



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:06 PM UTC

PDB ID : 9I8M / pdb_00009i8m
EMDB ID : EMD-52729
Title : NEDD1-bound native vertebrate gamma-tubulin ring complex from *Xenopus laevis*, focused reconstruction
Authors : Vermeulen, B.J.A.; Pfeffer, S.
Deposited on : 2025-02-05
Resolution : 4.30 Å(reported)

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

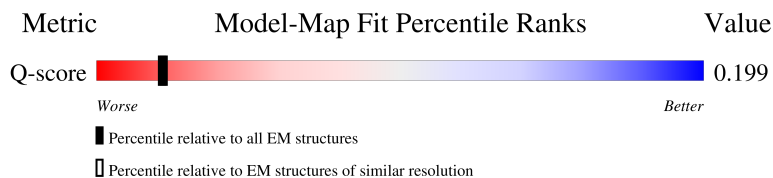
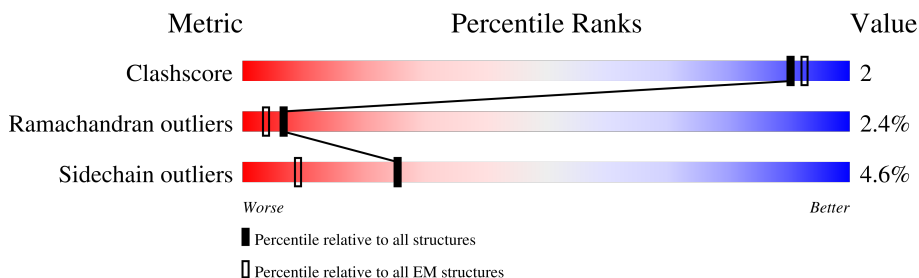
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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 (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	896	13% 14% 14% . 69%
1	C	896	7% 13% 13% . 72%
1	E	896	16% 12% 14% . 72%
1	G	896	7% 14% 12% . 72%

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Mol	Chain	Length	Quality of chain
2	B	906	
2	D	906	
2	F	906	
2	H	906	
2	O	906	
2	Q	906	
2	R	906	
2	S	906	
2	T	906	
3	I	666	
3	K	666	
4	J	1019	
5	L	1698	
6	U	671	
6	V	671	
6	W	671	
6	X	671	
7	o	72	
7	p	72	
7	q	72	
7	r	72	
7	s	72	
7	t	72	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 37358 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	275	Total	C	N	O	S	0	0
			2211	1412	369	421	9		
1	C	250	Total	C	N	O	S	0	0
			2014	1289	336	382	7		
1	E	253	Total	C	N	O	S	0	0
			2038	1306	340	385	7		
1	G	250	Total	C	N	O	S	0	0
			2014	1289	336	382	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	294	Total	C	N	O	S	0	0
			2363	1517	401	434	11		
2	D	254	Total	C	N	O	S	0	0
			2059	1324	351	375	9		
2	F	242	Total	C	N	O	S	0	0
			1964	1263	337	355	9		
2	H	263	Total	C	N	O	S	0	0
			2135	1374	363	389	9		
2	O	93	Total	C	N	O	S	0	0
			753	480	137	134	2		
2	Q	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	R	98	Total	C	N	O	S	0	0
			794	503	144	145	2		
2	S	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	T	93	Total	C	N	O	S	0	0
			753	480	137	134	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	287	Total	C	N	O	S	0	0
			2325	1500	394	418	13		
3	K	287	Total	C	N	O	S	0	0
			2325	1500	394	418	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	352	Total	C	N	O	S	0	0
			2909	1881	493	522	13		

- Molecule 5 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	478	Total	C	N	O	S	0	0
			3794	2449	613	713	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	392	ASP	GLU	conflict	UNP A0A974HT83
L	394	VAL	ILE	conflict	UNP A0A974HT83

- Molecule 6 is a protein called NEDD1 gamma-tubulin ring complex targeting factor L homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	V	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	W	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	X	75	Total	C	N	O	S	0	0
			634	396	112	122	4		

- Molecule 7 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	52	Total	C	N	O	S	0	0
			403	248	71	79	5		
7	p	56	Total	C	N	O	S	0	0
			429	263	73	89	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	56	Total	C	N	O	S	0	0
			432	266	76	86	4		
7	r	59	Total	C	N	O	S	0	0
			454	278	80	91	5		
7	s	59	Total	C	N	O	S	0	0
			451	277	79	90	5		
7	t	58	Total	C	N	O	S	0	0
			446	274	78	89	5		



ASN
GLN
LYS
SER
ALA
PRO
LEU
LEU
GLY
PRO
ALA
GLN
HIS
ALA
VAL
SER
THR
LYS

- Molecule 1: Gamma-tubulin complex component



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

[illegible]

Tyr	GLU	ARG	PRO	ALA	LEU	THR	GLY	ASP	PHE	MET	SER	PHE	SER	ASN	PRO	SER	THR	ASP	VAL	THR	VAL	SER	ILE	GLY	THR	LEU	PRO			
L209	P210	S211	Q212	E213	T214	C215	L216	V217	E218	D219	L220	L221	Y222	L223	L224	L225	V226	D228	G229	R230	Y231	L232	L233	V234	Q235	P236	L237	V238	G239	A240

Q241	S242	R243	S244	F245	S246	E247	E248	Q249	N250	D252	S253	S254	V255	K256	E257	R260	T261	T262	L263	P264	V265	A266	Y269	V272	T273	R274	F275	V276	E277	E278	N279	S280	S281	F282	G285	Q286	V287	N288	H289	A290	L291	G292	A293	A294	H295	L298	G299	K300	E301	Y302	M303	L304	S305
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T306	S307	E310	H311	L312	Q313	R314	Q315	G316	L317	L318	S319	L320	L321	Q321	K322	L323	W324	Q328	P329	T330	L331	R332	T333	K334	E335	V336	L337	A338	S339	T340	A341	N345	R346	G347	E348	C349	F350	G351	L355	S356	L357	L358	H359	D360	R361	T362	F363	G364	F365	T366	G367	D368	S369	Q370	A371	T372
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E373	L374	C375	A381	A382	A383	A384	A385	A386	F387	D388	L389	L390	E391	R392	A393	L394	Y395	R396	G397	L398	L399	M400	D401	P402	Y403	Y404	A405	F406	M407	V408	E409	E410	H411	GLU	LEU	GLN	LYS	GLU	GLU	LYS	ILE	GLN	GLU	ASP	TYR	ASN	ASP	LYS	TYR	W427	D428	Q429	R430	Y431	T432	T433	L434	Q435	Q436
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Q437	I438	P439	S440	F441	L442	Q443	K444	V445	A446	D447	K448	I449	L450	S451	T452	G453	K454	V455	L456	N457	V458	VAL	ARG	GLU	CYS	GLY	GLY	HIS	ASP	ASP	ALA	LYS	GLU	ILE	THR	TYR	TYR	LEU	LYS	GLU	GLU	Q481	A482	V483	V484	E485	R486	I487	E488	A489	Y491	N492	Y493	A494	S495
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V497	LEU	ASP	ASP	ASP	PHE	PHE	MET	GLU	GLU	GLU	GLU	LEU	VAL	ALA	HIS	HIS	LEU	ARG	SER	ILE	LYS	HIS	TYR	PHE	PHE	LEU	MET	ASP	GLN	GLY	ASP	ASP	PHE	PHE	VAL	HIS	HIS	PHE	MET	MET	ASP	LEU	THR	GLU	GLU	GLU	GLU	LYS	LYS	PRO	PRO	VAL	ASP	ASP	ILE	ILE	PRO	THR	THR	ARG	LEU	GLU	ALA	LEU	LEU	GLU
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ALA LEU ARG MET SER THR ALA ASN ASP PRO PHE LYS ASP ASP LEU LYS ILE GLU LEU MET PRO PRO ASP LEU LEU ARG VAL LEU ALA ILE GLU THR HIS GLN GLU LYS ALA LEU LEU SER GLY THR THR GLU LEU ALA LEU SER GLY THR THR GLU LEU LEU SER PHE THR

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

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

- Molecule 1: Gamma-tubulin complex component



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

ALA	PRO	ASN	THR	SER	LYS	ILE	SER	MET	GLN	GLU	LEU	GLU	GLU	LEU	ARG	ARG	GLN	LEU	LEU	THR	ALA	THR	THR	VAL	ALA	VAL	SER	SER	SER	HIS	GLN	PRO	PRO	GLU	VAL	VAL	LEU	ARG	ASP	LYS	LEU	LEU	ASN	LYS	LYS	HIS	THR	GLY	HIS	PRO	PRO	VAL	VAL	PHE	PRO	SER	SER	TRP	VAL
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Tyr	Leu	Val	Met	Ala	Pro	Arg	Glu	Thr	Asp	Ser	Asn	Pro	Ser	Thr	Val	Leu	Thr	Gly	Leu	Val	Met	Ala	Pro	Arg	Glu	Tyr													
L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248

Q249	N250	L251	D252	V255	V259	N260	R261	L262	L263	N268	V269	S270	T273	R274	E277	N279	S280	S281	V284	G285	T287	N288	H289	A294	M295	R296	T297	L298	G299	K300	E301	T302	M303	T304	S307	Q308	L309	E310	H311	L312	Q313	R314	Q315	L318	Q321	K322	L323
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W324	F325	V326	Z327	Q328	P329	T330	L331	R332	T333	M334	E335	V336	L337	T340	A341	T342	L344	N345	G346	E348	F349	G351	G352	A353	T354	L357	L358	H359	D360	F363	G364	G367	D368	S369	Q370	A371	Q372	C375	L376	V377	A381	A382	S383	A384	F385	V386	F387	D388	T389
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[illegible]

L456	L457	V458	ARG	ARG	GLU	CYS	GLY	HIS	ASP	VAL	THR	CYS	PRO	ASP	ALA	LYS	GLU	ILE	THR	TYR	THR	LEU	LYS	GLU	Q481	A482	V483	V484	E485	R486	L487	E488	K489	A490	V491	H492	V493	A494	S495	LYS	VAL	LEU	LEU	ASP	ASP	PHE	LEU	LEU	MET	MET	GLU	GLU	GLU	GLU	VAL	ALA	HIS	ARG	LEU	ARG	SER	ILE
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LYS HIS TYR PHE LEU MET ASP GLN GLY GLU ASP PHE PHE VAL HIS HIS PHE MET ASP LEU THR GLU GLU GLU LEU LYS LYS PRO VAL ASP ASP ILE ILE ILE PRO THR ARG ARG LEU LEU ALA LEU LEU LEU ALA LEU LEU MET SER THR THR ALA ASN THR THR ASP ASP PHE PHE LYS LYS ASP ASP LEU LEU LYS ILE THR

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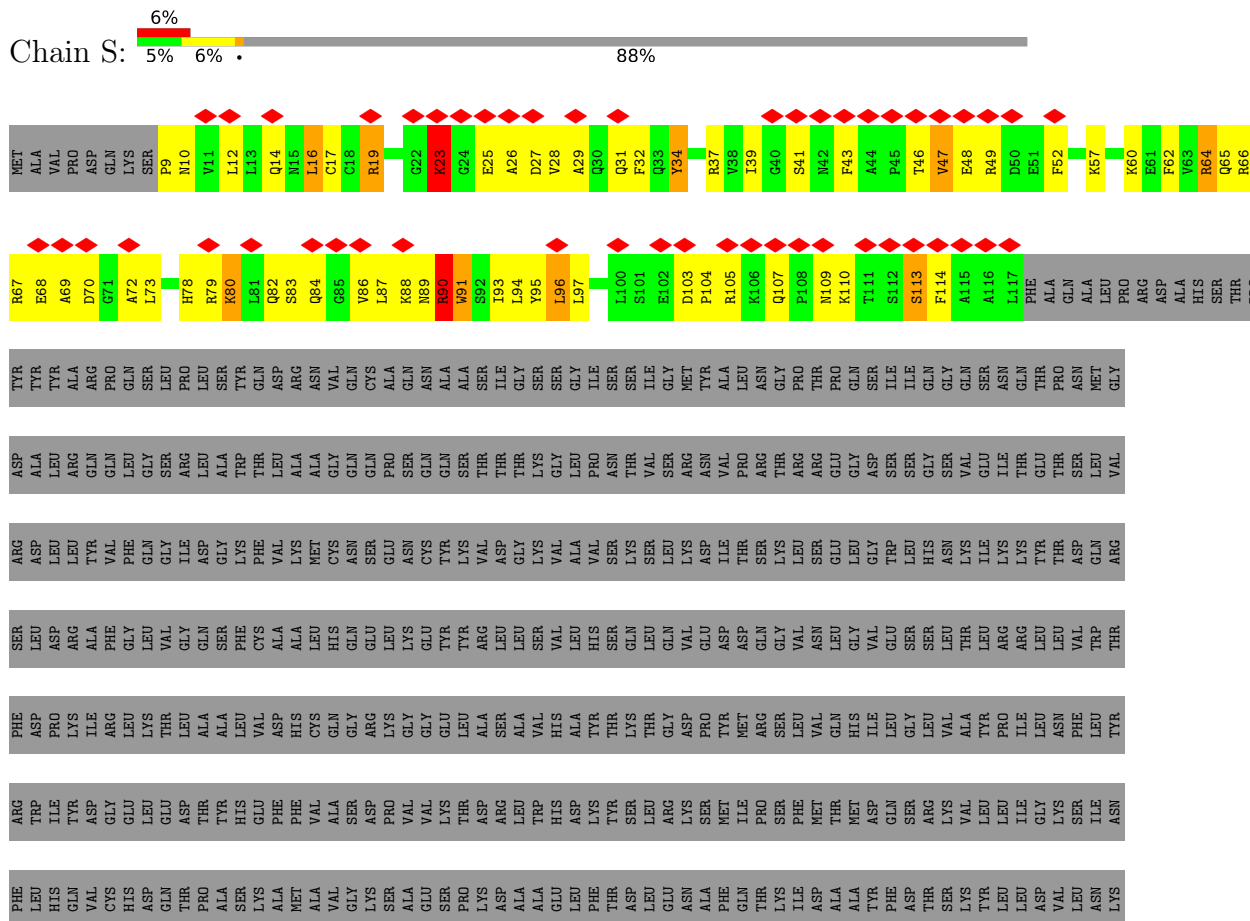
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GLU PHE VAL VAL ARG ARG ARG GLU GLU ALA ALA ASP ASP GLY GLY ALA ALA LEU LEU PHE PHE SER SER GLU GLU HIS HIS ARG ARG LYS LYS LEU LEU GLN GLN SER SER GLN GLN GLY GLY VAL VAL LEU LEU LYS LYS ASN ASN ARG ARG TRP TRP SER SER ILE ILE LEU LEU TYR TYR LEU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

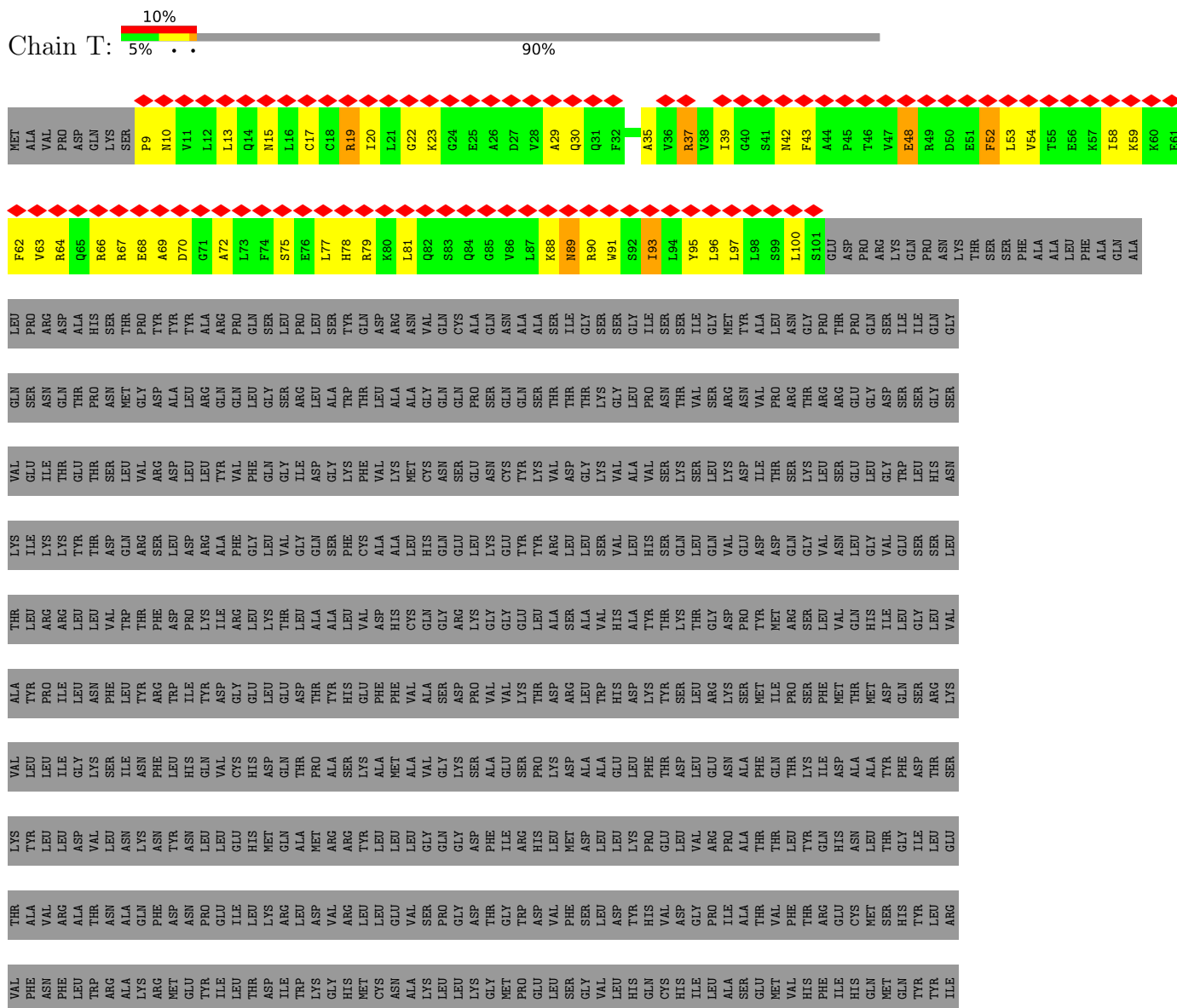


[illegible]

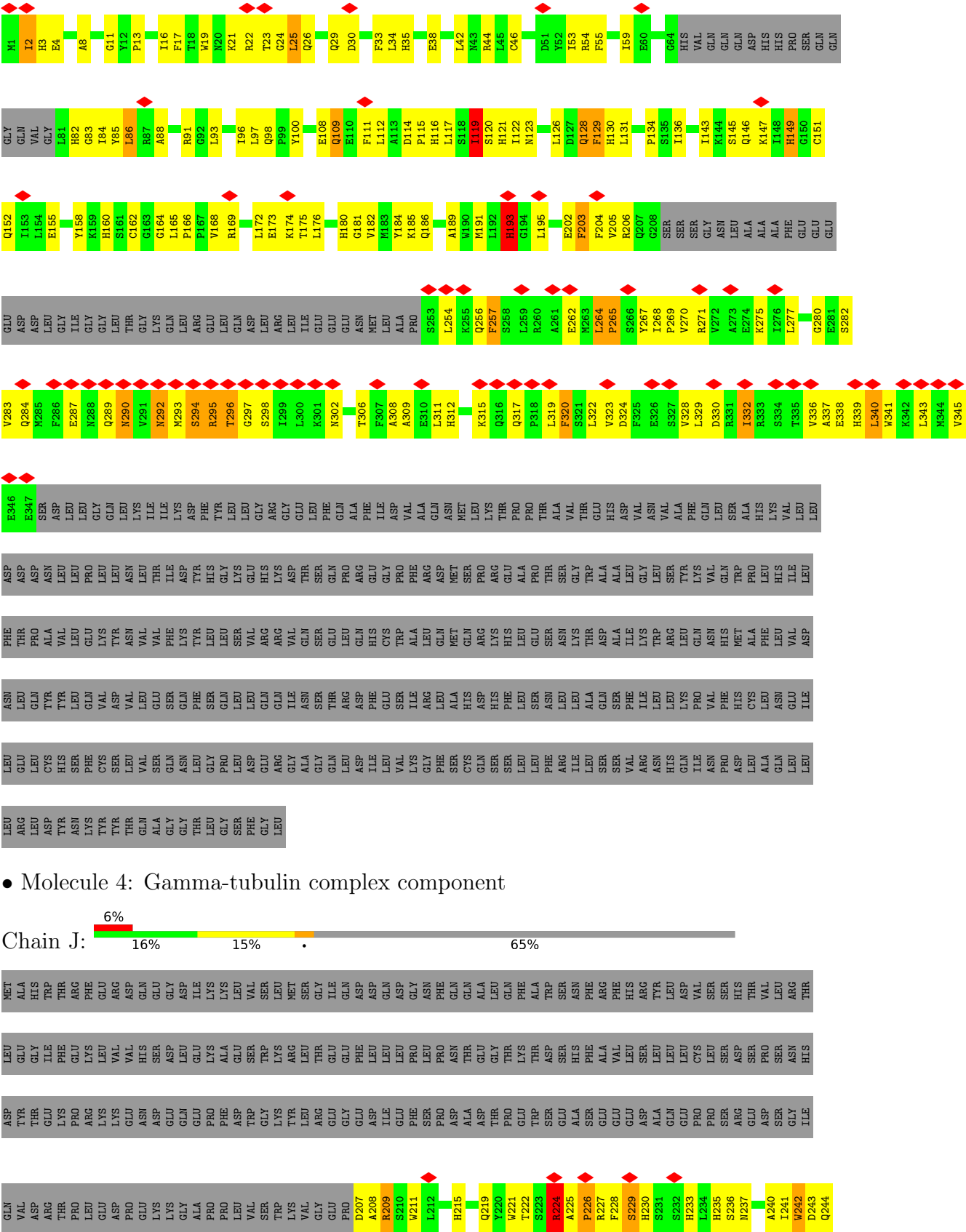
- Molecule 2: Gamma-tubulin complex component 3 homolog



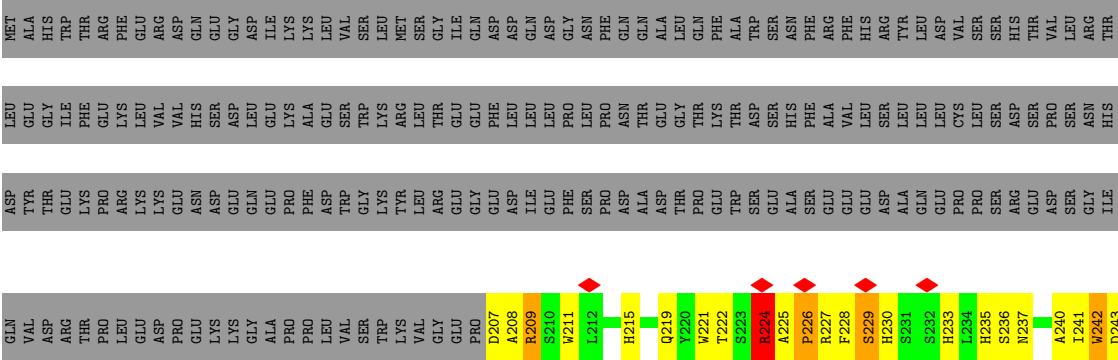
- Molecule 2: Gamma-tubulin complex component 3 homolog

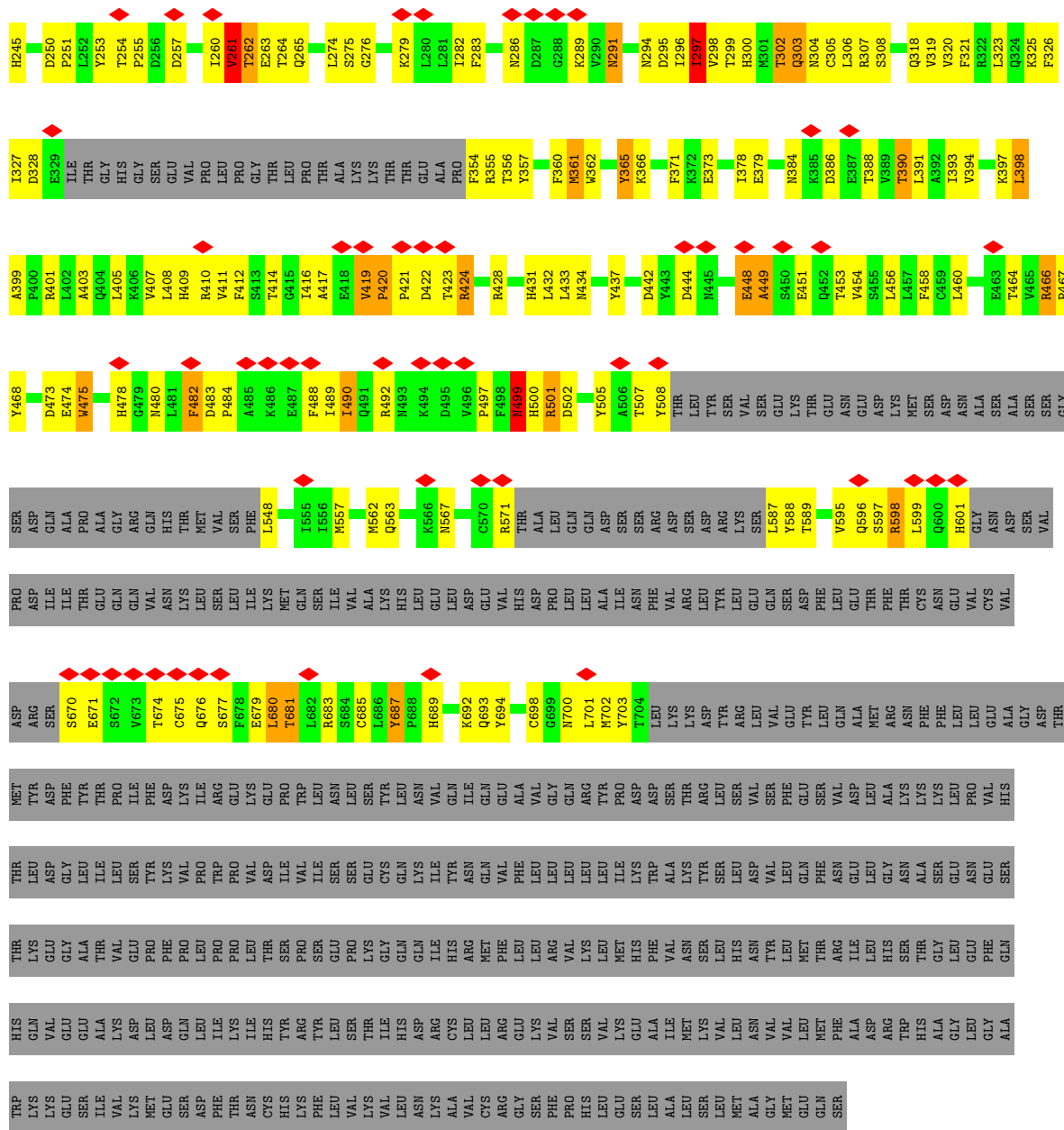




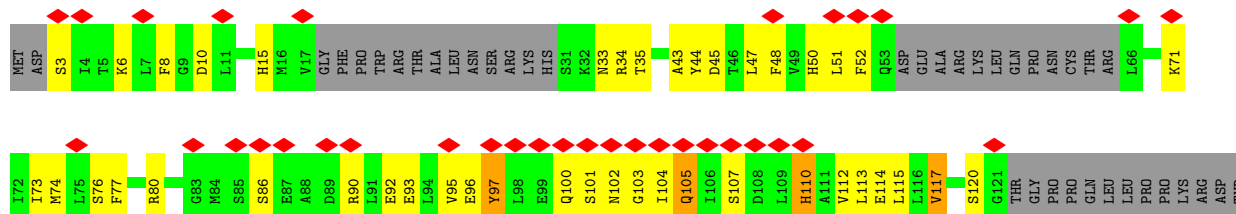


● Molecule 4: Gamma-tubulin complex component



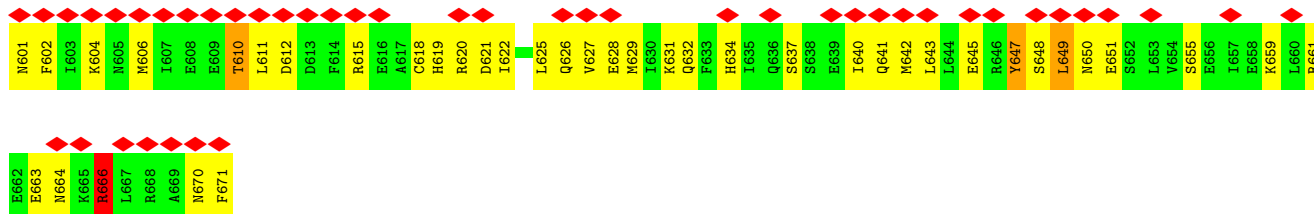


• Molecule 5: Gamma-tubulin complex component 6

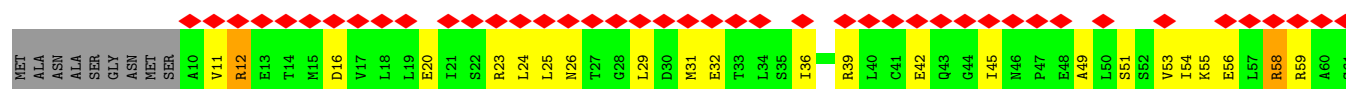
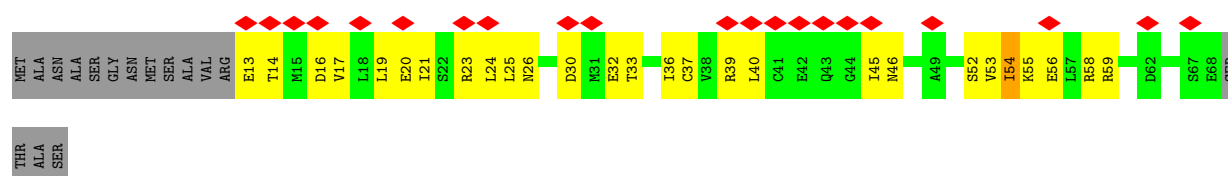
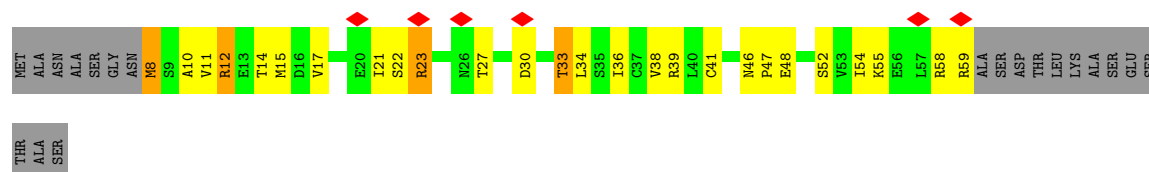
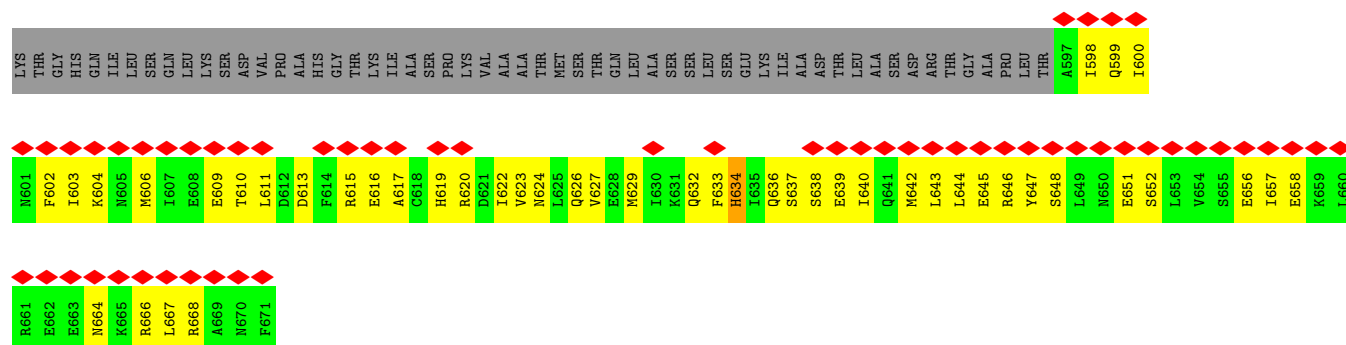


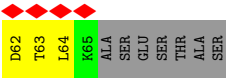




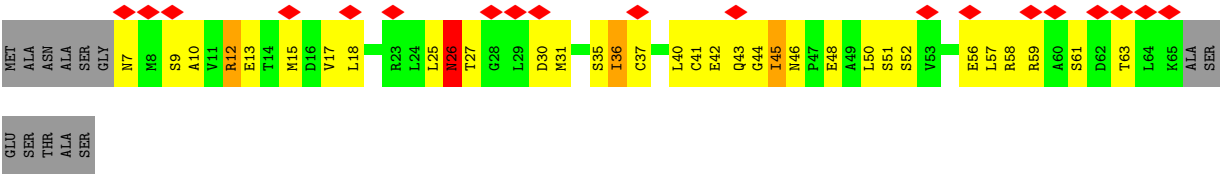




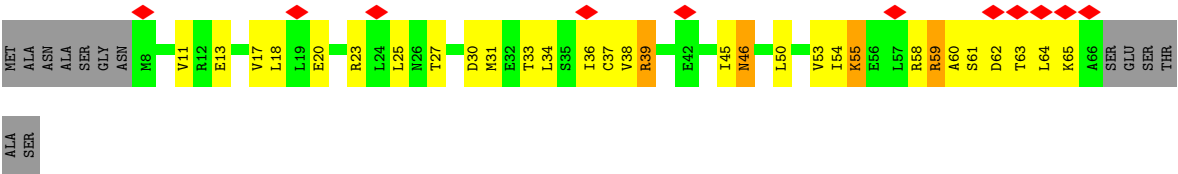




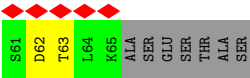
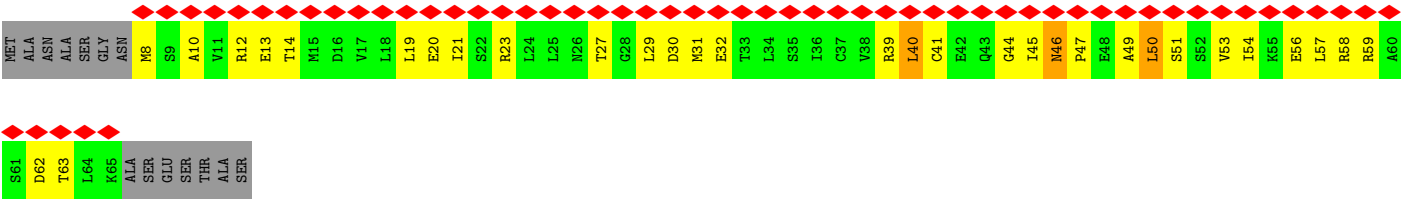
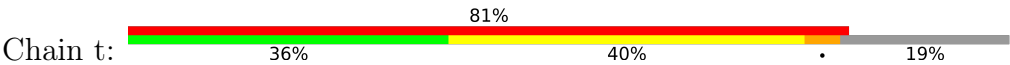
• Molecule 7: Mitotic-spindle organizing protein 1



• Molecule 7: Mitotic-spindle organizing protein 1



• Molecule 7: Mitotic-spindle organizing protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0421	Depositor
Map size (Å)	365.9392, 365.9392, 365.9392	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.42945, 1.42945, 1.42945	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	2.24	75/2254 (3.3%)	2.41	150/3055 (4.9%)
1	C	2.26	80/2053 (3.9%)	2.42	121/2781 (4.4%)
1	E	2.24	63/2077 (3.0%)	2.38	135/2813 (4.8%)
1	G	2.22	64/2053 (3.1%)	2.35	112/2781 (4.0%)
2	B	2.22	81/2413 (3.4%)	2.32	113/3257 (3.5%)
2	D	2.20	68/2101 (3.2%)	2.33	121/2831 (4.3%)
2	F	2.18	71/2004 (3.5%)	2.33	101/2700 (3.7%)
2	H	2.18	71/2178 (3.3%)	2.34	108/2936 (3.7%)
2	O	2.21	21/764 (2.7%)	2.60	69/1026 (6.7%)
2	Q	2.23	27/892 (3.0%)	2.61	82/1199 (6.8%)
2	R	2.30	30/805 (3.7%)	2.45	41/1081 (3.8%)
2	S	2.23	25/892 (2.8%)	2.53	69/1199 (5.8%)
2	T	2.27	25/764 (3.3%)	2.59	53/1026 (5.2%)
3	I	2.25	70/2377 (2.9%)	2.38	154/3212 (4.8%)
3	K	2.24	81/2377 (3.4%)	2.30	116/3212 (3.6%)
4	J	2.45	98/2976 (3.3%)	2.43	176/4037 (4.4%)
5	L	2.22	143/3862 (3.7%)	2.42	257/5228 (4.9%)
6	U	2.24	19/640 (3.0%)	2.66	62/854 (7.3%)
6	V	2.18	18/640 (2.8%)	2.65	53/854 (6.2%)
6	W	2.27	21/640 (3.3%)	2.44	41/854 (4.8%)
6	X	2.29	26/640 (4.1%)	2.61	49/854 (5.7%)
7	o	2.26	14/403 (3.5%)	2.45	27/541 (5.0%)
7	p	2.27	12/429 (2.8%)	2.66	42/577 (7.3%)
7	q	2.32	18/432 (4.2%)	2.50	24/581 (4.1%)
7	r	2.28	16/454 (3.5%)	2.65	41/610 (6.7%)
7	s	2.38	25/451 (5.5%)	2.40	31/606 (5.1%)
7	t	2.24	12/446 (2.7%)	2.72	41/599 (6.8%)
All	All	2.25	1274/38017 (3.4%)	2.42	2389/51304 (4.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	C	0	6
1	E	0	8
1	G	0	10
2	B	0	5
2	D	0	6
2	F	0	10
2	H	0	11
2	O	0	2
2	Q	0	2
2	R	0	3
2	S	0	3
2	T	0	2
3	I	0	9
3	K	0	6
4	J	0	16
5	L	0	20
6	U	0	4
6	V	0	2
6	W	0	4
6	X	0	4
7	o	0	2
7	q	0	2
7	r	0	1
7	s	0	1
7	t	0	1
All	All	0	146

The worst 5 of 1274 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	16	ILE	CG1-CD1	33.79	2.83	1.51
4	J	242	TRP	CD2-CE3	33.30	1.93	1.40
4	J	242	TRP	CZ2-CH2	26.19	1.87	1.37
4	J	242	TRP	CE2-CZ2	24.86	1.92	1.39
4	J	242	TRP	CD2-CE2	22.39	1.79	1.41

The worst 5 of 2389 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	86	VAL	N-CA-C	-11.89	101.07	112.96
2	D	361	LEU	N-CA-C	-11.25	99.54	113.38
4	J	228	PHE	CA-CB-CG	11.13	124.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	441	PHE	CA-CB-CG	-11.03	102.77	113.80
1	A	327	ILE	N-CA-C	-10.53	102.54	111.91

There are no chirality outliers.

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Sidechain
1	A	284	TYR	Sidechain
1	A	326	TYR	Sidechain
1	A	365	TYR	Sidechain
1	A	395	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2211	0	2199	6	0
1	C	2014	0	1998	5	0
1	E	2038	0	2031	5	0
1	G	2014	0	1998	6	0
2	B	2363	0	2379	6	0
2	D	2059	0	2080	8	0
2	F	1964	0	1988	8	0
2	H	2135	0	2160	3	0
2	O	753	0	779	1	0
2	Q	878	0	903	1	0
2	R	794	0	814	2	0
2	S	878	0	903	4	0
2	T	753	0	779	4	0
3	I	2325	0	2335	34	0
3	K	2325	0	2335	9	0
4	J	2909	0	2916	42	0
5	L	3794	0	3844	6	0
6	U	634	0	635	3	0
6	V	634	0	635	1	0
6	W	634	0	635	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	634	0	635	0	0
7	o	403	0	426	0	0
7	p	429	0	446	1	0
7	q	432	0	457	0	0
7	r	454	0	477	1	0
7	s	451	0	476	0	0
7	t	446	0	471	4	0
All	All	37358	0	37734	126	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 2.

The worst 5 of 126 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)
4:J:242:TRP:CZ3	4:J:242:TRP:CE3	1.83	1.66
4:J:242:TRP:CZ2	4:J:242:TRP:CH2	1.87	1.61
4:J:242:TRP:CZ3	4:J:242:TRP:CH2	1.82	1.59
4:J:242:TRP:CZ2	4:J:242:TRP:CE2	1.92	1.57
4:J:242:TRP:CE3	4:J:242:TRP:CD2	1.93	1.56

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/896 (30%)	250 (92%)	14 (5%)	7 (3%)	4	25
1	C	244/896 (27%)	217 (89%)	21 (9%)	6 (2%)	4	26
1	E	247/896 (28%)	229 (93%)	12 (5%)	6 (2%)	4	27
1	G	244/896 (27%)	232 (95%)	11 (4%)	1 (0%)	30	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	290/906 (32%)	261 (90%)	20 (7%)	9 (3%)	3	22
2	D	248/906 (27%)	224 (90%)	17 (7%)	7 (3%)	4	24
2	F	236/906 (26%)	214 (91%)	13 (6%)	9 (4%)	2	19
2	H	257/906 (28%)	227 (88%)	20 (8%)	10 (4%)	2	19
2	O	91/906 (10%)	85 (93%)	5 (6%)	1 (1%)	11	45
2	Q	107/906 (12%)	97 (91%)	6 (6%)	4 (4%)	2	20
2	R	96/906 (11%)	90 (94%)	4 (4%)	2 (2%)	5	30
2	S	107/906 (12%)	96 (90%)	8 (8%)	3 (3%)	4	24
2	T	91/906 (10%)	85 (93%)	4 (4%)	2 (2%)	5	29
3	I	281/666 (42%)	255 (91%)	20 (7%)	6 (2%)	5	30
3	K	281/666 (42%)	259 (92%)	13 (5%)	9 (3%)	3	21
4	J	342/1019 (34%)	317 (93%)	15 (4%)	10 (3%)	3	23
5	L	462/1698 (27%)	422 (91%)	26 (6%)	14 (3%)	3	22
6	U	73/671 (11%)	73 (100%)	0	0	100	100
6	V	73/671 (11%)	72 (99%)	0	1 (1%)	9	39
6	W	73/671 (11%)	71 (97%)	1 (1%)	1 (1%)	9	39
6	X	73/671 (11%)	72 (99%)	1 (1%)	0	100	100
7	o	50/72 (69%)	50 (100%)	0	0	100	100
7	p	54/72 (75%)	54 (100%)	0	0	100	100
7	q	54/72 (75%)	53 (98%)	1 (2%)	0	100	100
7	r	57/72 (79%)	54 (95%)	1 (2%)	2 (4%)	3	20
7	s	57/72 (79%)	54 (95%)	3 (5%)	0	100	100
7	t	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
All	All	4515/18903 (24%)	4168 (92%)	237 (5%)	110 (2%)	7	27

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	428	ASP
2	B	312	LEU
2	D	314	ARG
2	F	281	ALA

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	A	244/824 (30%)	230 (94%)	14 (6%)	18	41
1	C	221/824 (27%)	210 (95%)	11 (5%)	22	44
1	E	224/824 (27%)	214 (96%)	10 (4%)	24	47
1	G	221/824 (27%)	211 (96%)	10 (4%)	24	47
2	B	260/798 (33%)	249 (96%)	11 (4%)	26	48
2	D	227/798 (28%)	219 (96%)	8 (4%)	32	54
2	F	217/798 (27%)	202 (93%)	15 (7%)	14	37
2	H	236/798 (30%)	222 (94%)	14 (6%)	18	41
2	O	82/798 (10%)	80 (98%)	2 (2%)	43	63
2	Q	96/798 (12%)	94 (98%)	2 (2%)	47	65
2	R	87/798 (11%)	86 (99%)	1 (1%)	65	74
2	S	96/798 (12%)	87 (91%)	9 (9%)	8	27
2	T	82/798 (10%)	80 (98%)	2 (2%)	43	63
3	I	259/595 (44%)	245 (95%)	14 (5%)	20	43
3	K	259/595 (44%)	247 (95%)	12 (5%)	24	46
4	J	326/933 (35%)	308 (94%)	18 (6%)	19	43
5	L	431/1539 (28%)	414 (96%)	17 (4%)	28	50
6	U	72/598 (12%)	69 (96%)	3 (4%)	26	48
6	V	72/598 (12%)	70 (97%)	2 (3%)	38	59
6	W	72/598 (12%)	67 (93%)	5 (7%)	14	37
6	X	72/598 (12%)	70 (97%)	2 (3%)	38	59
7	o	48/62 (77%)	45 (94%)	3 (6%)	16	38
7	p	51/62 (82%)	51 (100%)	0	100	100
7	q	51/62 (82%)	51 (100%)	0	100	100
7	r	54/62 (87%)	52 (96%)	2 (4%)	30	51
7	s	53/62 (86%)	49 (92%)	4 (8%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	t	53/62 (86%)	53 (100%)	0	100	100
All	All	4166/16904 (25%)	3975 (95%)	191 (5%)	25	46

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	421	PRO
5	L	368	THR
4	J	598	ARG
3	K	134	PRO
5	L	573	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
6	U	619	HIS
6	V	632	GLN
7	r	7	ASN
2	F	300	HIS
1	E	481	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.

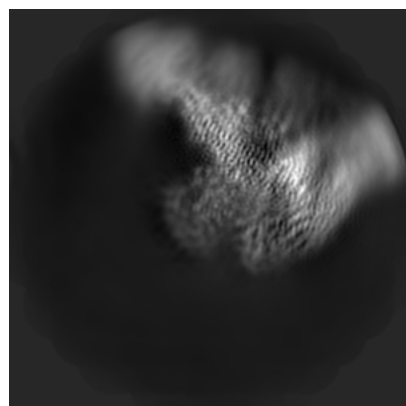
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52729. These allow visual inspection of the internal detail of the map and identification of artifacts.

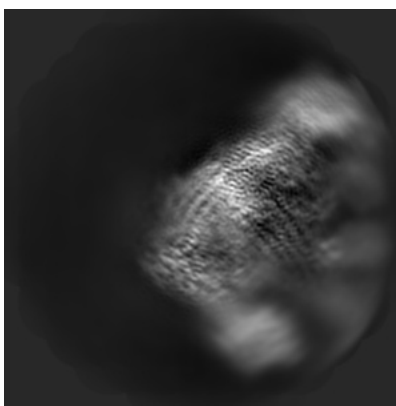
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

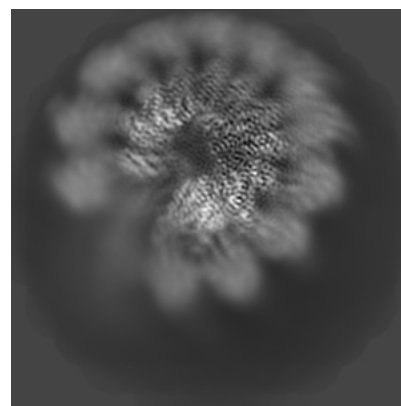
6.1.1 Primary map



X

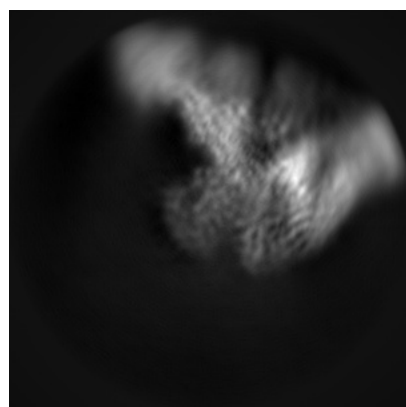


Y

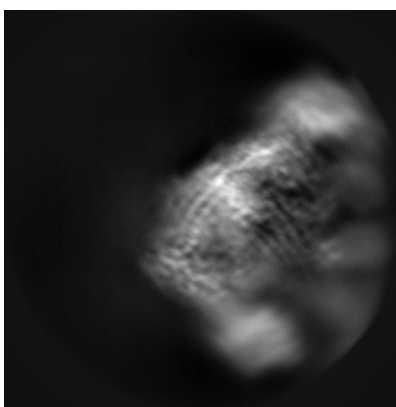


Z

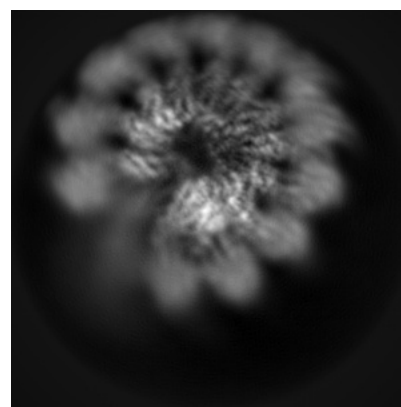
6.1.2 Raw map



X



Y

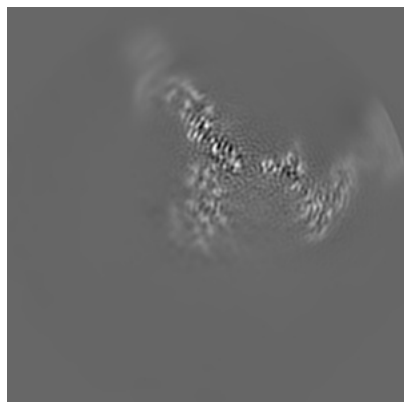


Z

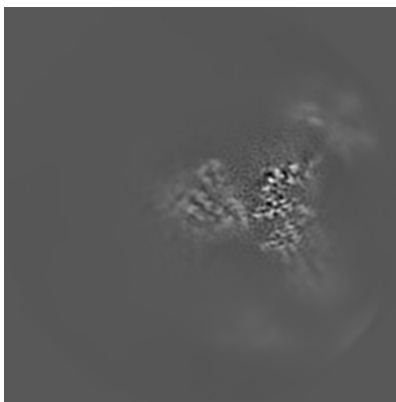
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

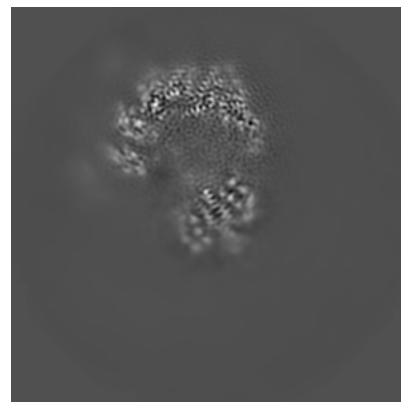
6.2.1 Primary map



X Index: 128

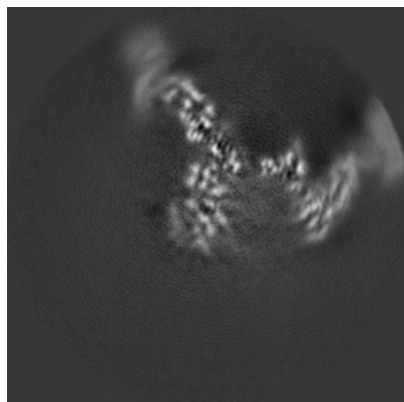


Y Index: 128

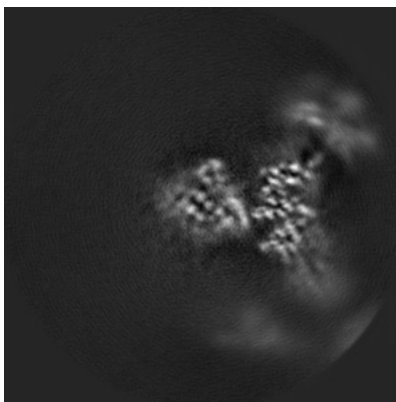


Z Index: 128

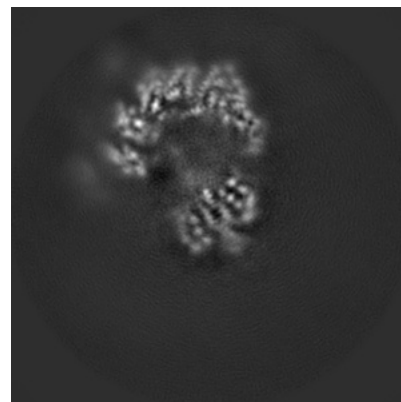
6.2.2 Raw map



X Index: 128



Y Index: 128

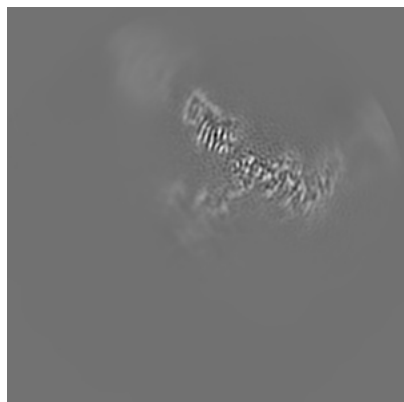


Z Index: 128

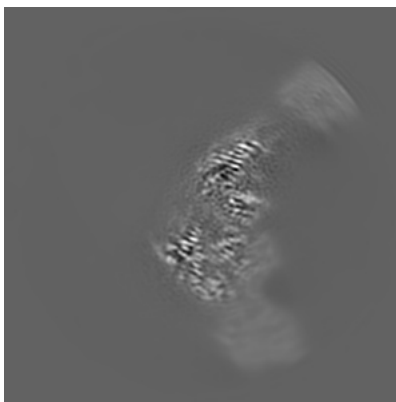
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

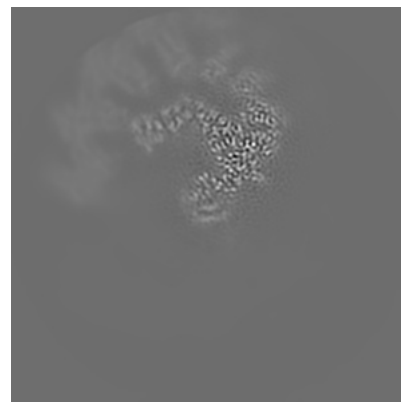
6.3.1 Primary map



X Index: 148

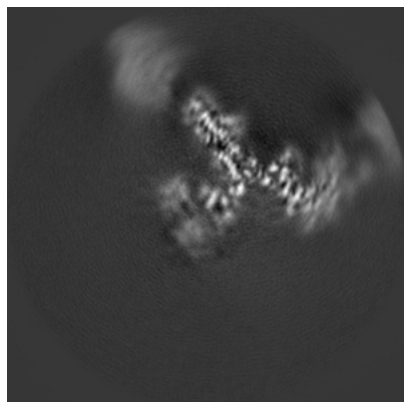


Y Index: 184

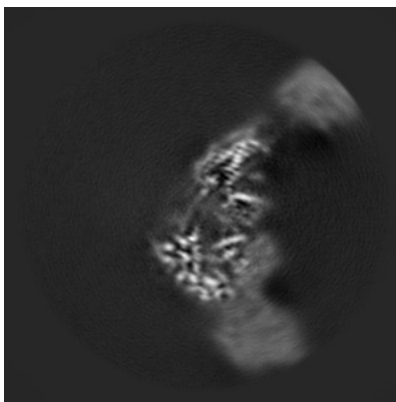


Z Index: 150

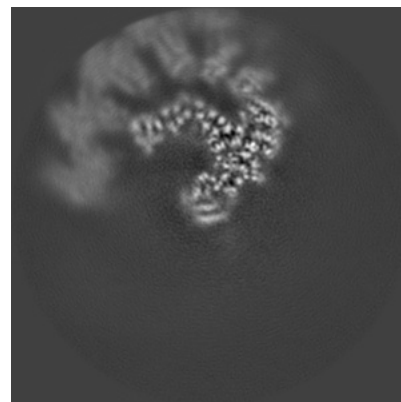
6.3.2 Raw map



X Index: 145



Y Index: 183

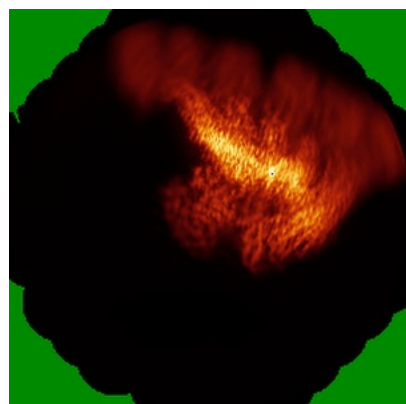


Z Index: 151

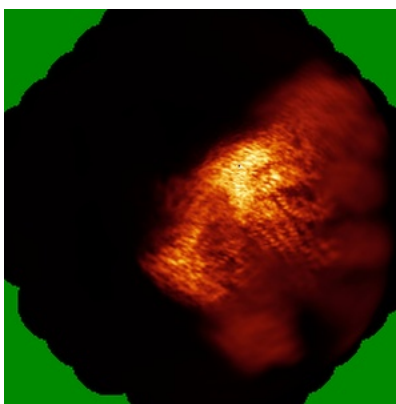
The images above show the largest variance slices of the map in three orthogonal directions.

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

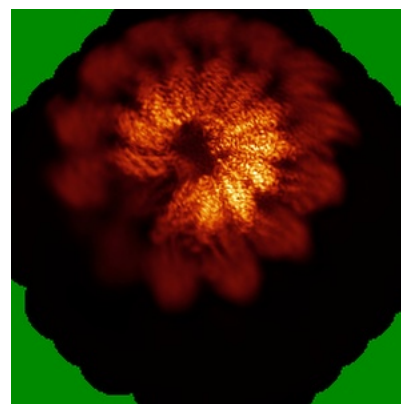
6.4.1 Primary map



X

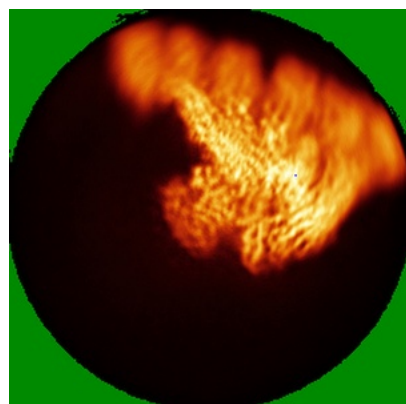


Y

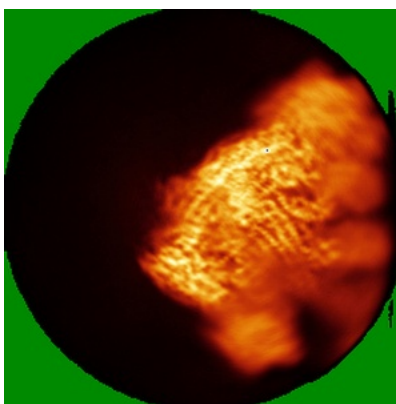


Z

6.4.2 Raw map



X



Y

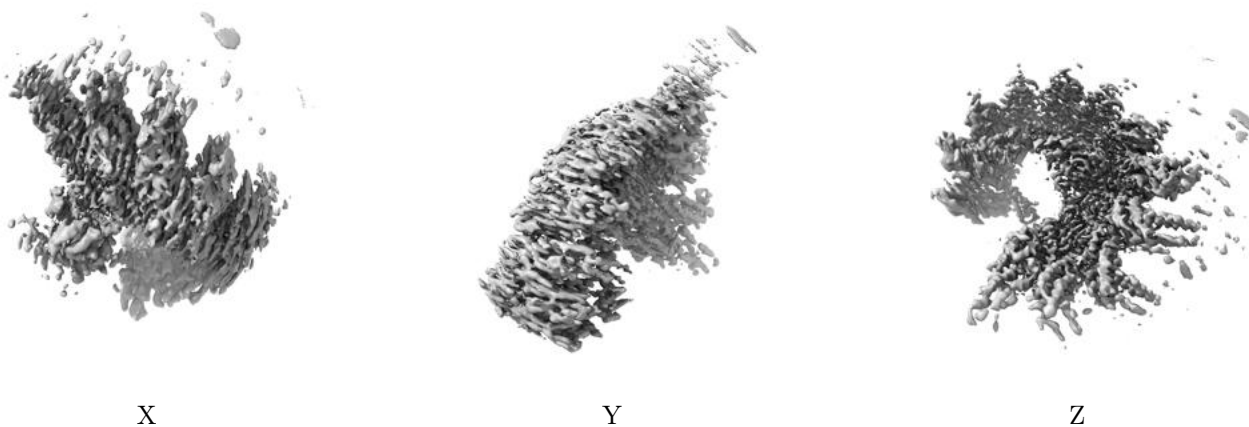


Z

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

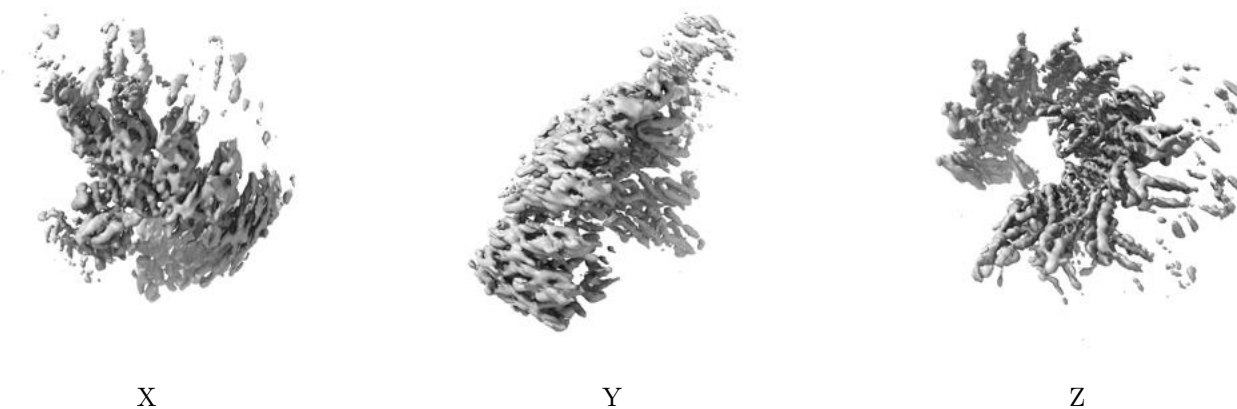
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0421. 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.

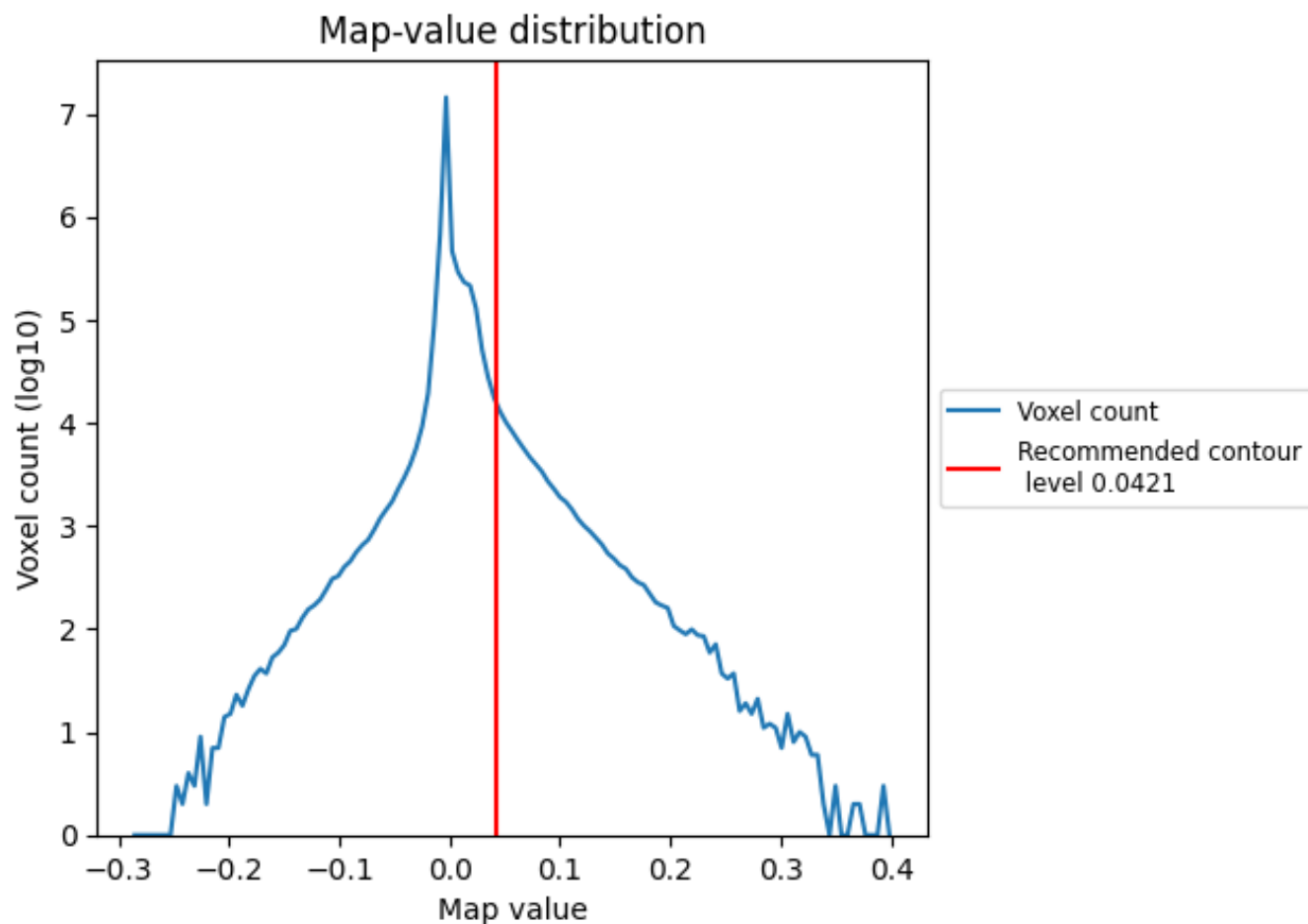
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

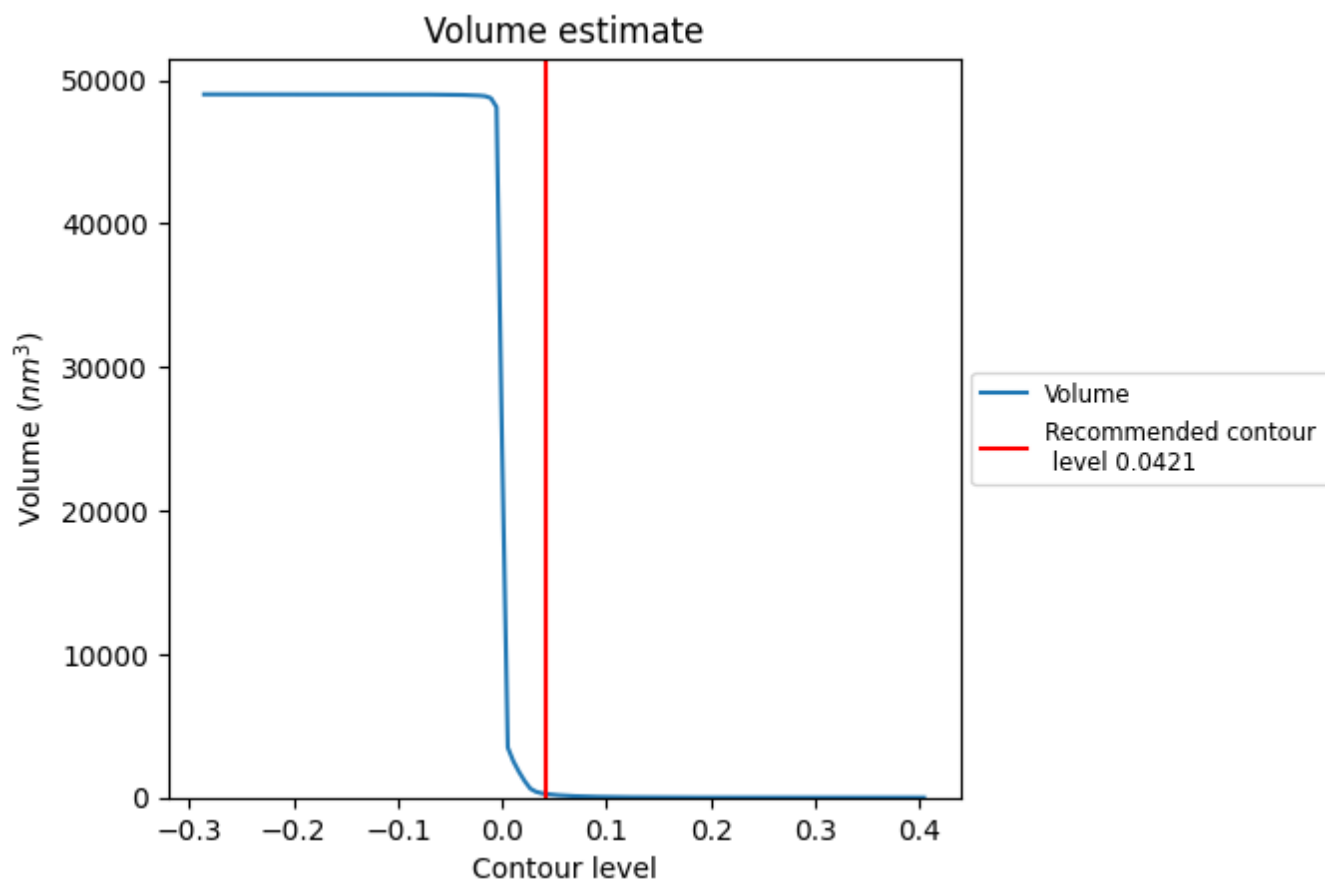
This section contains the results of statistical analysis of the map.

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.

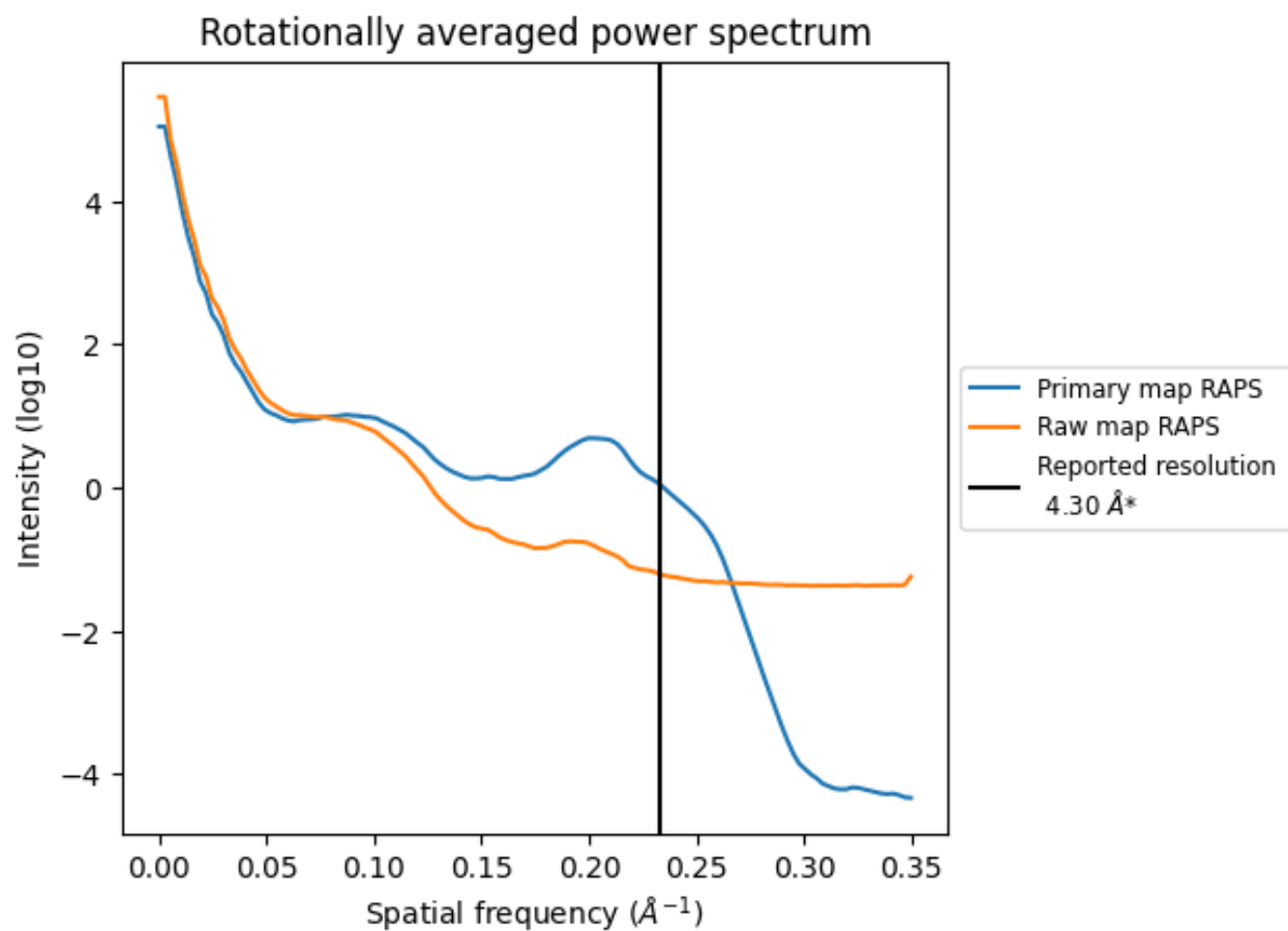
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm³; this corresponds to an approximate mass of 227 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 ⓘ

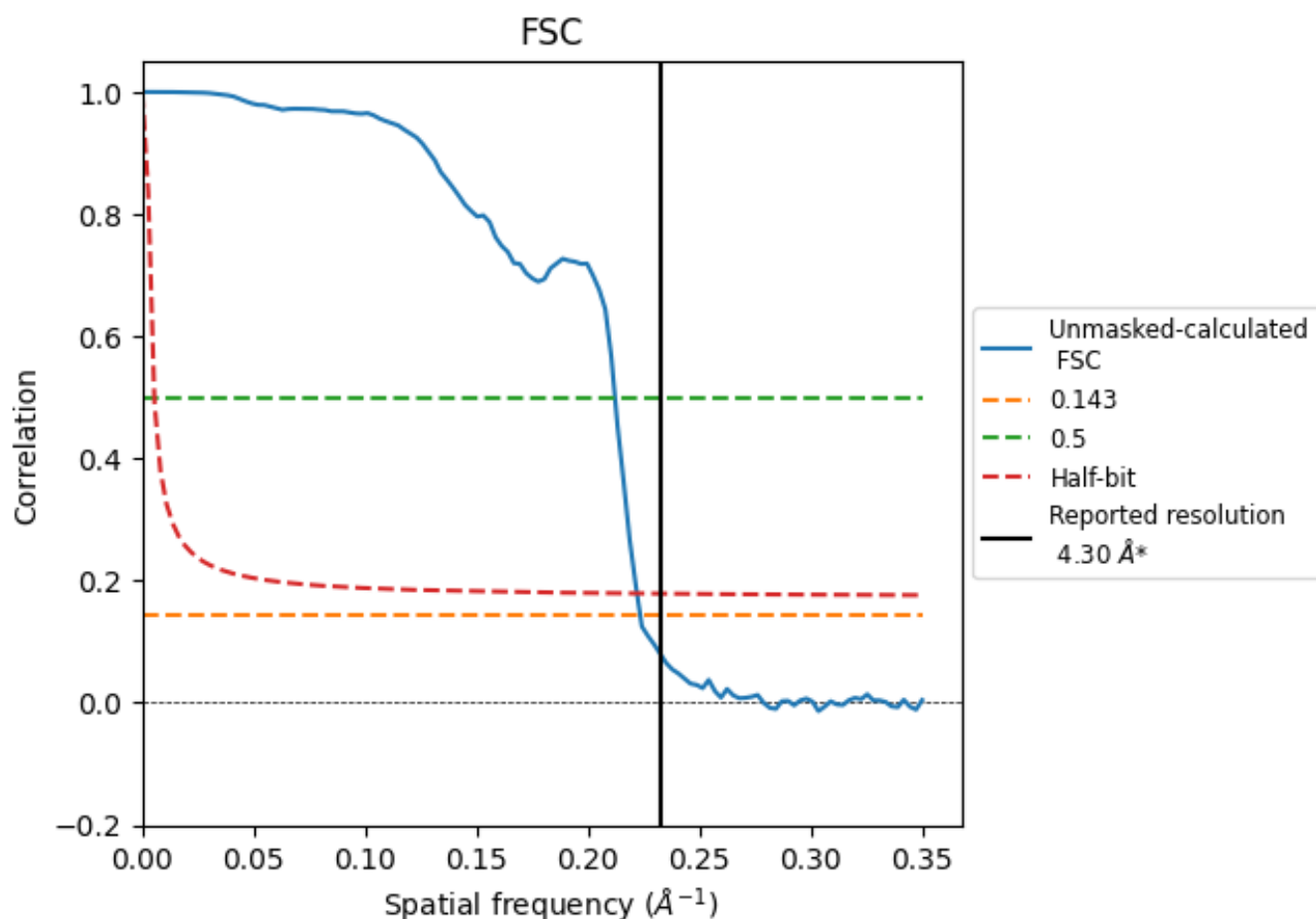


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 Å⁻¹

8.2 Resolution estimates [i](#)

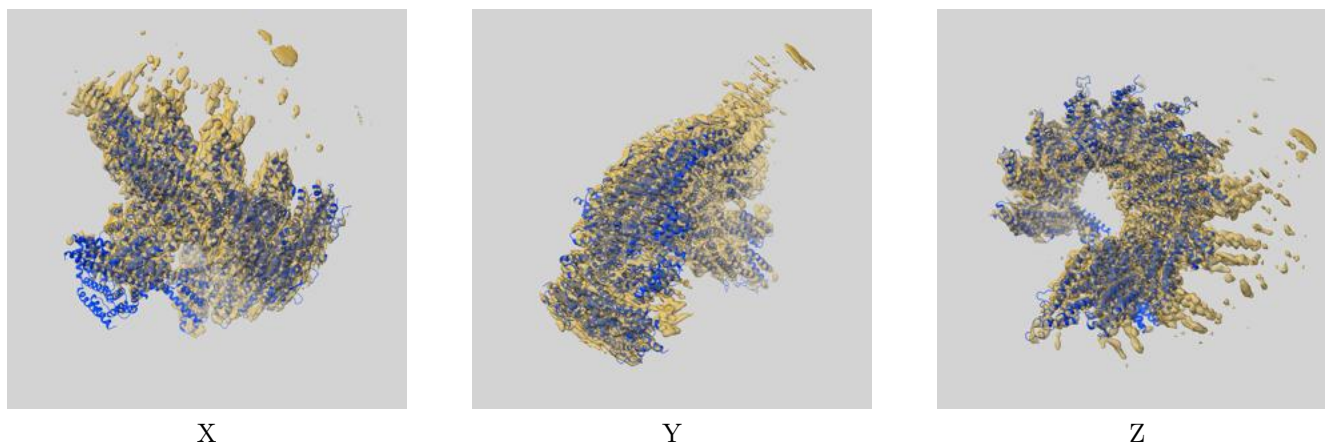
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	4.72	4.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

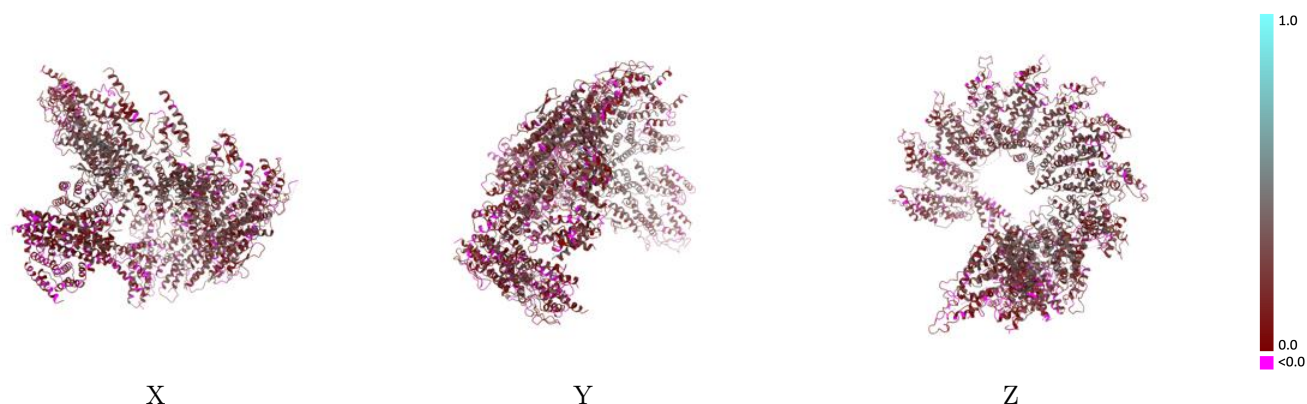
This section contains information regarding the fit between EMDB map EMD-52729 and PDB model 9I8M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



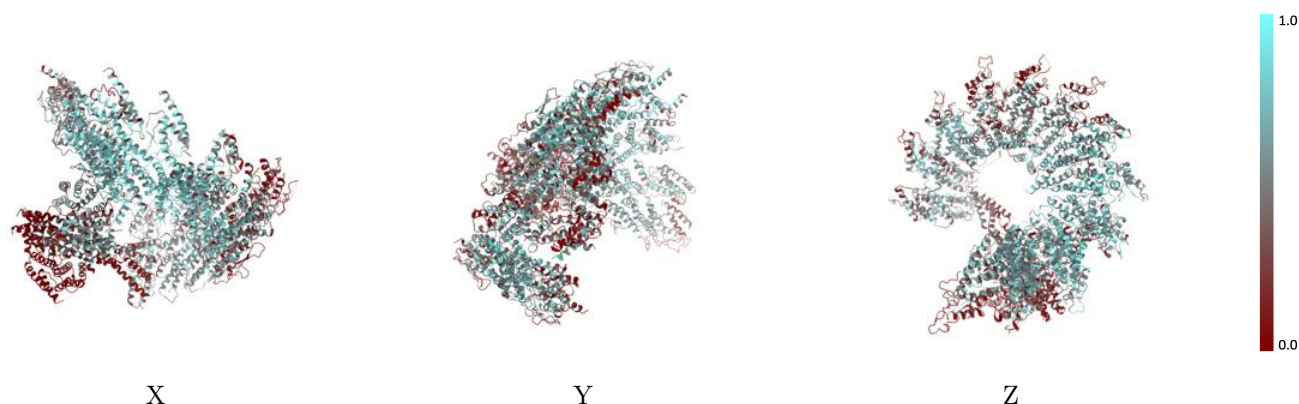
The images above show the 3D surface view of the map at the recommended contour level 0.0421 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



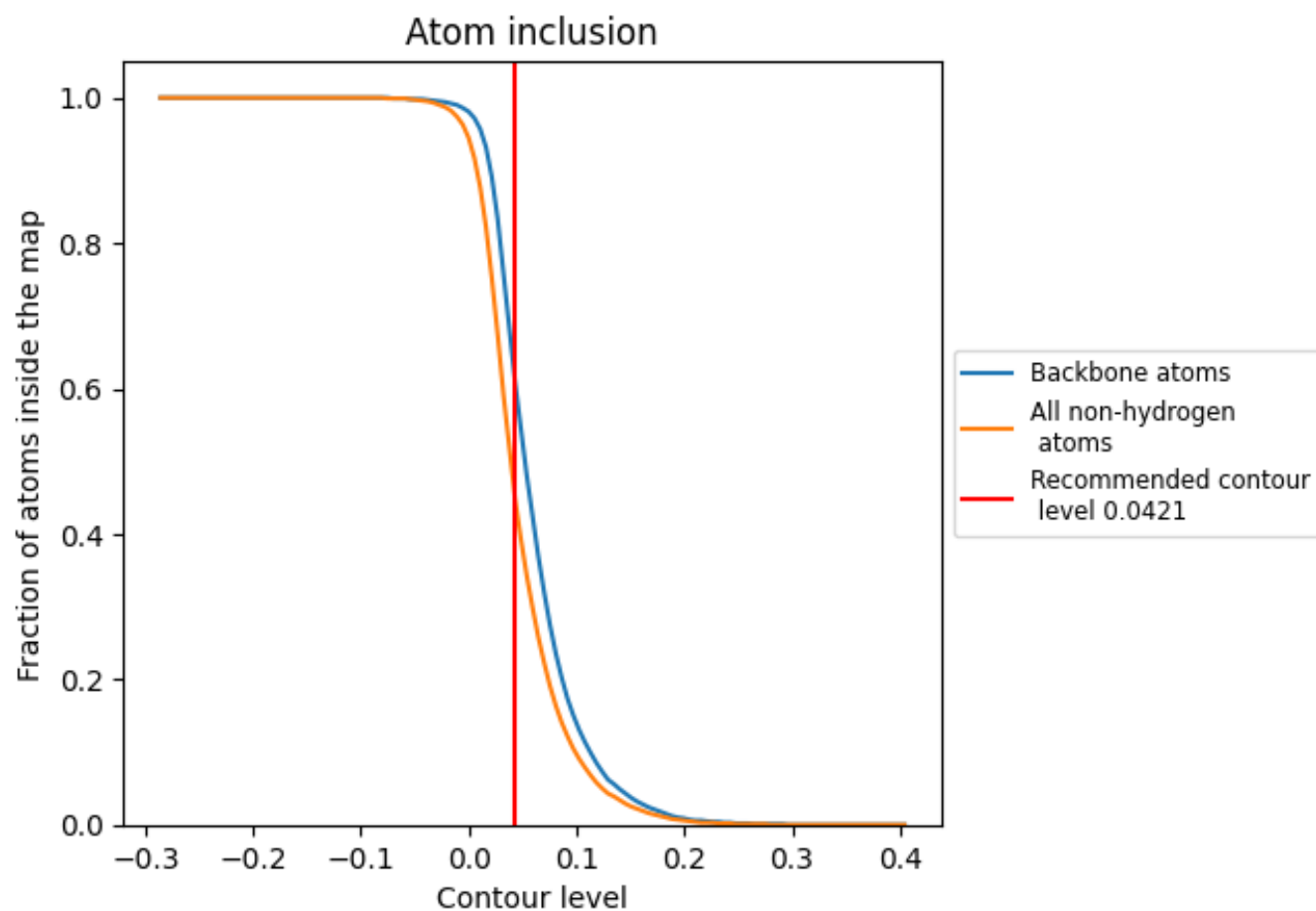
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0421).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 46% 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 (0.0421) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4610	 0.1990
A	 0.4370	 0.1340
B	 0.4790	 0.1530
C	 0.5550	 0.1810
D	 0.3590	 0.1690
E	 0.3630	 0.1960
F	 0.3810	 0.2020
G	 0.5550	 0.2200
H	 0.6540	 0.2460
I	 0.6440	 0.2650
J	 0.6320	 0.2690
K	 0.5640	 0.2530
L	 0.4320	 0.2020
O	 0.6400	 0.2920
Q	 0.1310	 0.1250
R	 0.3820	 0.1750
S	 0.4280	 0.1670
T	 0.0490	 0.0990
U	 0.3300	 0.1960
V	 0.2790	 0.1550
W	 0.2160	 0.1210
X	 0.1970	 0.1160
o	 0.6900	 0.3130
p	 0.4750	 0.2310
q	 0.1470	 0.0950
r	 0.4640	 0.1750
s	 0.5460	 0.1970
t	 0.0230	 0.1270

