



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:59 AM UTC

PDB ID : 7YWX / pdb_00007ywx
EMDB ID : EMD-14351
Title : Structure of the human CCAN CENP-A alpha-satellite complex
Authors : Yatskevich, S.; Muir, K.W.; Bellini, D.; Zhang, Z.; Yang, J.; Tischer, T.; Predin, M.; Dendooven, T.; McLaughlin, S.H.; Barford, D.
Deposited on : 2022-02-14
Resolution : 12.00 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:

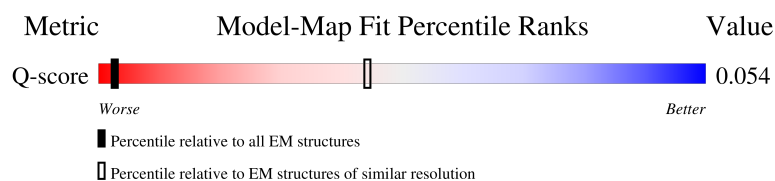
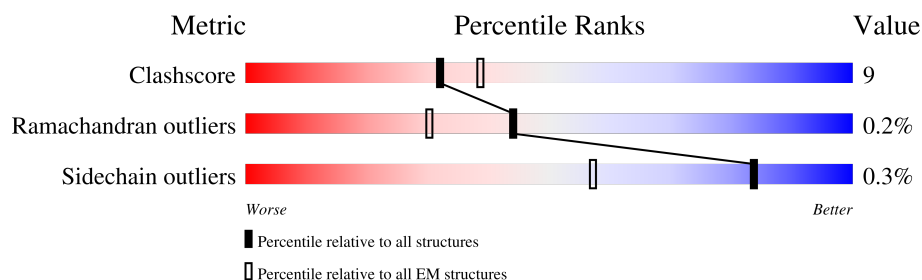
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 12.00 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.



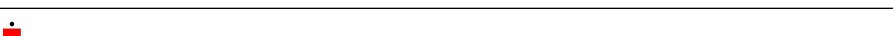
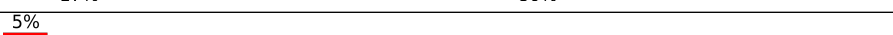
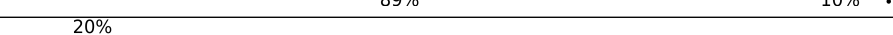
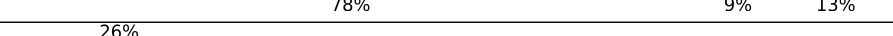
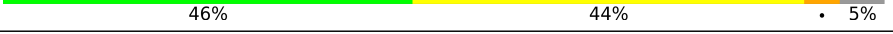
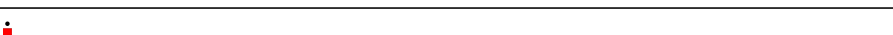
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	93 (11.50 - 12.50)

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	H	247	
2	I	756	
3	K	269	
4	L	344	

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Mol	Chain	Length	Quality of chain
5	M	180	
6	N	339	
7	O	300	
8	Q	268	
9	U	418	
10	P	288	
11	R	177	
12	T	561	
13	W	88	
14	S	138	
15	X	81	
16	i	171	
17	J	171	
18	A	140	
18	E	140	
19	B	103	
19	F	103	
20	C	130	
20	G	130	
21	D	126	
21	V	126	
22	a	544	
22	b	544	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 38294 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 H.

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

- Molecule 2 is a protein called Centromere protein I.

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

- Molecule 3 is a protein called Centromere protein K.

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

- Molecule 4 is a protein called Centromere protein L.

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

- Molecule 5 is a protein called Centromere protein M.

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

- Molecule 6 is a protein called Centromere protein N.

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

- Molecule 7 is a protein called Centromere protein O.

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

- Molecule 8 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	191	Total	C	N	O	S	0	0
			1526	953	258	304	11		

- Molecule 9 is a protein called Centromere protein U.

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

- 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 R.

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

- Molecule 12 is a protein called Centromere protein T.

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

- Molecule 13 is a protein called Centromere protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	88	Total	C	N	O	S	0	0
			704	445	143	112	4		

- Molecule 14 is a protein called Centromere protein S.

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

- Molecule 15 is a protein called Centromere protein X.

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

- Molecule 16 is a DNA chain called DNA (171-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	162	Total	C	N	O	P	0	0
			3320	1588	605	965	162		

- Molecule 17 is a DNA chain called DNA (171-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	162	Total	C	N	O	P	0	0
			3322	1591	590	979	162		

- Molecule 18 is a protein called Histone H3-like centromeric protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	99	Total	C	N	O	S	0	0
			799	518	147	133	1		
18	E	94	Total	C	N	O	S	0	0
			770	501	141	127	1		

- Molecule 19 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
19	F	80	Total	C	N	O	S	0	0
			641	405	125	110	1		

- Molecule 20 is a protein called Histone H2A type 1-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	C	98	Total	C	N	O	0	0
			755	474	149	132		

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Mol	Chain	Residues	Atoms				AltConf	Trace
20	G	103	Total	C	N	O	0	0
			784	491	155	138		

- Molecule 21 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	92	Total	C	N	O	S	0	0
			719	452	129	136	2		
21	V	92	Total	C	N	O	S	0	0
			719	452	129	136	2		

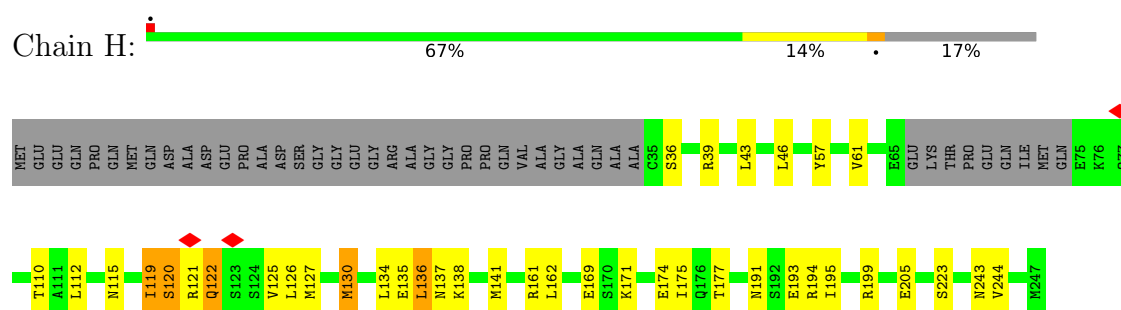
- Molecule 22 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	a	21	Total	C	N	O	0	0
			178	111	37	30		
22	b	57	Total	C	N	O	0	0
			476	298	85	93		

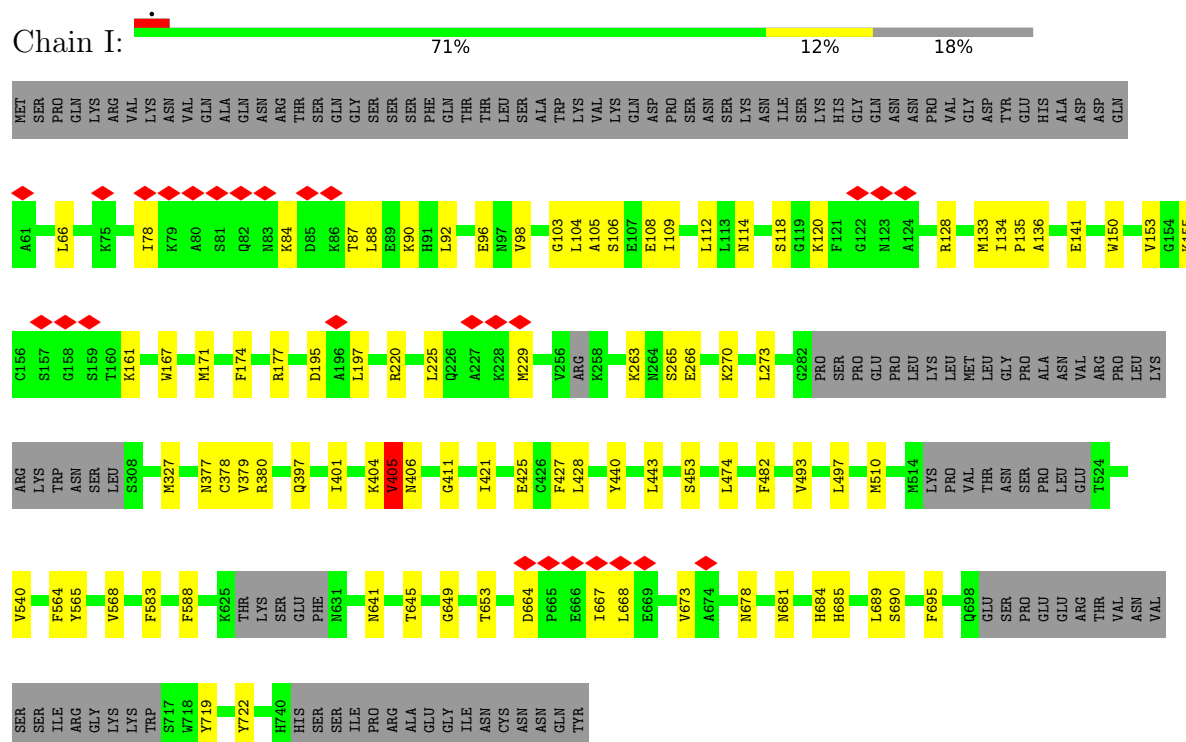
3 Residue-property plots

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.

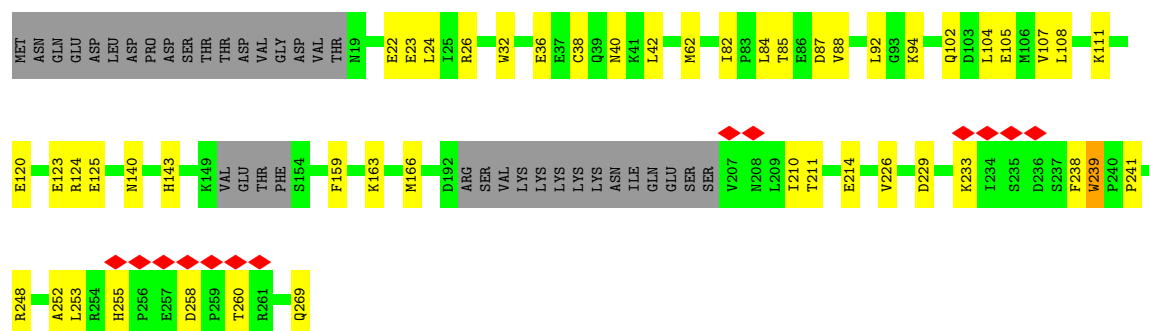
• Molecule 1: Centromere protein H



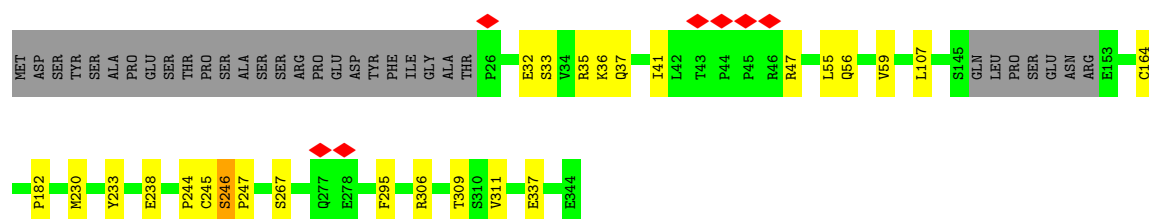
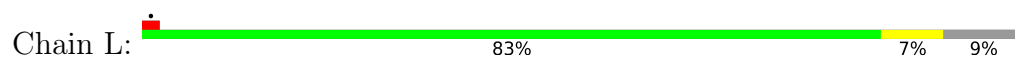
• Molecule 2: Centromere protein I



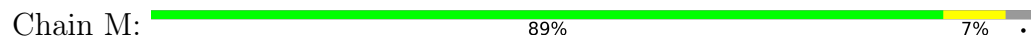
• Molecule 3: Centromere protein K



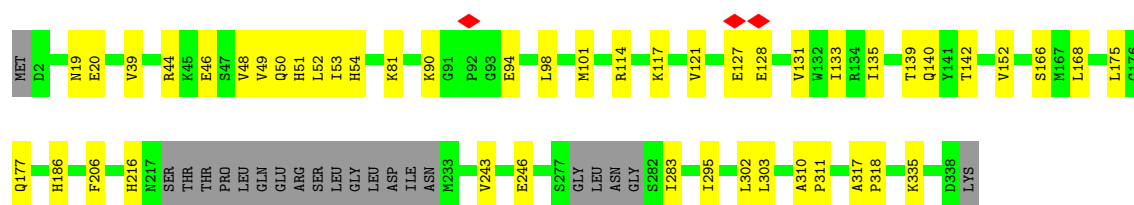
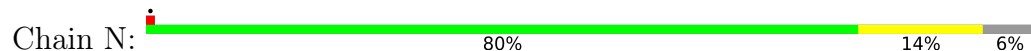
• Molecule 4: Centromere protein L



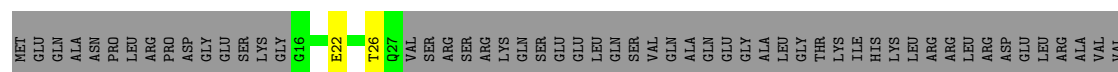
• Molecule 5: Centromere protein M

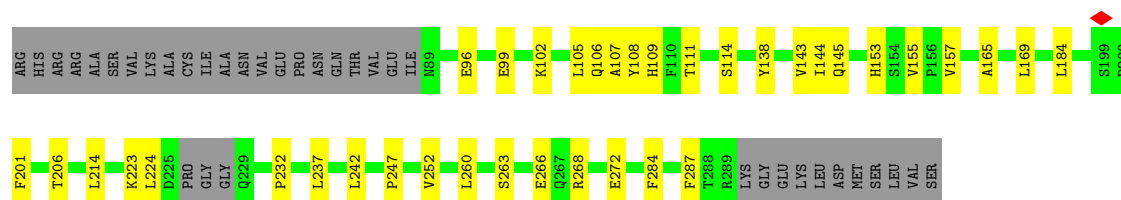


• Molecule 6: Centromere protein N

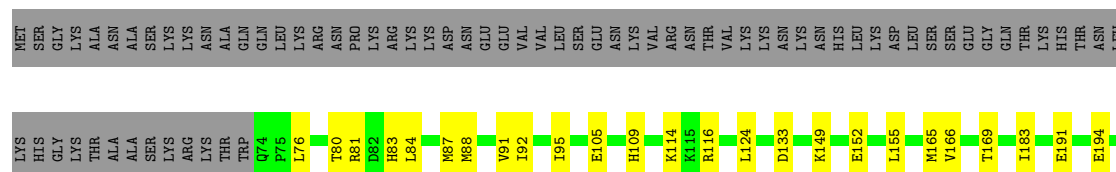


• Molecule 7: Centromere protein O

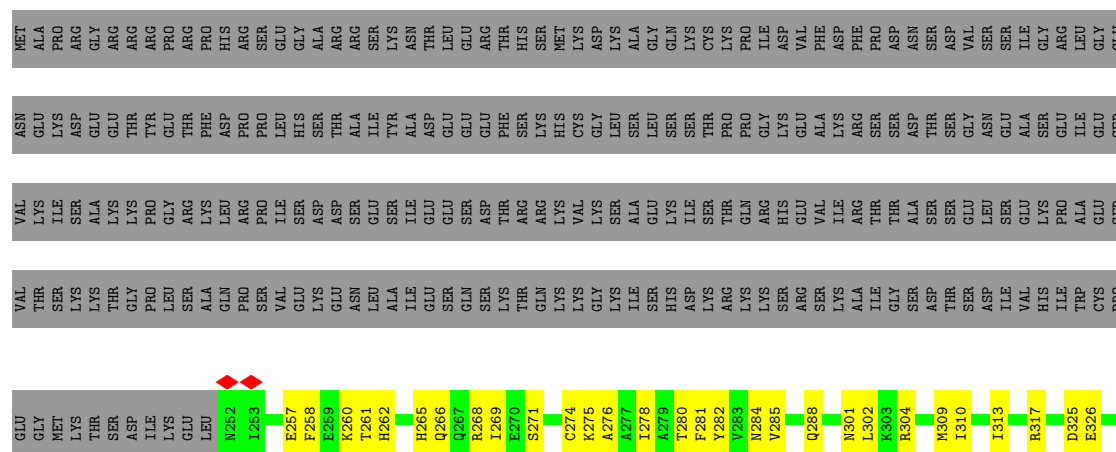




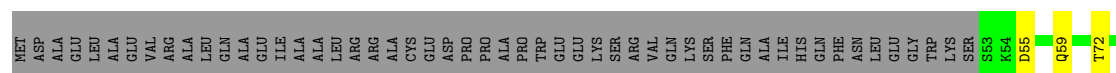
• Molecule 8: Centromere protein Q

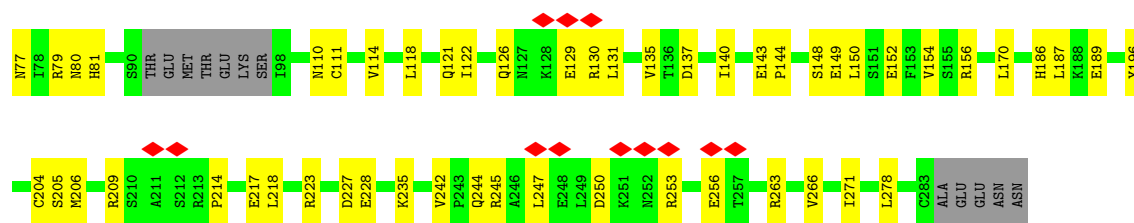


• Molecule 9: Centromere protein U

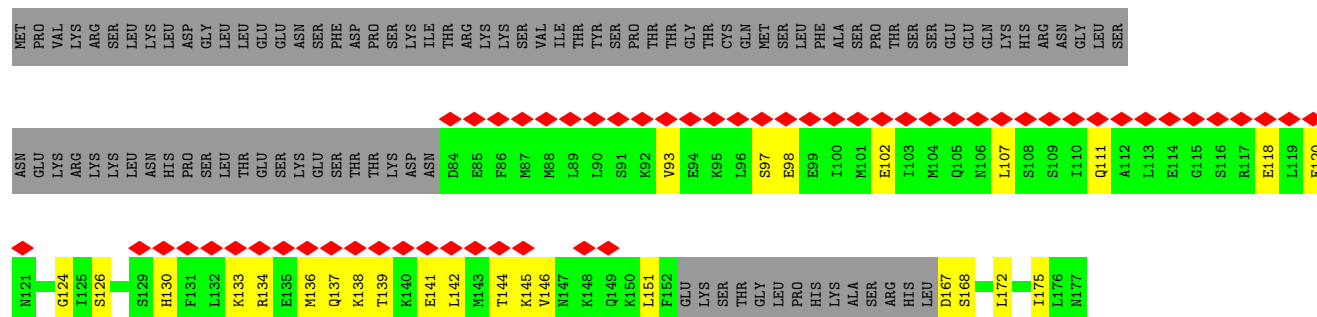
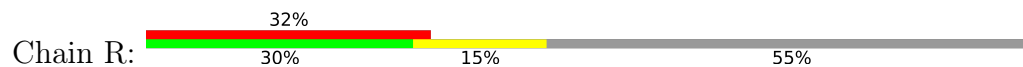


• Molecule 10: Centromere protein P

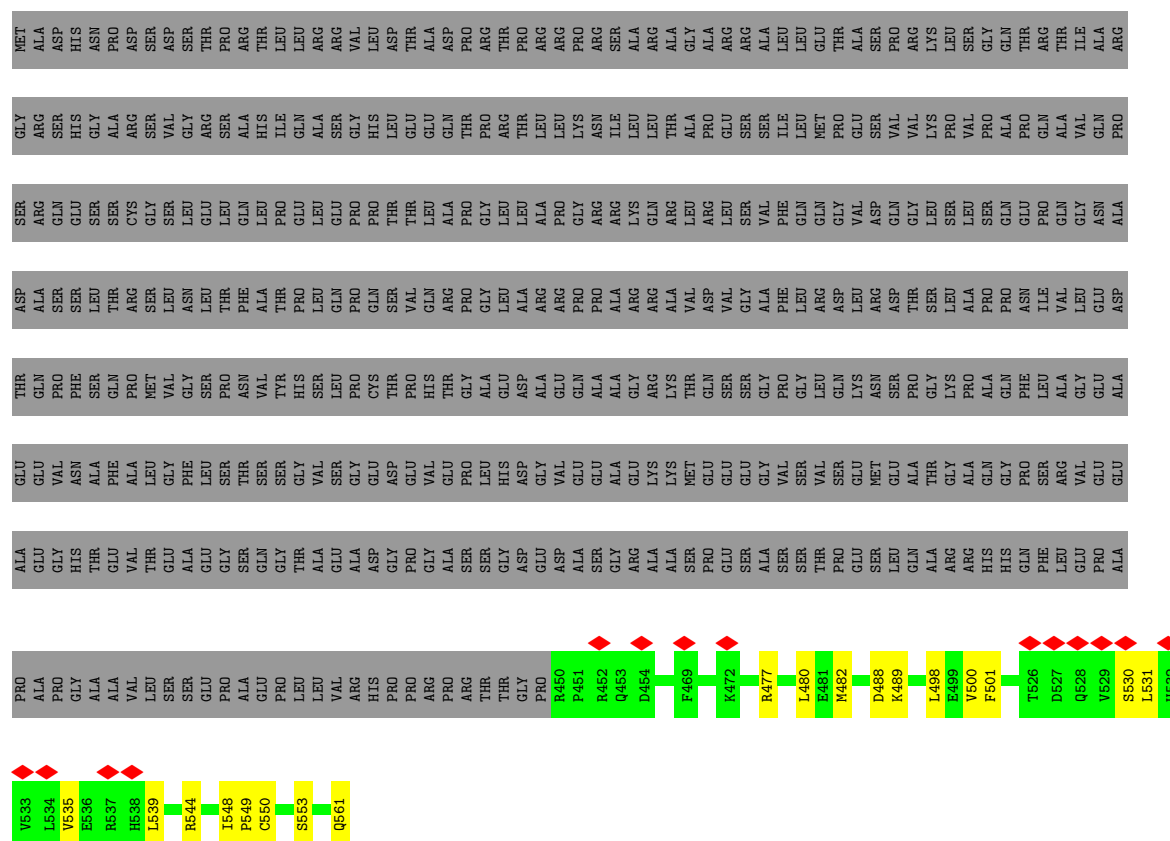




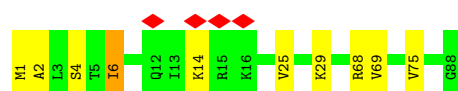
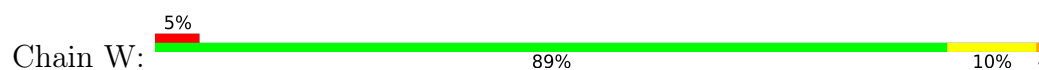
• Molecule 11: Centromere protein R



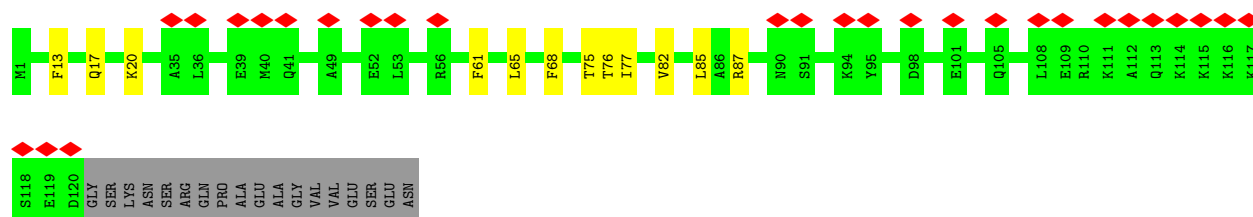
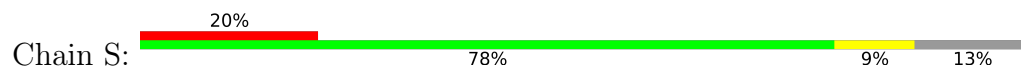
• Molecule 12: Centromere protein T



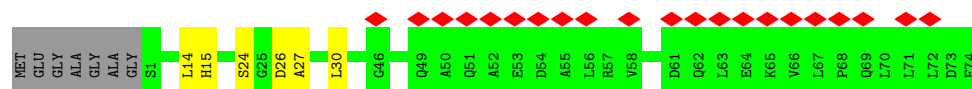
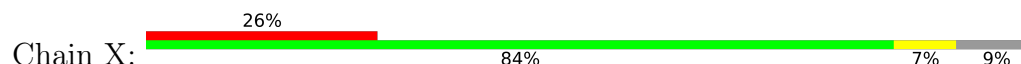
• Molecule 13: Centromere protein W



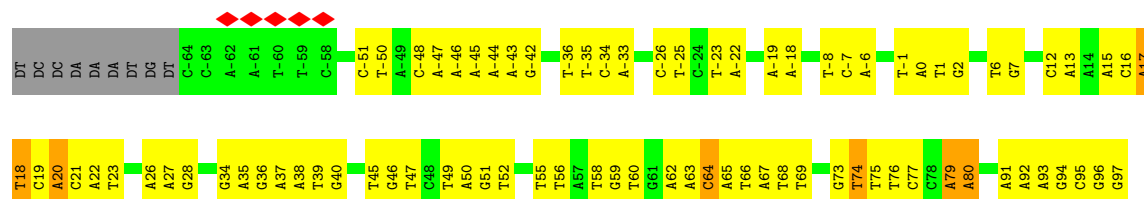
• Molecule 14: Centromere protein S



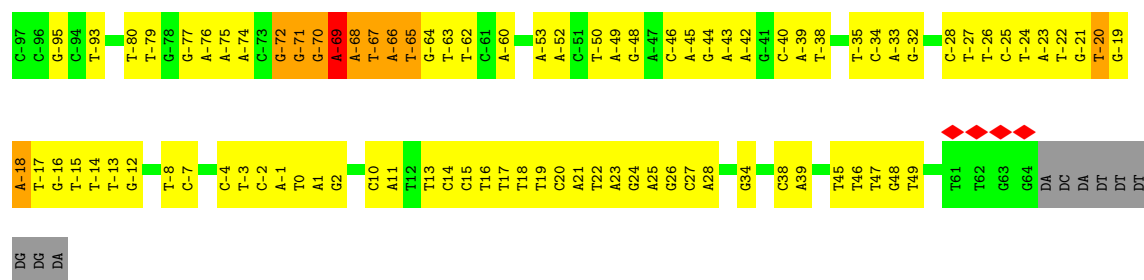
• Molecule 15: Centromere protein X



• Molecule 16: DNA (171-MER)

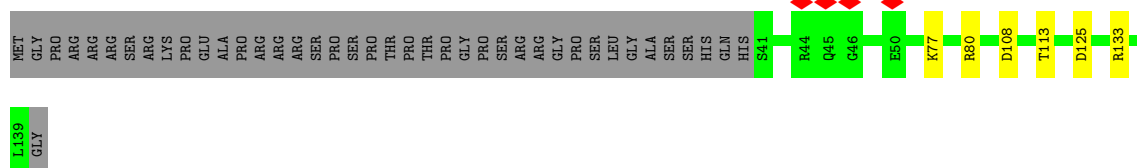


• Molecule 17: DNA (171-MER)



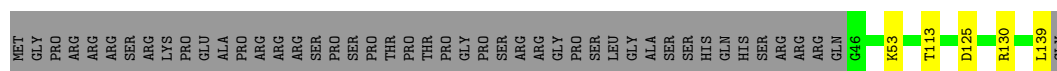
• Molecule 18: Histone H3-like centromeric protein A

Chain A:  66% 29%



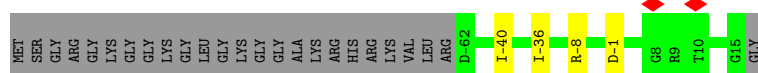
- Molecule 18: Histone H3-like centromeric protein A

Chain E:  64% 33%



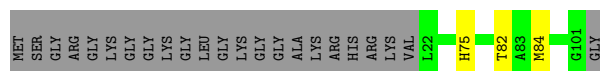
- Molecule 19: Histone H4

Chain B:  72% 24%



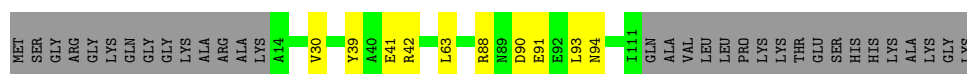
- Molecule 19: Histone H4

Chain F:  75% 22%



- Molecule 20: Histone H2A type 1-C

Chain C:  68% 8% 25%



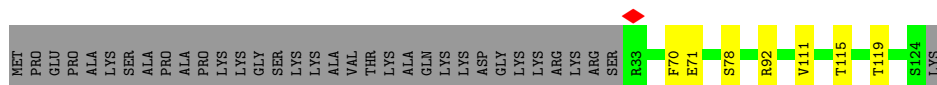
- Molecule 20: Histone H2A type 1-C

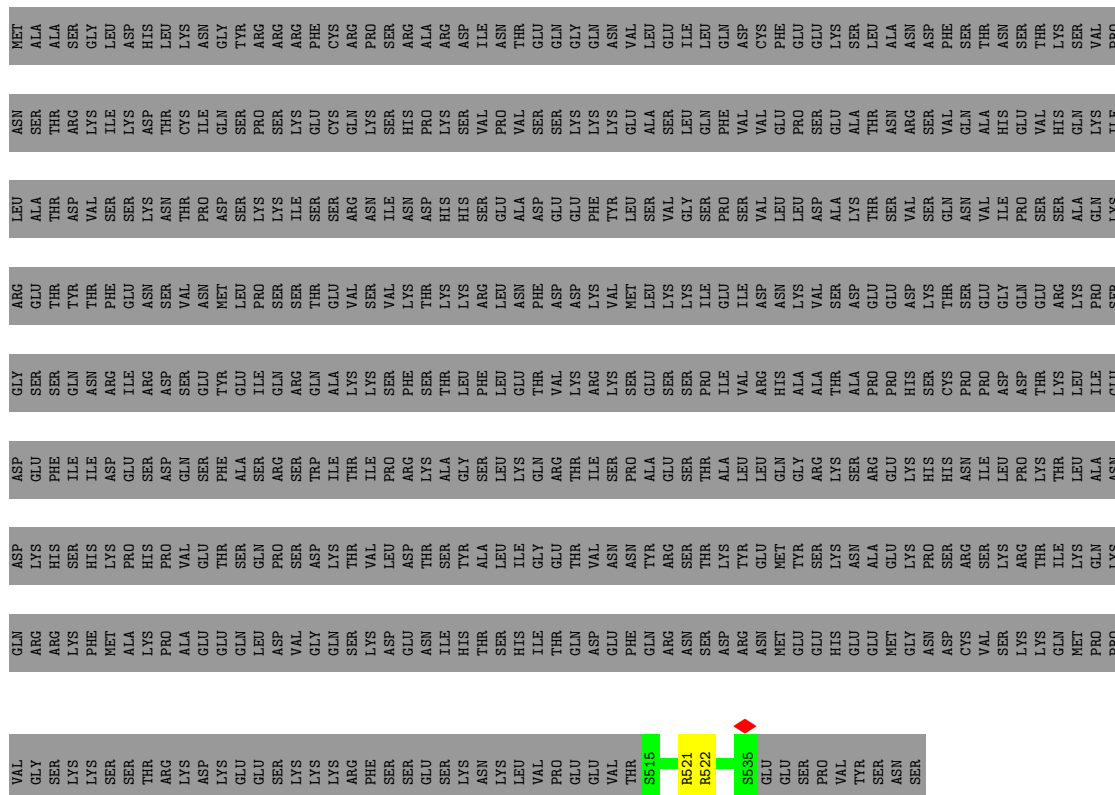
Chain G:  75% 21%

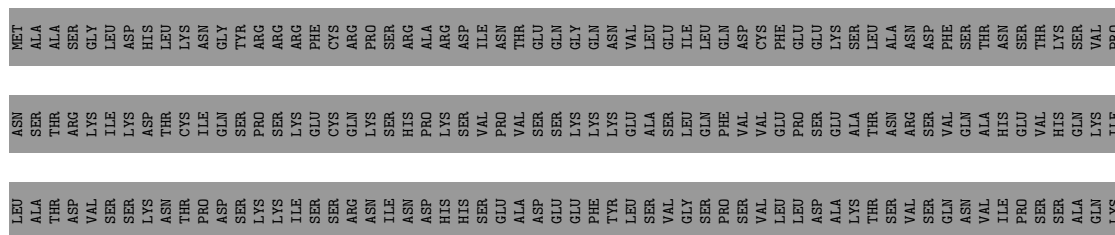


- Molecule 21: Histone H2B type 1-C/E/F/G/I

Chain D:  69% 27%







ARG	GLY	SER	THR	TYR	THR	PHE	GLU	ASN	SER	VAL	ASN	MET	LEU	PRO	SER	SER	THR	GLU	VAL	SER	VAL	LYS	THR	LYS	ARG	LEU	ASN	PHE	ASP	ASP	LYS	VAL	MET	LEU	LYS	LYS	ILE	GLU	ILE	ILE	ASP	ASN	LYS	VAL	SER	ASP	GLU	GLU	ASP	LYS	THR	SER	GLY	GLN	ARG	GLU	PRO	LYS	SER		
GLY	SER	GLN	ASN	ARG	ILE	ARG	ASP	SER	GLU	TYR	GLU	ILE	GLN	R256	Q257	A258	K259	K260	S261	F262	S263	T269	K270	K271	R272	K273	S274	E275	SER	SER	PRO	ILE	VAL	ARG	HIS	ALA	ALA	THR	ALA	PRO	HIS	HIS	SER	CYS	PRO	PRO	ASP	D295	K296	K297	L298	I299	E300	D301	I304	I305					
D306	E307	S308	D309	GLN	SER	PHE	ALA	SER	PRO	ARG	SER	TRP	ILE	THR	ILE	PRO	ARG	LYS	ALA	GLY	SER	LEU	LYS	GLN	ARG	T269	K270	K271	R272	K273	S274	E275	SER	THR	THR	ALA	LYS	LEU	GLN	GLY	ARG	LYS	ALA	ARG	GLU	LYS	HIS	HIS	SER	ARG	ILE	LYS	THR	LYS	LEU	ALA	L298	I299	E300	D301	HIS
LYS	PRO	HIS	VAL	GLU	THR	SER	GLN	LEU	ASP	PRO	VAL	ASP	THR	SER	TYR	ALA	SER	ILE	GLY	THR	GLN	THR	ILE	ASN	ASN	TYR	ALA	GLU	SER	THR	THR	ALA	LYS	LEU	GLN	GLY	SER	ARG	LYS	ASN	ILE	LYS	THR	LYS	PRO	SER	ARG	LYS	THR	ILE	LYS	GLN	LYS	PRO	VAL	GLY	SER	LYS	PHE		
MET	ALA	LYS	PRO	ALA	GLU	GLU	GLN	LEU	ASP	VAL	GLY	GLN	SER	LYS	PHE	LYS	ASP	GLU	ASN	ILE	HIS	THR	SER	HIS	LYS	LEU	VAL	PRO	THR	GLN	GLU	ASN	ASP	ASN	ASP	ASN	MET	GLU	GLU	HIS	GLU	GLU	GLY	ASN	ASN	ASP	CYS	VAL	SER	LYS	LYS	GLN	PRO	PRO	VAL	GLY	SER	LYS	LYS		
SER	SER	THR	ARG	LYS	LYS	GLU	LYS	SER	LYS	LYS	ARG	ARG	THR	VAL	T514	P527	S528	D529	S535	GLU	GLU	SER	PRO	VAL	TYR	SER	ASN	SER																																	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.038	Depositor
Minimum map value	-0.377	Depositor
Average map value	0.042	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	292.4, 292.4, 292.4	wwPDB
Map dimensions	170, 170, 170	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.7199999, 1.7199999, 1.7199999	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	H	0.38	1/1660 (0.1%)	0.65	4/2218 (0.2%)
2	I	0.23	0/5137	0.41	1/6955 (0.0%)
3	K	0.19	0/1953	0.35	0/2634
4	L	0.25	0/2569	0.43	0/3485
5	M	0.22	0/1347	0.35	0/1827
6	N	0.26	0/2670	0.44	0/3606
7	O	0.18	0/1678	0.36	0/2280
8	Q	0.17	0/1538	0.43	0/2062
9	U	0.17	0/1383	0.40	0/1856
10	P	0.16	0/1820	0.38	0/2451
11	R	0.10	0/653	0.31	0/865
12	T	0.15	0/937	0.34	0/1263
13	W	0.33	0/711	0.46	0/944
14	S	0.10	0/991	0.26	0/1322
15	X	0.09	0/596	0.30	0/801
16	i	0.35	3/3726 (0.1%)	0.83	14/5747 (0.2%)
17	J	0.41	2/3724 (0.1%)	0.86	27/5747 (0.5%)
18	A	0.12	0/814	0.27	0/1097
18	E	0.12	0/785	0.28	0/1057
19	B	0.14	0/629	0.30	0/843
19	F	0.14	0/648	0.31	0/868
20	C	0.13	0/764	0.32	0/1030
20	G	0.12	0/793	0.31	0/1070
21	D	0.12	0/730	0.26	0/982
21	V	0.12	0/730	0.27	0/982
22	a	0.13	0/182	0.34	0/245
22	b	1.29	10/481 (2.1%)	1.95	18/641 (2.8%)
All	All	0.29	16/39649 (0.0%)	0.56	64/54878 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
17	J	0	1
22	b	0	13
All	All	0	15

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	301	ASP	C-N	11.42	1.51	1.33
22	b	300	GLU	C-N	10.18	1.48	1.33
22	b	296	THR	C-N	9.87	1.47	1.33
22	b	299	ILE	C-N	9.10	1.46	1.33
17	J	-68	DA	O3'-P	-8.63	1.48	1.61

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	i	64	DC	OP1-P-O3'	-26.64	28.07	108.00
17	J	-66	DA	C2'-C3'-O3'	-26.13	72.31	111.50
22	b	274	SER	O-C-N	-19.41	95.62	121.83
16	i	64	DC	O3'-P-O5'	18.50	131.75	104.00
16	i	64	DC	P-O3'-C3'	-18.21	92.88	120.20

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	J	-69	DA	Sidechain
3	K	239	TRP	Peptide
22	b	256	ARG	Mainchain
22	b	257	GLN	Mainchain
22	b	258	ALA	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1652	0	1728	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	5014	0	5036	67	0
3	K	1922	0	1924	37	0
4	L	2502	0	2492	27	0
5	M	1325	0	1370	23	0
6	N	2613	0	2625	36	0
7	O	1642	0	1616	26	0
8	Q	1526	0	1586	35	0
9	U	1365	0	1396	38	0
10	P	1788	0	1791	40	0
11	R	649	0	673	20	0
12	T	915	0	924	21	0
13	W	704	0	789	46	0
14	S	982	0	987	8	0
15	X	590	0	623	5	0
16	i	3320	0	1830	126	0
17	J	3322	0	1837	138	0
18	A	799	0	823	4	0
18	E	770	0	807	3	0
19	B	622	0	663	2	0
19	F	641	0	684	2	0
20	C	755	0	800	7	0
20	G	784	0	815	4	0
21	D	719	0	738	5	0
21	V	719	0	738	5	0
22	a	178	0	185	2	0
22	b	476	0	483	29	0
All	All	38294	0	35963	630	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 9.

The worst 5 of 630 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:M:13:LEU:HD21	22:b:262:PHE:CE1	1.22	1.63
5:M:13:LEU:CD2	22:b:262:PHE:CE1	1.91	1.49
5:M:13:LEU:CG	22:b:262:PHE:HE1	1.40	1.34
5:M:13:LEU:CG	22:b:262:PHE:CE1	2.14	1.25
5:M:13:LEU:HD21	22:b:262:PHE:CD1	1.70	1.25

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	H	200/247 (81%)	196 (98%)	4 (2%)	0	100	100
2	I	610/756 (81%)	589 (97%)	19 (3%)	2 (0%)	36	72
3	K	227/269 (84%)	224 (99%)	3 (1%)	0	100	100
4	L	308/344 (90%)	299 (97%)	8 (3%)	1 (0%)	36	72
5	M	170/180 (94%)	168 (99%)	2 (1%)	0	100	100
6	N	312/339 (92%)	298 (96%)	14 (4%)	0	100	100
7	O	204/300 (68%)	199 (98%)	5 (2%)	0	100	100
8	Q	187/268 (70%)	184 (98%)	3 (2%)	0	100	100
9	U	164/418 (39%)	163 (99%)	1 (1%)	0	100	100
10	P	220/288 (76%)	212 (96%)	8 (4%)	0	100	100
11	R	76/177 (43%)	72 (95%)	4 (5%)	0	100	100
12	T	110/561 (20%)	109 (99%)	1 (1%)	0	100	100
13	W	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
14	S	118/138 (86%)	117 (99%)	1 (1%)	0	100	100
15	X	72/81 (89%)	72 (100%)	0	0	100	100
18	A	97/140 (69%)	93 (96%)	4 (4%)	0	100	100
18	E	92/140 (66%)	88 (96%)	4 (4%)	0	100	100
19	B	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
19	F	78/103 (76%)	78 (100%)	0	0	100	100
20	C	96/130 (74%)	94 (98%)	2 (2%)	0	100	100
20	G	101/130 (78%)	99 (98%)	2 (2%)	0	100	100
21	D	90/126 (71%)	89 (99%)	1 (1%)	0	100	100
21	V	90/126 (71%)	89 (99%)	1 (1%)	0	100	100
22	a	19/544 (4%)	15 (79%)	4 (21%)	0	100	100
22	b	51/544 (9%)	46 (90%)	1 (2%)	4 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3854/6540 (59%)	3752 (97%)	95 (2%)	7 (0%)	44 78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	405	VAL
2	I	411	GLY
4	L	246	SER
22	b	257	GLN
22	b	258	ALA

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	H	188/224 (84%)	184 (98%)	4 (2%)	47 65
2	I	560/691 (81%)	558 (100%)	2 (0%)	84 84
3	K	221/260 (85%)	221 (100%)	0	100 100
4	L	277/306 (90%)	276 (100%)	1 (0%)	84 84
5	M	151/158 (96%)	151 (100%)	0	100 100
6	N	287/311 (92%)	287 (100%)	0	100 100
7	O	177/263 (67%)	177 (100%)	0	100 100
8	Q	179/248 (72%)	179 (100%)	0	100 100
9	U	152/379 (40%)	152 (100%)	0	100 100
10	P	197/259 (76%)	197 (100%)	0	100 100
11	R	75/166 (45%)	75 (100%)	0	100 100
12	T	100/461 (22%)	100 (100%)	0	100 100
13	W	77/77 (100%)	76 (99%)	1 (1%)	61 74
14	S	107/121 (88%)	107 (100%)	0	100 100
15	X	65/67 (97%)	65 (100%)	0	100 100
18	A	80/118 (68%)	80 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	E	79/118 (67%)	79 (100%)	0	100	100
19	B	64/79 (81%)	64 (100%)	0	100	100
19	F	66/79 (84%)	66 (100%)	0	100	100
20	C	76/99 (77%)	76 (100%)	0	100	100
20	G	77/99 (78%)	76 (99%)	1 (1%)	61	74
21	D	79/106 (74%)	79 (100%)	0	100	100
21	V	79/106 (74%)	78 (99%)	1 (1%)	61	74
22	a	21/508 (4%)	21 (100%)	0	100	100
22	b	56/508 (11%)	54 (96%)	2 (4%)	31	52
All	All	3490/5811 (60%)	3478 (100%)	12 (0%)	84	86

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

Mol	Chain	Res	Type
13	W	6	ILE
20	G	19	SER
22	b	296	THR
21	V	71	GLU
1	H	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
9	U	409	HIS
18	A	87	GLN
21	V	84	ASN
10	P	59	GLN
12	T	456	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

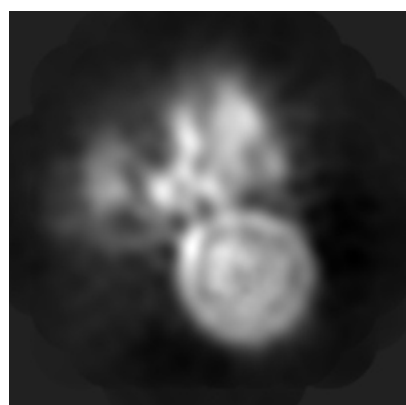
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14351. These allow visual inspection of the internal detail of the map and identification of artifacts.

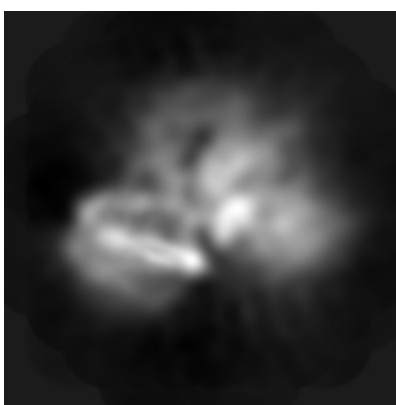
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

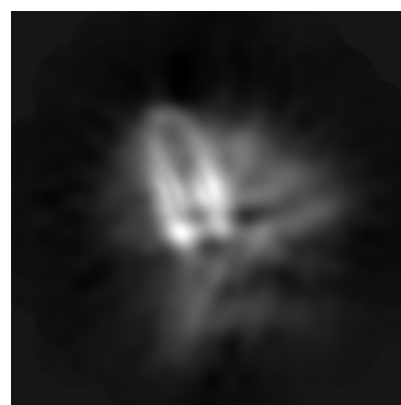
6.1.1 Primary map



X



Y

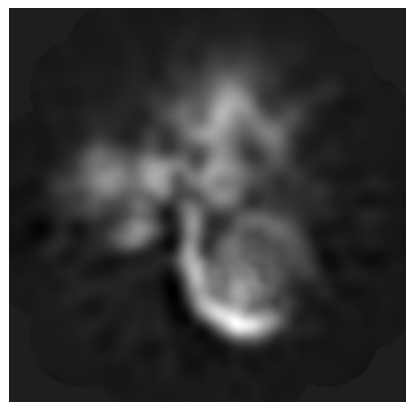


Z

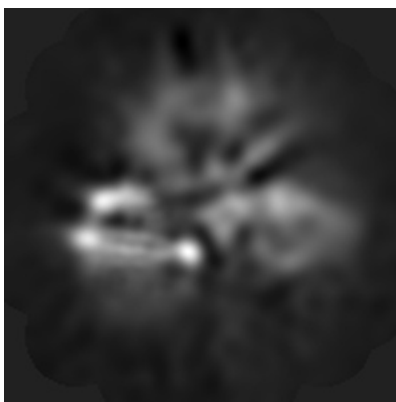
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

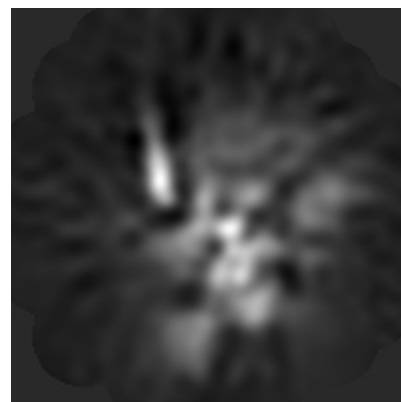
6.2.1 Primary map



X Index: 85



Y Index: 85

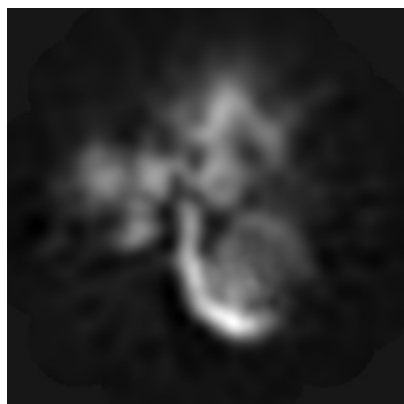


Z Index: 85

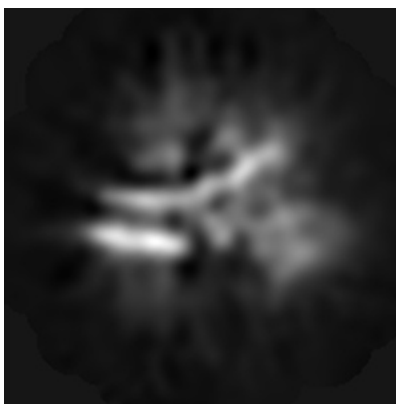
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

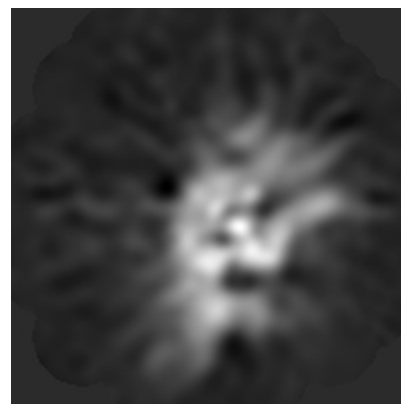
6.3.1 Primary map



X Index: 86



Y Index: 76

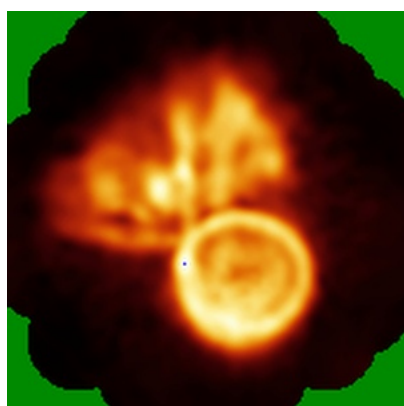


Z Index: 96

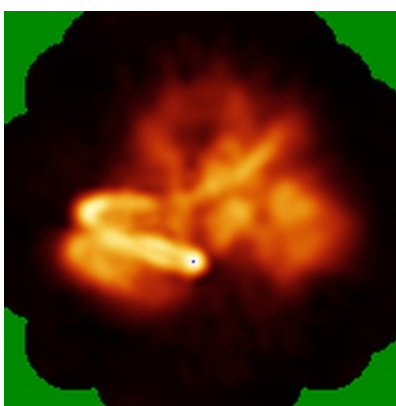
The images above show the largest variance slices of the map in three orthogonal directions.

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

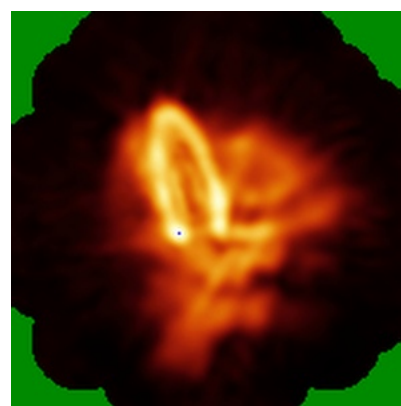
6.4.1 Primary map



X



Y

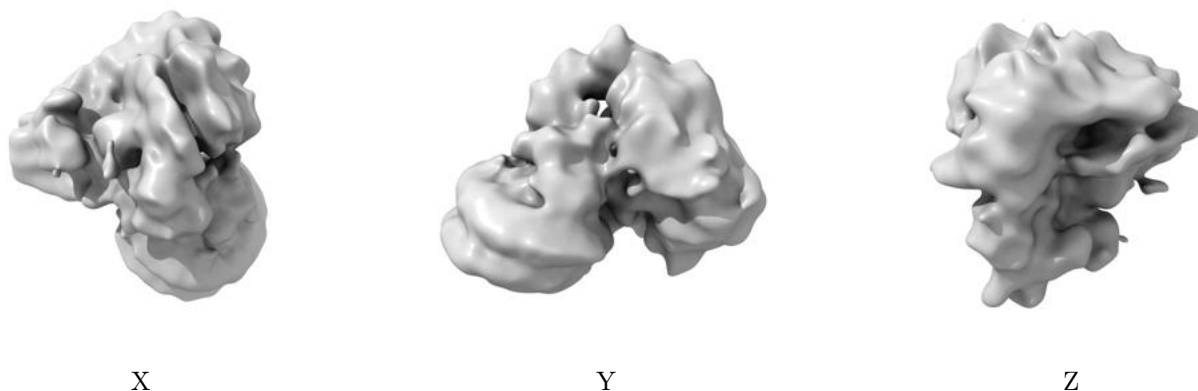


Z

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

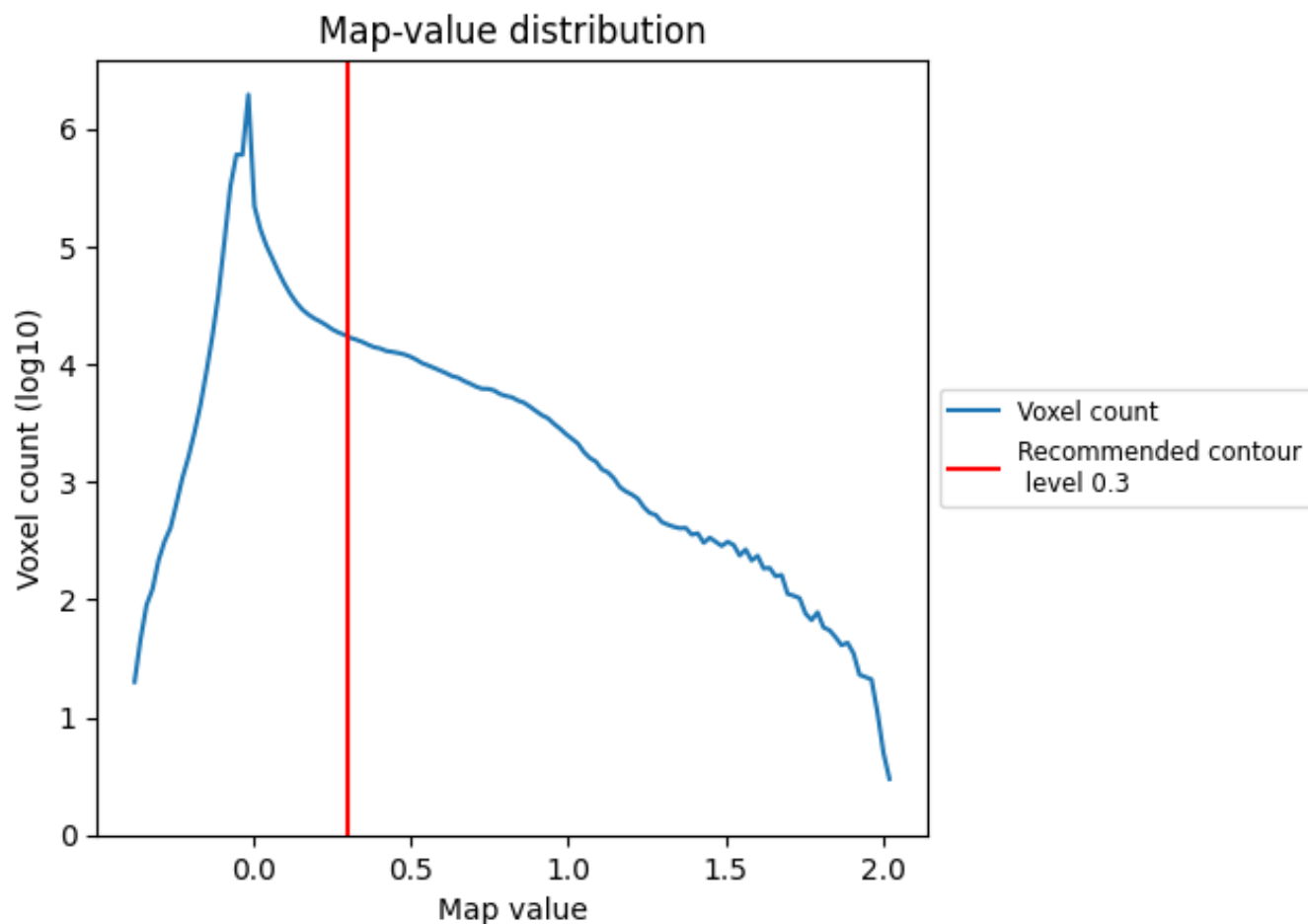
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

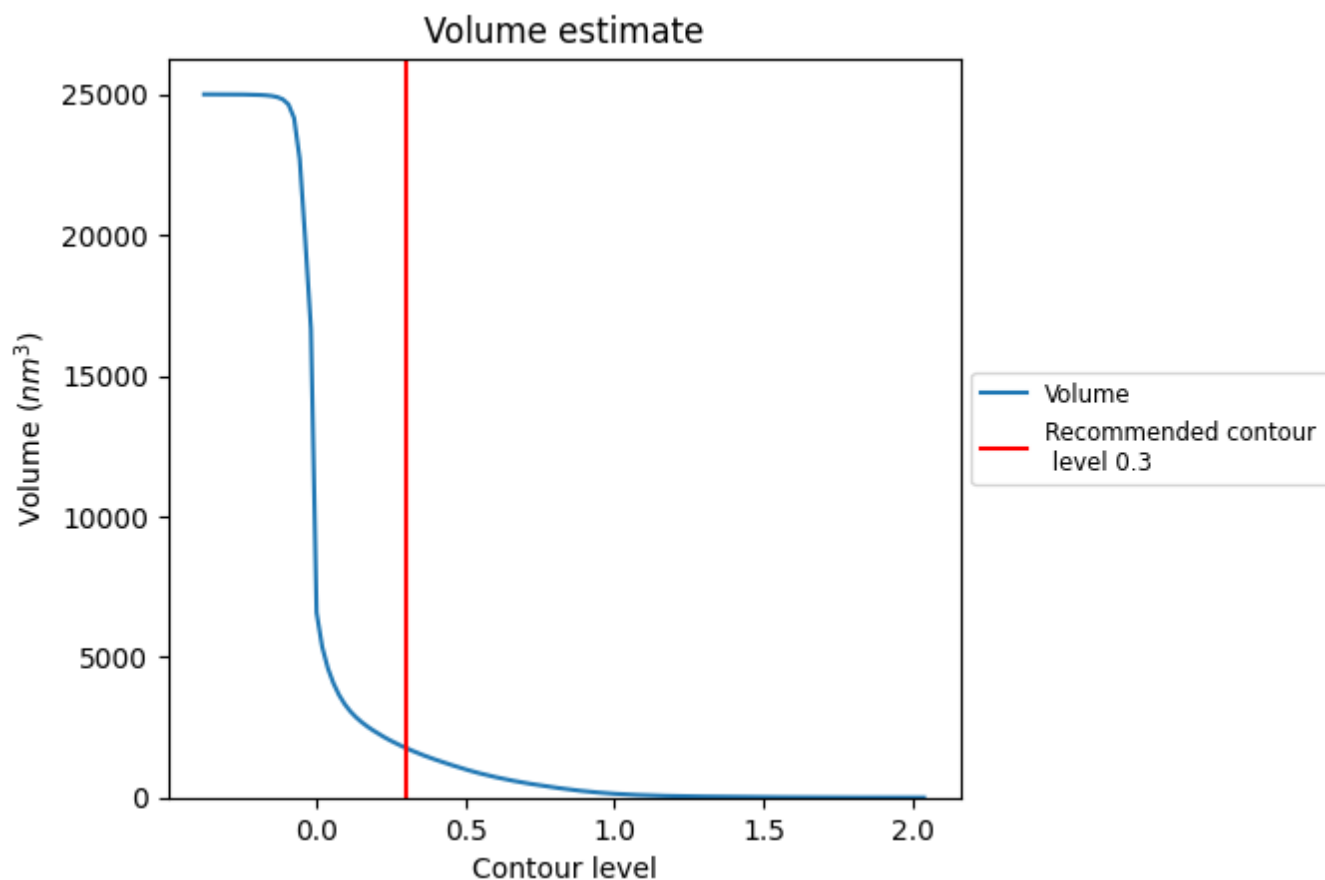
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

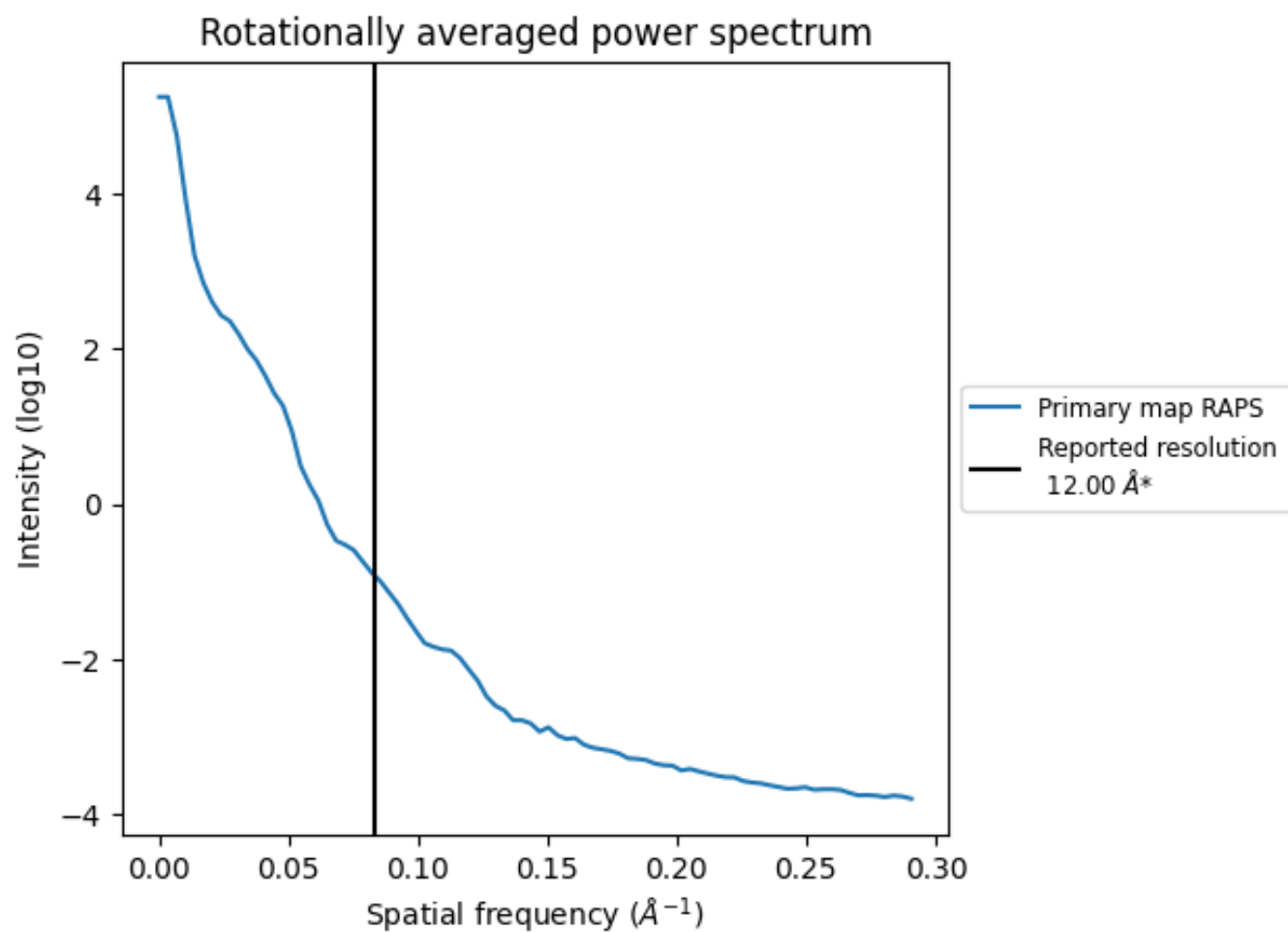
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1765 nm^3 ; this corresponds to an approximate mass of 1594 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 ⓘ

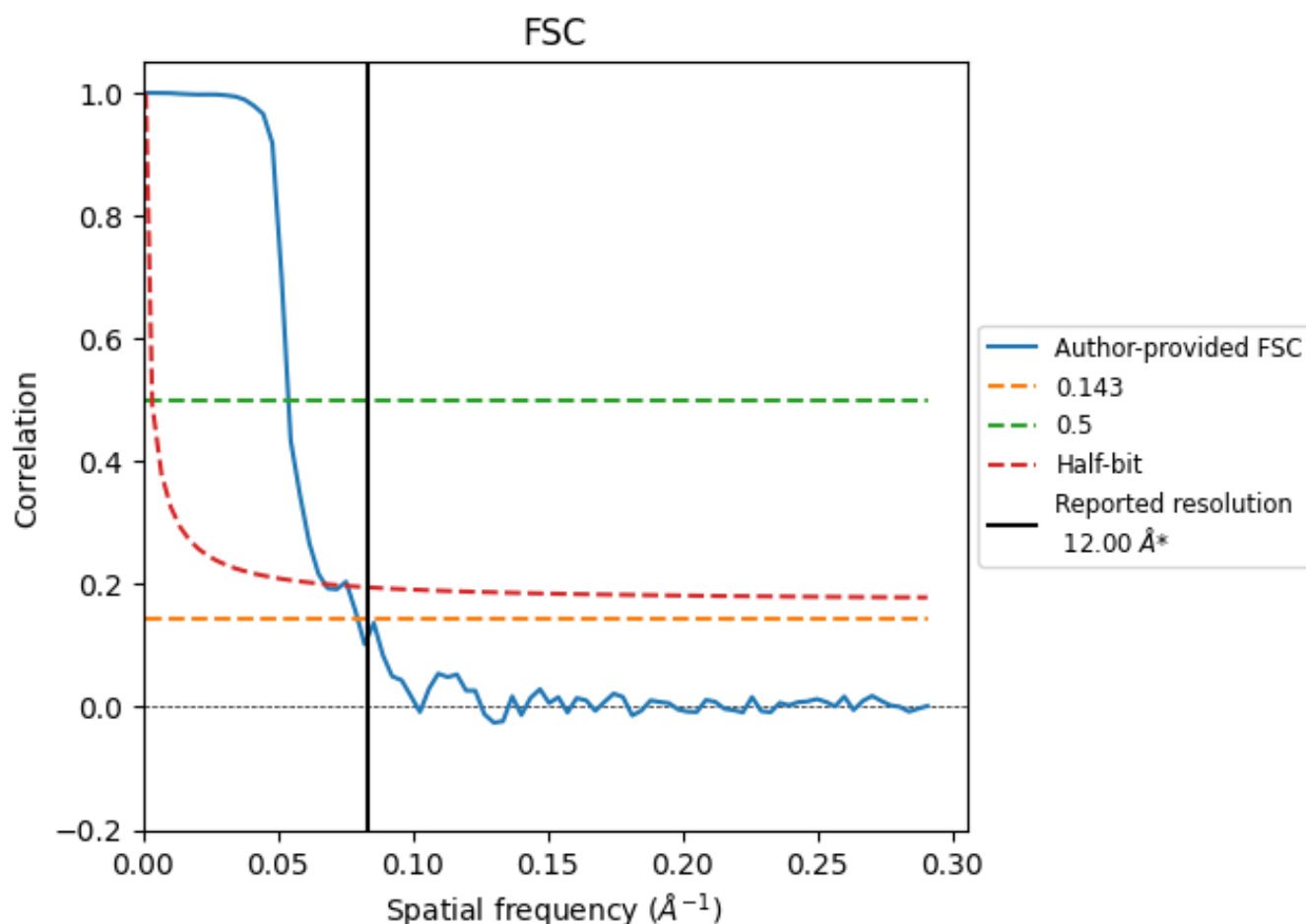


*Reported resolution corresponds to spatial frequency of 0.083 Å⁻¹

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 0.083 Å⁻¹

8.2 Resolution estimates [i](#)

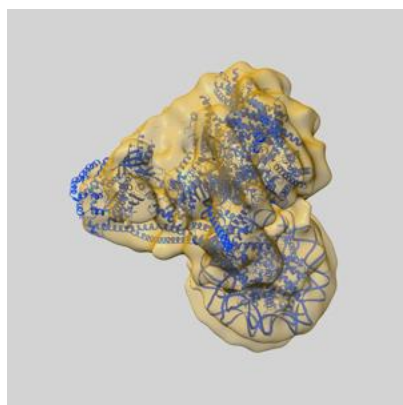
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	12.00	-	-
Author-provided FSC curve	12.58	18.55	14.84
Unmasked-calculated*	-	-	-

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

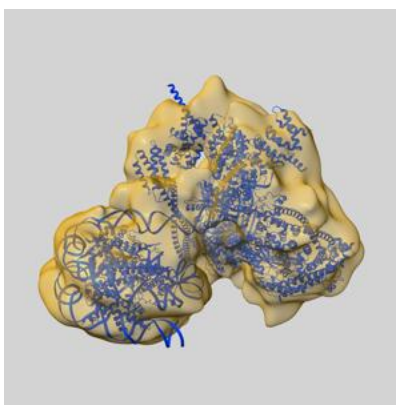
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14351 and PDB model 7YWX. Per-residue inclusion information can be found in section [3](#) on page [8](#).

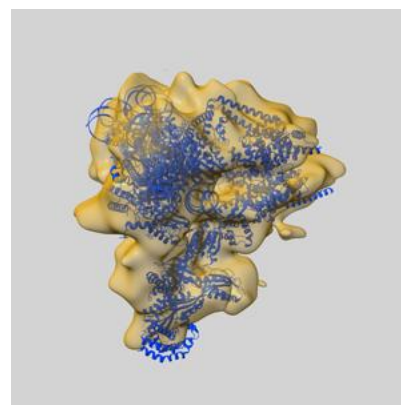
9.1 Map-model overlay [i](#)



X



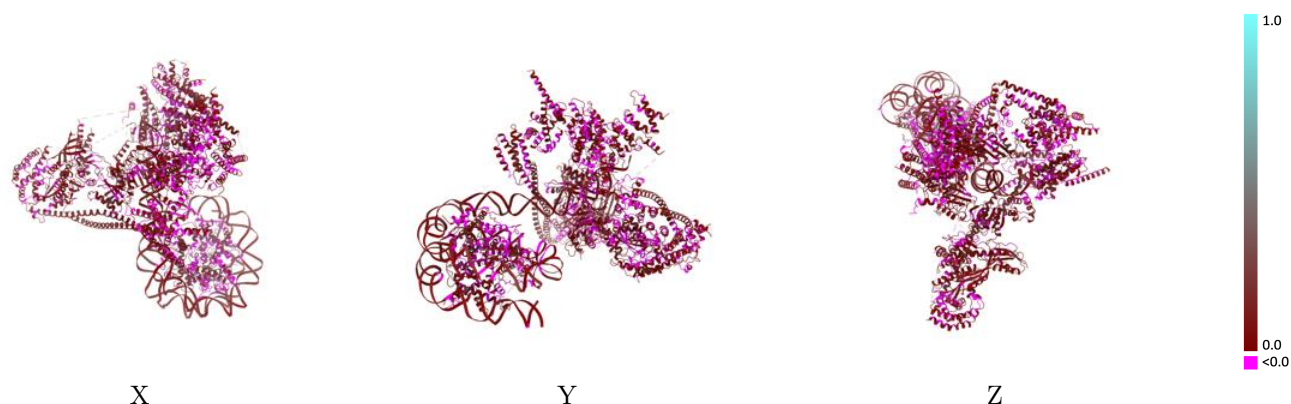
Y



Z

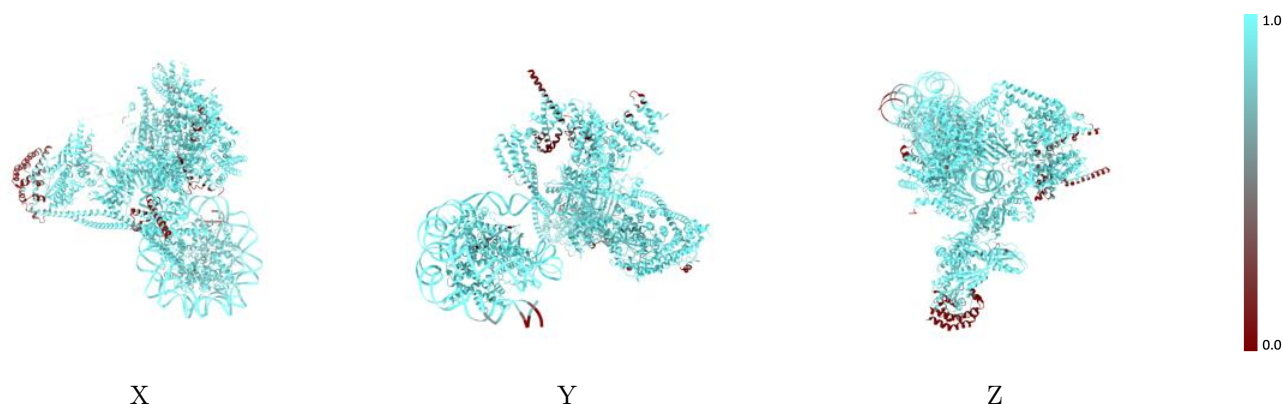
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



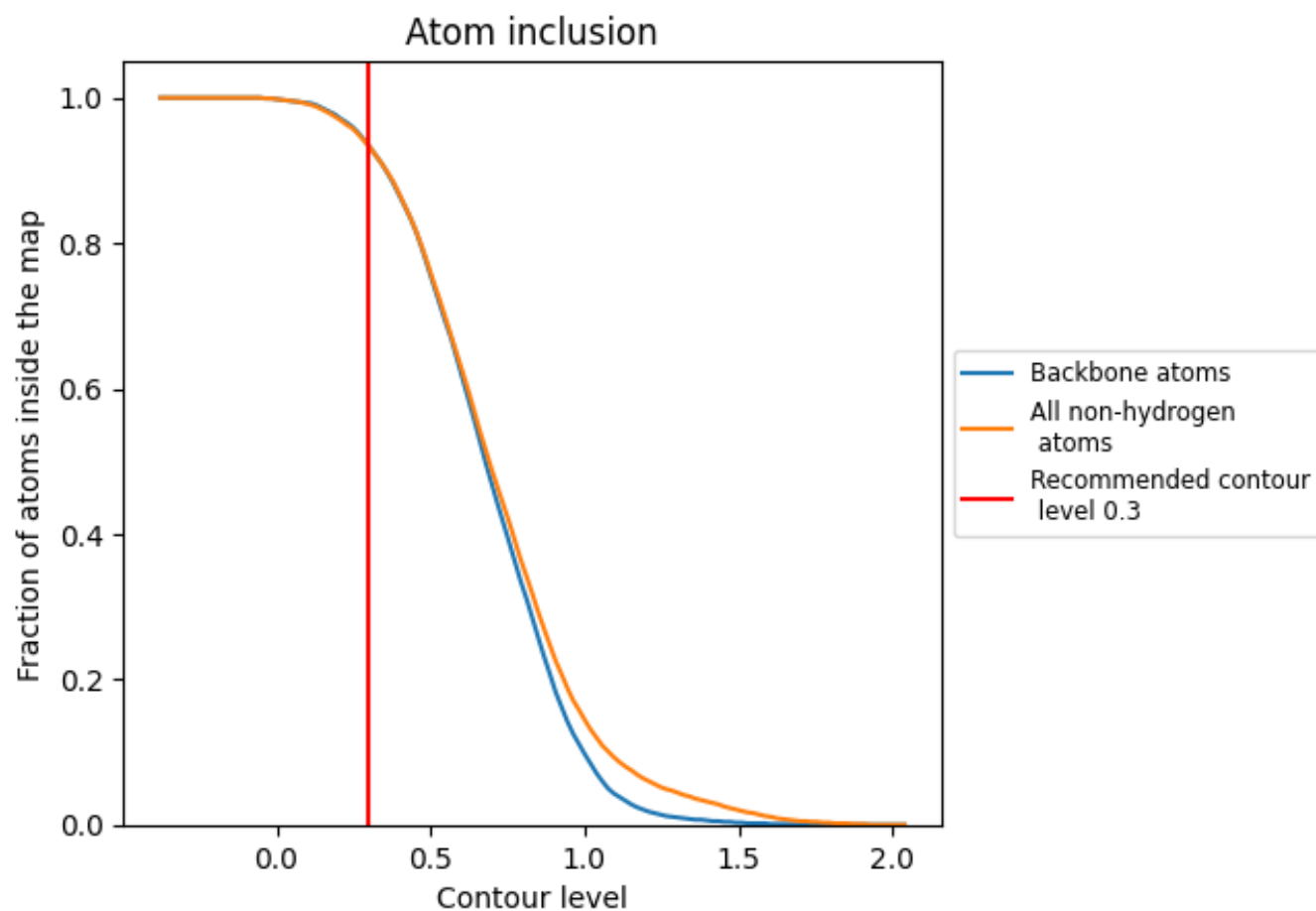
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.0540
A	 0.9460	 0.0390
B	 0.9700	 0.0300
C	 1.0000	 0.0620
D	 1.0000	 0.0550
E	 0.9790	 0.0230
F	 0.9840	 0.0370
G	 0.9510	 0.0200
H	 0.9850	 0.0420
I	 0.9540	 0.0320
J	 0.9620	 0.1020
K	 0.9410	 0.0540
L	 0.9700	 0.0480
M	 0.9950	 0.0280
N	 0.9890	 0.0660
O	 0.9940	 0.0640
P	 0.9440	 0.0620
Q	 0.8310	 0.0860
R	 0.2750	 0.0270
S	 0.7440	 0.0120
T	 0.8430	 0.0140
U	 0.8790	 0.0790
V	 0.9770	 0.0240
W	 0.9280	 0.0410
X	 0.7050	 0.0450
a	 0.9760	 0.0230
b	 0.9500	 0.0050
i	 0.9520	 0.0830

