



wwPDB EM Validation Summary Report ⓘ

Dec 15, 2022 – 12:19 PM JST

PDB ID : 7XHO
EMDB ID : EMD-33197
Title : Structure of human inner kinetochore CCAN complex
Authors : Tian, T.; Wang, C.L.; Yang, Z.S.; Sun, L.F.; Zang, J.Y.
Deposited on : 2022-04-09
Resolution : 3.29 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.dev43
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) : 2.31.3

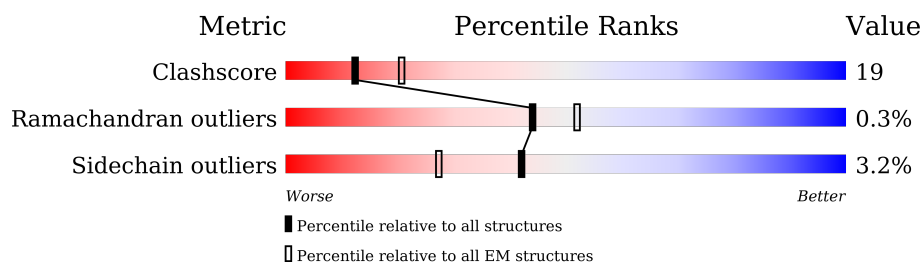
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 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.





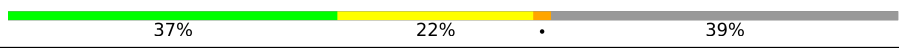
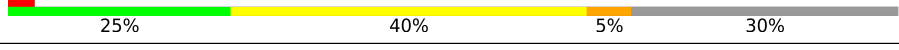



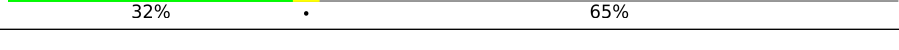
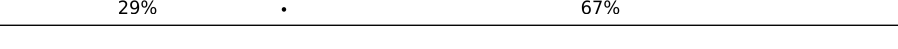
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	943	
1	c	943	
2	H	247	
3	I	756	
4	K	269	
5	L	344	
6	M	180	
7	N	339	

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Mol	Chain	Length	Quality of chain
8	O	300	
9	P	288	
10	Q	268	
11	S	138	
12	T	561	
13	W	88	
14	X	81	
15	R	177	
16	U	418	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 22243 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 protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	5	Total	C	N	O	0	0
			40	28	5	7		
1	c	13	Total	C	N	O	0	0
			105	69	17	19		

- Molecule 2 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	195	Total	C	N	O	S	0	0
			1560	980	273	299	8		

- Molecule 3 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	517	Total	C	N	O	S	0	0
			4111	2700	661	724	26		

- Molecule 4 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	230	Total	C	N	O	S	0	0
			1869	1183	312	364	10		

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	302	Total	C	N	O	S	0	0
			2422	1576	395	437	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	116	ASP	ASN	engineered mutation	UNP Q8N0S6

- Molecule 6 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	168	Total	C	N	O	S	0	0
			1298	825	232	234	7		

- Molecule 7 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	305	Total	C	N	O	S	0	0
			2492	1600	434	448	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	84	ASP	GLU	variant	UNP Q96H22

- Molecule 8 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	206	Total	C	N	O	S	0	0
			1588	1017	269	294	8		

- Molecule 9 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	224	Total	C	N	O	S	0	0
			1808	1144	311	344	9		

- Molecule 10 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	164	Total	C	N	O	S	0	0
			1175	718	207	242	8		

- Molecule 11 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	97	Total	C	N	O	S	0	0
			790	494	141	150	5		

- Molecule 12 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	99	Total	C	N	O	S	0	0
			804	516	139	142	7		

- Molecule 13 is a protein called CENP-W.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	75	Total	C	N	O	S	0	0
			584	367	119	95	3		

- Molecule 14 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	74	Total	C	N	O	S	0	0
			590	378	104	107	1		

- Molecule 15 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	62	Total	C	N	O	0	0
			308	184	62	62		

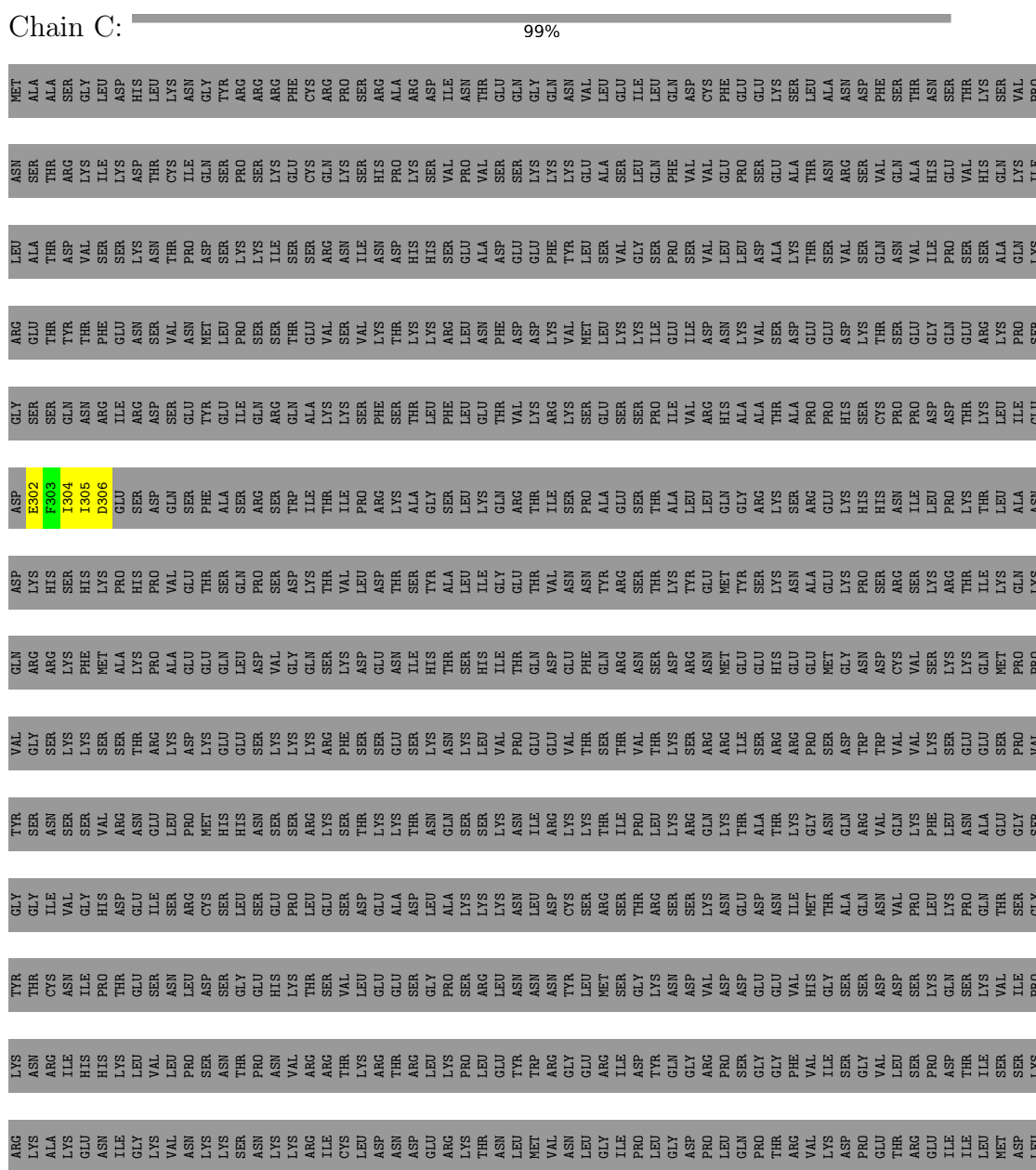
- Molecule 16 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	U	140	Total	C	N	O	0	0
			699	419	140	140		

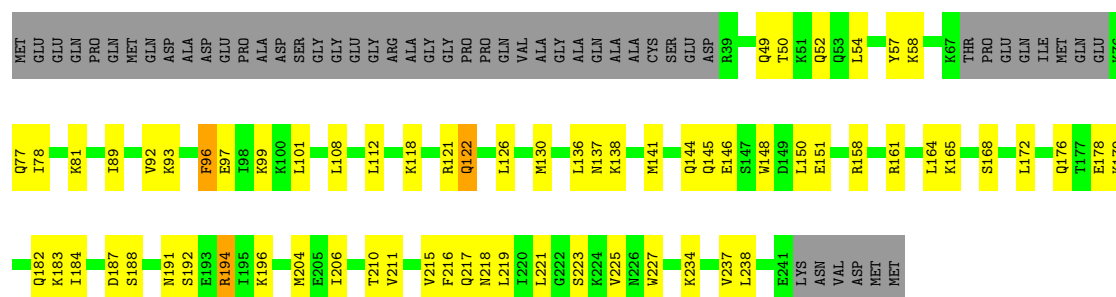
3 Residue-property plots

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: Centromere protein C

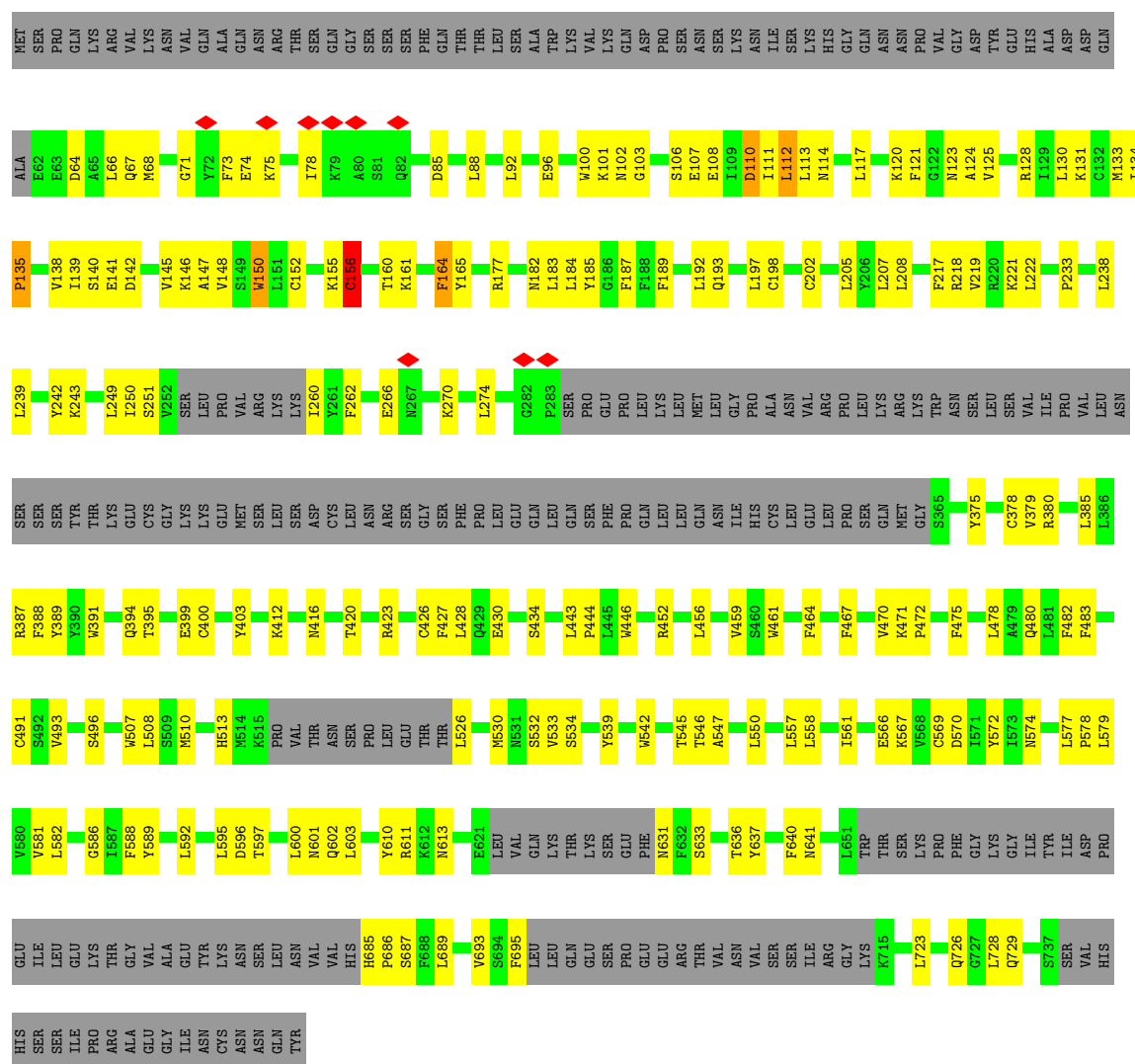


Chain H: 



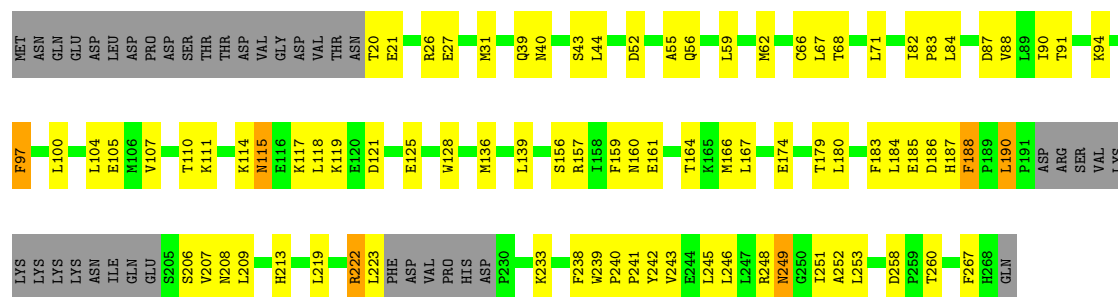
• Molecule 3: Centromere protein I

Chain I: 



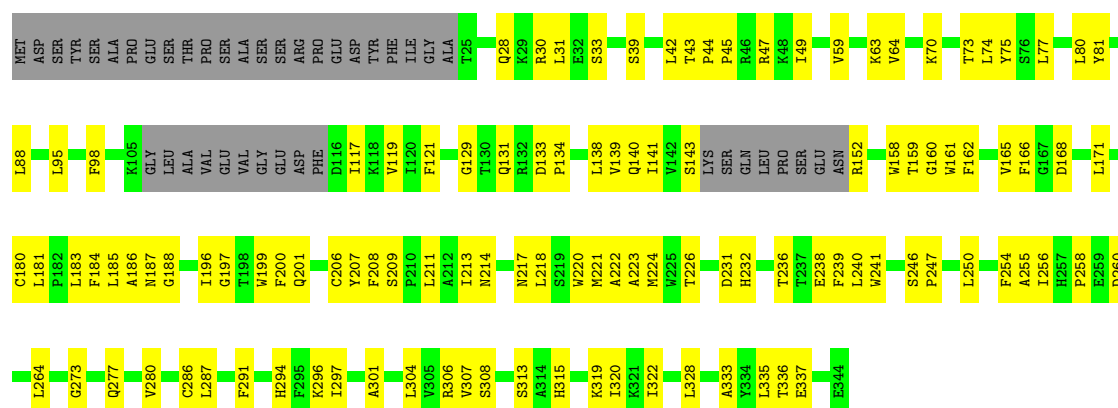
• Molecule 4: Centromere protein K

Chain K: 



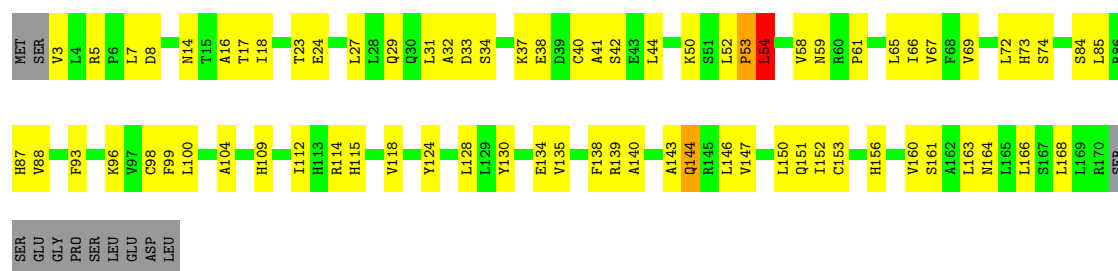
• Molecule 5: Centromere protein L

Chain L: 55% 33% 12%



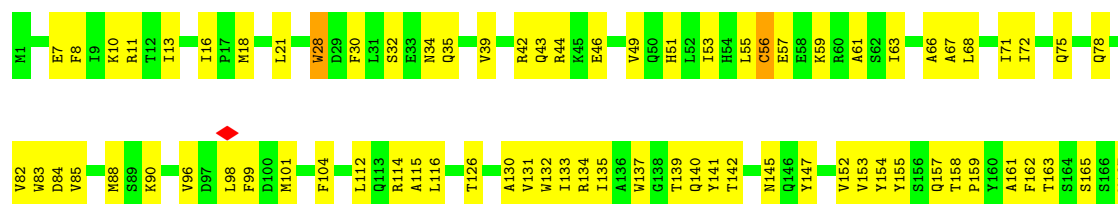
• Molecule 6: Centromere protein M

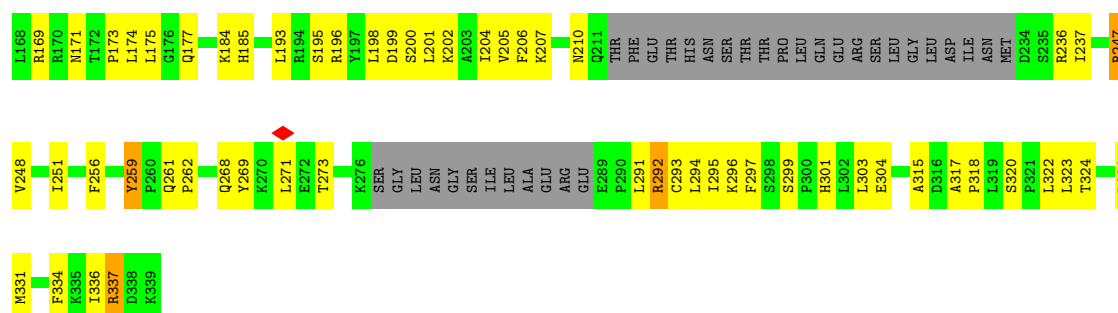
Chain M: 52% 39% 7%



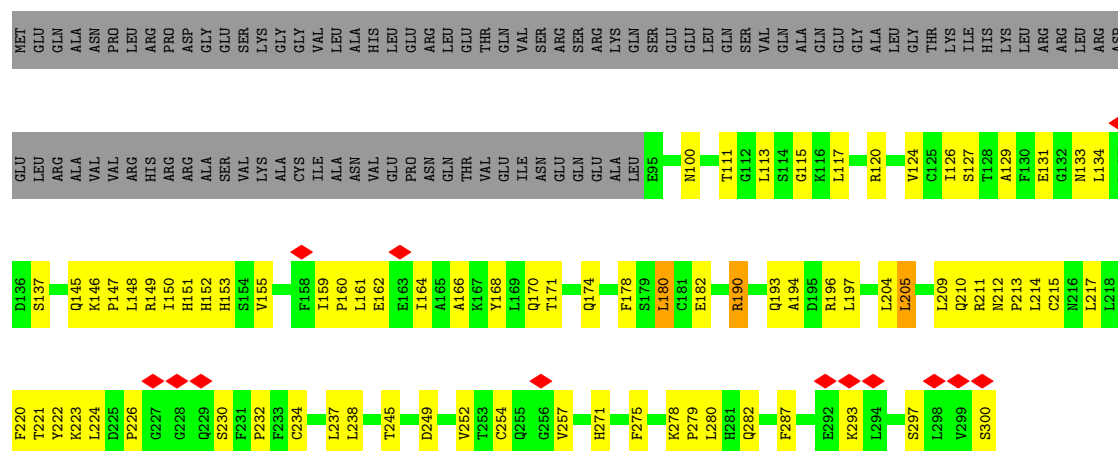
• Molecule 7: Centromere protein N

Chain N: 51% 37% 10%

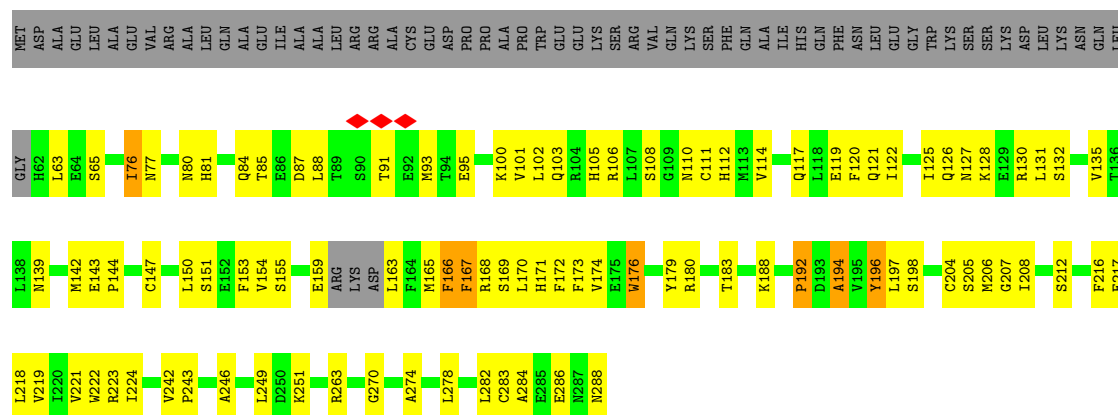




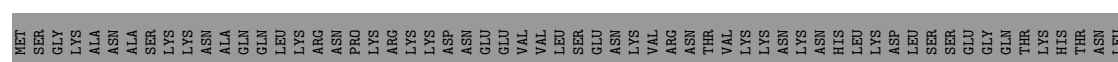
• Molecule 8: Centromere protein O



• Molecule 9: Centromere protein P



• Molecule 10: Centromere protein Q



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.448	Depositor
Minimum map value	-2.649	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	380.64, 380.64, 380.64	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.22, 1.22, 1.22	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	C	0.26	0/40	0.61	0/53
1	c	0.28	0/106	0.88	0/141
2	H	0.24	0/1566	0.50	0/2093
3	I	0.26	0/4210	0.49	1/5704 (0.0%)
4	K	0.25	0/1897	0.57	0/2558
5	L	0.26	0/2487	0.50	0/3379
6	M	0.27	0/1320	0.53	0/1791
7	N	0.27	0/2546	0.56	0/3439
8	O	0.27	0/1624	0.57	0/2208
9	P	0.28	0/1839	0.61	1/2474 (0.0%)
10	Q	0.26	0/1175	0.69	2/1580 (0.1%)
11	S	0.27	0/799	0.63	0/1070
12	T	0.28	0/821	0.63	0/1105
13	W	0.27	0/590	0.60	0/785
14	X	0.26	0/596	0.60	0/801
15	R	0.25	0/306	0.36	0/424
16	U	0.24	0/697	0.46	3/972 (0.3%)
All	All	0.26	0/22619	0.55	7/30577 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	194	ALA	CB-CA-C	6.13	119.29	110.10
16	U	256	PRO	N-CA-CB	5.79	110.25	103.30
16	U	388	PRO	N-CA-CB	5.78	110.24	103.30
16	U	332	PRO	N-CA-CB	5.72	110.16	103.30
10	Q	222	PRO	N-CA-CB	5.61	110.03	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	C	40	0	36	6	0
1	c	105	0	106	0	0
2	H	1560	0	1633	79	0
3	I	4111	0	4032	161	0
4	K	1869	0	1857	70	0
5	L	2422	0	2396	100	0
6	M	1298	0	1349	68	0
7	N	2492	0	2509	113	0
8	O	1588	0	1540	68	0
9	P	1808	0	1810	72	0
10	Q	1175	0	1058	43	0
11	S	790	0	798	74	0
12	T	804	0	814	46	0
13	W	584	0	631	29	0
14	X	590	0	620	43	0
15	R	308	0	127	4	0
16	U	699	0	303	10	0
All	All	22243	0	21619	827	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 19.

The worst 5 of 827 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:I:155:LYS:O	3:I:156:CYS:O	1.86	0.92
12:T:515:LEU:HD13	13:W:42:LEU:HB3	1.53	0.90
2:H:101:LEU:HD21	3:I:586:GLY:HA2	1.57	0.85
9:P:111:CYS:SG	9:P:112:HIS:N	2.49	0.84
7:N:269:TYR:HB2	7:N:295:ILE:HB	1.58	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	3/943 (0%)	2 (67%)	1 (33%)	0	100	100
1	c	11/943 (1%)	9 (82%)	2 (18%)	0	100	100
2	H	191/247 (77%)	181 (95%)	10 (5%)	0	100	100
3	I	503/756 (66%)	470 (93%)	31 (6%)	2 (0%)	34	66
4	K	224/269 (83%)	204 (91%)	17 (8%)	3 (1%)	12	40
5	L	296/344 (86%)	272 (92%)	24 (8%)	0	100	100
6	M	166/180 (92%)	148 (89%)	17 (10%)	1 (1%)	25	57
7	N	299/339 (88%)	271 (91%)	28 (9%)	0	100	100
8	O	204/300 (68%)	183 (90%)	21 (10%)	0	100	100
9	P	220/288 (76%)	196 (89%)	21 (10%)	3 (1%)	11	38
10	Q	156/268 (58%)	153 (98%)	3 (2%)	0	100	100
11	S	95/138 (69%)	93 (98%)	2 (2%)	0	100	100
12	T	97/561 (17%)	95 (98%)	2 (2%)	0	100	100
13	W	73/88 (83%)	72 (99%)	1 (1%)	0	100	100
14	X	72/81 (89%)	72 (100%)	0	0	100	100
15	R	58/177 (33%)	55 (95%)	3 (5%)	0	100	100
16	U	136/418 (32%)	132 (97%)	4 (3%)	0	100	100
All	All	2804/6340 (44%)	2608 (93%)	187 (7%)	9 (0%)	44	71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	156	CYS
9	P	76	ILE
9	P	192	PRO
4	K	190	LEU
4	K	207	VAL

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	C	4/875 (0%)	4 (100%)	0	100	100
1	c	12/875 (1%)	10 (83%)	2 (17%)	2	10
2	H	174/224 (78%)	170 (98%)	4 (2%)	50	73
3	I	440/691 (64%)	433 (98%)	7 (2%)	62	79
4	K	211/260 (81%)	202 (96%)	9 (4%)	29	59
5	L	268/306 (88%)	264 (98%)	4 (2%)	65	81
6	M	147/158 (93%)	142 (97%)	5 (3%)	37	65
7	N	273/311 (88%)	265 (97%)	8 (3%)	42	69
8	O	170/263 (65%)	164 (96%)	6 (4%)	36	64
9	P	204/259 (79%)	197 (97%)	7 (3%)	37	65
10	Q	109/248 (44%)	100 (92%)	9 (8%)	11	36
11	S	86/121 (71%)	79 (92%)	7 (8%)	11	36
12	T	88/461 (19%)	85 (97%)	3 (3%)	37	65
13	W	61/77 (79%)	60 (98%)	1 (2%)	62	79
14	X	65/67 (97%)	62 (95%)	3 (5%)	27	58
All	All	2312/5196 (44%)	2237 (97%)	75 (3%)	42	67

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	Q	172	MET
14	X	24	LYS
11	S	12	ARG
11	S	92	LEU
6	M	53	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
7	N	103	GLN
8	O	175	HIS
14	X	69	GLN
7	N	106	ASN
8	O	100	ASN

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.

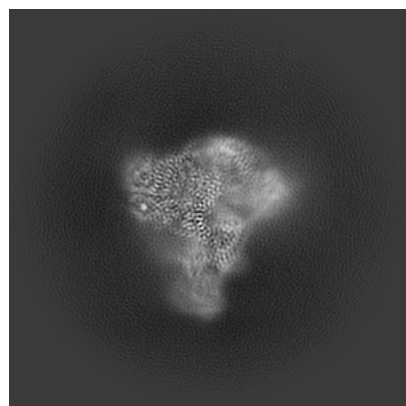
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33197. These allow visual inspection of the internal detail of the map and identification of artifacts.

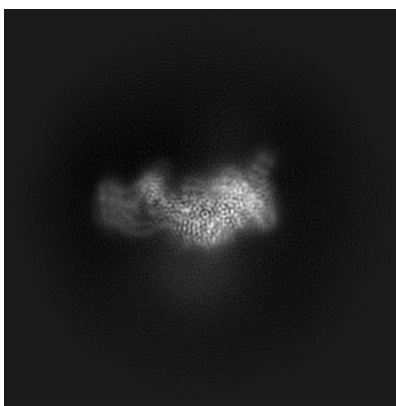
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

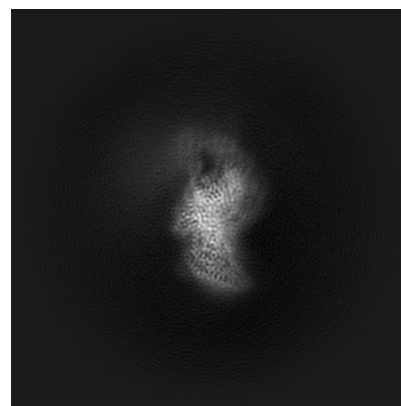
6.1.1 Primary map



X

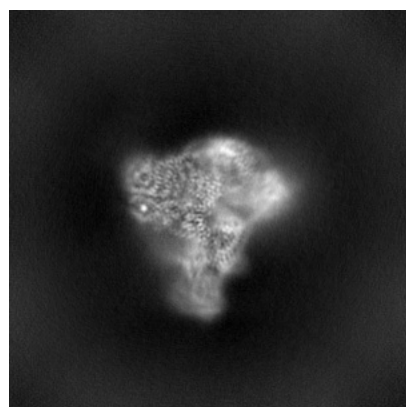


Y

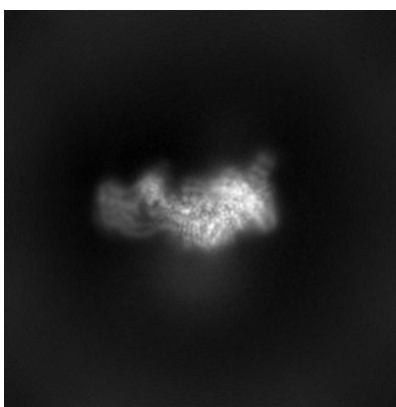


Z

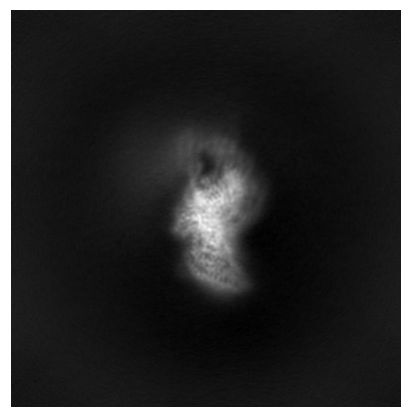
6.1.2 Raw map



X



Y

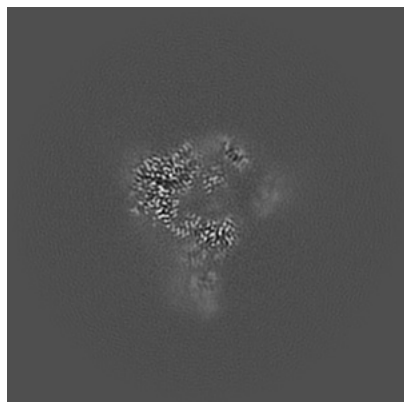


Z

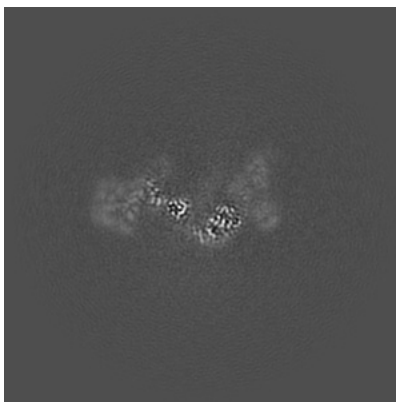
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

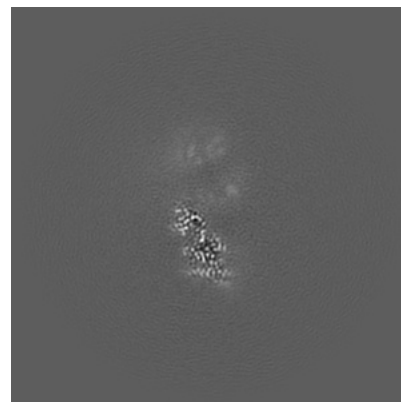
6.2.1 Primary map



X Index: 156

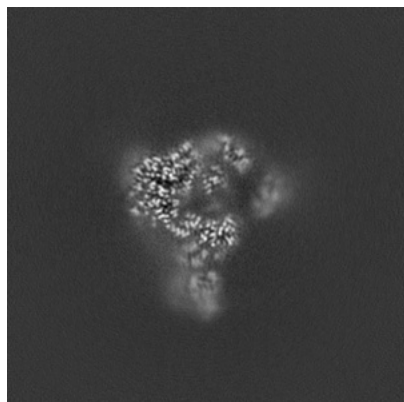


Y Index: 156

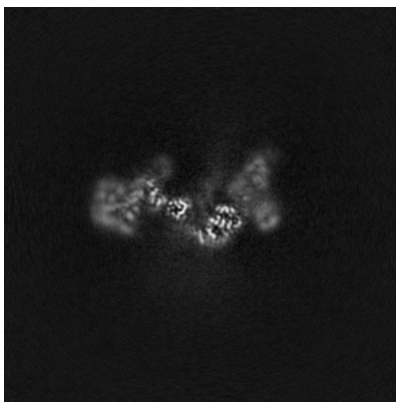


Z Index: 156

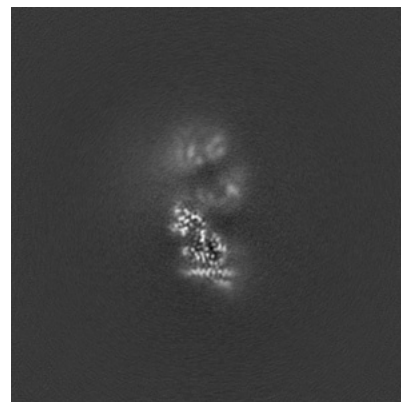
6.2.2 Raw map



X Index: 156



Y Index: 156

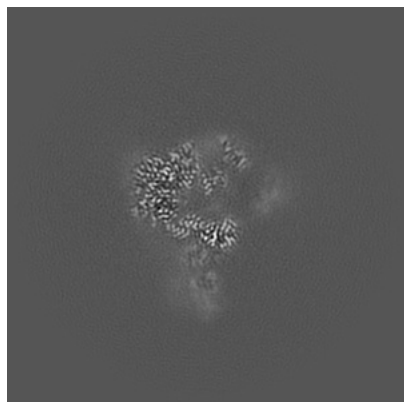


Z Index: 156

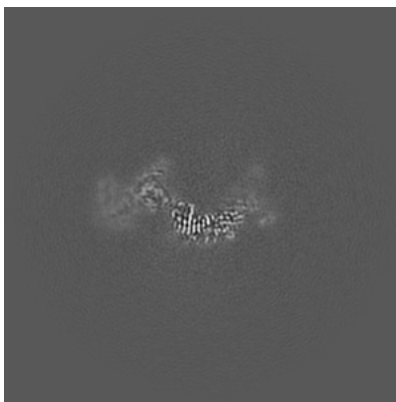
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

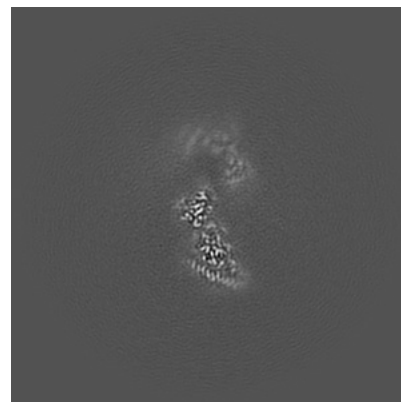
6.3.1 Primary map



X Index: 155

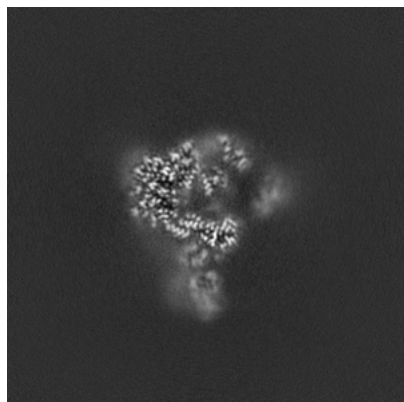


Y Index: 149

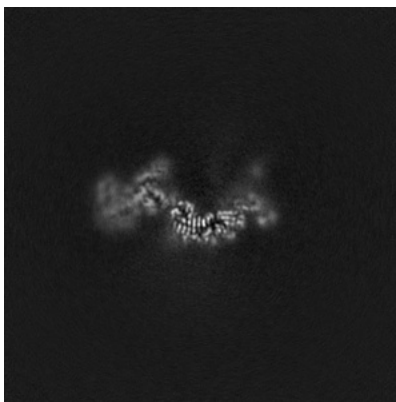


Z Index: 171

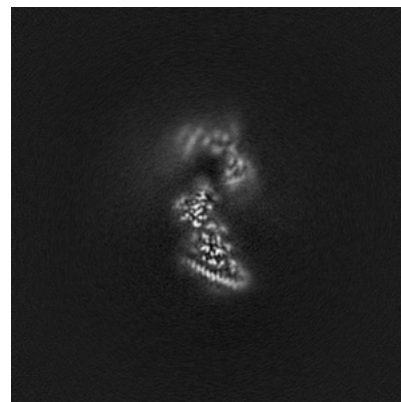
6.3.2 Raw map



X Index: 155



Y Index: 148

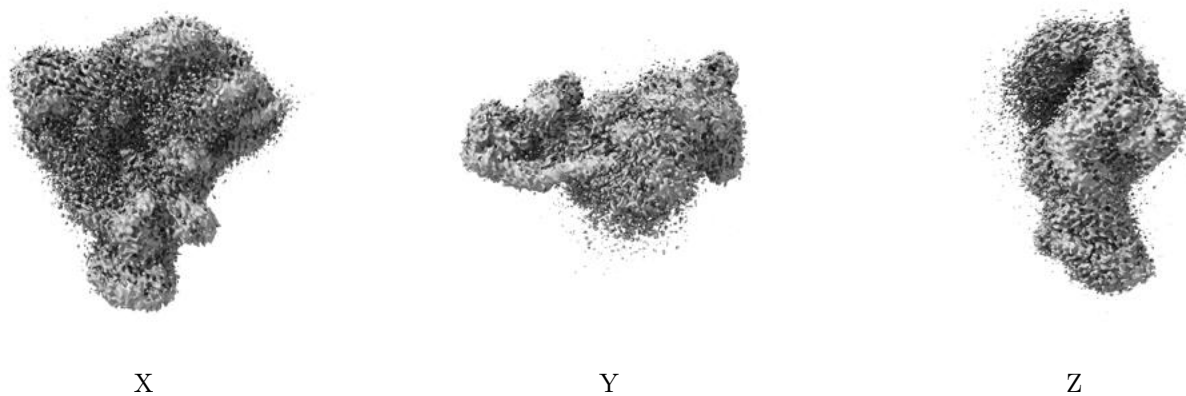


Z Index: 171

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

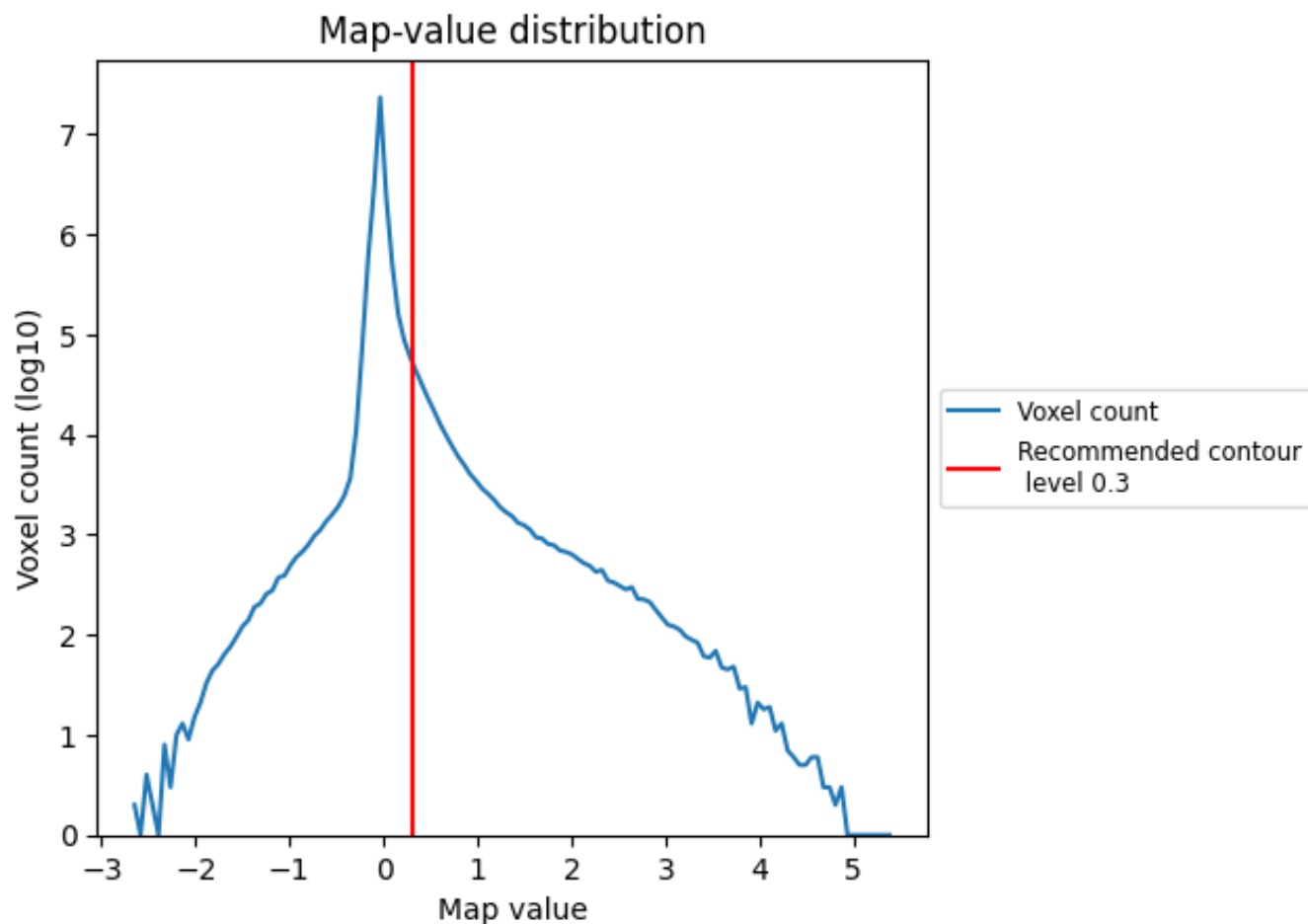
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

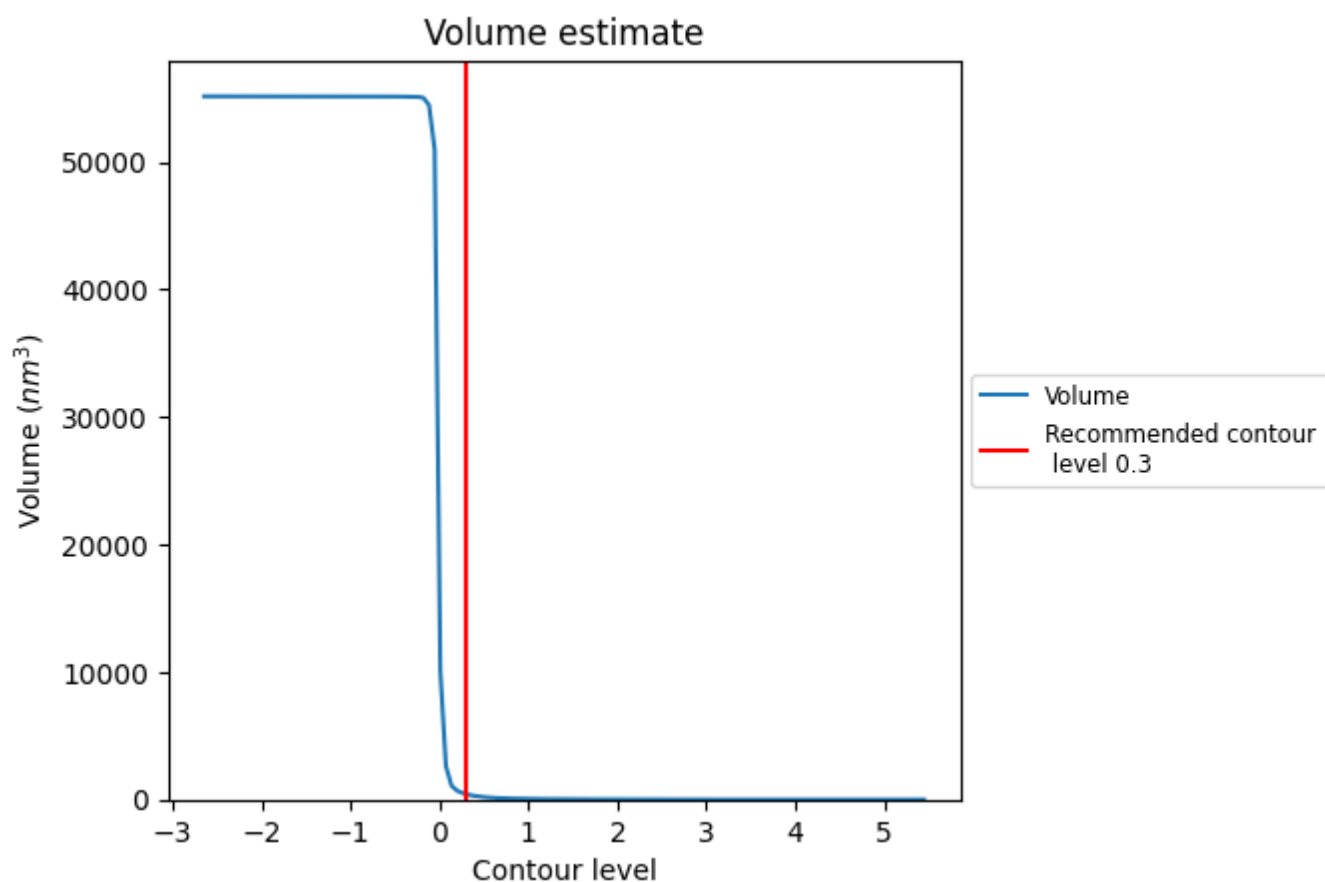
This section contains the results of statistical analysis of the map.

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.

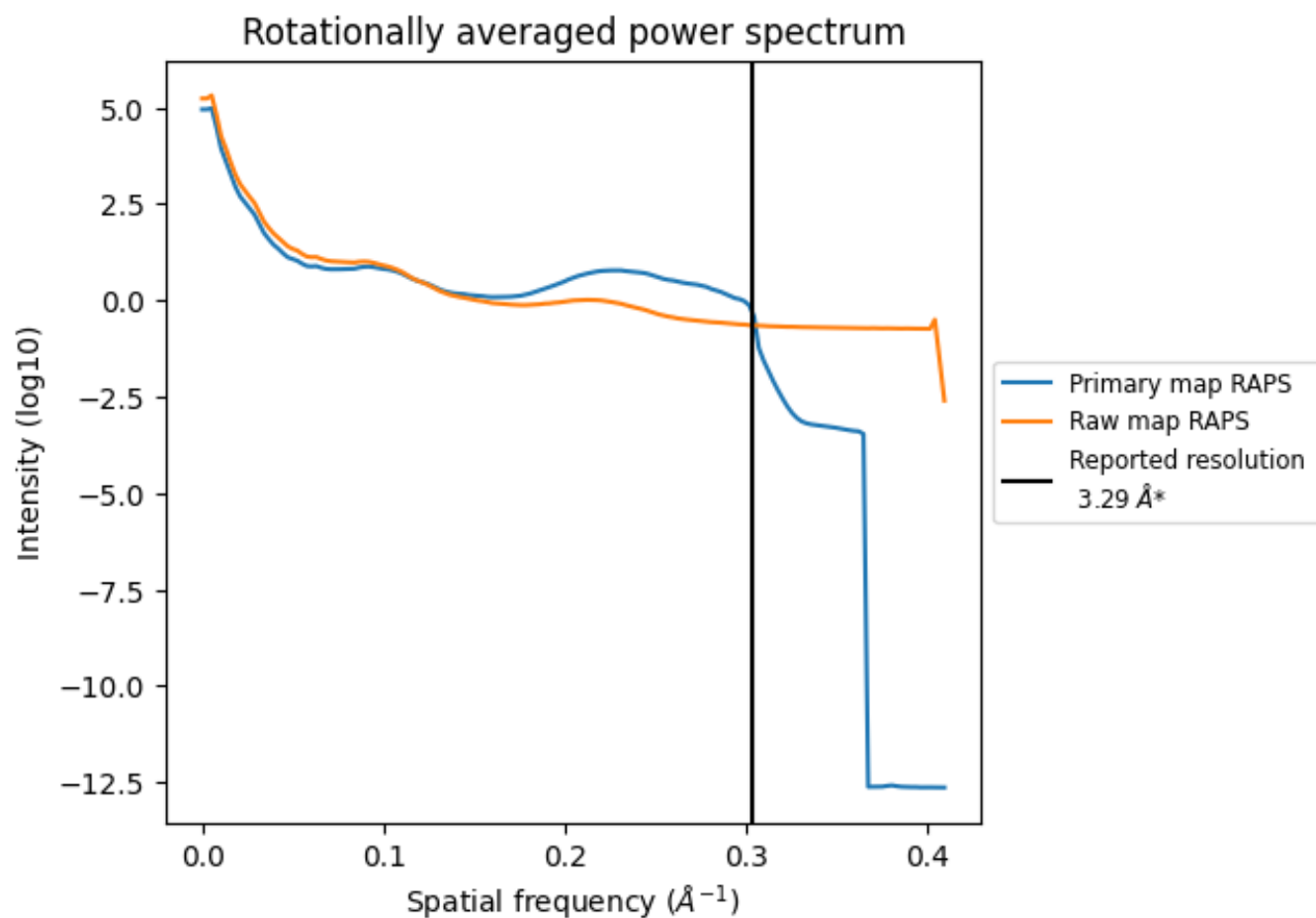
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 427 nm^3 ; this corresponds to an approximate mass of 385 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 ⓘ

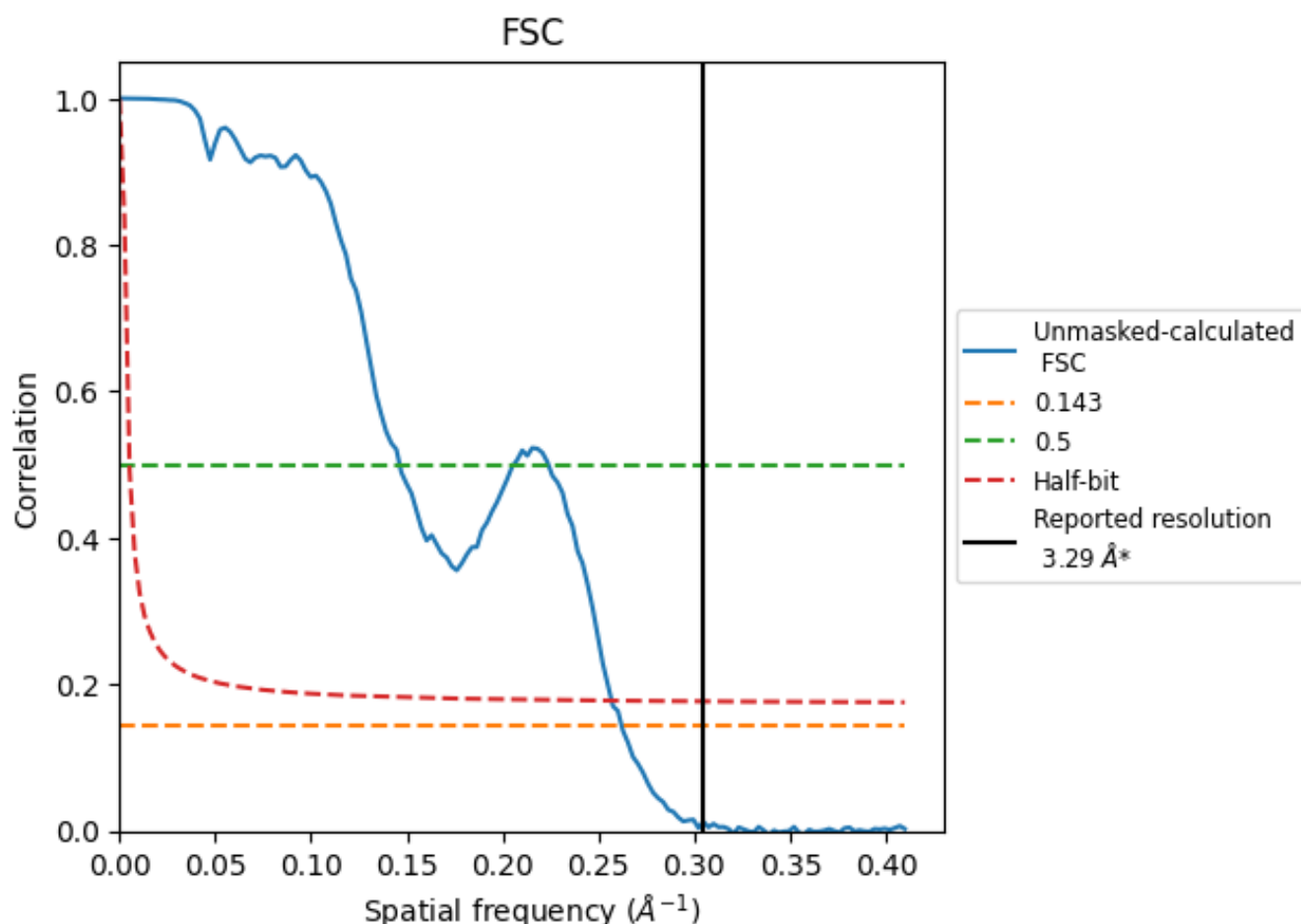


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

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 0.304 Å⁻¹

8.2 Resolution estimates [i](#)

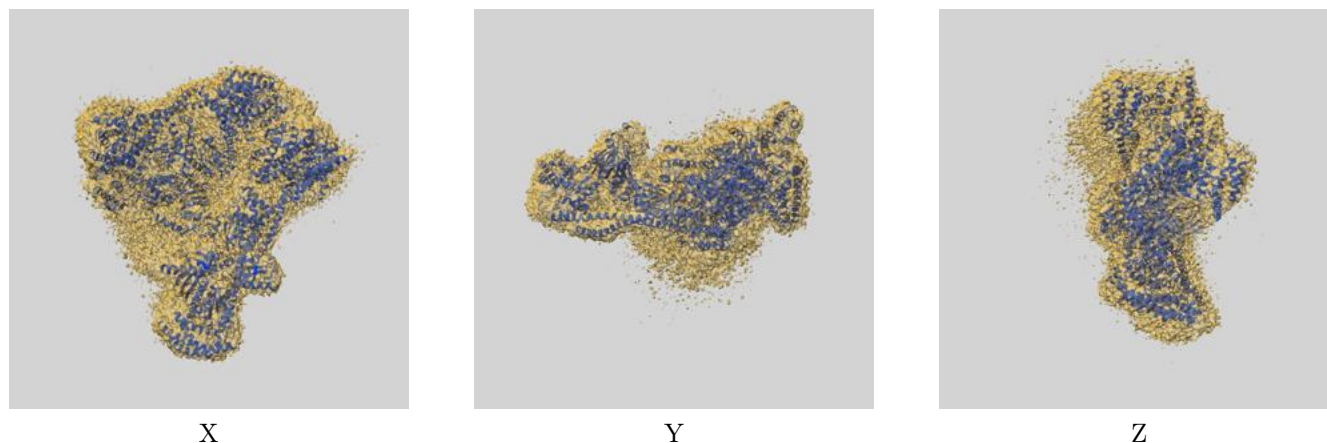
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	6.84	3.89

*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 3.82 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

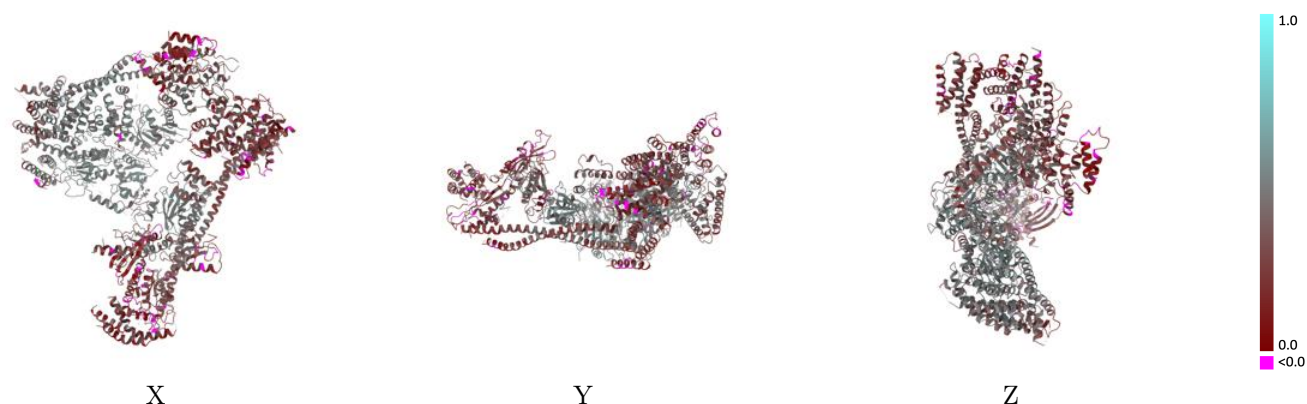
This section contains information regarding the fit between EMDB map EMD-33197 and PDB model 7XHO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



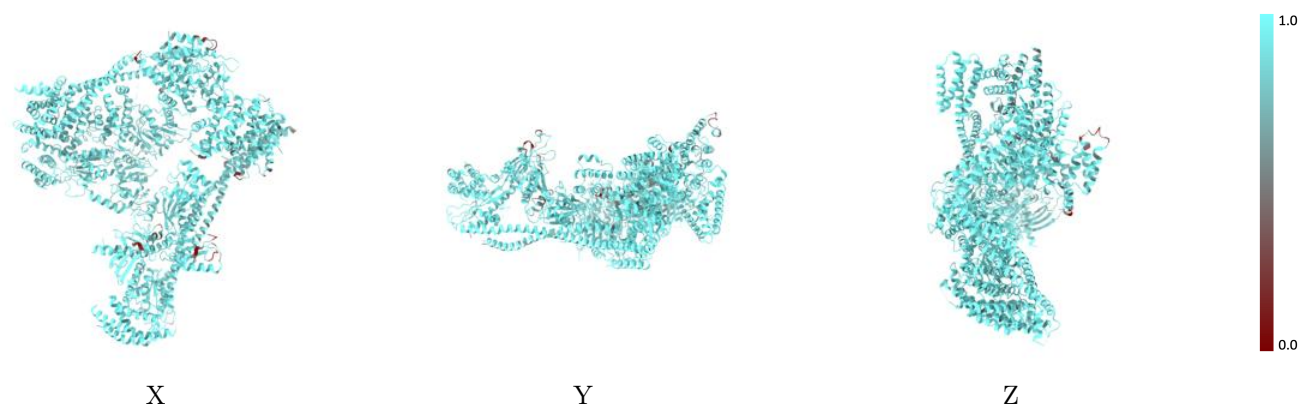
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



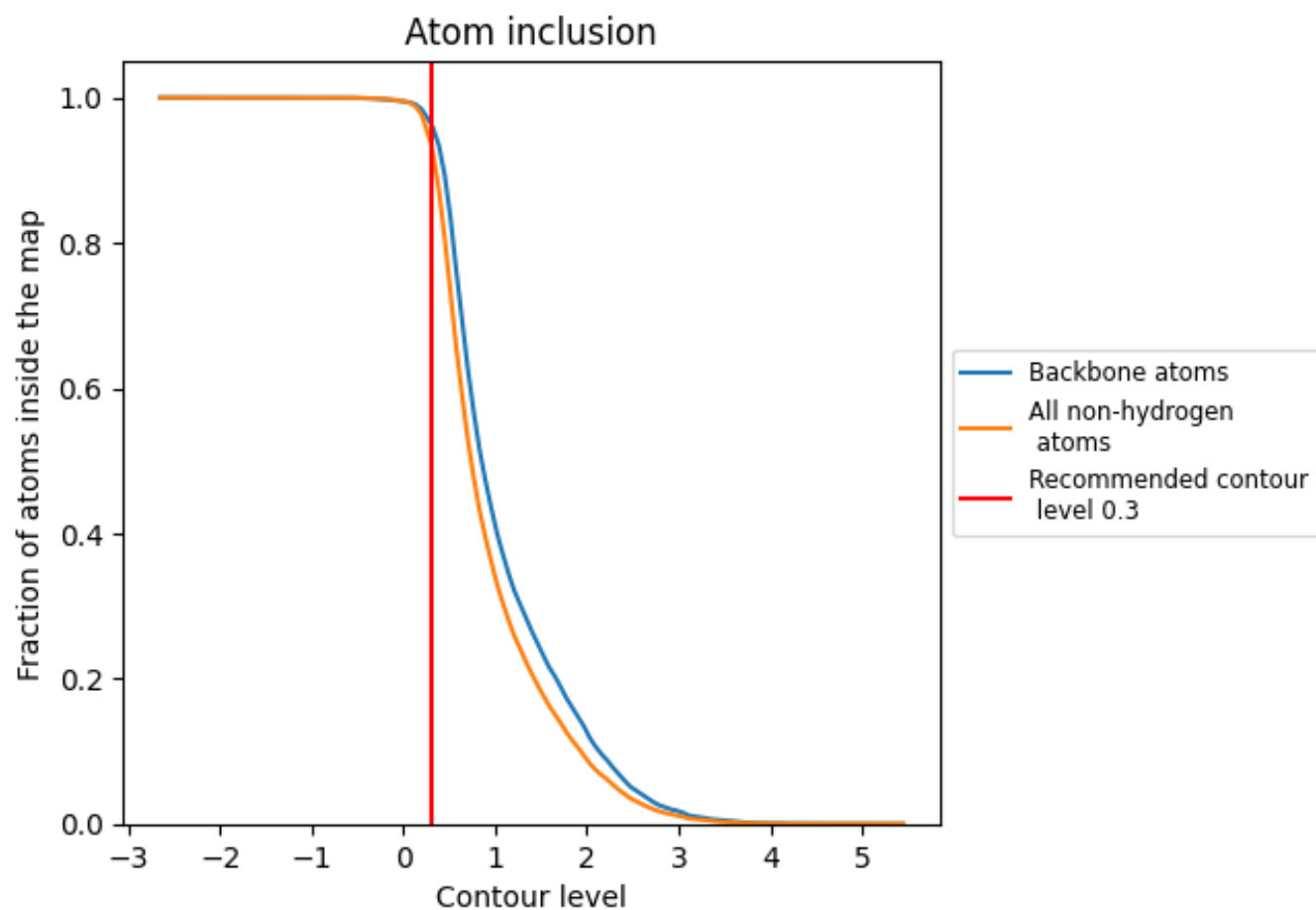
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9375	 0.3660
C	 0.6250	 0.1220
H	 0.9545	 0.4220
I	 0.9314	 0.3890
K	 0.9593	 0.4110
L	 0.9594	 0.4880
M	 0.9655	 0.5110
N	 0.9497	 0.4450
O	 0.8868	 0.3260
P	 0.9222	 0.1920
Q	 0.9416	 0.2480
R	 0.9675	 0.2460
S	 0.9082	 0.2200
T	 0.9530	 0.3360
U	 0.9914	 0.2830
W	 0.9243	 0.2730
X	 0.8207	 0.1640
c	 0.8738	 0.3170

