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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

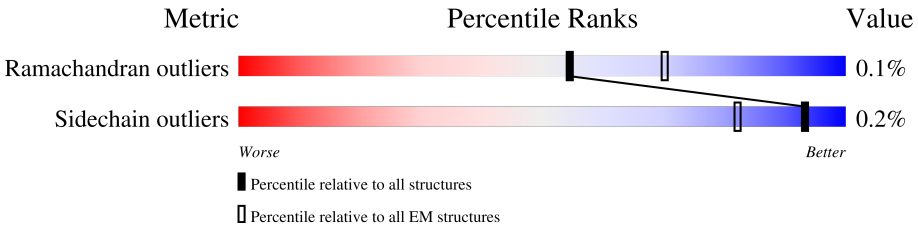
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 <=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	7% 93% 7%
1	k	451	20% 93% 7%
1	l	451	26% 92% 7%
1	m	451	40% 92% 7%
1	n	451	49% 93% 7%
2	J	1024	6% 58% 42%
3	I	667	8% 78% 22%
3	K	667	14% 83% 17%
4	B	907	17% 67% 33%
4	D	907	6% 64% 36%
4	F	907	5% 66% 34%
4	H	907	5% 65% 35%
4	N	907	44% 65% 35%
5	A	902	31% 68% 32%
5	C	902	7% 68% 31%
5	E	902	5% 71% 29%
5	G	902	5% 70% 29%
5	M	902	27% 71% 29%
6	L	1819	12% 34% 66%

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
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
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
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.

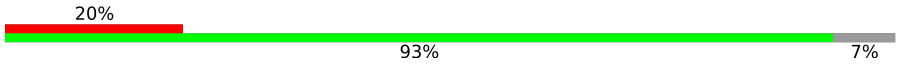
Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	616	Total	C	H	N	O	S	0	0
			9869	3211	4951	826	855	26		

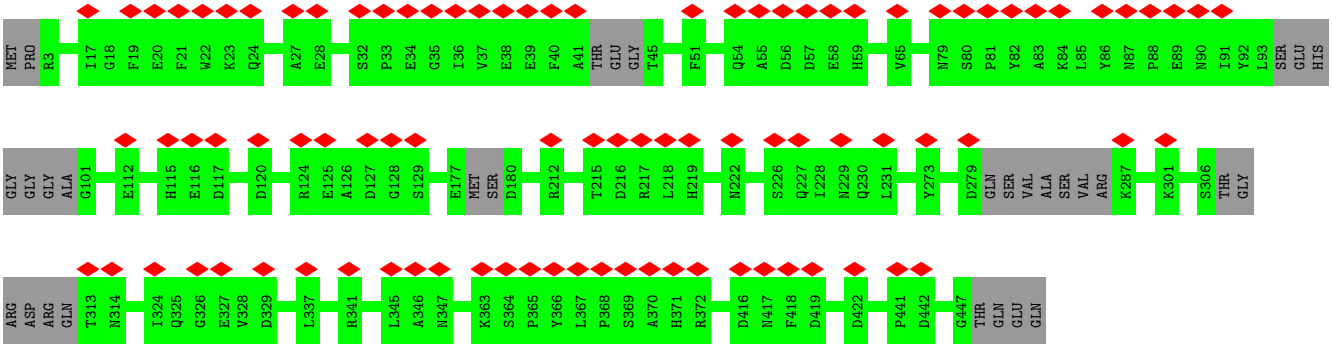
3 Residue-property plots (i)

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

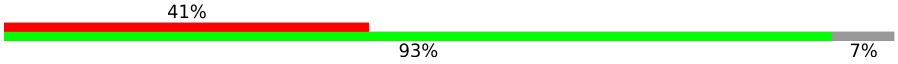
Chain k:

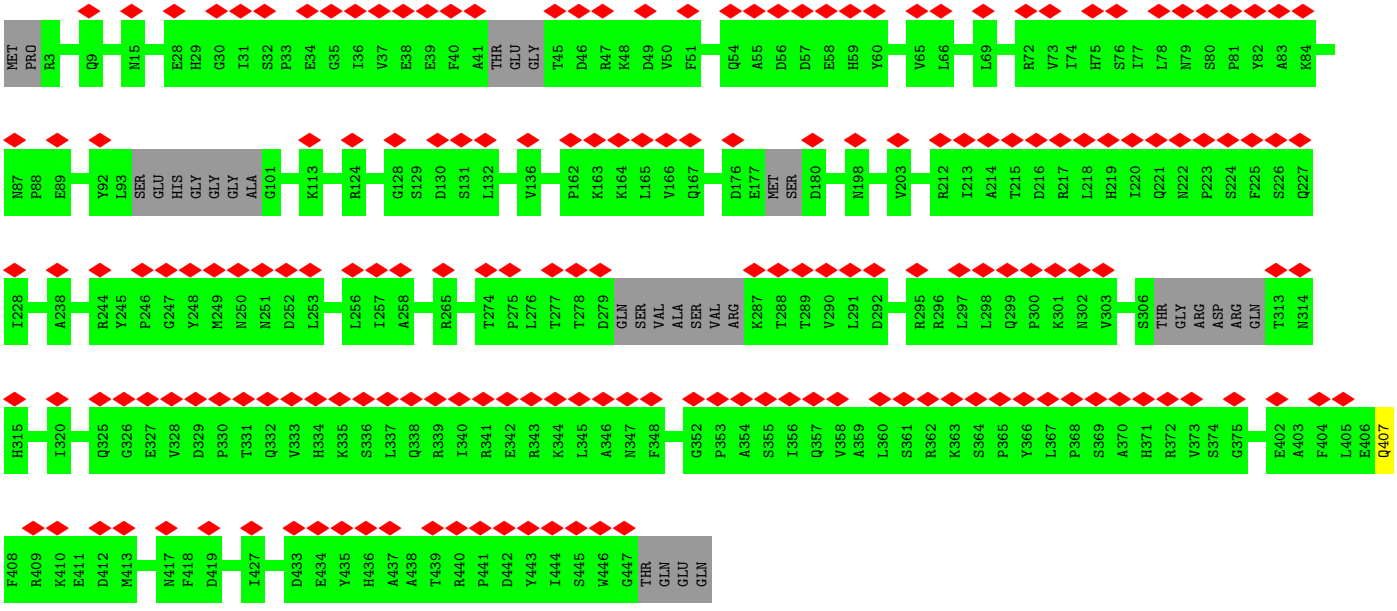




• Molecule 1: Tubulin gamma-1 chain

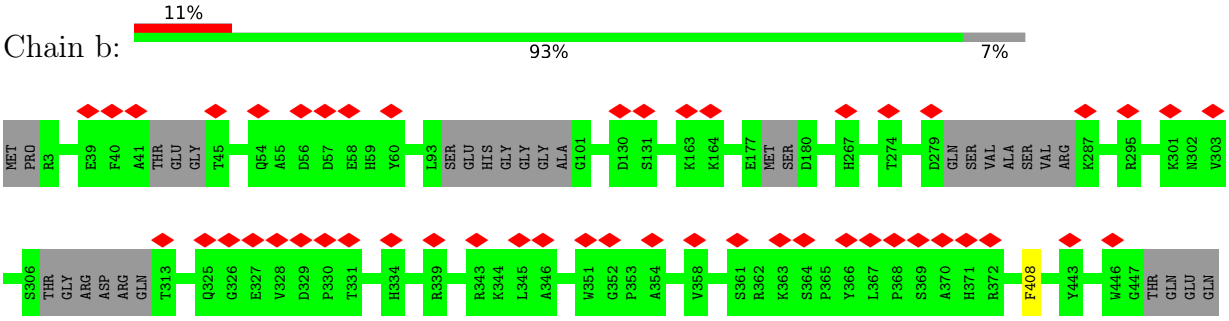
Chain a:





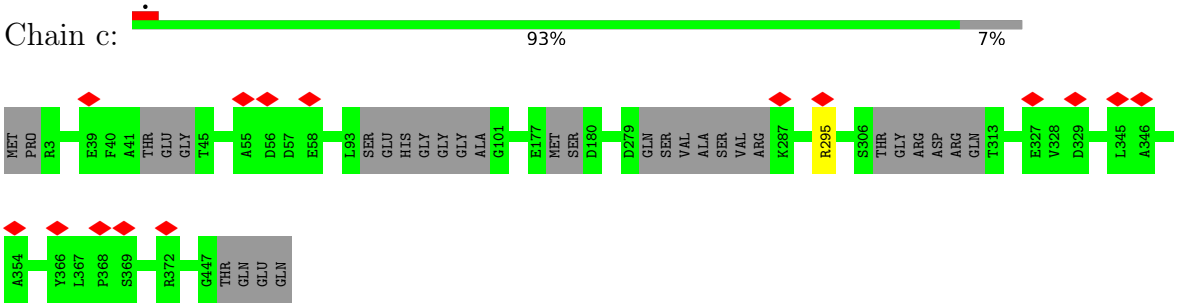
• Molecule 1: Tubulin gamma-1 chain

Chain b:



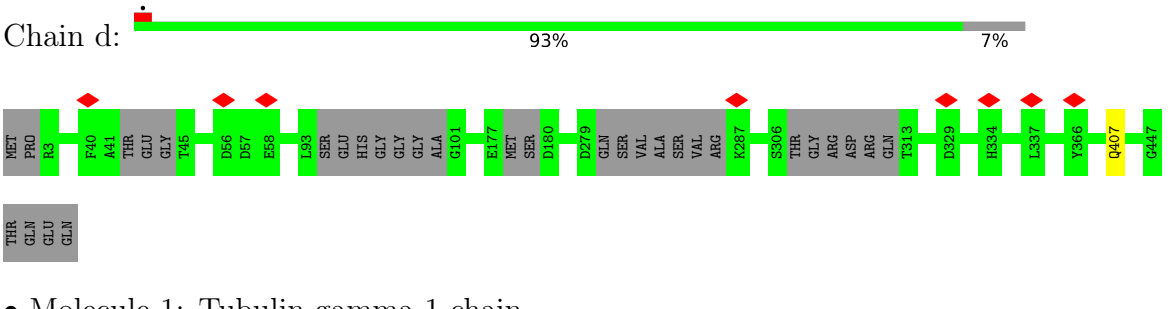
• Molecule 1: Tubulin gamma-1 chain

Chain c:



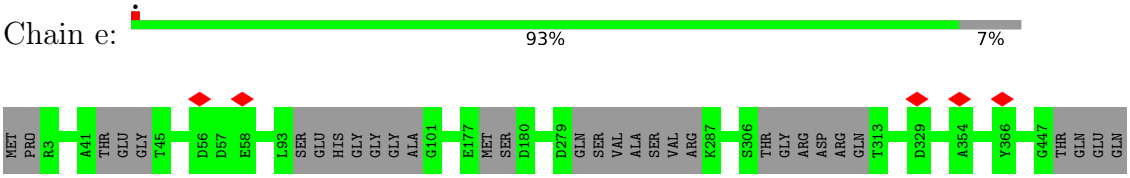
• Molecule 1: Tubulin gamma-1 chain

Chain d:



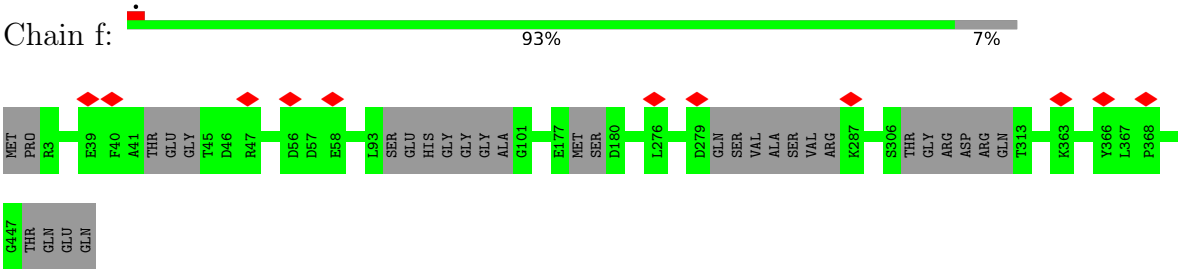
• Molecule 1: Tubulin gamma-1 chain

Chain e:



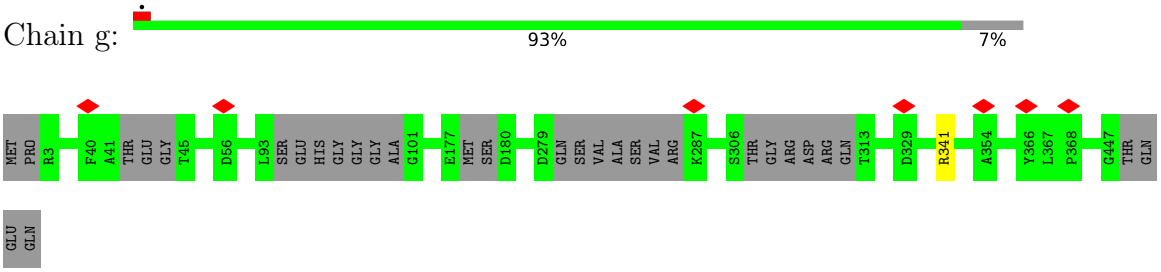
• Molecule 1: Tubulin gamma-1 chain

Chain f:



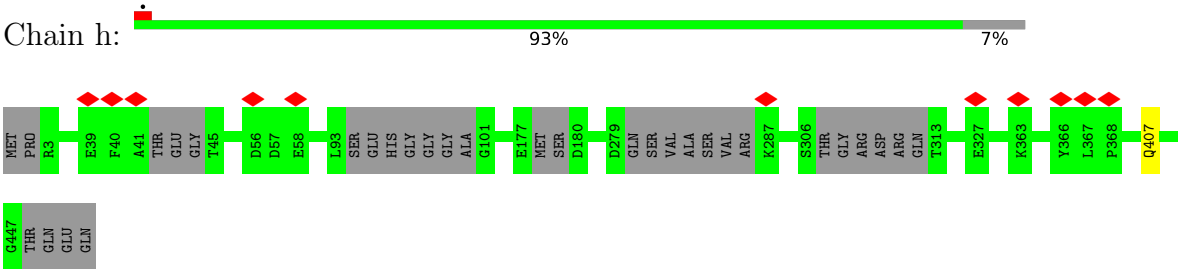
• Molecule 1: Tubulin gamma-1 chain

Chain g:



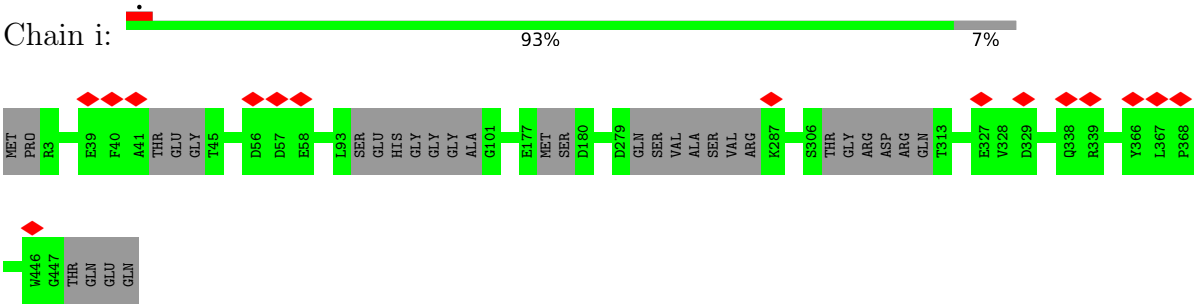
• Molecule 1: Tubulin gamma-1 chain

Chain h:



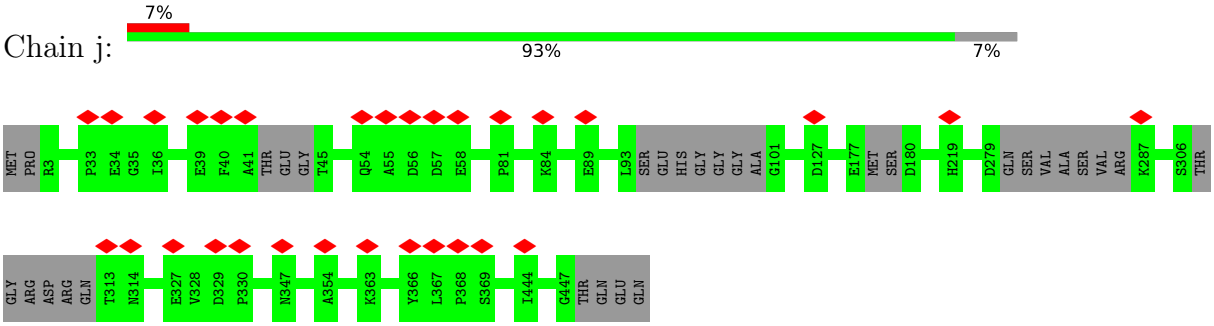
• Molecule 1: Tubulin gamma-1 chain

Chain i:



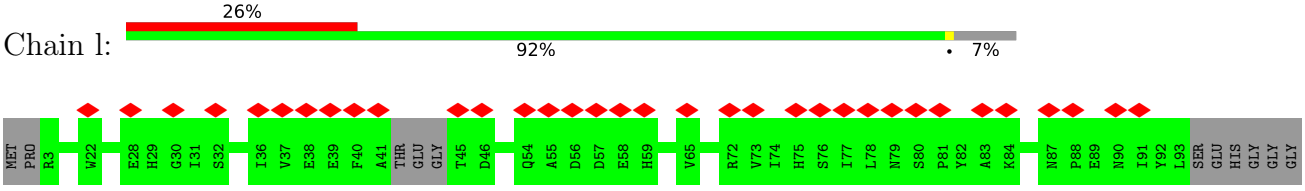
• Molecule 1: Tubulin gamma-1 chain

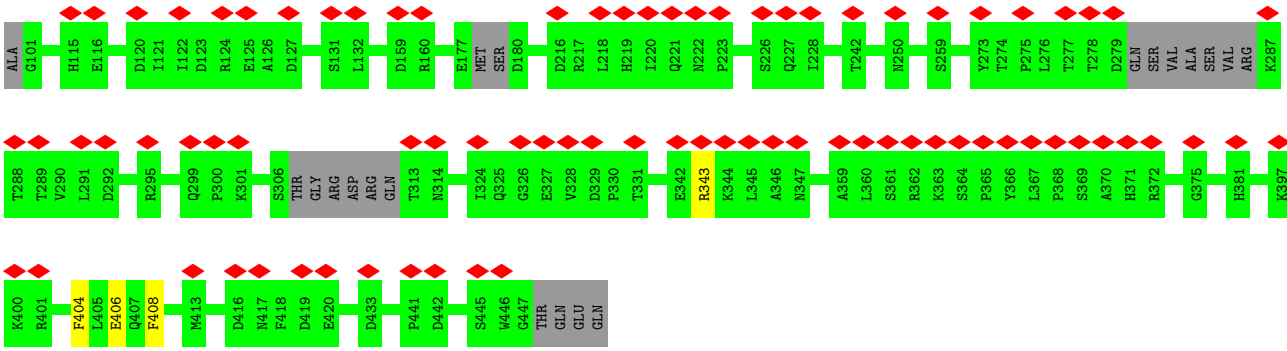
Chain j:



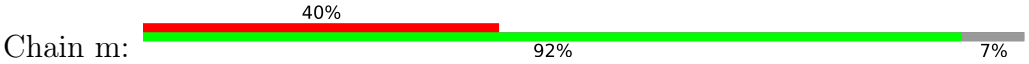
• Molecule 1: Tubulin gamma-1 chain

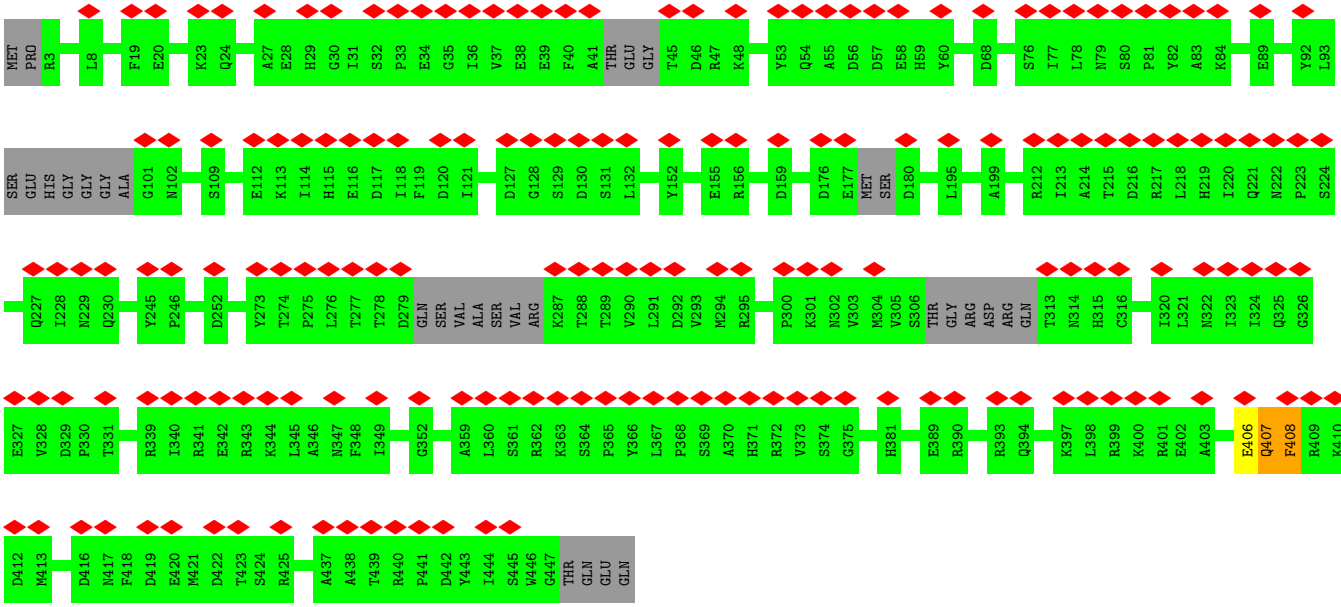
Chain l:



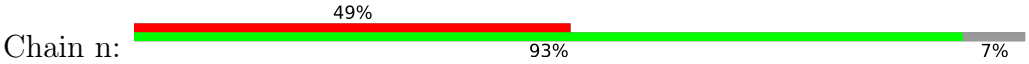


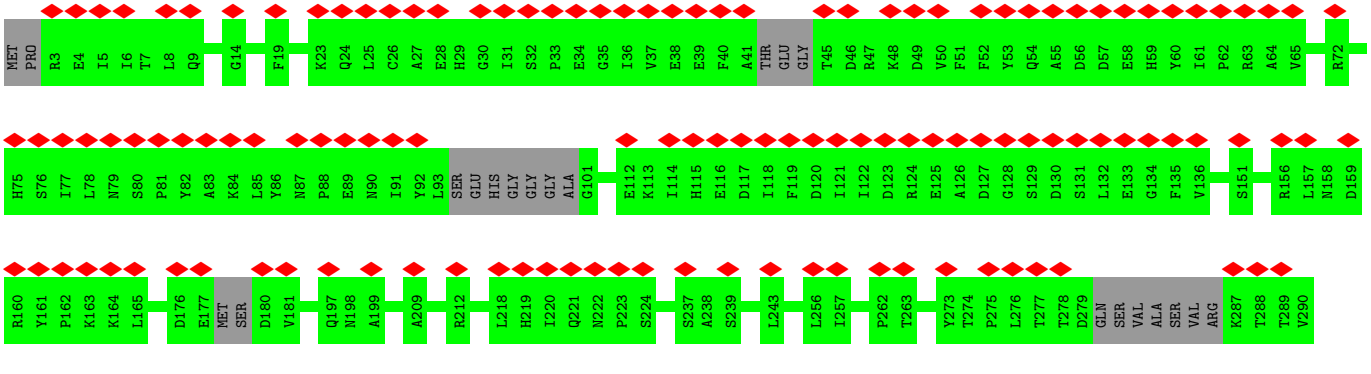
• Molecule 1: Tubulin gamma-1 chain

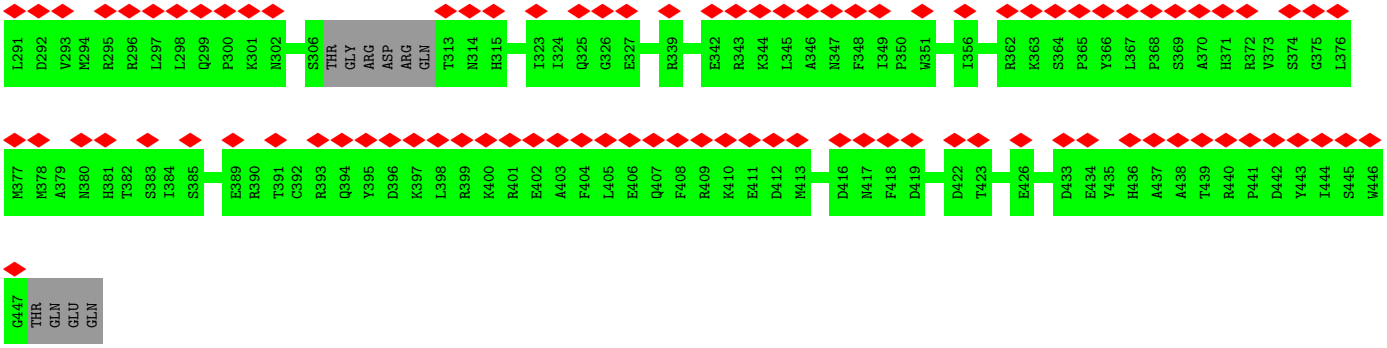




• Molecule 1: Tubulin gamma-1 chain

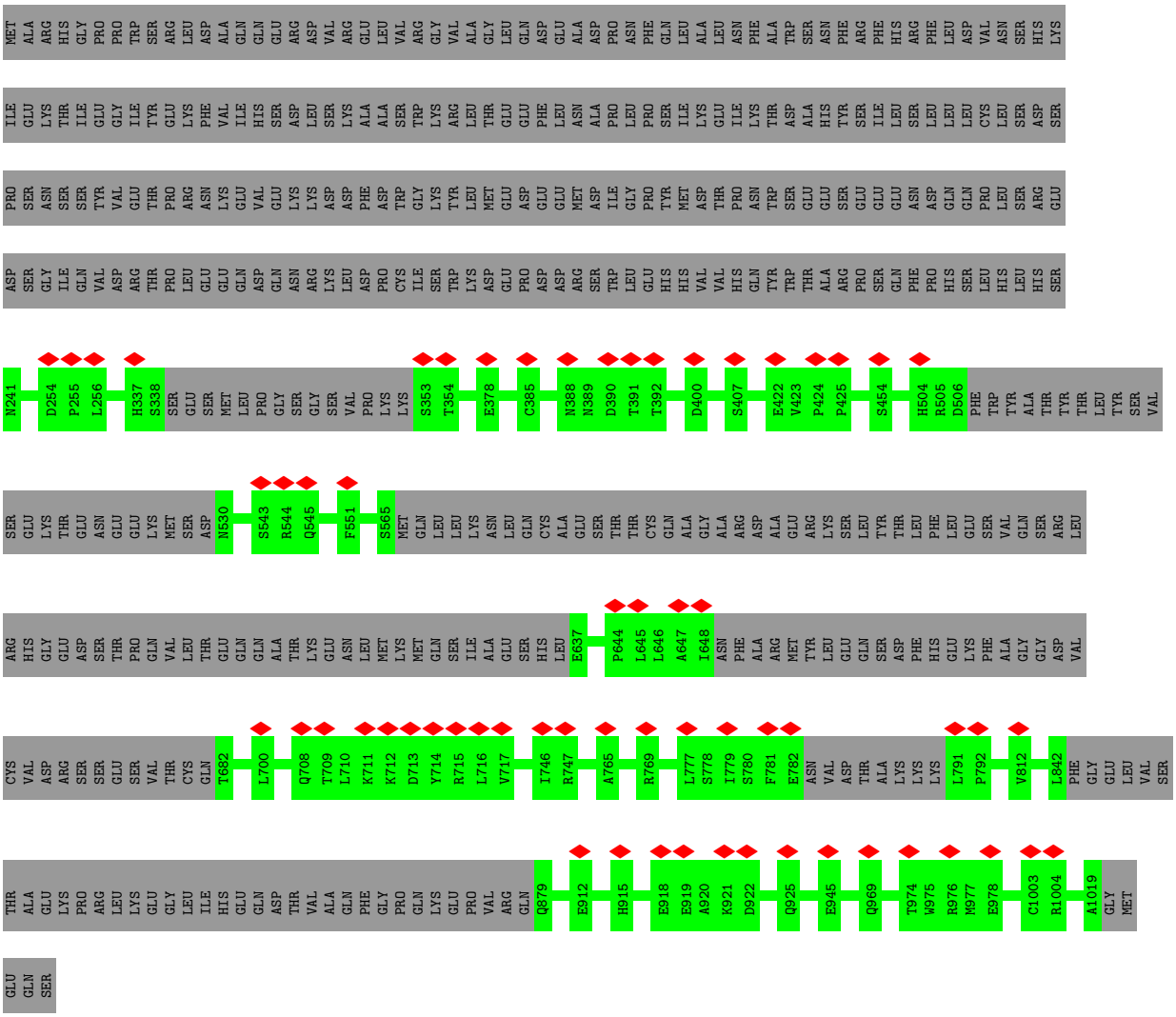






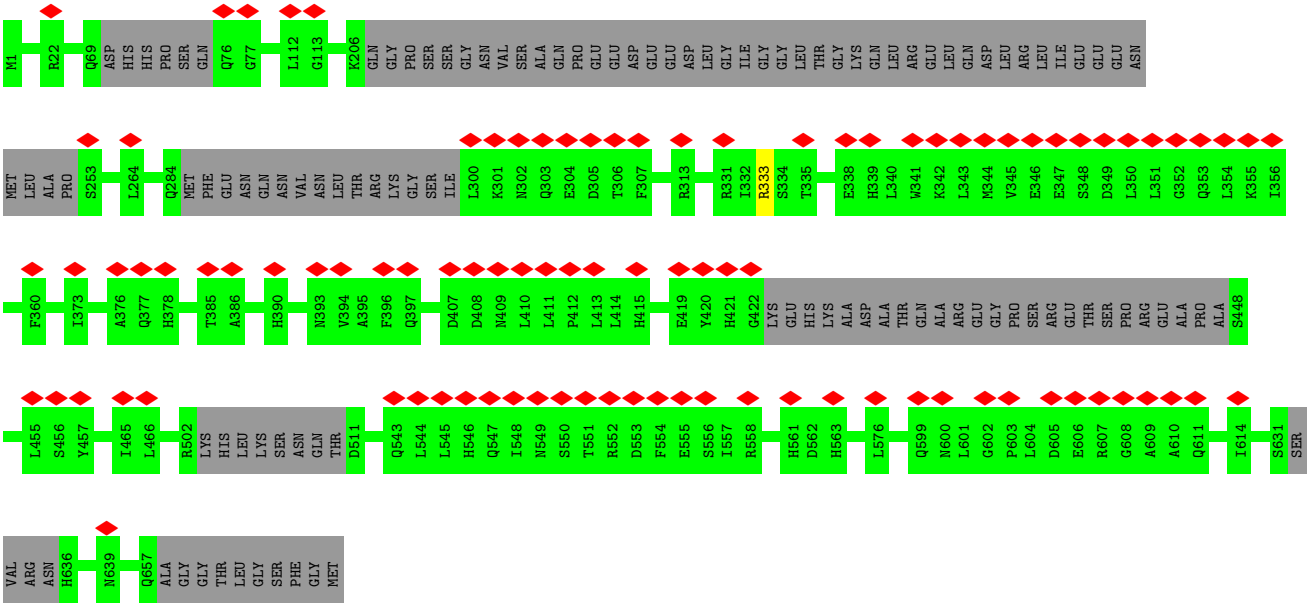
• Molecule 2: Gamma-tubulin complex component 5

Chain J:



• Molecule 3: Gamma-tubulin complex component 4

Chain K:

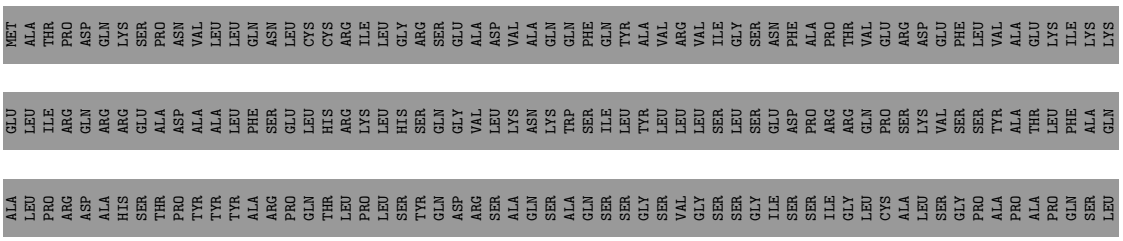


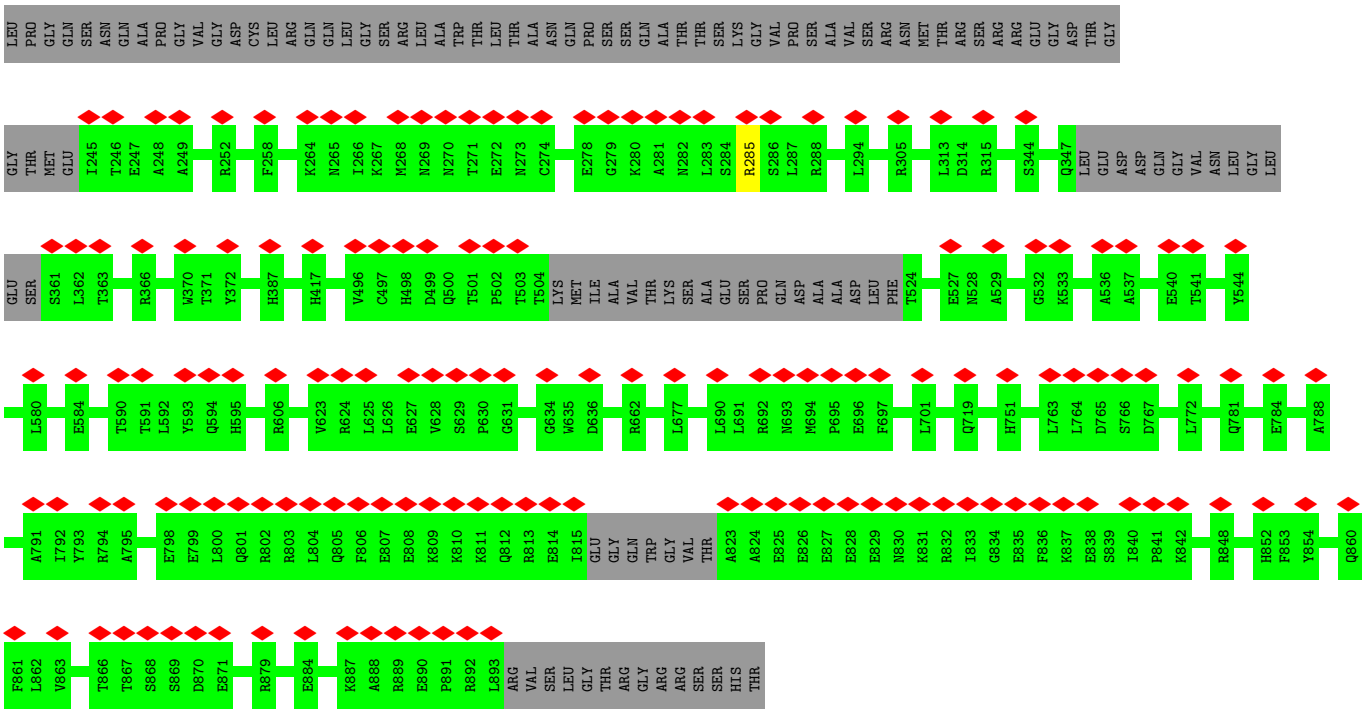
• Molecule 3: Gamma-tubulin complex component 4

Chain I:

• Molecule 4: Gamma-tubulin complex component 3

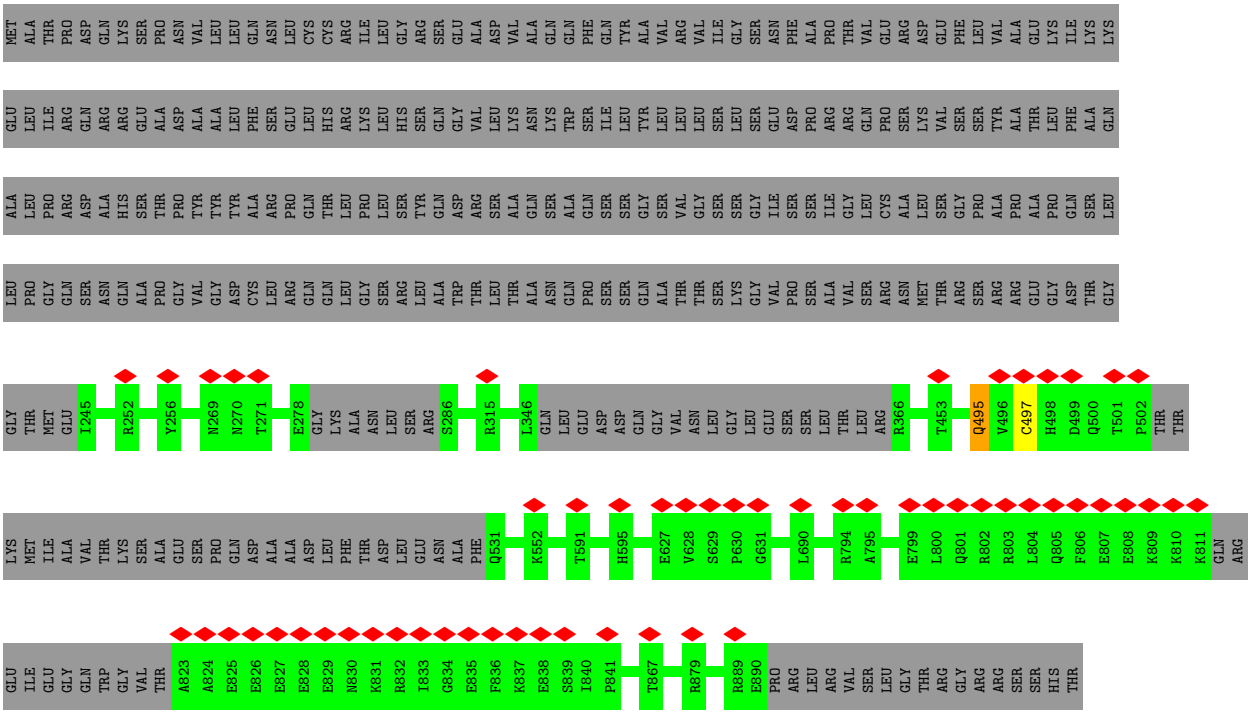
Chain B:





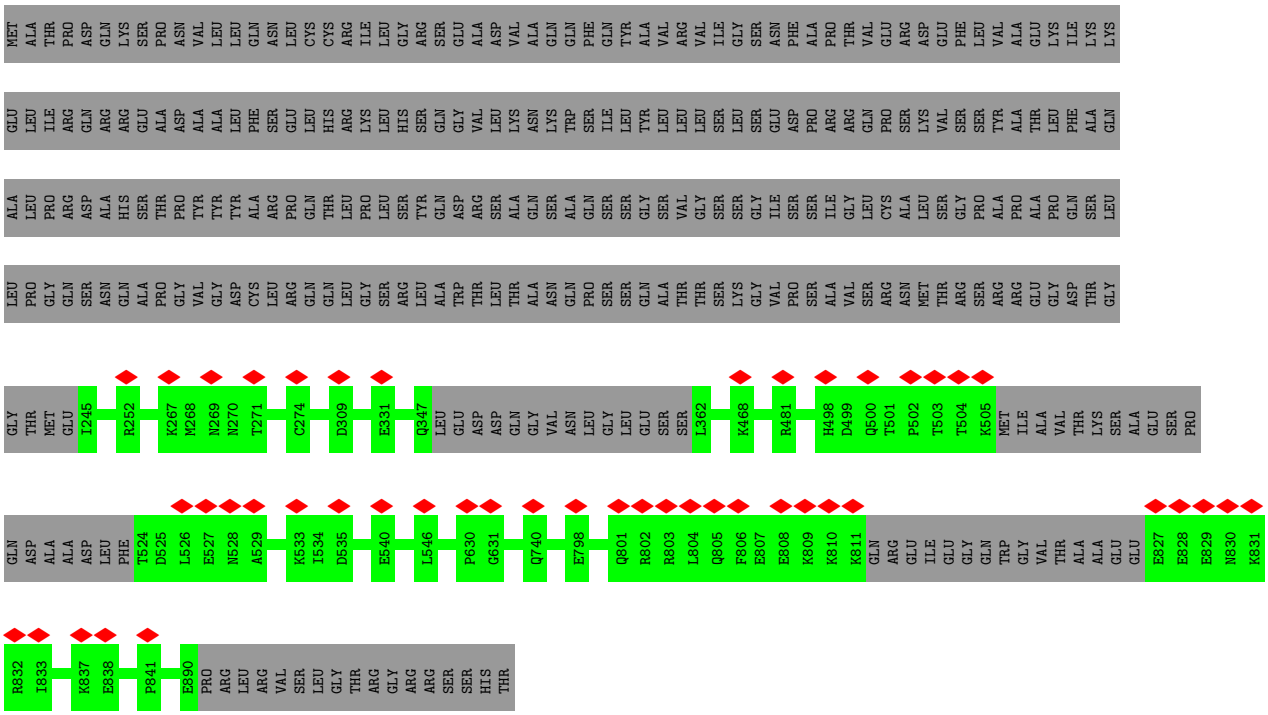
• Molecule 4: Gamma-tubulin complex component 3

Chain D:



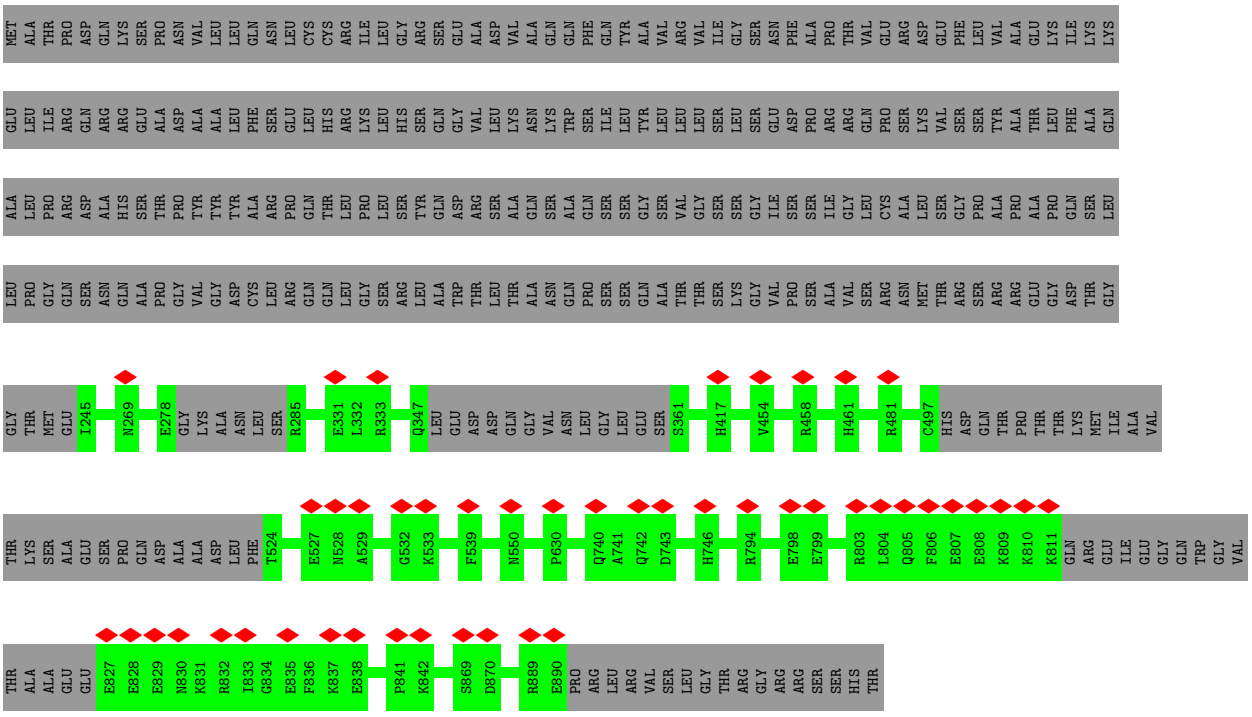
• Molecule 4: Gamma-tubulin complex component 3

Chain F:



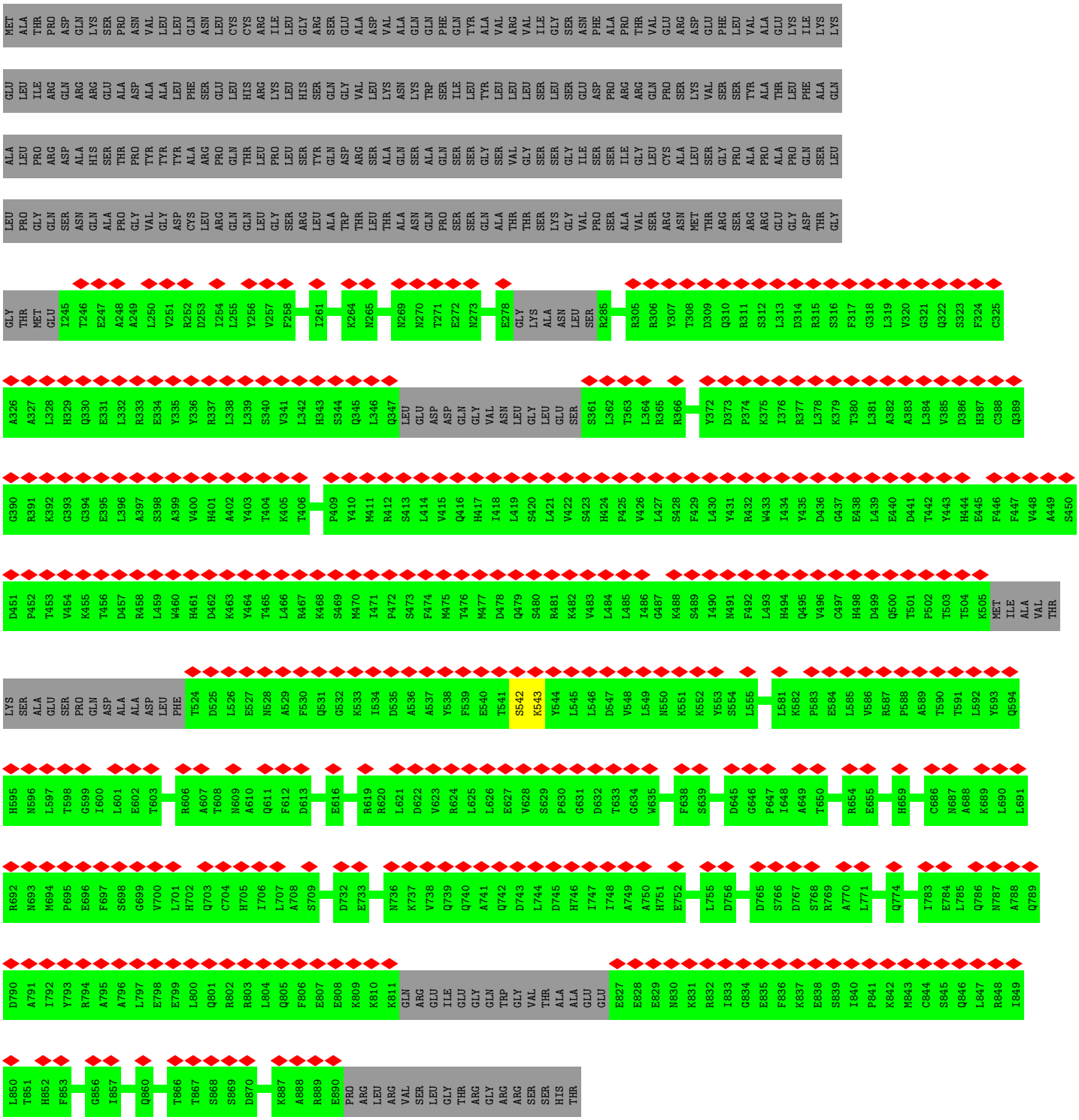
• Molecule 4: Gamma-tubulin complex component 3

Chain H:



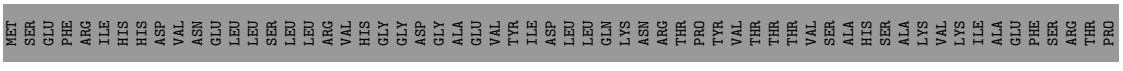
• Molecule 4: Gamma-tubulin complex component 3

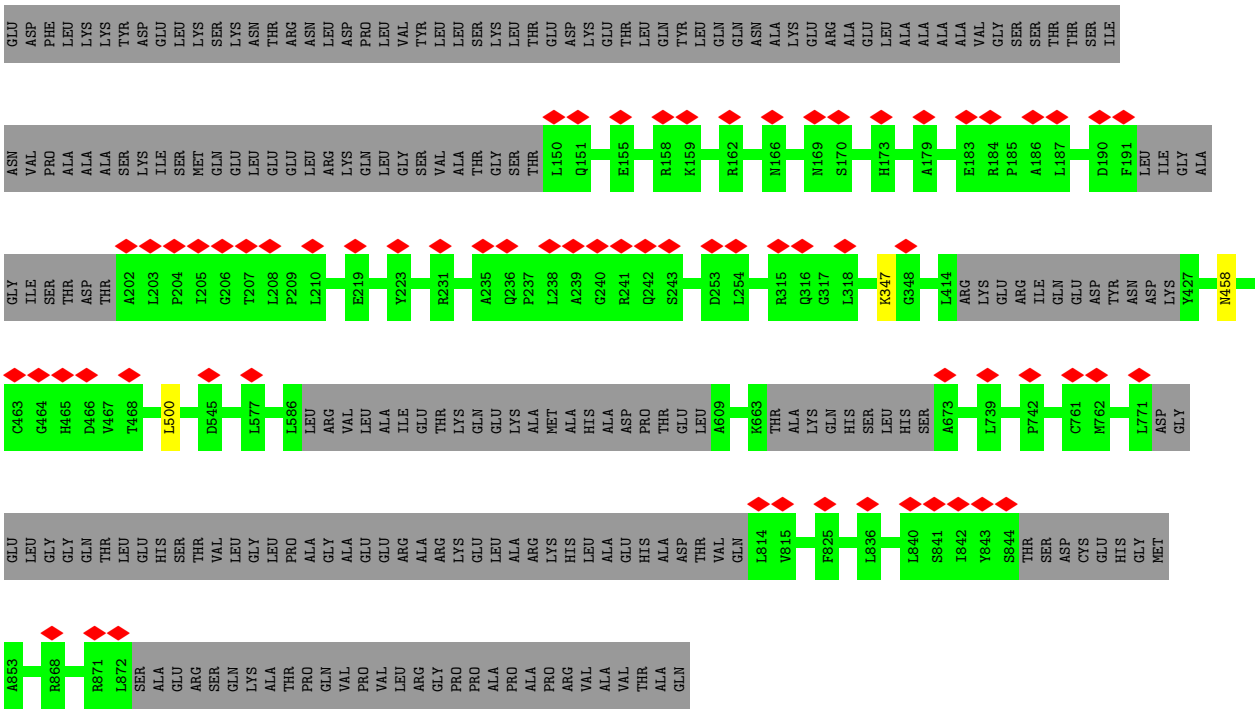
Chain N:



• Molecule 5: Gamma-tubulin complex component 2

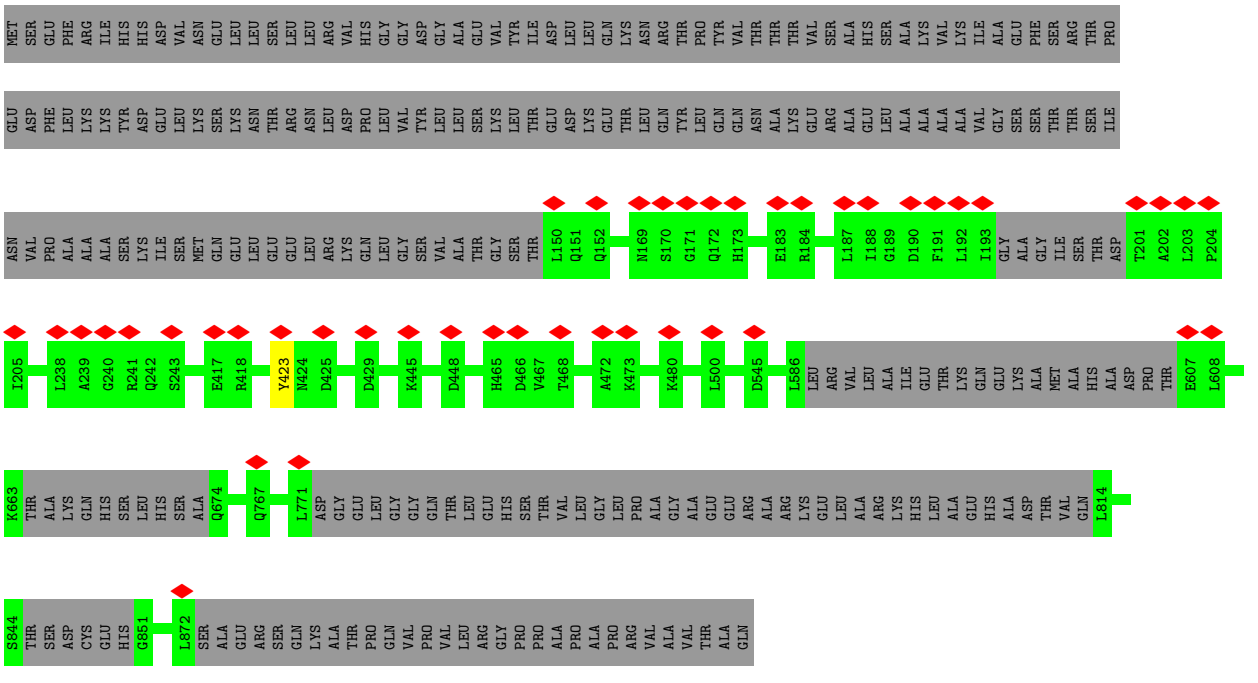
Chain C:





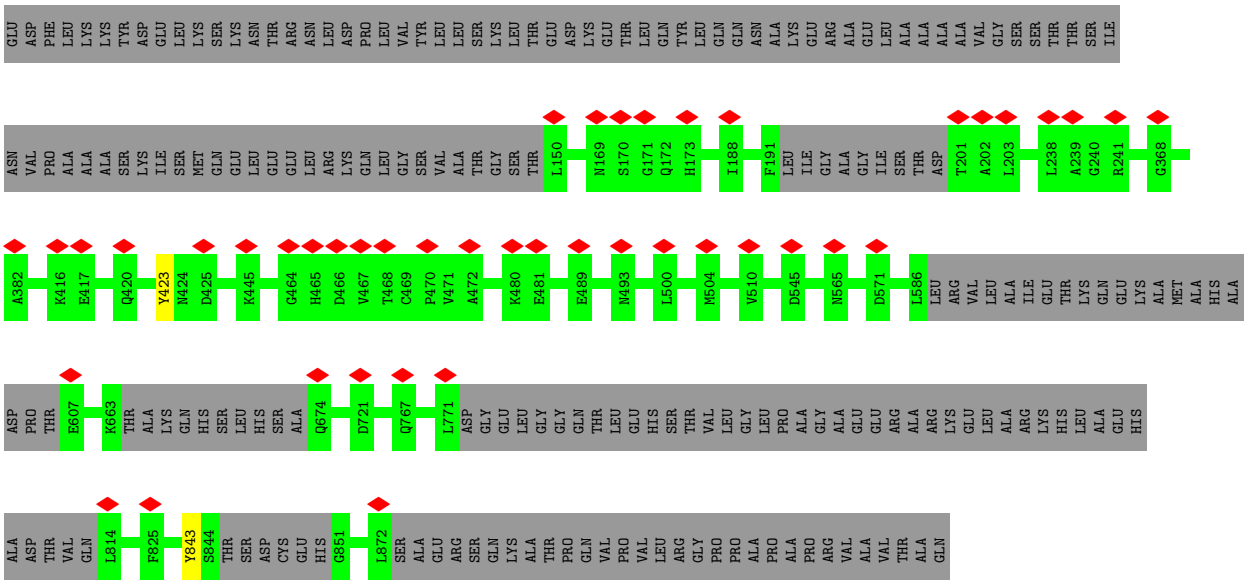
• Molecule 5: Gamma-tubulin complex component 2

Chain E:



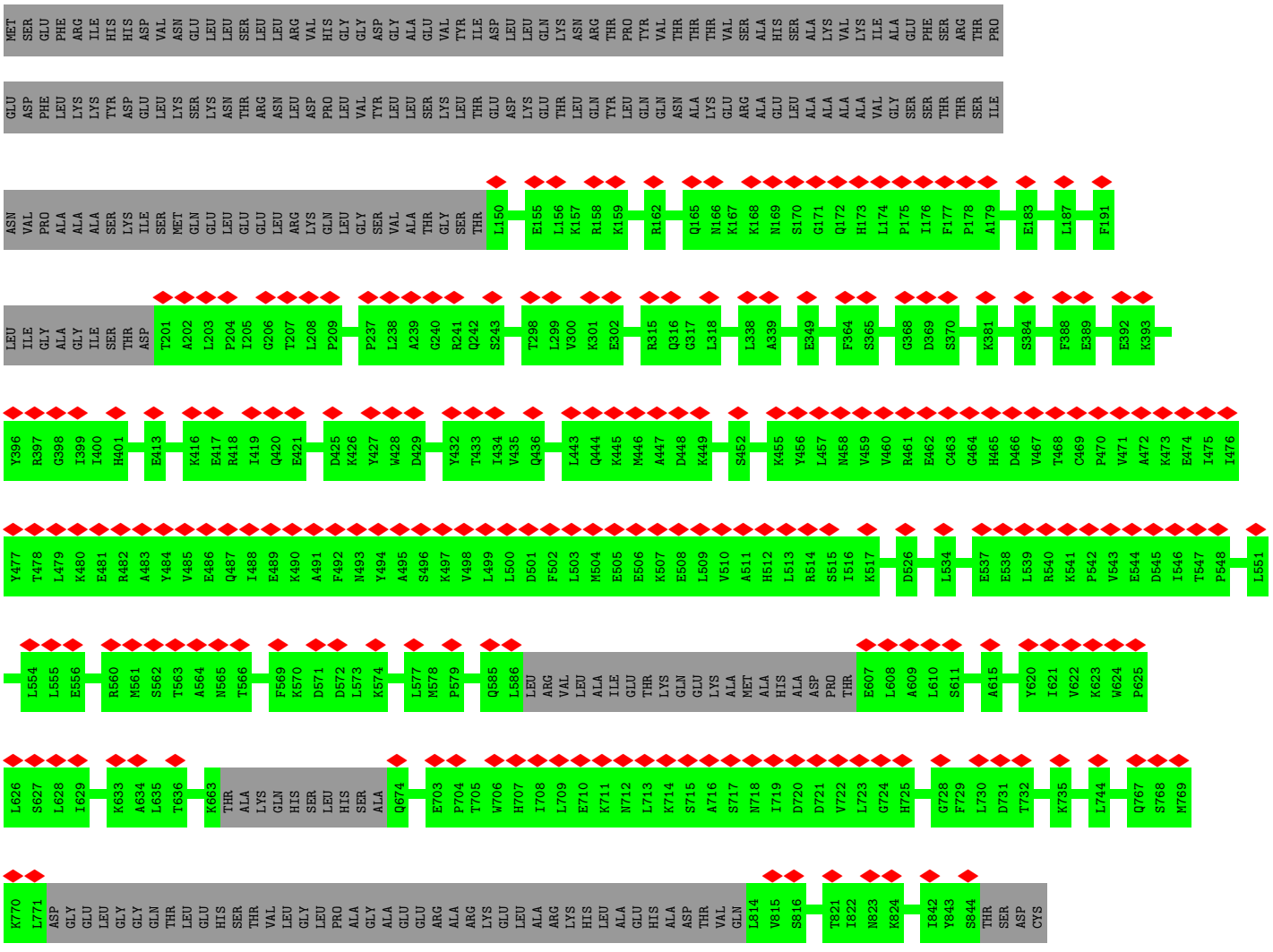
• Molecule 5: Gamma-tubulin complex component 2

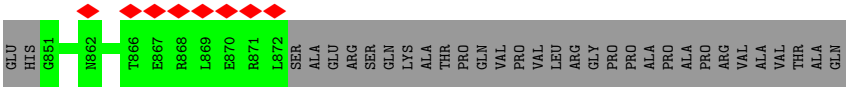
Chain G:



• Molecule 5: Gamma-tubulin complex component 2

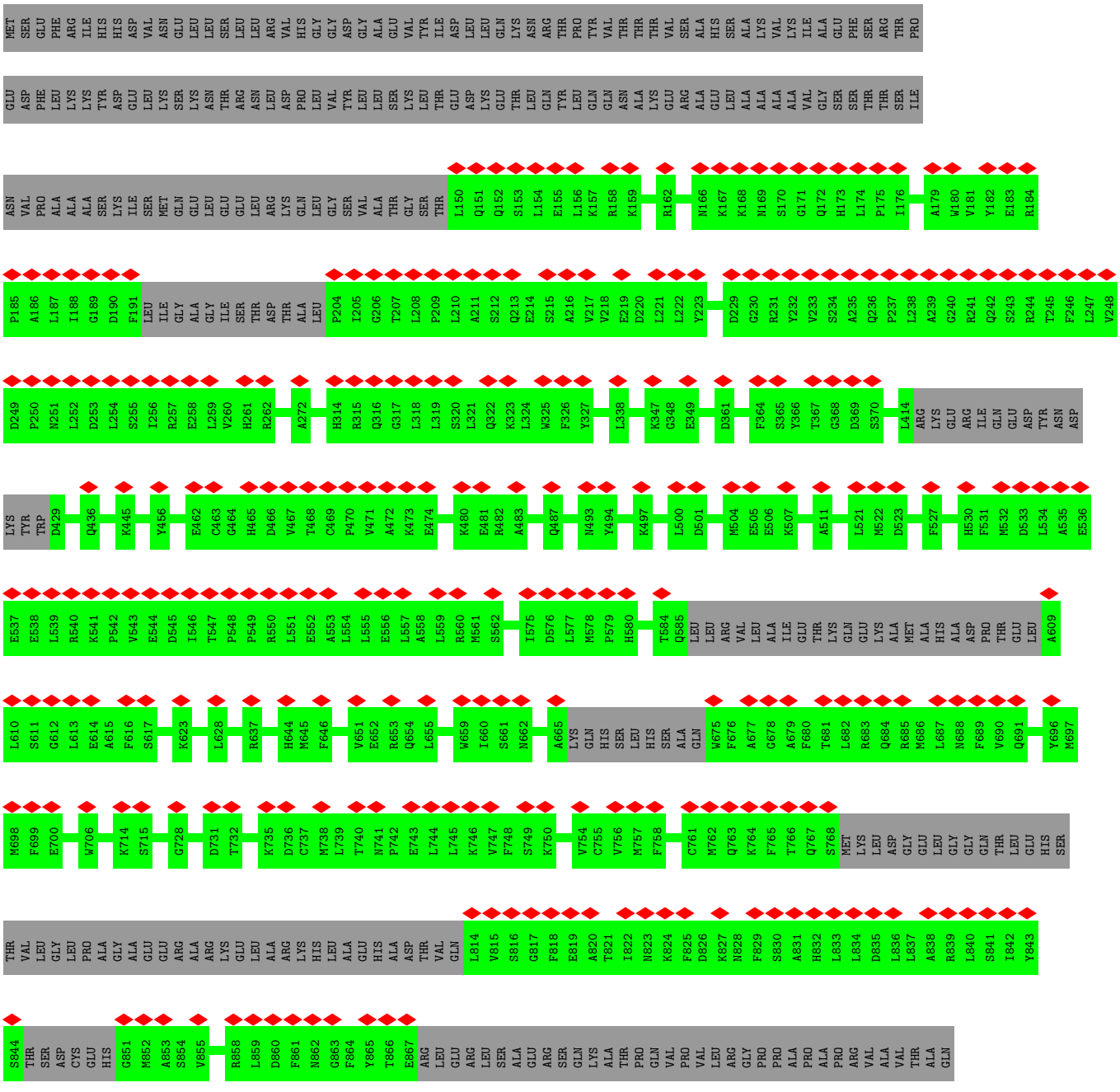
Chain M:





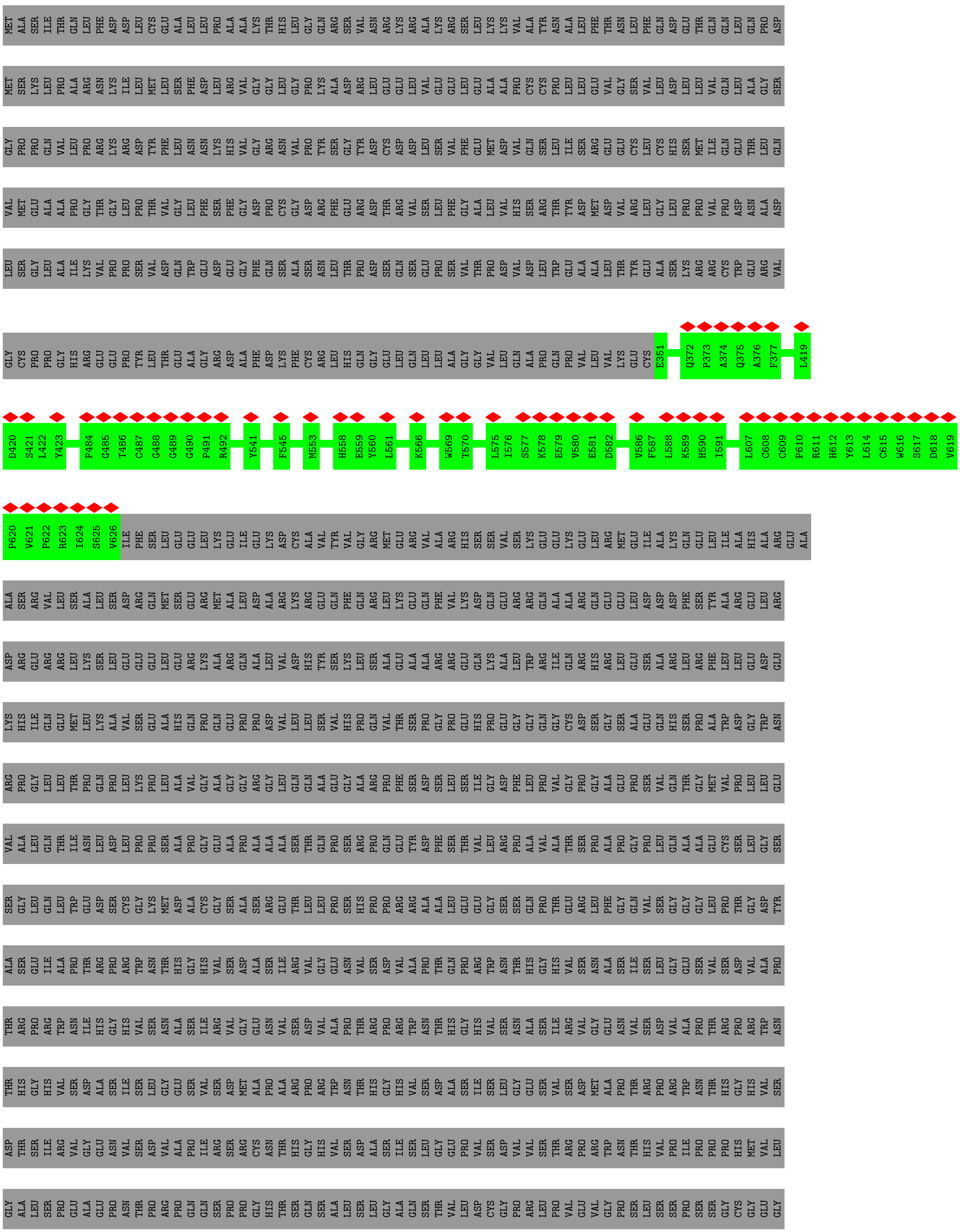
• Molecule 5: Gamma-tubulin complex component 2

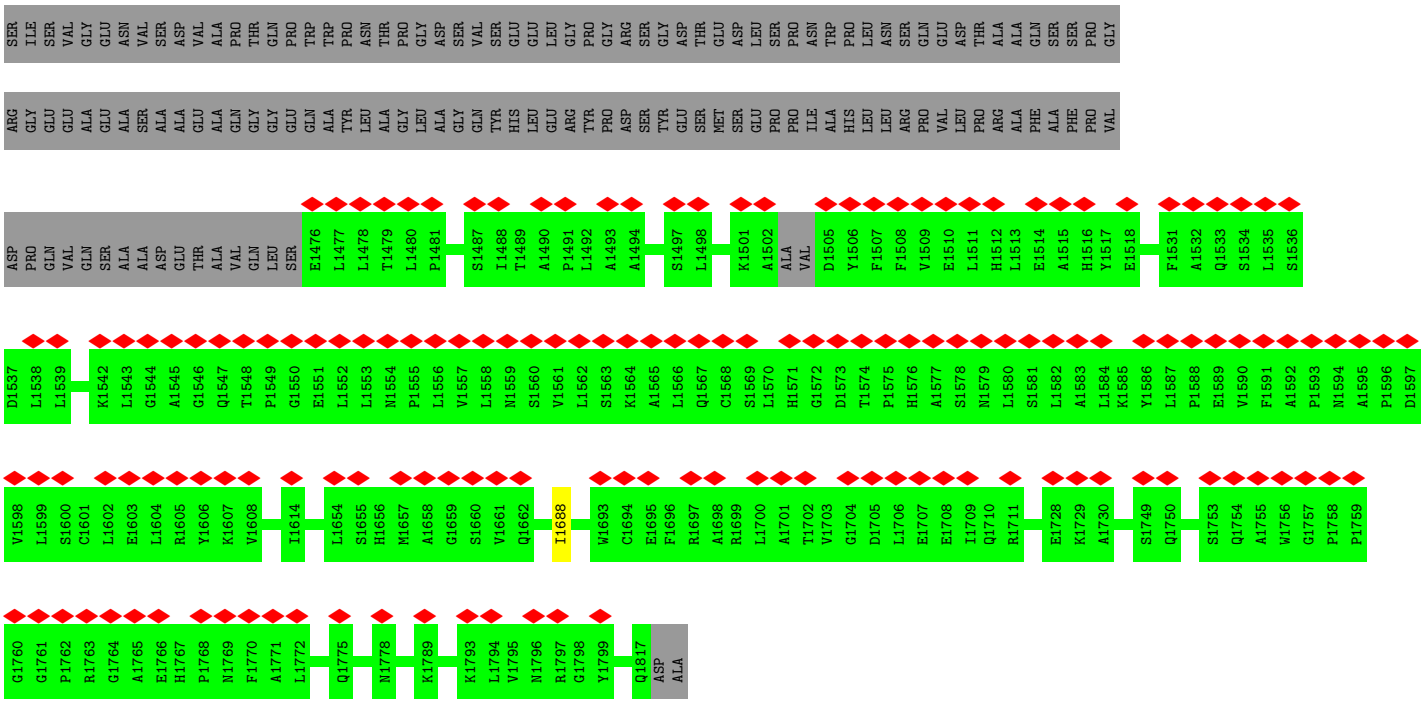
Chain A:



• Molecule 6: Gamma-tubulin complex component 6

Chain L:




SER ILE SER VAL GLY GLU ASN VAL SER ASP VAL ALA PRO THR GLN PRO TRP TRP PRO ASN THR PRO GLY ASP SER VAL SER GLU GLU LEU GLY PRO GLY ARG SER GLY ASP THR GLU ASP LEU SER PRO ASN TRP PRO LEU LEU ASN SER GLN GLU ASP THR ALA ALA GLN SER SER PRO GLY
ARG GLY GLU GLU ALA GLU ALA SER ALA ALA GLU GLU ALA GLN GLY GLY GLU GLN ALA TYR LEU ALA GLY LEU ALA GLY GLN TYR HIS LEU GLU GLU ARG TYR PRO ASP SER TYR GLU SER MET SER GLU PRO PRO ILE ALA HIS LEU LEU ARG PRO VAL LEU PRO ARG ALA PHE ALA PHE PRO PRO VAL
ASP PRO GLN VAL GLN SER ALA ALA ASP GLU THR ALA VAL GLN LEU SER E1476 L1477 L1478 T1479 L1480 P1481 S1487 I1488 T1489 A1490 P1491 L1492 A1493 A1494 S1497 L1498 K1501 A1502 ALA VAL D1505 Y1506 F1507 F1508 V1509 E1510 L1511 H1512 L1513 E1514 A1515 H1516 Y1517 E1518 F1531 A1532 Q1533 S1534 L1535 S1536
D1537 L1538 L1539 K1542 L1543 G1544 A1545 G1546 Q1547 T1548 P1549 G1550 E1551 L1552 L1553 N1554 P1555 L1556 V1557 L1558 N1559 S1560 V1561 L1562 S1563 K1564 A1565 L1566 Q1567 C1568 S1569 L1570 H1571 G1572 D1573 T1574 P1575 H1576 A1577 S1578 N1579 L1580 S1581 L1582 A1583 L1584 K1585 Y1586 L1587 P1588 E1589 V1590 F1591 A1592 P1593 N1594 A1595 P1596 D1597
V1598 L1599 S1600 C1601 L1602 E1603 L1604 R1605 Y1606 K1607 V1608 I1614 L1654 S1655 H1656 M1657 A1658 G1659 S1660 V1661 Q1662 I1688 W1693 C1694 E1695 F1696 R1697 A1698 R1699 L1700 A1701 T1702 V1703 G1704 D1705 L1706 E1707 E1708 I1709 Q1710 R1711 E1728 K1729 A1730 S1749 Q1750 S1753 Q1754 A1755 W1756 G1757 P1758 P1759
G1760 G1761 P1762 R1763 G1764 A1765 E1766 H1767 P1768 N1769 F1770 A1771 L1772 Q1775 N1778 K1789 K1793 L1794 V1795 N1796 R1797 G1798 Y1799 Q1817 ASP ALA

4 Experimental information (i)

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 ($e^-/Å^2$)	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

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	0.33	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

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	343	ARG
1	m	406	GLU
1	m	408	PHE
1	m	407	GLN
5	G	423	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	371	HIS
1	h	357	GLN
1	f	198	ASN
1	g	347	ASN
1	j	198	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

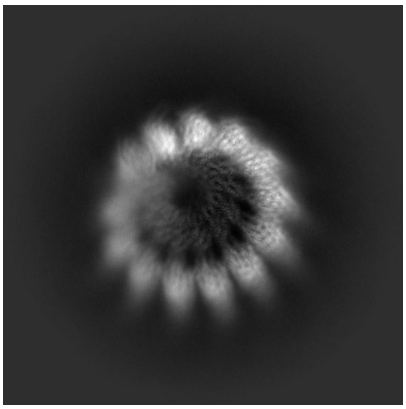
6 Map visualisation

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.

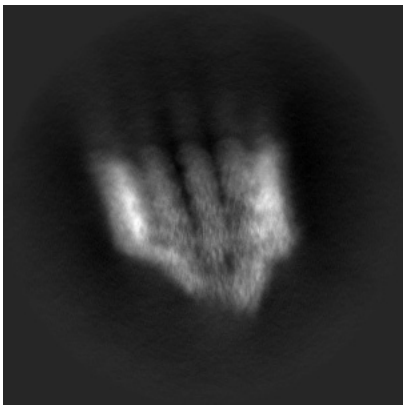
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

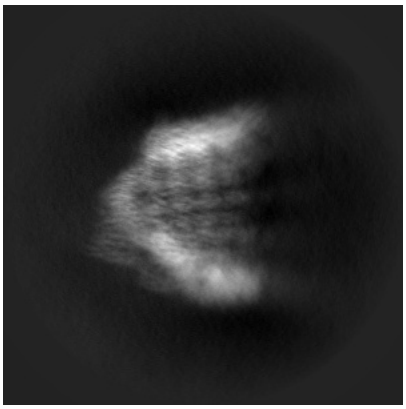
6.1.1 Primary map



X

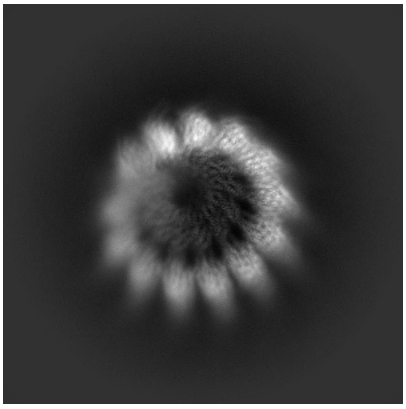


Y

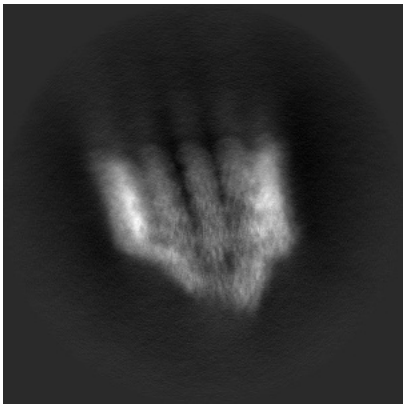


Z

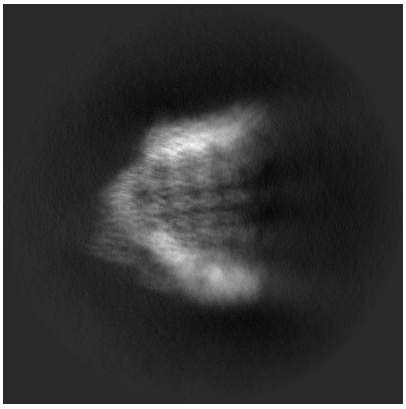
6.1.2 Raw map



X



Y

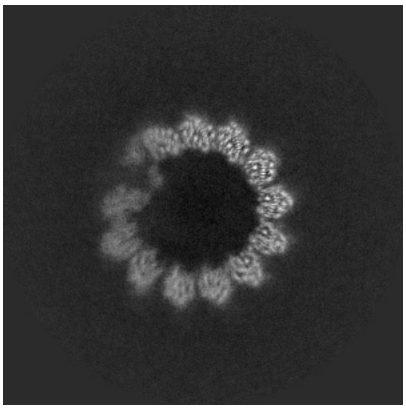


Z

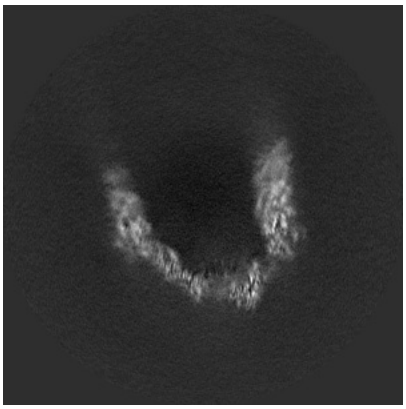
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

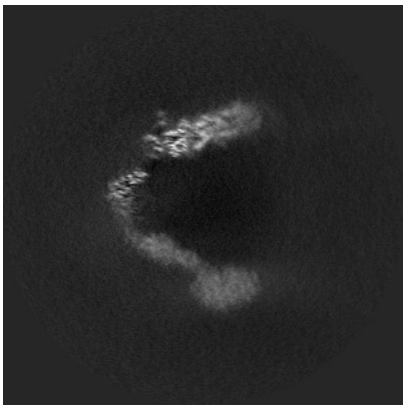
6.2.1 Primary map



X Index: 215

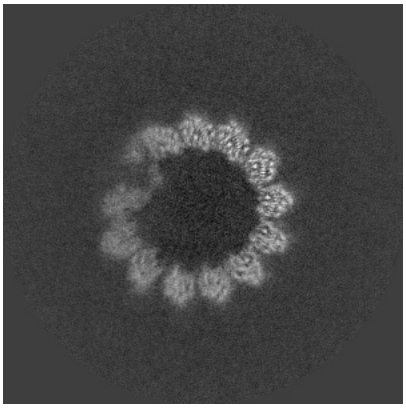


Y Index: 215

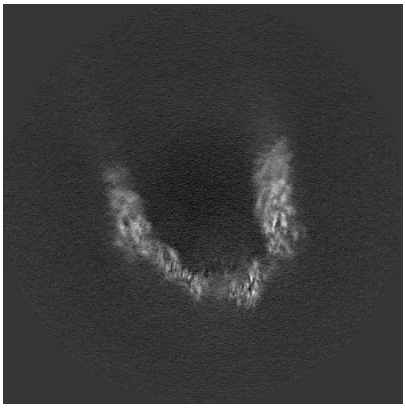


Z Index: 215

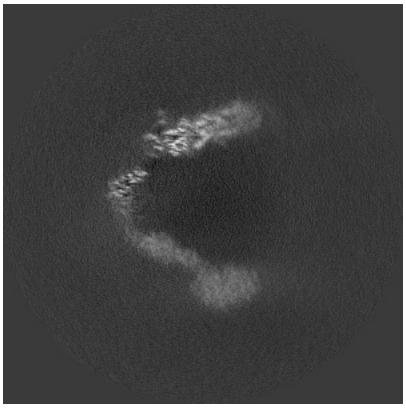
6.2.2 Raw map



X Index: 215



Y Index: 215

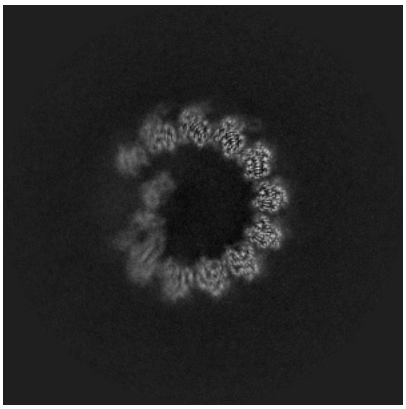


Z Index: 215

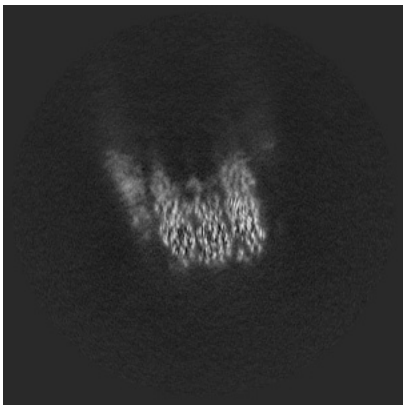
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

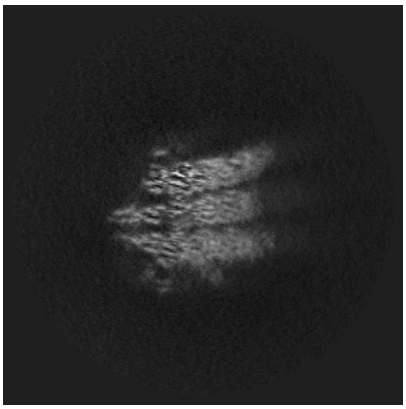
6.3.1 Primary map



X Index: 189

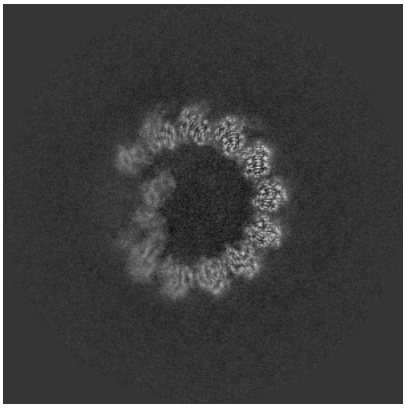


Y Index: 280

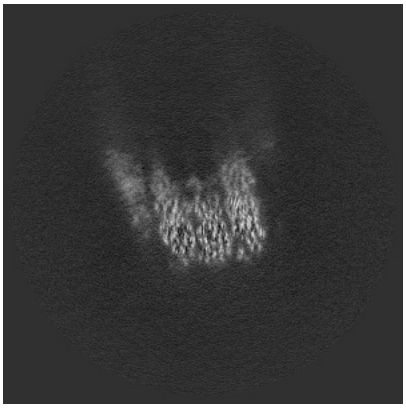


Z Index: 284

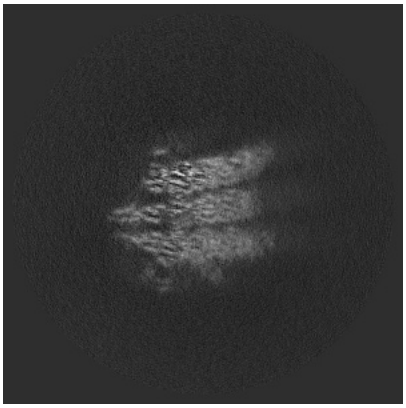
6.3.2 Raw map



X Index: 188



Y Index: 280

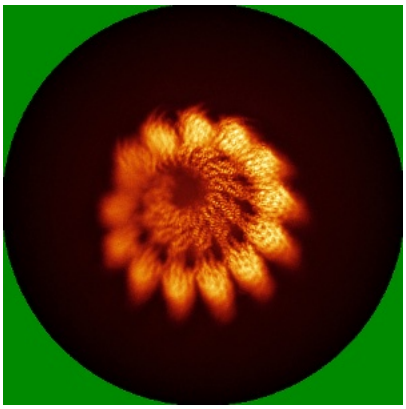


Z Index: 284

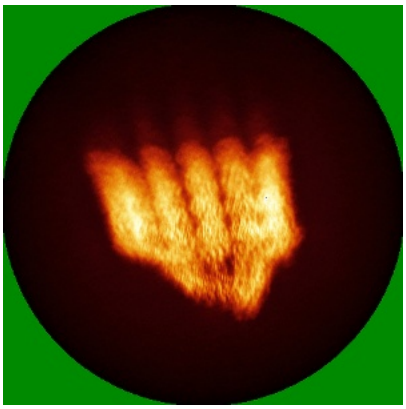
The images above show the largest variance slices of the map in three orthogonal directions.

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

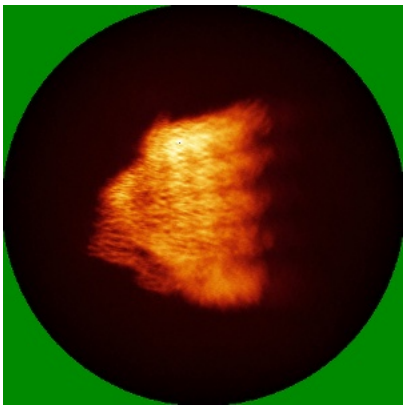
6.4.1 Primary map



X

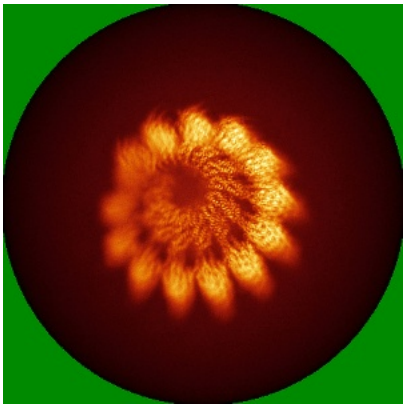


Y

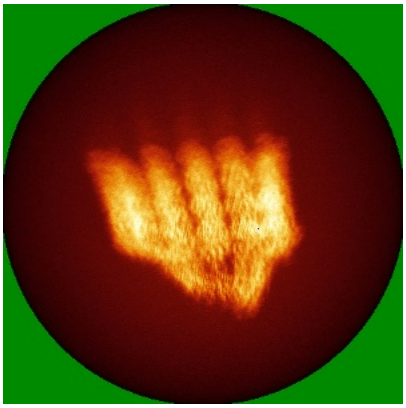


Z

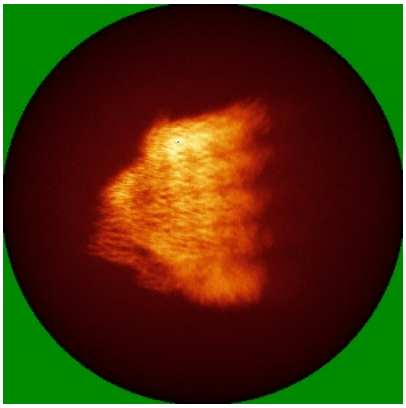
6.4.2 Raw map



X



Y

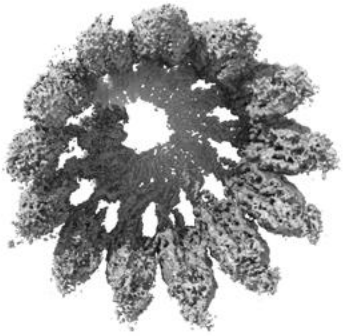


Z

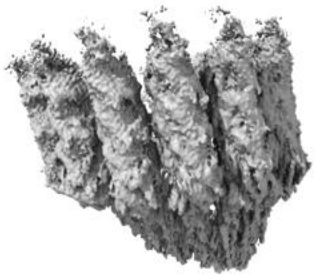
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



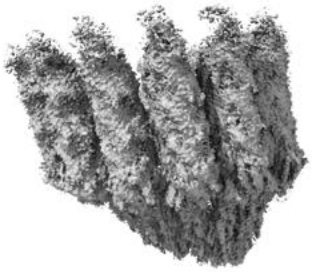
Y

Z

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

X



Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

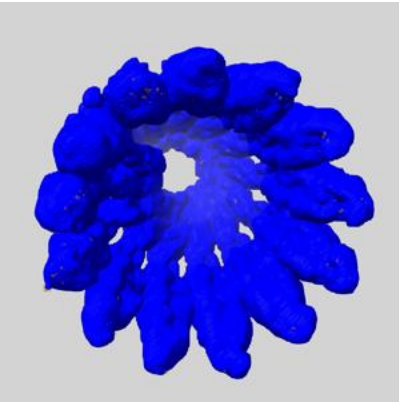
6.6 Mask visualisation (i)

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

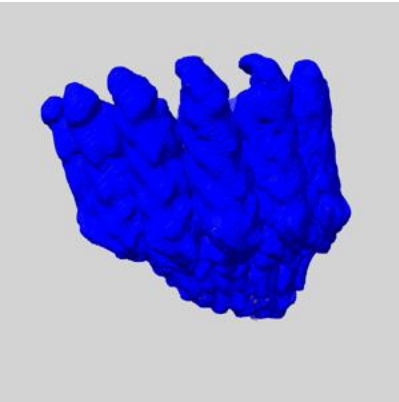
A mask typically either:

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

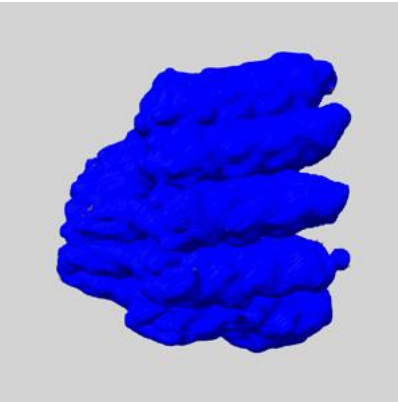
6.6.1 emd_18181_msk_1.map (i)



X



Y

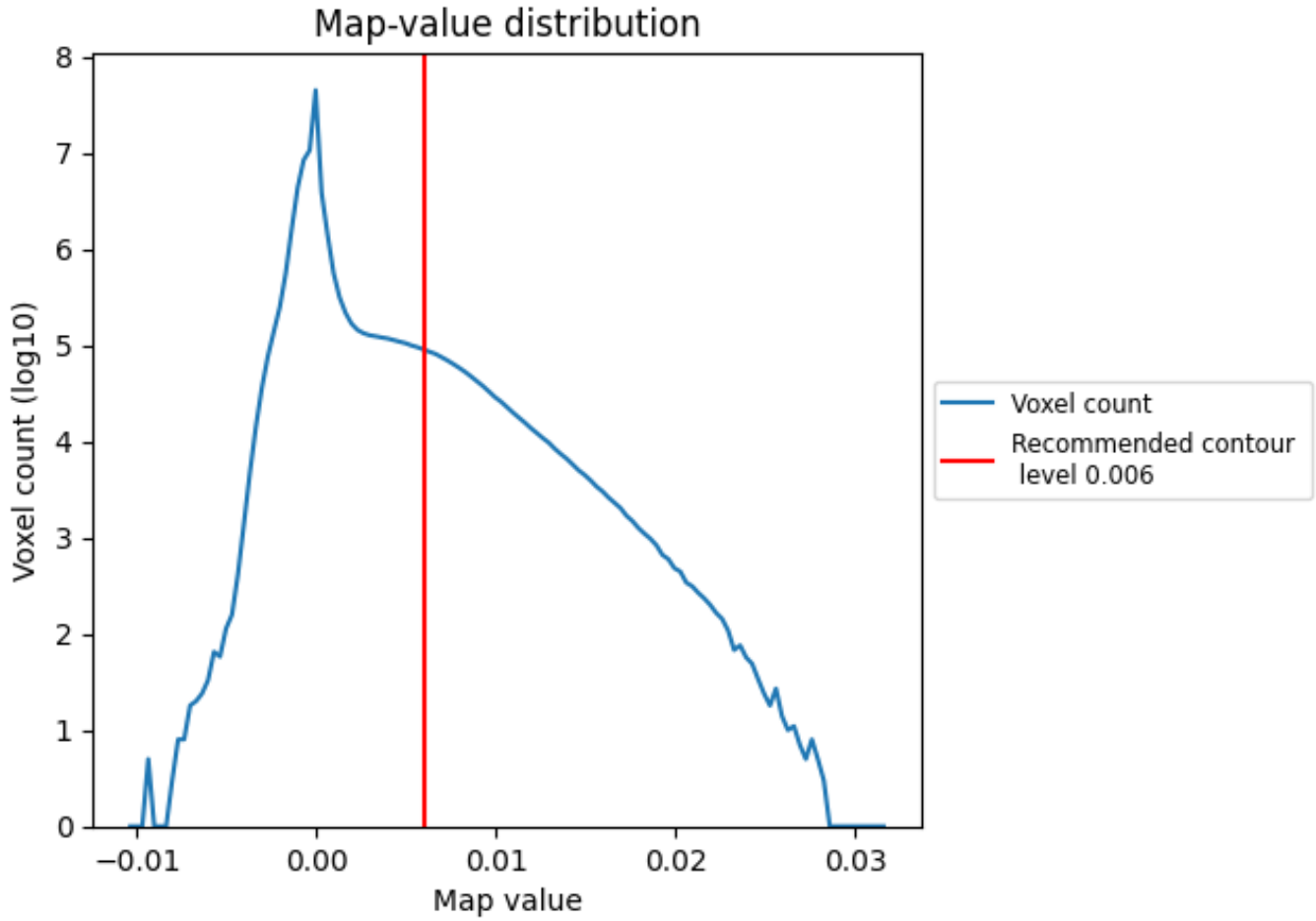


Z

7 Map analysis

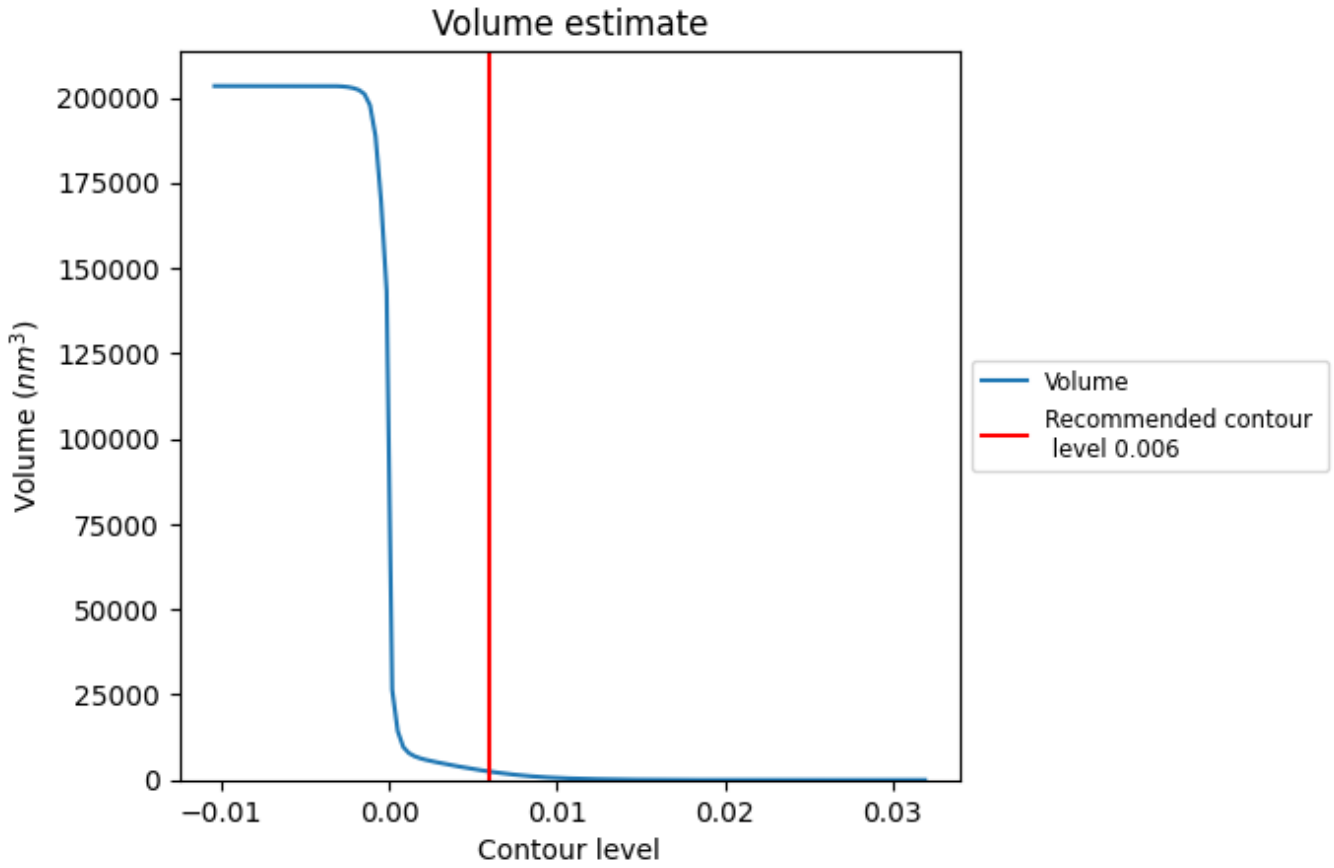
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

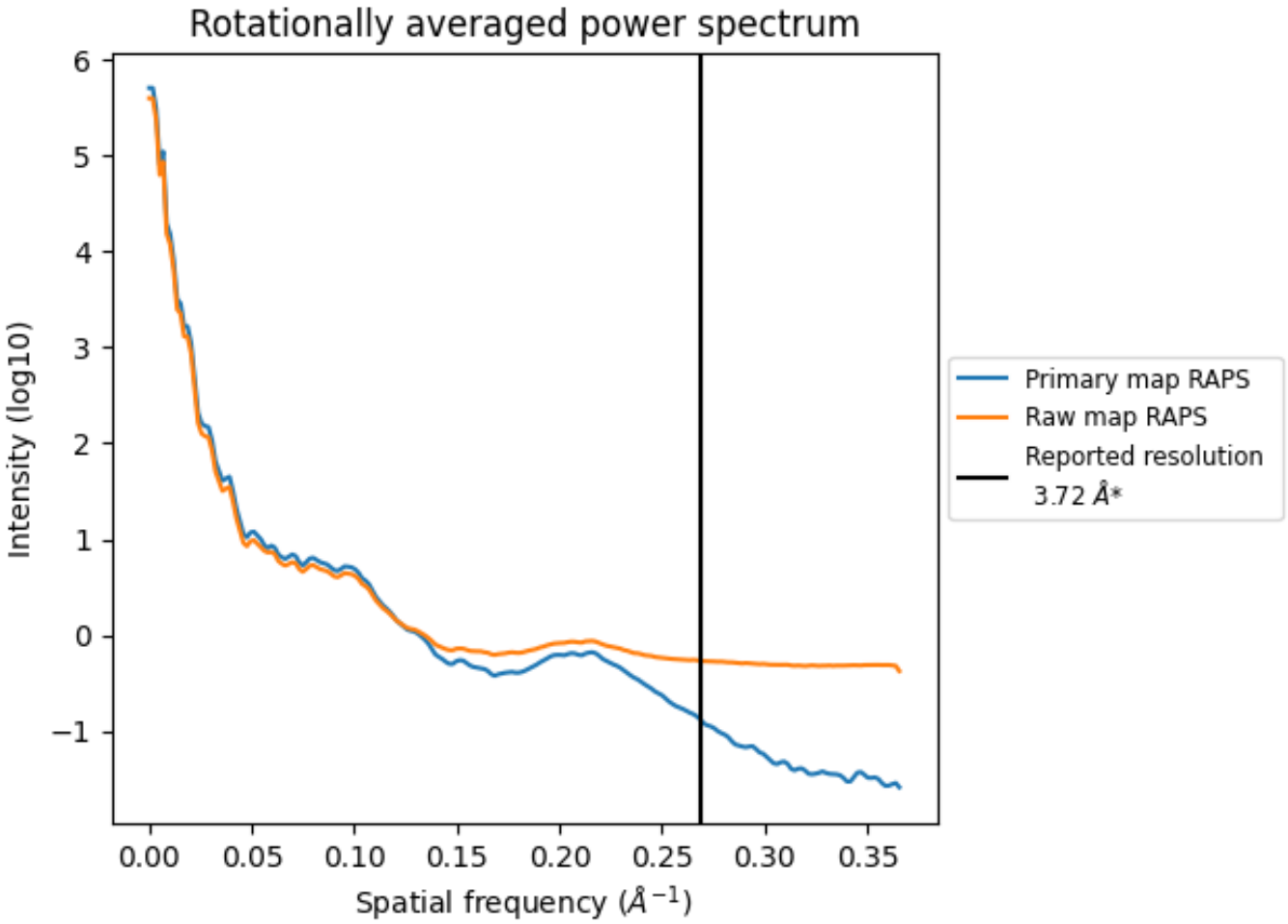
7.2 Volume estimate (i)



The volume at the recommended contour level is 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)

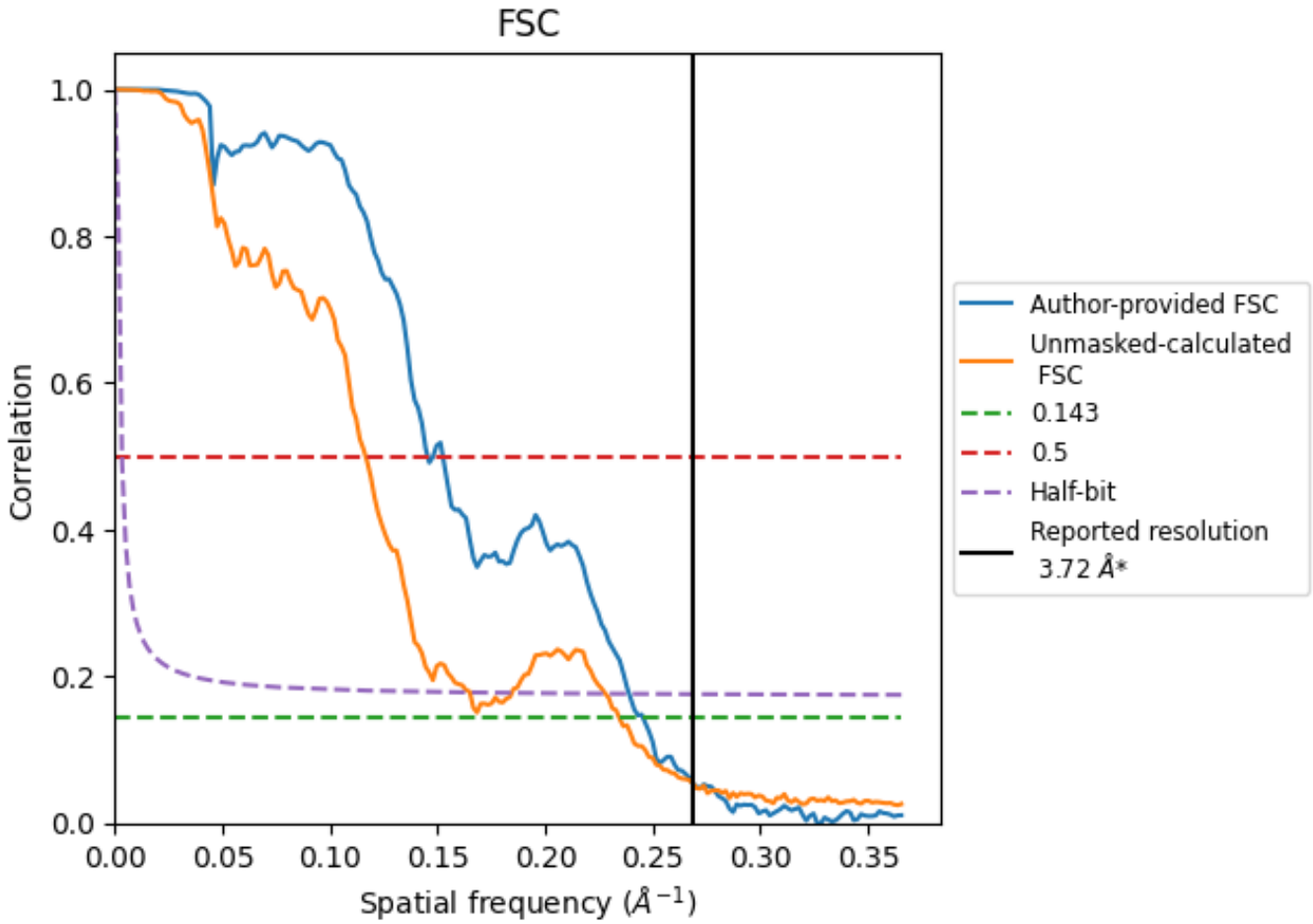


*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8.2 Resolution estimates (i)

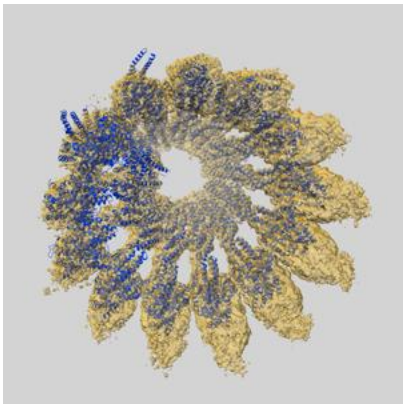
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	4.07	6.87	4.18
Unmasked-calculated*	4.26	8.58	6.06

*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 %

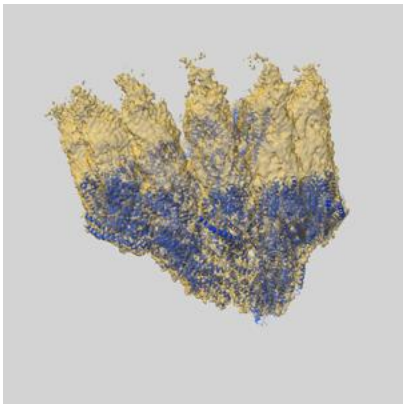
9 Map-model fit

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.

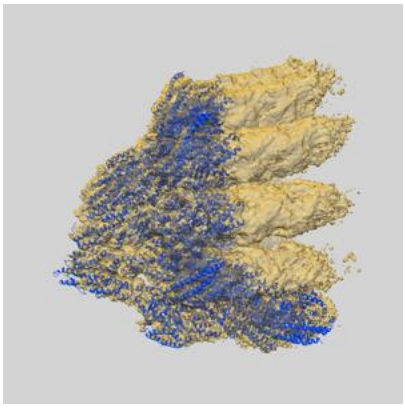
9.1 Map-model overlay



X



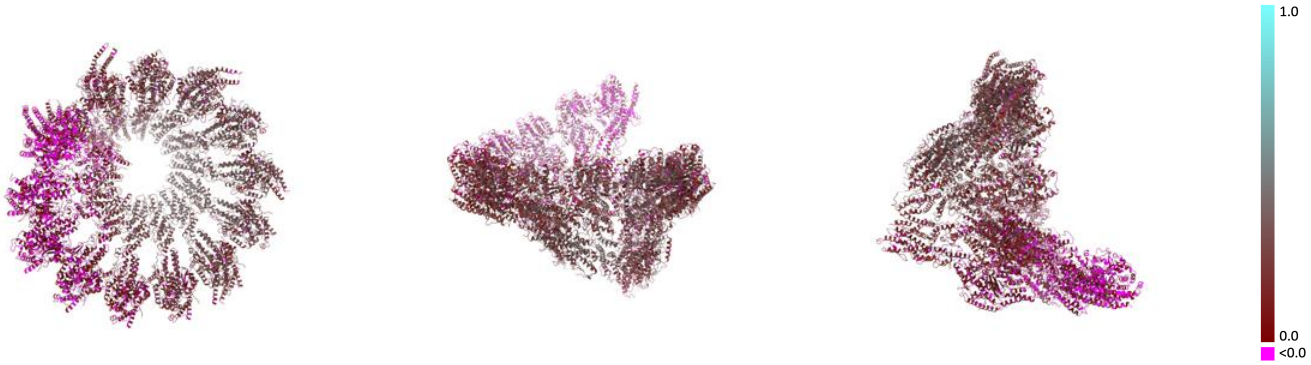
Y



Z

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.

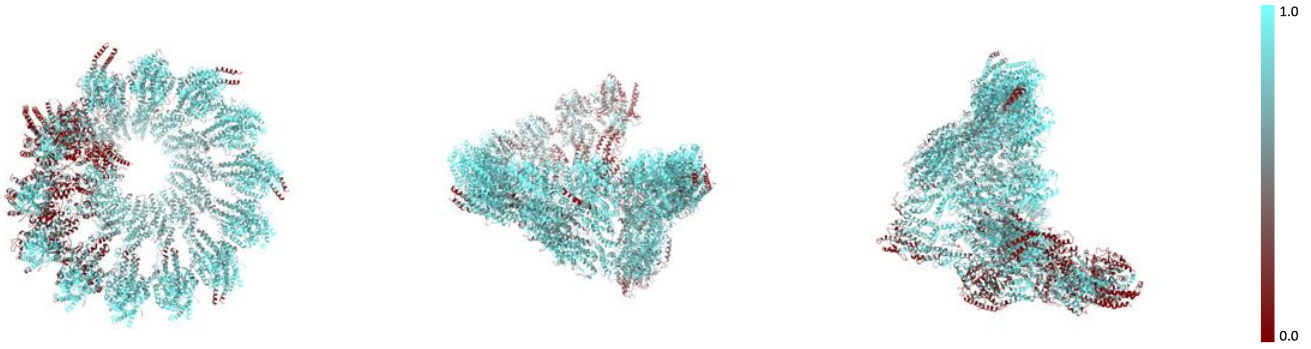
9.2 Q-score mapped to coordinate model (i)



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.

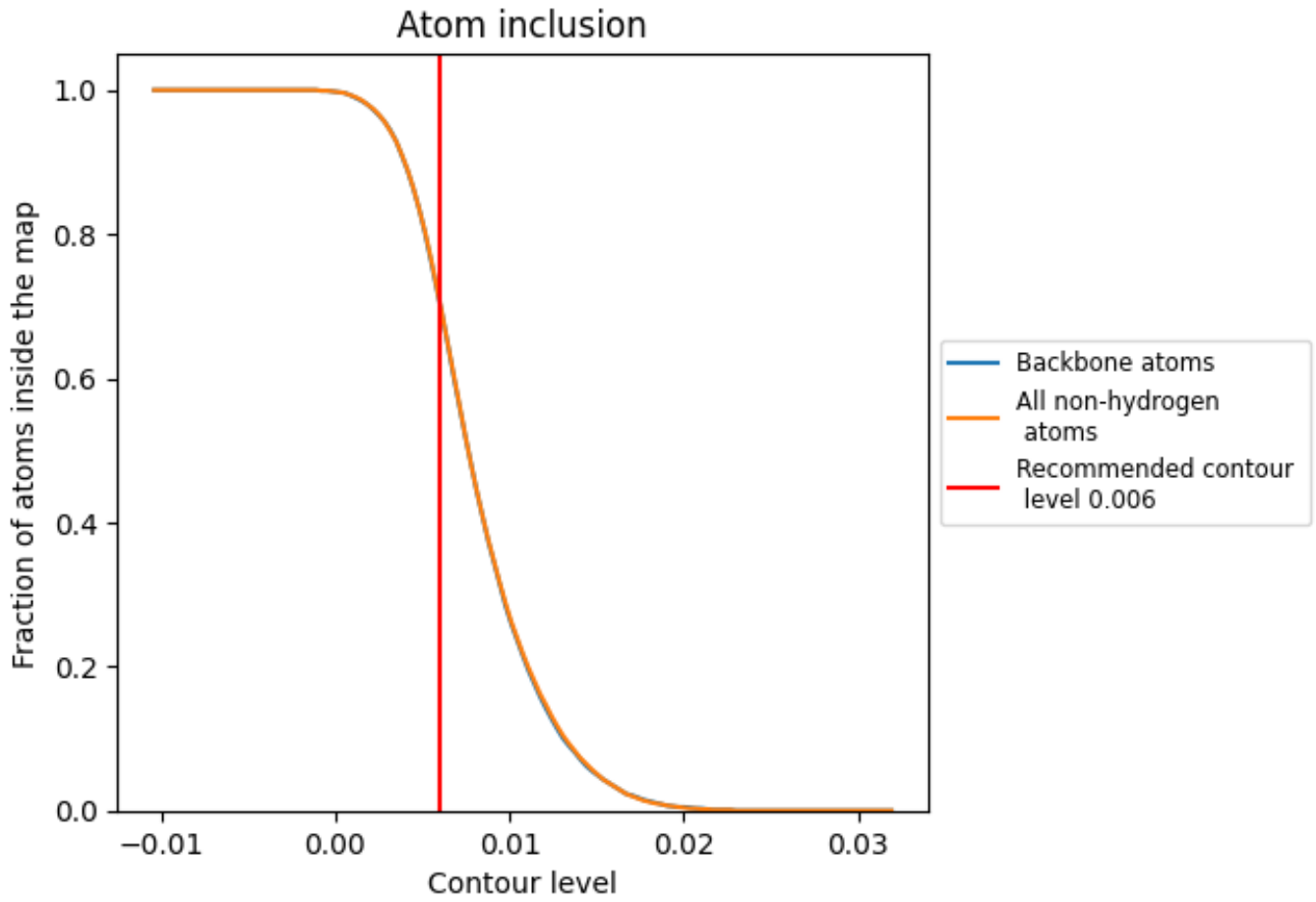
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

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