wwPDB EM Validation Summary Report

Sep 19, 2023 – 08:56 AM EDT

PDB ID	:	8TH8
EMDB ID	:	EMD-41251
Title	:	Linker domain of Nexin-dynein regulatory complex from Tetrahymena thermophila
Authors	:	Ghanaeian, A.G.; Bui, K.H.
Deposited on	:	2023-07-14
Resolution	:	7.40 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:

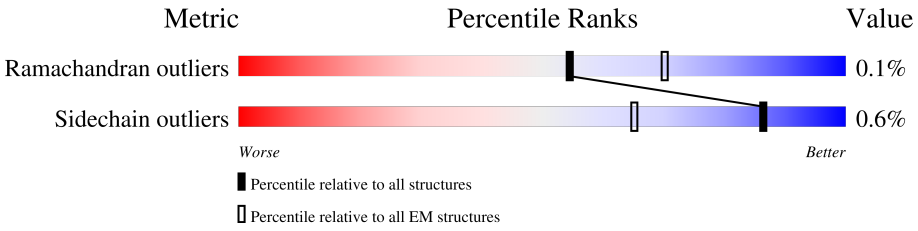
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 7.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	826	35% 65%
2	B	506	12% 54% 45%
3	C	575	92% 7%
4	D	472	10% 61% 38%
5	E	468	11% 61% 38%
6	F	461	33% 99%
7	G	345	10% 99%
8	H	852	19% 95%
9	I	185	11% 99%

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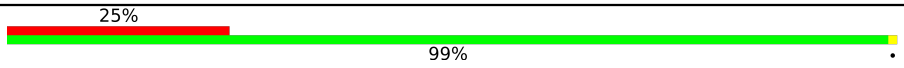
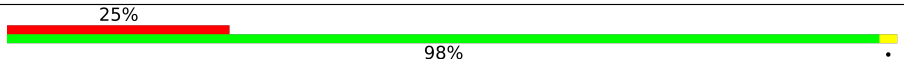
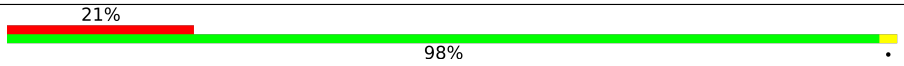
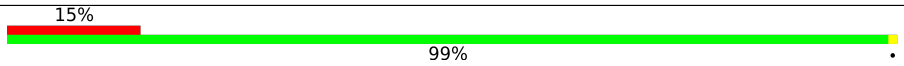
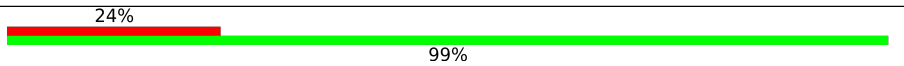
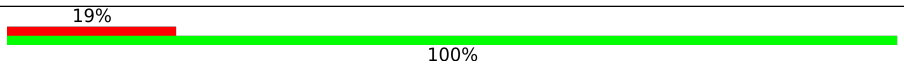
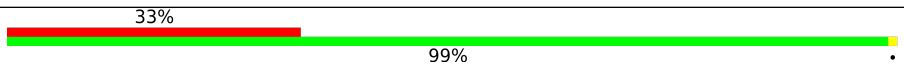
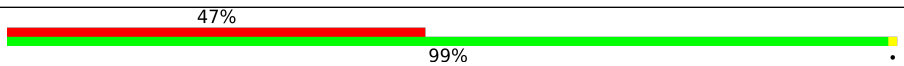
Mol	Chain	Length	Quality of chain
9	i	185	
10	J	372	
11	K	434	
12	L	862	
13	P	794	
14	Q	202	
14	R	202	
15	S	187	
15	s	187	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 58466 atoms, of which 5024 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 Dynein regulatory complex protein 1/2 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	290	2460	1524	439	483	14	0	0

- Molecule 2 is a protein called Coiled-coil protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	276	2329	1451	421	447	10	0	0

- Molecule 3 is a protein called LRRC48 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	533	4433	2771	760	890	12	0	0

- Molecule 4 is a protein called Growth-arrest-specific microtubule-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	292	4976	1536	2515	435	482	8	0	0

- Molecule 5 is a protein called Growth-arrest-specific microtubule-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	291	4952	1528	2509	430	478	7	0	0

- Molecule 6 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	461	3714	2351	632	714	17	0	0

- Molecule 7 is a protein called Kinase domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	345	Total	C	N	O	S	0	0
			2780	1763	474	527	16		

- Molecule 8 is a protein called Coiled-coil lobo-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	820	Total	C	N	O	S	0	0
			6857	4318	1192	1314	33		

- Molecule 9 is a protein called EF-hand calcium-binding domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	185	Total	C	N	O	S	0	0
			1553	1002	244	301	6		
9	i	185	Total	C	N	O	S	0	0
			1553	1002	244	301	6		

- Molecule 10 is a protein called Dynein regulatory complex protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	372	Total	C	N	O	S	0	0
			3151	1949	574	620	8		

- Molecule 11 is a protein called Dynein regulatory complex protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	434	Total	C	N	O	S	0	0
			3588	2229	647	699	13		

- Molecule 12 is a protein called AAA family ATPase CDC48 subfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	862	Total	C	N	O	S	0	0
			7102	4513	1213	1345	31		

- Molecule 13 is a protein called DUF4201 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	305	Total	C	N	O	S	0	0
			2576	1624	442	502	8		

- Molecule 14 is a protein called Calmodulin 7-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	202	Total	C	N	O	S	0	0
			1679	1061	276	338	4		
14	R	202	Total	C	N	O	S	0	0
			1679	1061	276	338	4		

- Molecule 15 is a protein called Coiled-coil domain-containing protein 153.

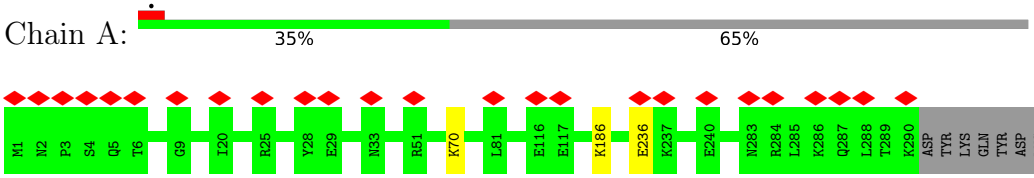
Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	187	Total	C	N	O	S	0	0
			1542	943	274	314	11		
15	s	187	Total	C	N	O	S	0	0
			1542	943	274	314	11		

3 Residue-property plots (i)

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

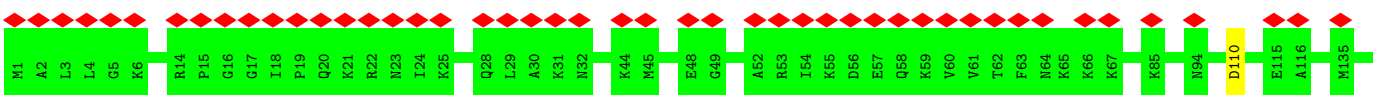
• Molecule 1: Dynein regulatory complex protein 1/2 N-terminal domain-containing protein

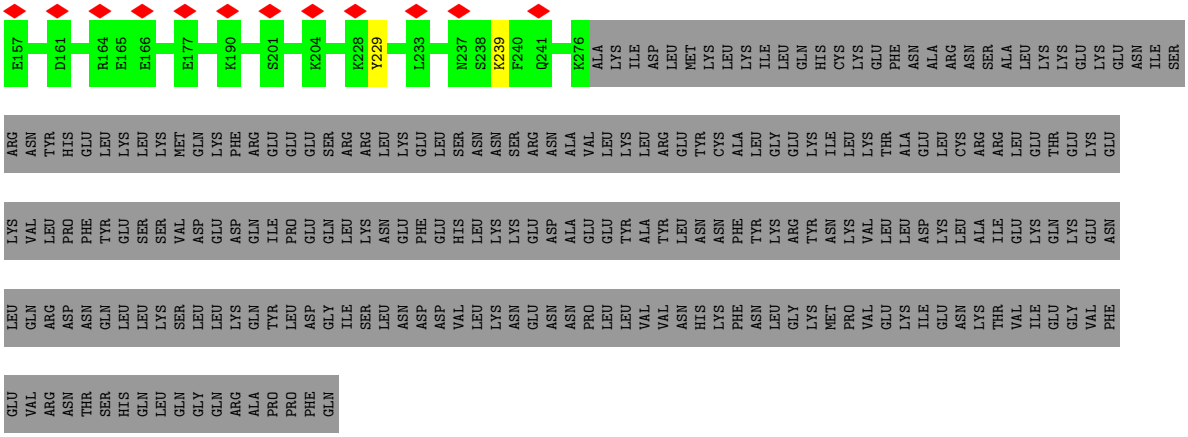
Chain A:



• Molecule 2: Coiled-coil protein, putative

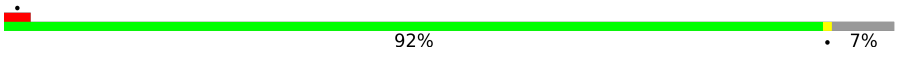
Chain B:

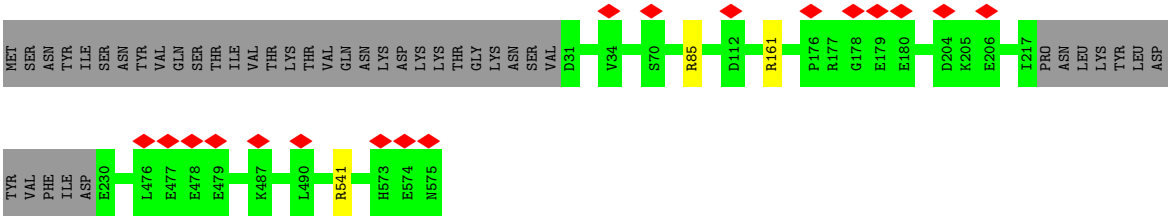




• Molecule 3: LRRC48 protein

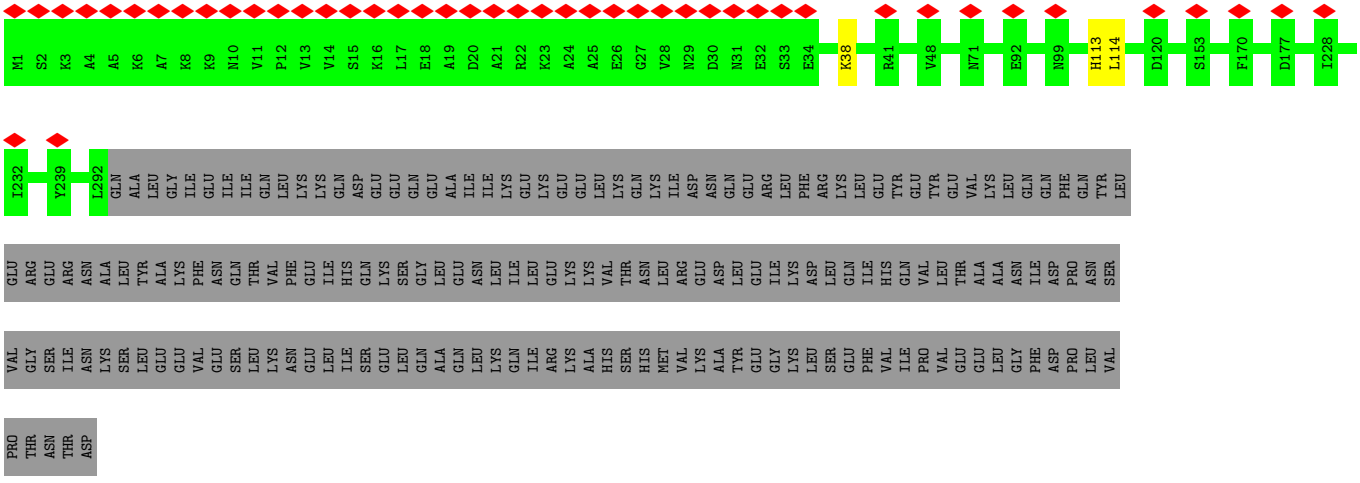
Chain C:





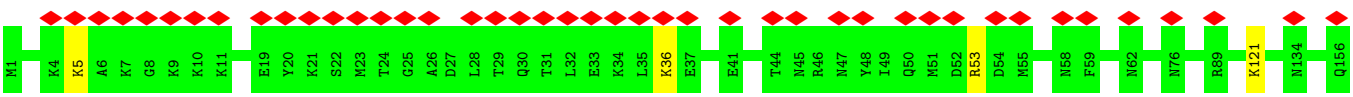
• Molecule 4: Growth-arrest-specific microtubule-binding protein

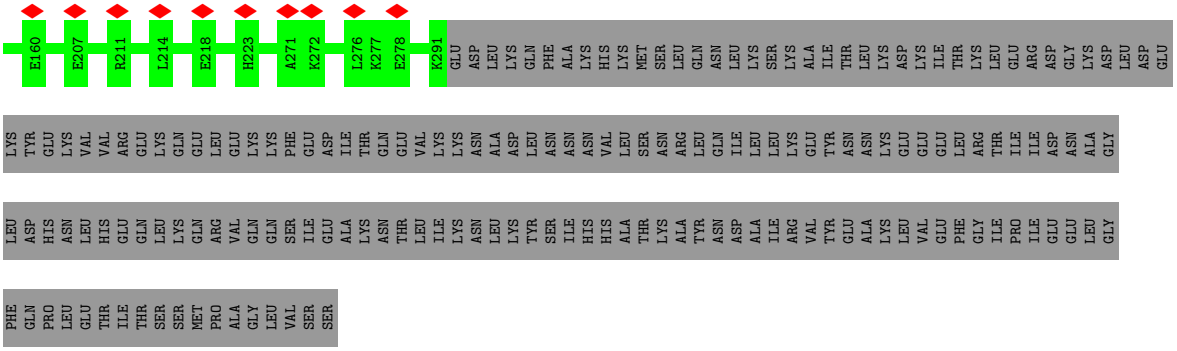
Chain D:



• Molecule 5: Growth-arrest-specific microtubule-binding protein

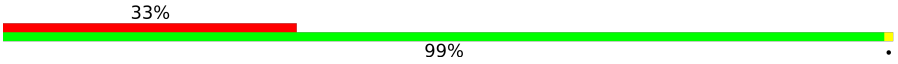
Chain E:

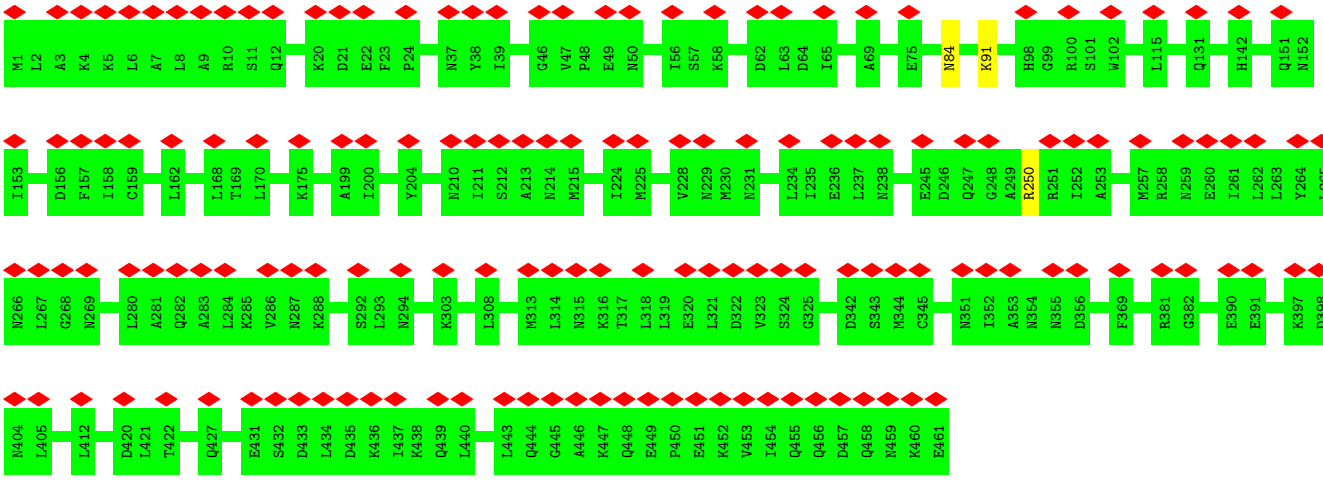




• Molecule 6: Flagellar associated protein

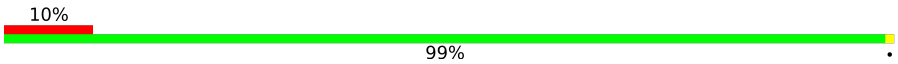
Chain F:

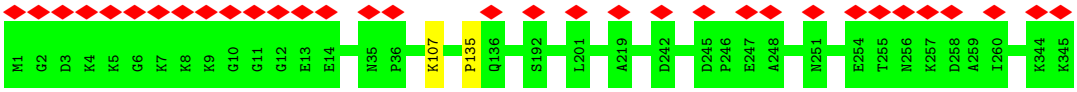




• Molecule 7: Kinase domain protein

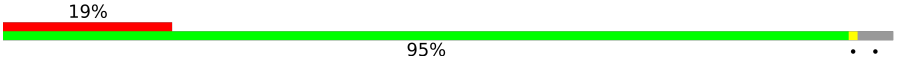
Chain G:

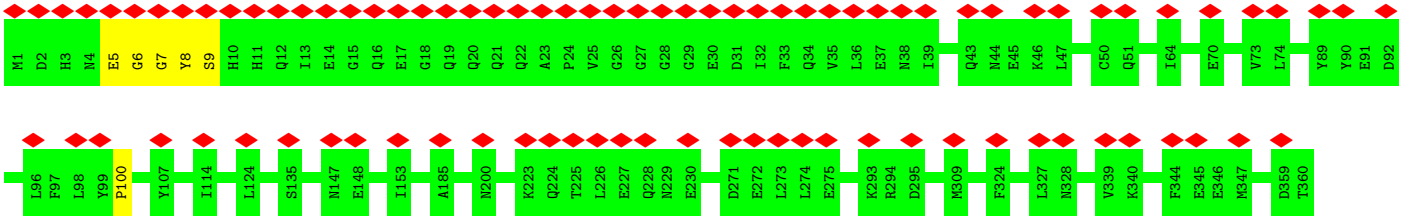


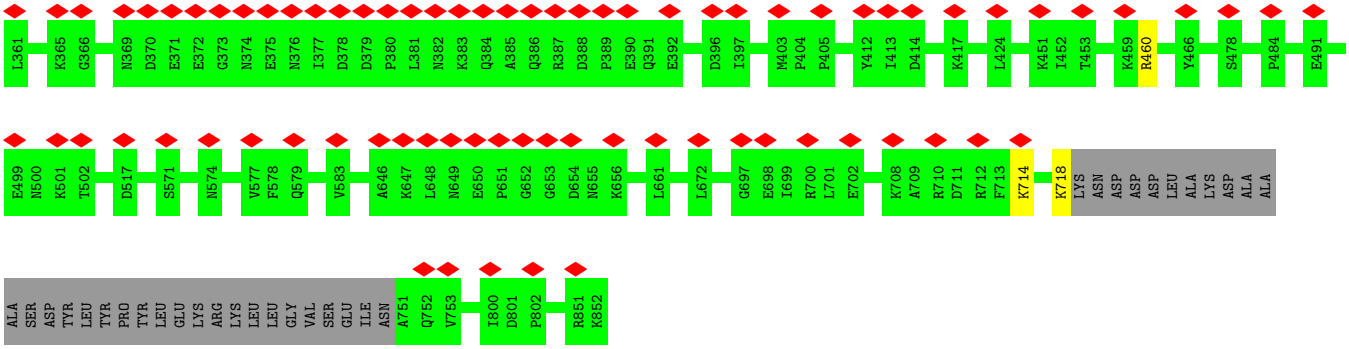


• Molecule 8: Coiled-coil lobo-like protein, putative

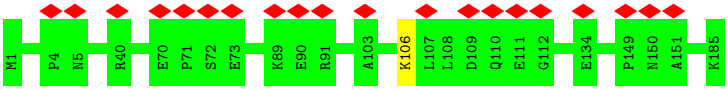
Chain H:



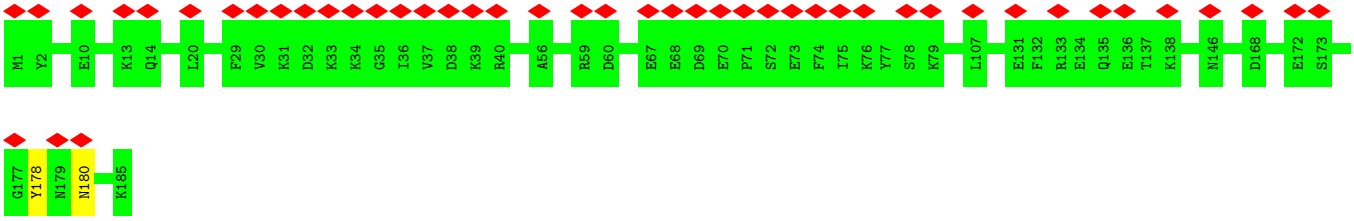




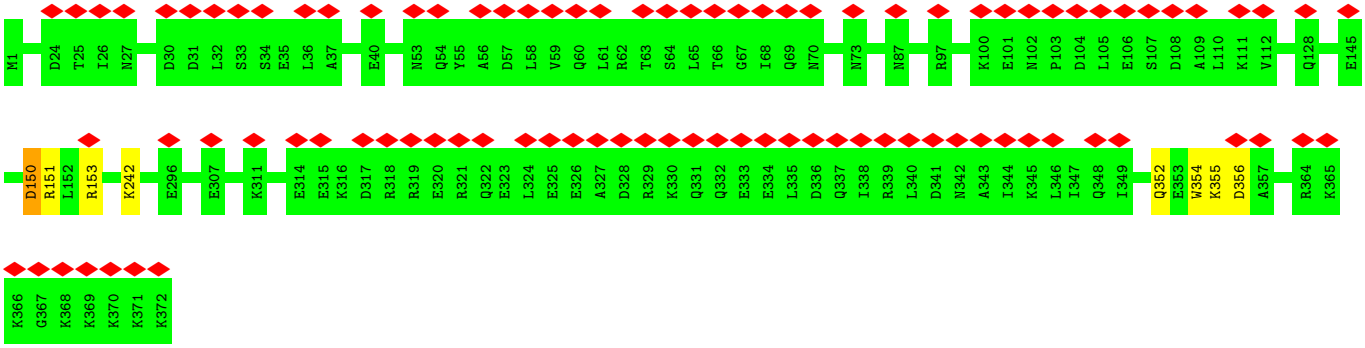
• Molecule 9: EF-hand calcium-binding domain protein



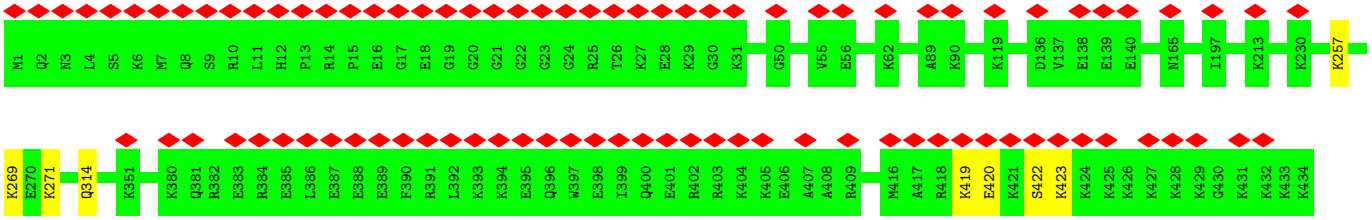
• Molecule 9: EF-hand calcium-binding domain protein



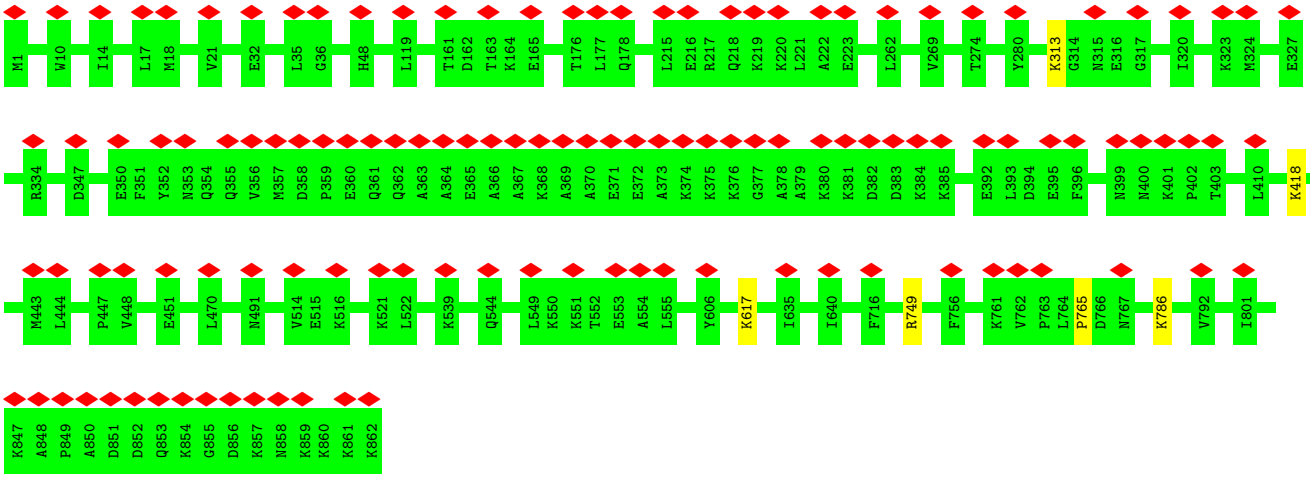
• Molecule 10: Dynein regulatory complex protein 9



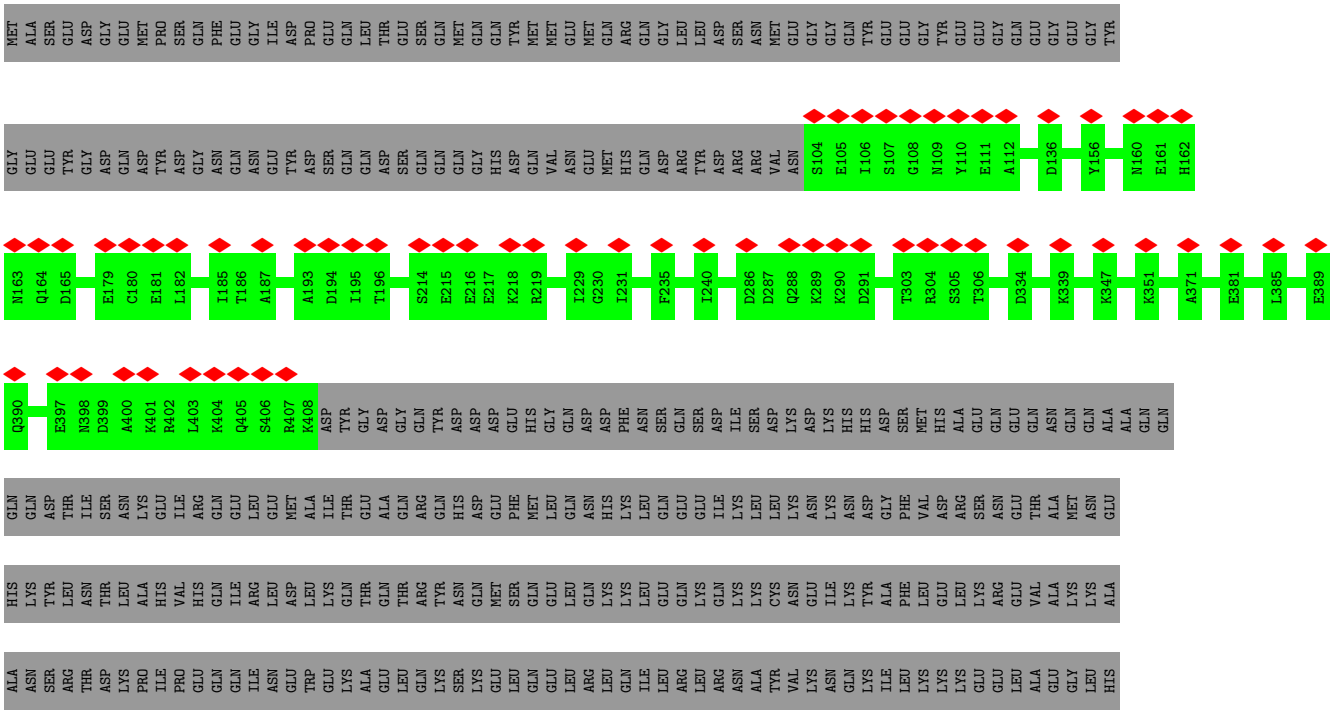
• Molecule 11: Dynein regulatory complex protein 10



• Molecule 12: AAA family ATPase CDC48 subfamily protein

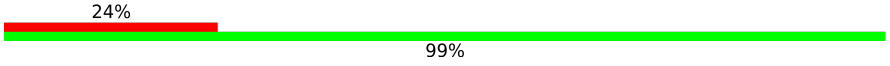


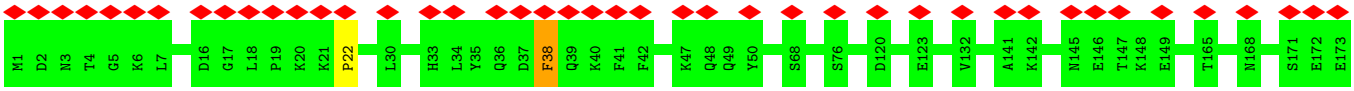
• Molecule 13: DUF4201 domain-containing protein



• Molecule 14: Calmodulin 7-2

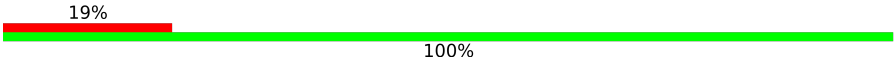
Chain Q:

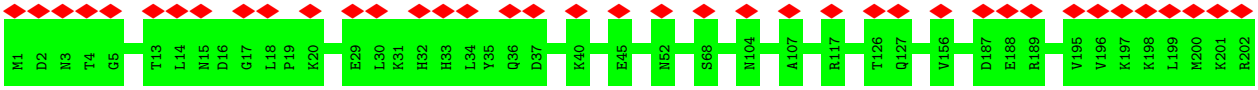




• Molecule 14: Calmodulin 7-2

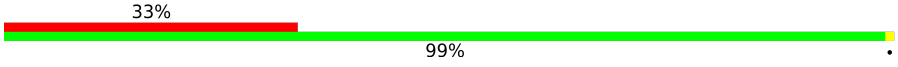
Chain R:

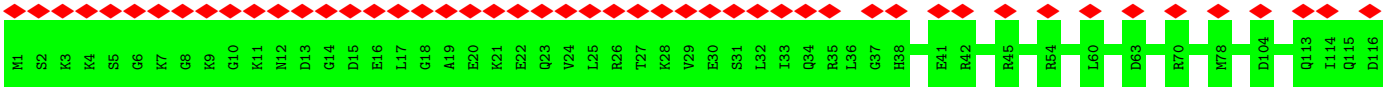




• Molecule 15: Coiled-coil domain-containing protein 153

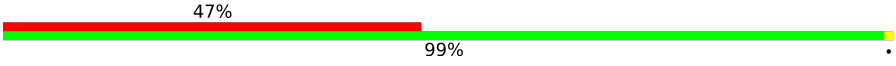
Chain S:

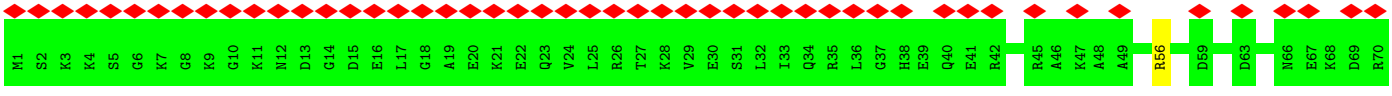




• Molecule 15: Coiled-coil domain-containing protein 153

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211502	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.174	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0217	Depositor
Map size (Å)	706.92, 578.14, 569.92	wwPDB
Map dimensions	258, 211, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.74, 2.74, 2.74	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/2485	0.47	0/3301
2	B	0.26	0/2356	0.52	0/3138
3	C	0.25	0/4482	0.44	0/6008
4	D	0.26	0/2487	0.47	0/3314
5	E	0.27	0/2470	0.47	1/3290 (0.0%)
6	F	0.24	0/3768	0.44	0/5071
7	G	0.24	0/2821	0.45	1/3772 (0.0%)
8	H	1.20	8/6994 (0.1%)	0.53	3/9419 (0.0%)
9	I	0.25	0/1586	0.41	0/2128
9	i	0.25	0/1586	0.42	0/2128
10	J	0.35	2/3173 (0.1%)	0.53	2/4219 (0.0%)
11	K	0.25	0/3620	0.44	0/4803
12	L	0.29	1/7234 (0.0%)	0.47	3/9693 (0.0%)
13	P	0.27	0/2623	0.50	0/3530
14	Q	1.98	6/1705 (0.4%)	0.61	3/2290 (0.1%)
14	R	0.25	0/1705	0.47	0/2290
15	S	0.24	0/1552	0.44	0/2057
15	s	0.24	0/1552	0.46	0/2057
All	All	0.61	17/54199 (0.0%)	0.48	13/72508 (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
2	B	0	1
4	D	0	1
8	H	0	2
9	i	0	2
10	J	0	2
11	K	0	3
14	Q	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	12

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	8	TYR	CD2-CE2	53.51	2.19	1.39
8	H	8	TYR	CD1-CE1	51.18	2.16	1.39
14	Q	38	PHE	CD1-CE1	38.85	2.17	1.39
14	Q	38	PHE	CE1-CZ	37.73	2.09	1.37
14	Q	38	PHE	CE2-CZ	37.26	2.08	1.37

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	5	GLU	C-N-CA	15.07	153.94	122.30
12	L	765	PRO	N-CD-CG	-13.65	82.72	103.20
10	J	355	LYS	C-N-CA	13.37	155.12	121.70
14	Q	38	PHE	CB-CG-CD2	-10.76	113.27	120.80
8	H	6	GLY	N-CA-C	8.49	134.33	113.10

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	229	TYR	Peptide
4	D	113	HIS	Peptide
8	H	7	GLY	Peptide
8	H	9	SER	Peptide
10	J	352	GLN	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	Percentiles
1	A	288/826 (35%)	275 (96%)	11 (4%)	2 (1%)	22 63
2	B	274/506 (54%)	243 (89%)	31 (11%)	0	100 100
3	C	529/575 (92%)	505 (96%)	24 (4%)	0	100 100
4	D	290/472 (61%)	284 (98%)	5 (2%)	1 (0%)	41 77
5	E	289/468 (62%)	277 (96%)	12 (4%)	0	100 100
6	F	459/461 (100%)	424 (92%)	35 (8%)	0	100 100
7	G	343/345 (99%)	321 (94%)	22 (6%)	0	100 100
8	H	816/852 (96%)	729 (89%)	87 (11%)	0	100 100
9	I	183/185 (99%)	181 (99%)	2 (1%)	0	100 100
9	i	183/185 (99%)	174 (95%)	9 (5%)	0	100 100
10	J	370/372 (100%)	349 (94%)	20 (5%)	1 (0%)	41 77
11	K	432/434 (100%)	394 (91%)	37 (9%)	1 (0%)	47 81
12	L	860/862 (100%)	823 (96%)	37 (4%)	0	100 100
13	P	303/794 (38%)	283 (93%)	20 (7%)	0	100 100
14	Q	200/202 (99%)	181 (90%)	18 (9%)	1 (0%)	29 69
14	R	200/202 (99%)	180 (90%)	20 (10%)	0	100 100
15	S	185/187 (99%)	175 (95%)	10 (5%)	0	100 100
15	s	185/187 (99%)	183 (99%)	2 (1%)	0	100 100
All	All	6389/8115 (79%)	5981 (94%)	402 (6%)	6 (0%)	54 86

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	LYS
4	D	114	LEU
11	K	419	LYS
1	A	236	GLU
10	J	150	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/766 (35%)	270 (100%)	1 (0%)	91 94
2	B	258/473 (54%)	256 (99%)	2 (1%)	81 89
3	C	499/540 (92%)	496 (99%)	3 (1%)	86 92
4	D	272/438 (62%)	271 (100%)	1 (0%)	91 94
5	E	272/434 (63%)	269 (99%)	3 (1%)	73 84
6	F	414/414 (100%)	411 (99%)	3 (1%)	84 90
7	G	310/310 (100%)	309 (100%)	1 (0%)	92 95
8	H	759/786 (97%)	756 (100%)	3 (0%)	91 94
9	I	170/170 (100%)	169 (99%)	1 (1%)	86 92
9	i	170/170 (100%)	170 (100%)	0	100 100
10	J	350/350 (100%)	346 (99%)	4 (1%)	73 84
11	K	403/403 (100%)	399 (99%)	4 (1%)	76 86
12	L	776/776 (100%)	771 (99%)	5 (1%)	86 92
13	P	284/733 (39%)	284 (100%)	0	100 100
14	Q	189/189 (100%)	189 (100%)	0	100 100
14	R	189/189 (100%)	189 (100%)	0	100 100
15	S	172/172 (100%)	170 (99%)	2 (1%)	71 83
15	s	172/172 (100%)	170 (99%)	2 (1%)	71 83
All	All	5930/7485 (79%)	5895 (99%)	35 (1%)	86 92

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	617	LYS
12	L	749	ARG
15	S	127	LYS
6	F	250	ARG
6	F	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
13	P	362	GLN
14	Q	145	ASN
9	i	182	GLN
5	E	223	HIS
5	E	206	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

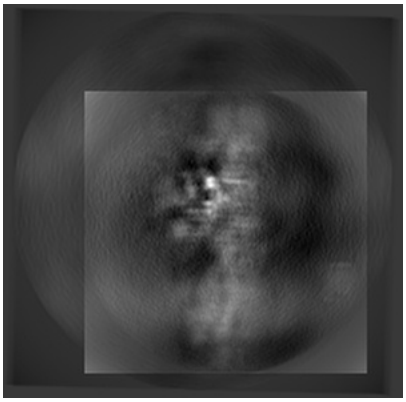
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41251. These allow visual inspection of the internal detail of the map and identification of artifacts.

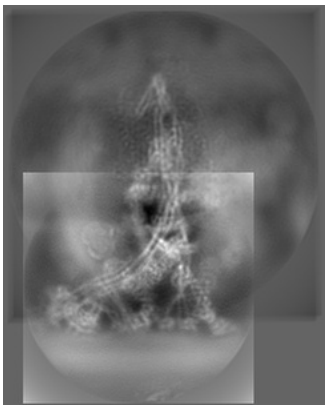
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

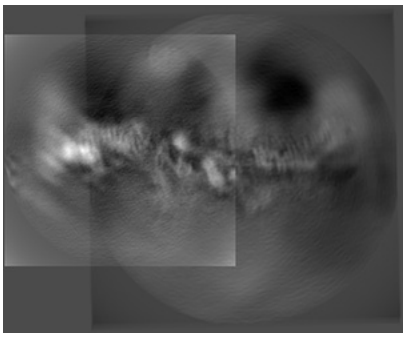
6.1.1 Primary map



X

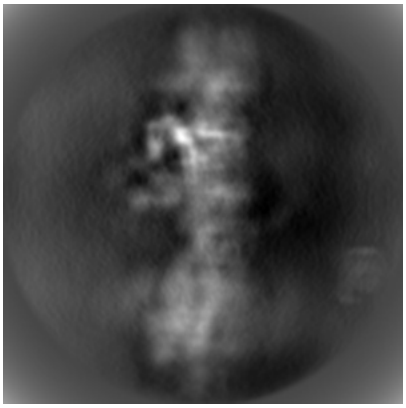


Y

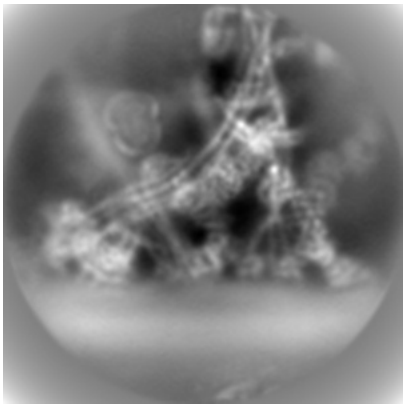


Z

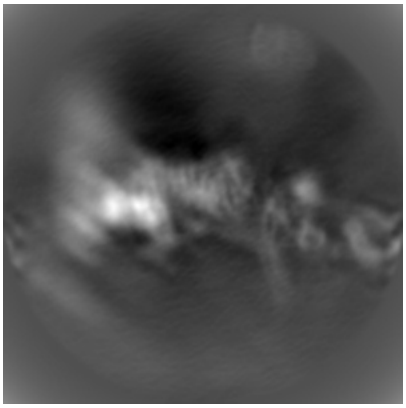
6.1.2 Raw map



X



Y

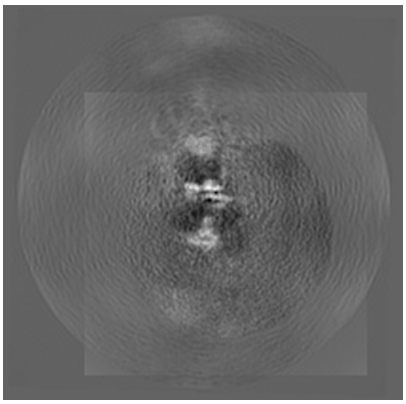


Z

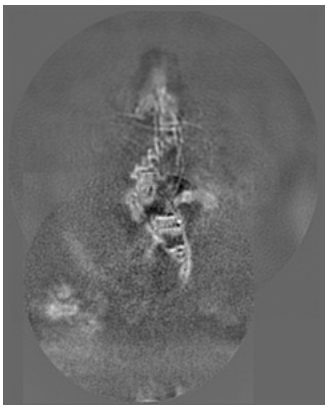
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

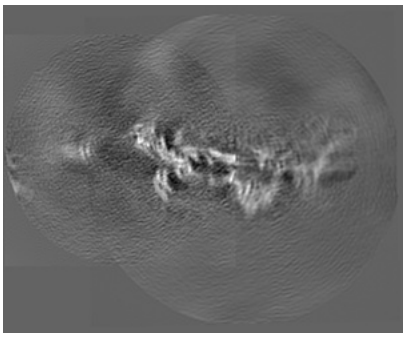
6.2.1 Primary map



X Index: 129

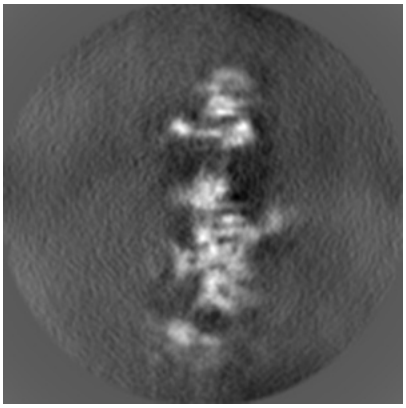


Y Index: 105

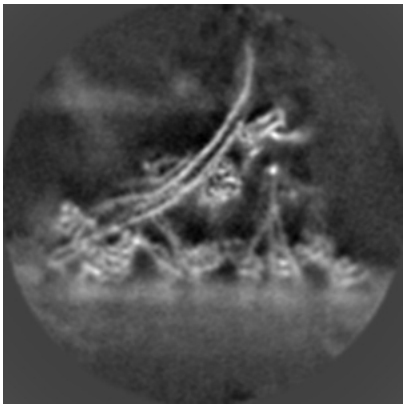


Z Index: 104

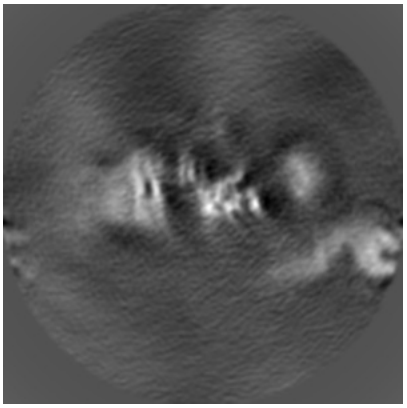
6.2.2 Raw map



X Index: 75



Y Index: 75

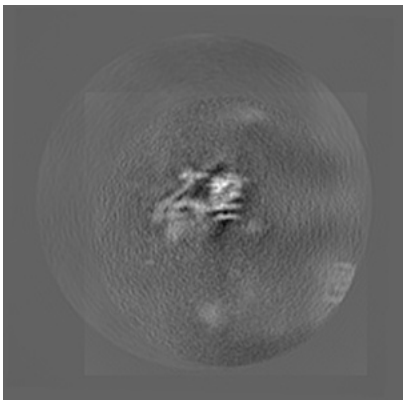


Z Index: 75

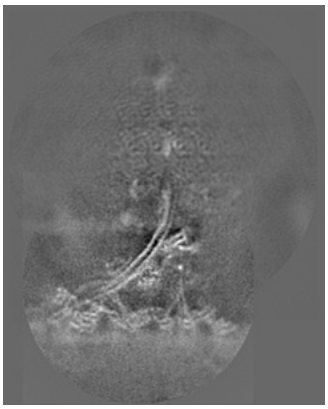
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

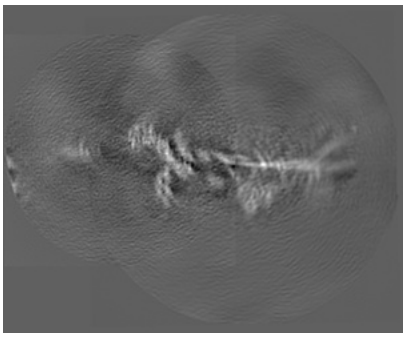
6.3.1 Primary map



X Index: 105

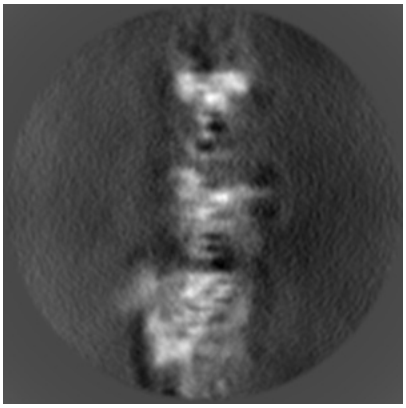


Y Index: 117

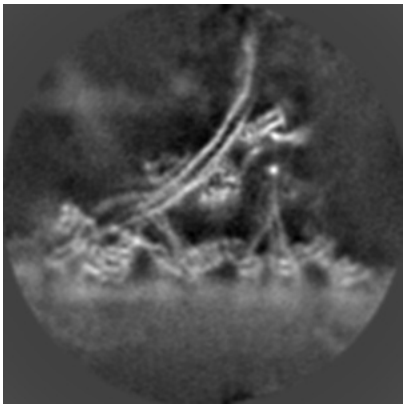


Z Index: 102

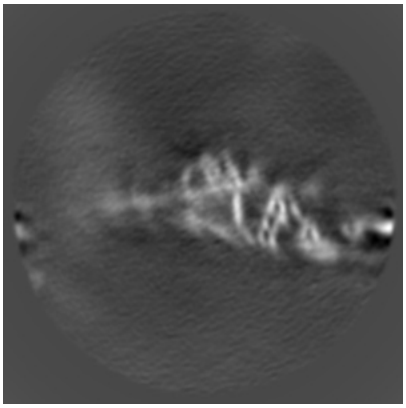
6.3.2 Raw map



X Index: 56



Y Index: 74

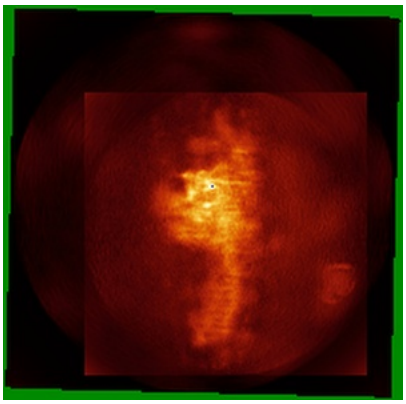


Z Index: 101

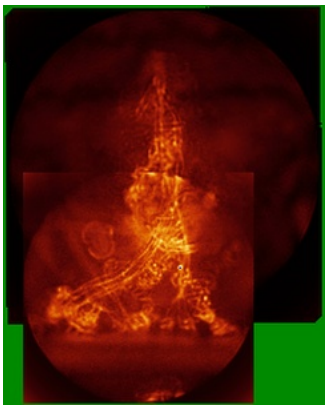
The images above show the largest variance slices of the map in three orthogonal directions.

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

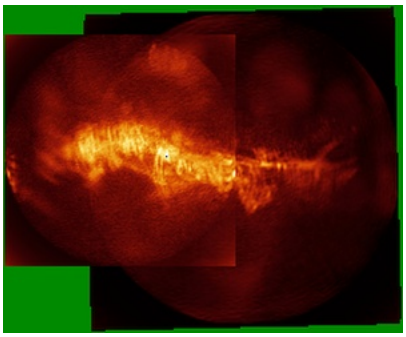
6.4.1 Primary map



X

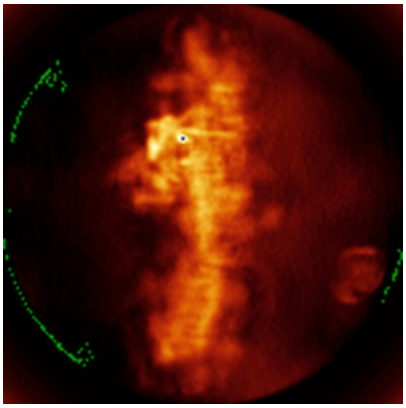


Y

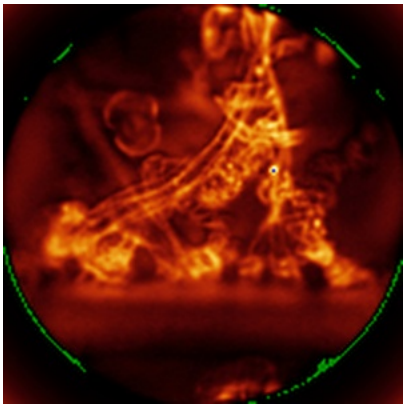


Z

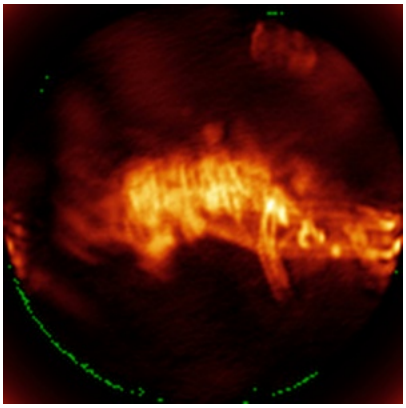
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0217. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

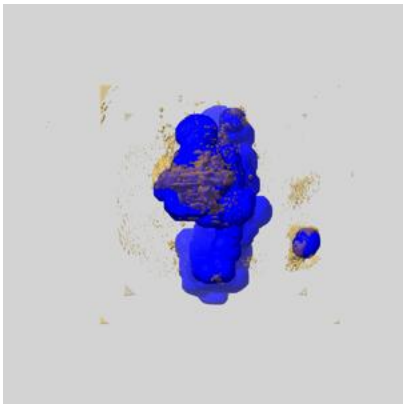
6.6 Mask visualisation (i)

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

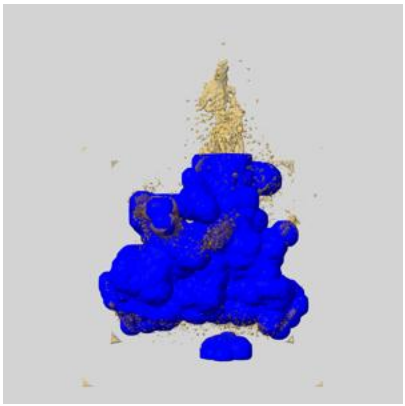
A mask typically either:

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

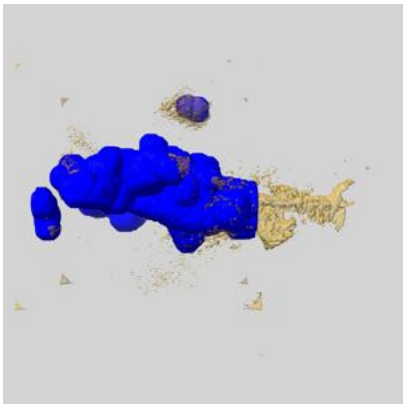
6.6.1 emd_41251_msk_1.map (i)



X



Y

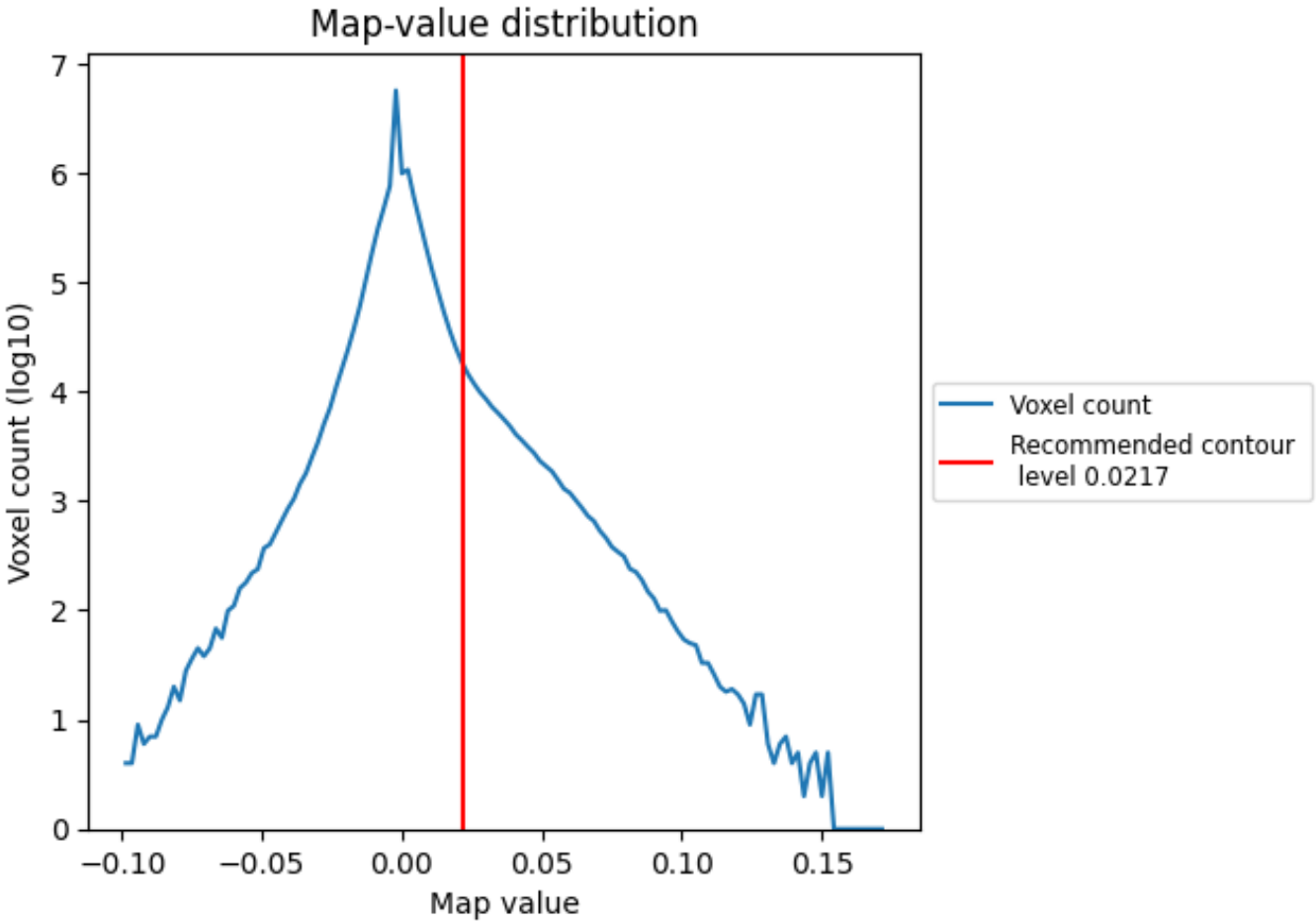


Z

7 Map analysis

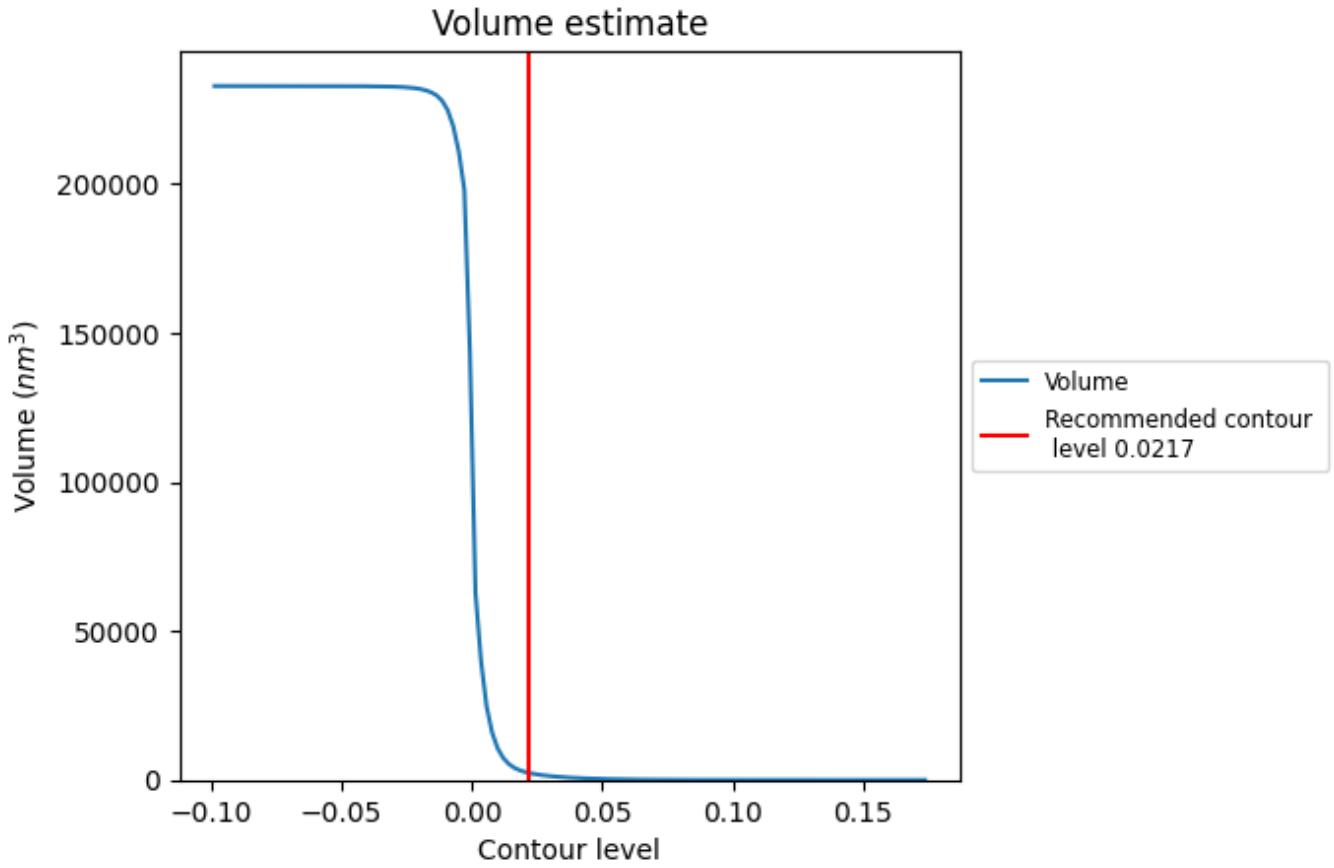
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 2392 nm^3; this corresponds to an approximate mass of 2161 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.

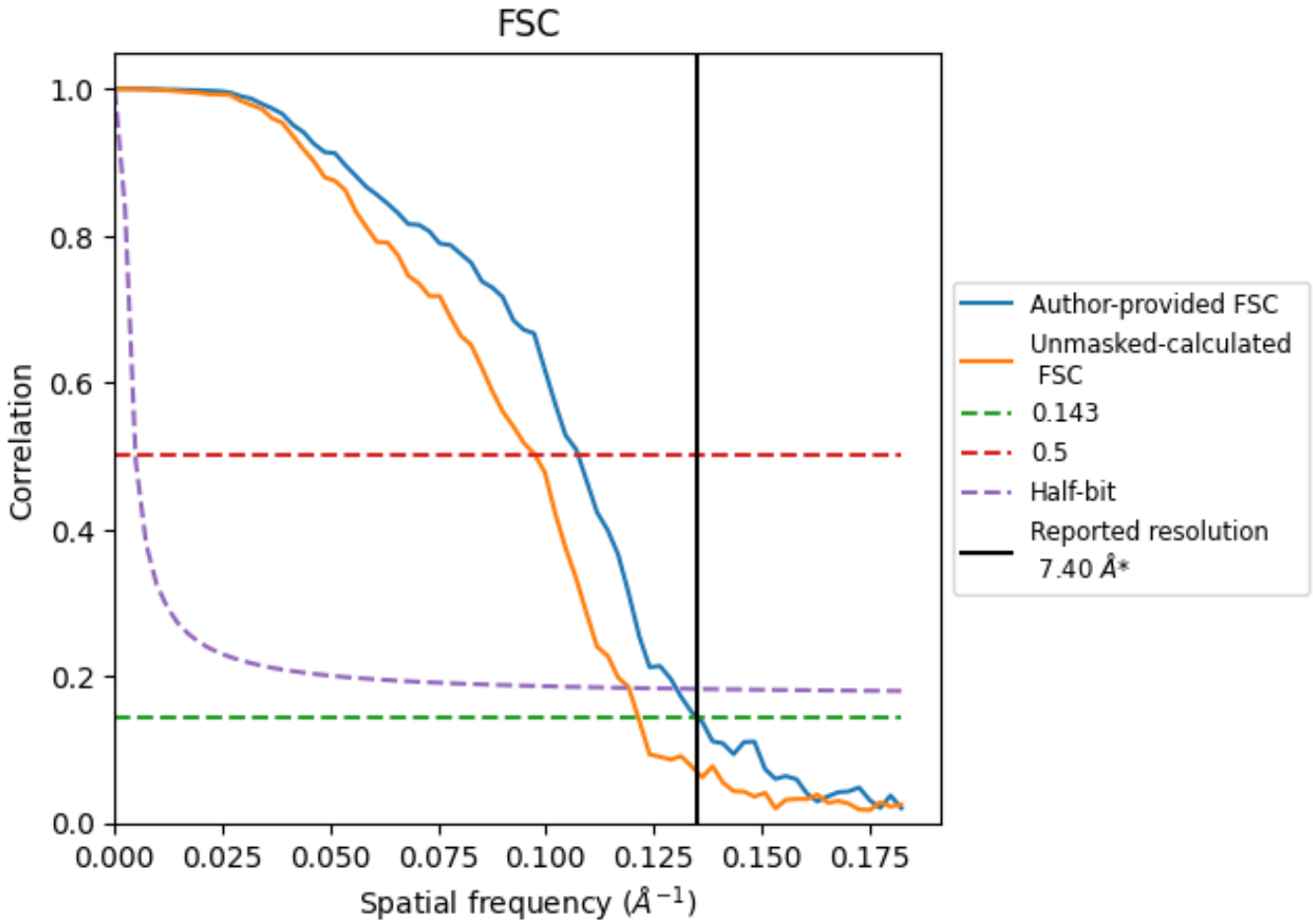
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.135 Å^{-1}

8.2 Resolution estimates (i)

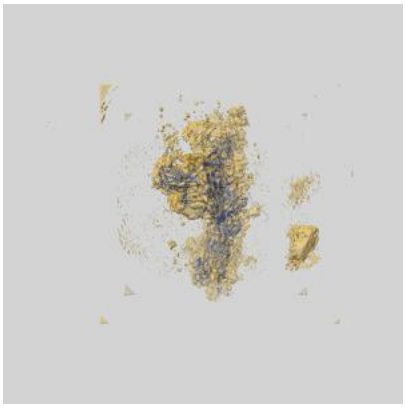
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	7.40
Author-provided FSC curve	7.39	9.30	7.67	-
Unmasked-calculated*	8.23	10.25	8.38	-

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

9 Map-model fit

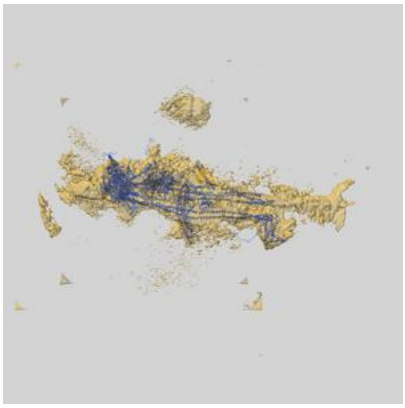
This section contains information regarding the fit between EMDB map EMD-41251 and PDB model 8TH8. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay



X

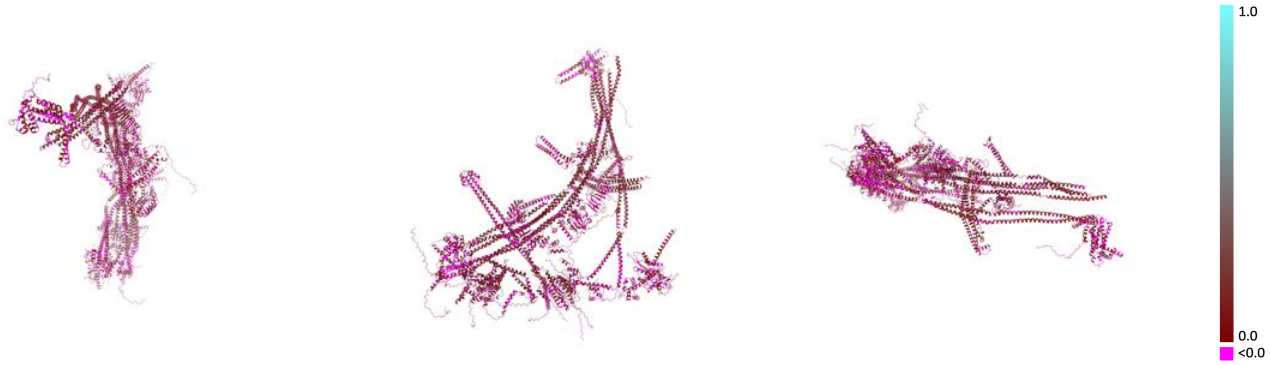
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0217 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

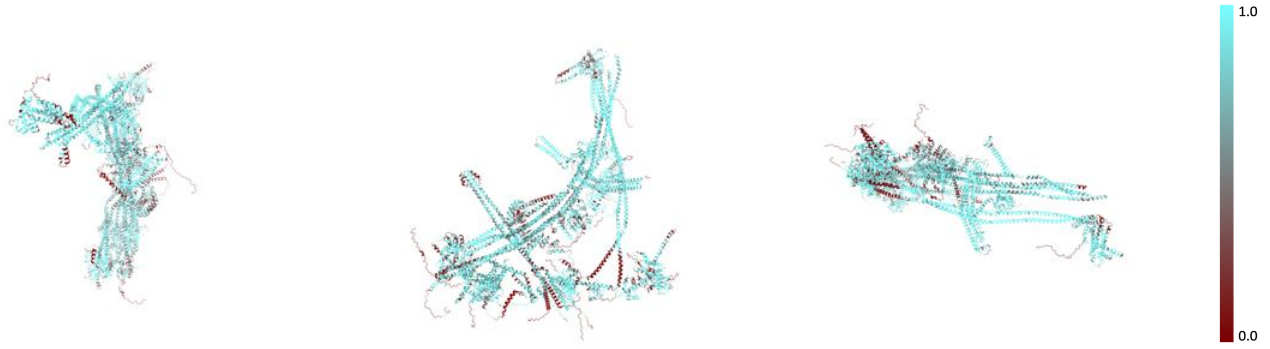
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

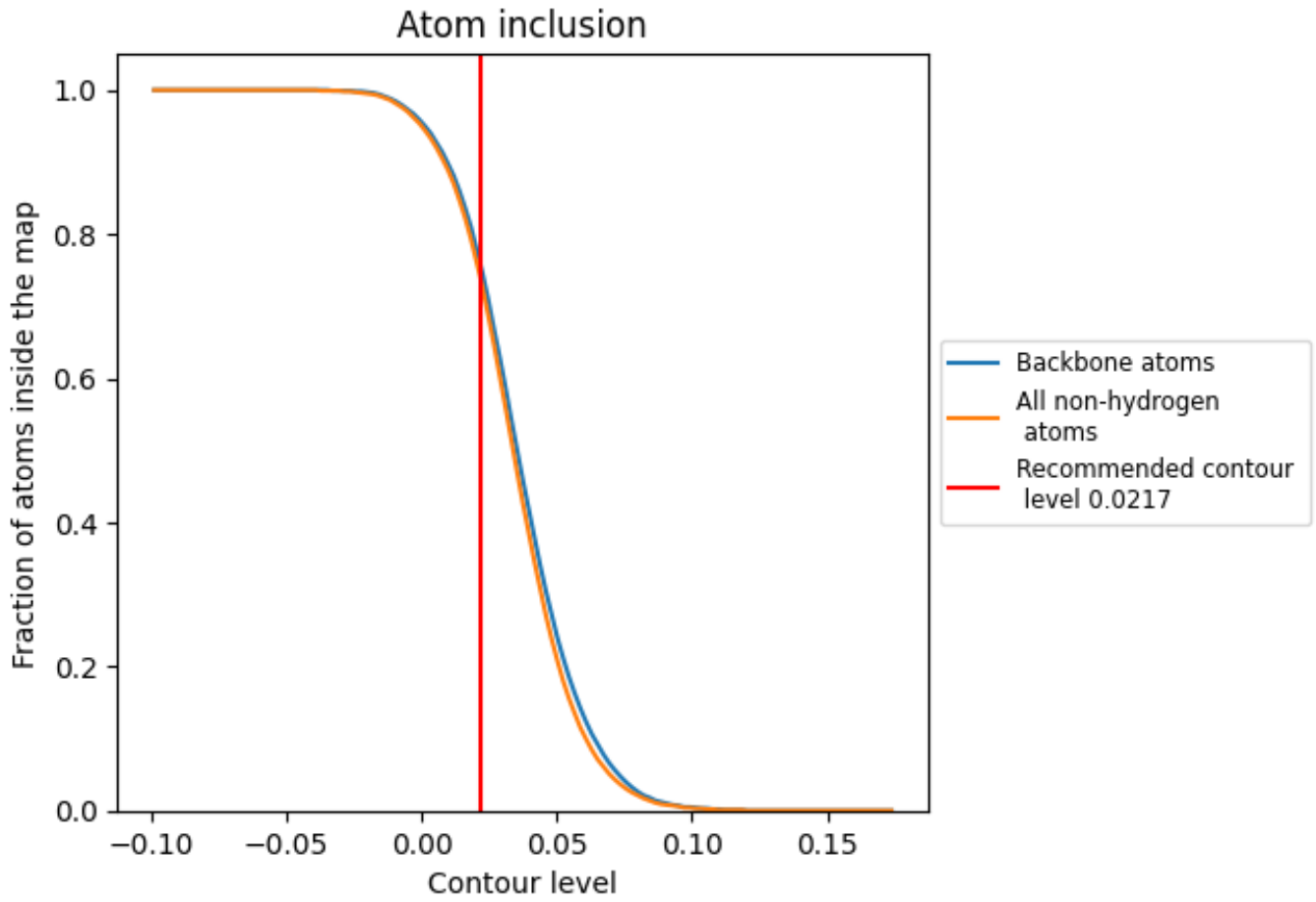
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0217).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.0217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.0870
A	0.8020	0.1410
B	0.6920	0.1080
C	0.8960	0.1310
D	0.7720	0.1100
E	0.7300	0.0830
F	0.5790	0.0990
G	0.8340	0.0890
H	0.7290	0.0720
I	0.8710	0.0610
J	0.6900	0.0730
K	0.7400	0.0670
L	0.7820	0.0980
P	0.7140	0.0590
Q	0.6980	0.0600
R	0.7690	0.0630
S	0.5770	0.0790
i	0.7130	0.0500
s	0.4810	0.0570