



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:22 AM UTC

PDB ID : 7QOO / pdb_00007qoo
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

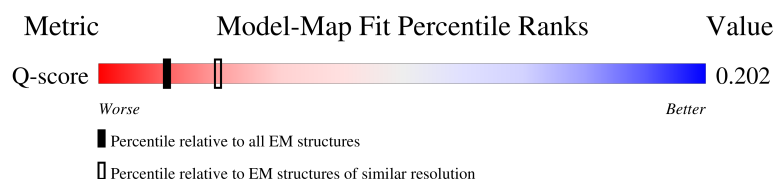
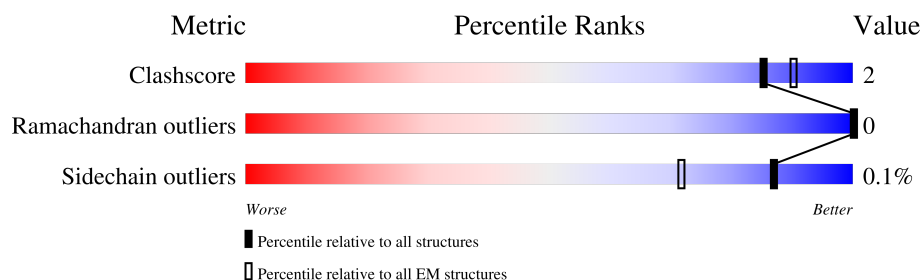
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

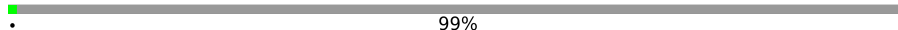
The reported resolution of this entry is 4.60 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	 99%
2	H	247	 9% 78% 7% 15%
3	I	756	 16% 75% 6% 18%
4	K	269	 12% 89% 5% 6%

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Mol	Chain	Length	Quality of chain
5	L	344	
6	M	180	
7	N	339	
8	O	300	
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.

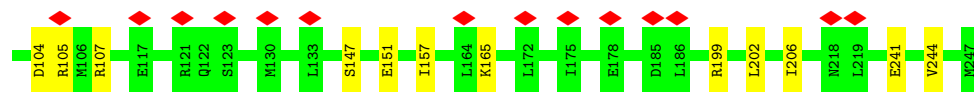
Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	108	Total	C	N	O	S	0	0
			878	564	152	155	7		

- Molecule 14 is a protein called Centromere protein W.

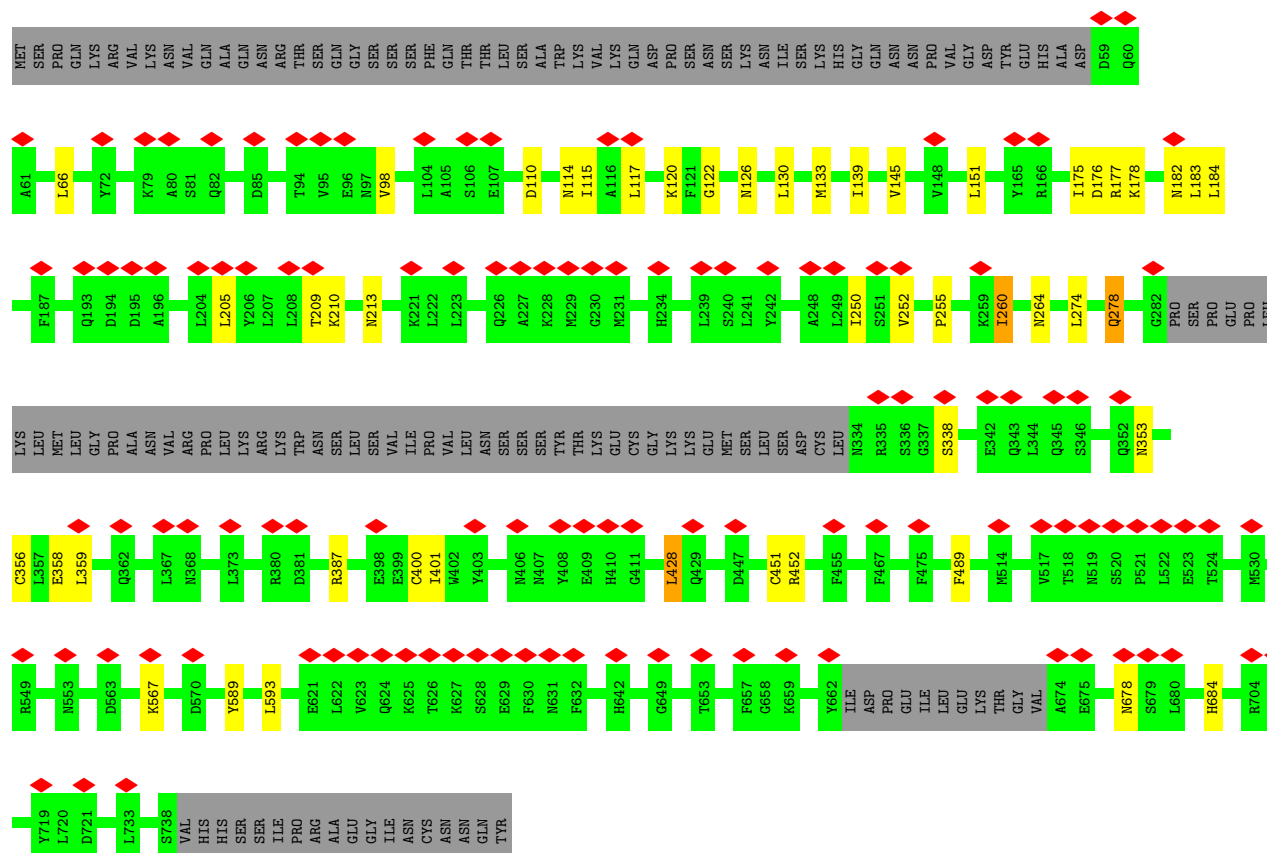
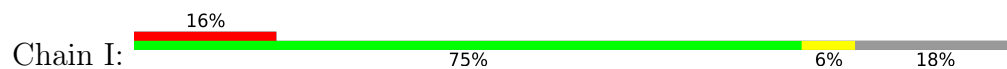
Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	72	Total	C	N	O	S	0	0
			575	364	116	92	3		

- Molecule 15 is a protein called Unknown protein.

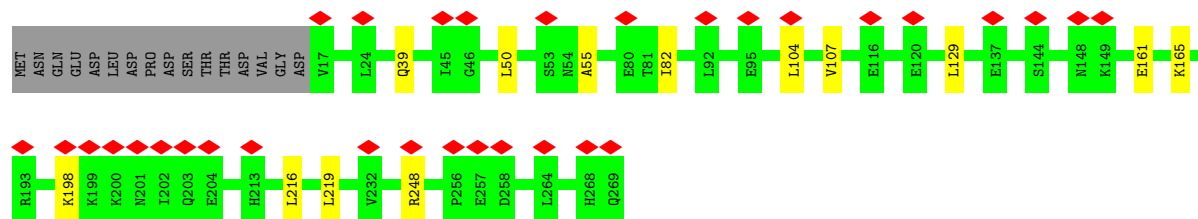
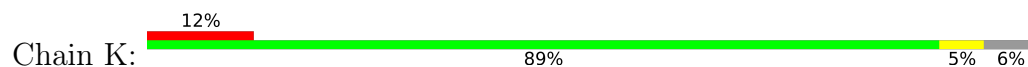
Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	15	Total	C	N	O	0	0
			76	45	15	16		



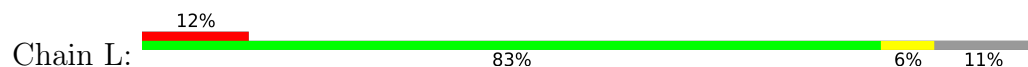
• Molecule 3: Centromere protein I

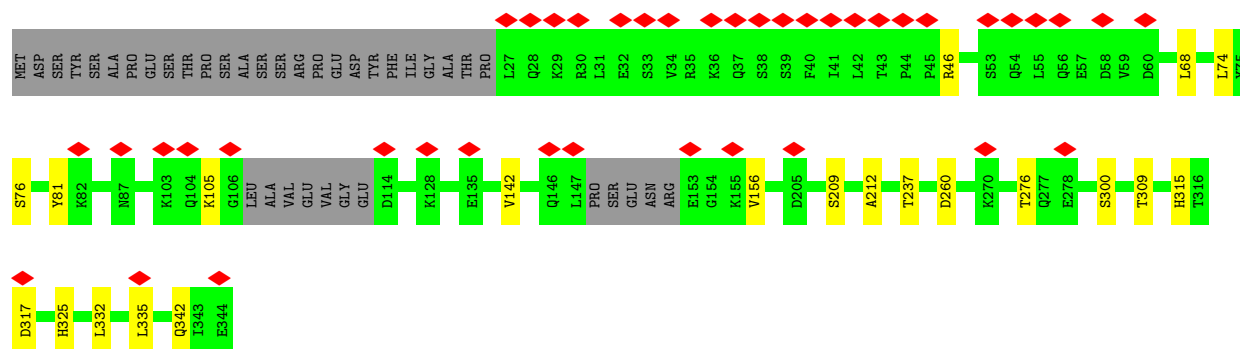


• Molecule 4: Centromere protein K

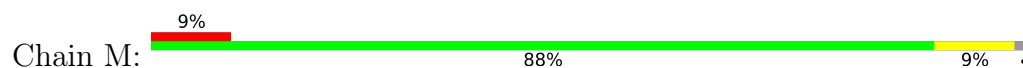


• Molecule 5: Centromere protein L

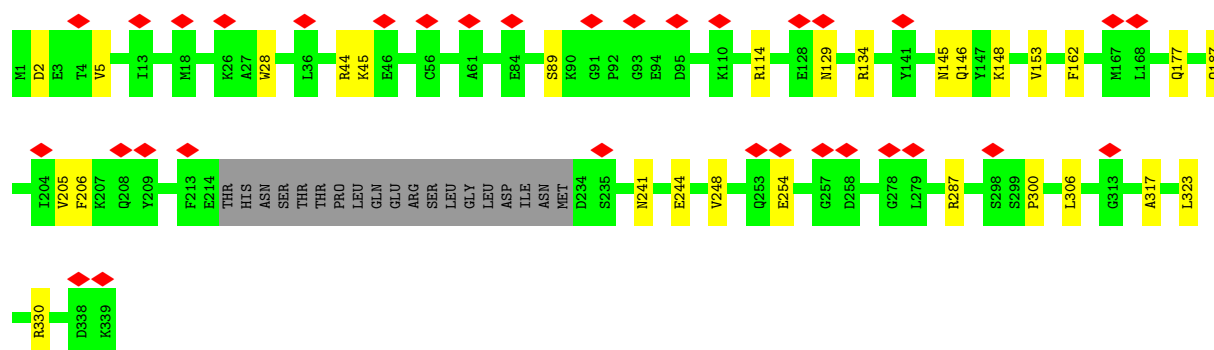
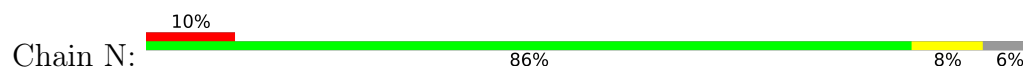




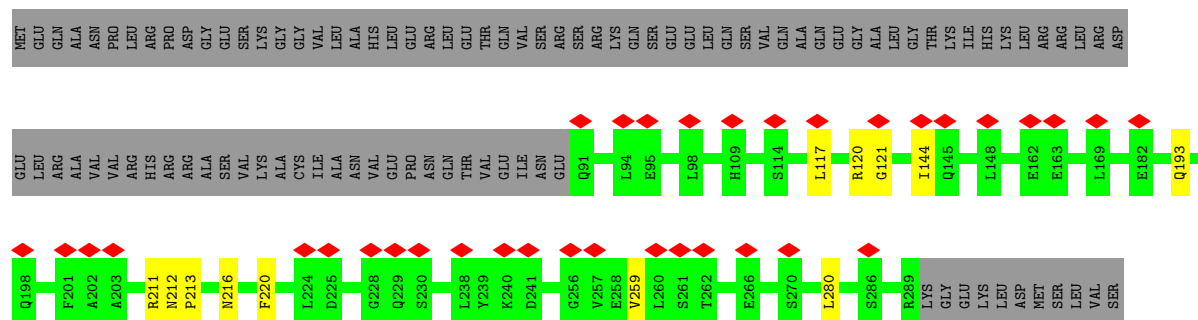
• Molecule 6: Centromere protein M



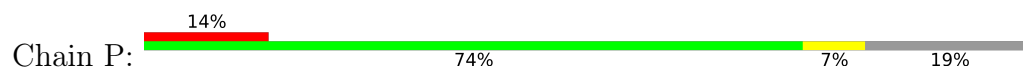
• Molecule 7: Centromere protein N

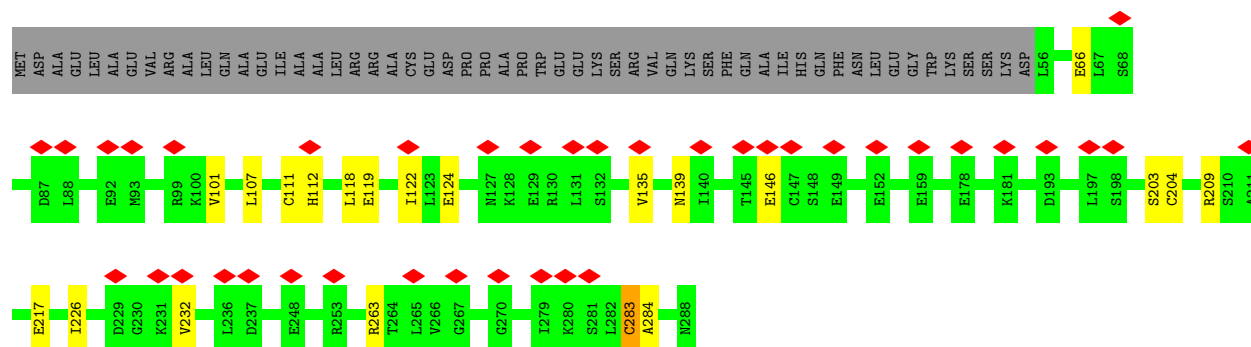


• Molecule 8: Centromere protein O

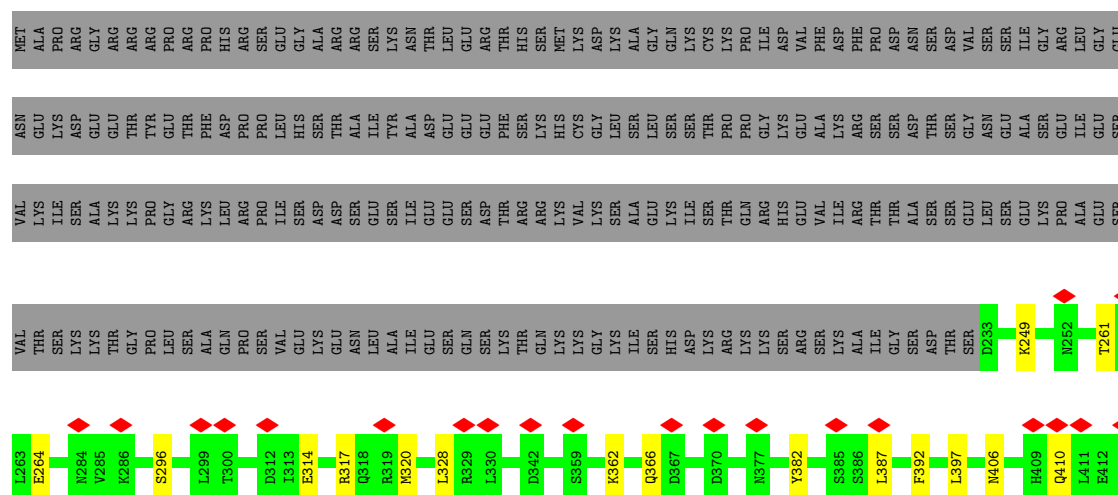
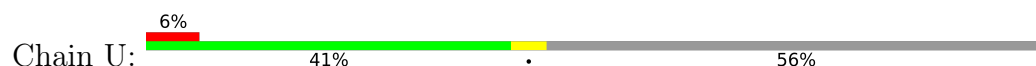


• Molecule 9: Centromere protein P

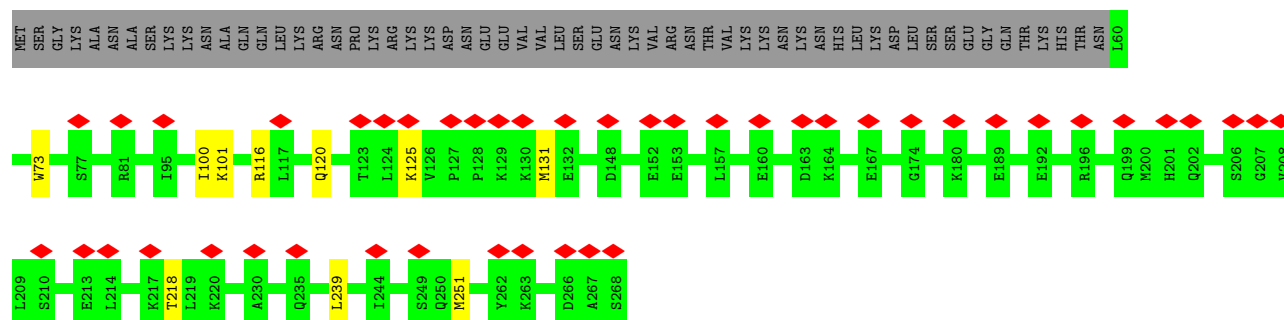
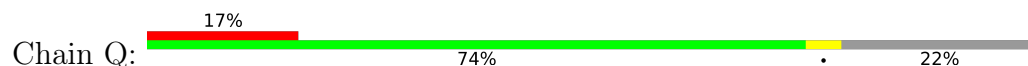




- Molecule 10: Centromere protein U

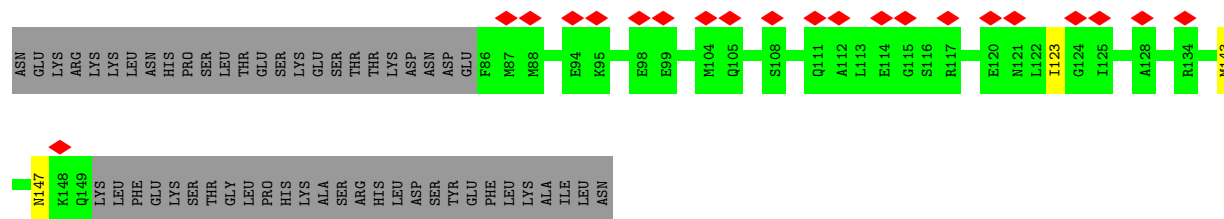


- Molecule 11: Centromere protein Q

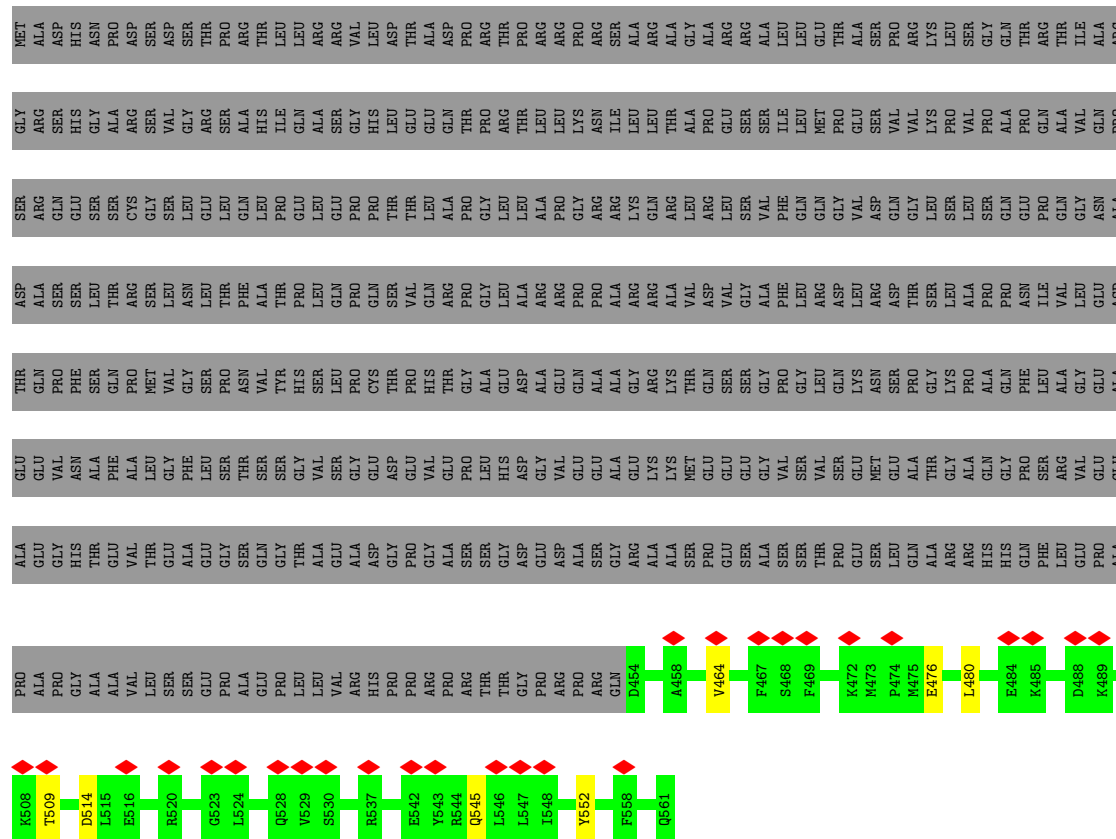


- Molecule 12: Centromere protein R

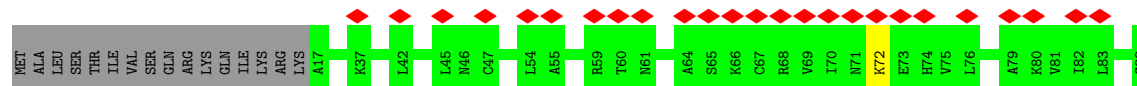
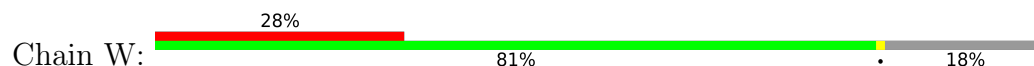




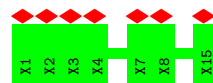
- Molecule 13: Centromere protein T



- 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	0.38	0/35	0.53	0/46
2	H	0.34	0/1743	0.60	0/2324
3	I	0.28	0/5172	0.60	7/7002 (0.1%)
4	K	0.24	0/2134	0.55	2/2874 (0.1%)
5	L	0.25	0/2532	0.52	2/3432 (0.1%)
6	M	0.24	0/1373	0.56	0/1862
7	N	0.31	0/2697	0.64	6/3637 (0.2%)
8	O	0.27	0/1622	0.51	0/2204
9	P	0.24	0/1924	0.53	2/2587 (0.1%)
10	U	0.27	0/1557	0.57	0/2087
11	Q	0.22	0/1683	0.55	0/2255
12	R	0.19	0/514	0.51	0/680
13	T	0.26	0/899	0.51	0/1211
14	W	0.22	0/582	0.55	0/773
All	All	0.27	0/24467	0.57	19/32974 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	278	GLN	CA-C-N	5.91	130.76	122.08
3	I	278	GLN	C-N-CA	5.91	130.76	122.08
3	I	260	ILE	CA-C-N	5.89	132.79	121.54
3	I	260	ILE	C-N-CA	5.89	132.79	121.54
7	N	28	TRP	CA-C-N	5.59	132.21	121.54
7	N	28	TRP	C-N-CA	5.59	132.21	121.54
3	I	451	CYS	CA-CB-SG	5.51	127.08	114.40
5	L	81	TYR	CA-C-N	5.46	129.88	122.07
5	L	81	TYR	C-N-CA	5.46	129.88	122.07
7	N	300	PRO	CA-C-N	5.34	130.40	122.82
7	N	300	PRO	C-N-CA	5.34	130.40	122.82
7	N	206	PHE	CA-C-N	5.20	129.51	122.07
7	N	206	PHE	C-N-CA	5.20	129.51	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	283	CYS	CA-C-N	5.10	129.80	122.40
9	P	283	CYS	C-N-CA	5.10	129.80	122.40
4	K	198	LYS	CA-C-N	5.10	131.28	121.54
4	K	198	LYS	C-N-CA	5.10	131.28	121.54
3	I	428	LEU	CA-C-N	5.06	130.99	123.05
3	I	428	LEU	C-N-CA	5.06	130.99	123.05

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	27	0
4	K	2100	0	2129	9	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	14	0
11	Q	1667	0	1740	9	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	109	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.

All (109) 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
7:N:241:ASN:HB3	7:N:244:GLU:HB3	1.89	0.54
6:M:67:VAL:HG12	6:M:98:CYS:HB3	1.90	0.53
5:L:68:LEU:HD11	5:L:325:HIS:HB3	1.90	0.53
8:O:121:GLY:HA2	8:O:144:ILE:HG12	1.91	0.53
6:M:40:CYS:SG	6:M:41:ALA:N	2.82	0.52
9:P:111:CYS:SG	9:P:112:HIS:N	2.82	0.52
2:H:107:ARG:HH12	4:K:82:ILE:HB	1.75	0.52
9:P:146:GLU:HA	10:U:406:ASN:HD21	1.75	0.52
3:I:400:CYS:SG	3:I:401:ILE:N	2.81	0.52
7:N:205:VAL:HG13	7:N:330:ARG:HD2	1.92	0.52
13:T:507:ARG:NH2	13:T:514:ASP:OD2	2.44	0.51
8:O:193:GLN:HB3	8:O:280:LEU:HD22	1.91	0.51
3:I:359:LEU:HD13	3:I:387:ARG:HH22	1.77	0.50
10:U:406:ASN:O	10:U:410:GLN:NE2	2.44	0.50
7:N:153:VAL:HB	7:N:162:PHE:HB2	1.92	0.50
7:N:129:ASN:HD22	8:O:213:PRO:HD3	1.76	0.50
7:N:254:GLU:O	8:O:120:ARG:NH1	2.44	0.50
2:H:199:ARG:HH21	2:H:202:LEU:HD22	1.77	0.50
10:U:362:LYS:O	10:U:366:GLN:NE2	2.45	0.50
9:P:101:VAL:HB	9:P:124:GLU:HB2	1.93	0.50
6:M:142:MET:SD	6:M:145:ARG:NH2	2.85	0.49
2:H:151:GLU:OE2	3:I:567:LYS:NZ	2.46	0.49
9:P:119:GLU:HB3	9:P:139:ASN:HB3	1.94	0.49
9:P:209:ARG:NH1	9:P:217:GLU:OE2	2.46	0.48
13:T:507:ARG:NH1	13:T:509:THR:O	2.45	0.48
4:K:104:LEU:HA	4:K:107:VAL:HG12	1.95	0.48
9:P:283:CYS:SG	9:P:284:ALA:N	2.80	0.48
2:H:147:SER:O	2:H:151:GLU:HB2	2.13	0.48
2:H:165:LYS:NZ	3:I:428:LEU:O	2.45	0.47
10:U:249:LYS:HD3	11:Q:131:MET:HE3	1.95	0.47
5:L:237:THR:HG23	5:L:309:THR:HG22	1.96	0.47
3:I:66:LEU:HD22	3:I:98:VAL:HG11	1.96	0.47
2:H:57:TYR:OH	6:M:62:ARG:NH1	2.48	0.47
5:L:142:VAL:HG22	5:L:156:VAL:HG22	1.96	0.47
5:L:260:ASP:OD1	7:N:287:ARG:NH2	2.48	0.47
9:P:122:ILE:HG12	9:P:135:VAL:HG22	1.95	0.47
10:U:264:GLU:OE1	11:Q:116:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:134:ARG:NH2	7:N:146:GLN:OE1	2.47	0.47
2:H:104:ASP:OD1	2:H:107:ARG:NH2	2.49	0.46
3:I:678:ASN:O	3:I:684:HIS:ND1	2.46	0.46
4:K:248:ARG:NH1	13:T:545:GLN:OE1	2.48	0.46
3:I:110:ASP:O	3:I:114:ASN:ND2	2.48	0.46
6:M:20:LEU:HB3	6:M:28:LEU:HD23	1.96	0.46
12:R:143:MET:O	12:R:147:ASN:ND2	2.49	0.46
10:U:249:LYS:NZ	10:U:296:SER:OG	2.48	0.46
10:U:261:THR:HG21	11:Q:120:GLN:HG3	1.98	0.46
3:I:130:LEU:HA	3:I:133:MET:HE3	1.98	0.46
9:P:263:ARG:NH2	11:Q:218:THR:O	2.48	0.46
3:I:353:ASN:HD21	3:I:356:CYS:HB2	1.79	0.46
9:P:203:SER:OG	9:P:204:CYS:N	2.49	0.46
10:U:382:TYR:HB2	11:Q:239:LEU:HD21	1.97	0.46
8:O:117:LEU:HD13	9:P:66:GLU:HG2	1.98	0.45
4:K:161:GLU:HG2	4:K:165:LYS:HZ1	1.81	0.45
8:O:212:ASN:ND2	8:O:216:ASN:OD1	2.49	0.45
3:I:210:LYS:H	3:I:213:ASN:HD22	1.65	0.45
7:N:248:VAL:HG12	7:N:317:ALA:HB2	1.99	0.45
3:I:117:LEU:HD22	3:I:151:LEU:HD21	1.99	0.45
3:I:260:ILE:O	3:I:264:ASN:ND2	2.50	0.45
11:Q:73:TRP:HB3	11:Q:125:LYS:HB3	1.98	0.44
3:I:176:ASP:OD1	3:I:177:ARG:NH1	2.51	0.44
5:L:46:ARG:HG2	5:L:276:THR:HG22	2.00	0.44
3:I:122:GLY:O	3:I:126:ASN:ND2	2.51	0.44
7:N:177:GLN:HE21	10:U:328:LEU:HD23	1.82	0.44
2:H:86:GLU:HA	2:H:89:ILE:HG22	1.99	0.43
10:U:397:LEU:HD22	11:Q:251:MET:HE3	1.99	0.43
3:I:178:LYS:O	3:I:182:ASN:ND2	2.50	0.43
5:L:315:HIS:ND1	5:L:317:ASP:OD1	2.49	0.43
4:K:216:LEU:HD23	4:K:219:LEU:HD12	2.00	0.43
3:I:255:PRO:HA	5:L:105:LYS:HE2	2.01	0.43
6:M:174:GLY:HA2	6:M:175:PRO:HD3	1.92	0.43
9:P:226:ILE:HG12	9:P:232:VAL:HG22	2.00	0.43
4:K:248:ARG:NH1	13:T:552:TYR:OH	2.51	0.43
10:U:314:GLU:OE1	10:U:317:ARG:NH2	2.52	0.43
5:L:76:SER:OG	5:L:209:SER:OG	2.37	0.43
10:U:387:LEU:HD13	11:Q:239:LEU:HD12	2.01	0.43
2:H:98:ILE:HD12	3:I:589:TYR:HB2	2.00	0.42
3:I:452:ARG:HD2	3:I:489:PHE:HD1	1.84	0.42
4:K:39:GLN:NE2	6:M:8:ASP:O	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:129:ASN:ND2	8:O:211:ARG:O	2.52	0.42
2:H:206:ILE:HG12	2:H:244:VAL:HG11	2.01	0.42
13:T:464:VAL:HG13	13:T:480:LEU:HD22	2.02	0.42
10:U:392:PHE:HE1	12:R:123:ILE:HG23	1.84	0.42
13:T:476:GLU:OE1	14:W:72:LYS:NZ	2.47	0.42
2:H:83:GLU:HA	2:H:86:GLU:HG2	2.02	0.42
3:I:250:ILE:HG22	3:I:252:VAL:H	1.84	0.42
5:L:74:LEU:HD21	5:L:335:LEU:HD13	2.01	0.42
2:H:241:GLU:HG2	3:I:183:LEU:HA	2.02	0.41
3:I:205:LEU:O	3:I:209:THR:OG1	2.37	0.41
7:N:44:ARG:HE	7:N:45:LYS:H	1.68	0.41
7:N:306:LEU:HD13	7:N:323:LEU:HD13	2.02	0.41
3:I:145:VAL:HA	3:I:184:LEU:HD11	2.01	0.41
3:I:274:LEU:HD22	3:I:278:GLN:HG2	2.01	0.41
7:N:89:SER:HB2	7:N:187:GLN:HB3	2.01	0.41
7:N:114:ARG:NH1	10:U:320:MET:SD	2.93	0.41
5:L:332:LEU:HD23	5:L:335:LEU:HD12	2.02	0.41
3:I:338:SER:HB2	3:I:358:GLU:HB3	2.02	0.41
4:K:50:LEU:HD11	4:K:55:ALA:HA	2.02	0.41
6:M:19:LEU:HB3	6:M:66:ILE:HG12	2.02	0.41
7:N:2:ASP:HB3	7:N:5:VAL:HG22	2.03	0.41
9:P:107:LEU:HB2	9:P:118:LEU:HB2	2.03	0.41
7:N:145:ASN:HD21	7:N:148:LYS:HE3	1.85	0.41
3:I:139:ILE:HB	3:I:175:ILE:HG12	2.02	0.41
2:H:157:ILE:HG23	4:K:129:LEU:HD22	2.02	0.40
11:Q:100:ILE:HG22	11:Q:101:LYS:HG3	2.03	0.40

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%)	3 (75%)	1 (25%)	0	4
2	H	200/224 (89%)	200 (100%)	0	100	100
3	I	565/691 (82%)	565 (100%)	0	100	100
4	K	245/260 (94%)	245 (100%)	0	100	100
5	L	274/306 (90%)	274 (100%)	0	100	100
6	M	154/158 (98%)	152 (99%)	2 (1%)	61	72
7	N	293/311 (94%)	293 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	O	176/263 (67%)	175 (99%)	1 (1%)	78	80
9	P	214/259 (83%)	214 (100%)	0	100	100
10	U	173/379 (46%)	173 (100%)	0	100	100
11	Q	194/248 (78%)	194 (100%)	0	100	100
12	R	60/166 (36%)	60 (100%)	0	100	100
13	T	96/461 (21%)	96 (100%)	0	100	100
14	W	62/77 (80%)	62 (100%)	0	100	100
All	All	2710/4311 (63%)	2706 (100%)	4 (0%)	87	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	304	ILE
6	M	7	LEU
6	M	146	LEU
8	O	259	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	115	ASN
2	H	122	GLN
2	H	163	GLN
2	H	180	ASN
2	H	191	ASN
3	I	114	ASN
3	I	182	ASN
3	I	193	GLN
3	I	213	ASN
3	I	226	GLN
3	I	278	GLN
3	I	353	ASN
3	I	394	GLN
3	I	502	GLN
3	I	503	ASN
3	I	559	HIS
3	I	642	HIS
4	K	63	GLN

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Mol	Chain	Res	Type
4	K	73	GLN
4	K	115	ASN
4	K	168	ASN
5	L	51	GLN
5	L	69	HIS
5	L	71	GLN
5	L	214	ASN
6	M	87	HIS
7	N	40	ASN
7	N	113	GLN
7	N	129	ASN
7	N	145	ASN
7	N	177	GLN
7	N	210	ASN
7	N	301	HIS
8	O	109	HIS
8	O	152	HIS
8	O	185	ASN
8	O	267	GLN
9	P	103	GLN
9	P	117	GLN
9	P	287	ASN
9	P	288	ASN
10	U	252	ASN
10	U	265	HIS
10	U	306	ASN
10	U	366	GLN
10	U	406	ASN
10	U	410	GLN
11	Q	151	ASN
11	Q	181	ASN
11	Q	202	GLN
11	Q	247	ASN
12	R	130	HIS
13	T	538	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

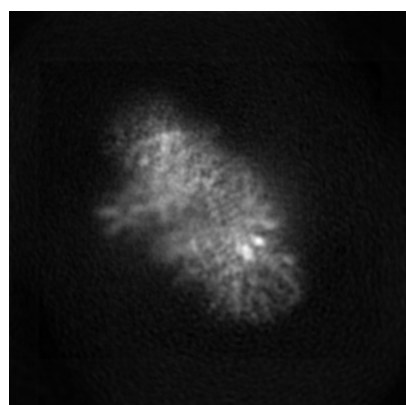
6 Map visualisation [i](#)

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

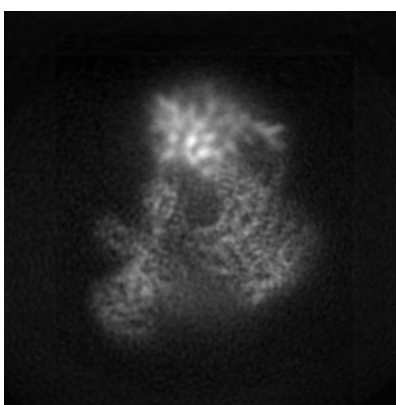
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

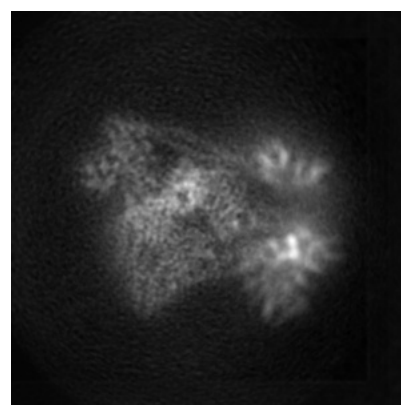
6.1.1 Primary map



X



Y

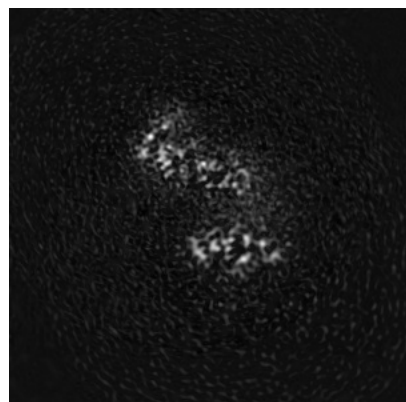


Z

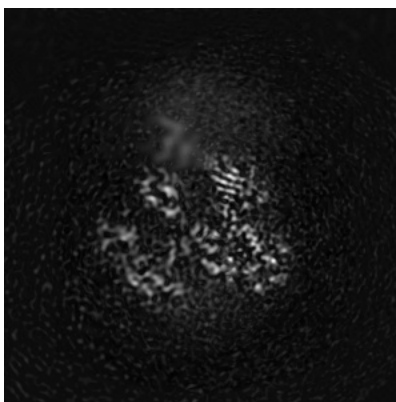
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

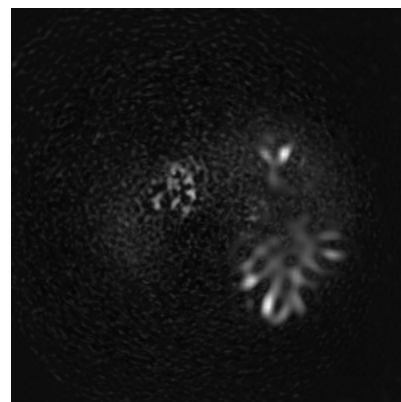
6.2.1 Primary map



X Index: 192



Y Index: 192

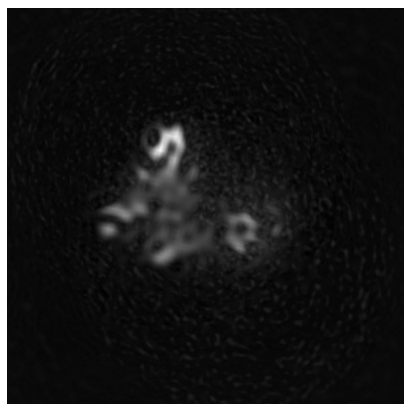


Z Index: 192

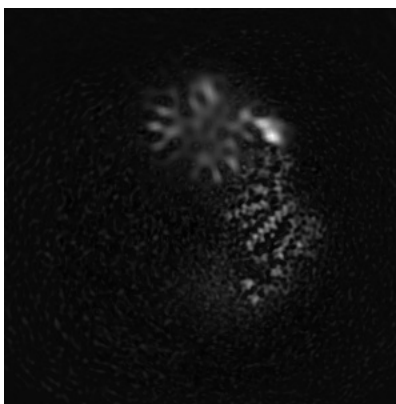
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

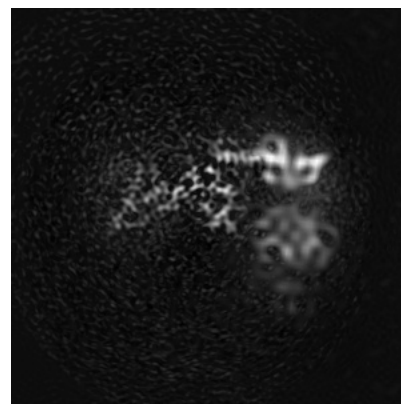
6.3.1 Primary map



X Index: 271



Y Index: 148

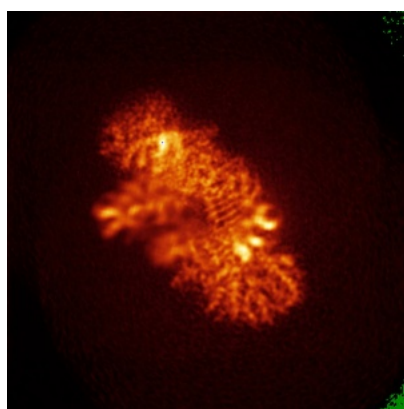


Z Index: 162

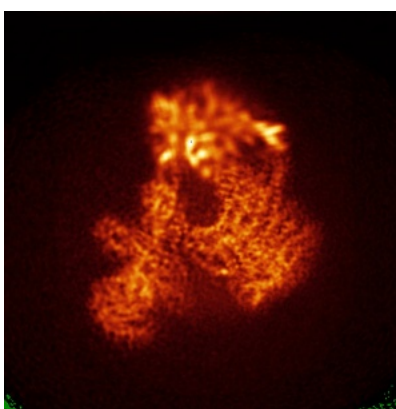
The images above show the largest variance slices of the map in three orthogonal directions.

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

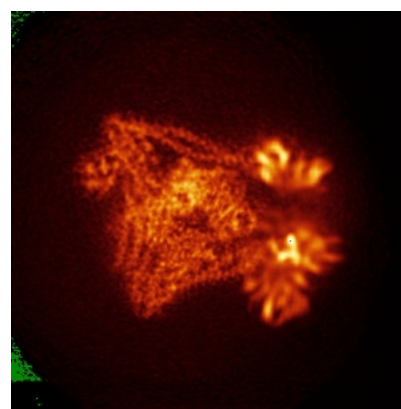
6.4.1 Primary map



X



Y

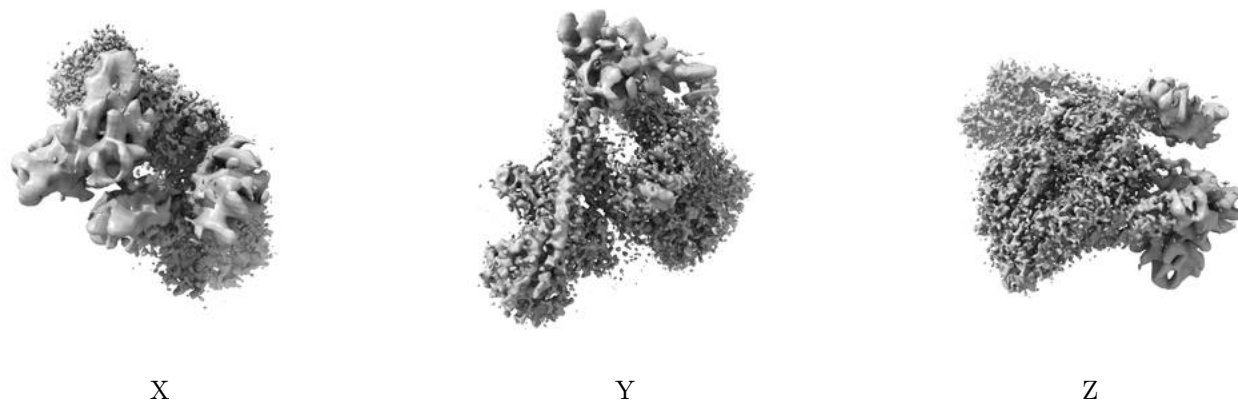


Z

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 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

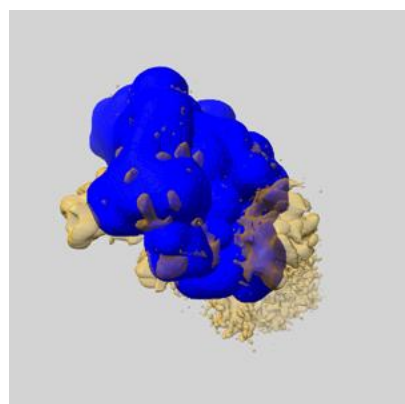
6.6 Mask visualisation [i](#)

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

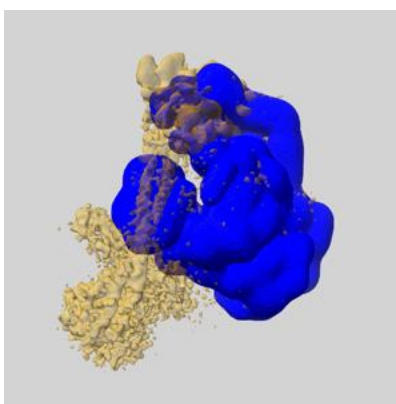
A mask typically either:

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

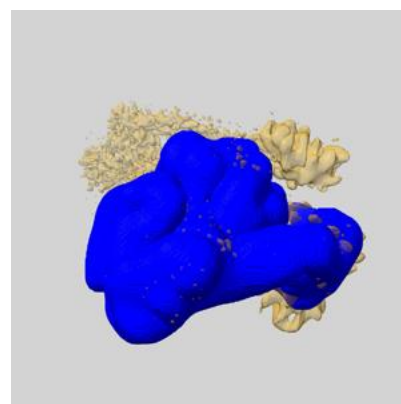
6.6.1 emd_14098_msk_1.map [i](#)



X

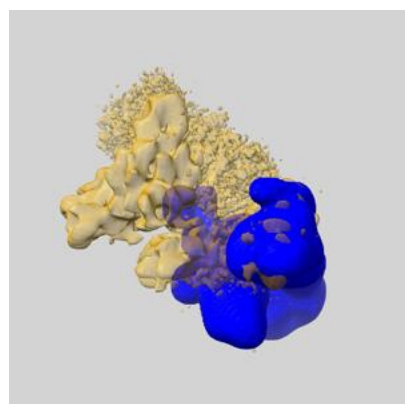


Y

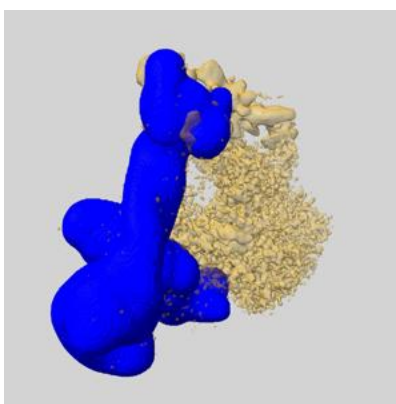


Z

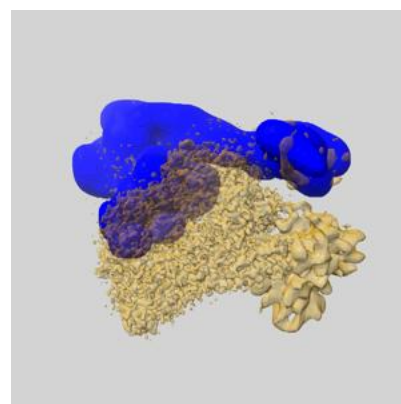
6.6.2 emd_14098_msk_2.map [i](#)



X

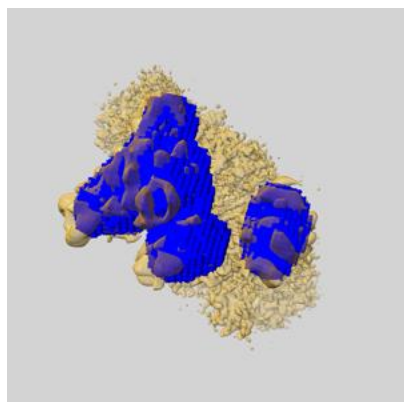


Y

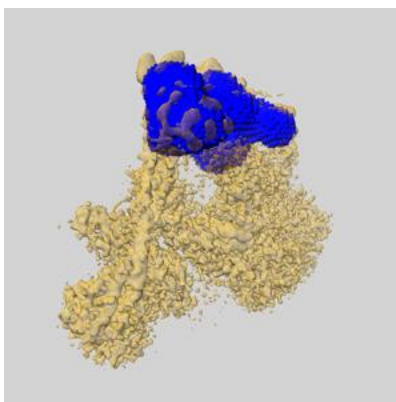


Z

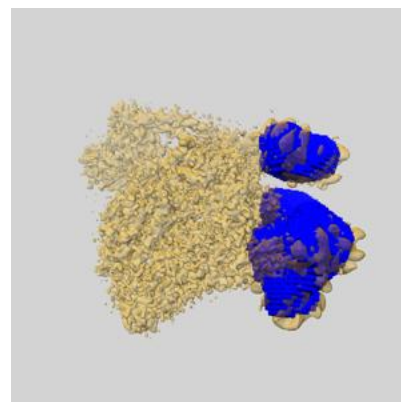
6.6.3 emd_14098_msk_3.map [i](#)



X



Y

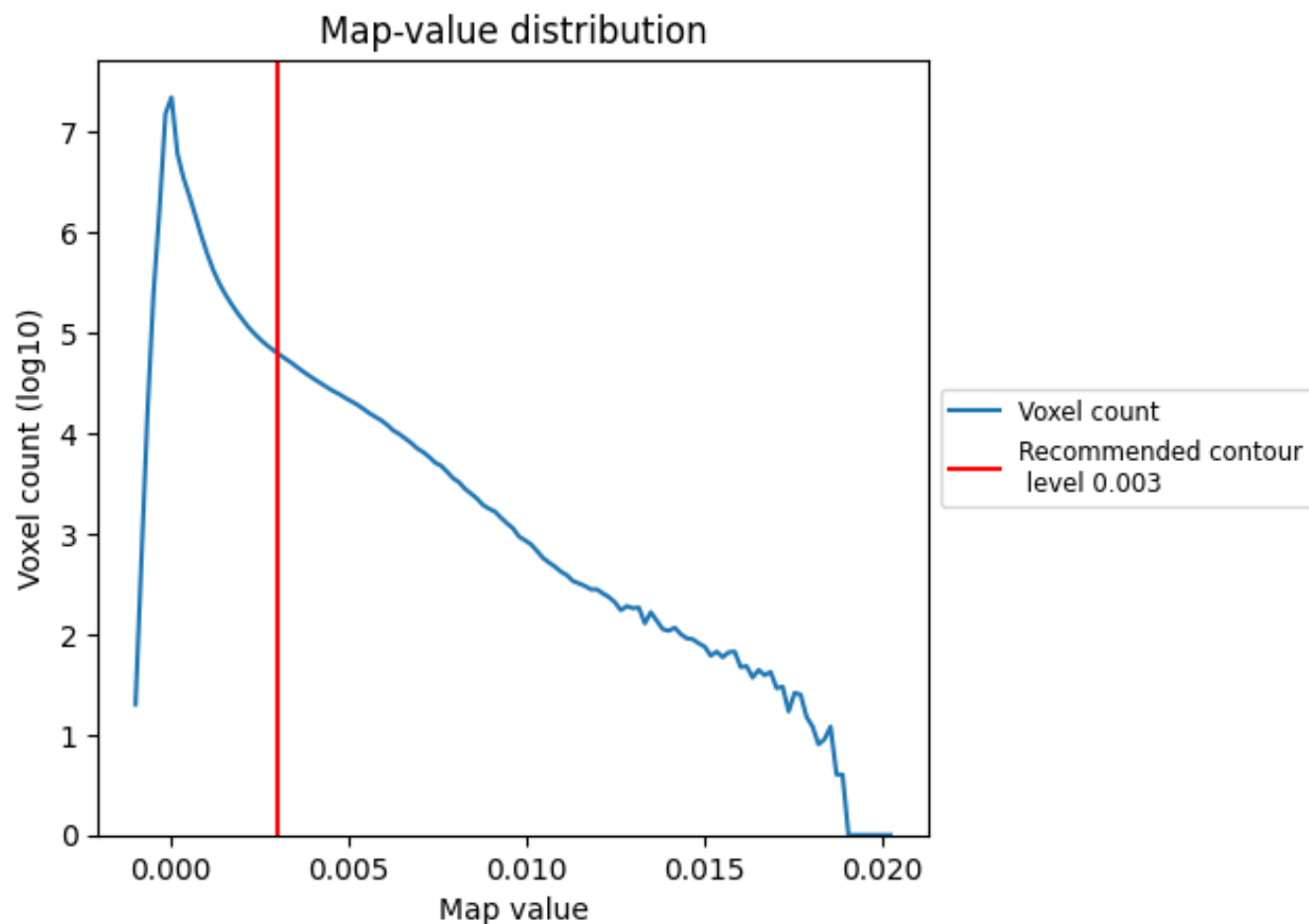


Z

7 Map analysis [i](#)

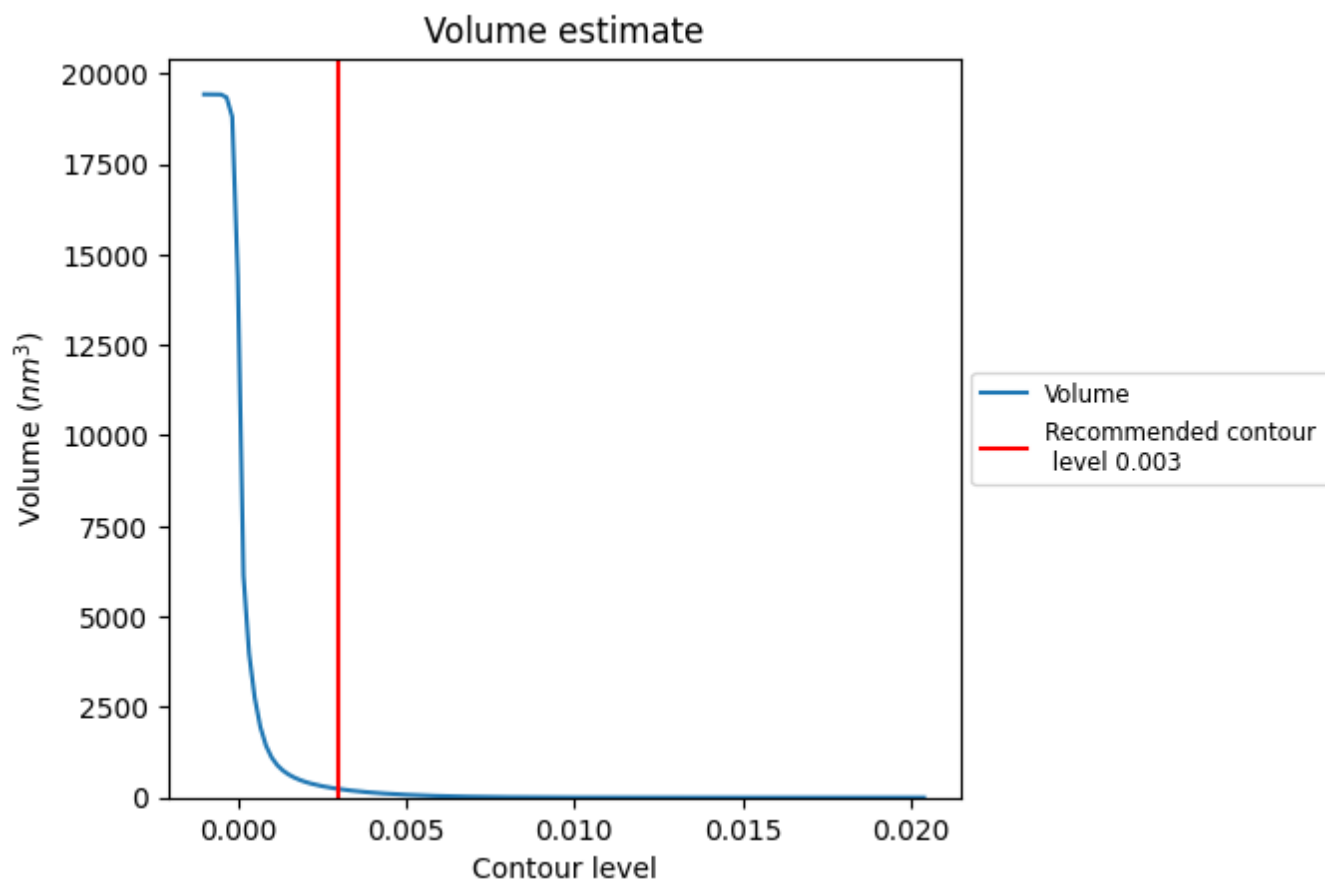
This section contains the results of statistical analysis of the map.

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.

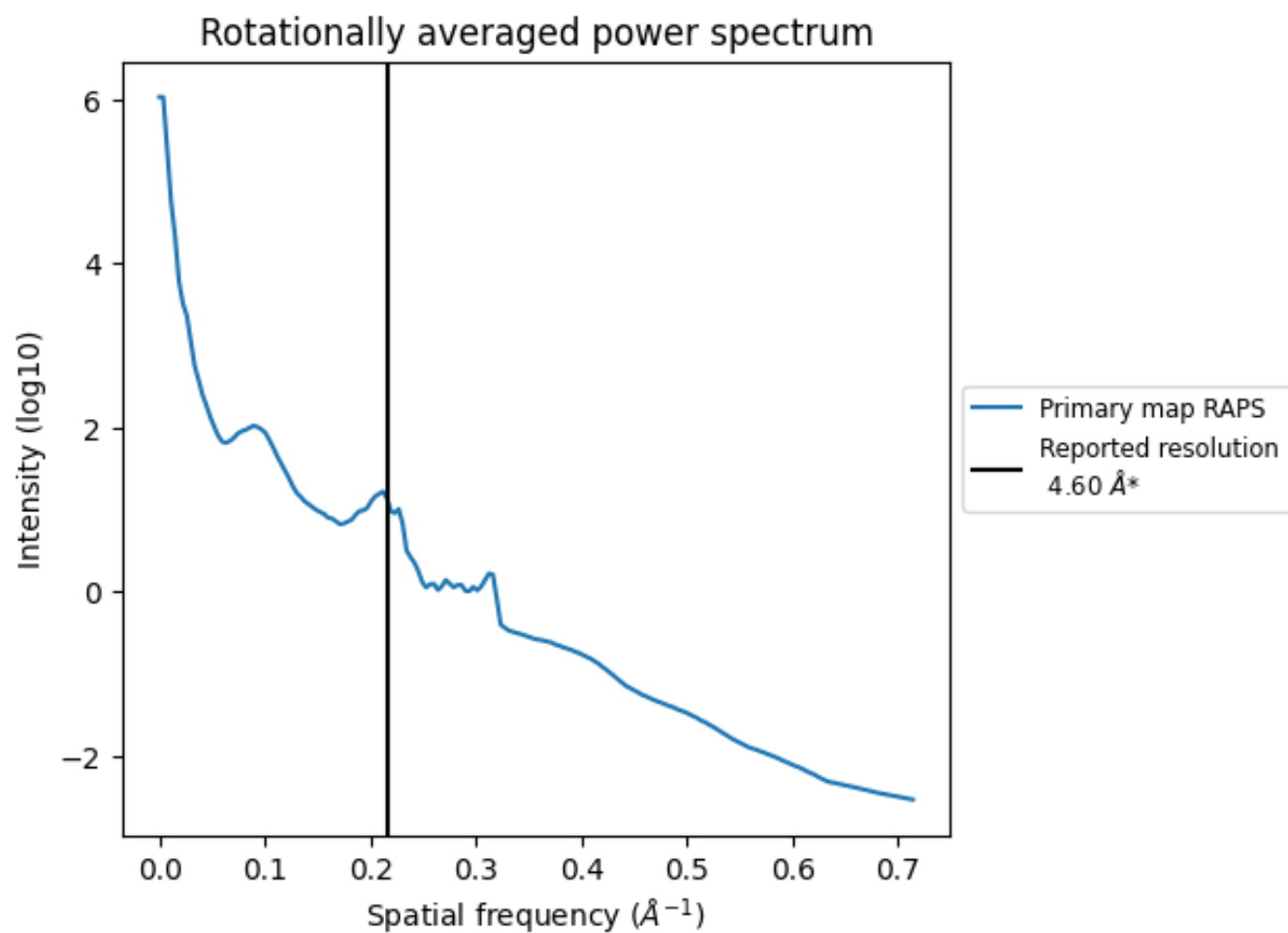
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm^3 ; 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 ⓘ

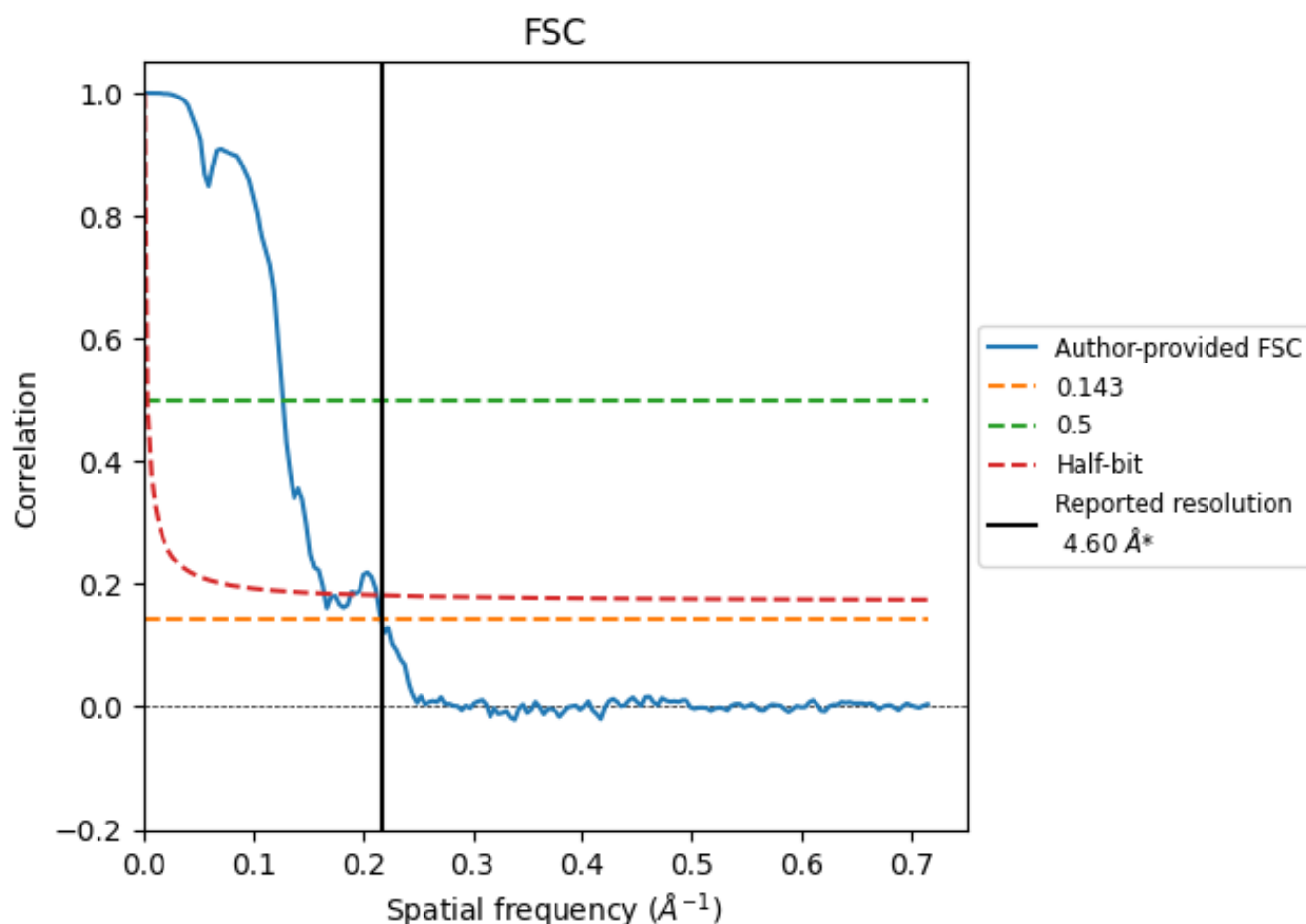


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

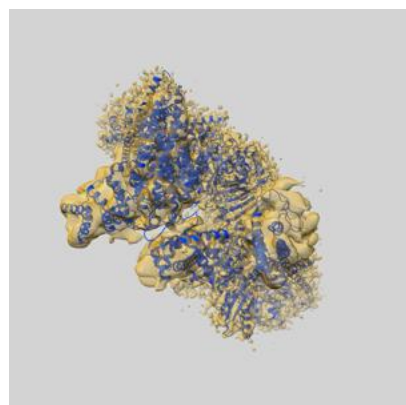
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	7.86	6.06
Unmasked-calculated*	-	-	-

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

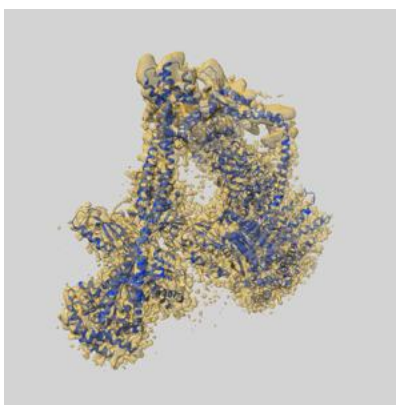
9 Map-model fit [i](#)

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](#).

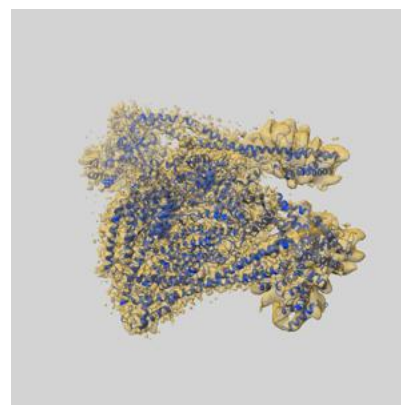
9.1 Map-model overlay [i](#)



X



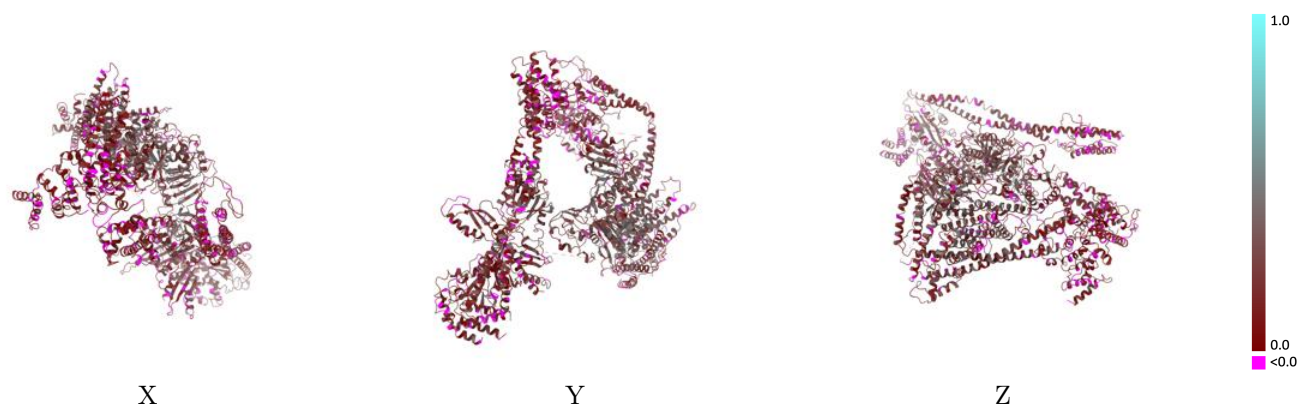
Y



Z

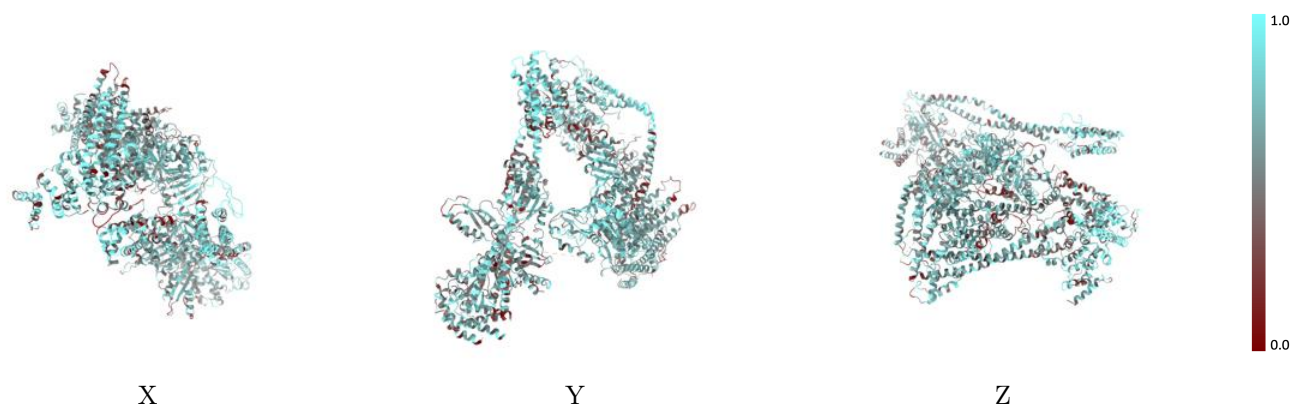
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



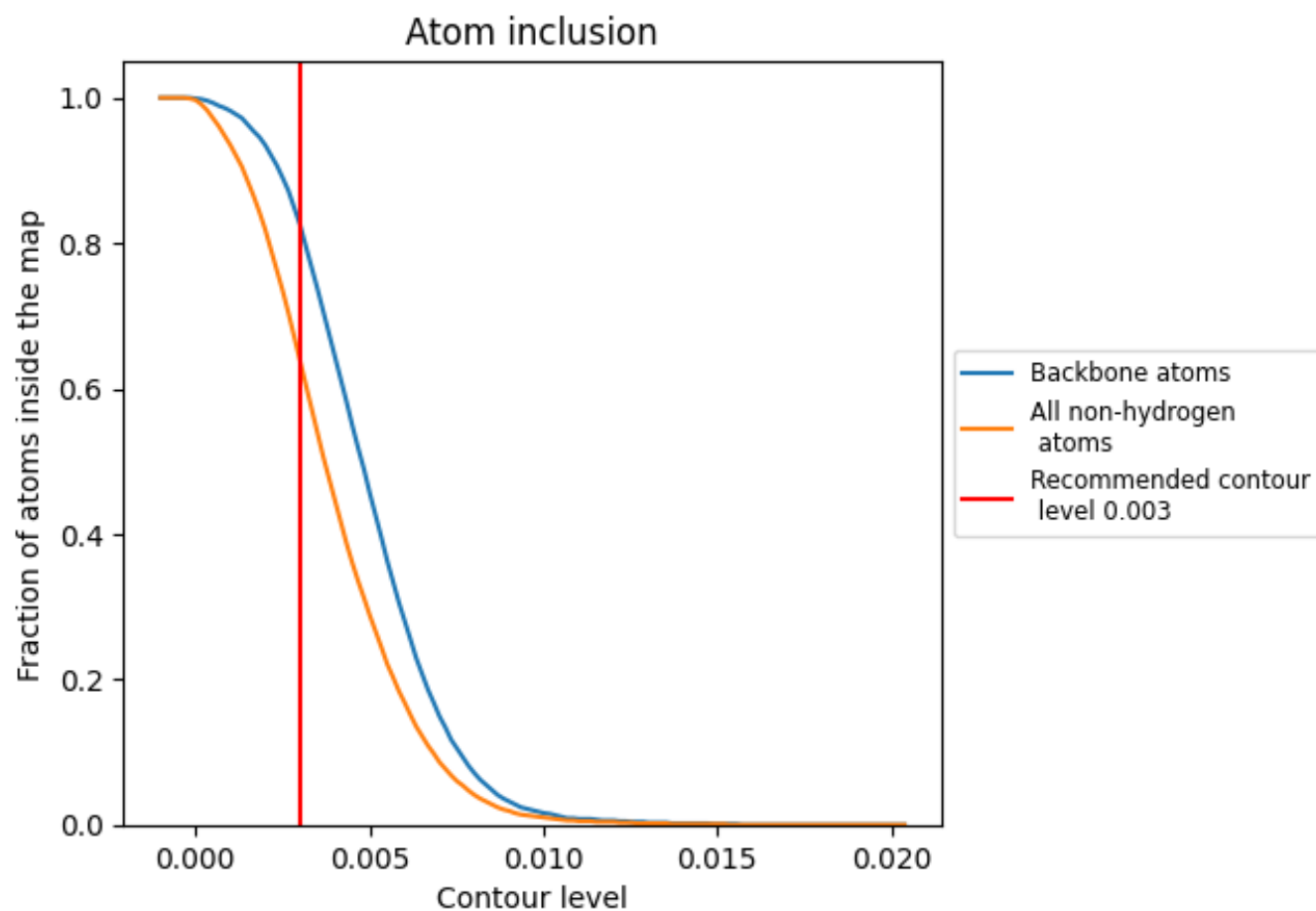
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 64% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.2020
C	 0.5710	 0.1940
H	 0.6590	 0.1950
I	 0.6290	 0.2040
K	 0.6800	 0.1770
L	 0.6450	 0.2620
M	 0.6700	 0.3220
N	 0.6510	 0.2430
O	 0.6040	 0.1960
P	 0.6200	 0.2050
Q	 0.6390	 0.1320
R	 0.5550	 0.1460
T	 0.6170	 0.1150
U	 0.6980	 0.1590
W	 0.5260	 0.0900
X	 0.4740	 0.2310

