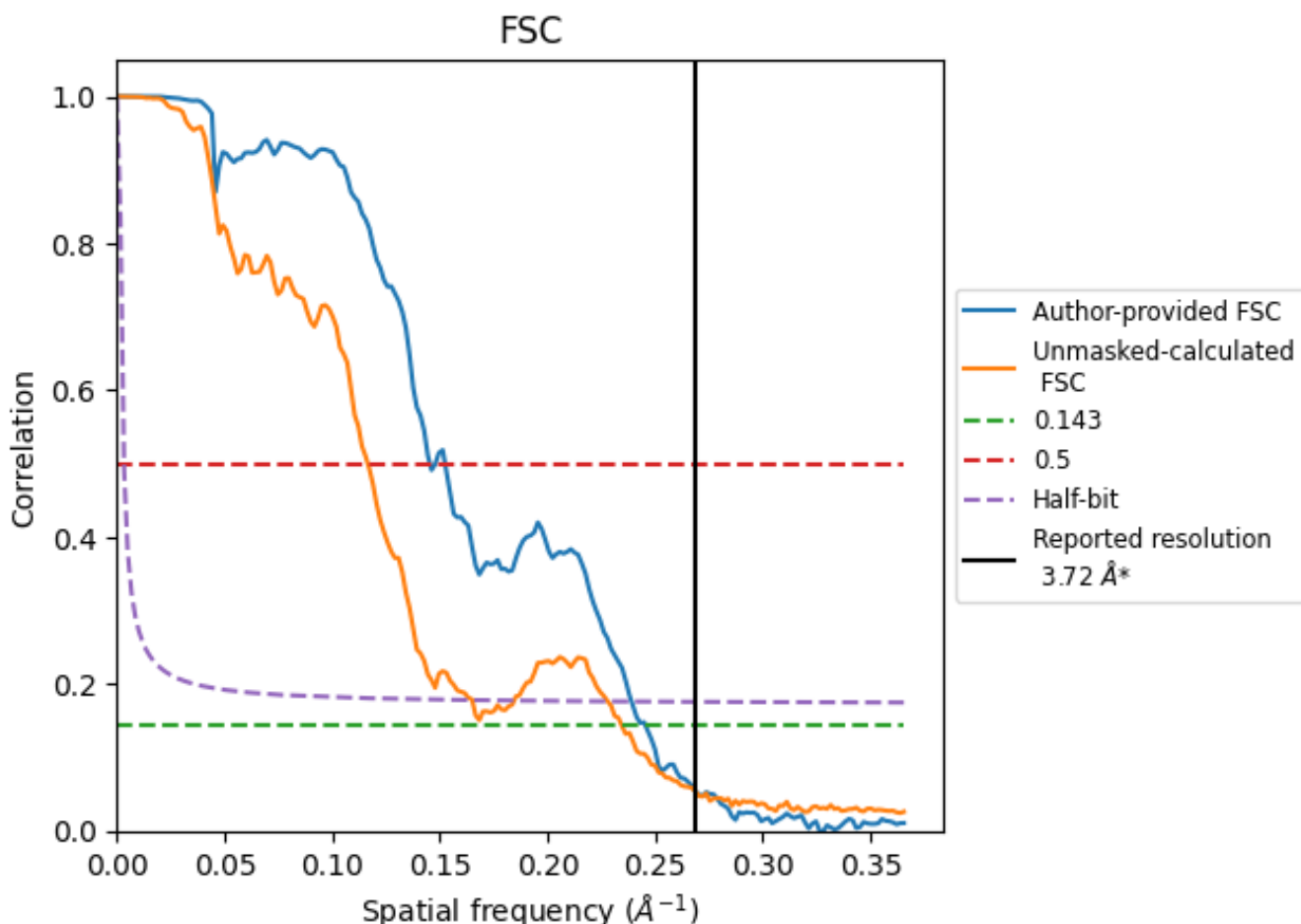


*Reported resolution corresponds to spatial frequency of 0.269 Å⁻¹

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 0.269 Å⁻¹

8.2 Resolution estimates [i](#)

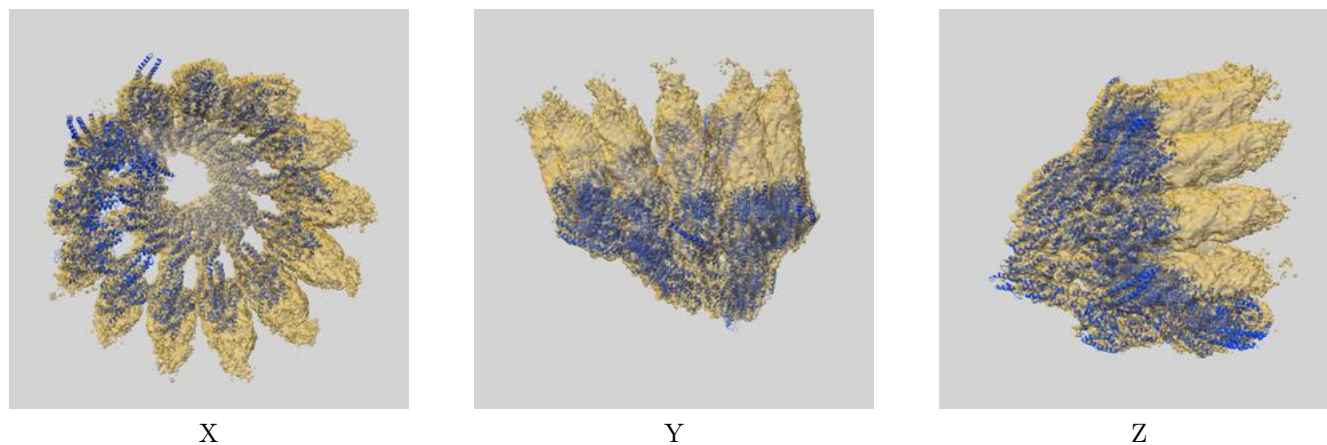
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	4.07	6.87	4.18
Unmasked-calculated*	4.26	8.58	6.06

*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 4.26 differs from the reported value 3.72 by more than 10 %

9 Map-model fit [i](#)

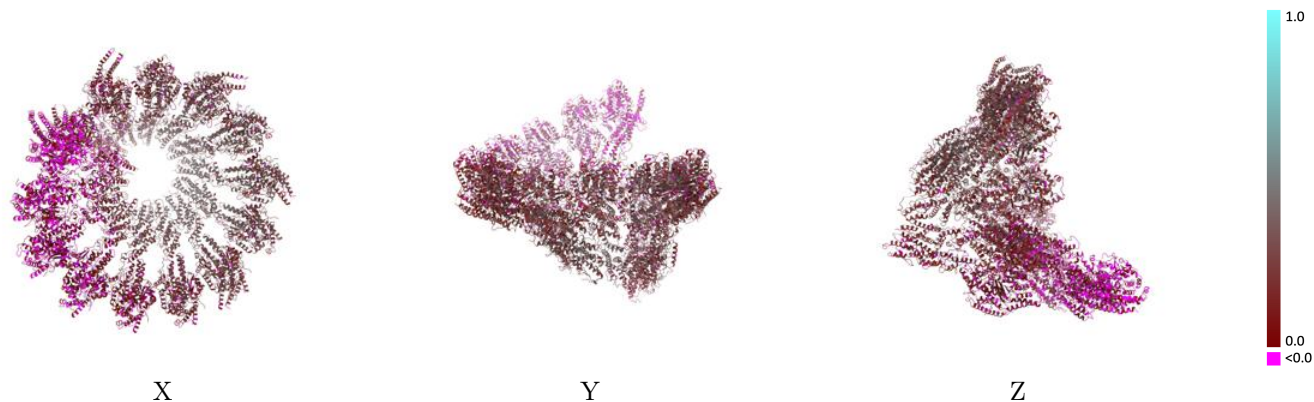
This section contains information regarding the fit between EMDB map EMD-18181 and PDB model 8Q62. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



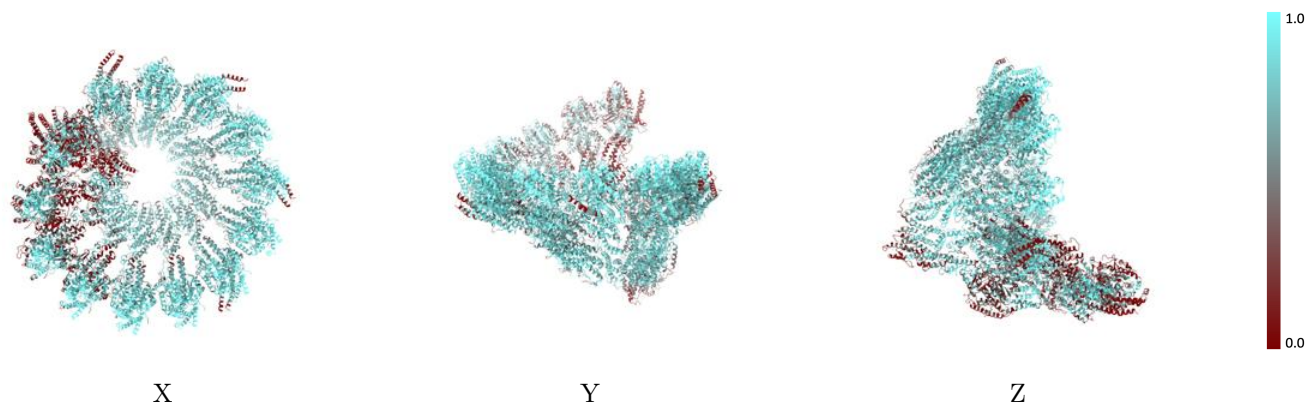
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



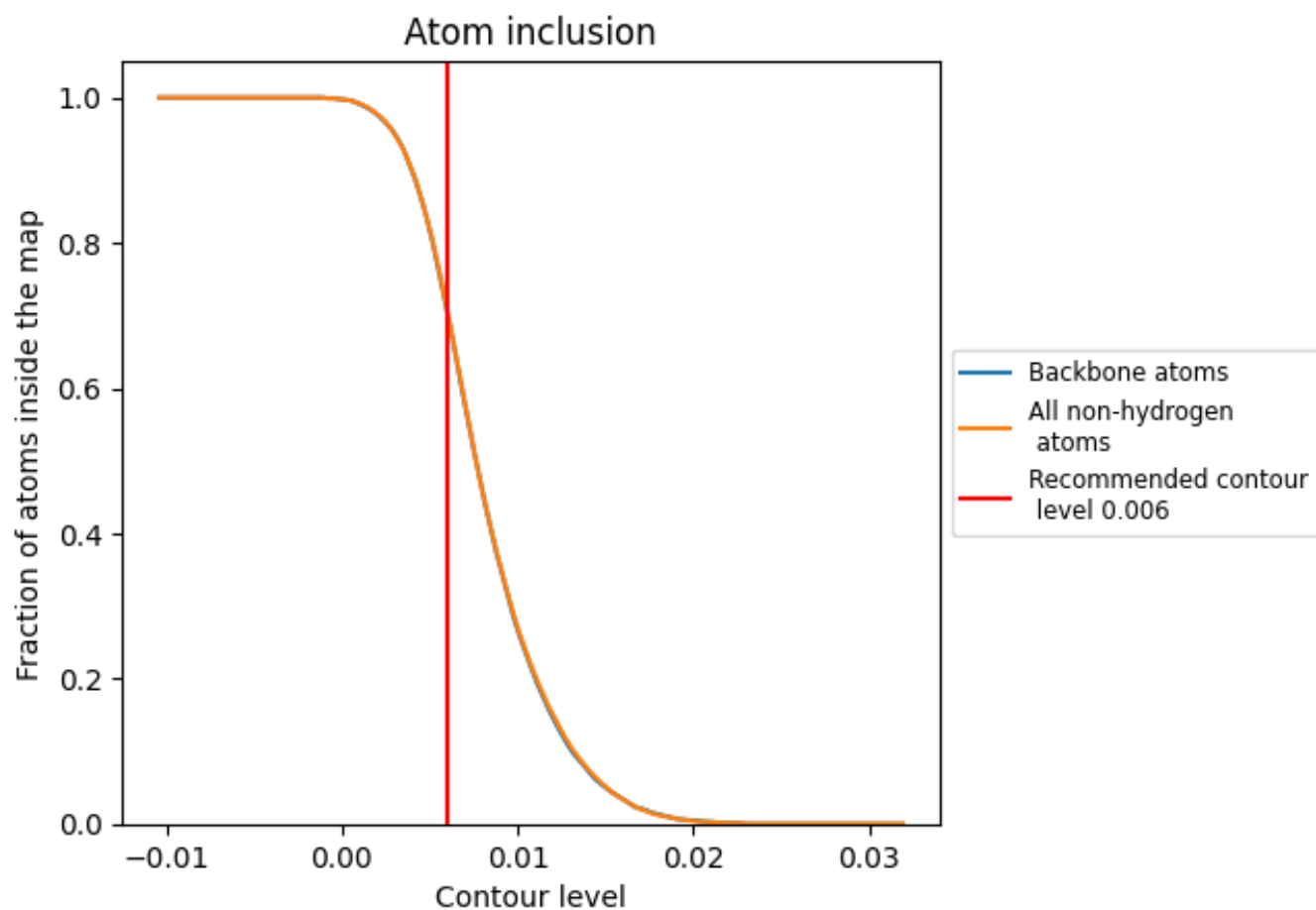
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 71% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.1770
A	 0.4680	 0.1320
B	 0.6230	 0.1790
C	 0.7620	 0.2330
D	 0.7560	 0.2680
E	 0.7890	 0.2940
F	 0.7840	 0.3040
G	 0.7700	 0.2970
H	 0.7740	 0.2800
I	 0.7560	 0.2340
J	 0.7860	 0.1890
K	 0.7270	 0.1210
L	 0.6040	 0.0830
M	 0.5480	 0.0630
N	 0.3180	 0.0450
a	 0.4800	 0.0950
b	 0.7720	 0.1630
c	 0.8480	 0.2190
d	 0.8830	 0.2490
e	 0.9100	 0.2680
f	 0.8890	 0.2630
g	 0.9070	 0.2570
h	 0.8810	 0.2240
i	 0.8840	 0.1740
j	 0.8490	 0.0990
k	 0.7360	 0.0480
l	 0.6620	 0.0250
m	 0.5100	 0.0220
n	 0.3960	 0.0060

