



wwPDB EM Validation Summary Report ⓘ

Jun 7, 2022 – 07:14 am BST

PDB ID : 7QOO
EMDB ID : EMD-14098
Title : Structure of the human inner kinetochore CCAN complex
Authors : Vetter, I.R.; Pesenti, M.; Raisch, T.
Deposited on : 2021-12-24
Resolution : 4.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev8
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

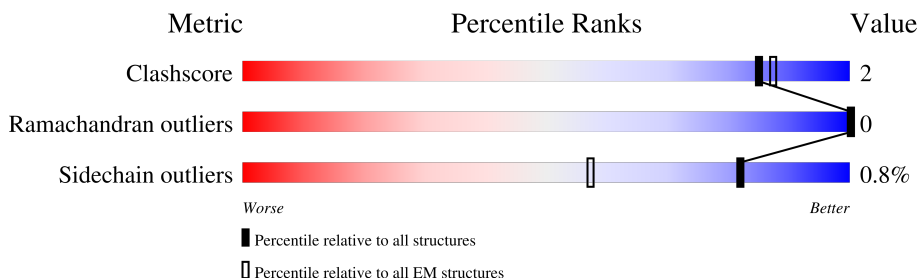
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	544	
2	H	247	
3	I	756	
4	K	269	
5	L	344	
6	M	180	
7	N	339	
8	O	300	

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Mol	Chain	Length	Quality of chain
9	P	288	
10	U	418	
11	Q	268	
12	R	177	
13	T	561	
14	W	88	
15	X	15	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 24085 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	4	Total	C	N	O	0	0
			35	25	4	6		

- Molecule 2 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	210	Total	C	N	O	S	0	0
			1733	1087	301	334	11		

- Molecule 3 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	618	Total	C	N	O	S	0	0
			5042	3297	824	893	28		

- Molecule 4 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	253	Total	C	N	O	S	0	0
			2100	1329	351	410	10		

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	306	Total	C	N	O	S	0	0
			2467	1605	404	444	14		

- Molecule 6 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	176	Total	C	N	O	S	0	0
			1350	854	240	248	8		

- Molecule 7 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	320	Total	C	N	O	S	0	0
			2640	1693	456	480	11		

- Molecule 8 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	199	Total	C	N	O	S	0	0
			1584	1020	265	292	7		

- Molecule 9 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	233	Total	C	N	O	S	0	0
			1891	1198	327	357	9		

- Molecule 10 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	186	Total	C	N	O	S	0	0
			1535	969	269	290	7		

- Molecule 11 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	209	Total	C	N	O	S	0	0
			1667	1040	287	329	11		

- Molecule 12 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	64	Total	C	N	O	S	0	0
			512	321	86	98	7		

- Molecule 13 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	108	Total	C	N	O	S	0	0
			878	564	152	155	7		

- Molecule 14 is a protein called Centromere protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	72	Total	C	N	O	S	0	0
			575	364	116	92	3		

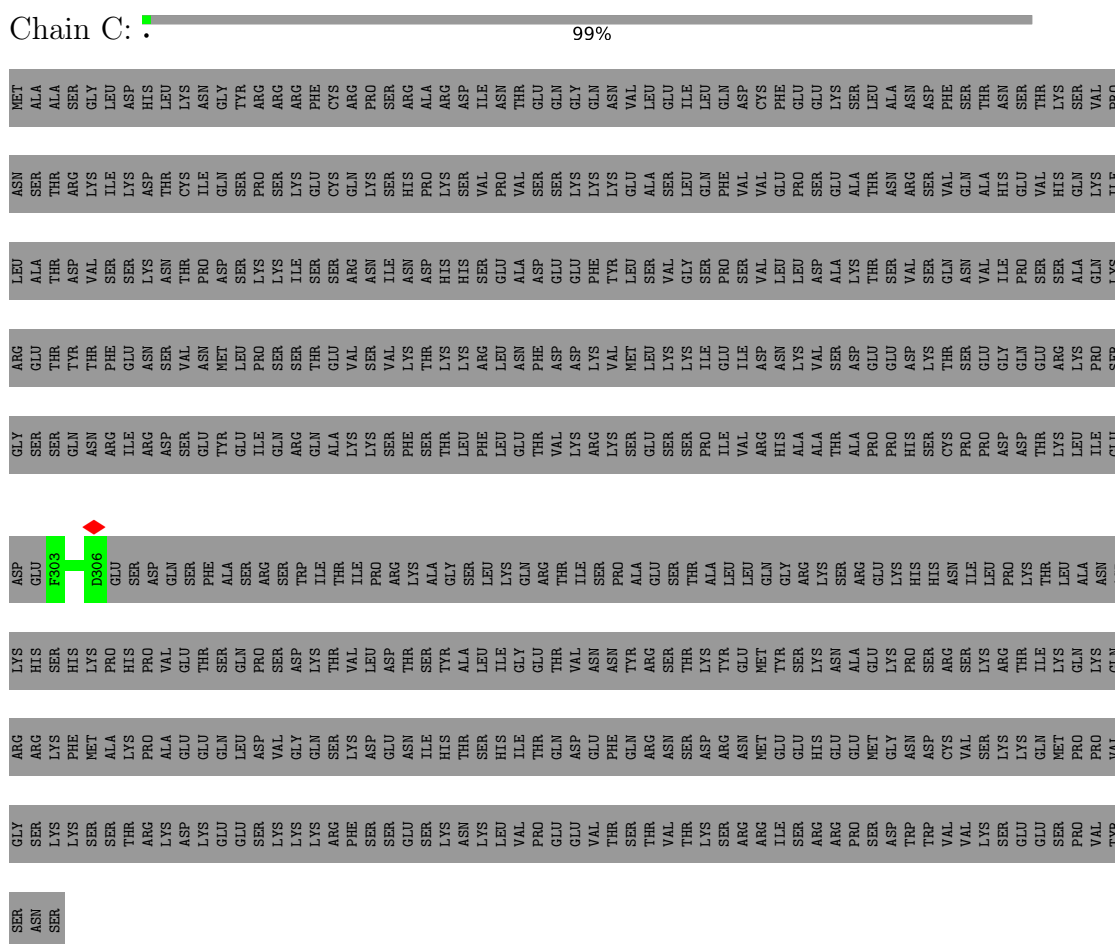
- Molecule 15 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	15	Total	C	N	O	0	0
			76	45	15	16		

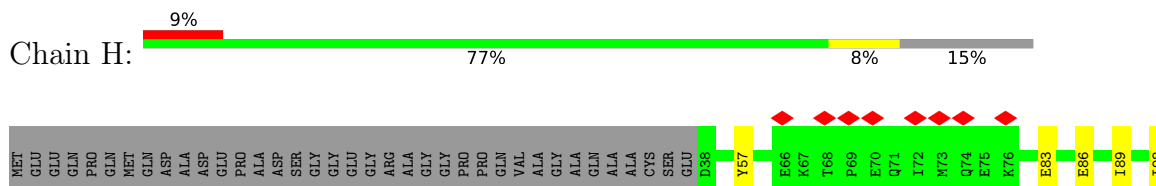
3 Residue-property plots

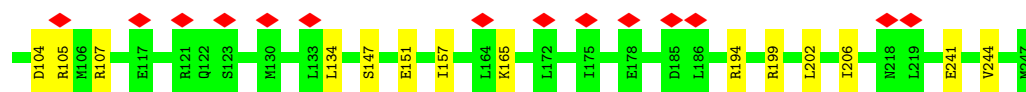
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

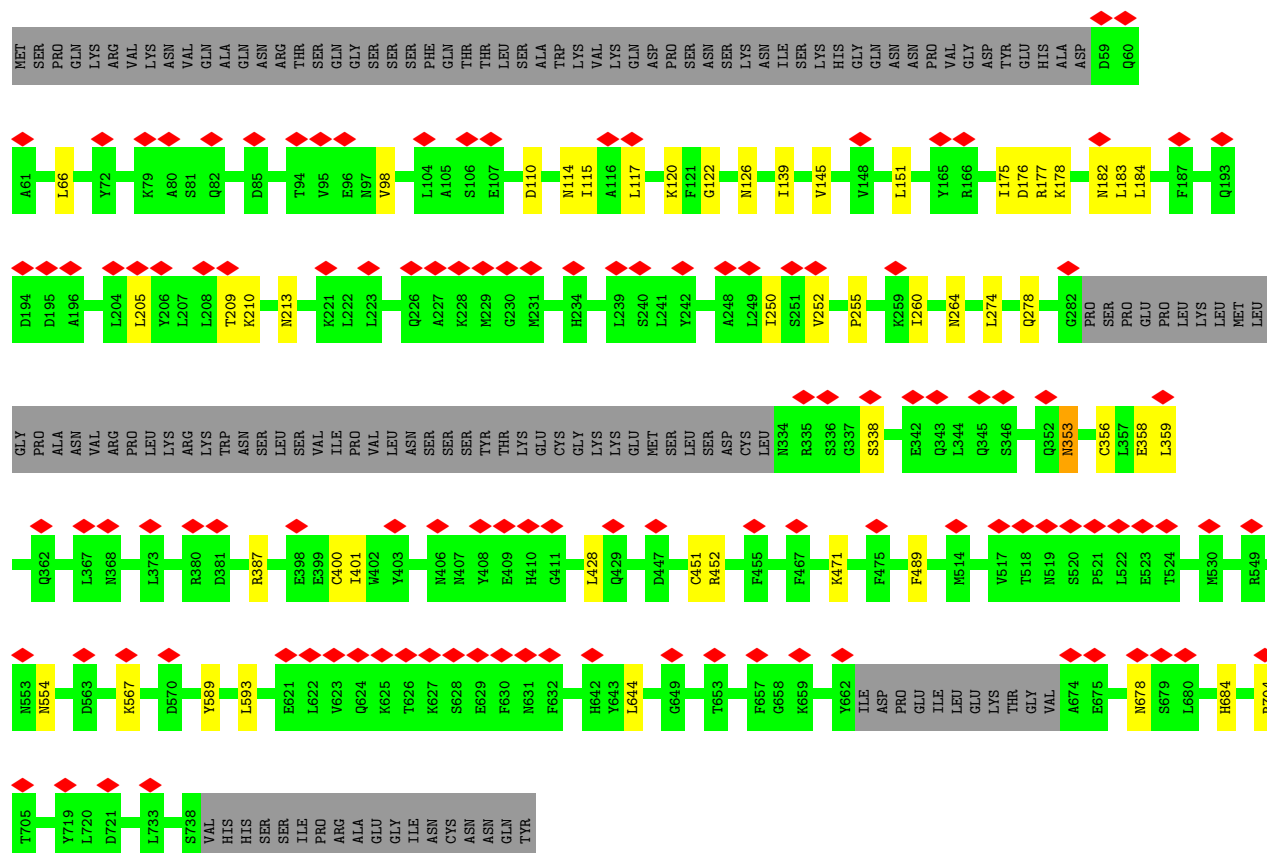
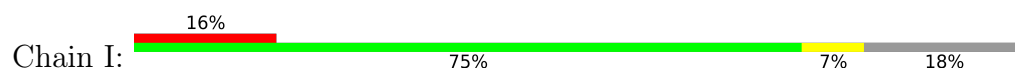


- Molecule 2: Centromere protein H

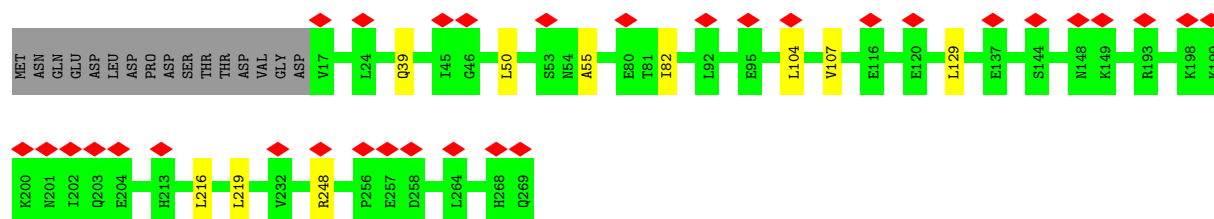
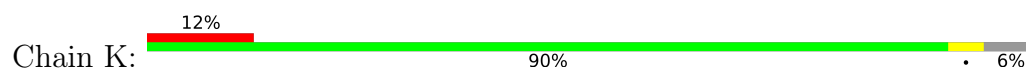




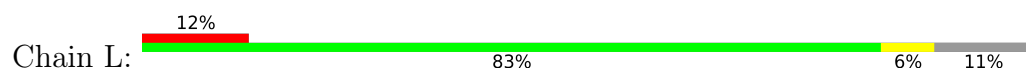
• Molecule 3: Centromere protein I

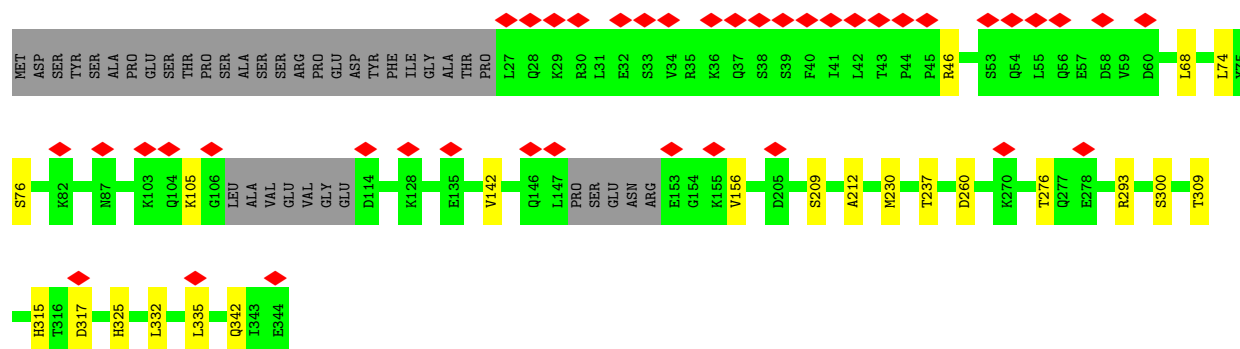


• Molecule 4: Centromere protein K

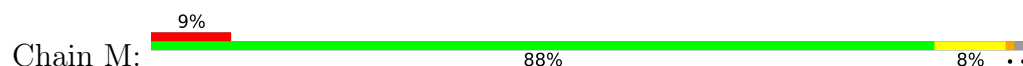


• Molecule 5: Centromere protein L

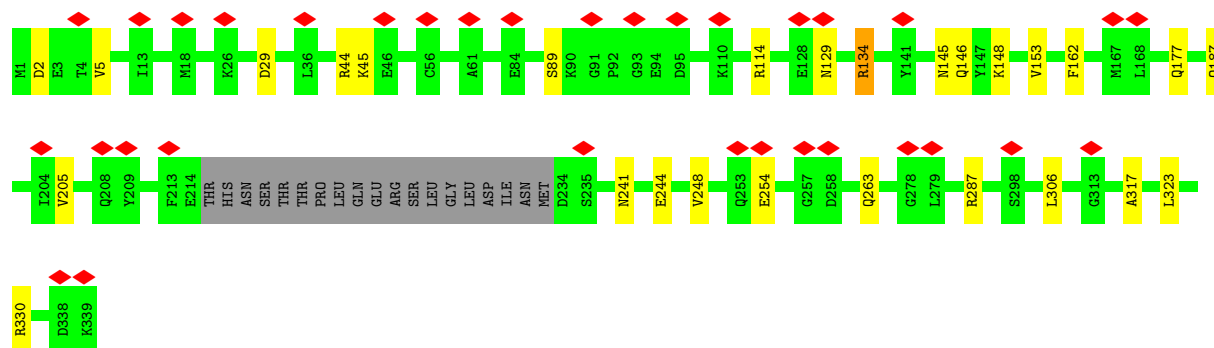
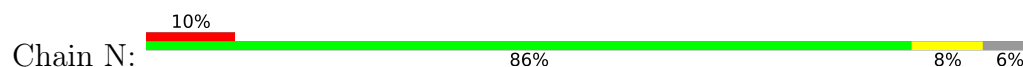




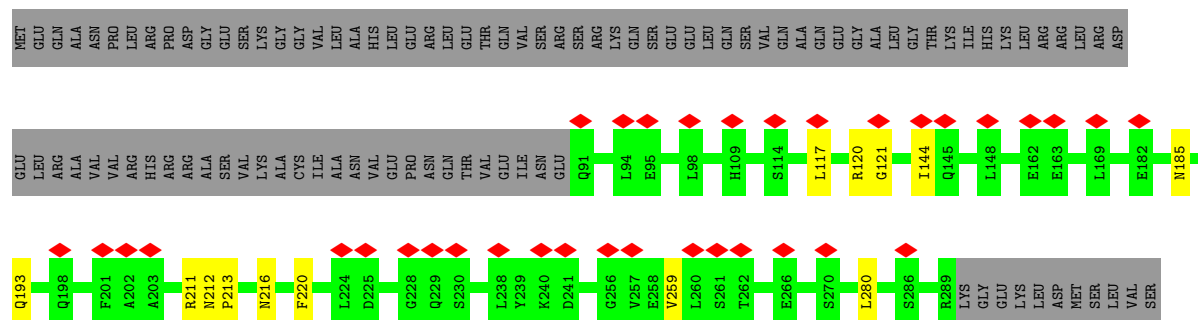
• Molecule 6: Centromere protein M



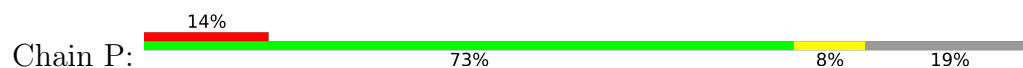
• Molecule 7: Centromere protein N

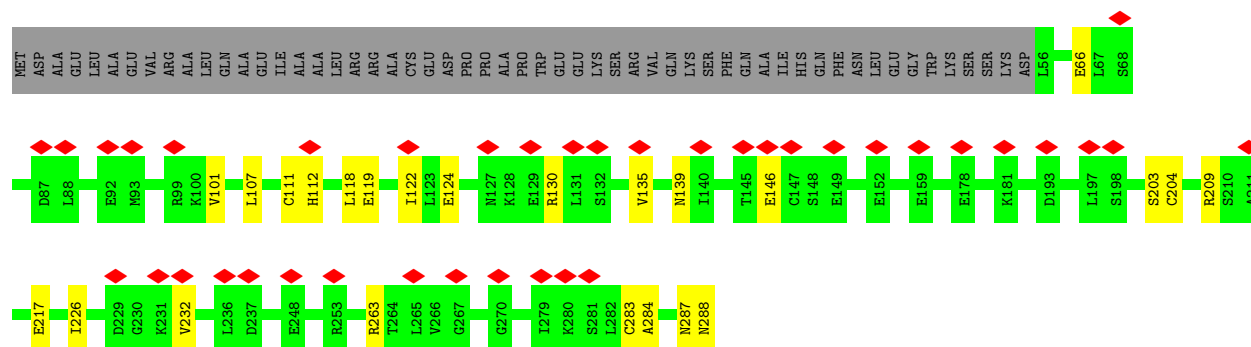


• Molecule 8: Centromere protein O

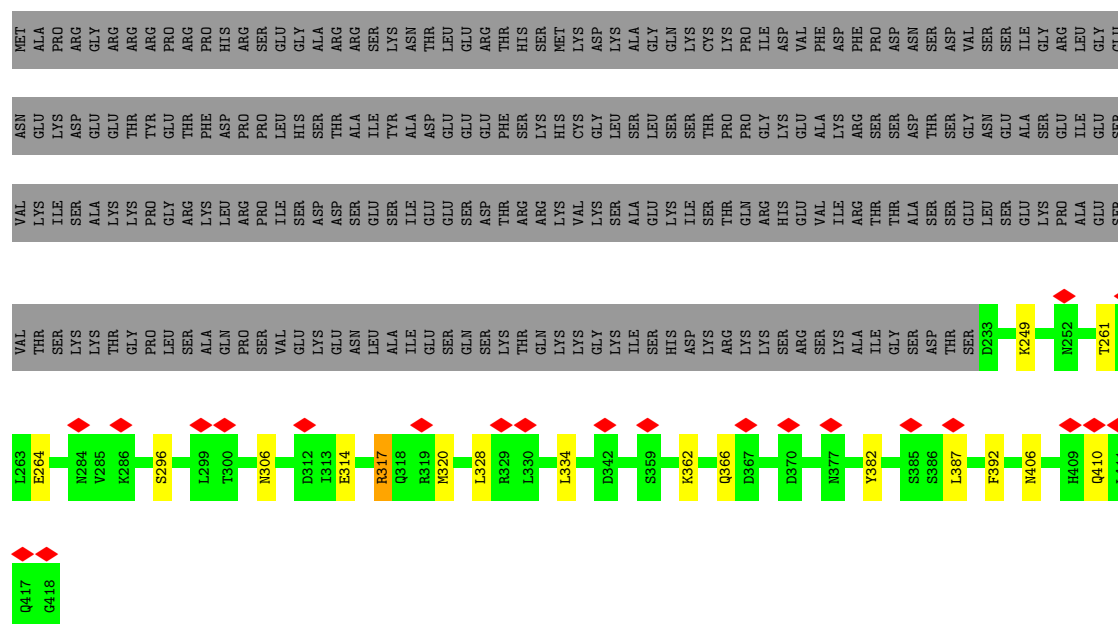
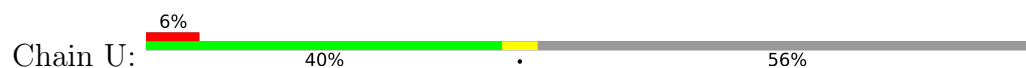


• Molecule 9: Centromere protein P

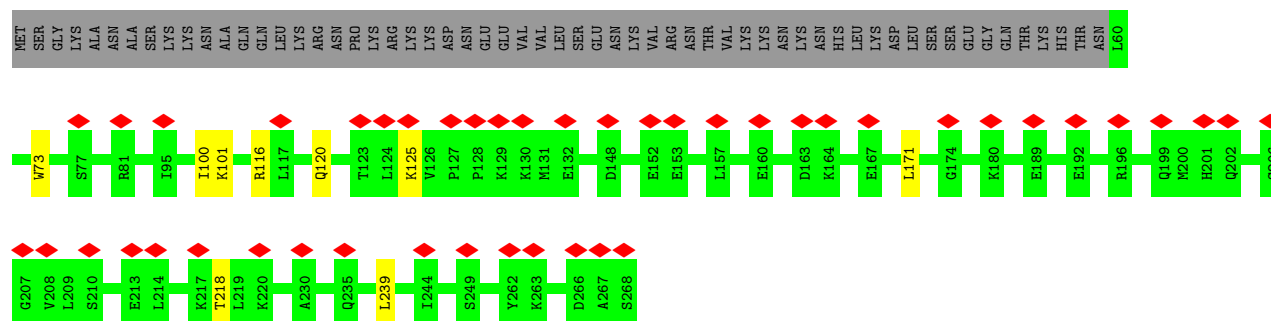
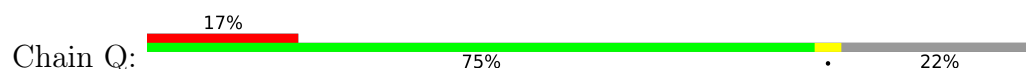




• Molecule 10: Centromere protein U

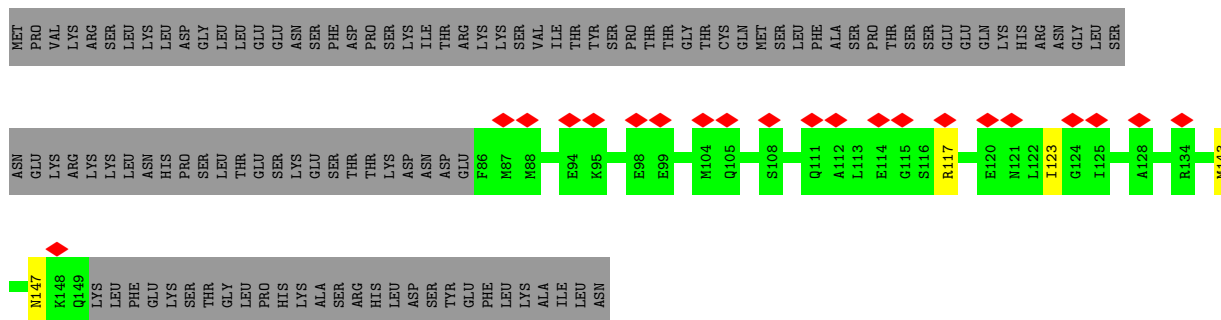


• Molecule 11: Centromere protein Q

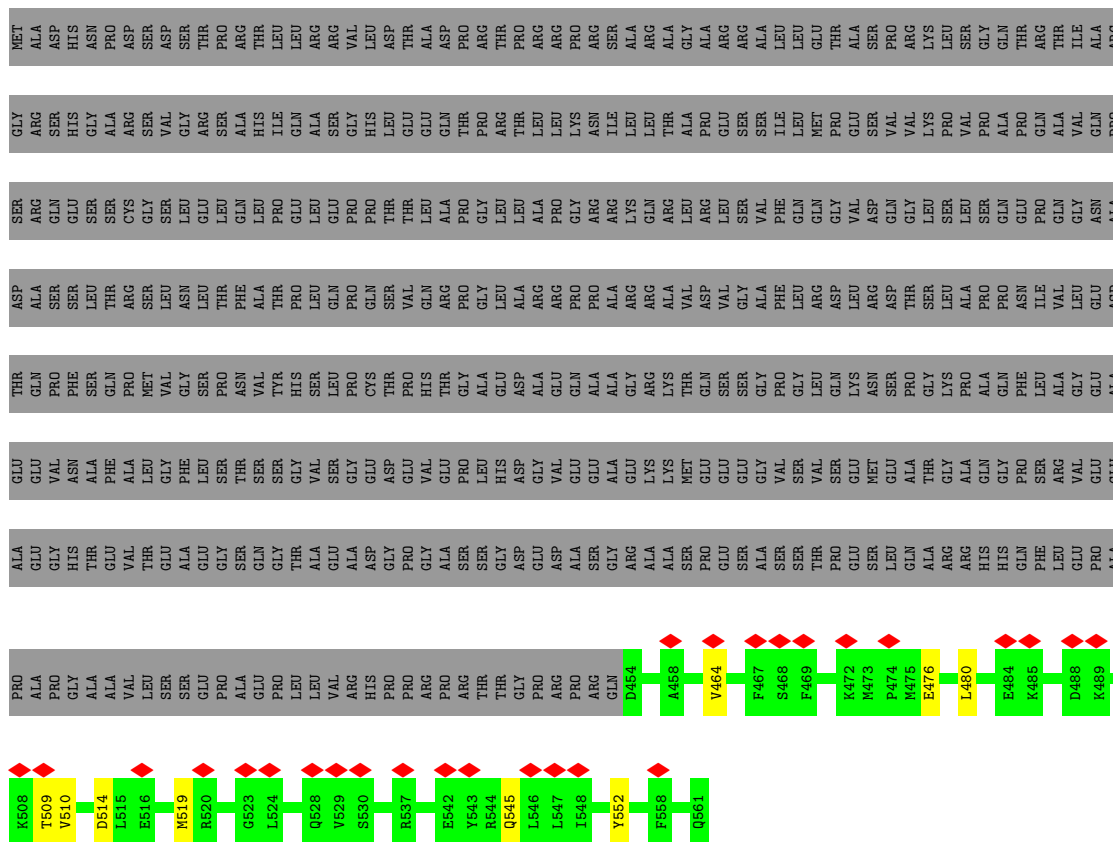


• Molecule 12: Centromere protein R

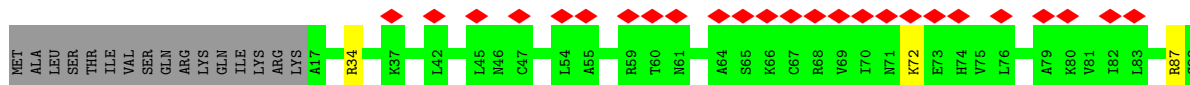
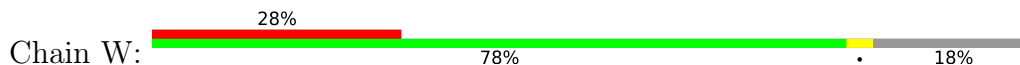




- Molecule 13: Centromere protein T

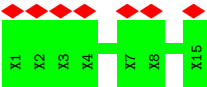


- Molecule 14: Centromere protein W



- Molecule 15: Unknown protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25206	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 ($e^-/\text{\AA}^2$)	76.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.020	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7, 0.7, 0.7	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	0.54	0/35	0.63	0/46
2	H	0.32	0/1743	0.58	1/2324 (0.0%)
3	I	0.38	0/5172	0.58	2/7002 (0.0%)
4	K	0.31	0/2134	0.53	0/2874
5	L	0.37	0/2532	0.55	0/3432
6	M	0.32	0/1373	0.59	1/1862 (0.1%)
7	N	0.38	0/2697	0.61	1/3637 (0.0%)
8	O	0.38	0/1622	0.61	0/2204
9	P	0.36	0/1924	0.55	0/2587
10	U	0.32	0/1557	0.58	1/2087 (0.0%)
11	Q	0.28	0/1683	0.56	1/2255 (0.0%)
12	R	0.29	0/514	0.52	0/680
13	T	0.36	0/899	0.51	1/1211 (0.1%)
14	W	0.31	0/582	0.48	0/773
All	All	0.35	0/24467	0.57	8/32974 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	451	CYS	CA-CB-SG	7.26	127.08	114.00
7	N	29	ASP	CB-CG-OD1	6.44	124.09	118.30
2	H	134	LEU	CA-CB-CG	5.76	128.55	115.30
13	T	510	VAL	C-N-CA	5.20	134.69	121.70
10	U	334	LEU	CA-CB-CG	5.17	127.18	115.30

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	35	0	34	0	0
2	H	1733	0	1840	14	0
3	I	5042	0	5077	26	0
4	K	2100	0	2129	8	0
5	L	2467	0	2457	12	0
6	M	1350	0	1397	9	0
7	N	2640	0	2678	16	0
8	O	1584	0	1574	8	0
9	P	1891	0	1909	12	0
10	U	1535	0	1577	13	0
11	Q	1667	0	1740	7	0
12	R	512	0	541	2	0
13	T	878	0	883	6	0
14	W	575	0	632	1	0
15	X	76	0	17	0	0
All	All	24085	0	24485	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 106 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)
5:L:212:ALA:H	5:L:342:GLN:HE22	1.44	0.63
8:O:211:ARG:HH22	8:O:220:PHE:HB3	1.69	0.57
5:L:300:SER:HB2	6:M:75:LYS:HB3	1.89	0.55
3:I:115:ILE:HG23	3:I:120:LYS:HD2	1.88	0.55
2:H:105:ARG:HG3	3:I:593:LEU:HB3	1.89	0.55

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	2/544 (0%)	2 (100%)	0	0	100	100
2	H	208/247 (84%)	207 (100%)	1 (0%)	0	100	100
3	I	612/756 (81%)	586 (96%)	26 (4%)	0	100	100
4	K	251/269 (93%)	241 (96%)	10 (4%)	0	100	100
5	L	300/344 (87%)	292 (97%)	8 (3%)	0	100	100
6	M	174/180 (97%)	169 (97%)	5 (3%)	0	100	100
7	N	316/339 (93%)	301 (95%)	15 (5%)	0	100	100
8	O	197/300 (66%)	192 (98%)	5 (2%)	0	100	100
9	P	231/288 (80%)	225 (97%)	6 (3%)	0	100	100
10	U	184/418 (44%)	182 (99%)	2 (1%)	0	100	100
11	Q	207/268 (77%)	200 (97%)	7 (3%)	0	100	100
12	R	62/177 (35%)	62 (100%)	0	0	100	100
13	T	106/561 (19%)	101 (95%)	5 (5%)	0	100	100
14	W	70/88 (80%)	67 (96%)	3 (4%)	0	100	100
All	All	2920/4779 (61%)	2827 (97%)	93 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	4/508 (1%)	4 (100%)	0	100	100
2	H	200/224 (89%)	199 (100%)	1 (0%)	88	93
3	I	565/691 (82%)	561 (99%)	4 (1%)	84	90
4	K	245/260 (94%)	245 (100%)	0	100	100
5	L	274/306 (90%)	272 (99%)	2 (1%)	84	90
6	M	154/158 (98%)	151 (98%)	3 (2%)	57	75
7	N	293/311 (94%)	291 (99%)	2 (1%)	84	90
8	O	176/263 (67%)	174 (99%)	2 (1%)	73	85
9	P	214/259 (83%)	211 (99%)	3 (1%)	67	81
10	U	173/379 (46%)	171 (99%)	2 (1%)	71	84
11	Q	194/248 (78%)	194 (100%)	0	100	100
12	R	60/166 (36%)	59 (98%)	1 (2%)	60	78
13	T	96/461 (21%)	95 (99%)	1 (1%)	76	86
14	W	62/77 (80%)	60 (97%)	2 (3%)	39	62
All	All	2710/4311 (63%)	2687 (99%)	23 (1%)	82	89

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	P	130	ARG
10	U	306	ASN
9	P	288	ASN
10	U	317	ARG
5	L	293	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
9	P	287	ASN
11	Q	247	ASN
10	U	366	GLN
3	I	642	HIS
7	N	177	GLN

5.3.3 RNA ⓘ

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.

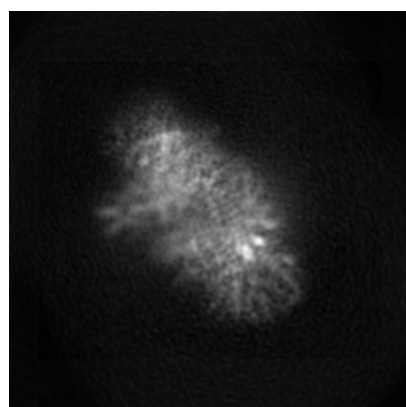
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14098. These allow visual inspection of the internal detail of the map and identification of artifacts.

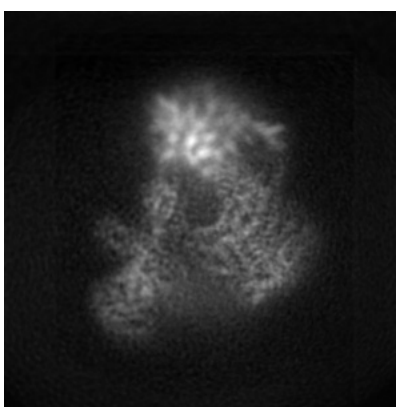
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

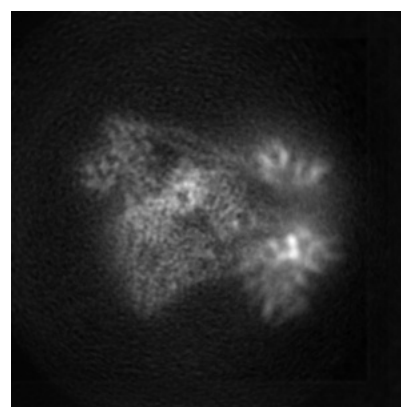
6.1.1 Primary map



X



Y

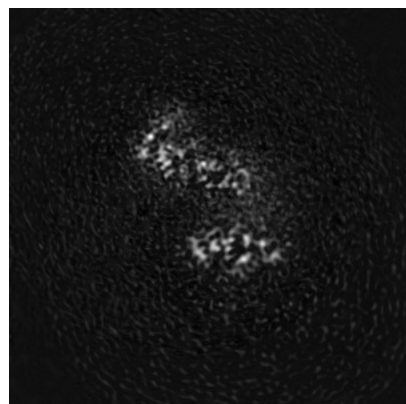


Z

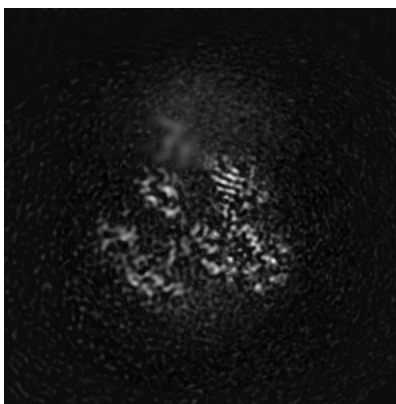
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

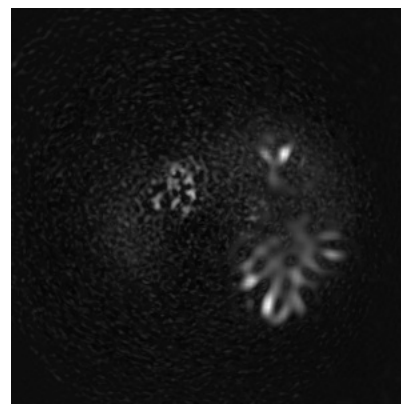
6.2.1 Primary map



X Index: 192



Y Index: 192

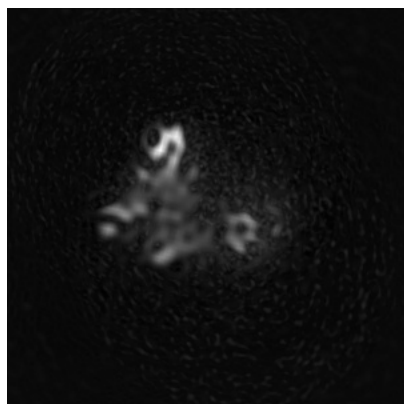


Z Index: 192

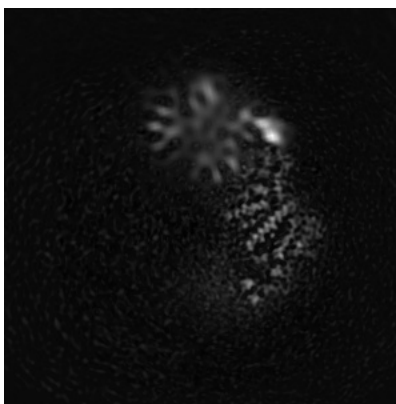
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

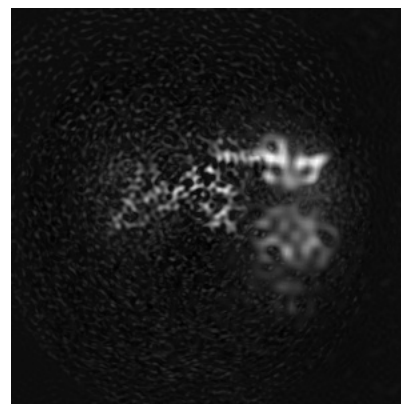
6.3.1 Primary map



X Index: 271



Y Index: 148

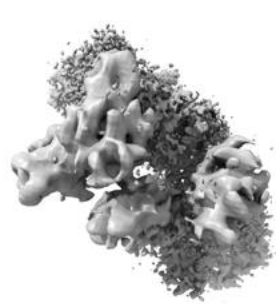


Z Index: 162

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

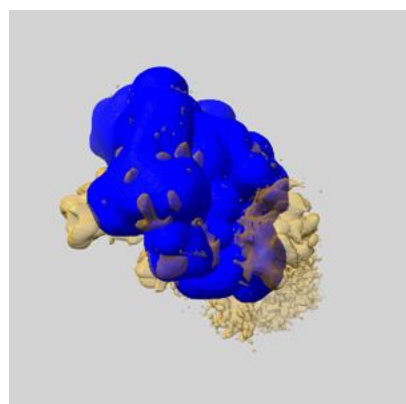
6.5 Mask visualisation [i](#)

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

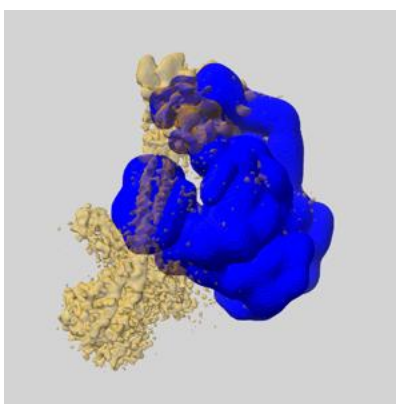
A mask typically either:

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

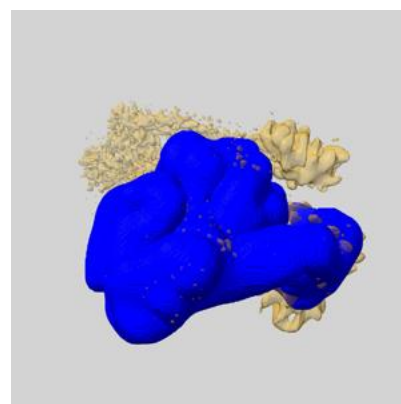
6.5.1 emd_14098_msk_1.map [i](#)



X

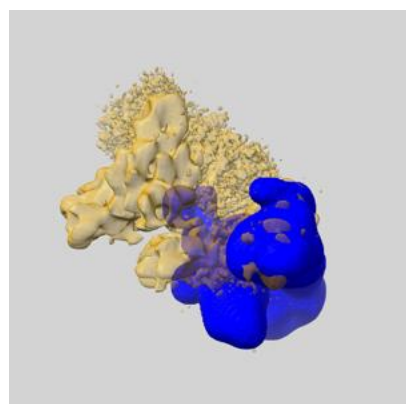


Y

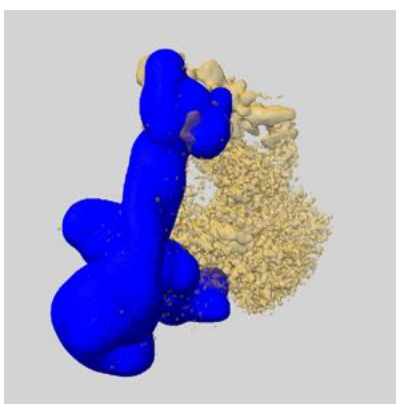


Z

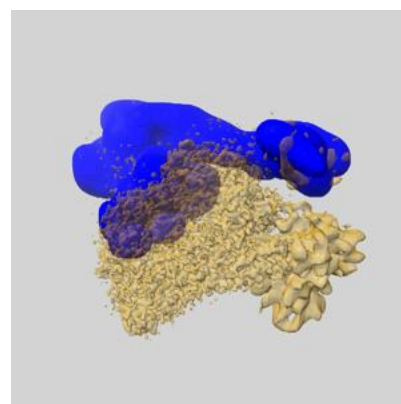
6.5.2 emd_14098_msk_2.map [i](#)



X

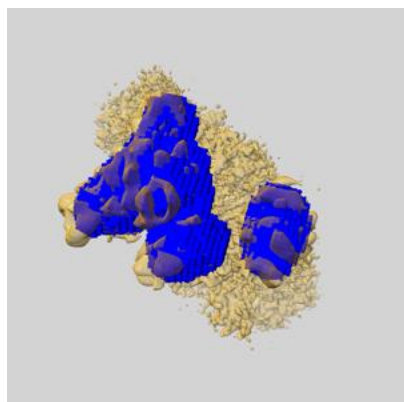


Y

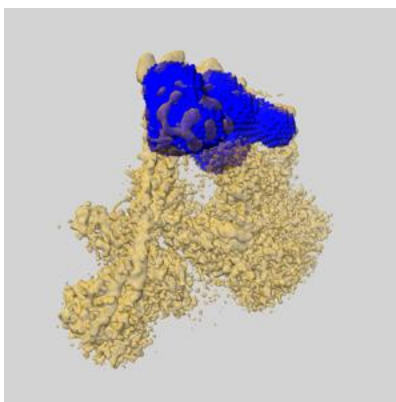


Z

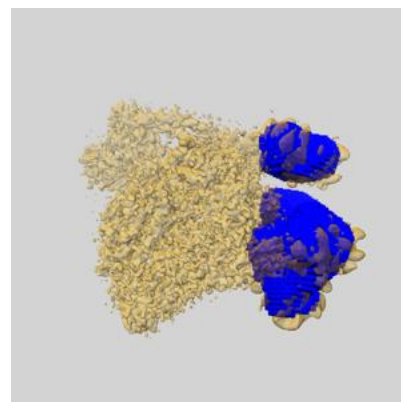
6.5.3 emd_14098_msk_3.map [i](#)



X



Y

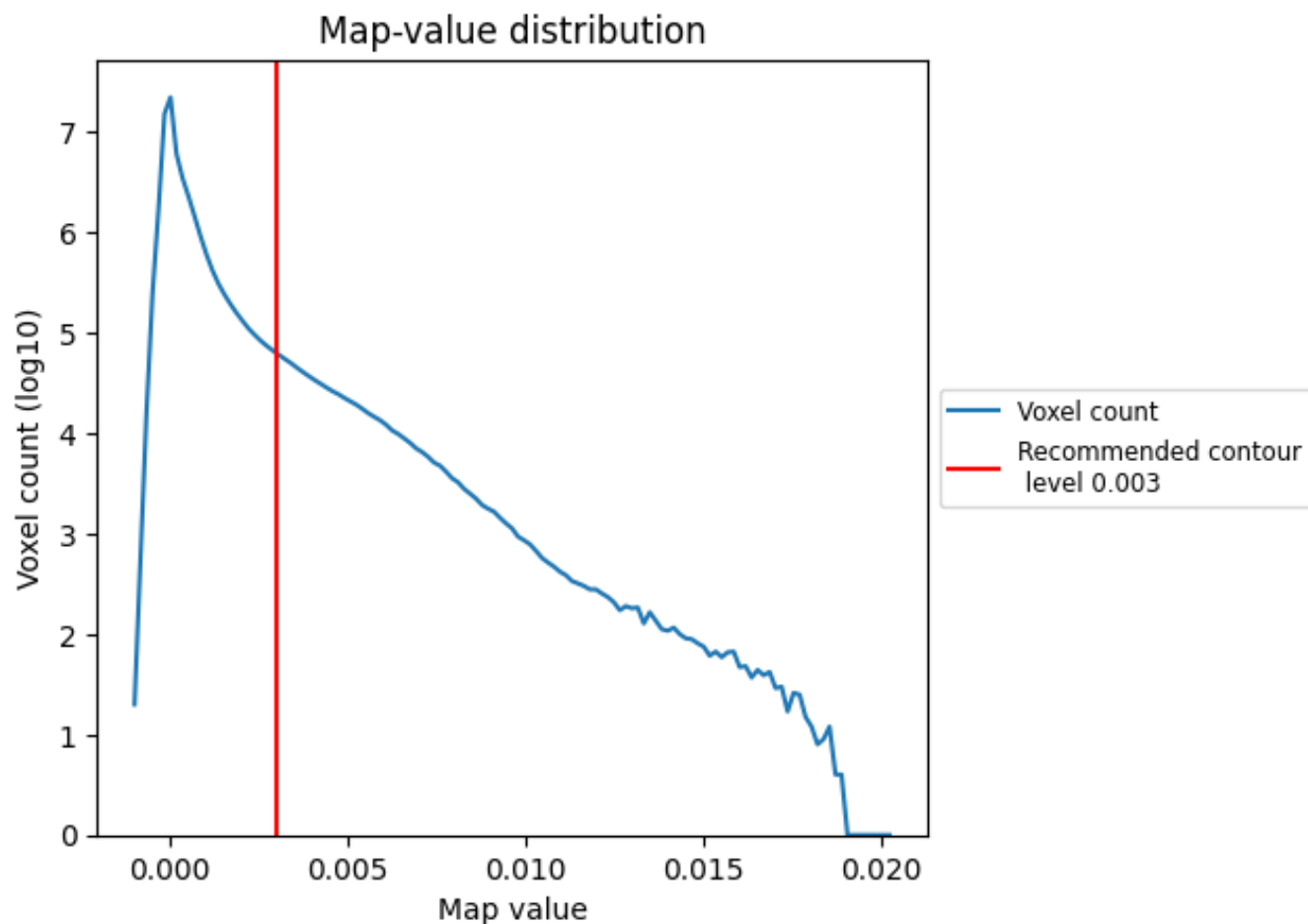


Z

7 Map analysis [i](#)

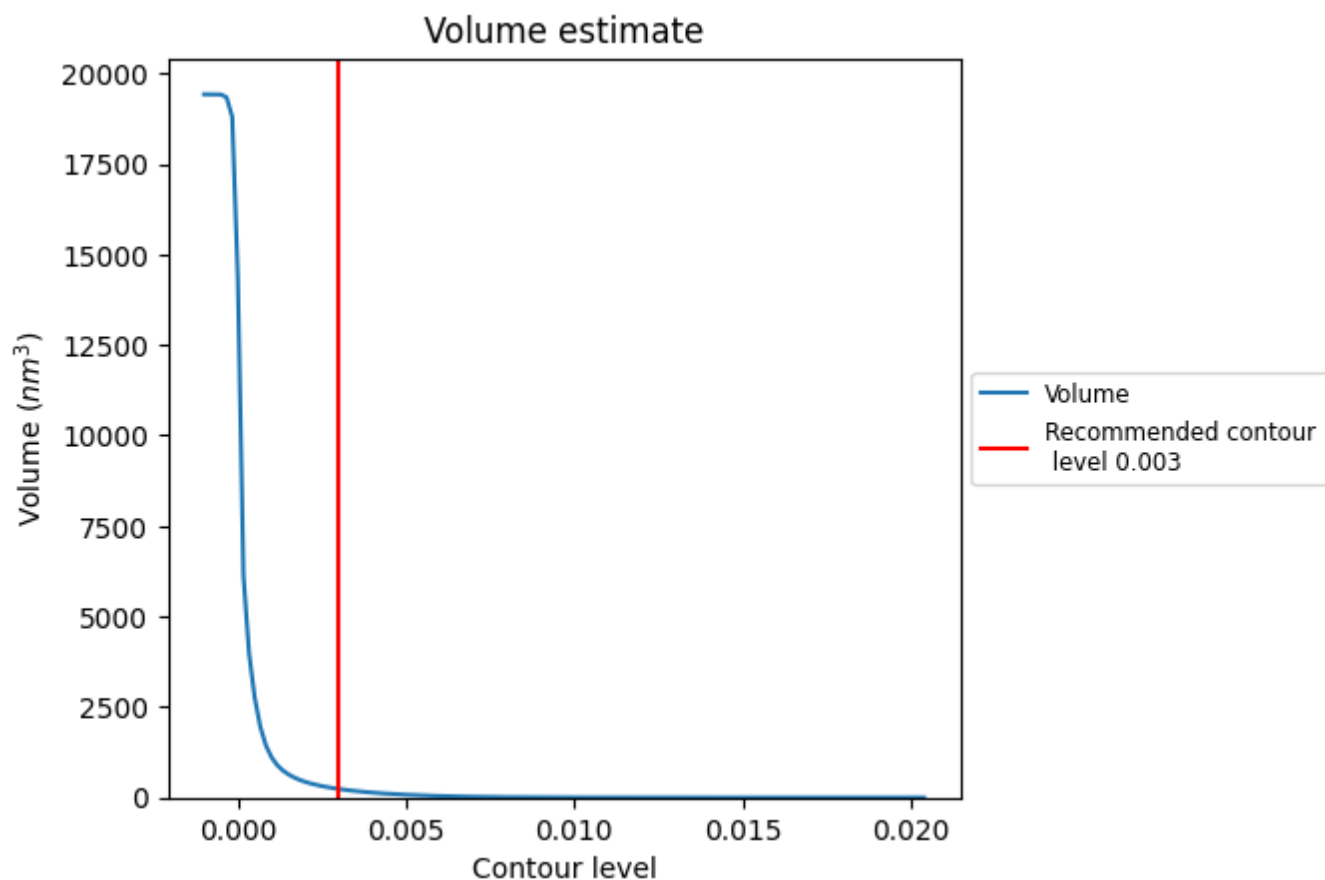
This section contains the results of statistical analysis of the map.

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.

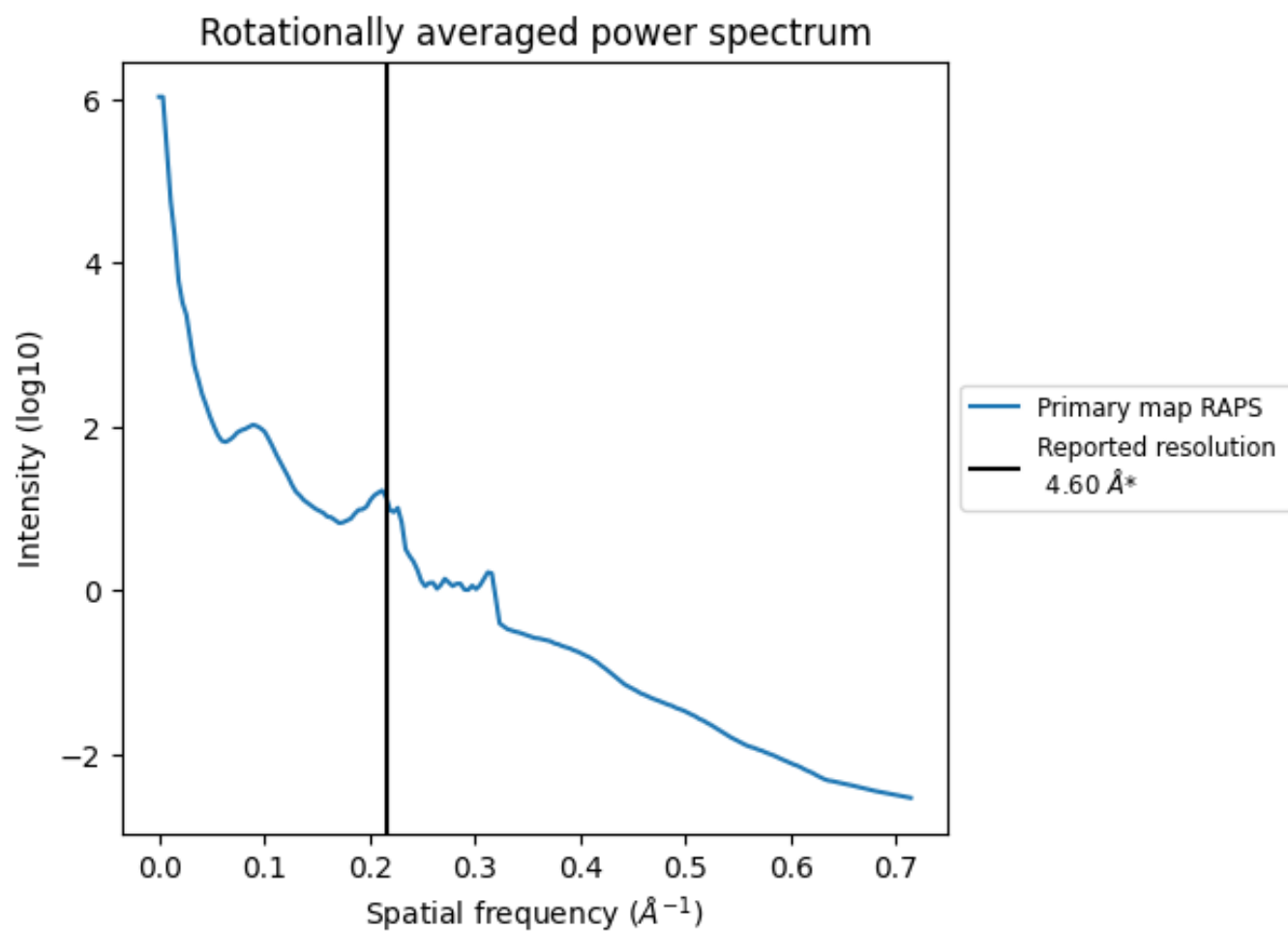
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm³; this corresponds to an approximate mass of 215 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 ⓘ

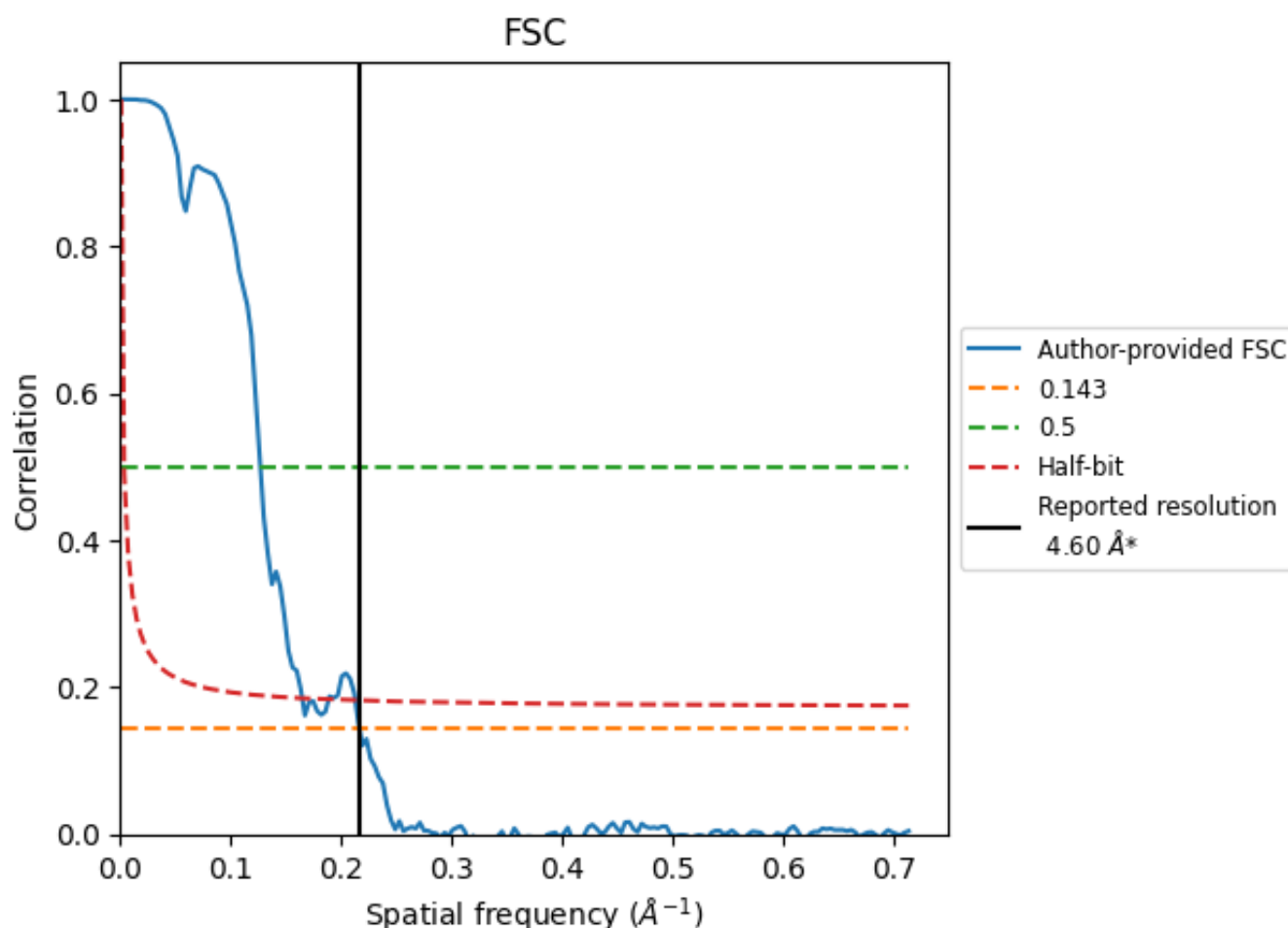


*Reported resolution corresponds to spatial frequency of 0.217 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

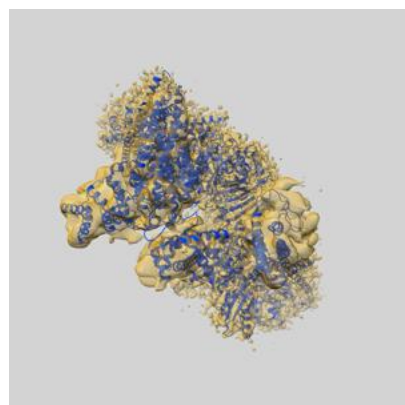
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	7.86	6.06
Unmasked-calculated*	-	-	-

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

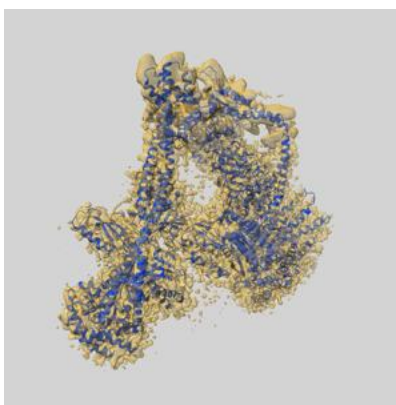
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14098 and PDB model 7QOO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

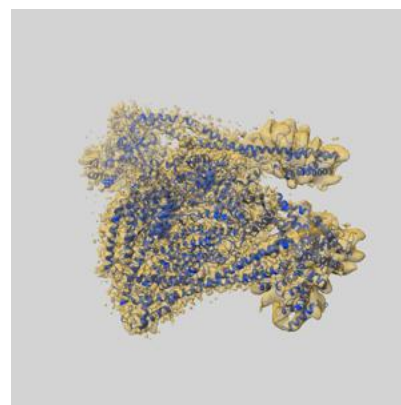
9.1 Map-model overlay [i](#)



X



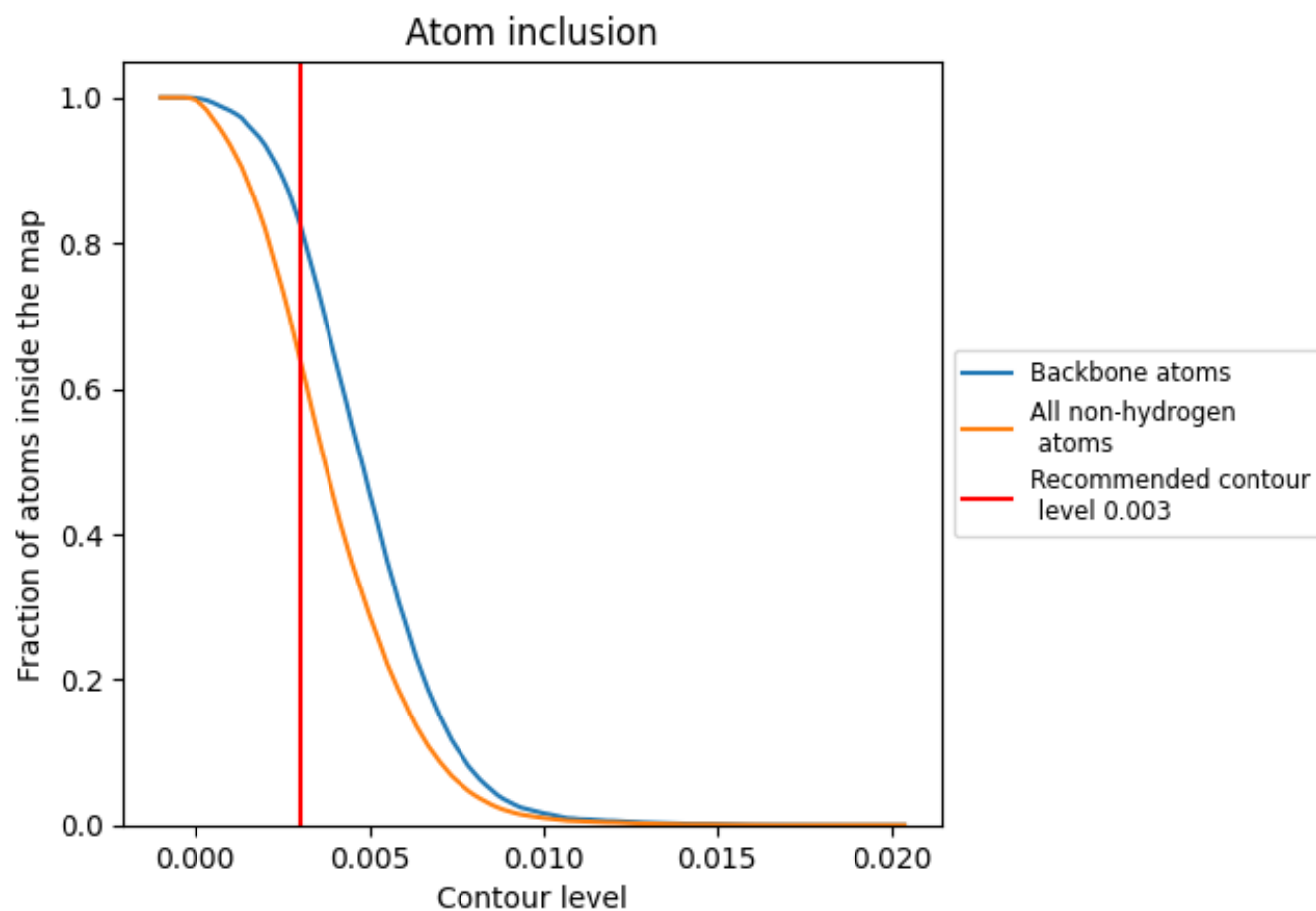
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 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 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.