



wwPDB EM Validation Summary Report ⓘ

Jul 8, 2024 – 05:46 am BST

PDB ID : 7QJ7
EMDB ID : EMD-14012
Title : Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 1-12 substoichiometric spokes 13-14)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 8.70 Å (reported)
Based on initial models : 6X0U, 7AS4, 6L81, 6V6S

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.dev92
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) : 2.37.1

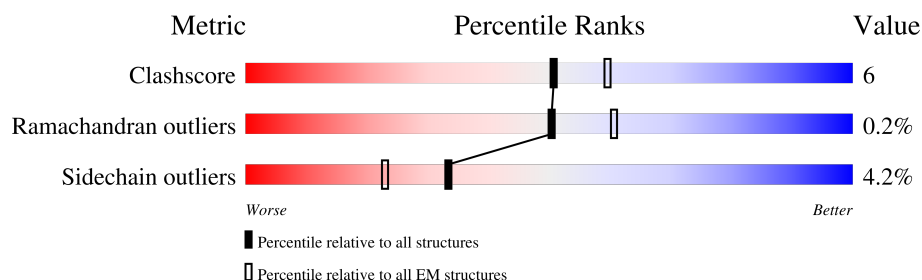
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













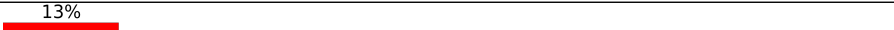

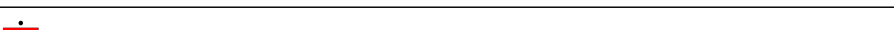
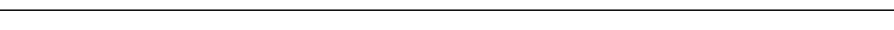











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	J	1024	
1	l	1024	
2	e	375	
3	A	902	
3	C	902	
3	E	902	
3	G	902	
4	B	907	

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Mol	Chain	Length	Quality of chain
4	D	907	
4	F	907	
4	H	907	
4	a	907	
4	f	907	
4	h	907	
4	j	907	
5	b	82	
5	d	82	
5	g	82	
5	i	82	
5	k	82	
5	m	82	
6	I	667	
6	K	667	
7	L	1819	
7	c	1819	
8	O	451	
8	P	451	
8	Q	451	
8	R	451	
8	S	451	
8	T	451	
8	U	451	
8	V	451	

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Mol	Chain	Length	Quality of chain
8	W	451	<div><div></div><div>63%</div><div>26%</div><div>• 7%</div></div>
8	X	451	<div><div></div><div>63%</div><div>27%</div><div>• 7%</div></div>
8	Y	451	<div><div></div><div>63%</div><div>27%</div><div>• 7%</div></div>
8	Z	451	<div><div></div><div>63%</div><div>26%</div><div>• 7%</div></div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 109579 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 Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	108	Total	C	N	O	S	0	0
			847	539	150	157	1		
1	J	534	Total	C	N	O	S	0	0
			4429	2893	737	776	23		

- Molecule 2 is a protein called actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	364	Total	C	N	O	S	0	0
			2847	1803	476	548	20		

- Molecule 3 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	613	Total	C	N	O	S	0	0
			4978	3212	831	903	32		
3	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
3	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		
3	E	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	610	Total	C	N	O	S	0	0
			5029	3203	888	913	25		
4	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		
4	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
4	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
4	f	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
4	h	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
4	j	107	Total	C	N	O	S	0	0
			843	533	156	152	2		

- Molecule 5 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
5	g	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
5	i	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
5	k	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
5	m	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
5	d	59	Total	C	N	O	S	0	0
			454	281	79	90	4		

- Molecule 6 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	521	Total	C	N	O	S	0	0
			4225	2737	720	750	18		
6	K	562	Total	C	N	O	S	0	0
			4579	2964	781	816	18		

- Molecule 7 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	566	Total	C	N	O	S	0	0
			4587	3000	773	789	25		
7	c	158	Total	C	N	O	S	0	0
			1220	771	209	232	8		

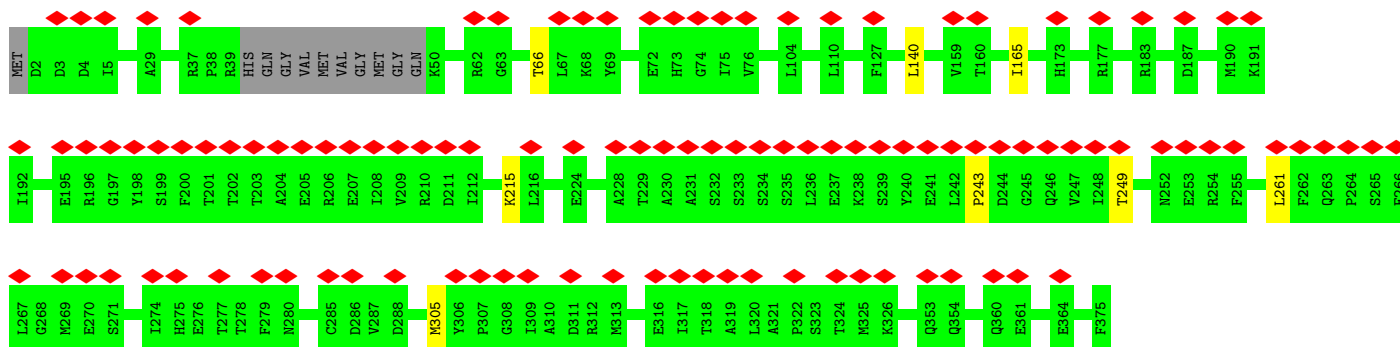
- Molecule 8 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	P	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	Q	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	R	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	S	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	T	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	U	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	V	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	W	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	X	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	Y	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	Z	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		

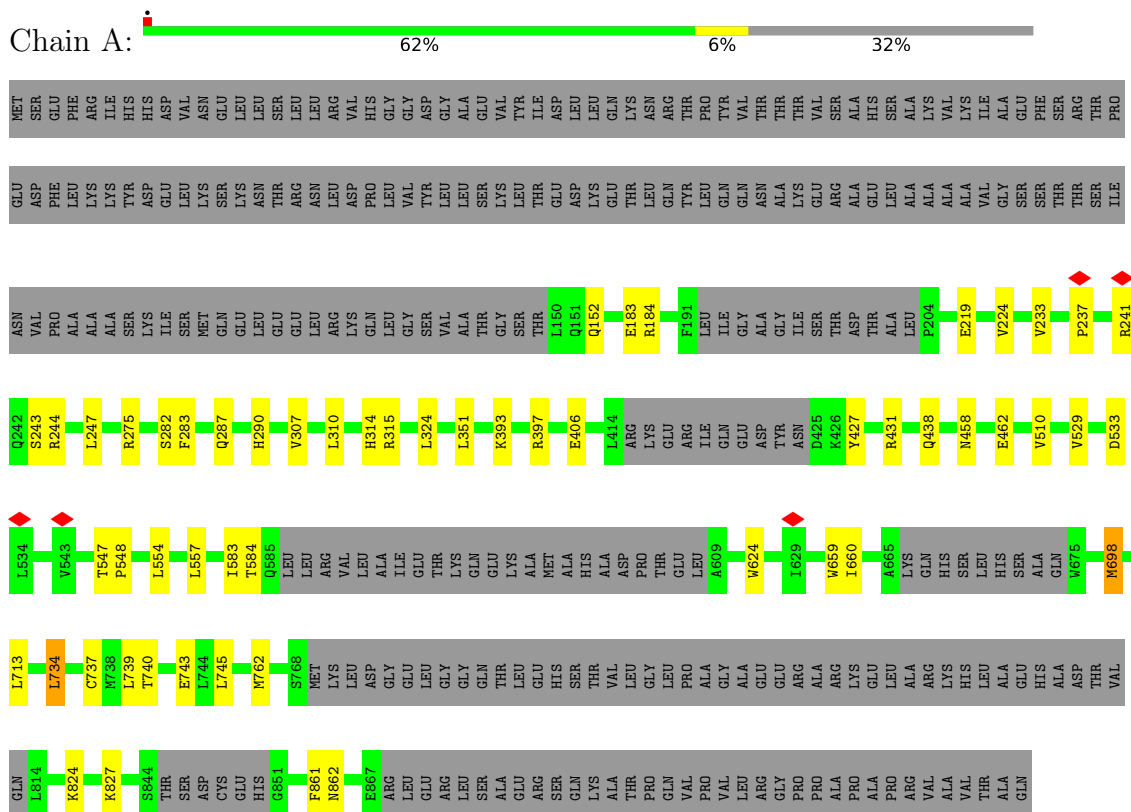
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	l	6	Total	O	0
			6	6	

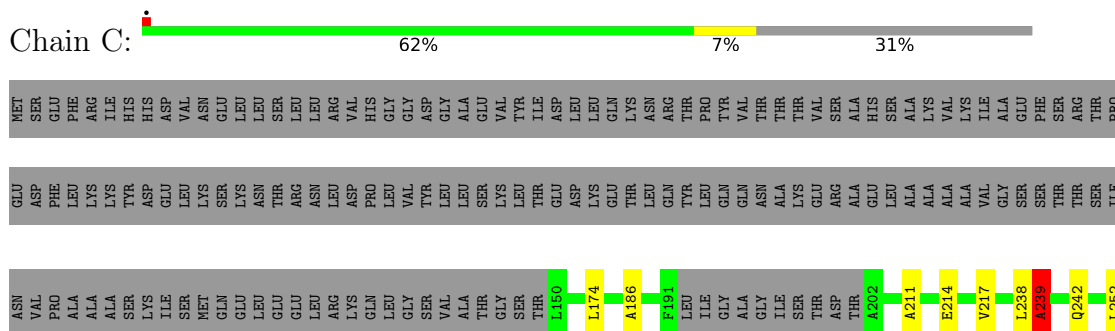


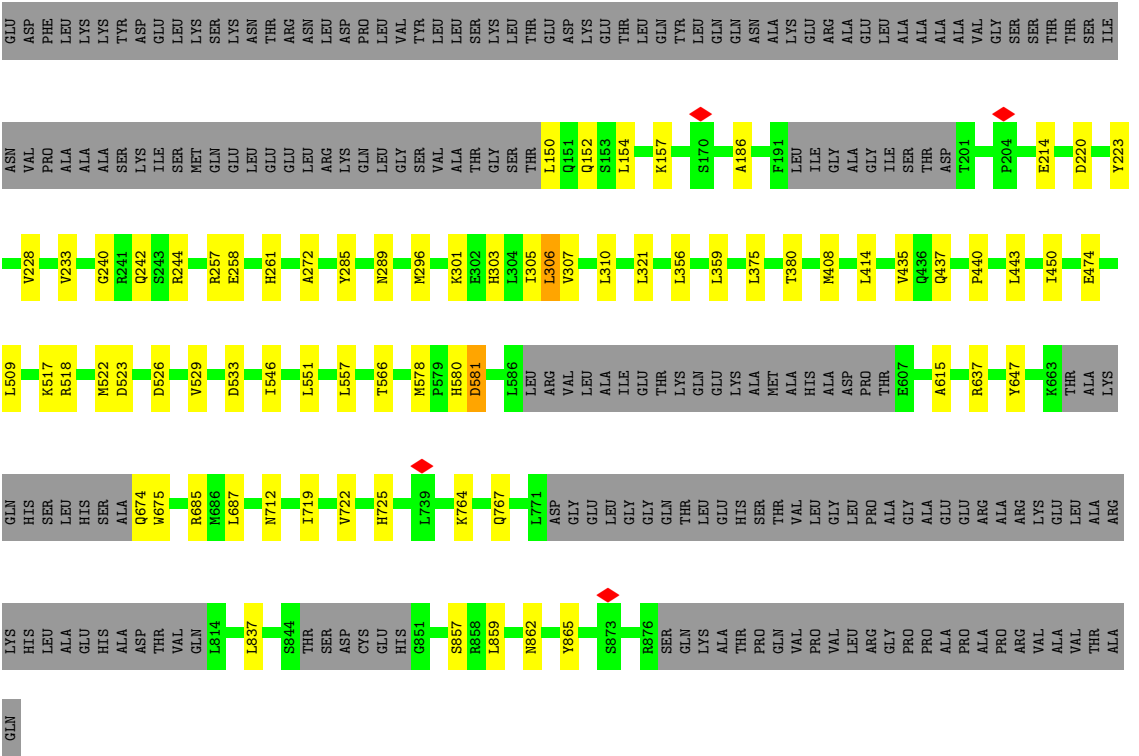


- Molecule 3: Gamma-tubulin complex component 2

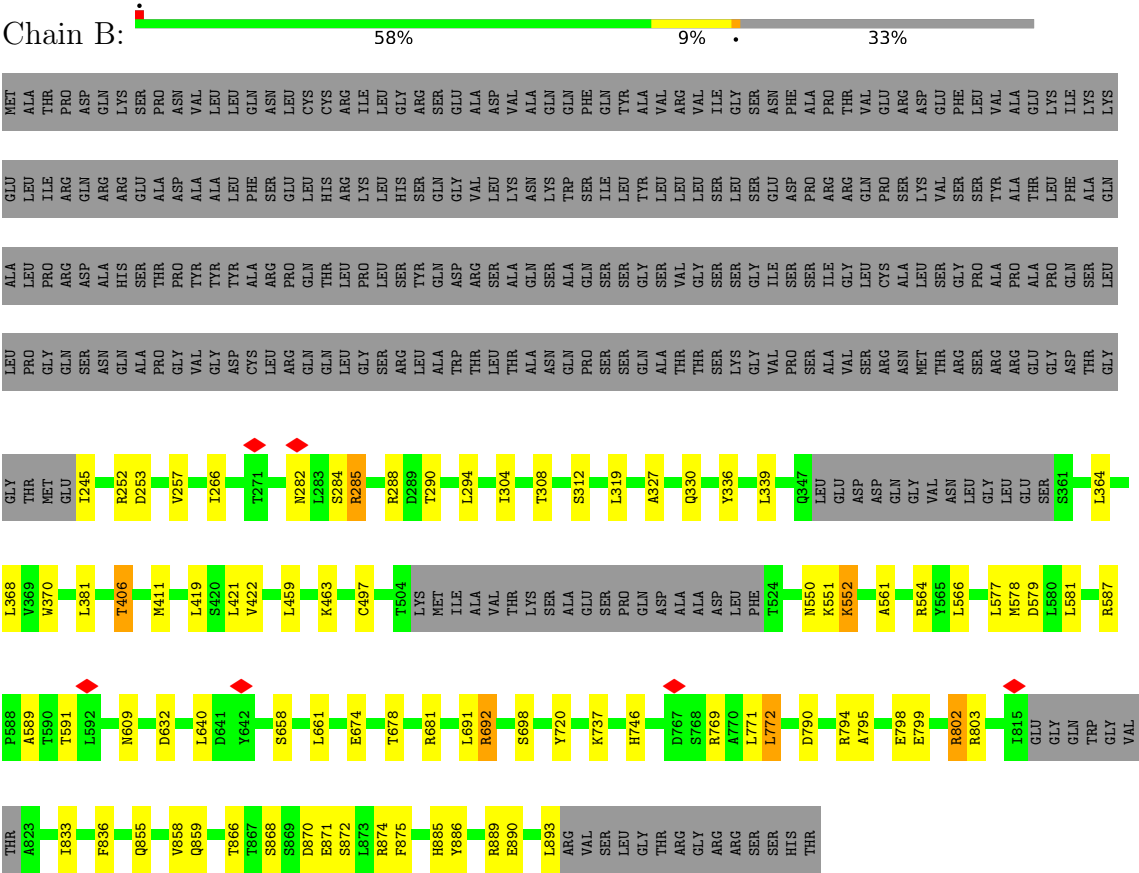


- Molecule 3: Gamma-tubulin complex component 2

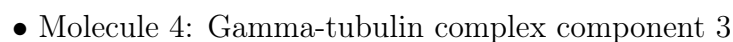




● Molecule 4: Gamma-tubulin complex component 3



● Molecule 4: Gamma-tubulin complex component 3

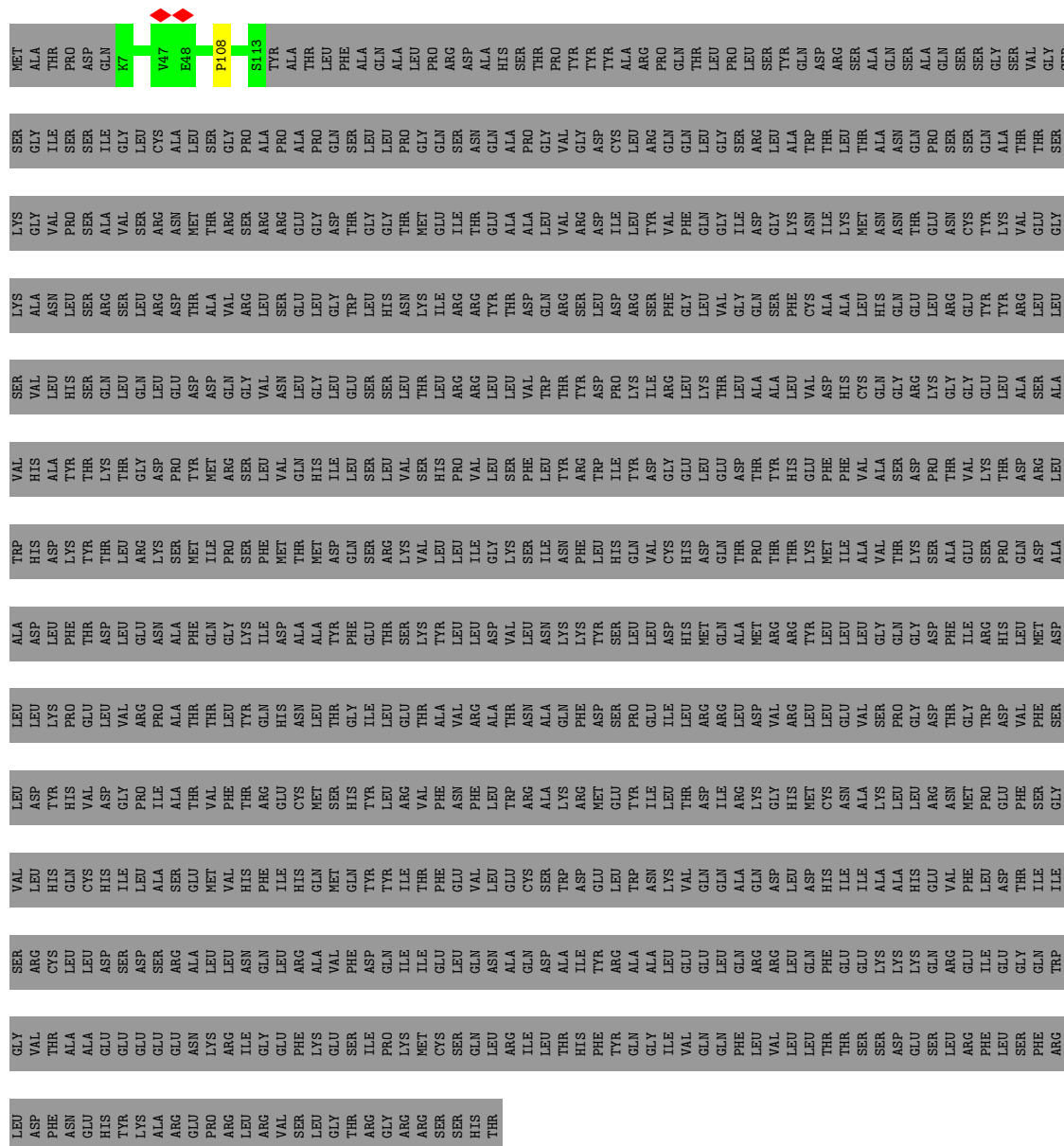


GLU	HIS	GLU	ALA	LEU	CYS	VAL	GLU	THR
HIS	TYR	GLU	GLU	ASP	HIS	ASP	LEU	ASP
LYS	ALA	GLU	GLU	ASP	LEU	LEU	ARG	VAL
ARG	GLU	GLU	GLU	SER	ALA	ILE	PRO	ALA
GLU	ASN	ASN	ALA	GLU	GLU	THR	THR	PHE
PRO	LYS	LEU	ARG	LEU	MET	VAL	THR	GLY
ARG	ARG	ASN	ILE	VAL	HIS	PHE	LEU	LYS
LEU	LEU	GLY	GLY	GLN	PHE	ARG	GLN	ILE
VAL	VAL	GLU	GLU	ILE	ILE	GLU	HIS	ASP
SER	SER	PHE	PHE	ARG	HIS	CYS	ASN	ALA
GLY	GLY	LYS	LYS	ALA	GLN	MET	LEU	ALA
THR	THR	GLU	GLU	VAL	MET	SER	THR	PHE
ARG	ARG	SER	SER	PHE	GLN	HIS	GLY	THR
GLY	GLY	ILE	ILE	ASP	TYR	TYR	ILE	THR
ARG	ARG	PRO	PRO	GLN	GLN	LEU	ARG	SER
ARG	ARG	LYS	LYS	ILE	ILE	VAL	GLU	LYS
THR	THR	MET	MET	ILE	THR	VAL	THR	VAL
		CYS	CYS	GLU	PHE	ASN	ALA	THR
		SER	SER	LEU	GLU	ASN	VAL	ASP
		HIS	HIS	GLN	VAL	PHE	ARG	ASP
		LEU	LEU	ASN	LEU	LEU	THR	VAL
		ARG	ARG	ALA	GLU	TRP	THR	ASP
		ILE	ILE	GLN	CYS	ALA	ASN	VAL
		THR	THR	GLN	SER	ALA	GLN	ASP
		ALA	ALA	ASP	TRP	LYS	LEU	ASP
		THR	THR	ILE	ASP	ARG	PHE	THR
		GLN	GLN	TYR	GLU	MET	ASP	LYS
		GLY	GLY	ARG	LEU	THR	GLU	THR
		VAL	VAL	GLU	VAL	THR	ILE	THR
		ASN	ASN	GLU	GLN	ILE	CYS	LEU
		GLU	GLU	GLN	GLN	GLN	ASN	GLY
		THR	THR	GLU	ASP	ARG	GLY	ASP
		GLY	GLY	LEU	GLN	ILE	VAL	LEU
		ARG	ARG	GLN	LEU	GLY	PRO	THR
		ASN	ASN	ASP	HIS	GLY	GLY	ASP
		THR	THR	GLU	ASP	THR	ASP	HIS
		LEU	LEU	GLY	THR	PHE	VAL	LEU
		PHE	PHE	GLN	ILE	SER	PHE	MET
		ARG	ARG	TRP	ILE	GLY	THR	ASP
		LEU	LEU	GLY	SER	VAL	LEU	LEU
		ASP	ASP	VAL	ARG	LEU	ASP	LEU
		PHE	PHE	THR	CYS	HIS	THR	THR
		ASN	ASN	ALA	LEU	GLN	PRO	PRO

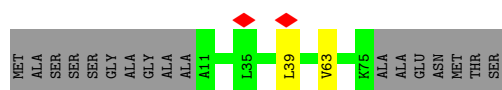
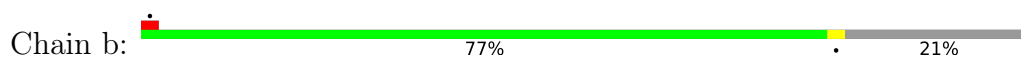
- Molecule 4: Gamma-tubulin complex component 3

Chain f:  11% 89%

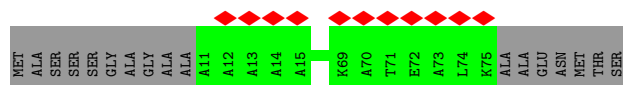
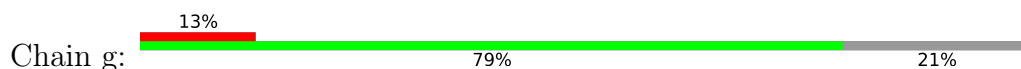
[illegible]



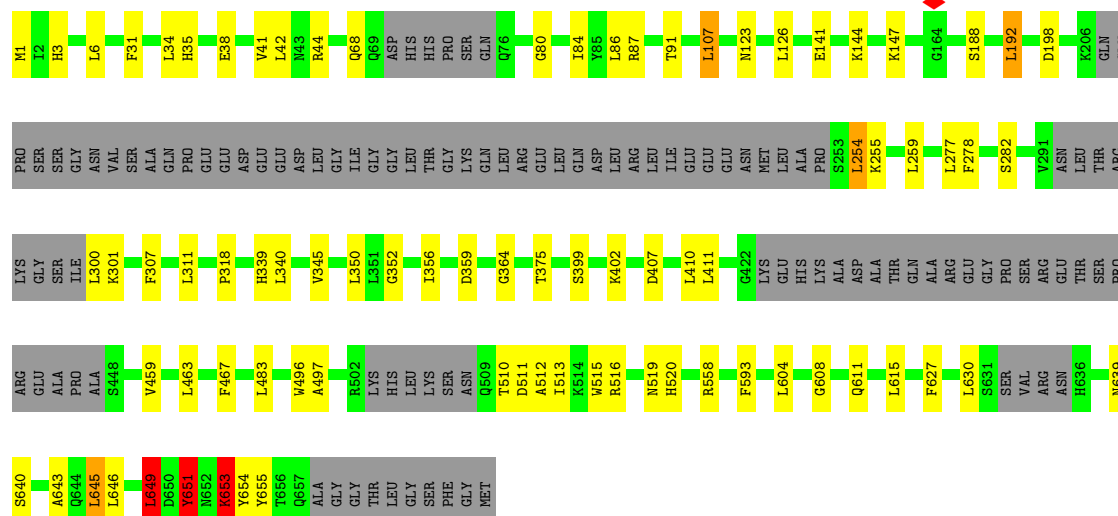
- Molecule 5: Mitotic-spindle organizing protein 1



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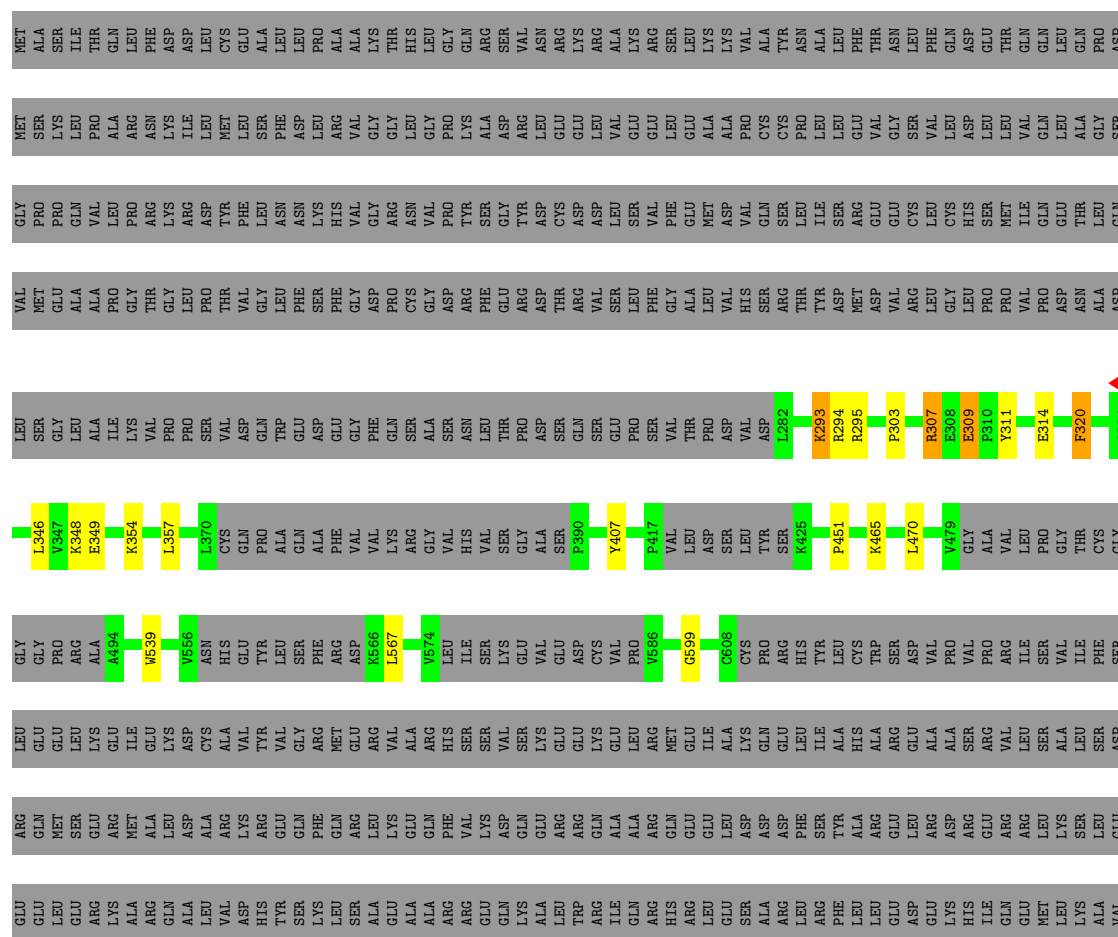


Chain K:  72% 11% 16%



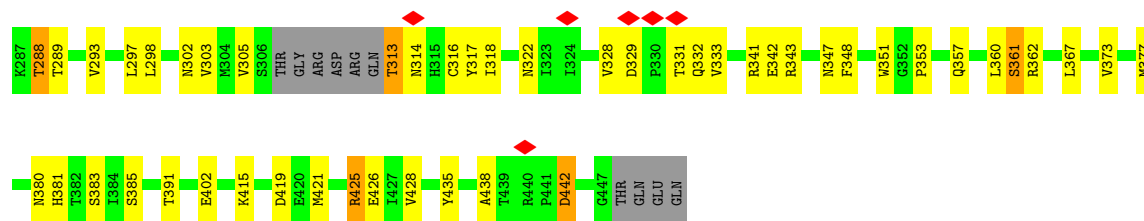
• Molecule 7: Gamma-tubulin complex component 6

Chain L:  28% 69%

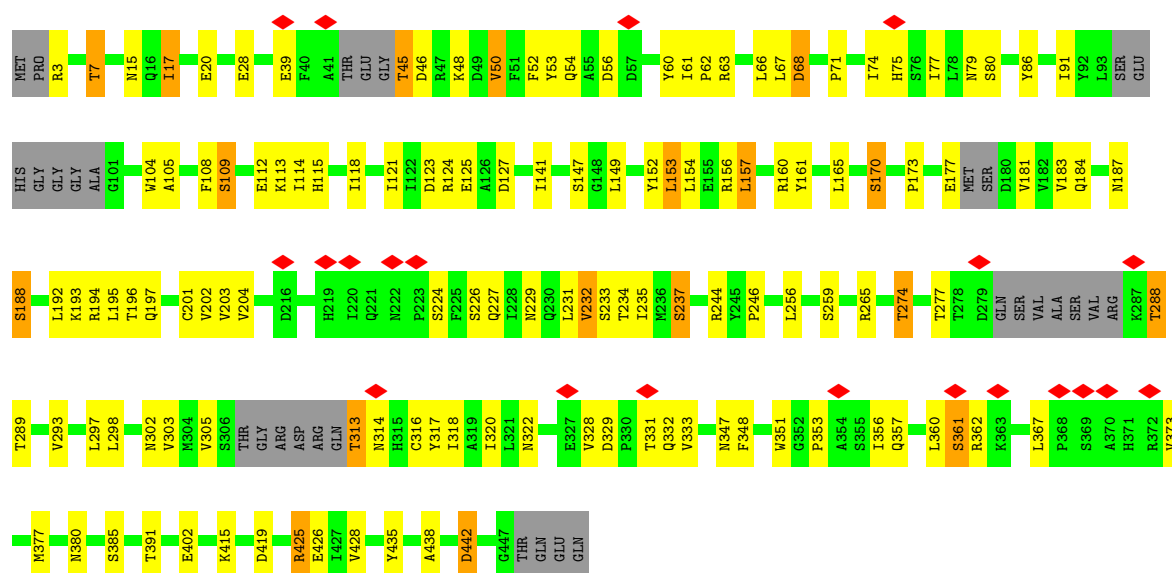




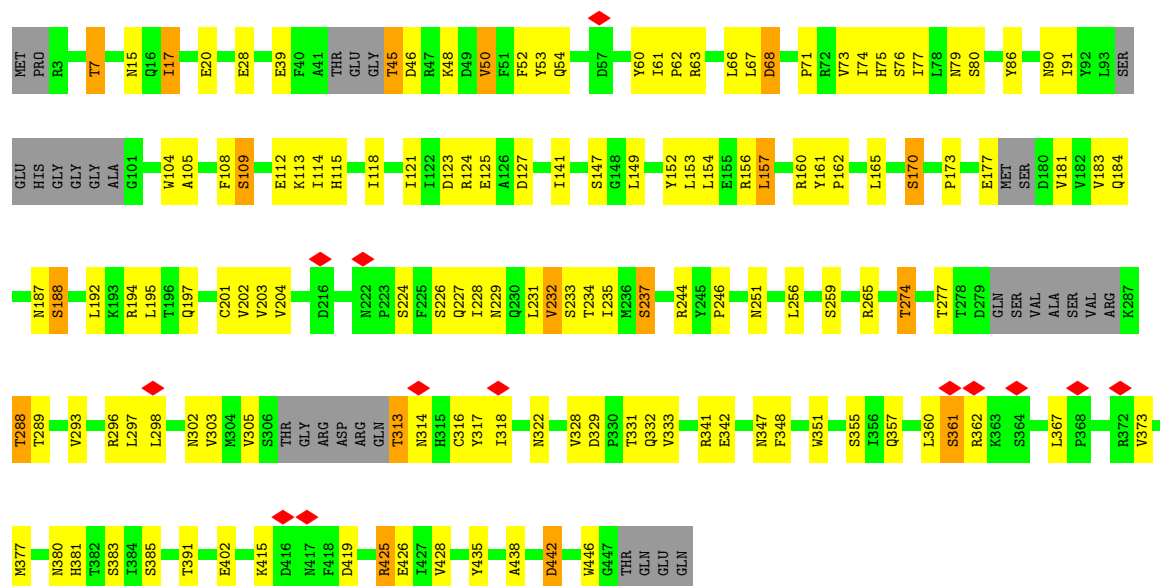




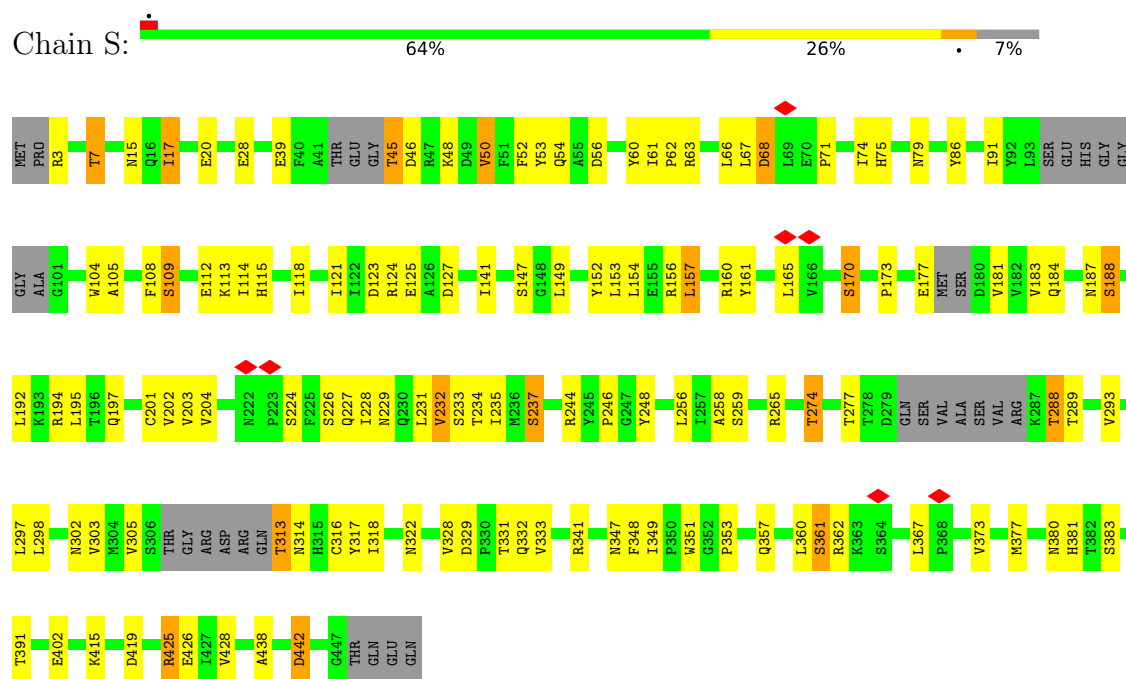
• Molecule 8: Tubulin gamma-1 chain



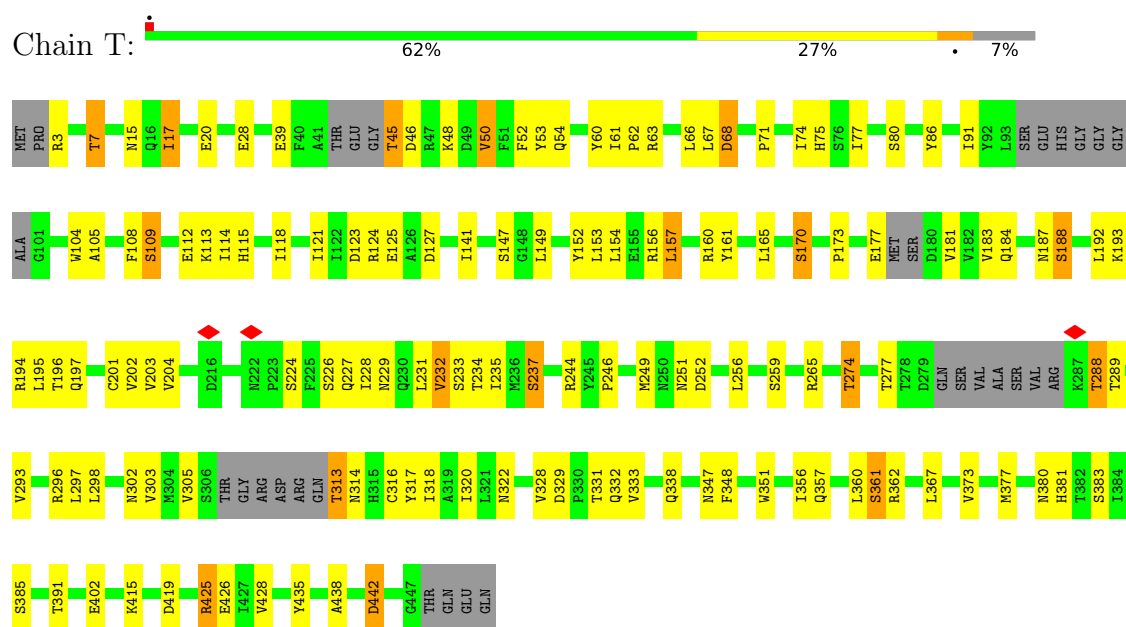
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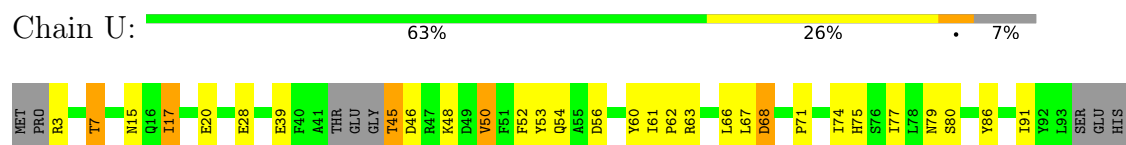
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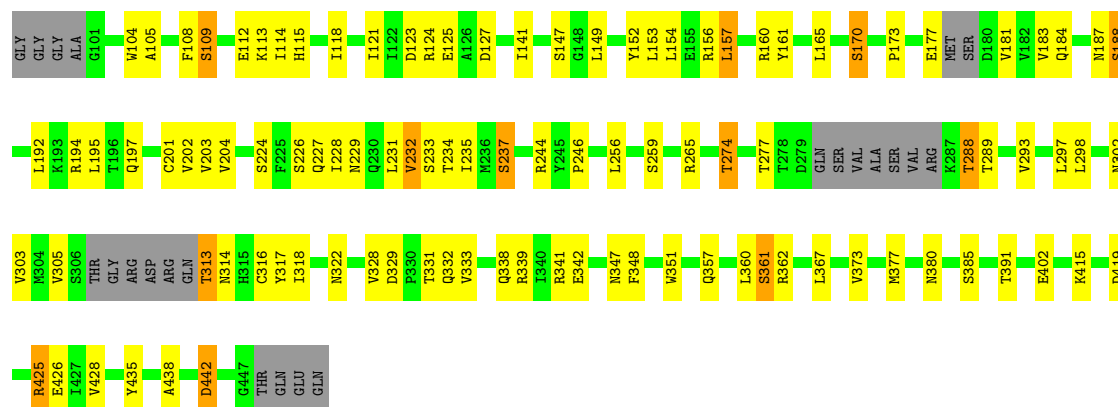


- Molecule 8: Tubulin gamma-1 chain

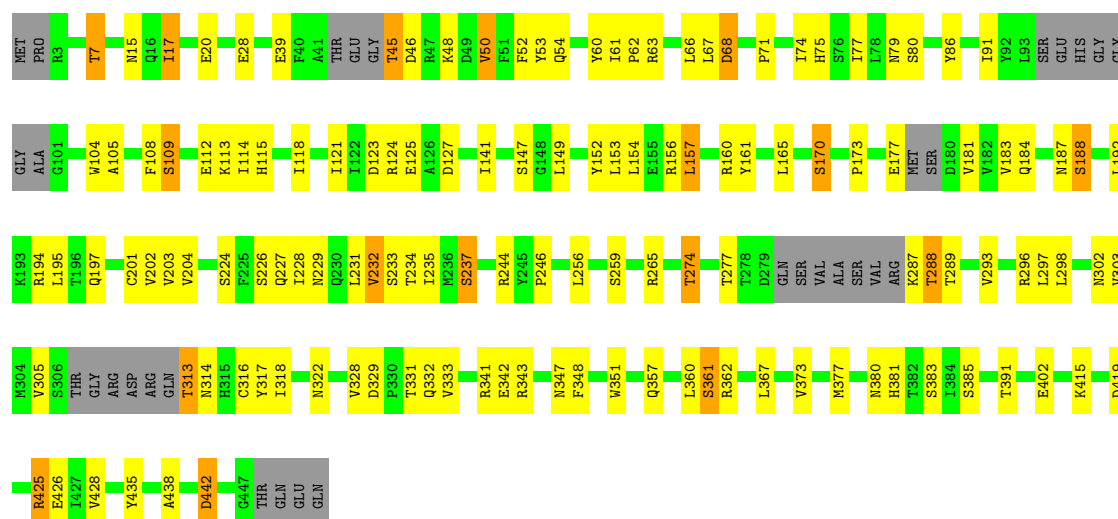


- Molecule 8: Tubulin gamma-1 chain

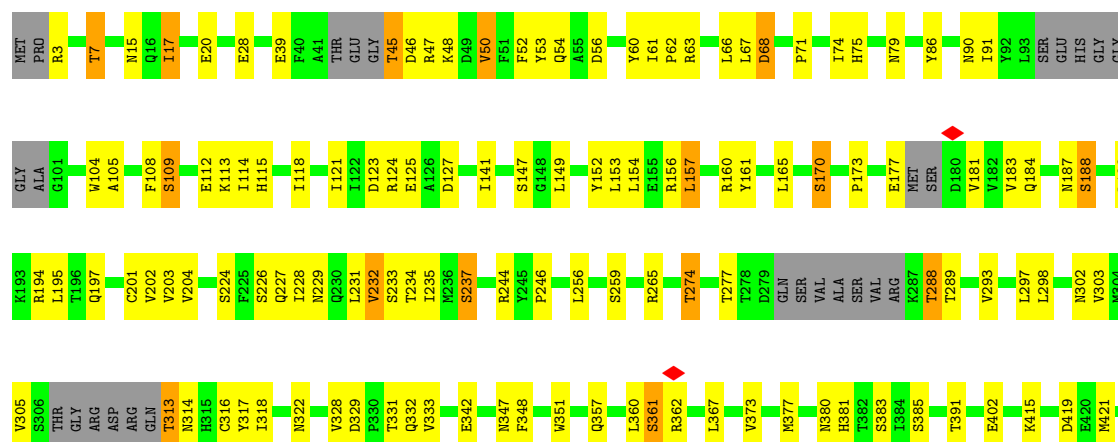




- Molecule 8: Tubulin gamma-1 chain



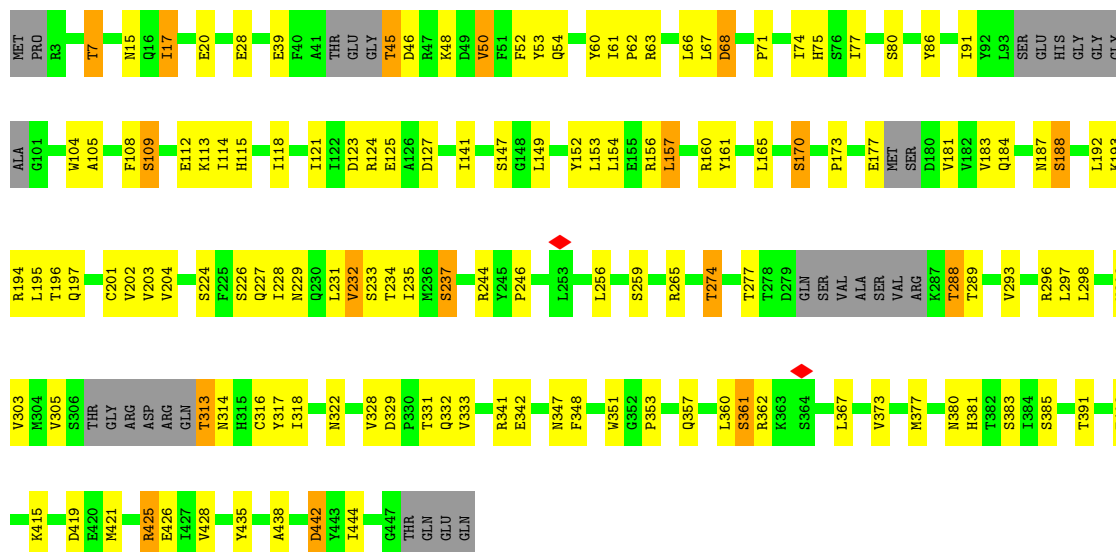
- Molecule 8: Tubulin gamma-1 chain





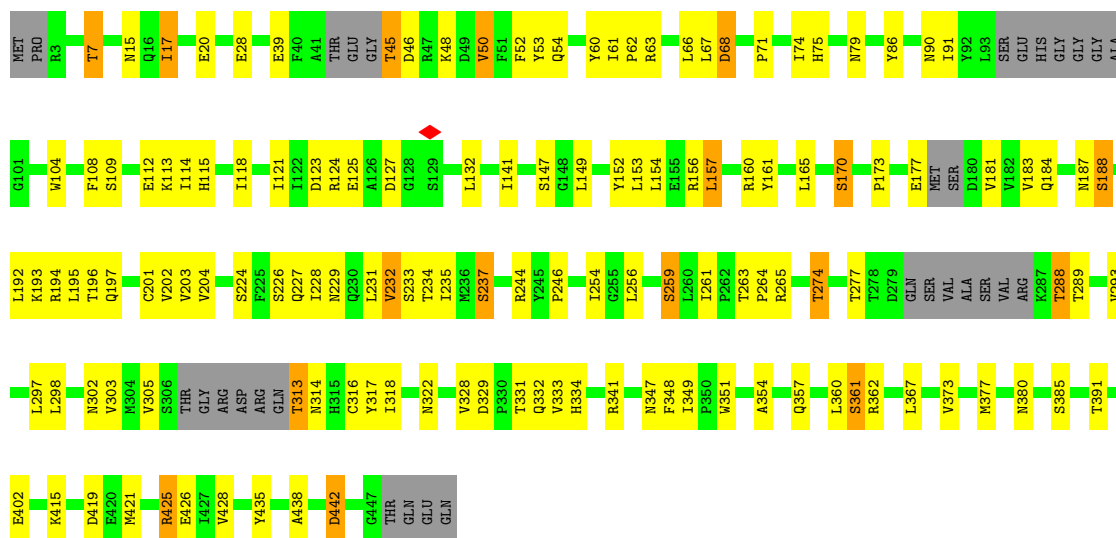
• Molecule 8: Tubulin gamma-1 chain

Chain X: 63% 27% 7%



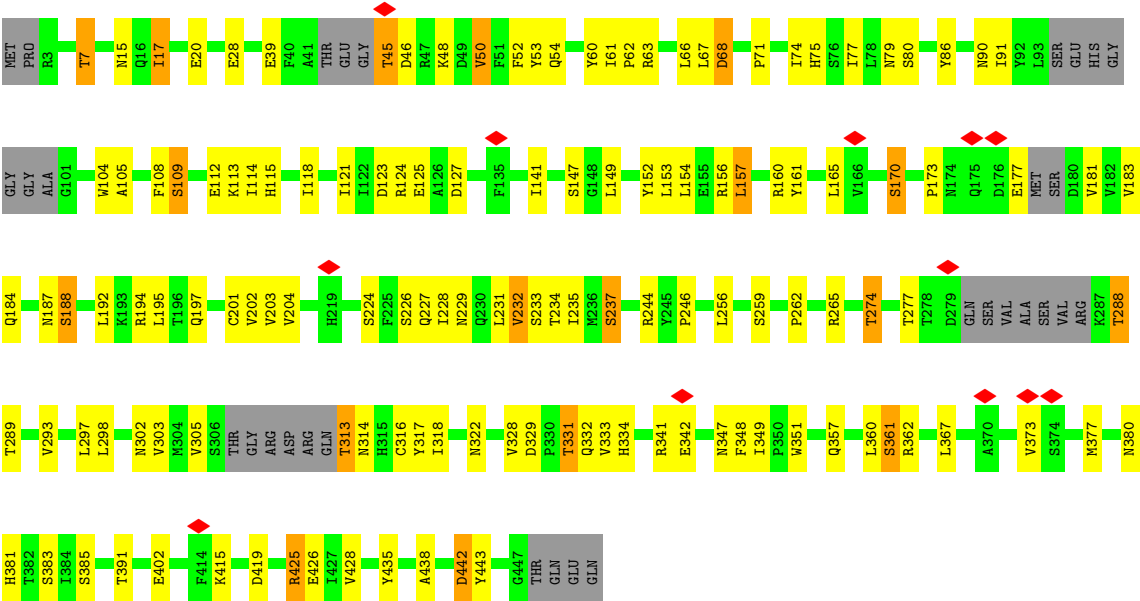
• Molecule 8: Tubulin gamma-1 chain

Chain Y: 63% 27% 7%



• Molecule 8: Tubulin gamma-1 chain

Chain Z: 63% 26% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8270	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0368	Depositor
Map size (\AA)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.66, 2.66, 2.66	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	J	0.38	0/4525	0.71	6/6119 (0.1%)
1	l	0.35	0/863	0.67	2/1166 (0.2%)
2	e	0.54	1/2908 (0.0%)	0.67	1/3938 (0.0%)
3	A	0.38	0/5085	0.61	4/6866 (0.1%)
3	C	0.35	0/5151	0.63	2/6955 (0.0%)
3	E	0.38	0/5315	0.66	5/7175 (0.1%)
3	G	0.37	0/5315	0.64	4/7175 (0.1%)
4	B	0.38	0/5133	0.67	6/6930 (0.1%)
4	D	0.38	1/4897 (0.0%)	0.62	3/6610 (0.0%)
4	F	0.36	0/5044	0.62	2/6809 (0.0%)
4	H	0.41	1/5009 (0.0%)	0.66	4/6761 (0.1%)
4	a	0.38	0/948	0.60	0/1277
4	f	0.30	0/815	0.50	0/1096
4	h	0.31	0/815	0.56	0/1096
4	j	0.37	0/855	0.64	1/1152 (0.1%)
5	b	0.34	0/484	0.70	1/653 (0.2%)
5	d	0.33	0/454	0.63	0/611
5	g	0.30	0/484	0.59	0/653
5	i	0.33	0/484	0.62	0/653
5	k	0.35	0/484	0.67	0/653
5	m	0.33	0/484	0.59	0/653
6	I	0.41	1/4322 (0.0%)	0.65	0/5853
6	K	0.46	3/4683 (0.1%)	0.70	10/6338 (0.2%)
7	L	0.38	2/4697 (0.0%)	0.65	8/6348 (0.1%)
7	c	0.30	0/1235	0.57	1/1664 (0.1%)
8	O	0.32	0/3441	0.56	1/4661 (0.0%)
8	P	0.32	0/3441	0.56	1/4661 (0.0%)
8	Q	0.32	0/3441	0.56	1/4661 (0.0%)
8	R	0.32	0/3441	0.56	1/4661 (0.0%)
8	S	0.32	0/3441	0.56	1/4661 (0.0%)
8	T	0.32	0/3441	0.56	1/4661 (0.0%)
8	U	0.32	0/3441	0.56	1/4661 (0.0%)
8	V	0.32	0/3441	0.56	1/4661 (0.0%)
8	W	0.32	0/3441	0.57	1/4661 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	X	0.32	0/3441	0.56	1/4661 (0.0%)
8	Y	0.32	0/3441	0.56	1/4661 (0.0%)
8	Z	0.32	0/3441	0.56	1/4661 (0.0%)
All	All	0.37	9/111781 (0.0%)	0.62	72/151136 (0.0%)

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	J	0	5
1	l	0	1
2	e	0	1
3	A	0	1
3	C	0	2
3	E	0	4
3	G	0	2
4	B	0	2
4	D	0	1
4	F	0	1
4	H	0	3
6	I	0	6
6	K	0	3
7	L	0	3
8	O	0	1
8	P	0	1
8	Q	0	1
8	R	0	1
8	S	0	1
8	T	0	1
8	U	0	1
8	V	0	1
8	W	0	1
8	X	0	1
8	Y	0	1
8	Z	0	1
All	All	0	47

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	243	PRO	N-CD	19.87	1.75	1.47
6	K	653	LYS	CD-CE	-8.02	1.31	1.51
7	L	1708	TYR	CD1-CE1	-6.35	1.29	1.39
7	L	1653	VAL	CB-CG1	-6.20	1.39	1.52
4	D	692	ARG	CB-CG	-5.95	1.36	1.52

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	238	LEU	CA-CB-CG	11.06	140.73	115.30
6	K	649	LEU	CA-CB-CG	10.51	139.47	115.30
1	J	238	LEU	CB-CG-CD1	-9.70	94.51	111.00
4	H	365	ARG	NE-CZ-NH1	-8.32	116.14	120.30
6	K	651	TYR	CB-CG-CD1	-7.91	116.26	121.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	583	ILE	Peptide
4	B	868	SER	Peptide
4	B	889	ARG	Peptide
2	e	249	THR	Peptide
1	l	121	PRO	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	J	4429	0	4482	34	0
1	l	847	0	789	0	0
2	e	2847	0	2810	0	0
3	A	4978	0	4996	32	0
3	C	5044	0	5081	40	0
3	E	5206	0	5230	40	0
3	G	5206	0	5230	29	0
4	B	5029	0	5018	47	0
4	D	4796	0	4775	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	4941	0	4935	45	0
4	H	4907	0	4896	34	0
4	a	933	0	953	0	0
4	f	803	0	831	0	0
4	h	803	0	831	0	0
4	j	843	0	846	0	0
5	b	484	0	512	0	0
5	d	454	0	482	0	0
5	g	484	0	512	0	0
5	i	484	0	512	0	0
5	k	484	0	512	0	0
5	m	484	0	512	0	0
6	I	4225	0	4259	28	0
6	K	4579	0	4586	60	0
7	L	4587	0	4636	26	0
7	c	1220	0	1231	0	0
8	O	3373	0	3325	71	0
8	P	3373	0	3325	74	0
8	Q	3373	0	3325	66	0
8	R	3373	0	3325	71	0
8	S	3373	0	3325	69	0
8	T	3373	0	3325	71	0
8	U	3373	0	3325	68	0
8	V	3373	0	3325	69	0
8	W	3373	0	3325	69	0
8	X	3373	0	3325	71	0
8	Y	3373	0	3325	80	0
8	Z	3373	0	3325	70	0
9	l	6	0	0	0	0
All	All	109579	0	109357	1214	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 6.

The worst 5 of 1214 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)
6:K:653:LYS:NZ	8:Y:349:ILE:O	2.13	0.80
3:G:222:LEU:HG	4:H:365:ARG:HH12	1.46	0.80
3:C:696:TYR:O	3:C:700:GLU:HB2	1.85	0.76
6:K:497:ALA:HB2	8:Y:254:ILE:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:572:ASP:OD1	8:T:251:ASN:ND2	2.21	0.74

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	J	506/1024 (49%)	465 (92%)	38 (8%)	3 (1%)	25	66
1	l	104/1024 (10%)	96 (92%)	4 (4%)	4 (4%)	3	24
2	e	360/375 (96%)	339 (94%)	21 (6%)	0	100	100
3	A	599/902 (66%)	576 (96%)	22 (4%)	1 (0%)	47	81
3	C	606/902 (67%)	568 (94%)	37 (6%)	1 (0%)	47	81
3	E	628/902 (70%)	594 (95%)	32 (5%)	2 (0%)	41	77
3	G	628/902 (70%)	587 (94%)	37 (6%)	4 (1%)	25	66
4	B	602/907 (66%)	573 (95%)	27 (4%)	2 (0%)	41	77
4	D	571/907 (63%)	547 (96%)	21 (4%)	3 (0%)	29	69
4	F	591/907 (65%)	555 (94%)	35 (6%)	1 (0%)	47	81
4	H	584/907 (64%)	559 (96%)	23 (4%)	2 (0%)	41	77
4	a	112/907 (12%)	107 (96%)	5 (4%)	0	100	100
4	f	97/907 (11%)	92 (95%)	5 (5%)	0	100	100
4	h	97/907 (11%)	93 (96%)	4 (4%)	0	100	100
4	j	105/907 (12%)	98 (93%)	7 (7%)	0	100	100
5	b	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
5	g	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	i	63/82 (77%)	60 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	k	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
5	m	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
6	I	511/667 (77%)	482 (94%)	24 (5%)	5 (1%)	15	55
6	K	548/667 (82%)	528 (96%)	19 (4%)	1 (0%)	47	81
7	L	540/1819 (30%)	493 (91%)	43 (8%)	4 (1%)	22	63
7	c	148/1819 (8%)	142 (96%)	6 (4%)	0	100	100
8	O	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	P	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Q	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	R	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	S	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	T	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	U	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	V	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	W	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	X	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Y	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Z	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
All	All	13205/24163 (55%)	12536 (95%)	636 (5%)	33 (0%)	50	81

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	121	PRO
3	A	584	THR
3	C	239	ALA
4	D	627	GLU
4	D	884	GLU

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	
1	J	498/933 (53%)	498 (100%)	0	100	100
1	l	84/933 (9%)	84 (100%)	0	100	100
2	e	310/318 (98%)	305 (98%)	5 (2%)	62	79
3	A	549/791 (69%)	546 (100%)	3 (0%)	88	93
3	C	556/791 (70%)	555 (100%)	1 (0%)	93	96
3	E	572/791 (72%)	571 (100%)	1 (0%)	93	96
3	G	572/791 (72%)	568 (99%)	4 (1%)	84	90
4	B	551/798 (69%)	546 (99%)	5 (1%)	78	87
4	D	525/798 (66%)	523 (100%)	2 (0%)	91	94
4	F	542/798 (68%)	537 (99%)	5 (1%)	78	87
4	H	539/798 (68%)	537 (100%)	2 (0%)	91	94
4	a	101/798 (13%)	100 (99%)	1 (1%)	76	86
4	f	88/798 (11%)	88 (100%)	0	100	100
4	h	88/798 (11%)	88 (100%)	0	100	100
4	j	88/798 (11%)	88 (100%)	0	100	100
5	b	53/62 (86%)	52 (98%)	1 (2%)	57	75
5	d	53/62 (86%)	53 (100%)	0	100	100
5	g	53/62 (86%)	53 (100%)	0	100	100
5	i	53/62 (86%)	53 (100%)	0	100	100
5	k	53/62 (86%)	53 (100%)	0	100	100
5	m	53/62 (86%)	53 (100%)	0	100	100
6	I	472/594 (80%)	471 (100%)	1 (0%)	93	96
6	K	509/594 (86%)	503 (99%)	6 (1%)	71	83
7	L	501/1546 (32%)	500 (100%)	1 (0%)	93	96
7	c	135/1546 (9%)	135 (100%)	0	100	100
8	O	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	P	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	Q	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	R	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	S	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	T	376/400 (94%)	337 (90%)	39 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	V	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	W	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	X	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	Y	376/400 (94%)	337 (90%)	39 (10%)	7	24
8	Z	376/400 (94%)	337 (90%)	39 (10%)	7	24
All	All	12110/21184 (57%)	11604 (96%)	506 (4%)	33	54

5 of 506 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	T	7	THR
8	Y	203	VAL
8	U	201	CYS
8	Y	165	LEU
8	Z	147	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 223 such sidechains are listed below:

Mol	Chain	Res	Type
8	R	187	ASN
3	E	763	GLN
8	T	334	HIS
3	E	725	HIS
8	Z	187	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 [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.

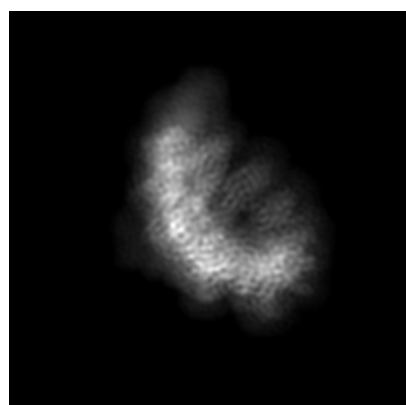
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14012. These allow visual inspection of the internal detail of the map and identification of artifacts.

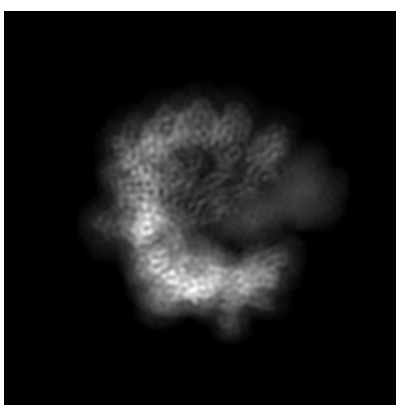
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

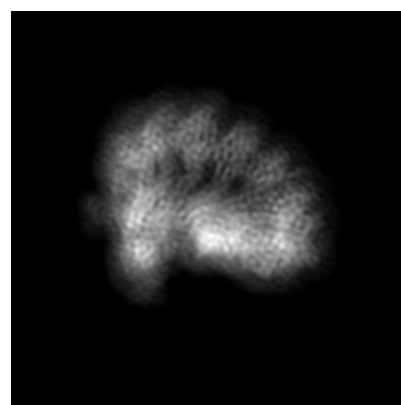
6.1.1 Primary map



X



Y



Z

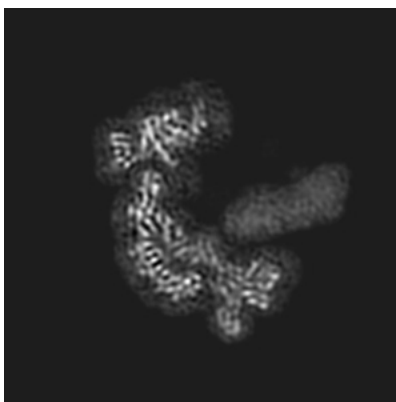
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

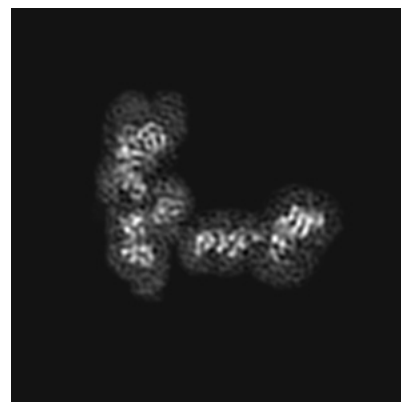
6.2.1 Primary map



X Index: 100



Y Index: 100

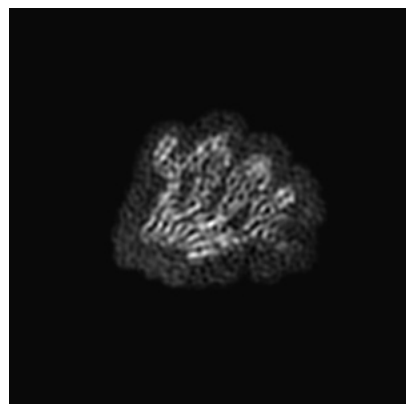


Z Index: 100

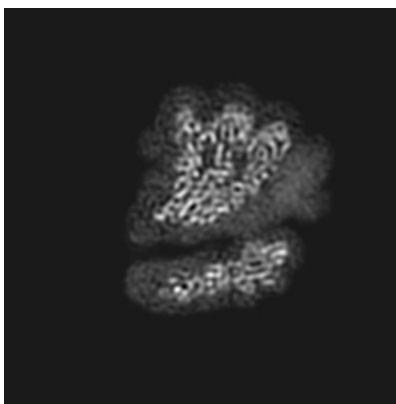
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

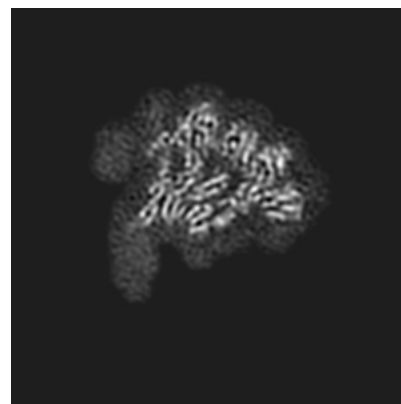
6.3.1 Primary map



X Index: 63



Y Index: 81



Z Index: 72

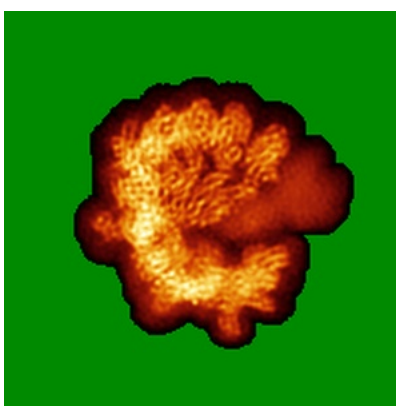
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

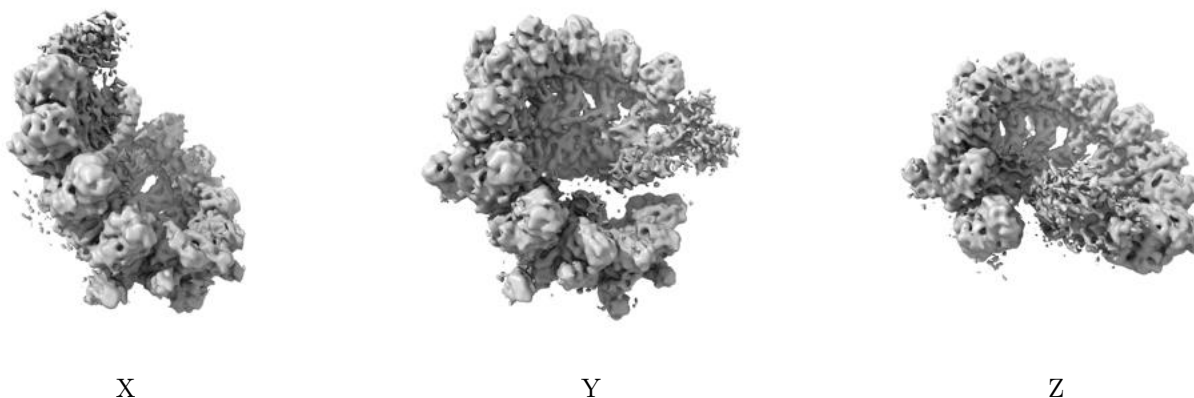


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0368. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

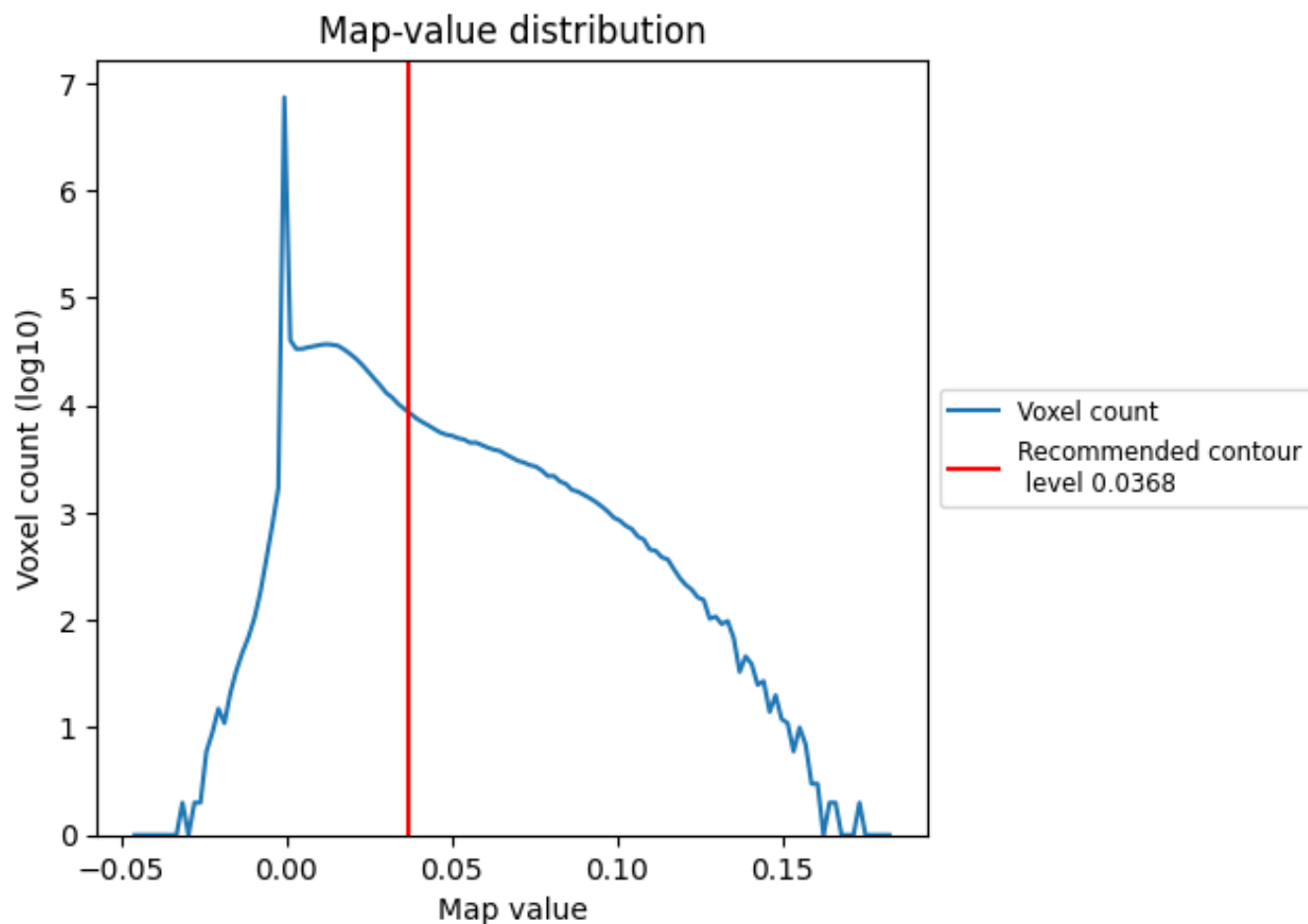
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

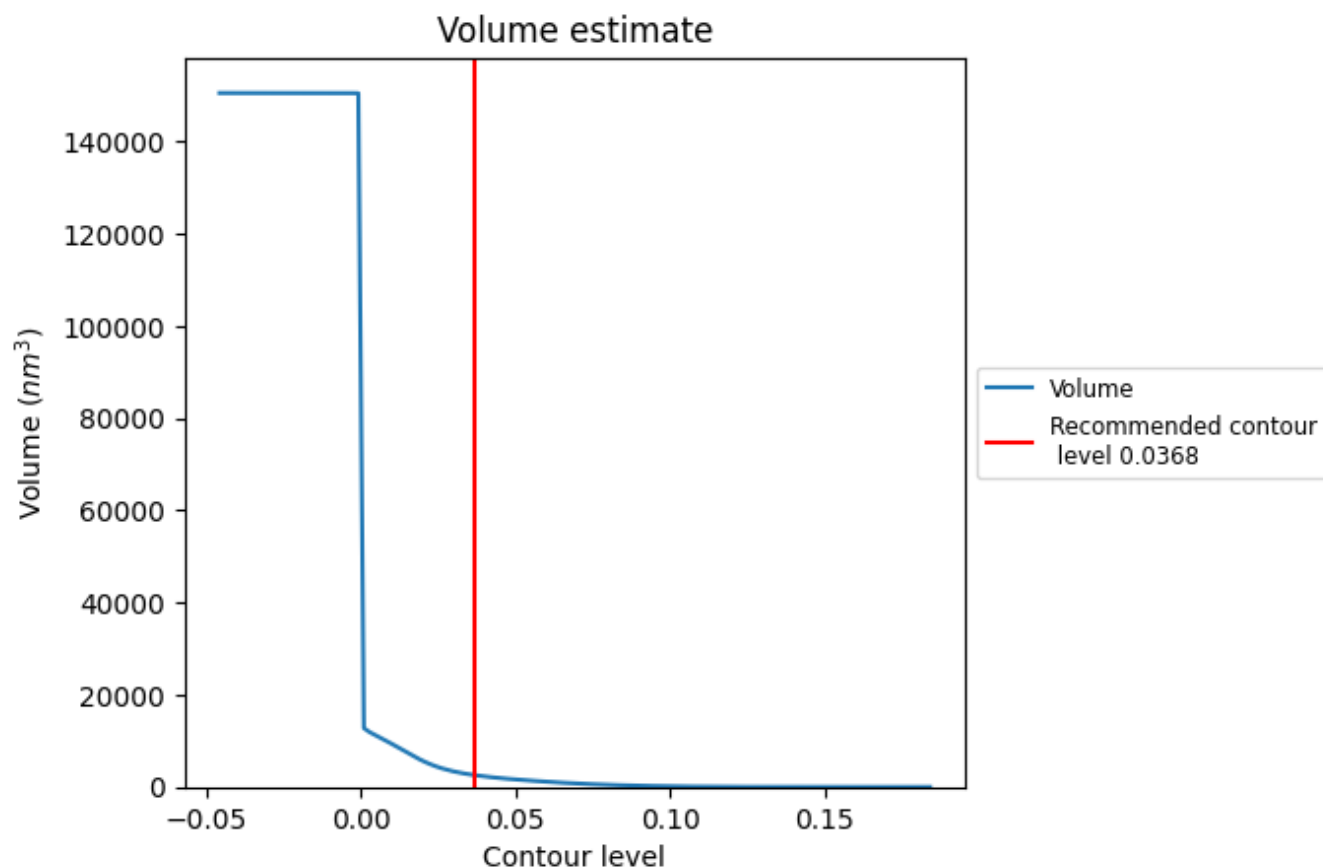
This section contains the results of statistical analysis of the map.

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.

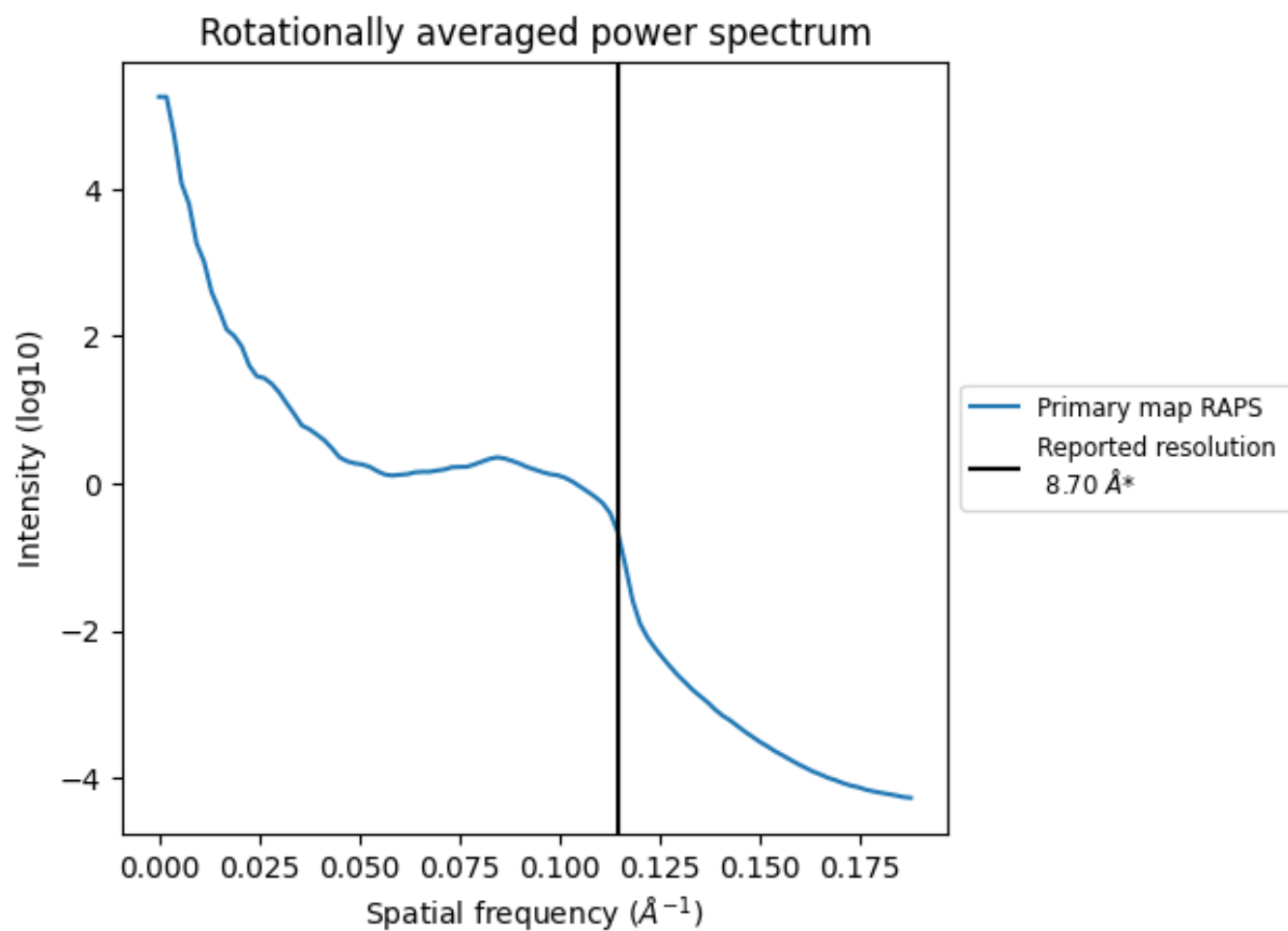
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2556 nm^3 ; this corresponds to an approximate mass of 2308 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 0.115 Å⁻¹

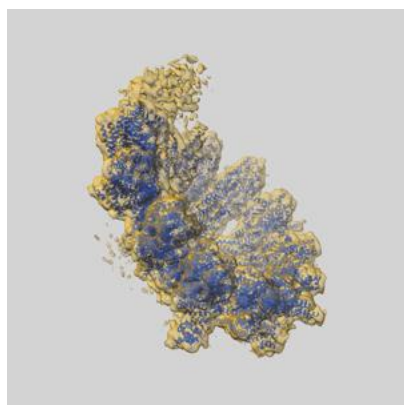
8 Fourier-Shell correlation ⓘ

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

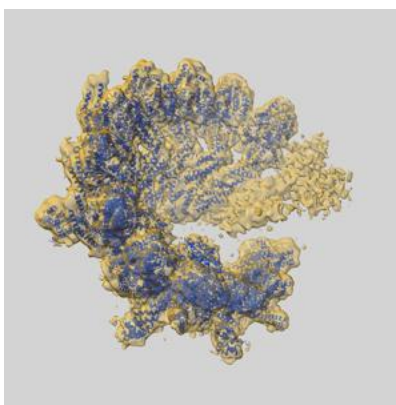
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14012 and PDB model 7QJ7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

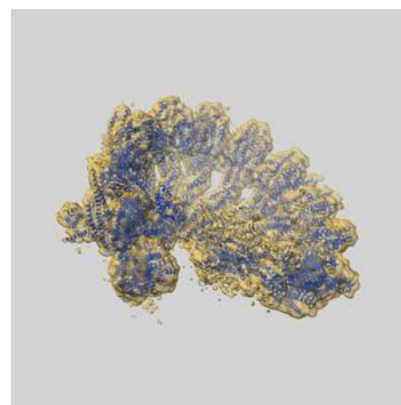
9.1 Map-model overlay [i](#)



X



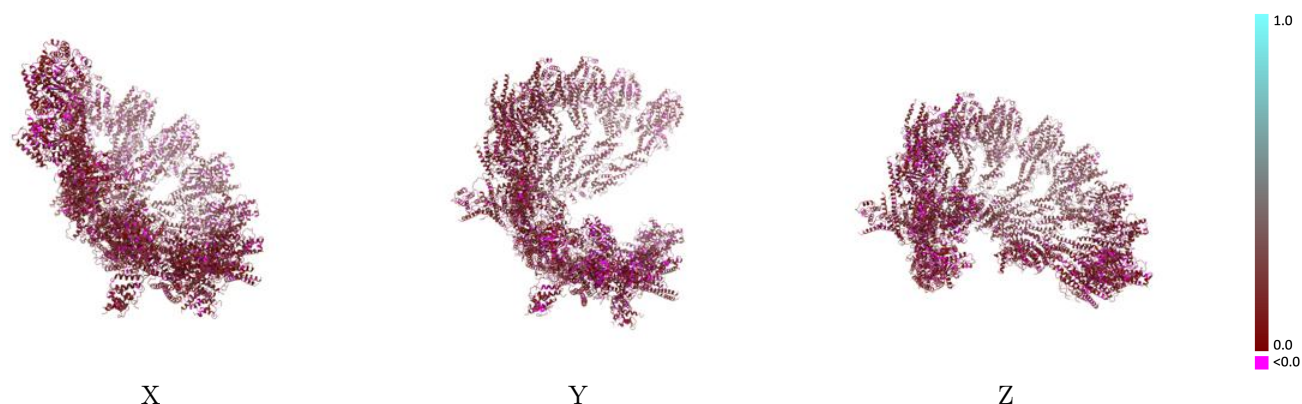
Y



Z

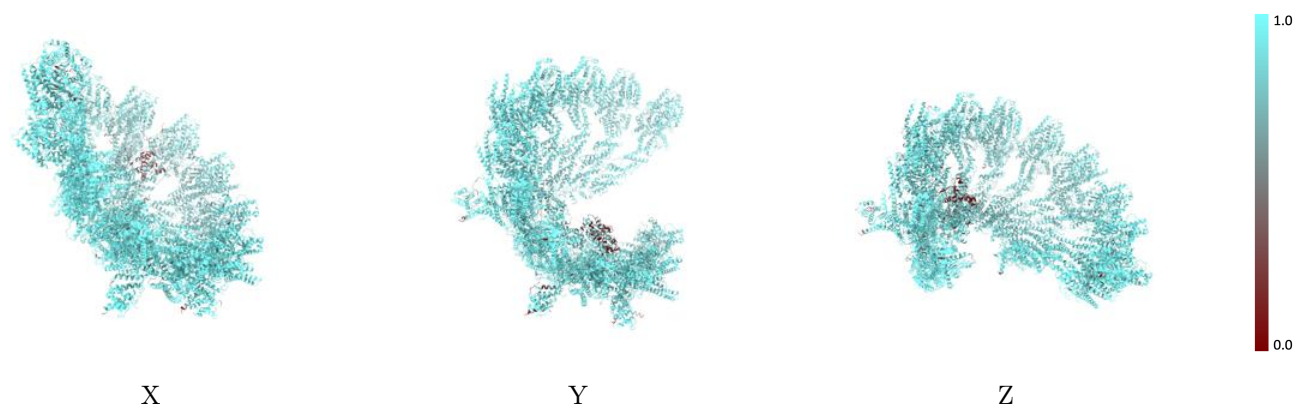
The images above show the 3D surface view of the map at the recommended contour level 0.0368 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



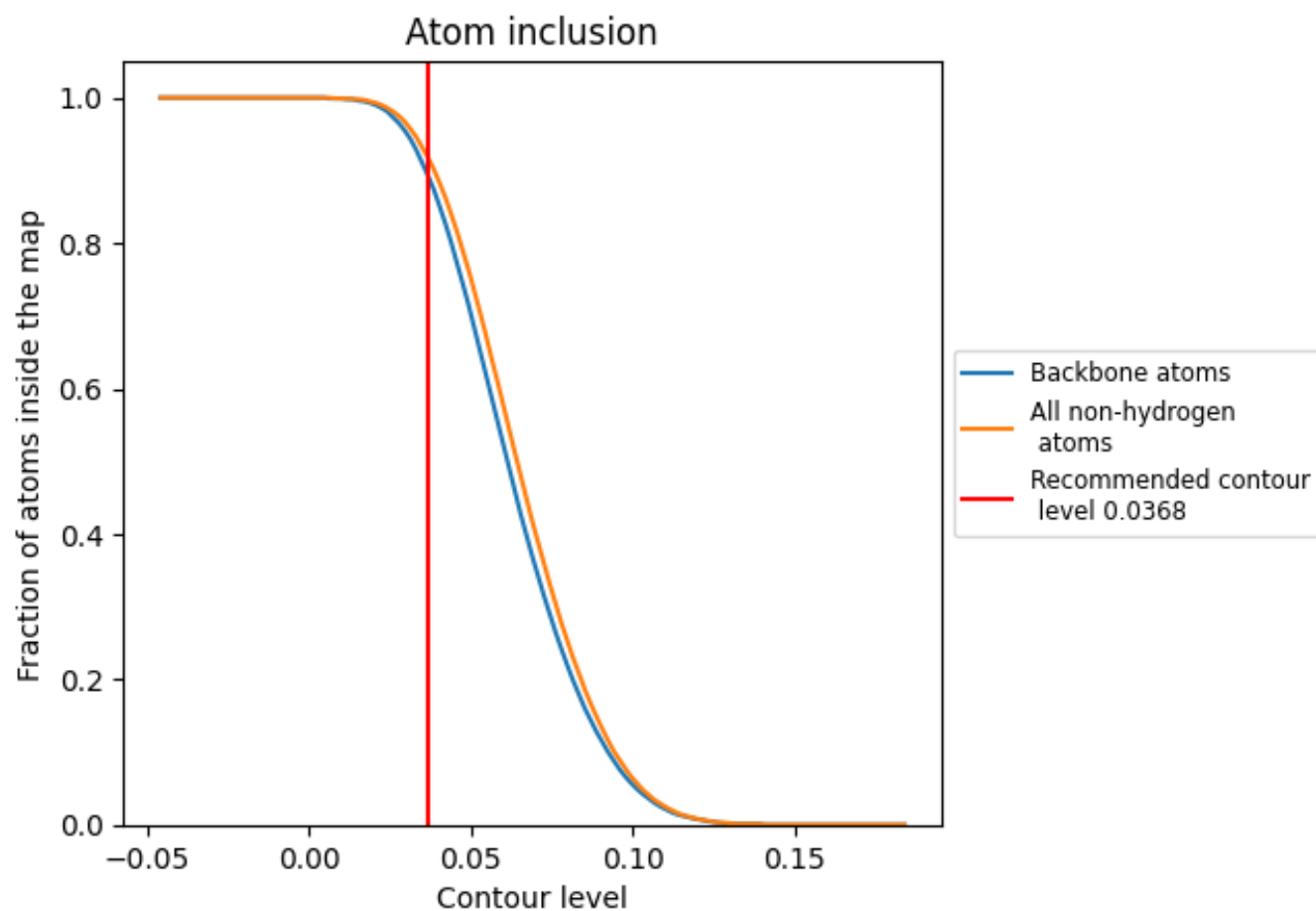
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0368).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 92% 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 (0.0368) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.1250
A	 0.9460	 0.1230
B	 0.9210	 0.1280
C	 0.9400	 0.1260
D	 0.9330	 0.1350
E	 0.9360	 0.1360
F	 0.9430	 0.1320
G	 0.9420	 0.1440
H	 0.9390	 0.1410
I	 0.9430	 0.1480
J	 0.9500	 0.1390
K	 0.9470	 0.1370
L	 0.9550	 0.1330
O	 0.9340	 0.0950
P	 0.8950	 0.1120
Q	 0.8780	 0.0970
R	 0.9080	 0.1030
S	 0.9300	 0.1010
T	 0.9440	 0.1230
U	 0.9450	 0.1250
V	 0.9530	 0.1420
W	 0.9530	 0.1300
X	 0.9600	 0.1240
Y	 0.9380	 0.1020
Z	 0.8930	 0.1080
a	 0.8410	 0.1240
b	 0.8700	 0.1620
c	 0.8360	 0.1090
d	 0.8360	 0.1670
e	 0.6190	 0.0790
f	 0.9030	 0.1040
g	 0.8070	 0.1270
h	 0.8360	 0.1190
i	 0.7580	 0.0870
j	 0.9330	 0.1090



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Chain	Atom inclusion	Q-score
k	 0.8870	 0.1210
l	 0.9300	 0.1370
m	 0.9180	 0.1680