



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 12:03 pm BST

PDB ID : 8OVW
EMDB ID : EMD-17224
Title : Cryo-EM structure of CBF1-CCAN bound topologically to centromeric DNA
Authors : Dendooven, T.D.; Zhang, Z.; Yang, J.; McLaughlin, S.; Schwabb, J.; Scheres, S.; Yatskevich, S.; Barford, D.
Deposited on : 2023-04-26
Resolution : 3.40 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

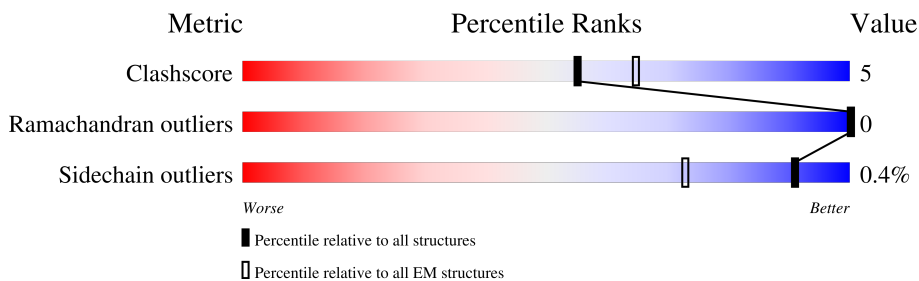
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



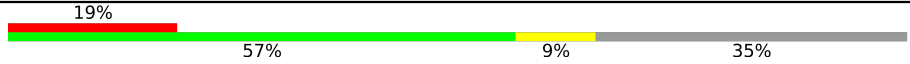
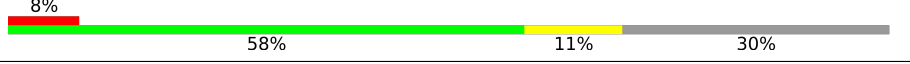


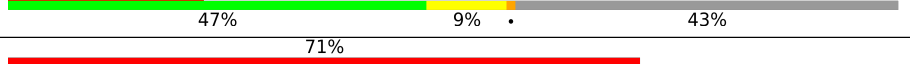
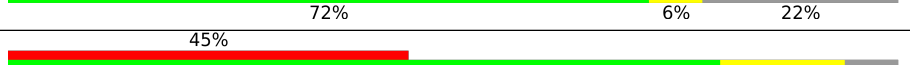

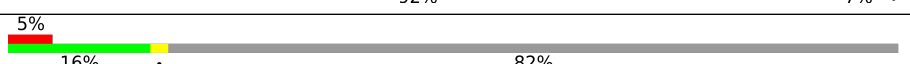

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	
2	D	153	
3	H	181	
4	I	733	
5	K	239	
6	L	245	
7	N	458	

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Mol	Chain	Length	Quality of chain
8	O	368	
9	P	369	
10	Q	406	
11	T	361	
12	U	324	
13	W	89	
14	Y	238	
15	Z	153	
16	E	153	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 28461 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 Centromere-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	101	Total	C	N	O	S	0	0
			822	507	152	161	2		
1	B	107	Total	C	N	O	S	0	0
			876	542	161	171	2		

- Molecule 2 is a DNA chain called C0N3 DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	D	27	Total	C	N	O	P	0	0
			553	262	101	163	27		

- Molecule 3 is a protein called Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	171	Total	C	N	O	S	0	0
			1412	890	247	273	2		

- Molecule 4 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	679	Total	C	N	O	S	0	0
			5496	3559	917	990	30		

- Molecule 5 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	219	Total	C	N	O	S	0	0
			1762	1113	304	340	5		

- Molecule 6 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	241	1941	1244	320	366	11	0	0

- Molecule 7 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	391	3166	2053	537	563	13	0	0

- Molecule 8 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	241	1979	1277	328	369	5	0	0

- Molecule 9 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	P	257	2116	1358	366	378	14	0	0

- Molecule 10 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Q	258	2144	1355	375	405	9	0	0

- Molecule 11 is a protein called Inner kinetochore subunit CNN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	T	92	761	488	125	144	4	0	0

- Molecule 12 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	184	1485	928	255	299	3	0	0

- Molecule 13 is a protein called Inner kinetochore subunit WIP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	W	69	551	348	96	105	2	0	0

- Molecule 14 is a protein called Inner kinetochore subunit NKP1.

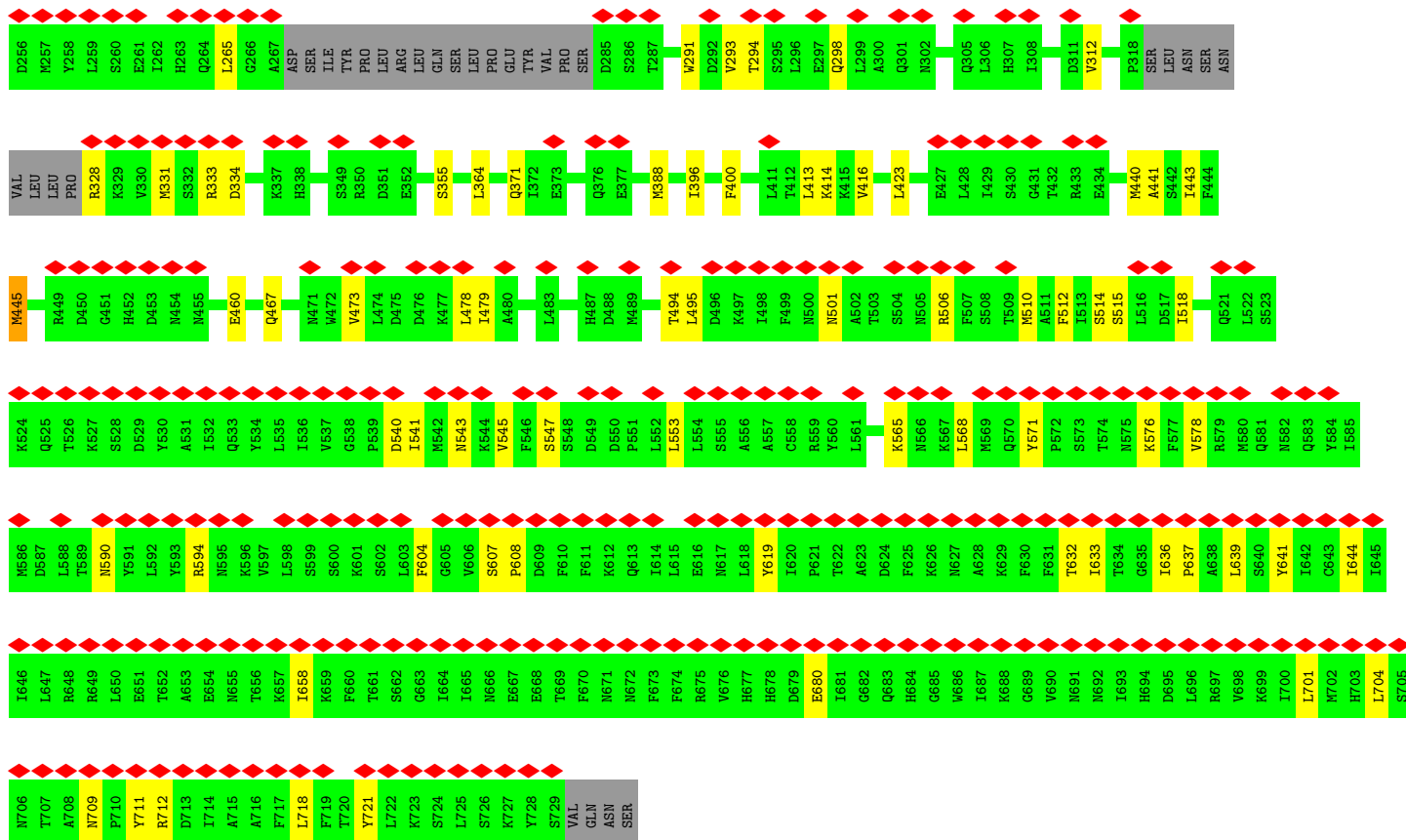
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Y	223	1663	1027	281	349	6	0	0

- Molecule 15 is a protein called Inner kinetochore subunit NKP2.

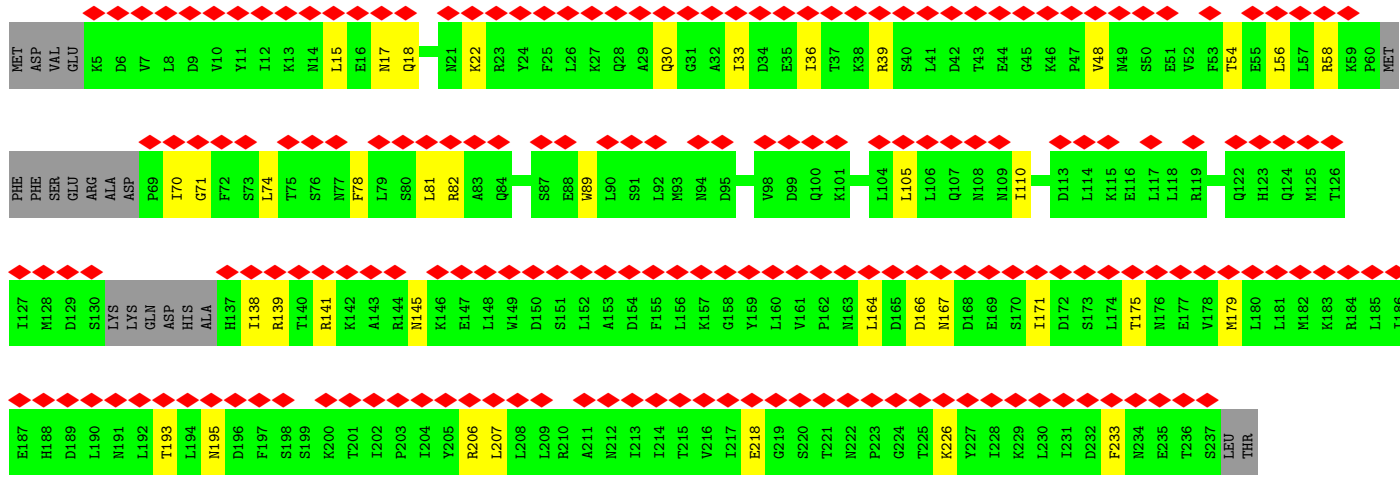
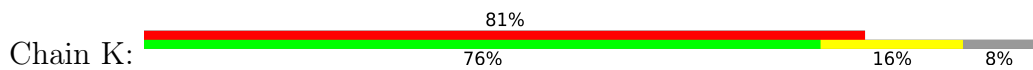
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Z	151	1180	740	204	235	1	0	0

- Molecule 16 is a DNA chain called C0N3 DNA.

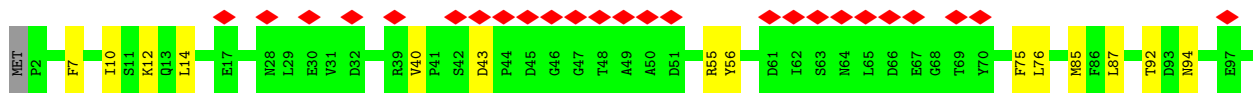
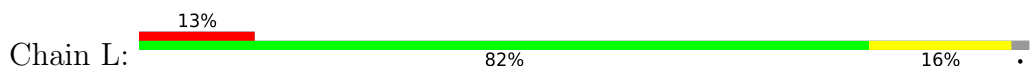
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	E	27	554	262	104	161	27	0	0



• Molecule 5: Inner kinetochore subunit MCM22

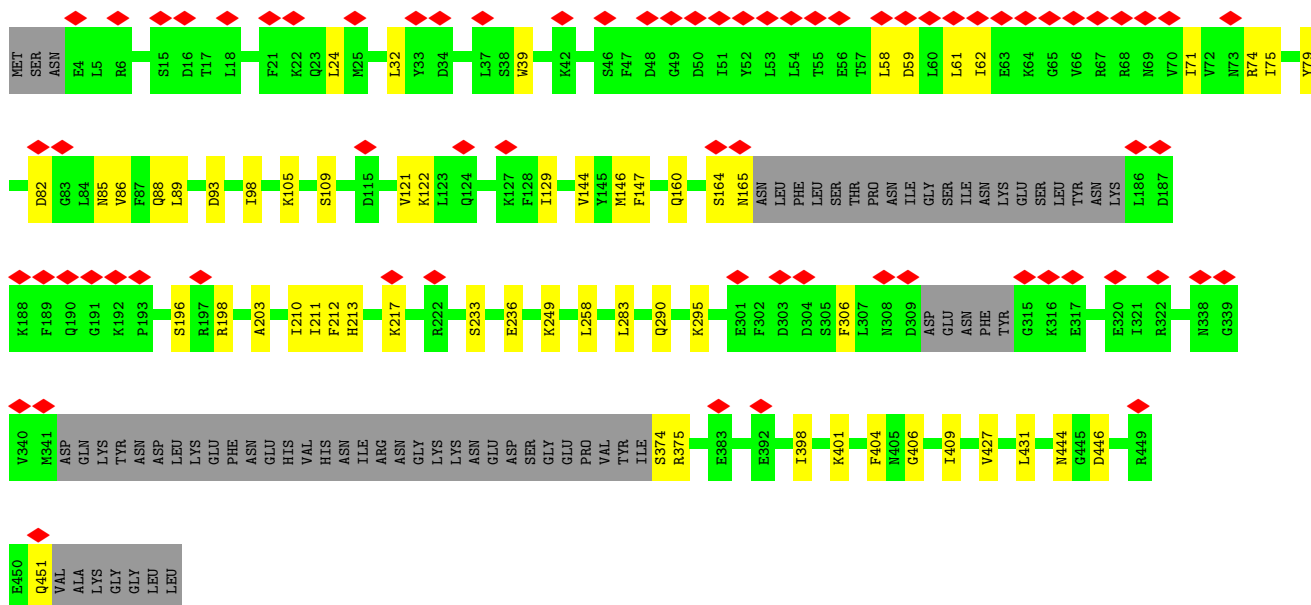
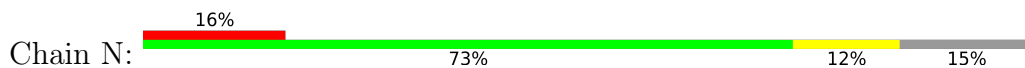


• Molecule 6: Inner kinetochore subunit IML3

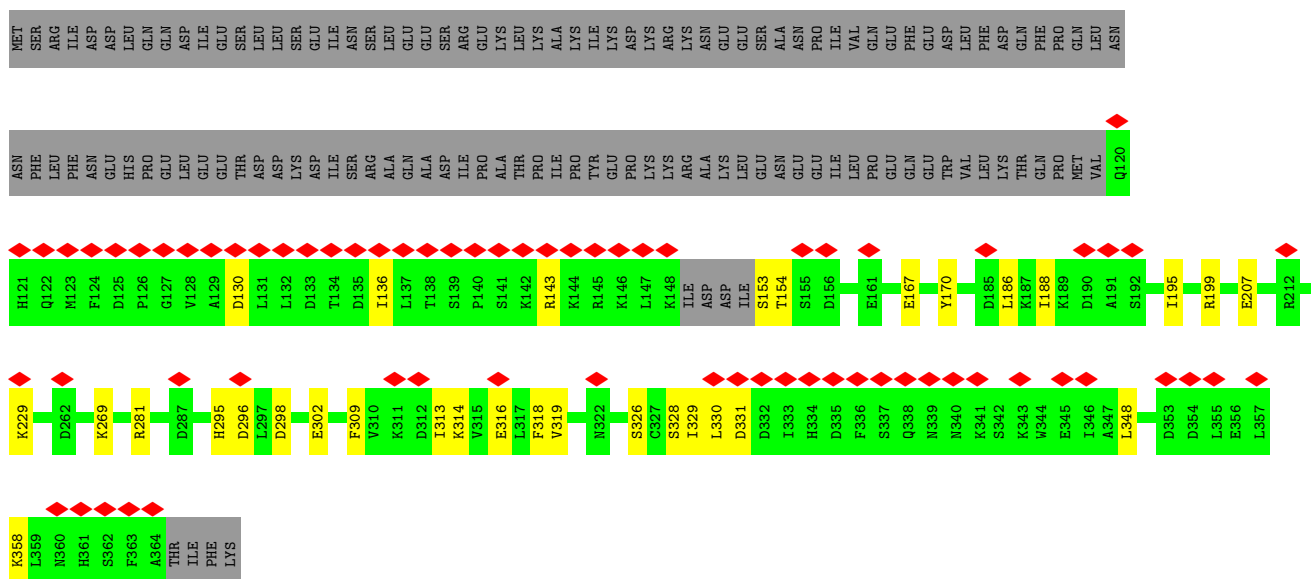




• Molecule 7: Inner kinetochore subunit CHL4

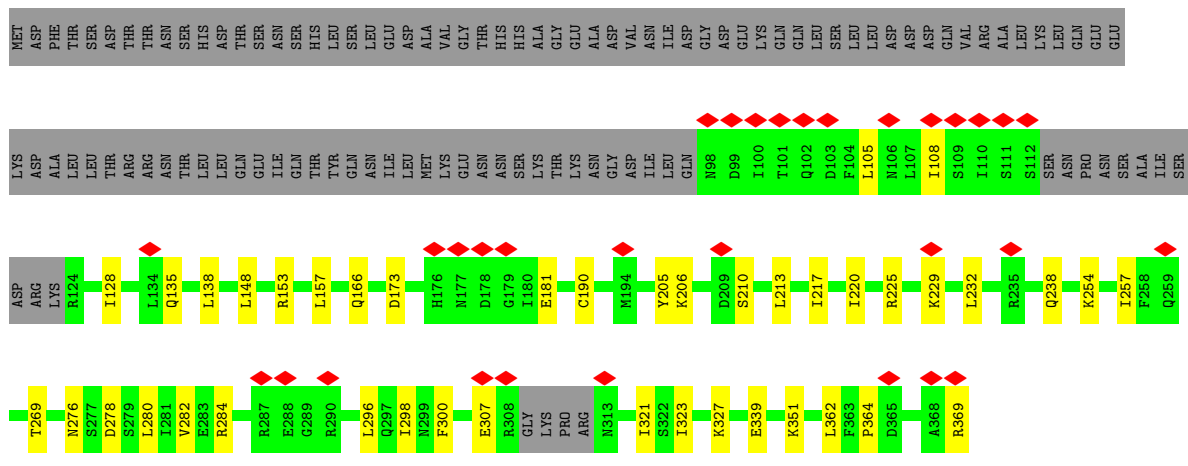


• Molecule 8: Inner kinetochore subunit MCM21

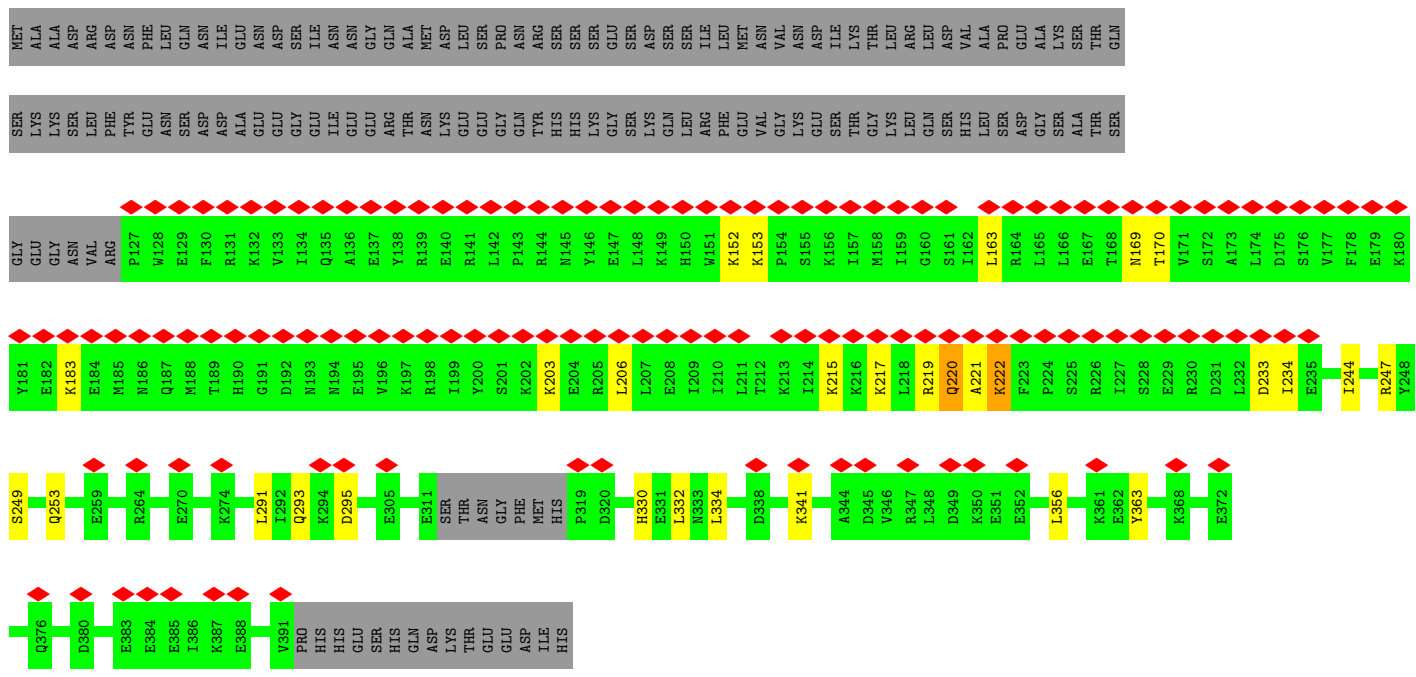


• Molecule 9: Inner kinetochore subunit CTF19





• Molecule 10: Inner kinetochore subunit OKP1



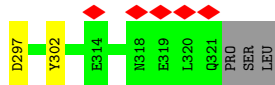
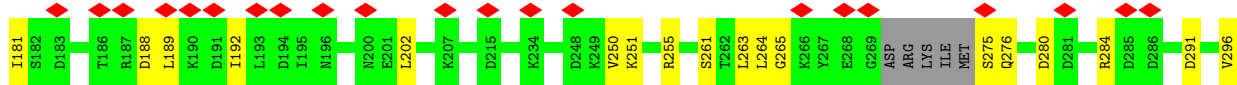
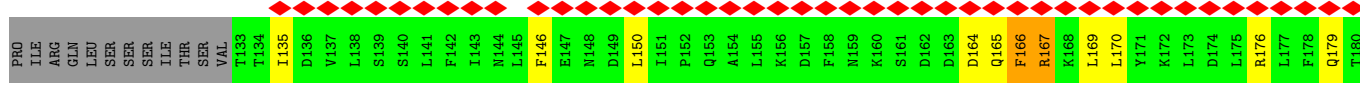
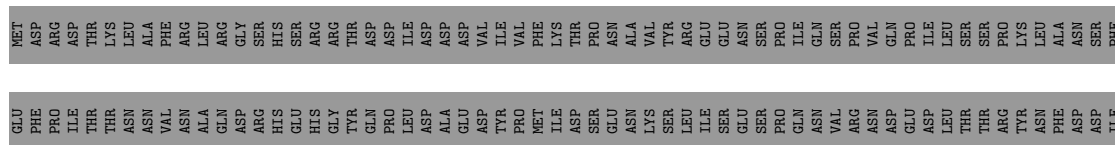
• Molecule 11: Inner kinetochore subunit CNN1



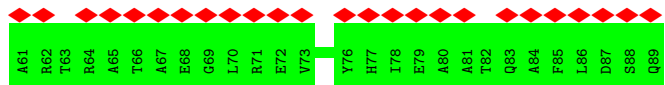
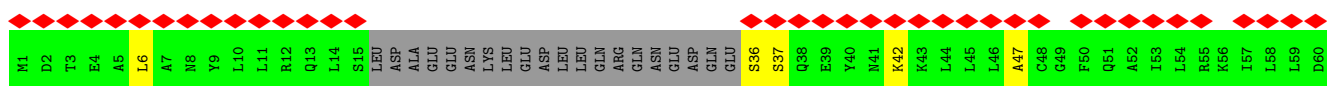


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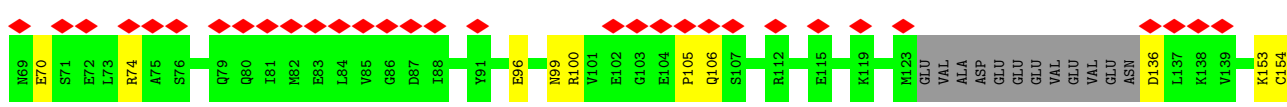
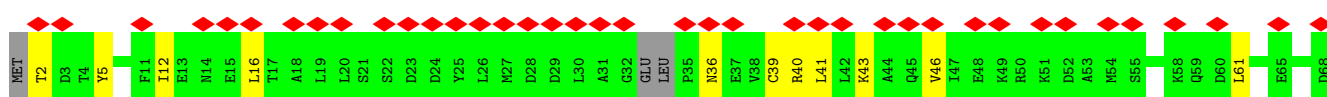
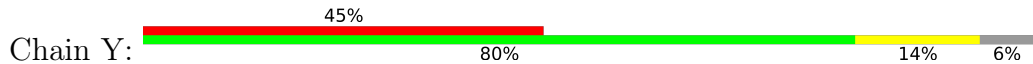
• Molecule 12: Inner kinetochore subunit AME1

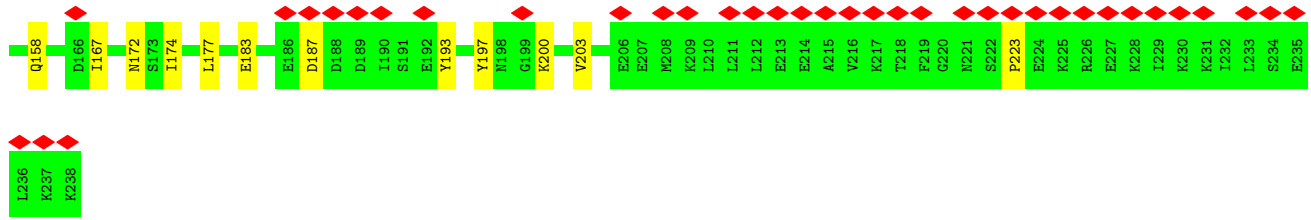


• Molecule 13: Inner kinetochore subunit WIP1

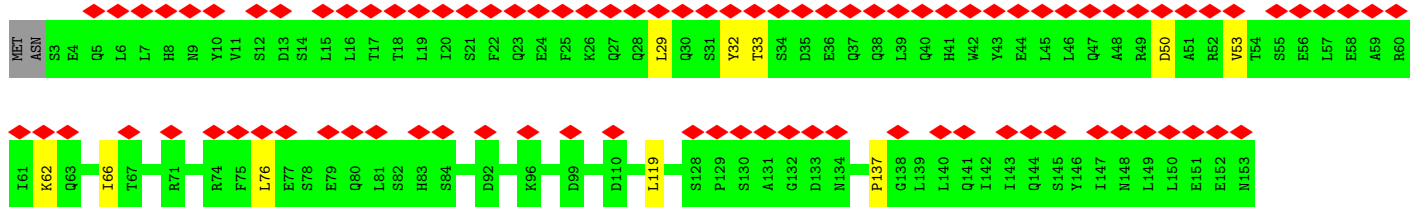
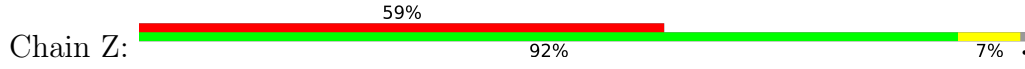


• Molecule 14: Inner kinetochore subunit NKP1

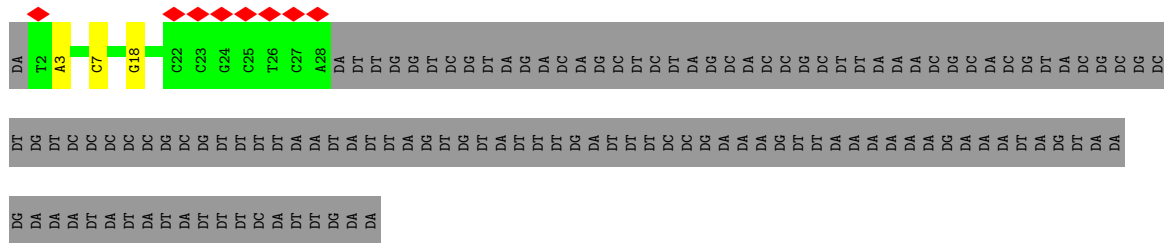




• Molecule 15: Inner kinetochore subunit NKP2



• Molecule 16: C0N3 DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0354	Depositor
Map size (Å)	327.88, 327.88, 327.88	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.171, 1.171, 1.171	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/828	0.41	0/1108
1	B	0.26	0/884	0.42	0/1182
2	D	0.51	0/619	0.90	0/953
3	H	0.26	0/1429	0.57	2/1923 (0.1%)
4	I	0.26	0/5620	0.48	2/7623 (0.0%)
5	K	0.26	0/1784	0.50	1/2404 (0.0%)
6	L	0.27	0/1981	0.52	0/2684
7	N	0.28	0/3239	0.51	1/4372 (0.0%)
8	O	0.27	0/2017	0.47	0/2713
9	P	0.27	0/2149	0.47	0/2888
10	Q	0.26	0/2175	0.46	0/2913
11	T	0.26	0/772	0.51	0/1040
12	U	0.30	0/1499	0.57	1/2018 (0.0%)
13	W	0.26	0/557	0.45	0/748
14	Y	0.27	0/1672	0.55	1/2252 (0.0%)
15	Z	0.25	0/1195	0.46	1/1616 (0.1%)
16	E	0.51	0/621	0.86	0/956
All	All	0.28	0/29041	0.52	9/39393 (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
4	I	0	3
9	P	0	1
10	Q	0	1
12	U	0	1
14	Y	0	1
All	All	0	7

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	I	478	LEU	CA-CB-CG	5.99	129.08	115.30
3	H	68	LEU	CA-CB-CG	5.89	128.86	115.30
3	H	114	LEU	CA-CB-CG	5.88	128.84	115.30
14	Y	223	PRO	N-CA-CB	5.62	110.05	103.30
15	Z	137	PRO	N-CA-CB	5.60	110.02	103.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	201	SER	Peptide
4	I	202	SER	Peptide
4	I	241	ALA	Peptide
9	P	307	GLU	Peptide
10	Q	219	ARG	Mainchain

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	822	0	845	7	0
1	B	876	0	896	10	0
2	D	553	0	304	1	0
3	H	1412	0	1451	36	0
4	I	5496	0	5615	83	0
5	K	1762	0	1796	33	0
6	L	1941	0	1946	28	0
7	N	3166	0	3220	40	0
8	O	1979	0	1995	24	0
9	P	2116	0	2189	30	0
10	Q	2144	0	2195	22	0
11	T	761	0	781	16	0
12	U	1485	0	1467	27	0
13	W	551	0	559	3	0
14	Y	1663	0	1588	25	0
15	Z	1180	0	1108	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	E	554	0	303	3	0
All	All	28461	0	28258	301	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 5.

The worst 5 of 301 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)
3:H:121:ARG:HH22	5:K:110:ILE:HG23	1.46	0.81
7:N:61:LEU:HD11	7:N:74:ARG:NH1	2.03	0.73
4:I:510:MET:HE2	5:K:89:TRP:CZ2	2.24	0.72
4:I:150:THR:HG21	4:I:186:SER:HB2	1.75	0.69
10:Q:341:LYS:HB2	14:Y:158:GLN:HE22	1.57	0.69

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	99/351 (28%)	98 (99%)	1 (1%)	0	100	100
1	B	105/351 (30%)	104 (99%)	1 (1%)	0	100	100
3	H	167/181 (92%)	163 (98%)	4 (2%)	0	100	100
4	I	669/733 (91%)	642 (96%)	27 (4%)	0	100	100
5	K	213/239 (89%)	211 (99%)	2 (1%)	0	100	100
6	L	239/245 (98%)	234 (98%)	5 (2%)	0	100	100
7	N	383/458 (84%)	368 (96%)	15 (4%)	0	100	100
8	O	237/368 (64%)	224 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	P	251/369 (68%)	239 (95%)	12 (5%)	0	100	100
10	Q	254/406 (63%)	252 (99%)	2 (1%)	0	100	100
11	T	90/361 (25%)	87 (97%)	3 (3%)	0	100	100
12	U	180/324 (56%)	173 (96%)	7 (4%)	0	100	100
13	W	65/89 (73%)	65 (100%)	0	0	100	100
14	Y	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
15	Z	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
All	All	3318/4866 (68%)	3214 (97%)	104 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	89/305 (29%)	89 (100%)	0	100	100
1	B	94/305 (31%)	94 (100%)	0	100	100
3	H	162/172 (94%)	162 (100%)	0	100	100
4	I	631/683 (92%)	630 (100%)	1 (0%)	93	98
5	K	202/223 (91%)	200 (99%)	2 (1%)	76	88
6	L	217/221 (98%)	217 (100%)	0	100	100
7	N	353/416 (85%)	352 (100%)	1 (0%)	92	97
8	O	226/347 (65%)	226 (100%)	0	100	100
9	P	241/344 (70%)	241 (100%)	0	100	100
10	Q	242/378 (64%)	239 (99%)	3 (1%)	71	85
11	T	89/339 (26%)	89 (100%)	0	100	100
12	U	168/308 (54%)	164 (98%)	4 (2%)	49	74
13	W	57/76 (75%)	57 (100%)	0	100	100
14	Y	175/219 (80%)	174 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	Z	121/143 (85%)	121 (100%)	0	100	100
All	All	3067/4479 (68%)	3055 (100%)	12 (0%)	91	95

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	U	164	ASP
12	U	165	GLN
14	Y	172	ASN
12	U	166	PHE
7	N	198	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
10	Q	220	GLN
12	U	165	GLN
5	K	18	GLN
6	L	78	ASN
9	P	166	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

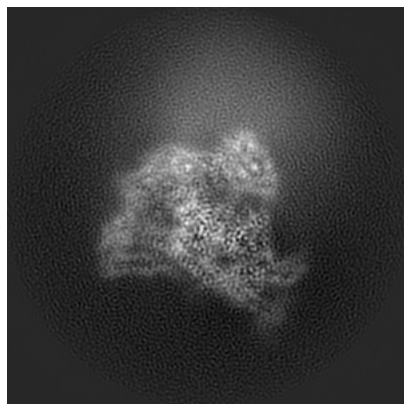
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17224. These allow visual inspection of the internal detail of the map and identification of artifacts.

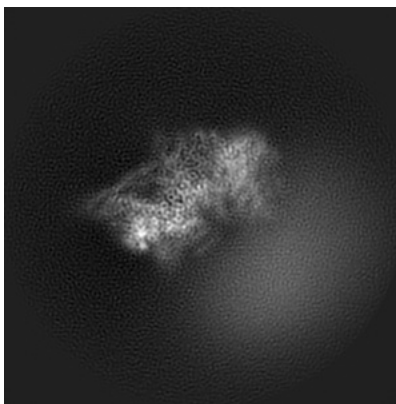
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

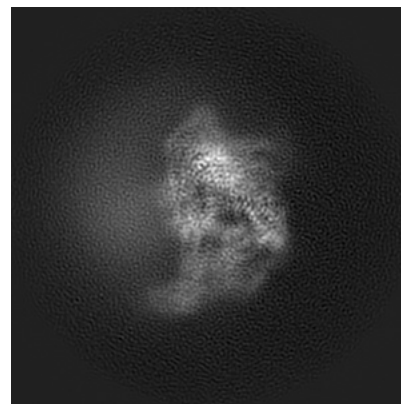
6.1.1 Primary map



X

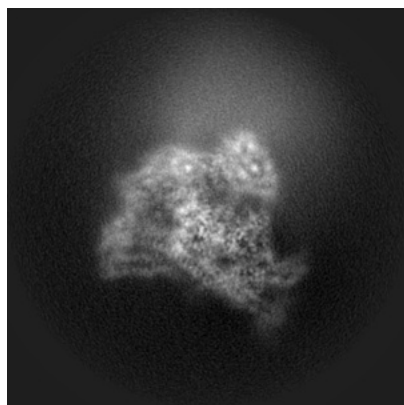


Y

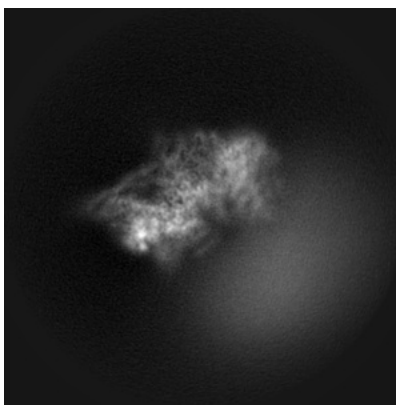


Z

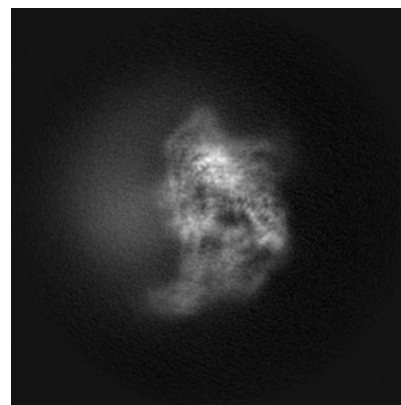
6.1.2 Raw map



X



Y

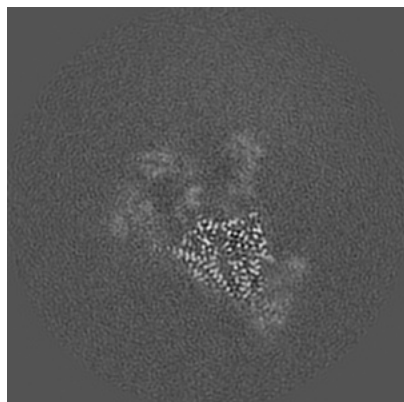


Z

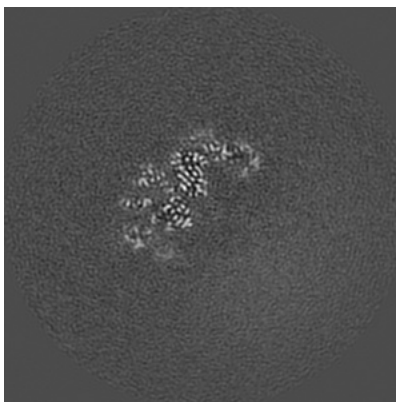
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

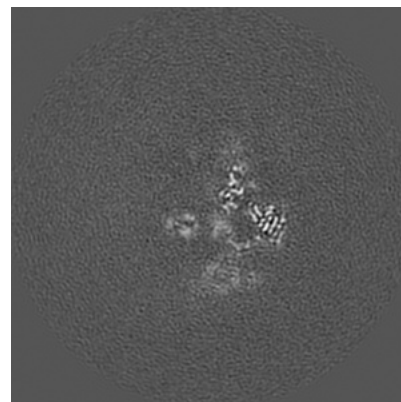
6.2.1 Primary map



X Index: 140

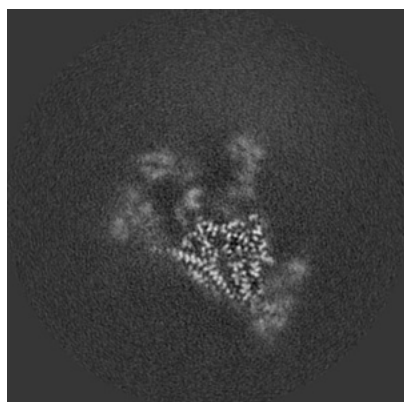


Y Index: 140

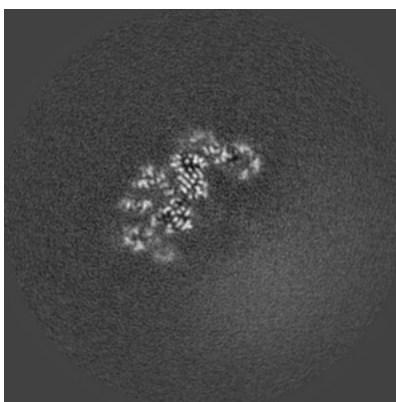


Z Index: 140

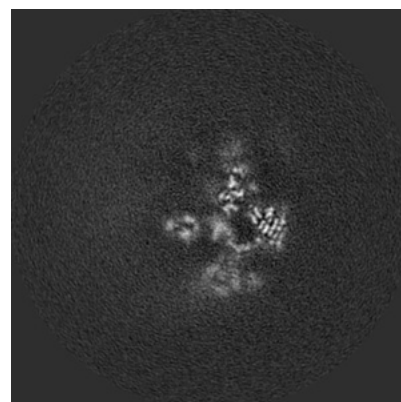
6.2.2 Raw map



X Index: 140



Y Index: 140

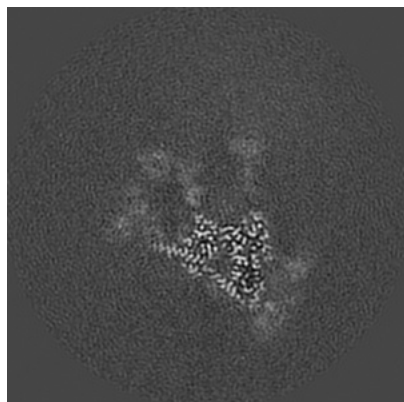


Z Index: 140

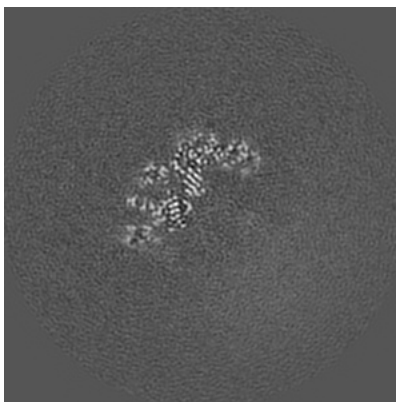
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

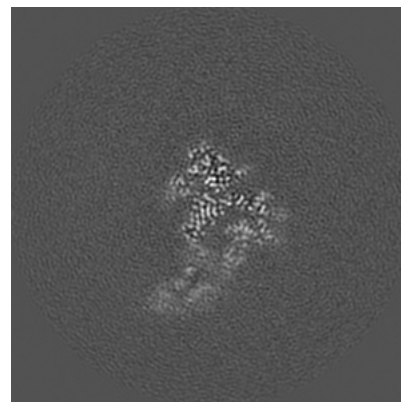
6.3.1 Primary map



X Index: 138

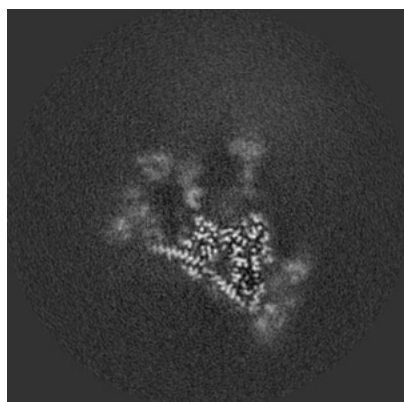


Y Index: 138

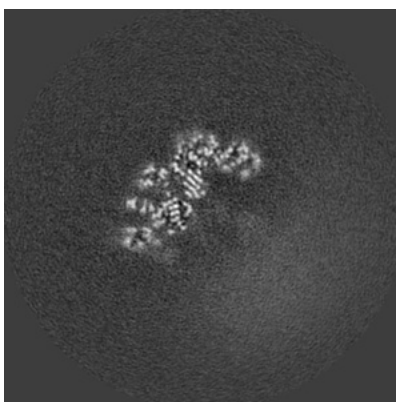


Z Index: 121

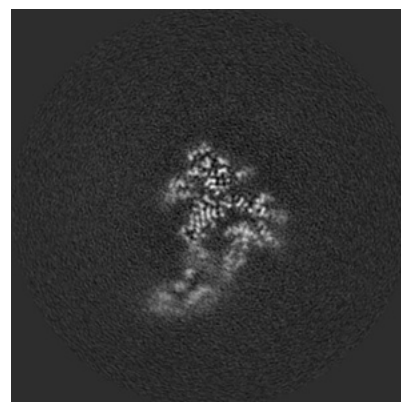
6.3.2 Raw map



X Index: 138



Y Index: 138

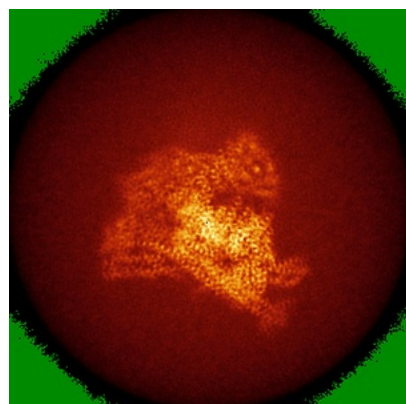


Z Index: 121

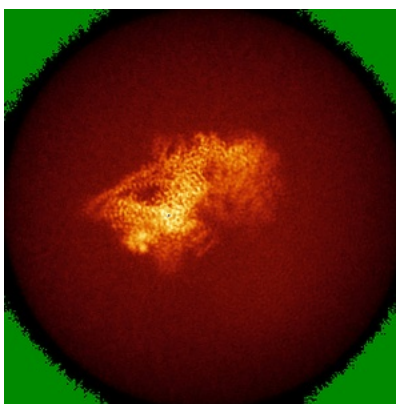
The images above show the largest variance slices of the map in three orthogonal directions.

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

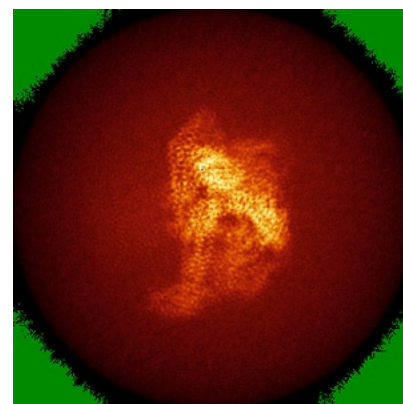
6.4.1 Primary map



X

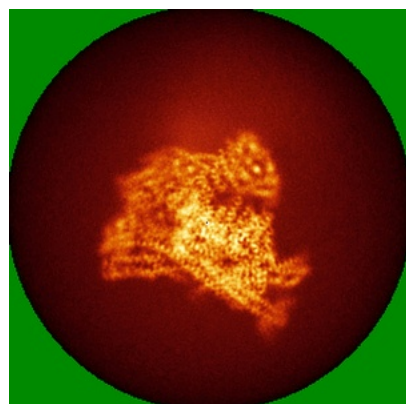


Y

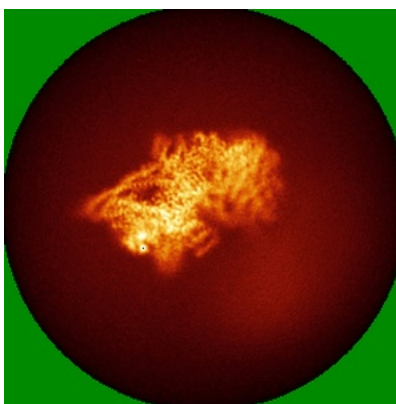


Z

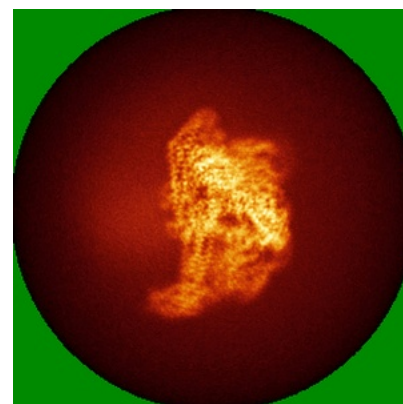
6.4.2 Raw map



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 0.0354. 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.

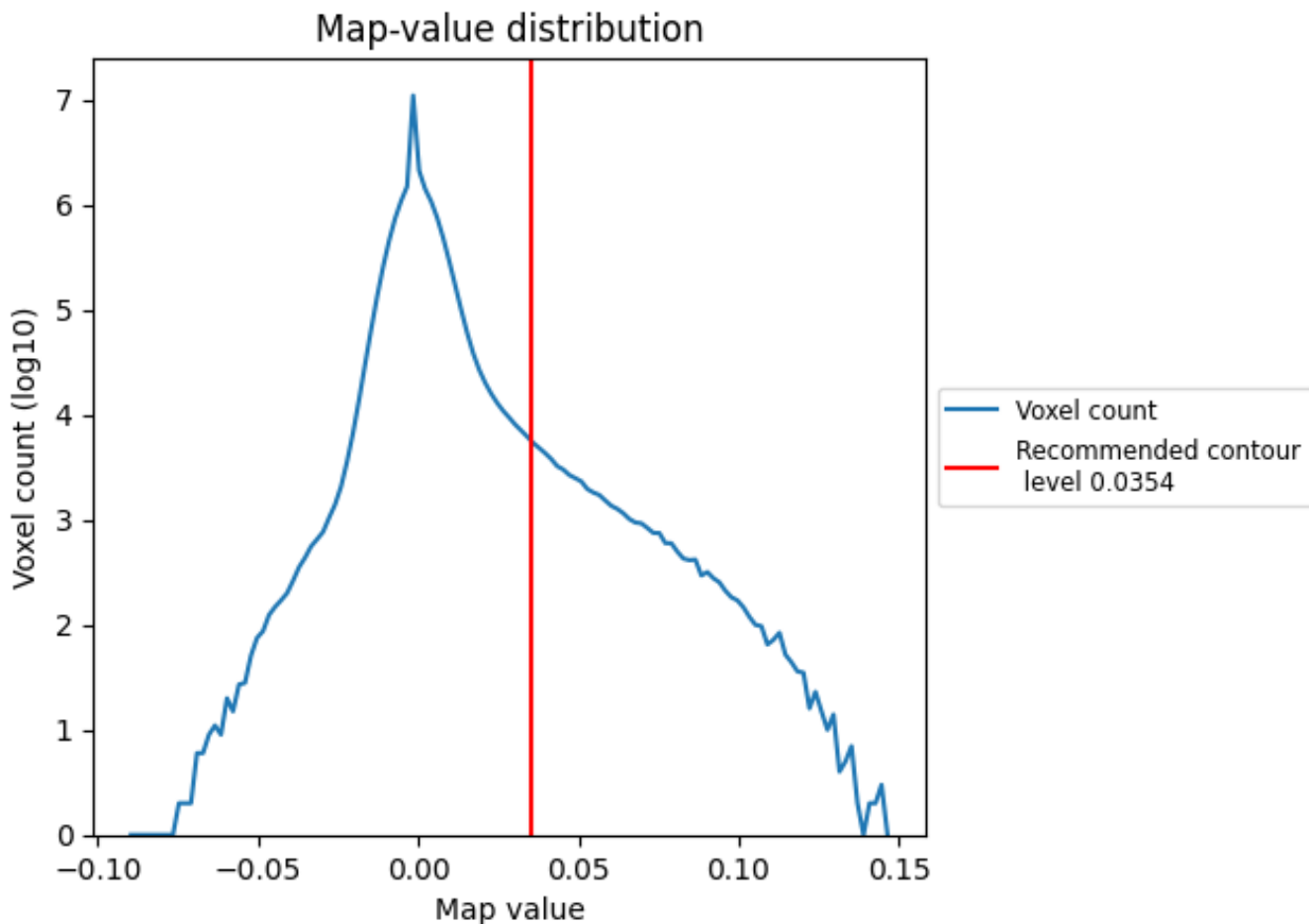
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

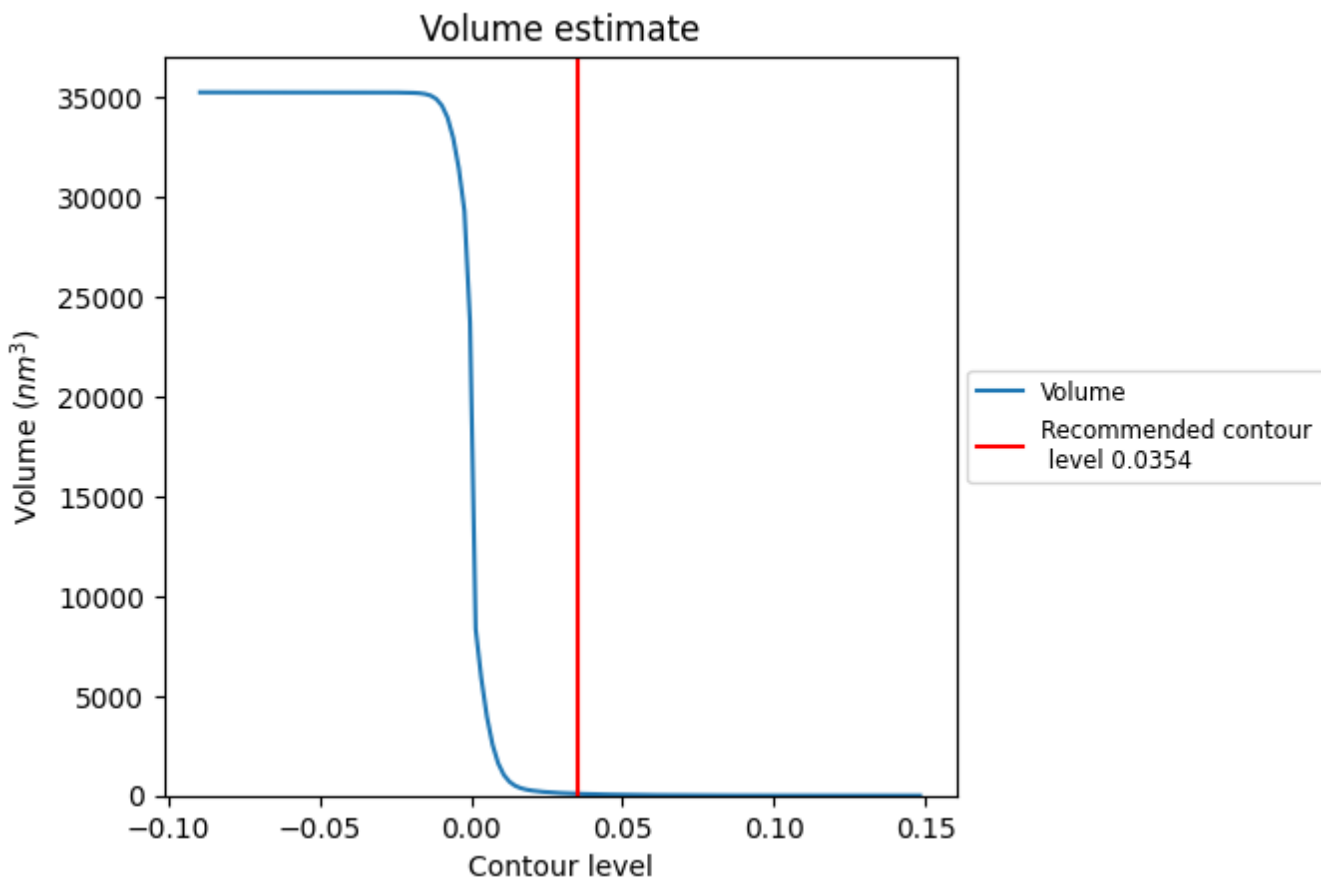
This section contains the results of statistical analysis of the map.

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.

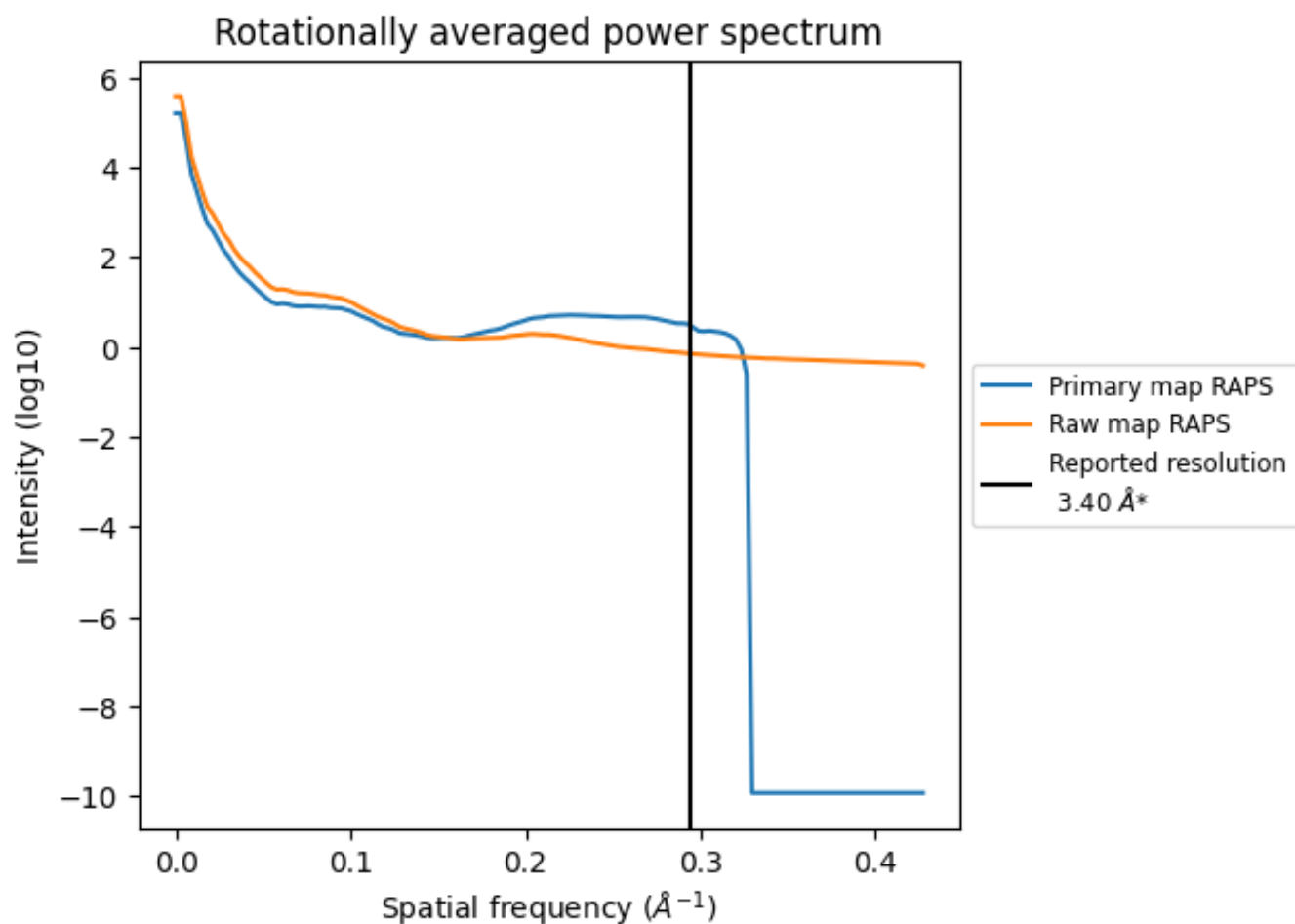
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 80 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](#)

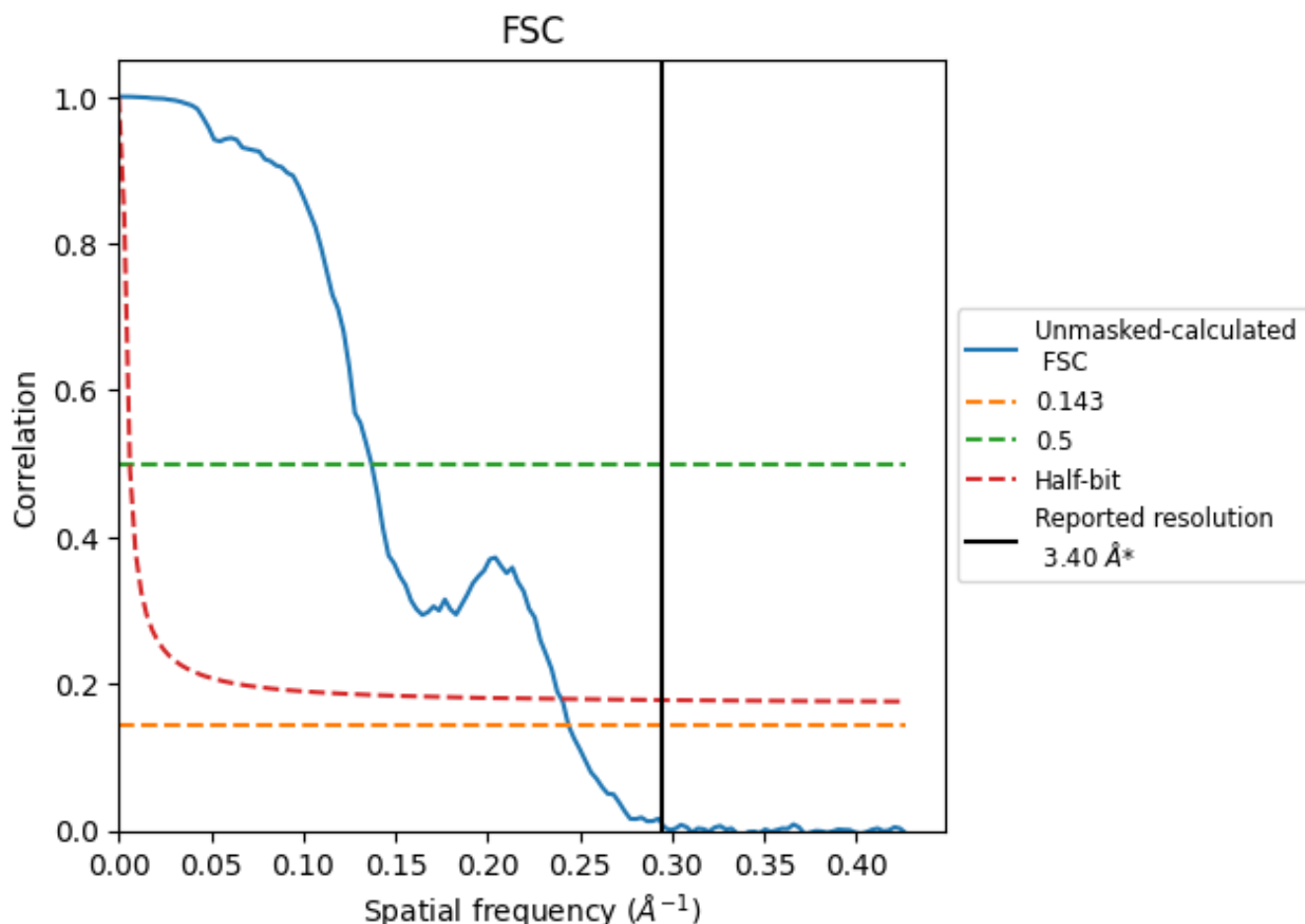


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

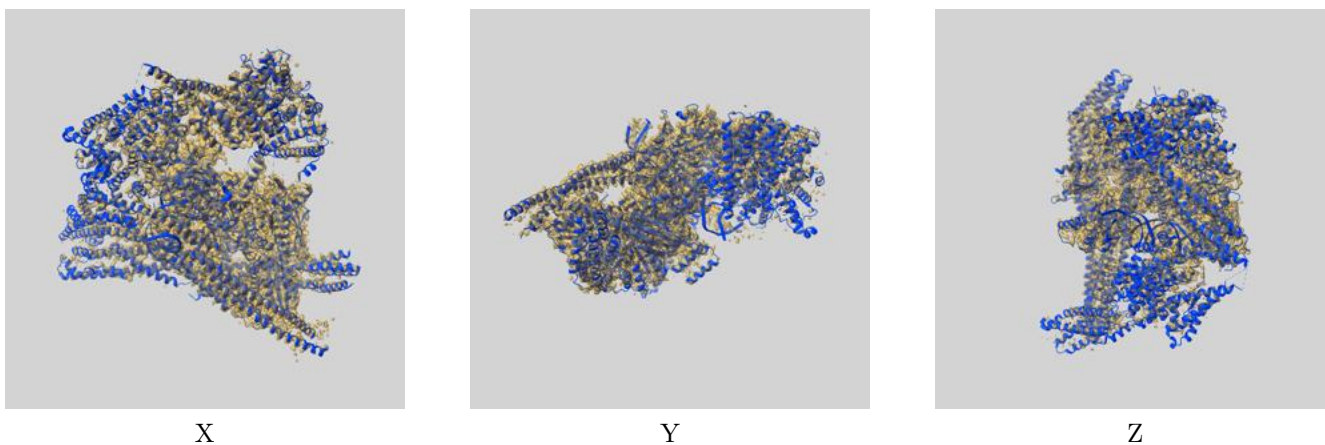
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	7.29	4.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.10 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

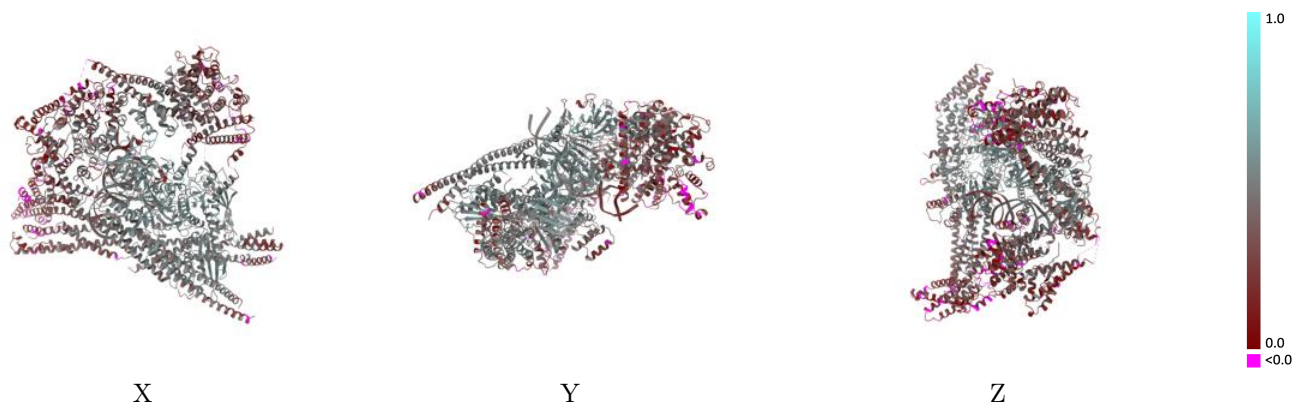
This section contains information regarding the fit between EMDB map EMD-17224 and PDB model 8OVW. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



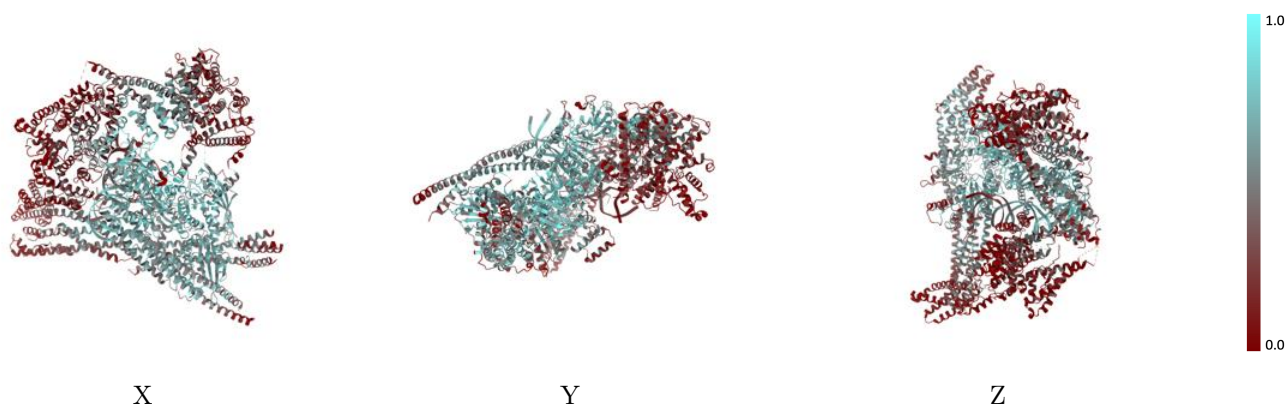
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



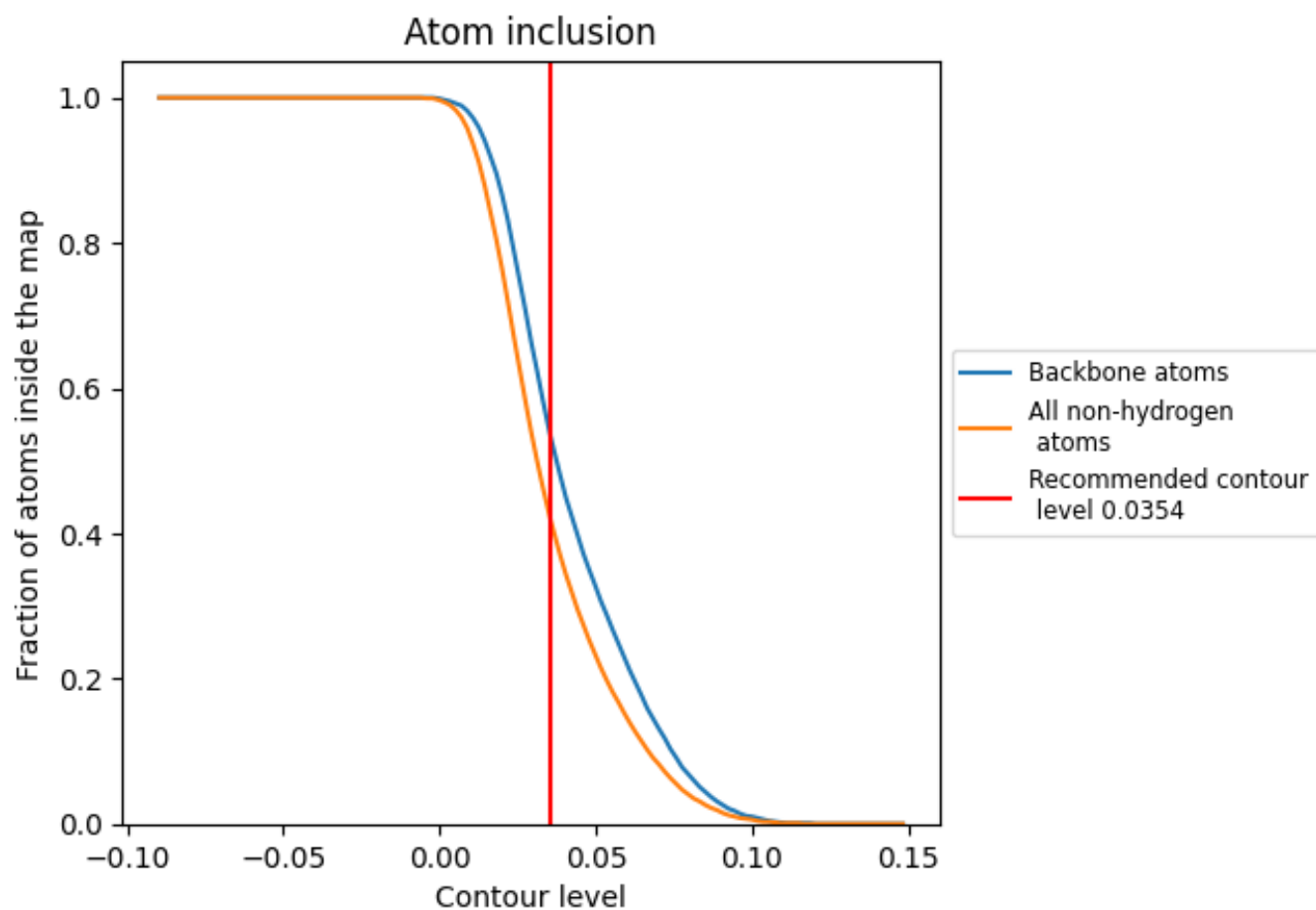
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0354).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 42% 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 (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4210	 0.3860
A	 0.5090	 0.4540
B	 0.5130	 0.4450
D	 0.5480	 0.3860
E	 0.5450	 0.3950
H	 0.2280	 0.3100
I	 0.2900	 0.3150
K	 0.1750	 0.2700
L	 0.6430	 0.4990
N	 0.6130	 0.4910
O	 0.5440	 0.4580
P	 0.6340	 0.4960
Q	 0.3620	 0.3260
T	 0.1430	 0.3370
U	 0.4390	 0.3690
W	 0.1730	 0.3330
Y	 0.3990	 0.3630
Z	 0.3340	 0.3280

