



wwPDB EM Validation Summary Report ⓘ

Jul 18, 2026 – 07:57 am BST

PDB ID : 9TAW / pdb_00009taw
EMDB ID : EMD-55757
Title : Structure of the human inner kinetochore CCAN bound to DNA
Authors : Yu, C.; Muir, K.W.; Barford, D.
Deposited on : 2025-11-18
Resolution : 3.54 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:

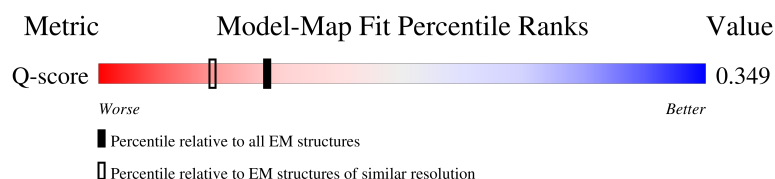
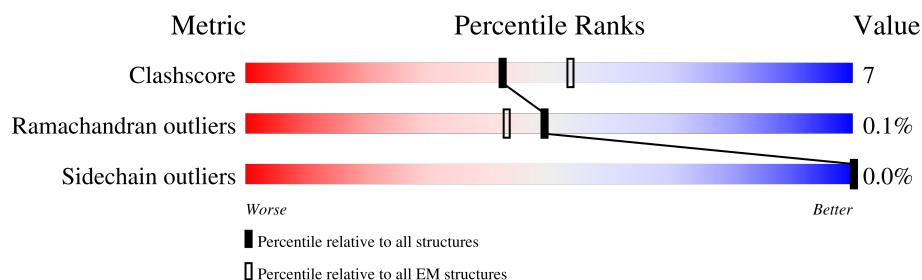
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.54 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	12891 (3.04 - 4.04)

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

Mol	Chain	Length	Quality of chain
1	A	171	 8% 22% 26% 52%
2	B	171	 5% 23% 23% 53%
3	H	247	 68% 15% 17%
4	I	762	 68% 13% 18%

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Mol	Chain	Length	Quality of chain
5	K	269	
6	L	348	
7	M	180	
8	N	339	
9	O	300	
10	P	288	
11	Q	215	
12	R	177	
13	S	138	
14	T	777	
15	U	211	
16	W	88	
17	X	81	
18	b	775	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 28846 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 DNA chain called DNA (82-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	82	Total	C	N	O	P	0	0
			1682	805	311	484	82		

- Molecule 2 is a DNA chain called DNA (80-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	80	Total	C	N	O	P	0	0
			1641	788	286	487	80		

- Molecule 3 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	204	Total	C	N	O	S	0	0
			1652	1036	286	319	11		

- Molecule 4 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	622	Total	C	N	O	S	0	0
			5014	3283	810	890	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	757	GLU	-	expression tag	UNP Q92674
I	758	ASN	-	expression tag	UNP Q92674
I	759	LEU	-	expression tag	UNP Q92674
I	760	TYR	-	expression tag	UNP Q92674
I	761	PHE	-	expression tag	UNP Q92674
I	762	GLN	-	expression tag	UNP Q92674

- Molecule 5 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	233	Total	C	N	O	S	0	0
			1922	1220	318	374	10		

- Molecule 6 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	312	Total	C	N	O	S	0	0
			2502	1628	409	451	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	expression tag	UNP Q8N0S6
L	-2	PRO	-	expression tag	UNP Q8N0S6
L	-1	LEU	-	expression tag	UNP Q8N0S6
L	0	GLY	-	expression tag	UNP Q8N0S6

- Molecule 7 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	172	Total	C	N	O	S	0	0
			1325	839	236	243	7		

- Molecule 8 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	318	Total	C	N	O	S	0	0
			2613	1678	453	472	10		

- Molecule 9 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	210	Total	C	N	O	S	0	0
			1642	1060	277	298	7		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1	MET	-	initiating methionine	UNP Q9BU64
O	2	GLU	-	expression tag	UNP Q9BU64
O	3	GLN	-	expression tag	UNP Q9BU64
O	4	ALA	-	expression tag	UNP Q9BU64

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Chain	Residue	Modelled	Actual	Comment	Reference
O	5	ASN	-	expression tag	UNP Q9BU64
O	6	PRO	-	expression tag	UNP Q9BU64
O	7	LEU	-	expression tag	UNP Q9BU64
O	8	ARG	-	expression tag	UNP Q9BU64
O	9	PRO	-	expression tag	UNP Q9BU64
O	10	ASP	-	expression tag	UNP Q9BU64
O	11	GLY	-	expression tag	UNP Q9BU64
O	12	GLU	-	expression tag	UNP Q9BU64
O	13	SER	-	expression tag	UNP Q9BU64
O	14	LYS	-	expression tag	UNP Q9BU64
O	15	GLY	-	expression tag	UNP Q9BU64
O	16	GLY	-	expression tag	UNP Q9BU64
O	17	VAL	-	expression tag	UNP Q9BU64
O	18	LEU	-	expression tag	UNP Q9BU64
O	19	ALA	-	expression tag	UNP Q9BU64
O	20	HIS	-	expression tag	UNP Q9BU64
O	21	LEU	-	expression tag	UNP Q9BU64
O	22	GLU	-	expression tag	UNP Q9BU64
O	23	ARG	-	expression tag	UNP Q9BU64
O	24	LEU	-	expression tag	UNP Q9BU64
O	25	GLU	-	expression tag	UNP Q9BU64
O	26	THR	-	expression tag	UNP Q9BU64
O	27	GLN	-	expression tag	UNP Q9BU64
O	28	VAL	-	expression tag	UNP Q9BU64
O	29	SER	-	expression tag	UNP Q9BU64
O	30	ARG	-	expression tag	UNP Q9BU64
O	31	SER	-	expression tag	UNP Q9BU64
O	32	ARG	-	expression tag	UNP Q9BU64
O	33	LYS	-	expression tag	UNP Q9BU64
O	34	GLN	-	expression tag	UNP Q9BU64
O	35	SER	-	expression tag	UNP Q9BU64
O	36	GLU	-	expression tag	UNP Q9BU64
O	37	GLU	-	expression tag	UNP Q9BU64
O	38	LEU	-	expression tag	UNP Q9BU64
O	39	GLN	-	expression tag	UNP Q9BU64
O	40	SER	-	expression tag	UNP Q9BU64
O	41	VAL	-	expression tag	UNP Q9BU64
O	42	GLN	-	expression tag	UNP Q9BU64
O	43	ALA	-	expression tag	UNP Q9BU64
O	44	GLN	-	expression tag	UNP Q9BU64
O	45	GLU	-	expression tag	UNP Q9BU64
O	46	GLY	-	expression tag	UNP Q9BU64

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Chain	Residue	Modelled	Actual	Comment	Reference
O	47	ALA	-	expression tag	UNP Q9BU64
O	48	LEU	-	expression tag	UNP Q9BU64
O	49	GLY	-	expression tag	UNP Q9BU64
O	50	THR	-	expression tag	UNP Q9BU64
O	51	LYS	-	expression tag	UNP Q9BU64
O	52	ILE	-	expression tag	UNP Q9BU64
O	53	HIS	-	expression tag	UNP Q9BU64
O	54	LYS	-	expression tag	UNP Q9BU64
O	55	LEU	-	expression tag	UNP Q9BU64
O	56	ARG	-	expression tag	UNP Q9BU64
O	57	ARG	-	expression tag	UNP Q9BU64
O	58	LEU	-	expression tag	UNP Q9BU64
O	59	ARG	-	expression tag	UNP Q9BU64
O	60	ASP	-	expression tag	UNP Q9BU64
O	61	GLU	-	expression tag	UNP Q9BU64
O	62	LEU	-	expression tag	UNP Q9BU64
O	63	ARG	-	expression tag	UNP Q9BU64
O	64	ALA	-	expression tag	UNP Q9BU64
O	65	VAL	-	expression tag	UNP Q9BU64
O	66	VAL	-	expression tag	UNP Q9BU64
O	67	ARG	-	expression tag	UNP Q9BU64
O	68	HIS	-	expression tag	UNP Q9BU64
O	69	ARG	-	expression tag	UNP Q9BU64
O	70	ARG	-	expression tag	UNP Q9BU64
O	71	ALA	-	expression tag	UNP Q9BU64
O	72	SER	-	expression tag	UNP Q9BU64
O	73	VAL	-	expression tag	UNP Q9BU64
O	74	LYS	-	expression tag	UNP Q9BU64
O	75	ALA	-	expression tag	UNP Q9BU64
O	76	CYS	-	expression tag	UNP Q9BU64
O	77	ILE	-	expression tag	UNP Q9BU64
O	78	ALA	-	expression tag	UNP Q9BU64
O	79	ASN	-	expression tag	UNP Q9BU64
O	80	VAL	-	expression tag	UNP Q9BU64
O	81	GLU	-	expression tag	UNP Q9BU64
O	82	PRO	-	expression tag	UNP Q9BU64
O	83	ASN	-	expression tag	UNP Q9BU64
O	84	GLN	-	expression tag	UNP Q9BU64
O	85	THR	-	expression tag	UNP Q9BU64
O	86	VAL	-	expression tag	UNP Q9BU64
O	87	GLU	-	expression tag	UNP Q9BU64
O	88	ILE	-	expression tag	UNP Q9BU64

- Molecule 10 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	224	Total	C	N	O	S	0	0
			1788	1141	310	329	8		

- Molecule 11 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	197	Total	C	N	O	S	0	0
			1582	989	270	312	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	54	MET	-	initiating methionine	UNP Q7L2Z9

- Molecule 12 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	80	Total	C	N	O	S	0	0
			649	412	105	125	7		

- Molecule 13 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	120	Total	C	N	O	S	0	0
			982	607	174	195	6		

- Molecule 14 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	112	Total	C	N	O	S	0	0
			915	586	163	159	7		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-215	MET	-	initiating methionine	UNP Q96BT3
T	-214	SER	-	expression tag	UNP Q96BT3
T	-213	TYR	-	expression tag	UNP Q96BT3
T	-212	TYR	-	expression tag	UNP Q96BT3
T	-211	HIS	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-210	HIS	-	expression tag	UNP Q96BT3
T	-209	HIS	-	expression tag	UNP Q96BT3
T	-208	HIS	-	expression tag	UNP Q96BT3
T	-207	HIS	-	expression tag	UNP Q96BT3
T	-206	HIS	-	expression tag	UNP Q96BT3
T	-205	ASP	-	expression tag	UNP Q96BT3
T	-204	TYR	-	expression tag	UNP Q96BT3
T	-203	ASP	-	expression tag	UNP Q96BT3
T	-202	ILE	-	expression tag	UNP Q96BT3
T	-201	PRO	-	expression tag	UNP Q96BT3
T	-200	THR	-	expression tag	UNP Q96BT3
T	-199	THR	-	expression tag	UNP Q96BT3
T	-198	GLU	-	expression tag	UNP Q96BT3
T	-197	ASN	-	expression tag	UNP Q96BT3
T	-196	LEU	-	expression tag	UNP Q96BT3
T	-195	TYR	-	expression tag	UNP Q96BT3
T	-194	PHE	-	expression tag	UNP Q96BT3
T	-193	GLN	-	expression tag	UNP Q96BT3
T	-192	GLY	-	expression tag	UNP Q96BT3
T	-191	MET	-	expression tag	UNP Q96BT3
T	-190	ASP	-	expression tag	UNP Q96BT3
T	-189	LYS	-	expression tag	UNP Q96BT3
T	-188	ASP	-	expression tag	UNP Q96BT3
T	-187	CYS	-	expression tag	UNP Q96BT3
T	-186	GLU	-	expression tag	UNP Q96BT3
T	-185	MET	-	expression tag	UNP Q96BT3
T	-184	LYS	-	expression tag	UNP Q96BT3
T	-183	ARG	-	expression tag	UNP Q96BT3
T	-182	THR	-	expression tag	UNP Q96BT3
T	-181	THR	-	expression tag	UNP Q96BT3
T	-180	LEU	-	expression tag	UNP Q96BT3
T	-179	ASP	-	expression tag	UNP Q96BT3
T	-178	SER	-	expression tag	UNP Q96BT3
T	-177	PRO	-	expression tag	UNP Q96BT3
T	-176	LEU	-	expression tag	UNP Q96BT3
T	-175	GLY	-	expression tag	UNP Q96BT3
T	-174	LYS	-	expression tag	UNP Q96BT3
T	-173	LEU	-	expression tag	UNP Q96BT3
T	-172	GLU	-	expression tag	UNP Q96BT3
T	-171	LEU	-	expression tag	UNP Q96BT3
T	-170	SER	-	expression tag	UNP Q96BT3
T	-169	GLY	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-168	CYS	-	expression tag	UNP Q96BT3
T	-167	GLU	-	expression tag	UNP Q96BT3
T	-166	GLN	-	expression tag	UNP Q96BT3
T	-165	GLY	-	expression tag	UNP Q96BT3
T	-164	LEU	-	expression tag	UNP Q96BT3
T	-163	HIS	-	expression tag	UNP Q96BT3
T	-162	ARG	-	expression tag	UNP Q96BT3
T	-161	ILE	-	expression tag	UNP Q96BT3
T	-160	ILE	-	expression tag	UNP Q96BT3
T	-159	PHE	-	expression tag	UNP Q96BT3
T	-158	LEU	-	expression tag	UNP Q96BT3
T	-157	GLY	-	expression tag	UNP Q96BT3
T	-156	LYS	-	expression tag	UNP Q96BT3
T	-155	GLY	-	expression tag	UNP Q96BT3
T	-154	THR	-	expression tag	UNP Q96BT3
T	-153	SER	-	expression tag	UNP Q96BT3
T	-152	ALA	-	expression tag	UNP Q96BT3
T	-151	ALA	-	expression tag	UNP Q96BT3
T	-150	ASP	-	expression tag	UNP Q96BT3
T	-149	ALA	-	expression tag	UNP Q96BT3
T	-148	VAL	-	expression tag	UNP Q96BT3
T	-147	GLU	-	expression tag	UNP Q96BT3
T	-146	VAL	-	expression tag	UNP Q96BT3
T	-145	PRO	-	expression tag	UNP Q96BT3
T	-144	ALA	-	expression tag	UNP Q96BT3
T	-143	PRO	-	expression tag	UNP Q96BT3
T	-142	ALA	-	expression tag	UNP Q96BT3
T	-141	ALA	-	expression tag	UNP Q96BT3
T	-140	VAL	-	expression tag	UNP Q96BT3
T	-139	LEU	-	expression tag	UNP Q96BT3
T	-138	GLY	-	expression tag	UNP Q96BT3
T	-137	GLY	-	expression tag	UNP Q96BT3
T	-136	PRO	-	expression tag	UNP Q96BT3
T	-135	GLU	-	expression tag	UNP Q96BT3
T	-134	PRO	-	expression tag	UNP Q96BT3
T	-133	LEU	-	expression tag	UNP Q96BT3
T	-132	MET	-	expression tag	UNP Q96BT3
T	-131	GLN	-	expression tag	UNP Q96BT3
T	-130	ALA	-	expression tag	UNP Q96BT3
T	-129	THR	-	expression tag	UNP Q96BT3
T	-128	ALA	-	expression tag	UNP Q96BT3
T	-127	TRP	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-126	LEU	-	expression tag	UNP Q96BT3
T	-125	ASN	-	expression tag	UNP Q96BT3
T	-124	ALA	-	expression tag	UNP Q96BT3
T	-123	TYR	-	expression tag	UNP Q96BT3
T	-122	PHE	-	expression tag	UNP Q96BT3
T	-121	HIS	-	expression tag	UNP Q96BT3
T	-120	GLN	-	expression tag	UNP Q96BT3
T	-119	PRO	-	expression tag	UNP Q96BT3
T	-118	GLU	-	expression tag	UNP Q96BT3
T	-117	ALA	-	expression tag	UNP Q96BT3
T	-116	ILE	-	expression tag	UNP Q96BT3
T	-115	GLU	-	expression tag	UNP Q96BT3
T	-114	GLU	-	expression tag	UNP Q96BT3
T	-113	PHE	-	expression tag	UNP Q96BT3
T	-112	PRO	-	expression tag	UNP Q96BT3
T	-111	VAL	-	expression tag	UNP Q96BT3
T	-110	PRO	-	expression tag	UNP Q96BT3
T	-109	ALA	-	expression tag	UNP Q96BT3
T	-108	LEU	-	expression tag	UNP Q96BT3
T	-107	HIS	-	expression tag	UNP Q96BT3
T	-106	HIS	-	expression tag	UNP Q96BT3
T	-105	PRO	-	expression tag	UNP Q96BT3
T	-104	VAL	-	expression tag	UNP Q96BT3
T	-103	PHE	-	expression tag	UNP Q96BT3
T	-102	GLN	-	expression tag	UNP Q96BT3
T	-101	GLN	-	expression tag	UNP Q96BT3
T	-100	GLU	-	expression tag	UNP Q96BT3
T	-99	SER	-	expression tag	UNP Q96BT3
T	-98	PHE	-	expression tag	UNP Q96BT3
T	-97	THR	-	expression tag	UNP Q96BT3
T	-96	ARG	-	expression tag	UNP Q96BT3
T	-95	GLN	-	expression tag	UNP Q96BT3
T	-94	VAL	-	expression tag	UNP Q96BT3
T	-93	LEU	-	expression tag	UNP Q96BT3
T	-92	TRP	-	expression tag	UNP Q96BT3
T	-91	LYS	-	expression tag	UNP Q96BT3
T	-90	LEU	-	expression tag	UNP Q96BT3
T	-89	LEU	-	expression tag	UNP Q96BT3
T	-88	LYS	-	expression tag	UNP Q96BT3
T	-87	VAL	-	expression tag	UNP Q96BT3
T	-86	VAL	-	expression tag	UNP Q96BT3
T	-85	LYS	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-84	PHE	-	expression tag	UNP Q96BT3
T	-83	GLY	-	expression tag	UNP Q96BT3
T	-82	GLU	-	expression tag	UNP Q96BT3
T	-81	VAL	-	expression tag	UNP Q96BT3
T	-80	ILE	-	expression tag	UNP Q96BT3
T	-79	SER	-	expression tag	UNP Q96BT3
T	-78	TYR	-	expression tag	UNP Q96BT3
T	-77	SER	-	expression tag	UNP Q96BT3
T	-76	HIS	-	expression tag	UNP Q96BT3
T	-75	LEU	-	expression tag	UNP Q96BT3
T	-74	ALA	-	expression tag	UNP Q96BT3
T	-73	ALA	-	expression tag	UNP Q96BT3
T	-72	LEU	-	expression tag	UNP Q96BT3
T	-71	ALA	-	expression tag	UNP Q96BT3
T	-70	GLY	-	expression tag	UNP Q96BT3
T	-69	ASN	-	expression tag	UNP Q96BT3
T	-68	PRO	-	expression tag	UNP Q96BT3
T	-67	ALA	-	expression tag	UNP Q96BT3
T	-66	ALA	-	expression tag	UNP Q96BT3
T	-65	THR	-	expression tag	UNP Q96BT3
T	-64	ALA	-	expression tag	UNP Q96BT3
T	-63	ALA	-	expression tag	UNP Q96BT3
T	-62	VAL	-	expression tag	UNP Q96BT3
T	-61	LYS	-	expression tag	UNP Q96BT3
T	-60	THR	-	expression tag	UNP Q96BT3
T	-59	ALA	-	expression tag	UNP Q96BT3
T	-58	LEU	-	expression tag	UNP Q96BT3
T	-57	SER	-	expression tag	UNP Q96BT3
T	-56	GLY	-	expression tag	UNP Q96BT3
T	-55	ASN	-	expression tag	UNP Q96BT3
T	-54	PRO	-	expression tag	UNP Q96BT3
T	-53	VAL	-	expression tag	UNP Q96BT3
T	-52	PRO	-	expression tag	UNP Q96BT3
T	-51	ILE	-	expression tag	UNP Q96BT3
T	-50	LEU	-	expression tag	UNP Q96BT3
T	-49	ILE	-	expression tag	UNP Q96BT3
T	-48	PRO	-	expression tag	UNP Q96BT3
T	-47	CYS	-	expression tag	UNP Q96BT3
T	-46	HIS	-	expression tag	UNP Q96BT3
T	-45	ARG	-	expression tag	UNP Q96BT3
T	-44	VAL	-	expression tag	UNP Q96BT3
T	-43	VAL	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-42	GLN	-	expression tag	UNP Q96BT3
T	-41	GLY	-	expression tag	UNP Q96BT3
T	-40	ASP	-	expression tag	UNP Q96BT3
T	-39	LEU	-	expression tag	UNP Q96BT3
T	-38	ASP	-	expression tag	UNP Q96BT3
T	-37	VAL	-	expression tag	UNP Q96BT3
T	-36	GLY	-	expression tag	UNP Q96BT3
T	-35	GLY	-	expression tag	UNP Q96BT3
T	-34	TYR	-	expression tag	UNP Q96BT3
T	-33	GLU	-	expression tag	UNP Q96BT3
T	-32	GLY	-	expression tag	UNP Q96BT3
T	-31	GLY	-	expression tag	UNP Q96BT3
T	-30	LEU	-	expression tag	UNP Q96BT3
T	-29	ALA	-	expression tag	UNP Q96BT3
T	-28	VAL	-	expression tag	UNP Q96BT3
T	-27	LYS	-	expression tag	UNP Q96BT3
T	-26	GLU	-	expression tag	UNP Q96BT3
T	-25	TRP	-	expression tag	UNP Q96BT3
T	-24	LEU	-	expression tag	UNP Q96BT3
T	-23	LEU	-	expression tag	UNP Q96BT3
T	-22	ALA	-	expression tag	UNP Q96BT3
T	-21	HIS	-	expression tag	UNP Q96BT3
T	-20	GLU	-	expression tag	UNP Q96BT3
T	-19	GLY	-	expression tag	UNP Q96BT3
T	-18	HIS	-	expression tag	UNP Q96BT3
T	-17	ARG	-	expression tag	UNP Q96BT3
T	-16	LEU	-	expression tag	UNP Q96BT3
T	-15	GLY	-	expression tag	UNP Q96BT3
T	-14	LYS	-	expression tag	UNP Q96BT3
T	-13	PRO	-	expression tag	UNP Q96BT3
T	-12	GLY	-	expression tag	UNP Q96BT3
T	-11	LEU	-	expression tag	UNP Q96BT3
T	-10	GLY	-	expression tag	UNP Q96BT3
T	-9	SER	-	expression tag	UNP Q96BT3
T	-8	ASP	-	expression tag	UNP Q96BT3
T	-7	LEU	-	expression tag	UNP Q96BT3
T	-6	GLU	-	expression tag	UNP Q96BT3
T	-5	VAL	-	expression tag	UNP Q96BT3
T	-4	LEU	-	expression tag	UNP Q96BT3
T	-3	PHE	-	expression tag	UNP Q96BT3
T	-2	GLN	-	expression tag	UNP Q96BT3
T	-1	GLY	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	0	PRO	-	expression tag	UNP Q96BT3

- Molecule 15 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	166	Total	C	N	O	S	0	0
			1365	861	242	257	5		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	419	GLU	-	expression tag	UNP Q71F23
U	420	ASN	-	expression tag	UNP Q71F23
U	421	LEU	-	expression tag	UNP Q71F23
U	422	TYR	-	expression tag	UNP Q71F23
U	423	PHE	-	expression tag	UNP Q71F23
U	424	GLN	-	expression tag	UNP Q71F23
U	425	SER	-	expression tag	UNP Q71F23
U	426	TRP	-	expression tag	UNP Q71F23
U	427	SER	-	expression tag	UNP Q71F23
U	428	HIS	-	expression tag	UNP Q71F23
U	429	PRO	-	expression tag	UNP Q71F23
U	430	GLN	-	expression tag	UNP Q71F23
U	431	PHE	-	expression tag	UNP Q71F23
U	432	GLU	-	expression tag	UNP Q71F23
U	433	LYS	-	expression tag	UNP Q71F23
U	434	GLY	-	expression tag	UNP Q71F23
U	435	GLY	-	expression tag	UNP Q71F23
U	436	GLY	-	expression tag	UNP Q71F23
U	437	SER	-	expression tag	UNP Q71F23
U	438	GLY	-	expression tag	UNP Q71F23
U	439	GLY	-	expression tag	UNP Q71F23
U	440	GLY	-	expression tag	UNP Q71F23
U	441	SER	-	expression tag	UNP Q71F23
U	442	GLY	-	expression tag	UNP Q71F23
U	443	GLY	-	expression tag	UNP Q71F23
U	444	GLY	-	expression tag	UNP Q71F23
U	445	SER	-	expression tag	UNP Q71F23
U	446	TRP	-	expression tag	UNP Q71F23
U	447	SER	-	expression tag	UNP Q71F23
U	448	HIS	-	expression tag	UNP Q71F23
U	449	PRO	-	expression tag	UNP Q71F23

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Chain	Residue	Modelled	Actual	Comment	Reference
U	450	GLN	-	expression tag	UNP Q71F23
U	451	PHE	-	expression tag	UNP Q71F23
U	452	GLU	-	expression tag	UNP Q71F23
U	453	LYS	-	expression tag	UNP Q71F23

- Molecule 16 is a protein called Centromere protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	86	Total	C	N	O	S	0	0
			691	437	141	110	3		

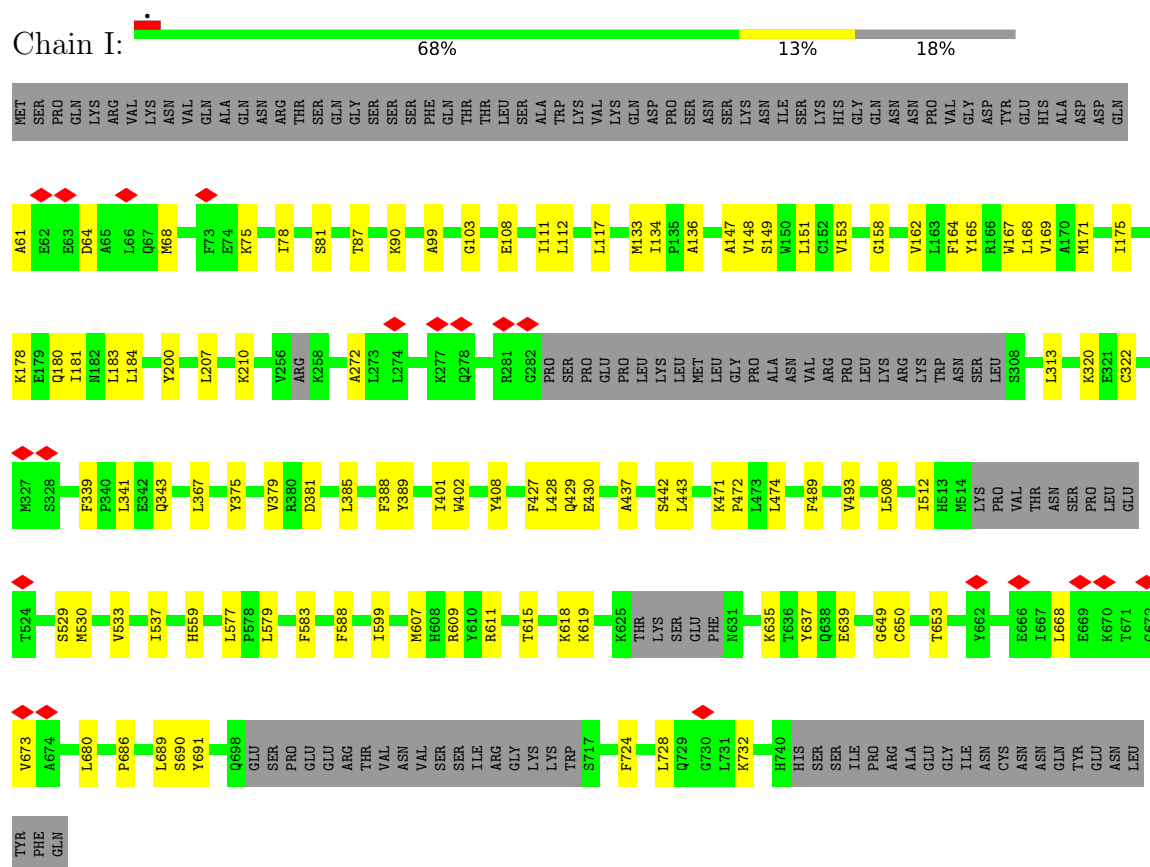
- Molecule 17 is a protein called Centromere protein X.

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

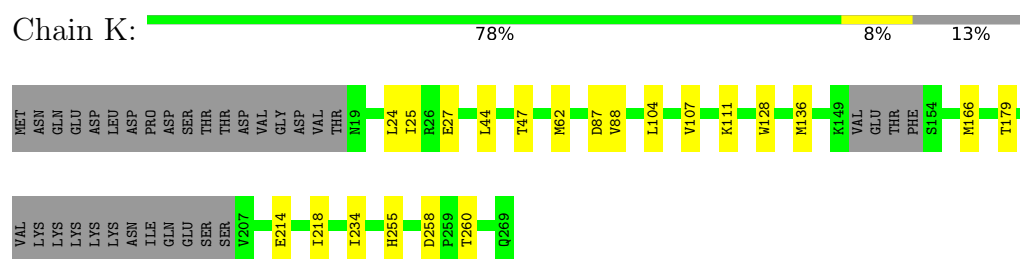
- Molecule 18 is a protein called Centromere protein C,Centromere protein C,Centromere protein C,Centromere protein C,Methylated-DNA--protein-cysteine methyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	b	35	Total	C	N	O	0	0
			291	183	47	61		

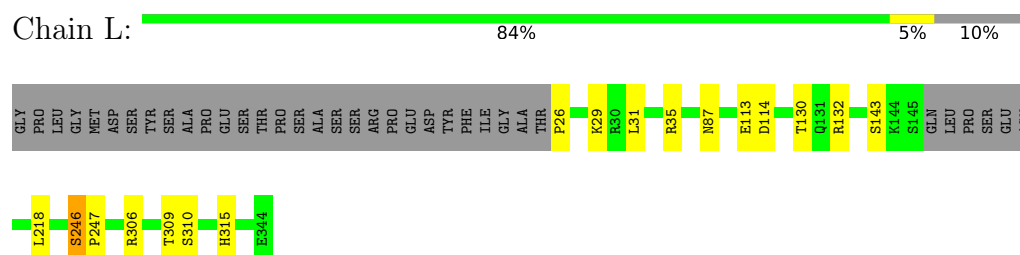
- Molecule 4: Centromere protein I



- Molecule 5: Centromere protein K



- Molecule 6: Centromere protein L



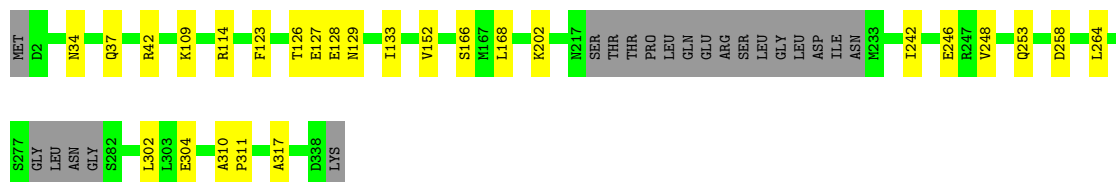
- Molecule 7: Centromere protein M





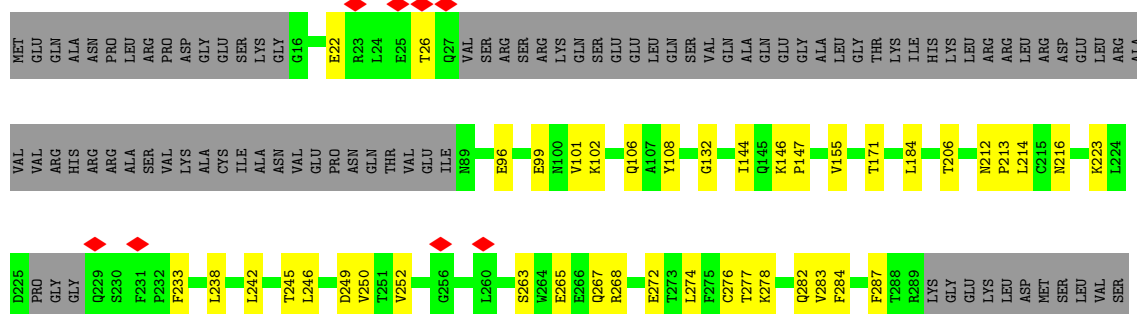
• Molecule 8: Centromere protein N

Chain N: 86% 8% 6%



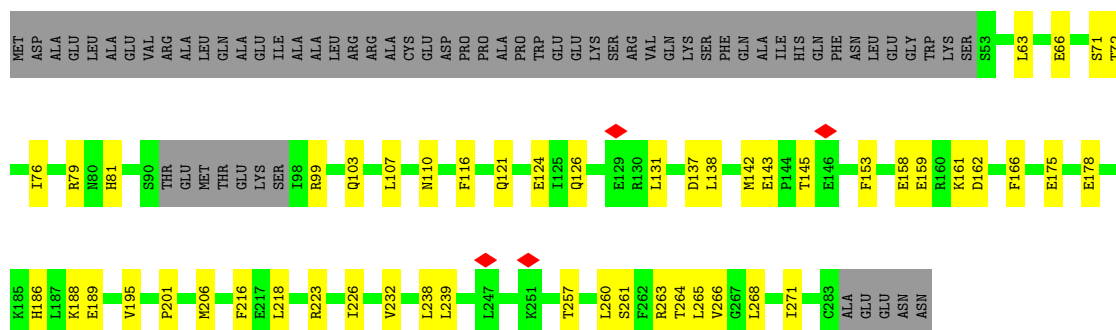
• Molecule 9: Centromere protein O

Chain O: 56% 14% 30%



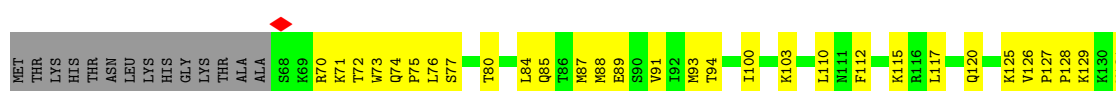
• Molecule 10: Centromere protein P

Chain P: 60% 18% 22%



• Molecule 11: Centromere protein Q

Chain Q: 16% 67% 25% 8%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.741	Depositor
Minimum map value	-0.461	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	261.0, 261.0, 261.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.17	0/1889	0.37	0/2912
2	B	0.19	0/1838	0.41	0/2836
3	H	0.21	0/1660	0.39	0/2218
4	I	0.19	0/5137	0.38	0/6955
5	K	0.22	0/1953	0.37	0/2634
6	L	0.19	0/2569	0.40	0/3485
7	M	0.16	0/1347	0.33	0/1827
8	N	0.19	0/2670	0.38	0/3606
9	O	0.22	0/1678	0.40	0/2280
10	P	0.16	0/1820	0.39	0/2451
11	Q	0.25	0/1596	0.57	0/2139
12	R	0.19	0/653	0.66	0/865
13	S	0.18	0/991	0.44	0/1322
14	T	0.19	0/937	0.39	0/1263
15	U	0.21	0/1383	0.38	0/1856
16	W	0.15	0/698	0.27	0/927
17	X	0.18	0/596	0.45	0/801
18	b	0.12	0/292	0.24	0/386
All	All	0.19	0/29707	0.40	0/40763

There are no bond length outliers.

There are no bond angle outliers.

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	A	1682	0	926	36	0
2	B	1641	0	911	23	0
3	H	1652	0	1728	28	0
4	I	5014	0	5036	71	0
5	K	1922	0	1924	17	0
6	L	2502	0	2492	14	0
7	M	1325	0	1370	7	0
8	N	2613	0	2627	17	0
9	O	1642	0	1616	28	0
10	P	1788	0	1791	43	0
11	Q	1582	0	1647	46	0
12	R	649	0	673	19	0
13	S	982	0	987	22	0
14	T	915	0	924	15	0
15	U	1365	0	1396	26	0
16	W	691	0	772	5	0
17	X	590	0	620	10	0
18	b	291	0	291	2	0
All	All	28846	0	27731	380	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 7.

The worst 5 of 380 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)
6:L:246:SER:HB3	6:L:247:PRO:HD3	1.53	0.90
10:P:72:THR:HG21	12:R:175:ILE:HG12	1.58	0.85
3:H:122:GLN:HG2	3:H:127:MET:HE2	1.64	0.78
11:Q:162:ILE:HD12	15:U:319:ARG:HG3	1.70	0.74
3:H:37:GLU:HA	3:H:40:MET:HE3	1.72	0.71

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	
3	H	200/247 (81%)	197 (98%)	3 (2%)	0	100	100
4	I	610/762 (80%)	586 (96%)	23 (4%)	1 (0%)	43	73
5	K	227/269 (84%)	223 (98%)	4 (2%)	0	100	100
6	L	308/348 (88%)	301 (98%)	6 (2%)	1 (0%)	36	66
7	M	170/180 (94%)	166 (98%)	4 (2%)	0	100	100
8	N	312/339 (92%)	296 (95%)	16 (5%)	0	100	100
9	O	204/300 (68%)	201 (98%)	3 (2%)	0	100	100
10	P	220/288 (76%)	214 (97%)	6 (3%)	0	100	100
11	Q	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
12	R	76/177 (43%)	71 (93%)	5 (7%)	0	100	100
13	S	118/138 (86%)	117 (99%)	1 (1%)	0	100	100
14	T	110/777 (14%)	105 (96%)	5 (4%)	0	100	100
15	U	164/211 (78%)	164 (100%)	0	0	100	100
16	W	84/88 (96%)	81 (96%)	3 (4%)	0	100	100
17	X	72/81 (89%)	71 (99%)	1 (1%)	0	100	100
18	b	31/775 (4%)	29 (94%)	2 (6%)	0	100	100
All	All	3099/5195 (60%)	3012 (97%)	85 (3%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	246	SER
4	I	429	GLN

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	
3	H	188/224 (84%)	188 (100%)	0	100	100
4	I	560/697 (80%)	560 (100%)	0	100	100
5	K	221/260 (85%)	221 (100%)	0	100	100
6	L	277/308 (90%)	277 (100%)	0	100	100
7	M	151/158 (96%)	151 (100%)	0	100	100
8	N	287/311 (92%)	287 (100%)	0	100	100
9	O	177/263 (67%)	176 (99%)	1 (1%)	78	80
10	P	197/259 (76%)	197 (100%)	0	100	100
11	Q	185/200 (92%)	185 (100%)	0	100	100
12	R	75/166 (45%)	75 (100%)	0	100	100
13	S	107/121 (88%)	107 (100%)	0	100	100
14	T	100/635 (16%)	100 (100%)	0	100	100
15	U	152/190 (80%)	152 (100%)	0	100	100
16	W	76/77 (99%)	76 (100%)	0	100	100
17	X	65/67 (97%)	65 (100%)	0	100	100
18	b	34/687 (5%)	34 (100%)	0	100	100
All	All	2852/4623 (62%)	2851 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	O	233	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	360	ASN
15	U	408	ASN
17	X	20	HIS
8	N	43	GLN
7	M	73	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.

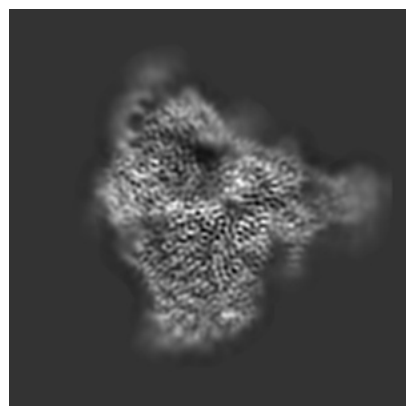
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55757. These allow visual inspection of the internal detail of the map and identification of artifacts.

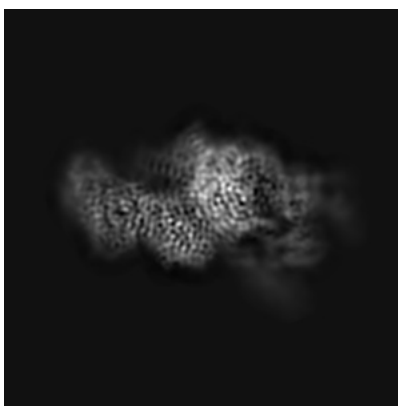
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

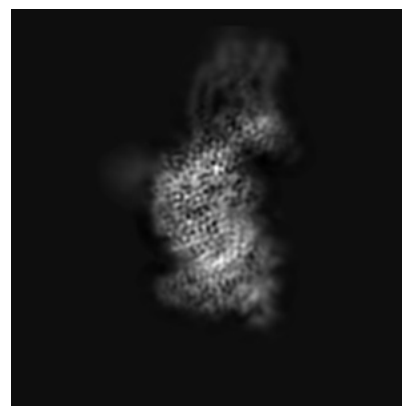
6.1.1 Primary map



X

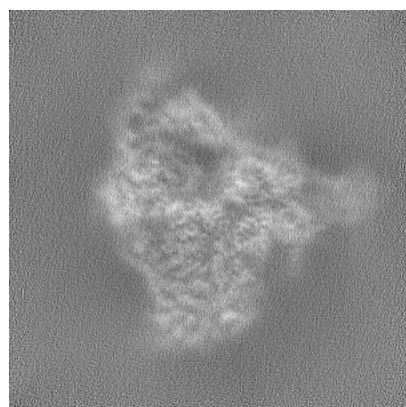


Y

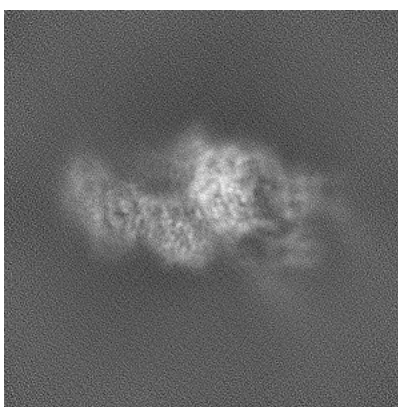


Z

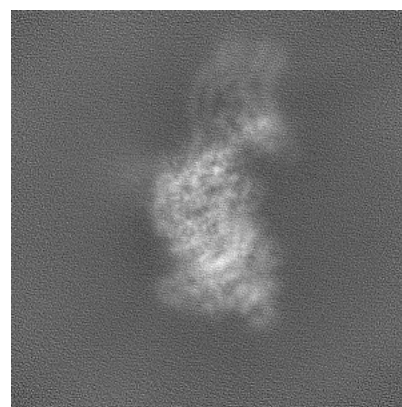
6.1.2 Raw map



X



Y

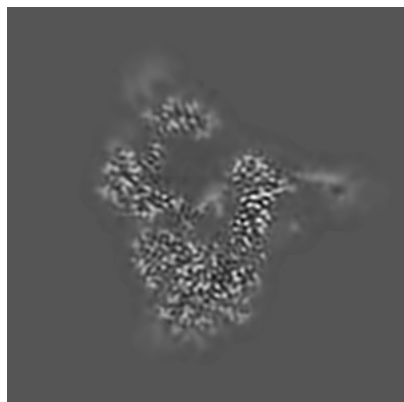


Z

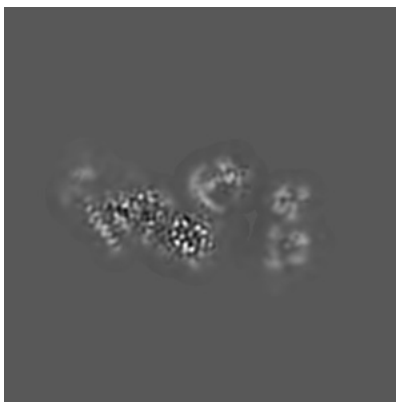
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

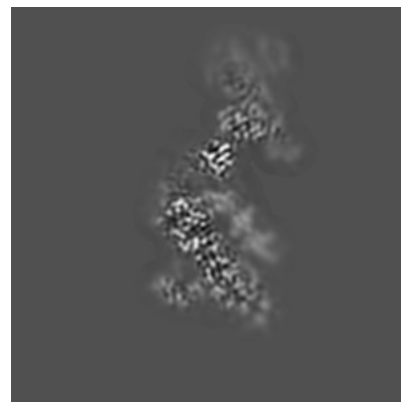
6.2.1 Primary map



X Index: 180

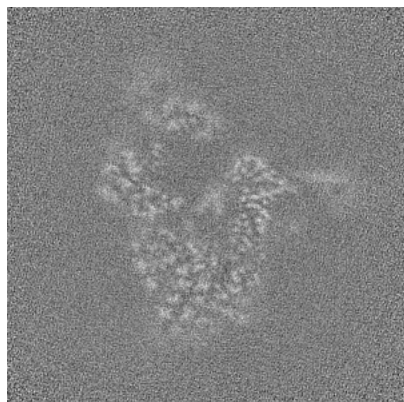


Y Index: 180



Z Index: 180

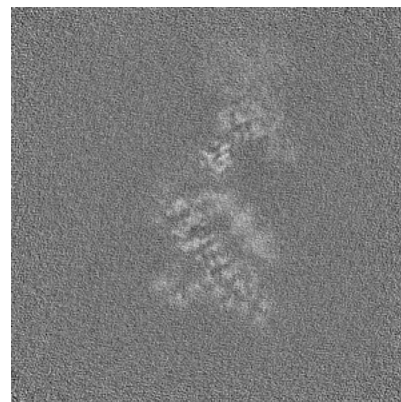
6.2.2 Raw map



X Index: 180



Y Index: 180

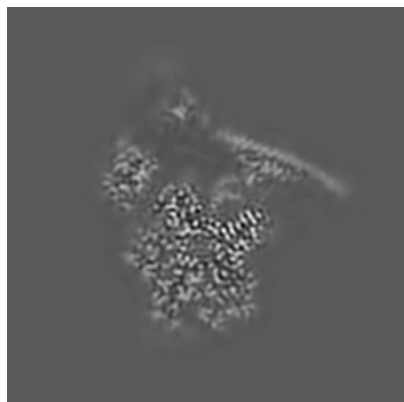


Z Index: 180

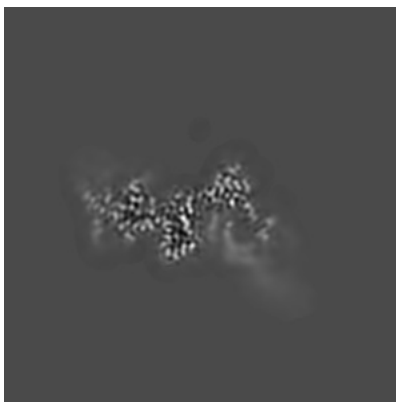
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

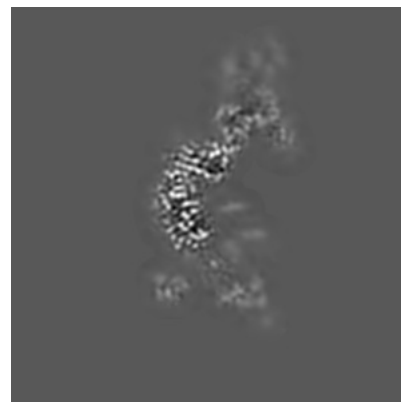
6.3.1 Primary map



X Index: 167

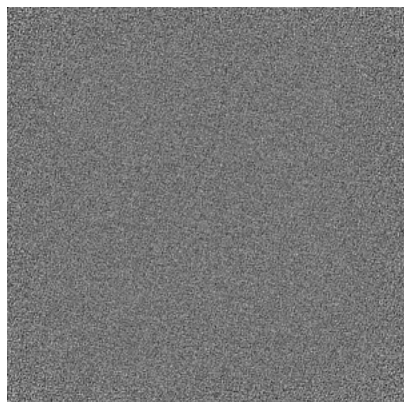


Y Index: 208

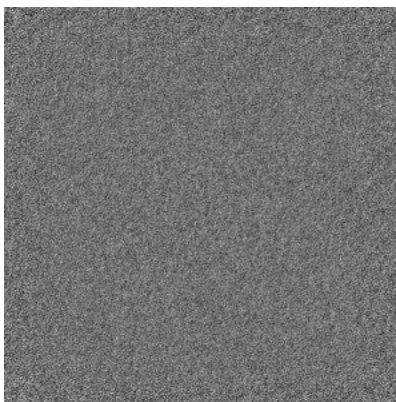


Z Index: 168

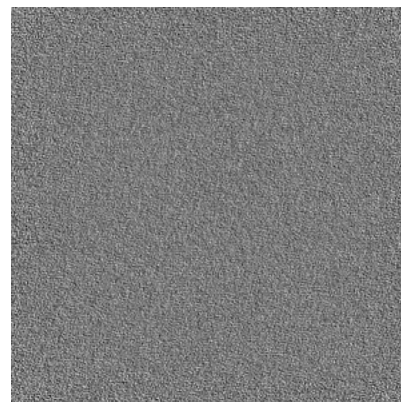
6.3.2 Raw map



X Index: 0



Y Index: 0

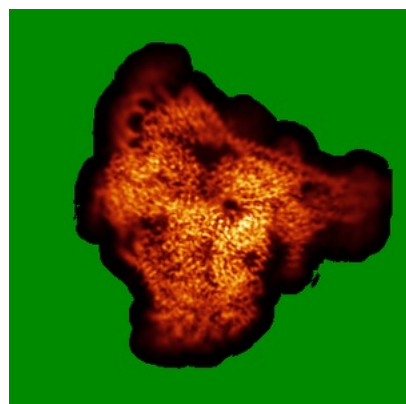


Z Index: 0

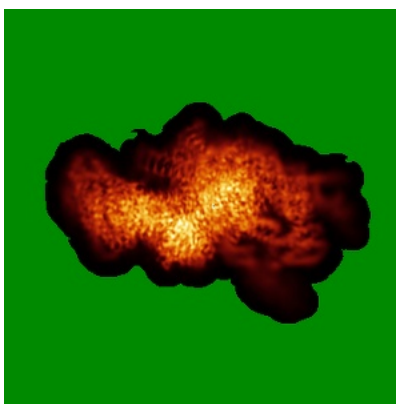
The images above show the largest variance slices of the map in three orthogonal directions.

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

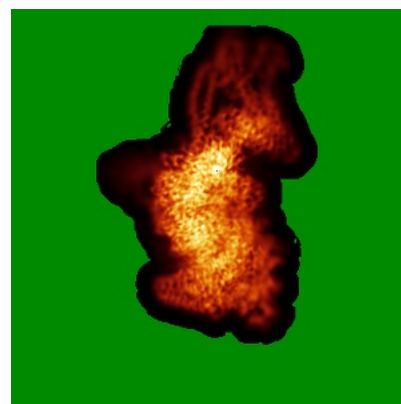
6.4.1 Primary map



X

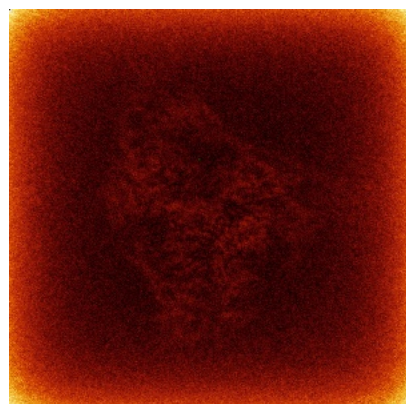


Y

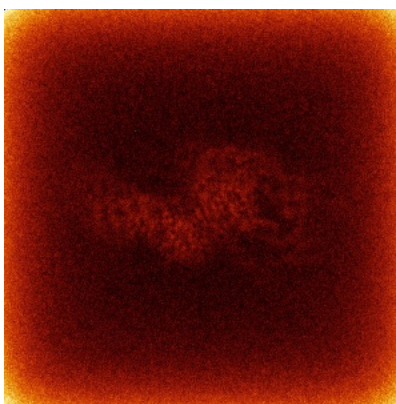


Z

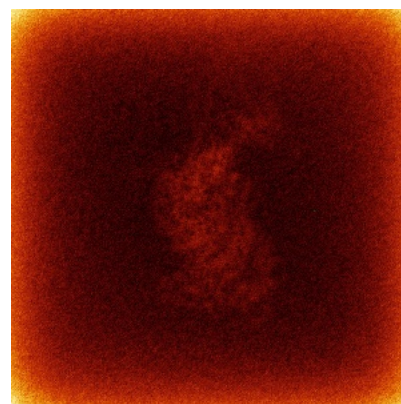
6.4.2 Raw map



X



Y

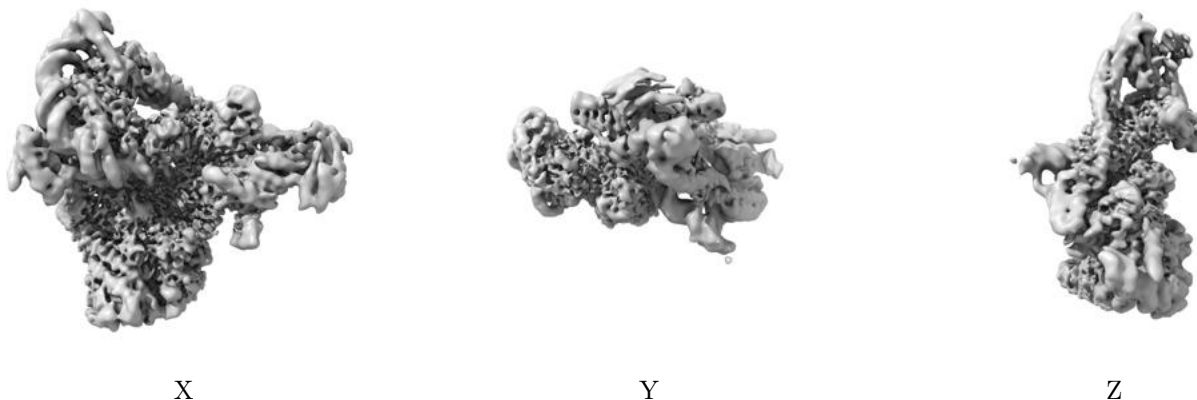


Z

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

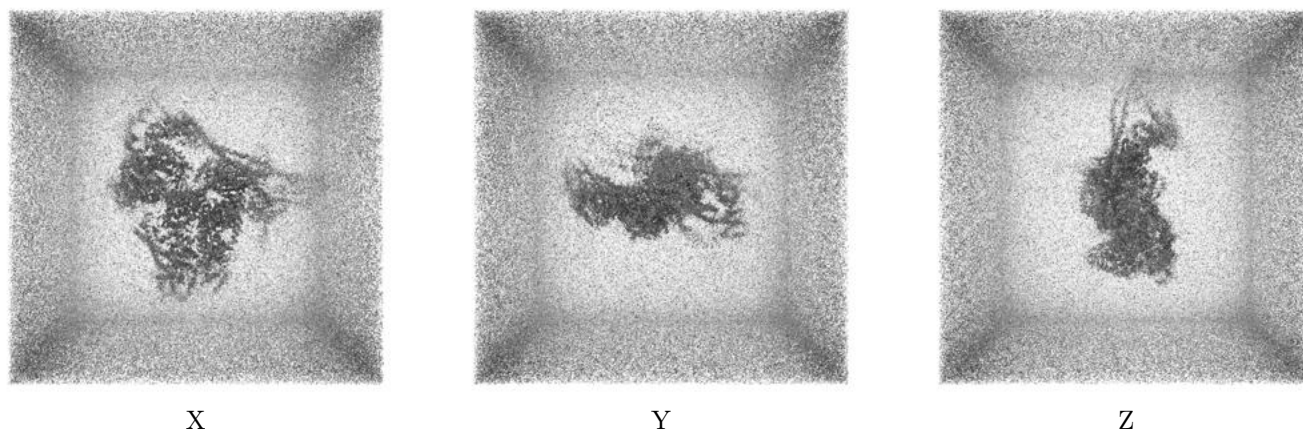
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

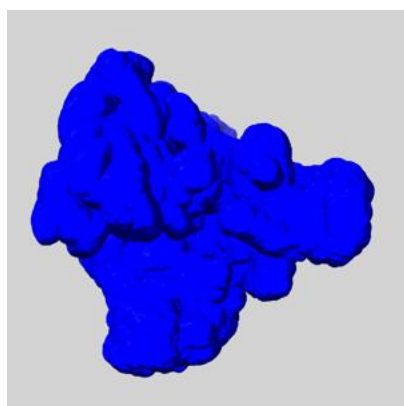
6.6 Mask visualisation [i](#)

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

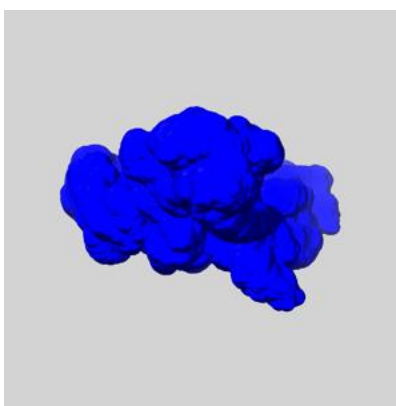
A mask typically either:

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

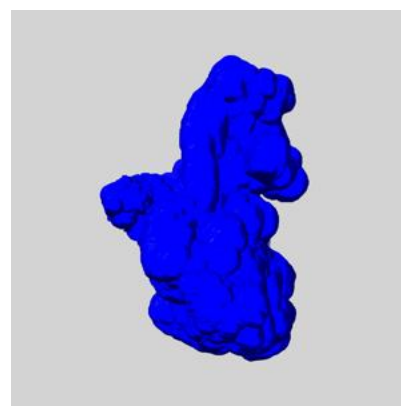
6.6.1 emd_55757_msk_1.map [i](#)



X



Y

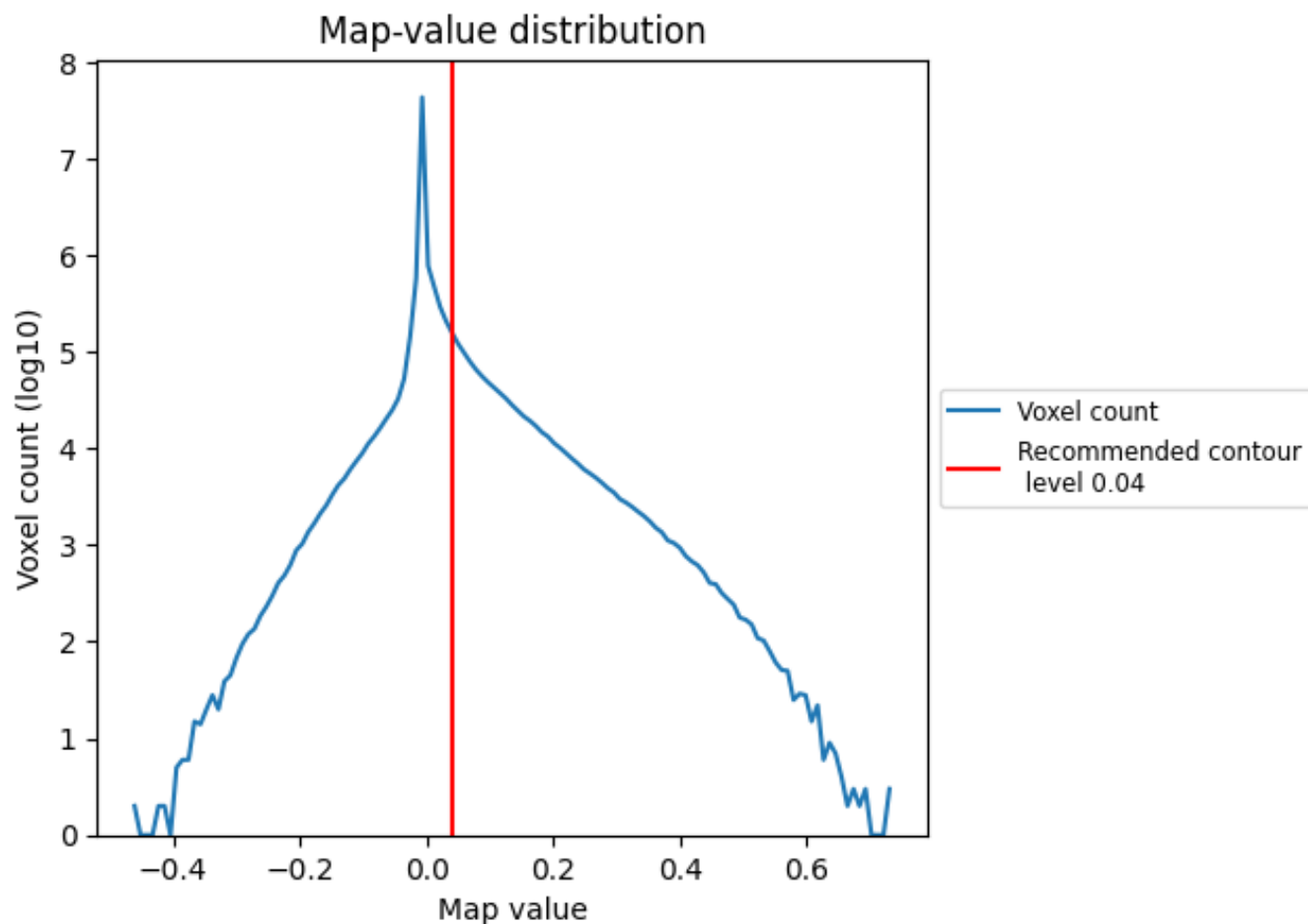


Z

7 Map analysis [i](#)

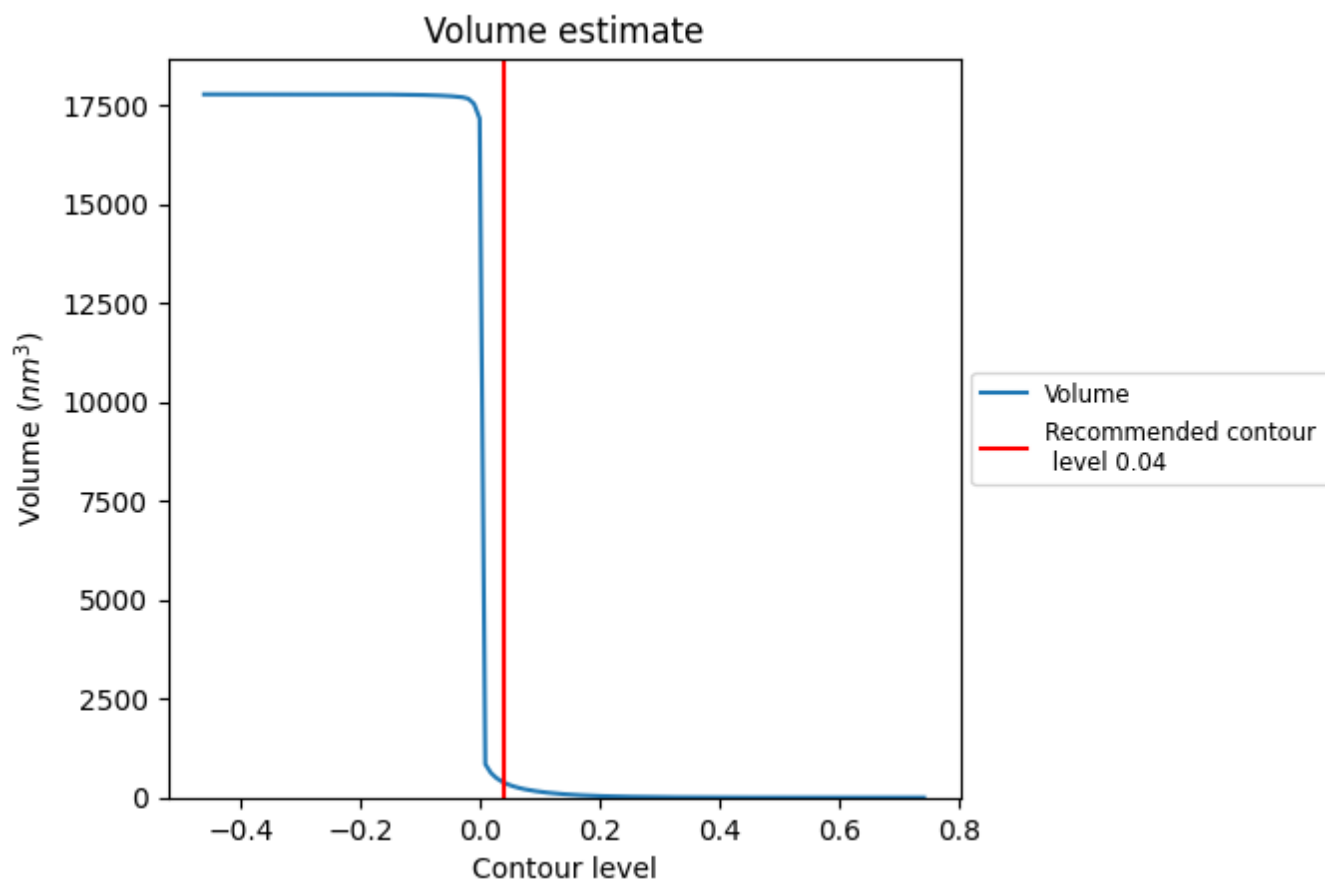
This section contains the results of statistical analysis of the map.

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.

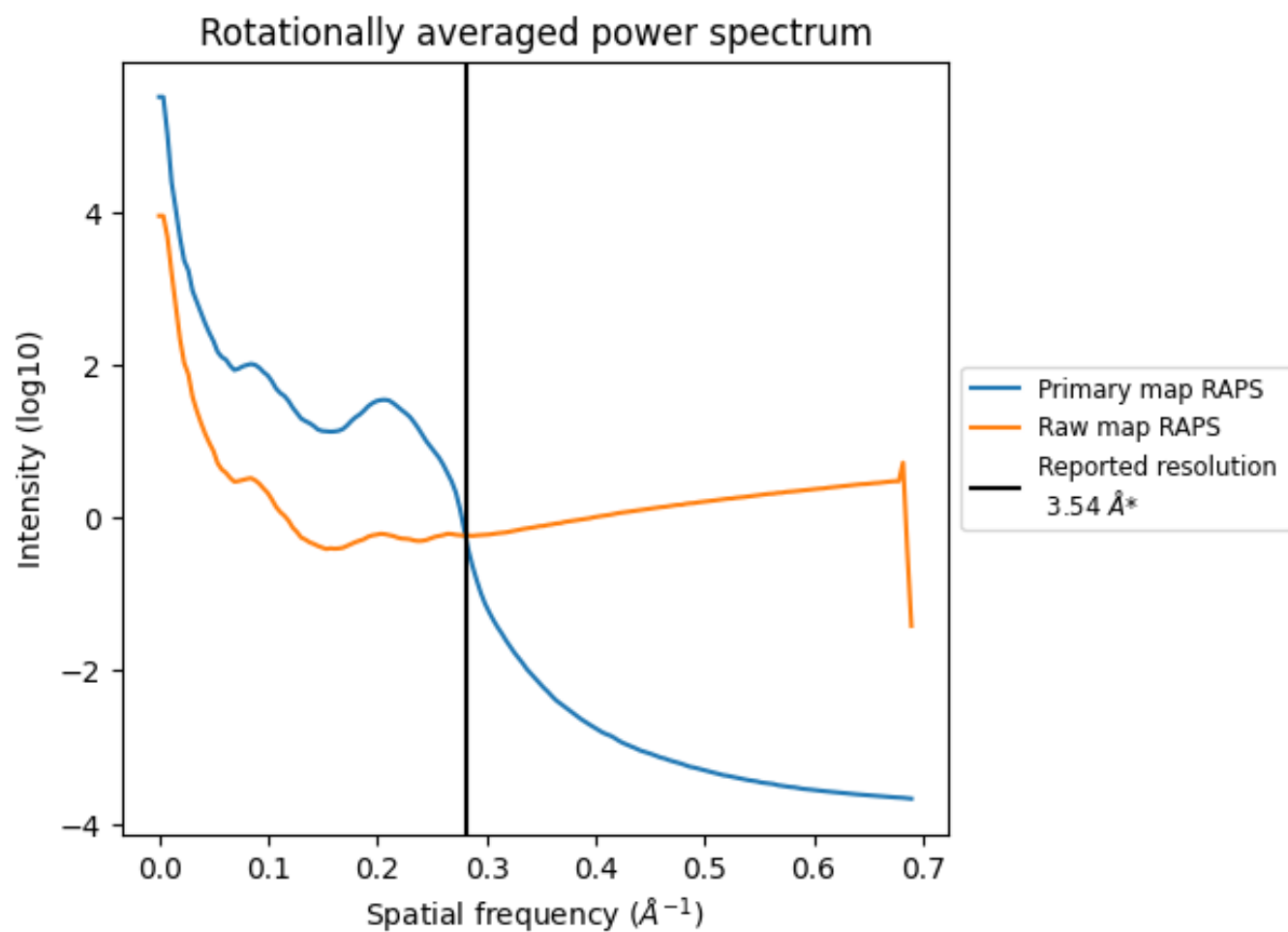
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm³; this corresponds to an approximate mass of 341 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 ⓘ

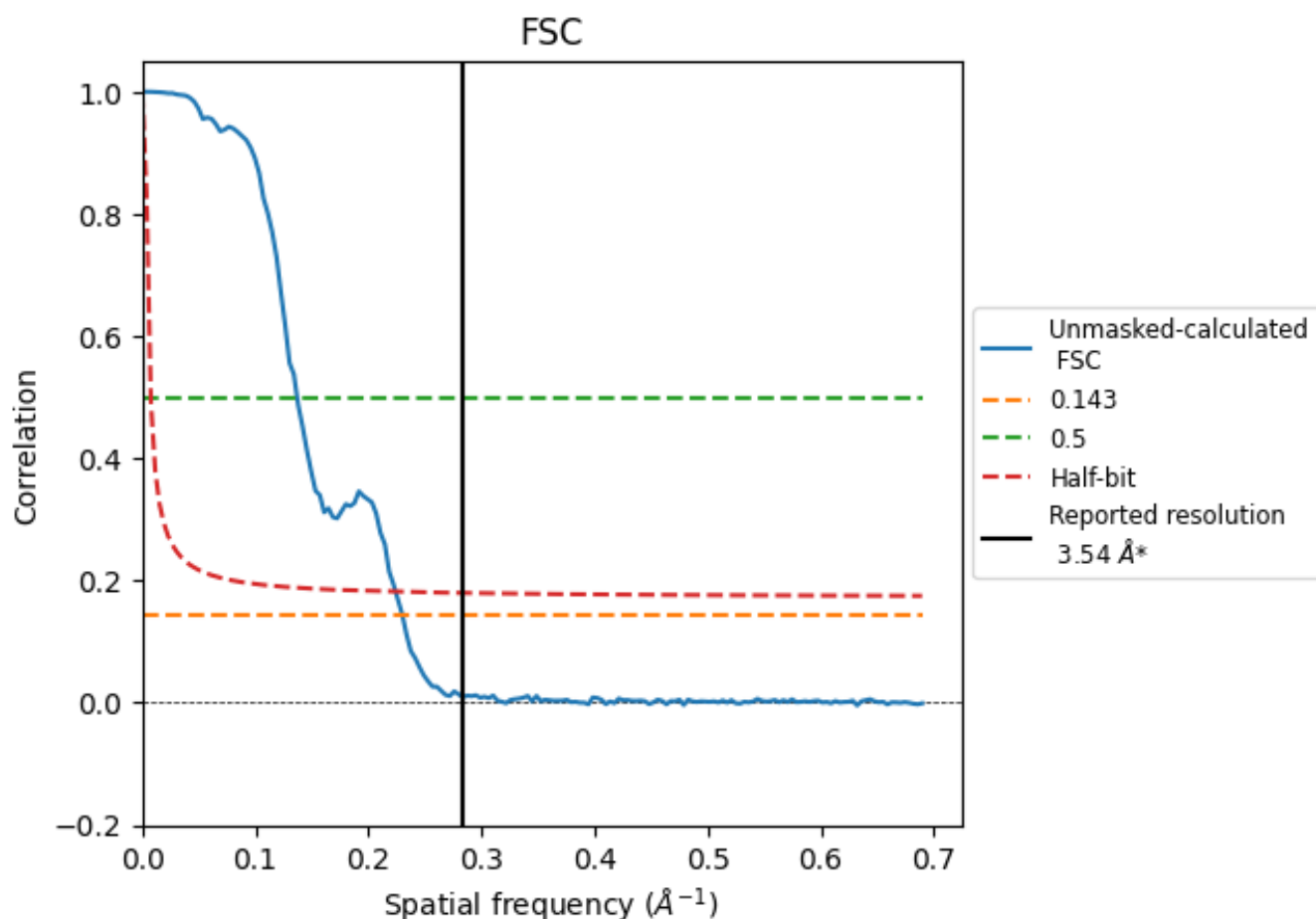


*Reported resolution corresponds to spatial frequency of 0.282 $\text{\AA}^{-1}$

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

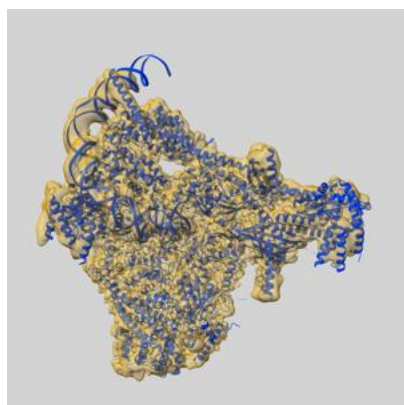
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.35	7.30	4.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.54 by more than 10 %

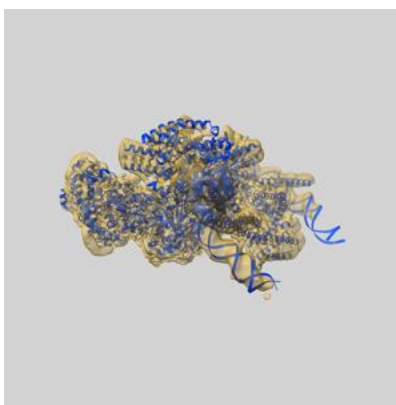
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55757 and PDB model 9TAW. Per-residue inclusion information can be found in section [3](#) on page [16](#).

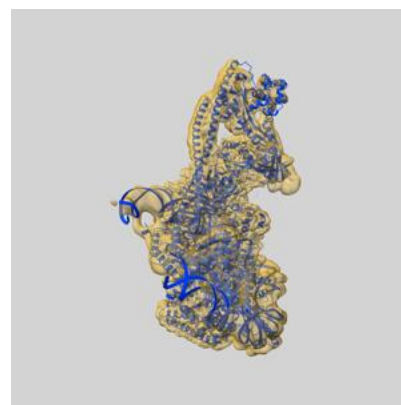
9.1 Map-model overlay [i](#)



X



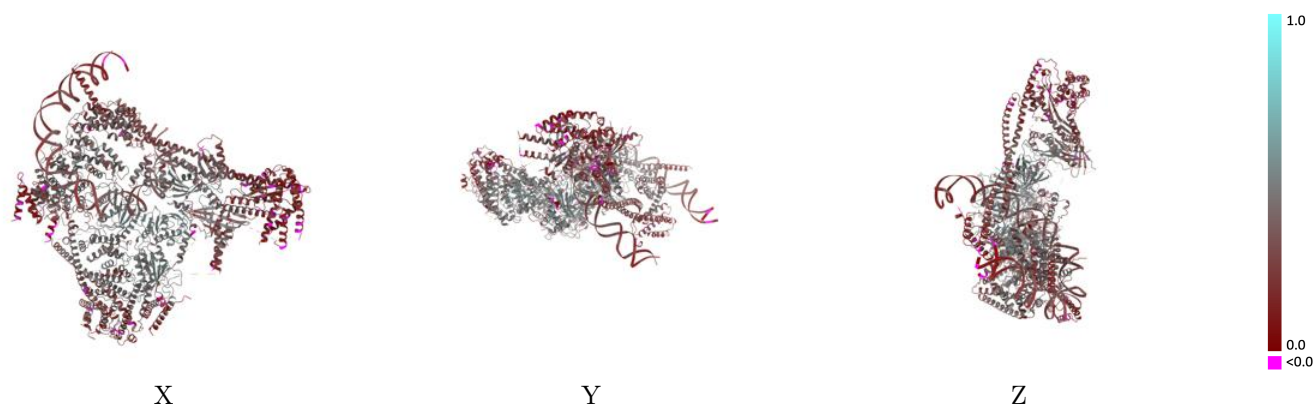
Y



Z

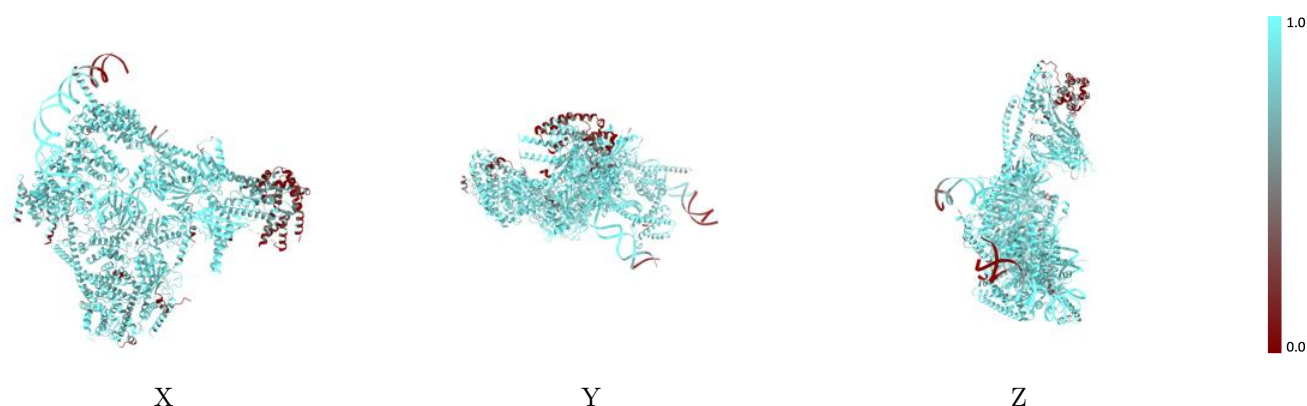
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



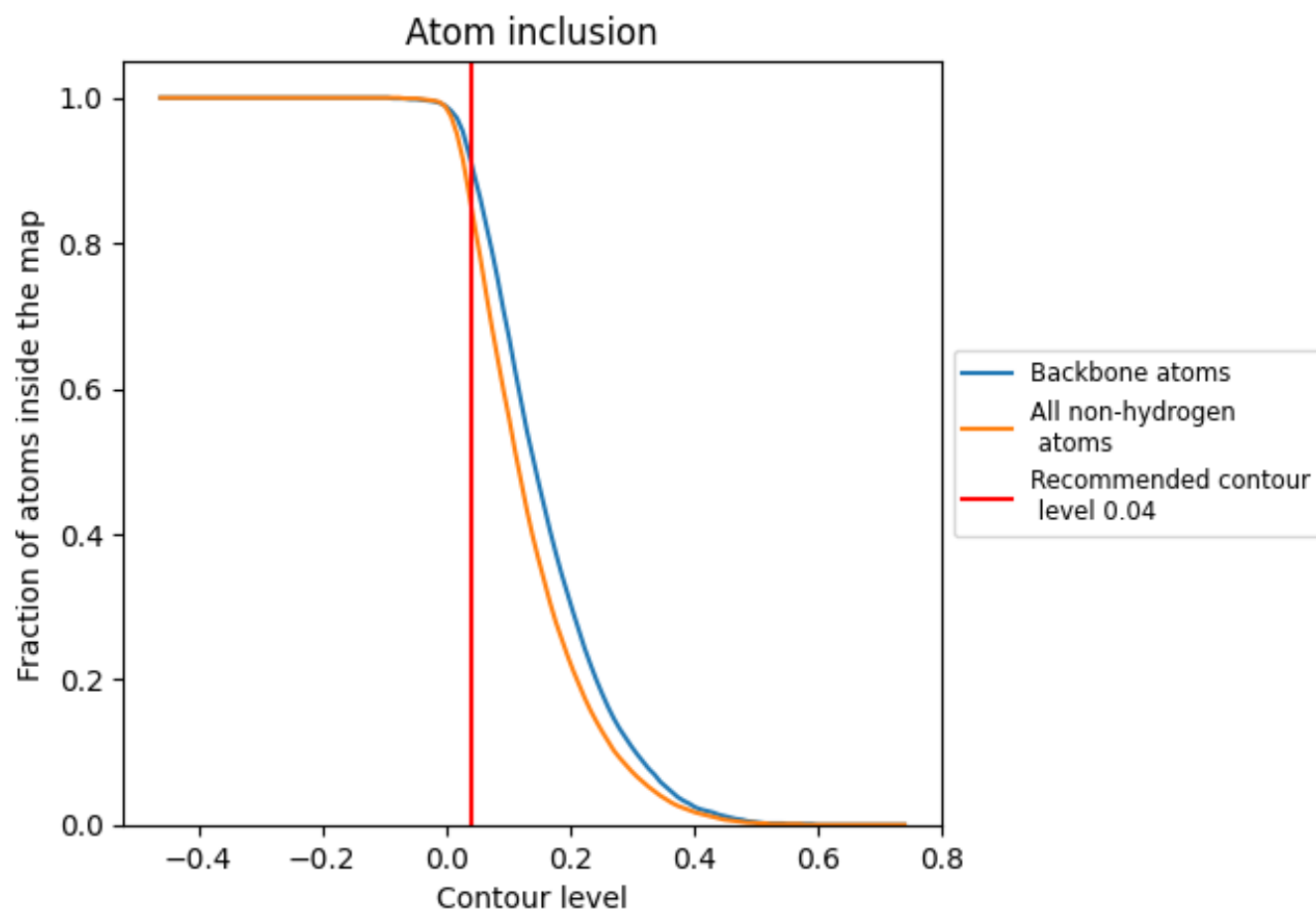
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.3490
A	 0.8060	 0.2450
B	 0.8390	 0.2540
H	 0.8960	 0.3370
I	 0.8700	 0.3540
K	 0.9110	 0.3760
L	 0.9420	 0.4760
M	 0.9560	 0.4920
N	 0.9450	 0.4670
O	 0.9160	 0.3890
P	 0.8550	 0.2820
Q	 0.7140	 0.2220
R	 0.2890	 0.1570
S	 0.8430	 0.3030
T	 0.9170	 0.4120
U	 0.7400	 0.2220
W	 0.9080	 0.4250
X	 0.9000	 0.3520
b	 0.2860	 0.1120

