

Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 07:52 am BST

PDB ID : 9G3Z

EMDB ID : EMD-51019

Title : Structure of the Open gamma-Tubulin Ring Complex from Pig Brain

Authors: Munoz-Hernandez, H.; Wieczorek, M.

Deposited on : 2024-07-12

Resolution : 4.30 Å(reported)

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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113

MolProbity : 4.02b-467

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

 $MapQ \quad : \quad 1.9.13$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

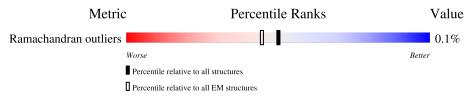
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 4.30 Å.

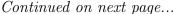
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \text{Entries})$	${ m EM~structures} \ (\#{ m Entries})$
	(11)	(11
Ramachandran outliers	207382	16835

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	
			62%	
1	О	79	85%	15%
1	Р	79	84%	• 15%
1	Q	79	81%	19%
2	Y	155	33% 67%	
3	a	451	98%	
3	b	451	98%	
3	c	451	98%	
3	d	451	94%	6%
3	e	451	96%	
3	f	451	96%	
3	g	451	96%	





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Mol	Chain	Length	Quality of chain	
3	h	451	97%	
3	i	451	97%	•
3	j	451	97%	
3	k	451	97%	
3	1	451	15%	•
3	m	451	95% 98%	·
3	n	451	92% 97%	•••
4	W	1663	• 98%	
4	X	1663	• 98%	
5	В	910	68%	32%
5	D	910	68%	32%
5	F	910	68%	32%
5	Н	910	81%	19%
5	N	910	38% 77%	22%
6	A	905	74%	26%
6	С	905	74%	26%
6	Е	905	74%	26%
6	G	905	74% 14%	26%
6	M	905	86%	14%
7	L	1715	45% 55	%
8	I	667	88%	12%
8	K	667	88%	12%
9	J	1042	64%	36%



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 113079 atoms, of which 34747 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 Mitotic spindle organizing protein 1.

Mol	Chain	Residues		At	oms		AltConf	Trace	
1	0	67	Total	С	Н	N	О	0	0
1		07	497	199	164	67	67	0	0
1	Р	67	Total	С	Н	N	О	0	0
1	1	07	497	199	164	67	67	U	U
1	0	64	Total	С	Н	N	О	0	0
1	Q	04	464	190	146	64	64	U	U

• Molecule 2 is a protein called Mitotic-spindle organizing protein 2A isoform X4.

Mol	Chain	Residues		At	oms			AltConf	Trace
2	Y	51	Total 379	C 150	H 127	N 51	O 51	0	0

• Molecule 3 is a protein called Tubulin gamma chain.

Mol	Chain	Residues		A	toms			AltConf	Trace
3		444	Total	С	Н	N	О	0	0
)	a	444	3161	1306	967	444	444	U	U
3	m	444	Total	С	Н	N	О	0	0
) 	m	444	3161	1306	967	444	444	0	U
3	b	442	Total	С	Н	N	О	0	0
) 	Ь	442	3146	1299	963	442	442	0	U
3	С	440	Total	С	Н	N	О	0	0
, J		440	3129	1293	956	440	440	0	0
3	d	426	Total	С	Н	N	О	0	0
, J	u	420	3030	1252	926	426	426	0	0
3	e	432	Total	С	Η	N	O	0	0
	C	402	3074	1270	940	432	432	U	U
3	f	433	Total	С	Η	N	O	0	0
	1	400	3081	1273	942	433	433	0	U
3	ď	433	Total	С	Η	N	O	0	0
	g	400	3081	1273	942	433	433	U	U
3	h	439	Total	С	Η	N	O	0	0
3	11	409	3122	1291	953	439	439		

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Mol	Chain	Residues		\mathbf{A}^{1}	toms			AltConf	Trace
3	;	438	Total	С	Н	N	О	0	0
)	1	430	3115	1288	951	438	438	0	U
3	10	442	Total	С	Н	N	О	0	0
)	n	442	3146	1299	963	442	442	0	U
3	k	438	Total	С	Н	N	О	0	0
)	K	430	3115	1288	951	438	438	U	0
3	;	439	Total	С	Н	N	О	0	0
)	J	409	3122	1292	952	439	439	0	
3	1	435	Total	С	Н	N	О	0	0
)		400	3094	1279	945	435	435		U

• Molecule 4 is a protein called CDK5 regulatory subunit-associated protein 2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	***	99	Total	С	Н	N	О	0	0
4	W	33	230	99	65	33	33	0	
1	37	2.4	Total	С	Н	N	О	0	0
4	X	34	237	102	67	34	34	U	U

• Molecule 5 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues		A	toms			AltConf	Trace
5	N	707	Total	С	Н	N	О	0	0
9	11	101	5082	2092	1576	707	707	0	U
5	В	621	Total	С	Н	N	О	0	0
	Ъ	021	4466	1839	1385	621	621		U
5	Н	739	Total	С	Н	N	О	0	0
	11	139	5322	2189	1655	739	739		U
5	D	621	Total	С	Н	N	О	0	0
9	ע	021	4466	1839	1385	621	621	0	U
5	F	621	Total	С	Н	N	О	0	0
3	Г	021	4466	1839	1385	621	621	U	U

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	782	Total 5606		H 1726		O 782	0	0
6	A	669	Total 4792		H 1471	N 669	O 669	0	0
6	С	669	Total 4792	C 1983	H 1471	N 669	O 669	0	0

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Mol	Chain	Residues	\mathbf{Atoms}					AltConf	Trace
6	E	660	Total	С	Н	N	О	0	0
0	15	669	4792	1983	1471	669	669	0	
6	С	669	Total	С	Н	N	О	0	0
	G	009	4792	1983	1471	669	669		U

• Molecule 7 is a protein called Tubulin gamma complex associated protein 6.

Mol	Chain	Residues		A	toms			AltConf	Trace
7	L	773	Total 5548	C 2269	H 1733	N 773	O 773	0	0

• Molecule 8 is a protein called Gamma-tubulin complex component.

\mathbf{N}	Iol	Chain	Residues	Atoms			AltConf	Trace		
	0	Т	587	Total	С	Н	N	О	0	0
	0	1	301	4180	1732	1274	587	587	0	U
	0	I/	587	Total	С	Н	N	О	0	0
	O	17	301	4180	1732	1274	587	587		U

• Molecule 9 is a protein called Gamma-tubulin complex component.

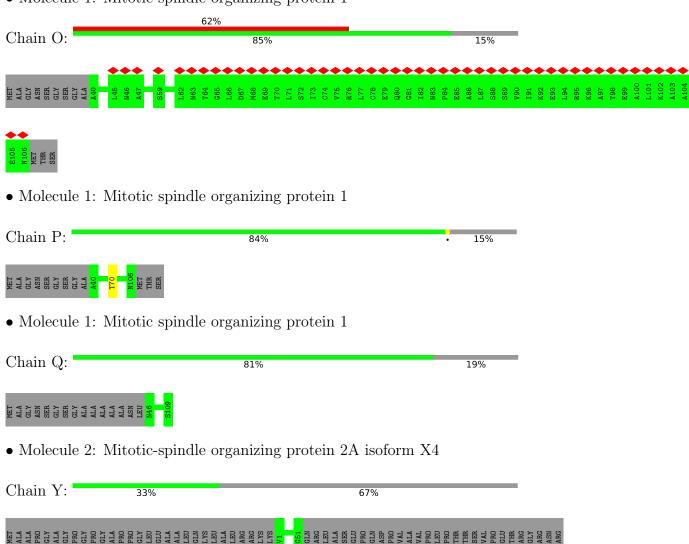
Mol	Chain	Residues	Atoms			AltConf	Trace		
9	J	664	Total 4714	C 1967	H 1419	N 664	O 664	0	0



3 Residue-property plots (i)

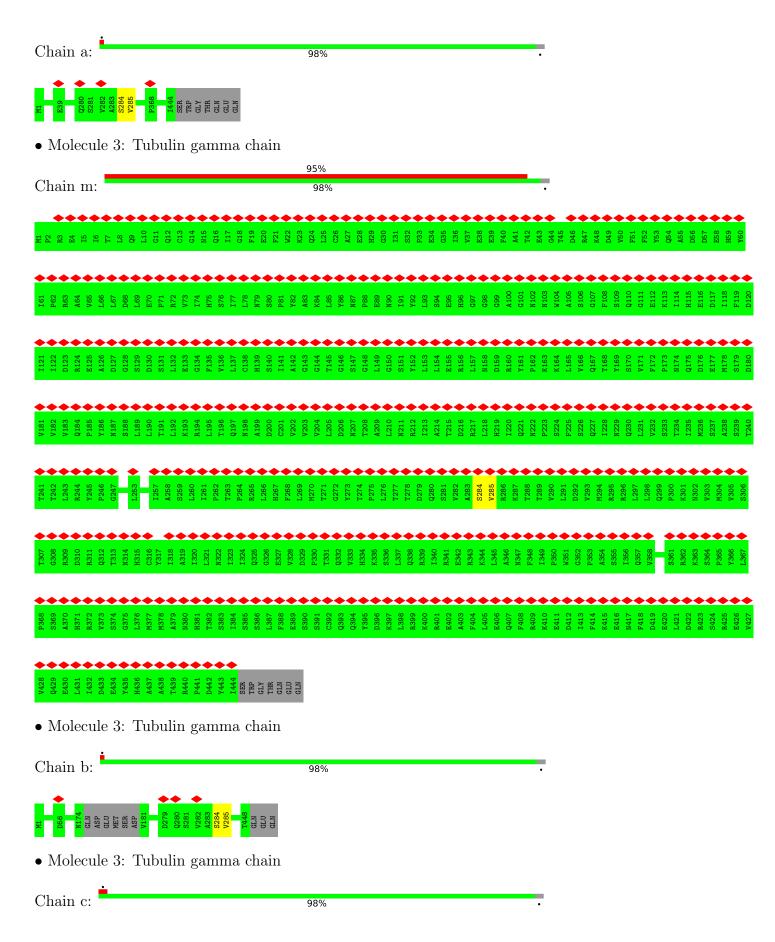
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



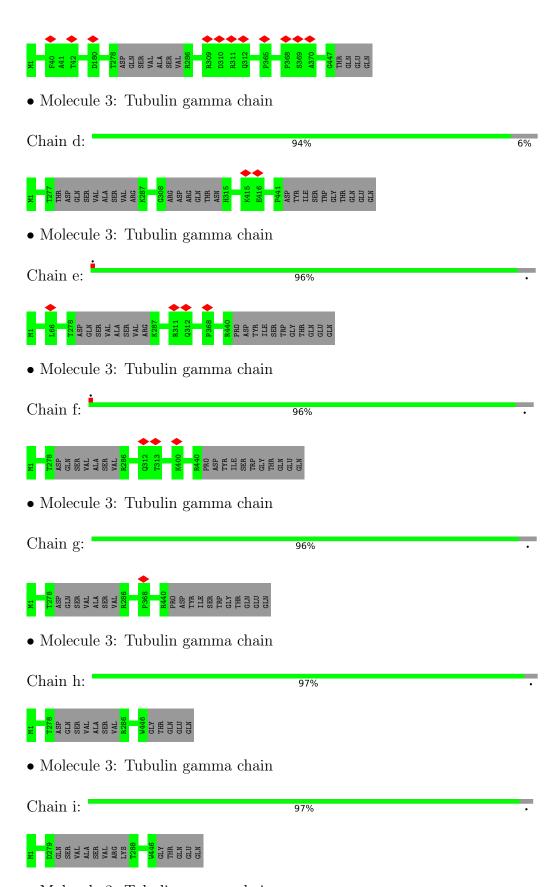


• Molecule 3: Tubulin gamma chain



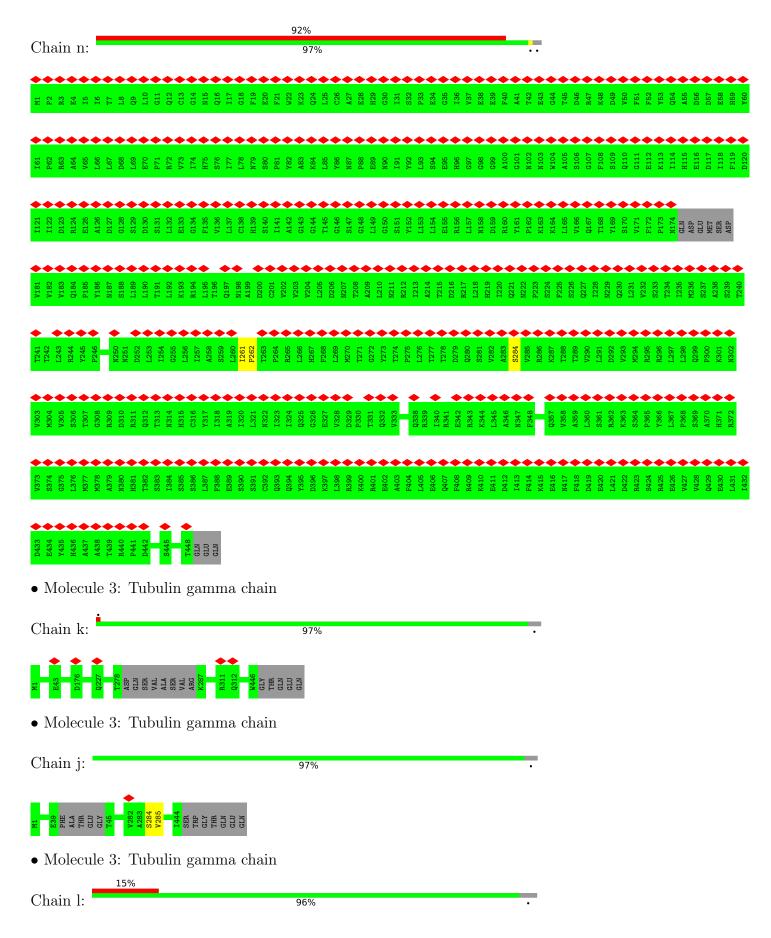




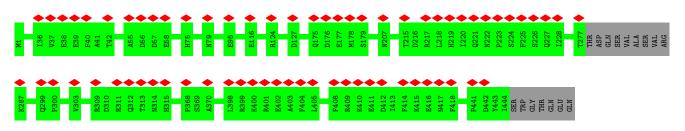


• Molecule 3: Tubulin gamma chain



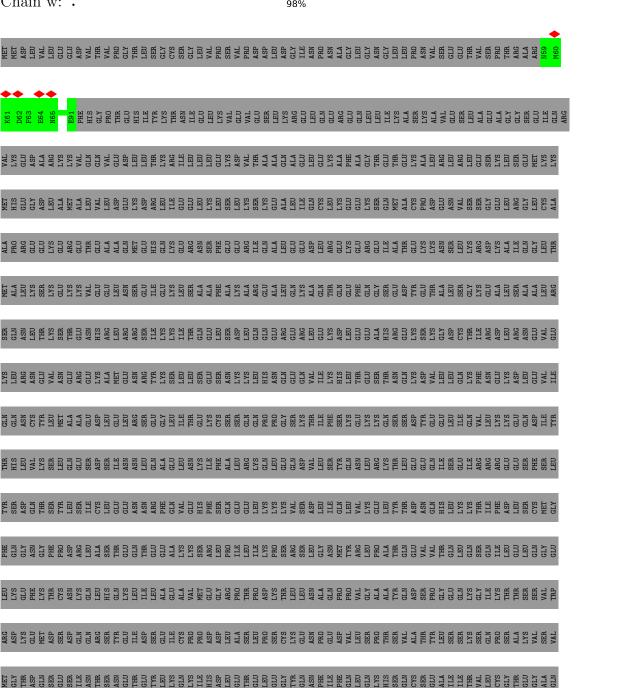




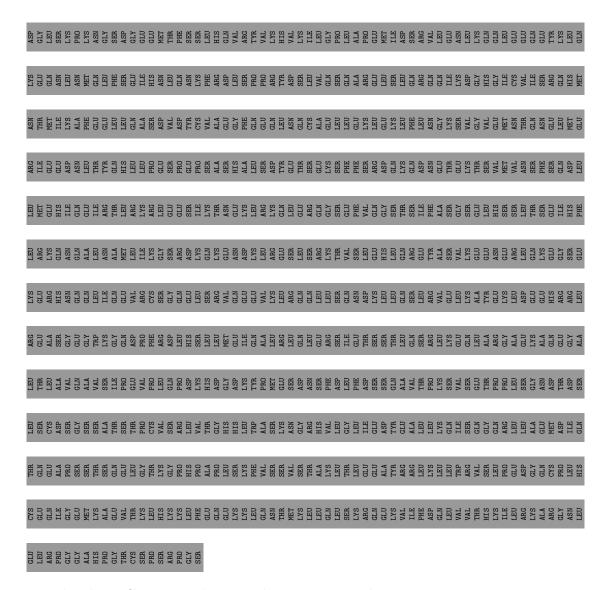


• Molecule 4: CDK5 regulatory subunit-associated protein 2

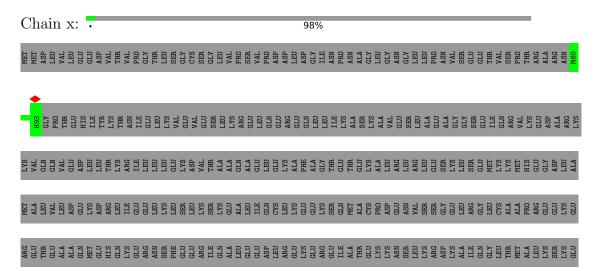
Chain w: 98%



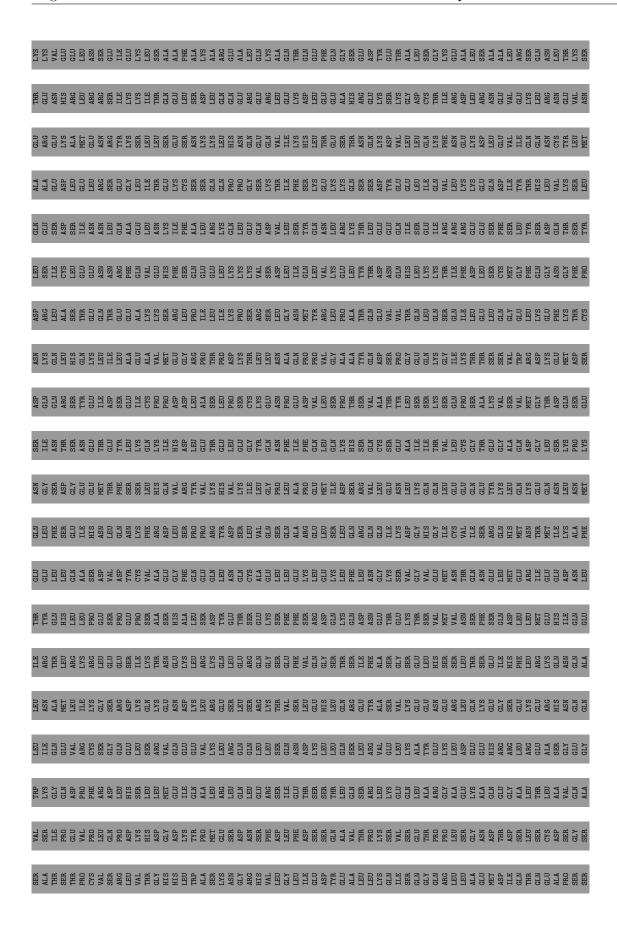




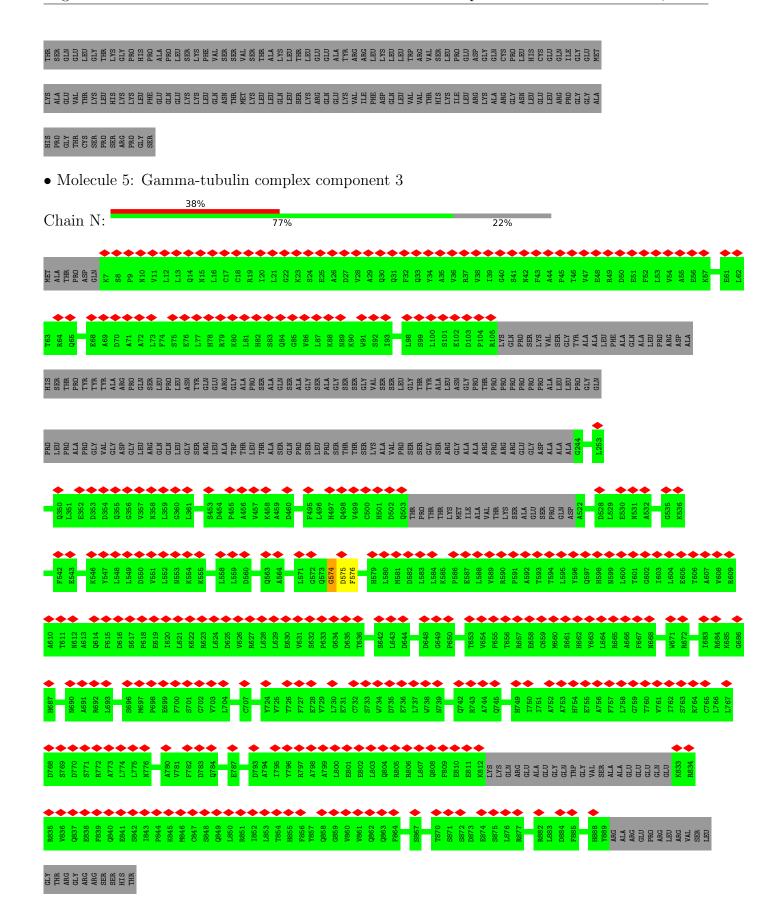
• Molecule 4: CDK5 regulatory subunit-associated protein 2





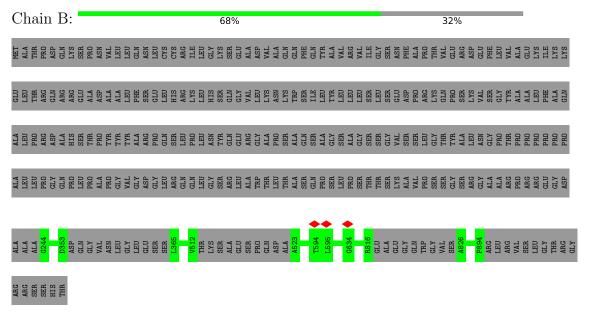






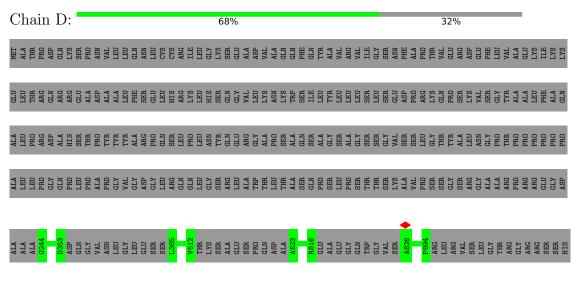
 \bullet Molecule 5: Gamma-tubulin complex component 3





• Molecule 5: Gamma-tubulin complex component 3

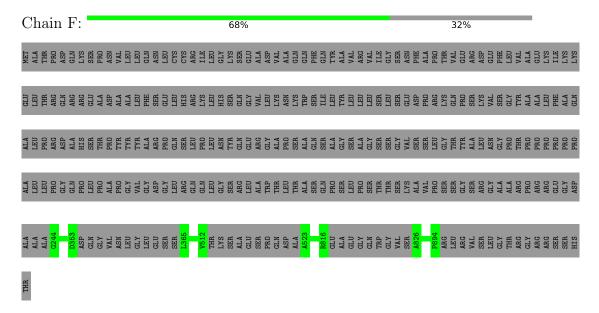
• Molecule 5: Gamma-tubulin complex component 3



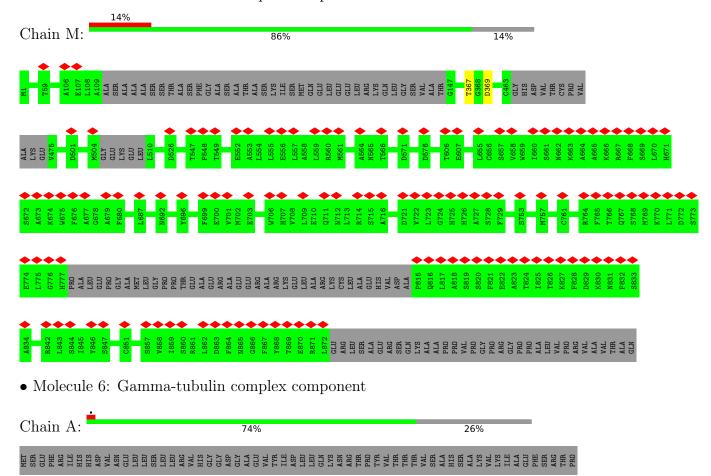




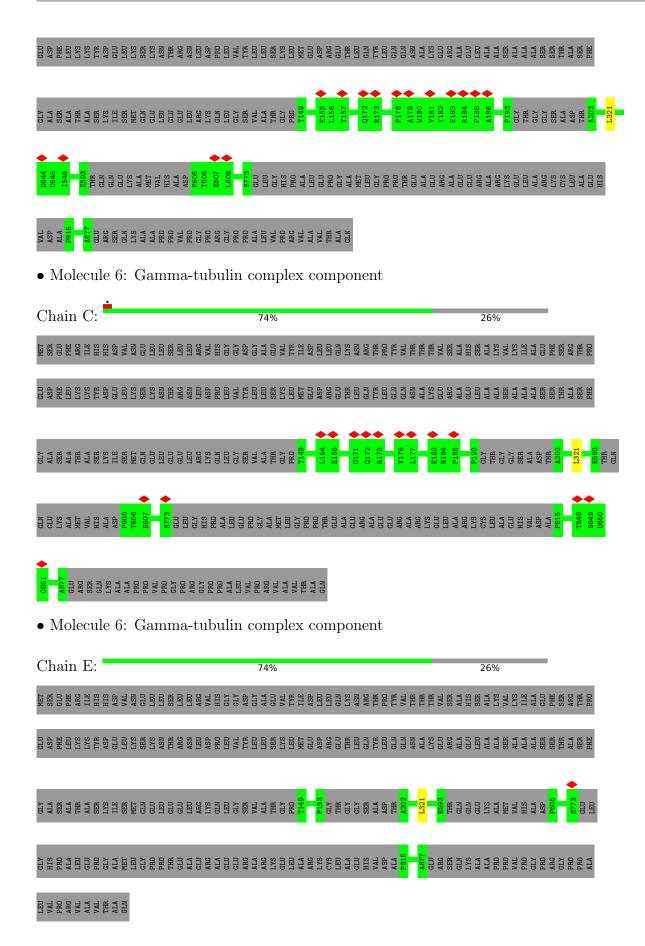
• Molecule 5: Gamma-tubulin complex component 3



• Molecule 6: Gamma-tubulin complex component

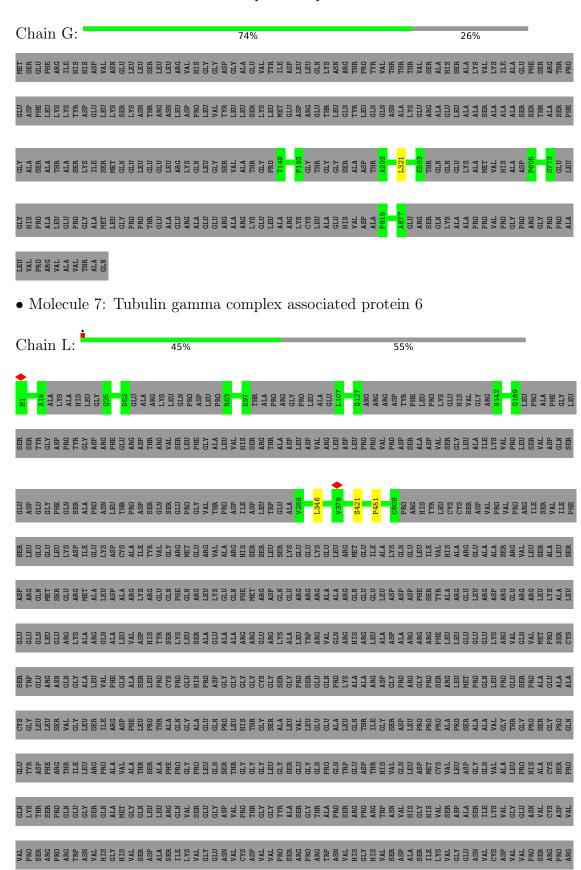




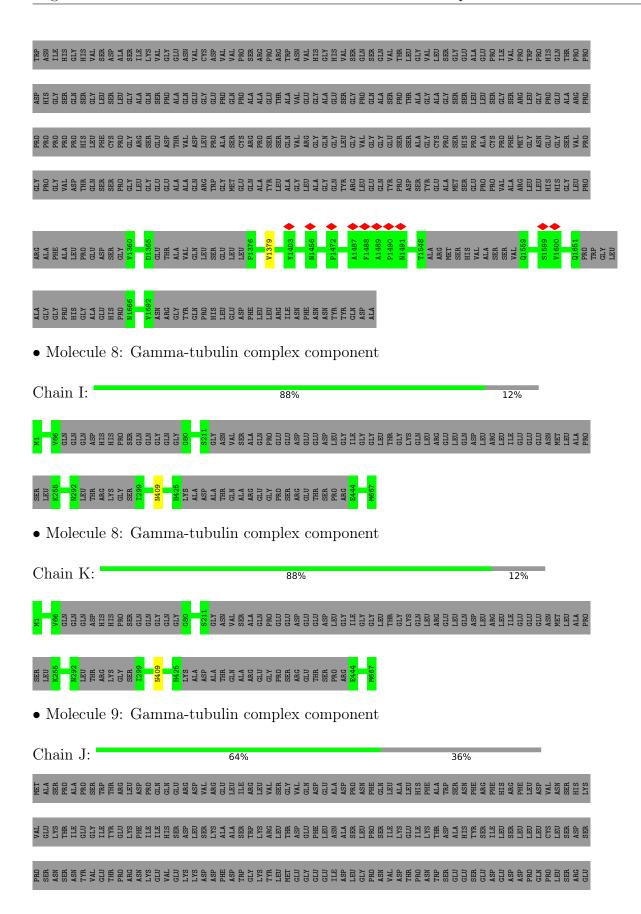




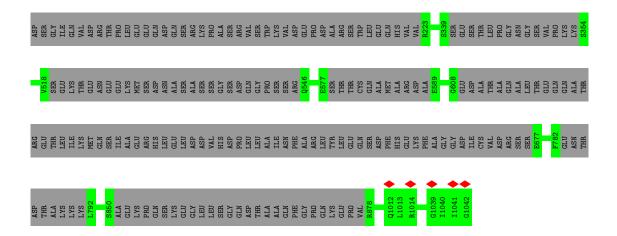
• Molecule 6: Gamma-tubulin complex component













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	55	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.846	Depositor
Minimum map value	-0.251	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	542.7187, 542.7187, 542.7187	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.41333, 1.41333, 1.41333	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).

N / L - 1	Cl :	Bond	lengths	В	ond angles
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	О	0.23	0/332	0.34	0/462
1	Р	0.26	0/332	0.45	0/462
1	Q	0.26	0/317	0.42	0/441
2	Y	0.25	0/251	0.39	0/348
3	a	0.26	0/2193	0.47	0/3053
3	b	0.26	0/2181	0.46	0/3034
3	С	0.27	0/2171	0.47	0/3020
3	d	0.26	0/2101	0.47	0/2921
3	е	0.25	0/2132	0.46	0/2966
3	f	0.26	0/2137	0.46	0/2973
3	g	0.26	0/2137	0.46	0/2973
3	h	0.27	0/2167	0.45	0/3015
3	i	0.27	0/2162	0.48	0/3008
3	j	0.27	0/2168	0.48	0/3017
3	k	0.26	0/2162	0.45	0/3008
3	1	0.25	0/2147	0.45	0/2987
3	m	0.25	0/2193	0.44	0/3053
3	n	0.25	0/2181	0.47	0/3034
4	W	0.22	0/164	0.34	0/228
4	X	0.21	0/169	0.34	0/235
5	В	0.26	0/3077	0.40	0/4287
5	D	0.26	0/3077	0.41	0/4287
5	F	0.27	0/3077	0.42	0/4287
5	Н	0.28	0/3662	0.43	0/5102
5	N	0.24	0/3502	0.44	2/4879~(0.0%)
6	A	0.26	0/3316	0.42	0/4620
6	С	0.27	0/3316	0.42	0/4620
6	Е	0.27	0/3316	0.44	0/4620
6	G	0.28	0/3316	0.44	0/4620
6	M	0.24	0/3875	0.41	0/5399
7	L	0.26	0/3805	0.48	0/5281
8	I	0.28	0/2901	0.44	0/4036
8	K	0.26	0/2901	0.43	0/4036
9	J	0.26	0/3288	0.44	0/4577



Mal	Chain	Bond	lengths	В	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
All	All	0.26	0/78226	0.44	$2/108889 \ (0.0\%)$

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	a	0	1
3	b	0	1
3	j	0	1
3	m	0	1
3	n	0	3
5	N	0	1
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
5	N	574	GLY	N-CA-C	6.72	129.91	113.10
5	N	576	PHE	N-CA-C	6.09	127.43	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	N	575	ASP	Peptide
3	a	284	SER	Peptide
3	b	284	SER	Peptide
3	j	284	SER	Peptide
3	m	284	SER	Peptide
3	n	261	ILE	Peptide
3	n	262	PRO	Peptide
3	n	284	SER	Peptide

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	Perce	ntiles
1	О	65/79~(82%)	65 (100%)	0	0	100	100
1	P	$65/79 \; (82\%)$	63 (97%)	1 (2%)	1 (2%)	8	39
1	Q	62/79 (78%)	59 (95%)	3 (5%)	0	100	100
2	Y	49/155~(32%)	49 (100%)	0	0	100	100
3	a	442/451 (98%)	431 (98%)	10 (2%)	1 (0%)	44	78
3	b	438/451 (97%)	429 (98%)	8 (2%)	1 (0%)	44	78
3	c	436/451 (97%)	429 (98%)	7 (2%)	0	100	100
3	d	420/451 (93%)	414 (99%)	6 (1%)	0	100	100
3	е	428/451 (95%)	422 (99%)	6 (1%)	0	100	100
3	f	429/451 (95%)	421 (98%)	8 (2%)	0	100	100
3	g	429/451 (95%)	421 (98%)	8 (2%)	0	100	100
3	h	435/451 (96%)	427 (98%)	8 (2%)	0	100	100
3	i	434/451 (96%)	426 (98%)	8 (2%)	0	100	100
3	j	435/451 (96%)	422 (97%)	12 (3%)	1 (0%)	44	78
3	k	434/451 (96%)	426 (98%)	8 (2%)	0	100	100
3	1	431/451 (96%)	423 (98%)	8 (2%)	0	100	100
3	m	442/451 (98%)	431 (98%)	10 (2%)	1 (0%)	44	78
3	n	438/451 (97%)	425 (97%)	13 (3%)	0	100	100
4	W	31/1663~(2%)	31 (100%)	0	0	100	100
4	X	32/1663~(2%)	32 (100%)	0	0	100	100
5	В	613/910 (67%)	608 (99%)	5 (1%)	0	100	100
5	D	613/910 (67%)	608 (99%)	5 (1%)	0	100	100
5	F	613/910 (67%)	607 (99%)	6 (1%)	0	100	100
5	Н	729/910 (80%)	718 (98%)	11 (2%)	0	100	100
5	N	699/910 (77%)	682 (98%)	16 (2%)	1 (0%)	48	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
6	A	659/905~(73%)	644 (98%)	14 (2%)	1 (0%)	44	78
6	С	659/905~(73%)	646 (98%)	12 (2%)	1 (0%)	44	78
6	E	659/905~(73%)	644 (98%)	14 (2%)	1 (0%)	44	78
6	G	659/905 (73%)	645 (98%)	13 (2%)	1 (0%)	44	78
6	M	772/905 (85%)	743 (96%)	27 (4%)	2 (0%)	37	72
7	L	753/1715 (44%)	677 (90%)	72 (10%)	4 (0%)	25	63
8	I	577/667 (86%)	567 (98%)	9 (2%)	1 (0%)	44	78
8	K	577/667 (86%)	568 (98%)	8 (1%)	1 (0%)	44	78
9	J	650/1042~(62%)	636 (98%)	14 (2%)	0	100	100
All	All	15607/23198 (67%)	15239 (98%)	350 (2%)	18 (0%)	50	83

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	321	LEU
6	С	321	LEU
6	Ε	321	LEU
6	G	321	LEU
5	N	574	GLY
7	L	421	SER
6	M	367	THR
6	M	369	ASP
7	L	451	PRO
7	L	1379	VAL
8	K	409	ASN
7	L	346	LEU
8	I	409	ASN
1	Р	70	THR
3	m	285	VAL
3	a	285	VAL
3	b	285	VAL
3	j	285	VAL

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.



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 oligosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	G	1
6	A	1
6	С	1
6	Ε	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	850:ASP	С	851:CYS	N	3.27
1	A	850:ASP	С	851:CYS	N	3.01
1	С	850:ASP	С	851:CYS	N	2.91
1	Е	850:ASP	С	851:CYS	N	2.88



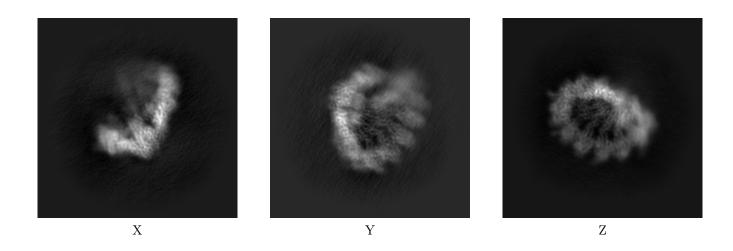
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-51019. 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



6.1.2 Raw map

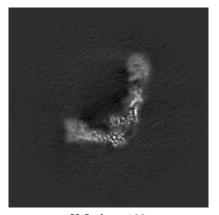


The images above show the map projected in three orthogonal directions.

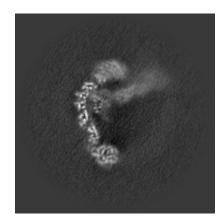


6.2 Central slices (i)

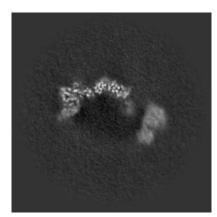
6.2.1 Primary map





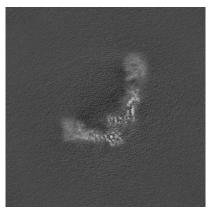


Y Index: 192



Z Index: 192

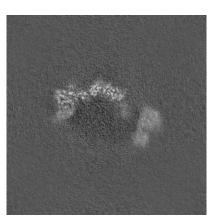
6.2.2 Raw map



X Index: 192



Y Index: 192



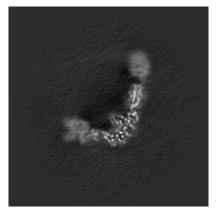
Z Index: 192

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

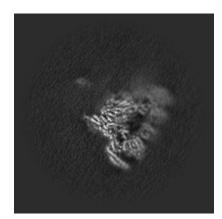


6.3 Largest variance slices (i)

6.3.1 Primary map





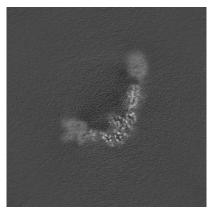


Y Index: 235



Z Index: 143

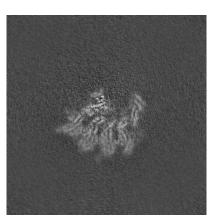
6.3.2 Raw map



X Index: 187



Y Index: 235



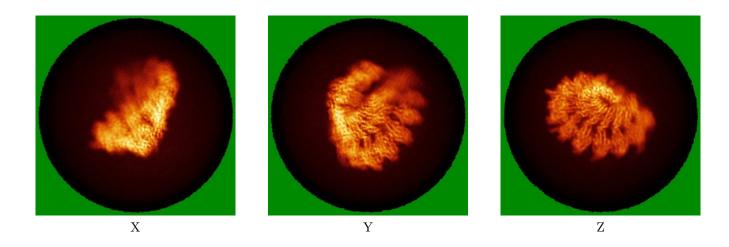
Z Index: 143

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

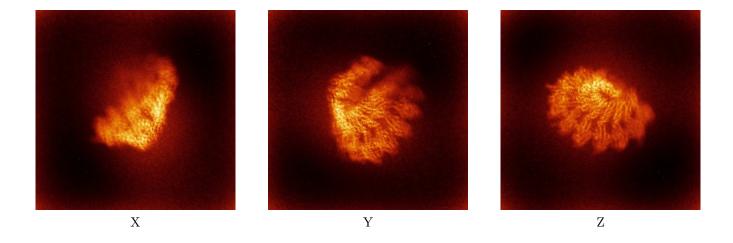


6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map

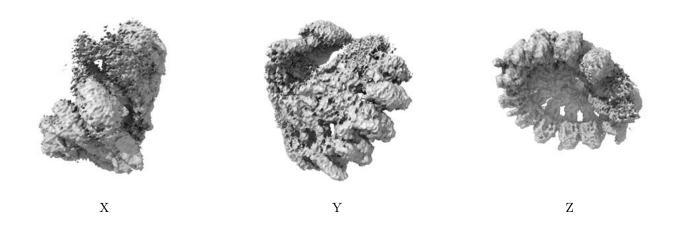


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



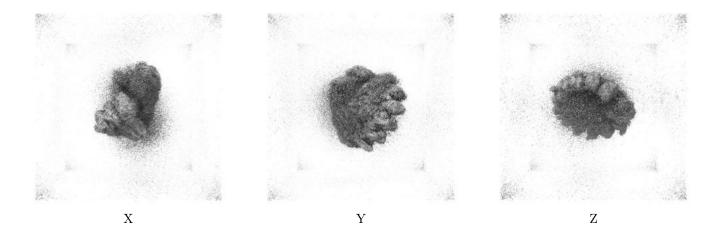
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.125. 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)

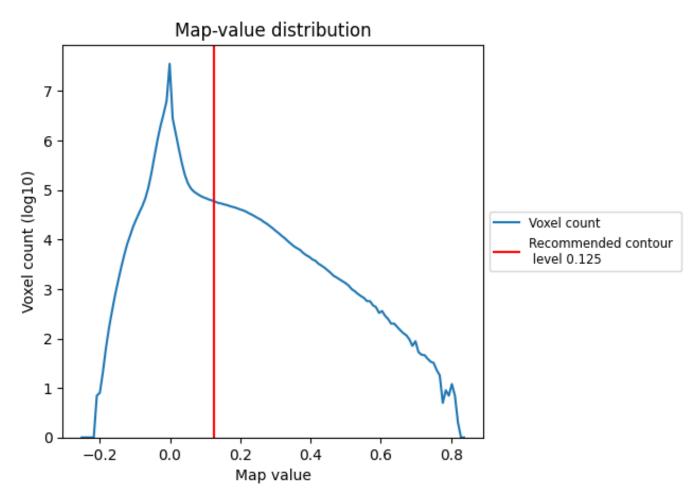
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

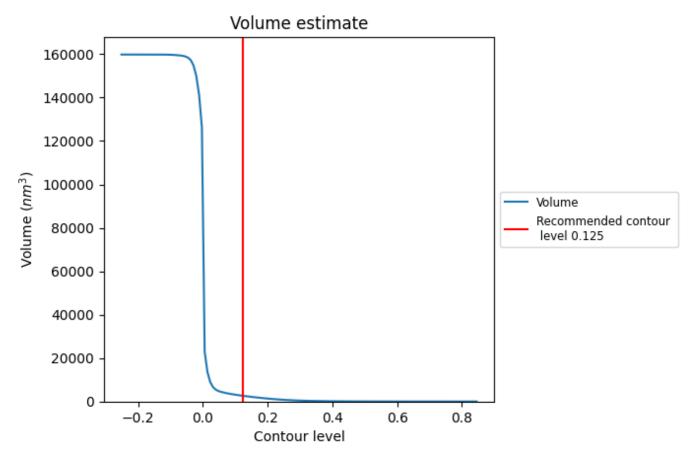
7.1 Map-value distribution (i)



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)

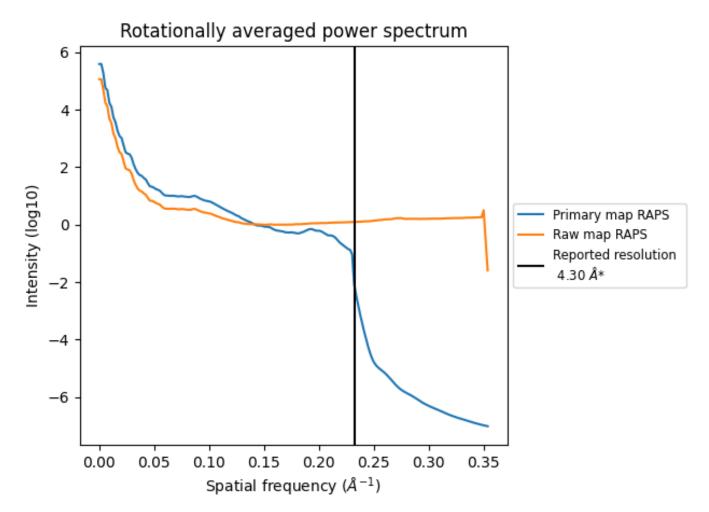


The volume at the recommended contour level is $2585~\mathrm{nm^3}$; this corresponds to an approximate mass of $2335~\mathrm{kDa}$.

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)



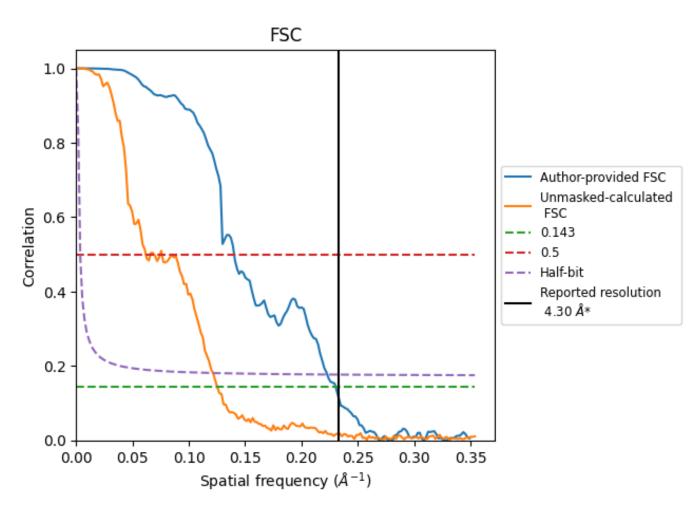
^{*}Reported resolution corresponds to spatial frequency of 0.233 $\rm \mathring{A}^{-1}$



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 0.233 $\rm \mathring{A}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
rtesolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	4.30	-	-	
Author-provided FSC curve	4.34	7.13	4.49	
Unmasked-calculated*	7.99	16.18	8.23	

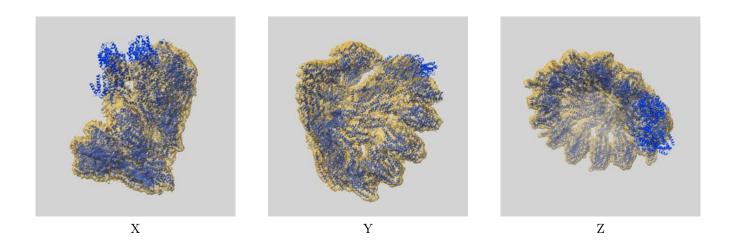
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 4.3 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-51019 and PDB model 9G3Z. Per-residue inclusion information can be found in section 3 on page 7.

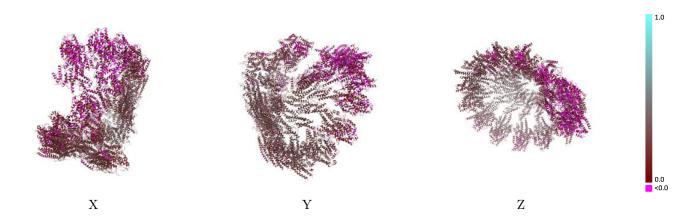
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

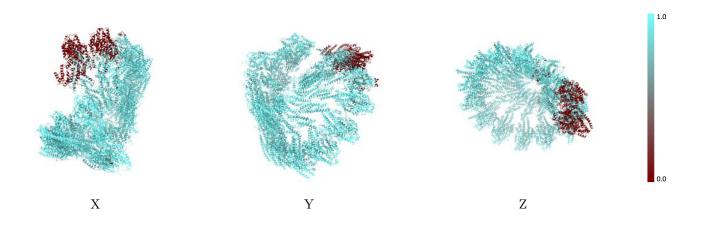


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

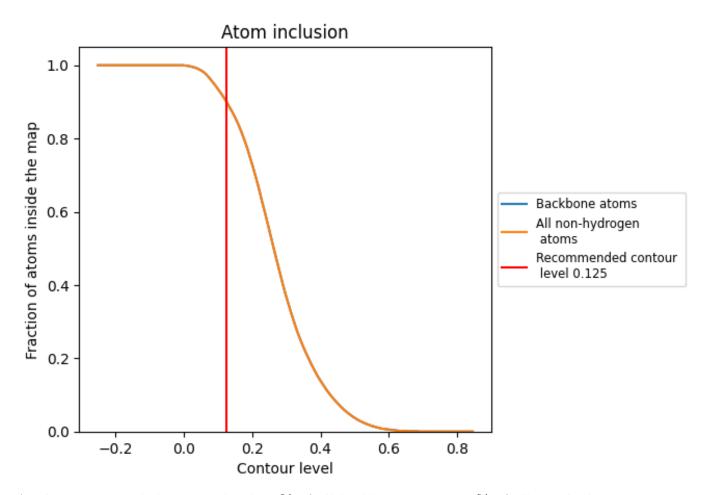
9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.125).



9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.2050
A	0.9730	0.1930
В	0.9930	0.2460
С	0.9750	0.2560
D	0.9950	0.2660
Е	0.9970	0.2850
F	0.9980	0.2920
G	0.9970	0.3080
Н	0.9970	0.3280
I	0.9980	0.3210
J	0.9930	0.2710
K	0.9990	0.2400
L	0.9780	0.1730
M	0.8300	0.0830
N	0.5200	0.0780
О	0.2550	0.1000
P	0.9880	0.3270
Q	0.9810	0.2500
Y	0.9880	0.1320
a	0.9900	0.1040
b	0.9840	0.1460
С	0.9720	0.1720
d	0.9900	0.1550
е	0.9870	0.1940
f	0.9910	0.2120
g	0.9950	0.2450
h	0.9980	0.3020
i	0.9990	0.2860
j	0.9910	0.1900
k	0.9850	0.1170
1	0.8240	0.0550
m	0.0430	0.0450
n	0.0710	0.0320
W	0.8610	-0.0210
X	0.9770	0.0520



