



## wwPDB EM Validation Summary Report ⓘ

Jul 8, 2024 – 01:14 pm BST

PDB ID : 7YWX  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

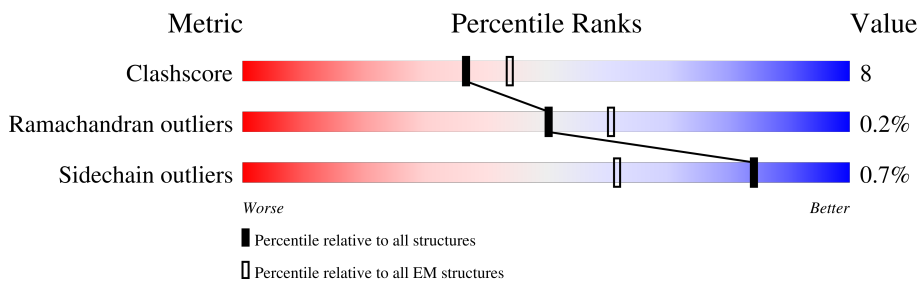
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
5	M	180	
6	N	339	
7	O	300	
8	Q	268	

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Mol	Chain	Length	Quality of chain
9	U	418	30% 10% 60%
10	P	288	59% 18% 22%
11	R	177	32% 15% 55%
12	T	561	17% 80%
13	W	88	5% 90% 9%
14	S	138	20% 78% 9% 13%
15	X	81	26% 84% 7% 9%
16	i	171	90% 5% 5%
17	J	171	49% 42% 5% 5%
18	A	140	66% 29%
18	E	140	64% 33%
19	B	103	71% 5% 24%
19	F	103	73% 5% 22%
20	C	130	67% 8% 25%
20	G	130	75% 21%
21	D	126	70% 27%
21	V	126	68% 5% 27%
22	a	544	96%
22	b	544	7% 90%

## 2 Entry composition [i](#)

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
			Total	C	N	O	S		
1	H	204	1652	1036	286	319	11	0	0

- Molecule 2 is a protein called Centromere protein I.

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

- Molecule 3 is a protein called Centromere protein K.

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

- Molecule 4 is a protein called Centromere protein L.

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

- Molecule 5 is a protein called Centromere protein M.

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

- Molecule 6 is a protein called Centromere protein N.

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

- Molecule 7 is a protein called Centromere protein O.

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

- Molecule 8 is a protein called Centromere protein Q.

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

- Molecule 9 is a protein called Centromere protein U.

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

- Molecule 10 is a protein called Centromere protein P.

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

- Molecule 11 is a protein called Centromere protein R.

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

- Molecule 12 is a protein called Centromere protein T.

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

- Molecule 13 is a protein called Centromere protein W.

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

- Molecule 14 is a protein called Centromere protein S.

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

- Molecule 15 is a protein called Centromere protein X.

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

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

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

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

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

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

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

- Molecule 19 is a protein called Histone H4.

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

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

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

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

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

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

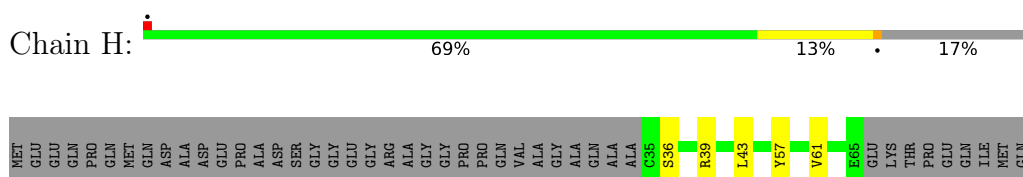
- Molecule 22 is a protein called Centromere protein C.

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

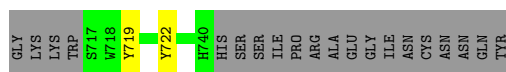
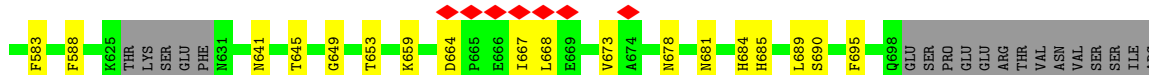
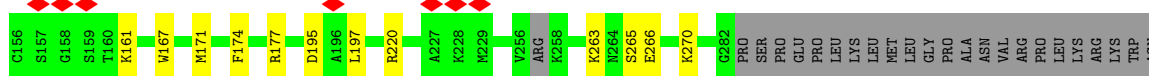
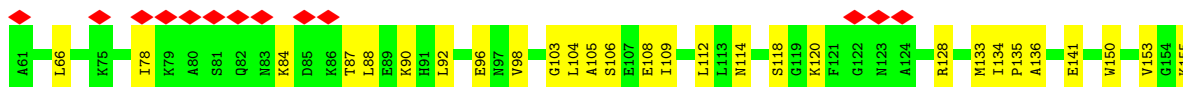
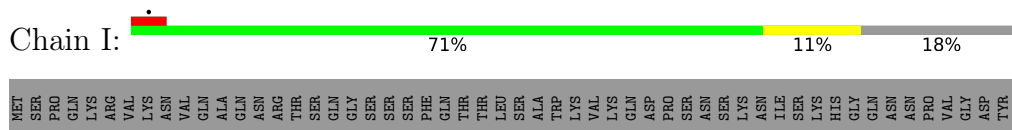
### 3 Residue-property plots [i](#)

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

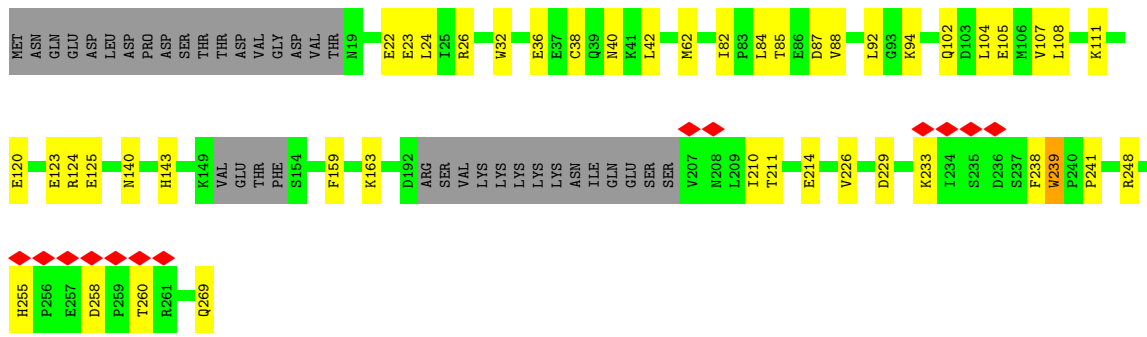


- Molecule 2: Centromere protein I

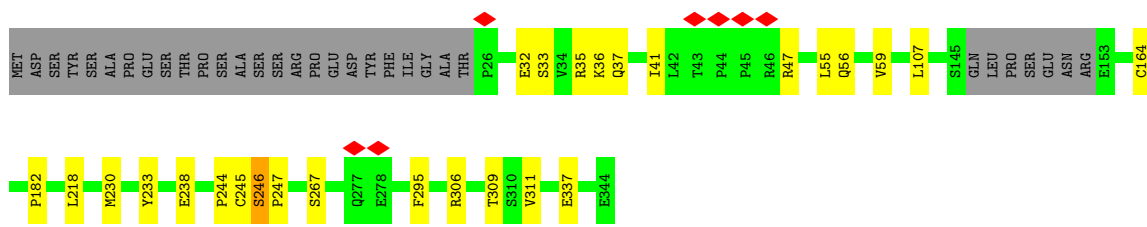
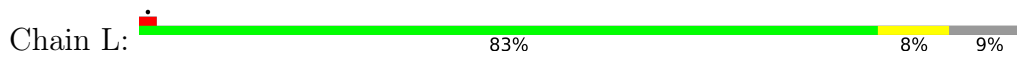


- Molecule 3: Centromere protein K

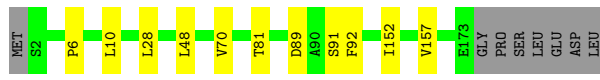
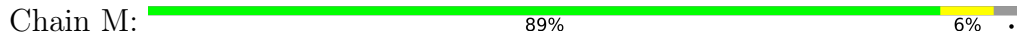




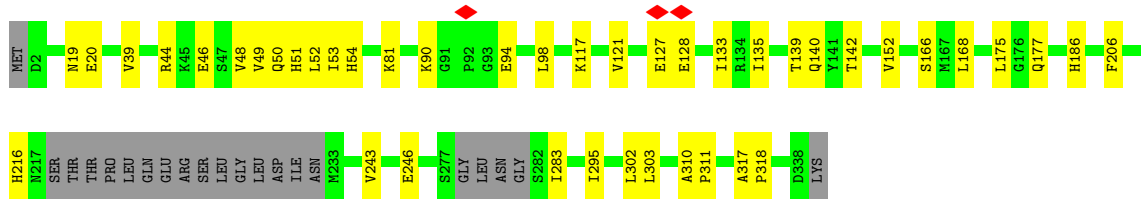
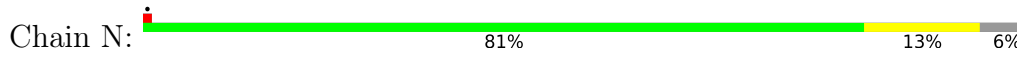
• Molecule 4: Centromere protein L



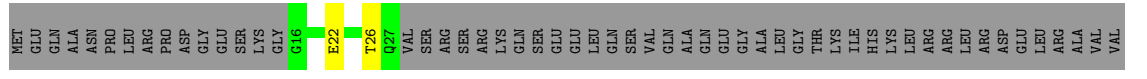
• Molecule 5: Centromere protein M



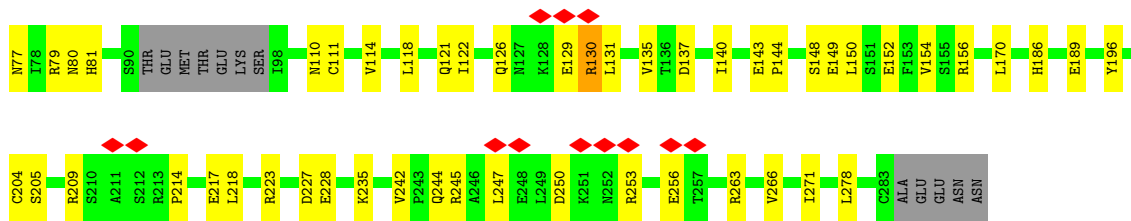
• Molecule 6: Centromere protein N



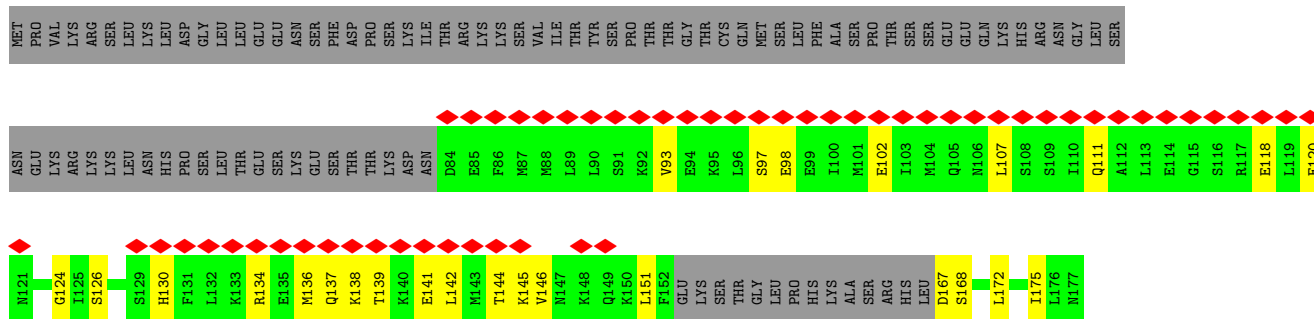
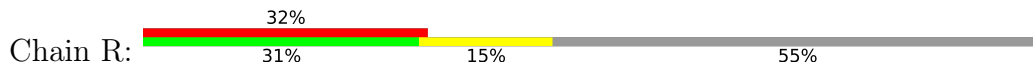
• Molecule 7: Centromere protein O



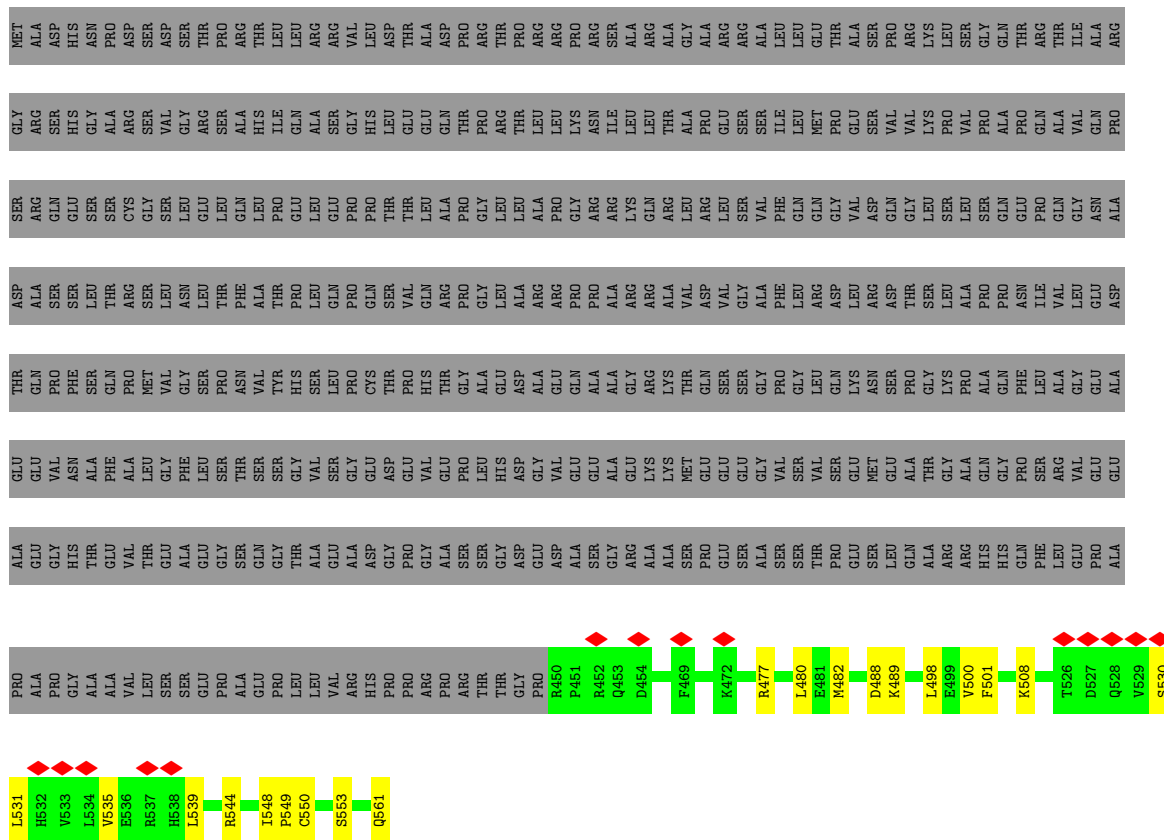




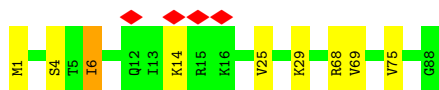
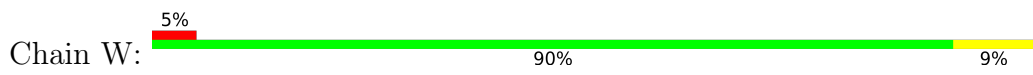
• Molecule 11: Centromere protein R



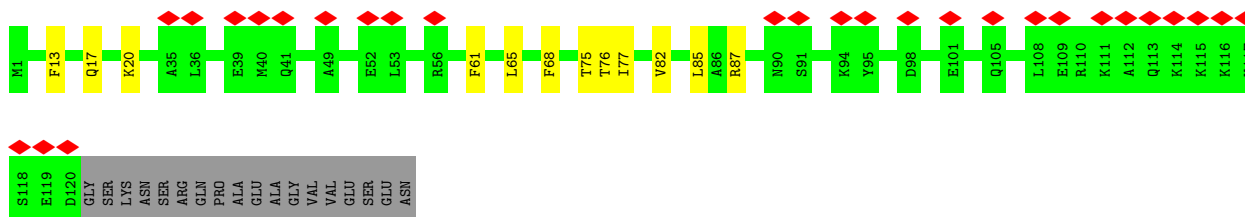
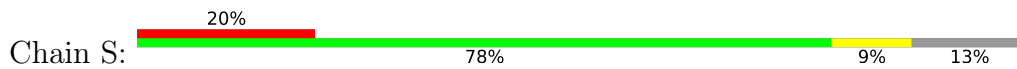
• Molecule 12: Centromere protein T



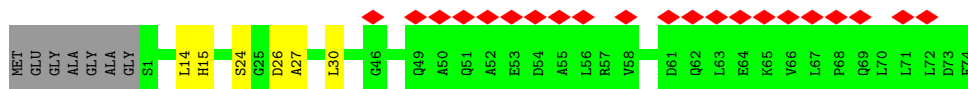
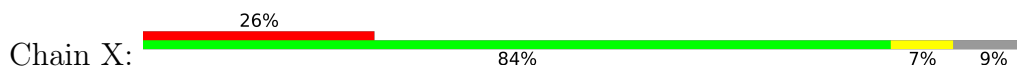
• Molecule 13: Centromere protein W



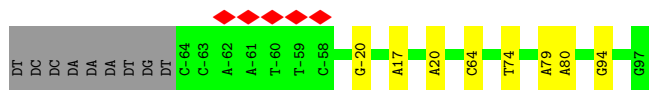
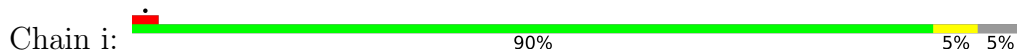
• Molecule 14: Centromere protein S



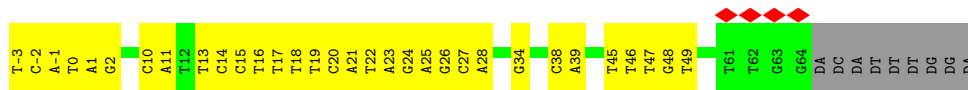
• Molecule 15: Centromere protein X



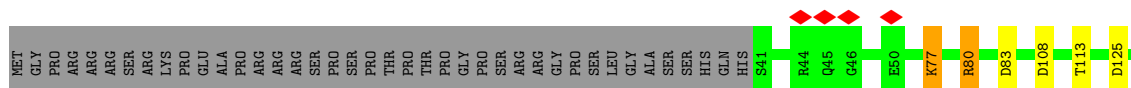
• Molecule 16: DNA (171-MER)



• Molecule 17: DNA (171-MER)



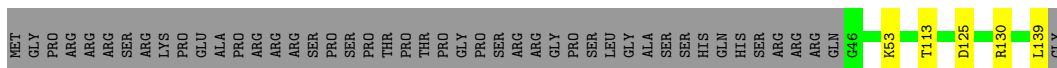
• Molecule 18: Histone H3-like centromeric protein A





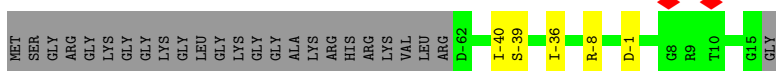
- Molecule 18: Histone H3-like centromeric protein A

Chain E: 64% 33%



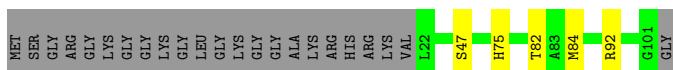
- Molecule 19: Histone H4

Chain B: 71% 5% 24%



- Molecule 19: Histone H4

Chain F: 73% 5% 22%



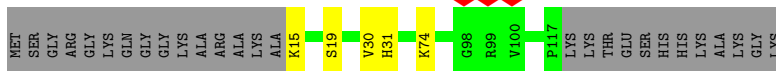
- Molecule 20: Histone H2A type 1-C

Chain C: 67% 8% 25%



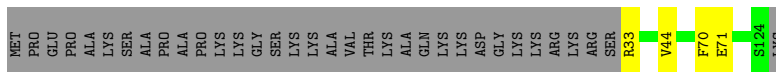
- Molecule 20: Histone H2A type 1-C

Chain G: 75% 21%



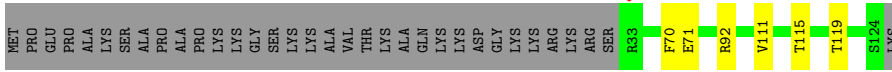
- Molecule 21: Histone H2B type 1-C/E/F/G/I

Chain D: 70% 27%



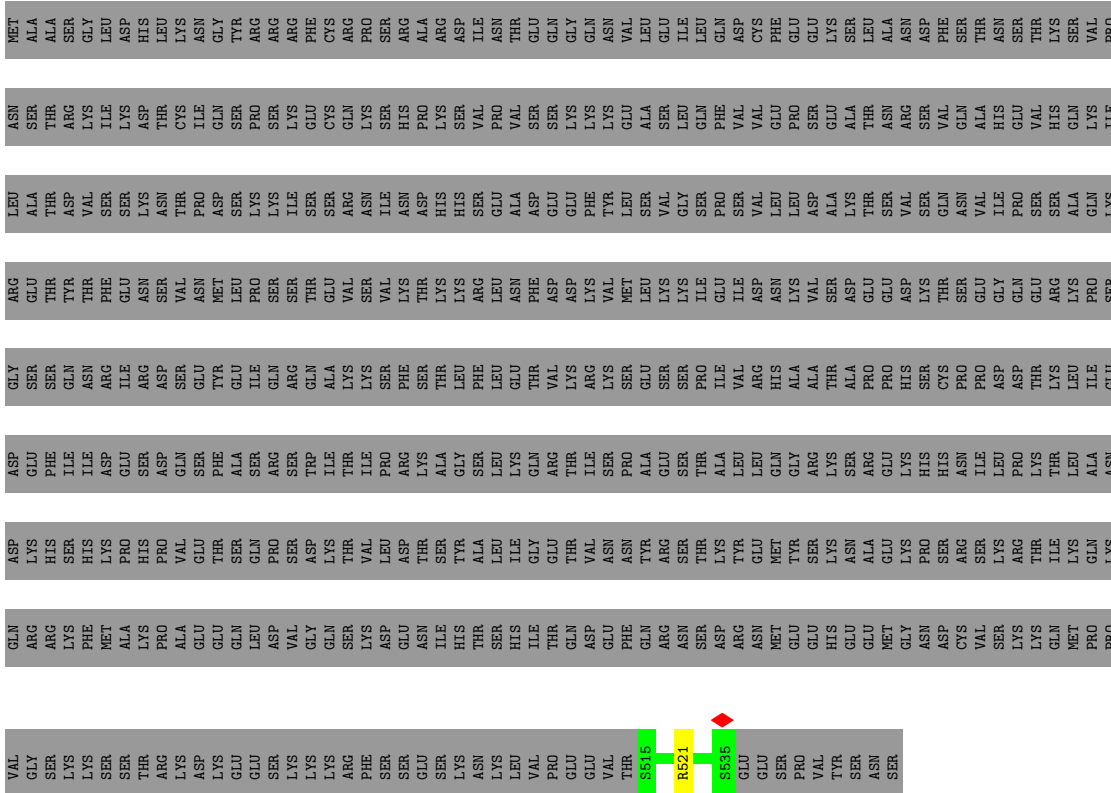
- Molecule 21: Histone H2B type 1-C/E/F/G/I

Chain V: 68% 5% 27%



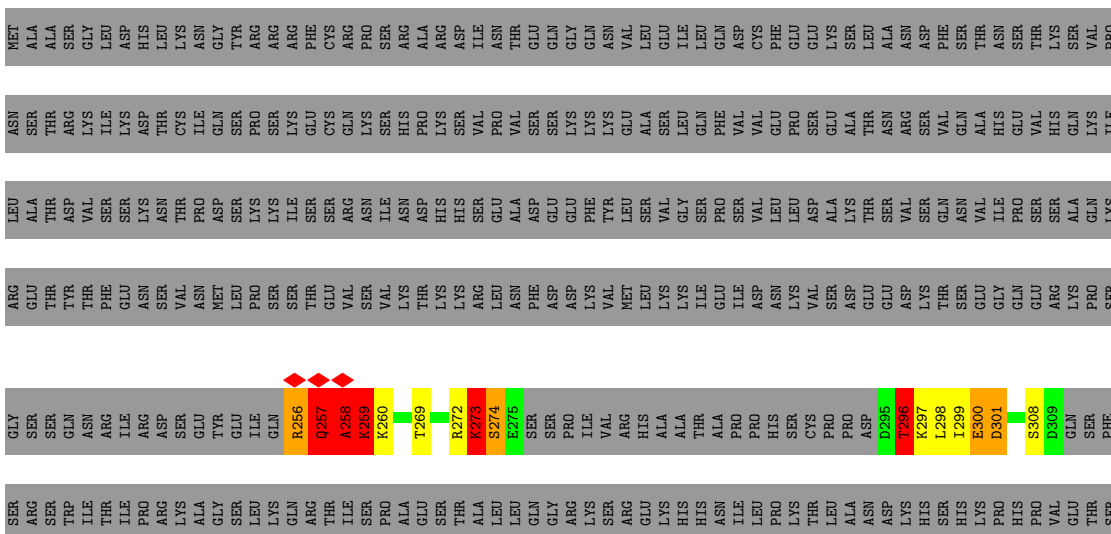
• Molecule 22: Centromere protein C

Chain a: . 96%



• Molecule 22: Centromere protein C

Chain b: 7% ... 90%



GLN PRO ASP VAL SER GLY ASP THR VAL LEU ASP THR ASN THR TYR ALA LEU ILE GLY THR VAL ASN THR ASP PHE ASN TYR ARG ARG ASN SER THR LYS TYR ARG

LEU ASP VAL GLY GLN SER LYS ASP ASP THR ASN ILE SER HIS THR SER HIS ILE THR GLN ASP GLU PHE GLN TYR ARG ASN SER ASP ARG ASN MET MET GLU TYR SER HIS GLU ASN MET GLY LYS ASN PRO ASP CYS VAL SER LYS ARG LYS THR ILE LYS MET PRO LYS VAL GLY SER LYS PHE SER ALA LYS THR ARG LYS ASP GLU

GLU SER LYS LYS ARG PHE SER SER GLU SER LYS ASN LYS LEU VAL PRO GLU VAL R514 R521 S535 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 (Å)	292.4, 292.4, 292.4	wwPDB
Map dimensions	170, 170, 170	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7199999, 1.7199999, 1.7199999	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

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	0.34	0/1660	0.52	0/2218
2	I	0.30	0/5137	0.46	0/6955
3	K	0.28	0/1953	0.46	0/2634
4	L	0.31	0/2569	0.49	1/3485 (0.0%)
5	M	0.30	0/1347	0.50	0/1827
6	N	0.32	0/2670	0.52	0/3606
7	O	0.30	0/1678	0.48	0/2280
8	Q	0.25	0/1538	0.49	0/2062
9	U	0.27	0/1383	0.49	0/1856
10	P	0.26	0/1820	0.51	0/2451
11	R	0.24	0/653	0.44	0/865
12	T	0.26	0/937	0.47	0/1263
13	W	0.31	0/711	0.53	0/944
14	S	0.24	0/991	0.45	0/1322
15	X	0.24	0/596	0.46	0/801
16	i	0.67	6/3726 (0.2%)	1.22	12/5747 (0.2%)
17	J	0.70	5/3724 (0.1%)	1.20	28/5747 (0.5%)
18	A	0.24	0/814	0.37	0/1097
18	E	0.24	0/785	0.37	0/1057
19	B	0.24	0/629	0.41	0/843
19	F	0.25	0/648	0.42	0/868
20	C	0.24	0/764	0.39	0/1030
20	G	0.24	0/793	0.38	0/1070
21	D	0.25	0/730	0.39	0/982
21	V	0.25	0/730	0.39	0/982
22	a	0.20	0/182	0.40	0/245
22	b	0.79	4/481 (0.8%)	1.62	8/641 (1.2%)
All	All	0.40	15/39649 (0.0%)	0.71	49/54878 (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 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	-68	DA	O3'-P	-10.79	1.48	1.61
17	J	-74	DA	O3'-P	7.96	1.70	1.61
22	b	301	ASP	C-N	7.48	1.51	1.34
16	i	74	DT	O3'-P	-7.07	1.52	1.61
17	J	-78	DG	C1'-N9	-7.05	1.37	1.47

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	i	64	DC	OP1-P-O3'	-35.06	28.07	105.20
16	i	64	DC	P-O3'-C3'	-22.35	92.88	119.70
17	J	-71	DG	O5'-P-OP1	-18.19	88.87	110.70
17	J	-67	DT	O5'-P-OP1	-17.57	89.61	110.70
22	b	274	SER	O-C-N	-16.92	95.62	122.70

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	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	5014	0	5036	64	0
3	K	1922	0	1924	35	0
4	L	2502	0	2492	26	0
5	M	1325	0	1370	8	0
6	N	2613	0	2625	31	0
7	O	1642	0	1616	27	0
8	Q	1526	0	1586	29	0
9	U	1365	0	1396	34	0
10	P	1788	0	1791	38	0
11	R	649	0	673	18	0
12	T	915	0	924	20	0
13	W	704	0	789	15	0
14	S	982	0	987	8	0
15	X	590	0	623	5	0
16	i	3320	0	1830	0	0
17	J	3322	0	1837	101	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	6	0
20	G	784	0	815	2	0
21	D	719	0	738	4	0
21	V	719	0	738	4	0
22	a	178	0	185	0	0
22	b	476	0	483	0	0
All	All	38294	0	35963	452	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 8.

The worst 5 of 452 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:N:94:GLU:OE1	6:N:186:HIS:CE1	1.90	1.24
4:L:246:SER:CB	4:L:247:PRO:HD3	1.70	1.18
12:T:480:LEU:HD11	13:W:6:ILE:HD11	1.16	1.13
1:H:126:LEU:HD12	3:K:94:LYS:HG2	1.30	1.13
4:L:246:SER:CB	4:L:247:PRO:CD	2.27	1.10

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	41	77
3	K	227/269 (84%)	224 (99%)	3 (1%)	0	100	100
4	L	308/344 (90%)	299 (97%)	8 (3%)	1 (0%)	41	77
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	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3854/6540 (59%)	3752 (97%)	95 (2%)	7 (0%)	50	81

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 [i](#)

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%)	185 (98%)	3 (2%)	62	79
2	I	560/691 (81%)	557 (100%)	3 (0%)	88	93
3	K	221/260 (85%)	221 (100%)	0	100	100
4	L	277/306 (90%)	276 (100%)	1 (0%)	91	94
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%)	196 (100%)	1 (0%)	88	93
11	R	75/166 (45%)	75 (100%)	0	100	100
12	T	100/461 (22%)	99 (99%)	1 (1%)	76	86
13	W	77/77 (100%)	76 (99%)	1 (1%)	69	81
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%)	77 (96%)	3 (4%)	33	57

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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%)	63 (98%)	1 (2%)	62	79
19	F	66/79 (84%)	64 (97%)	2 (3%)	41	63
20	C	76/99 (77%)	74 (97%)	2 (3%)	46	66
20	G	77/99 (78%)	74 (96%)	3 (4%)	32	56
21	D	79/106 (74%)	79 (100%)	0	100	100
21	V	79/106 (74%)	78 (99%)	1 (1%)	69	81
22	a	21/508 (4%)	20 (95%)	1 (5%)	25	51
22	b	56/508 (11%)	53 (95%)	3 (5%)	22	47
All	All	3490/5811 (60%)	3464 (99%)	26 (1%)	84	90

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	C	16	SER
19	F	92	ARG
22	b	296	THR
19	F	47	SER
20	G	19	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
21	V	84	ASN
20	G	94	ASN
19	B	-11	HIS
19	F	93	GLN
18	A	45	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

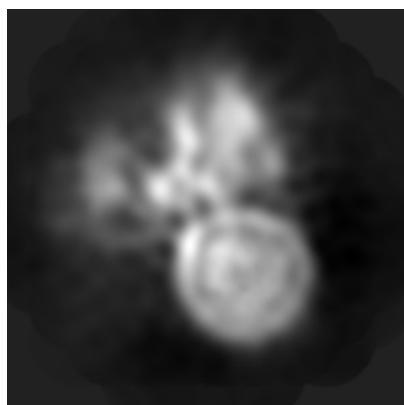
## 6 Map visualisation [i](#)

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

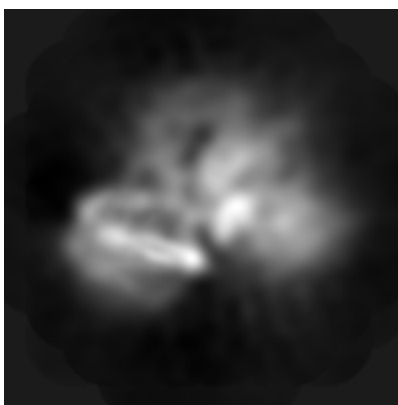
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

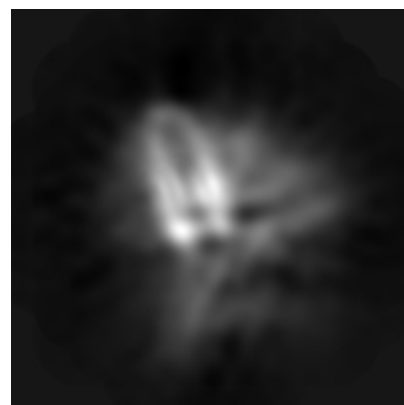
#### 6.1.1 Primary map



X



Y

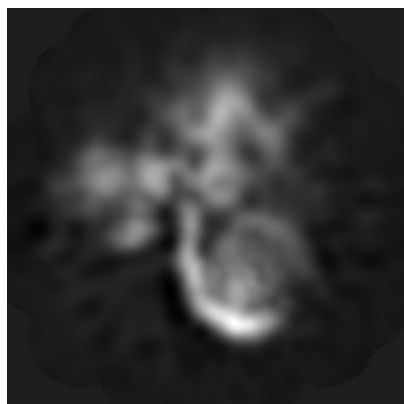


Z

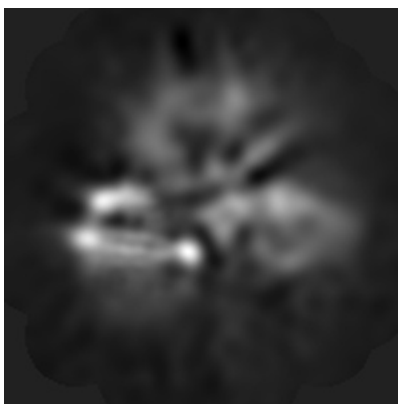
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

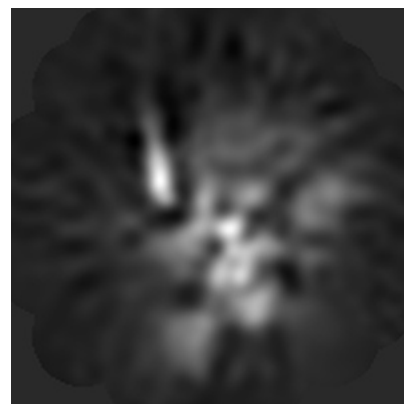
#### 6.2.1 Primary map



X Index: 85



Y Index: 85



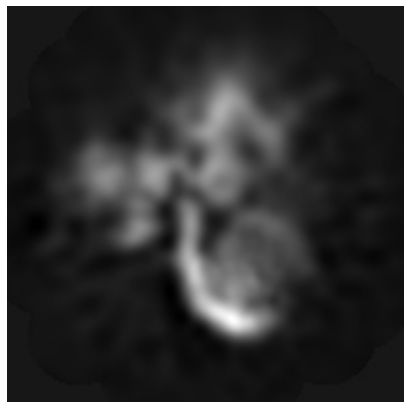
Z Index: 85



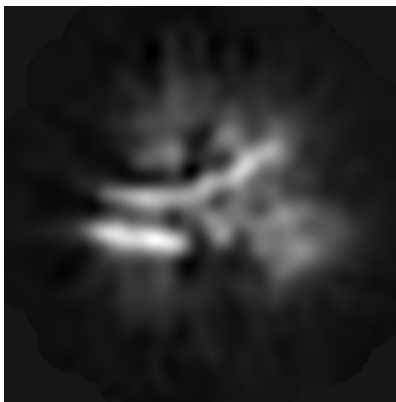
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

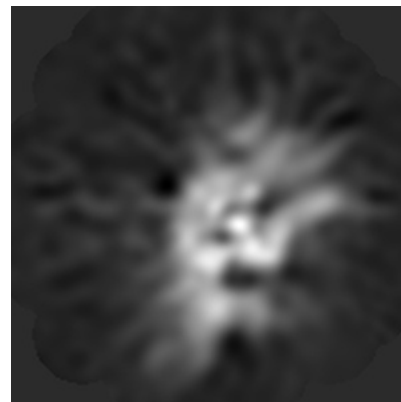
### 6.3.1 Primary map



X Index: 86



Y Index: 76

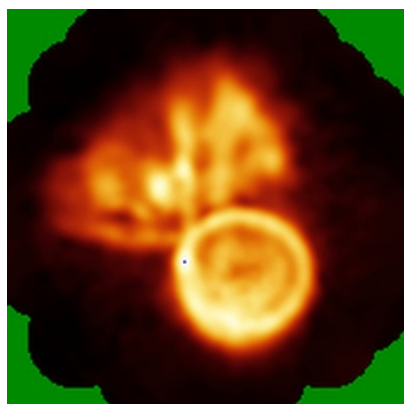


Z Index: 96

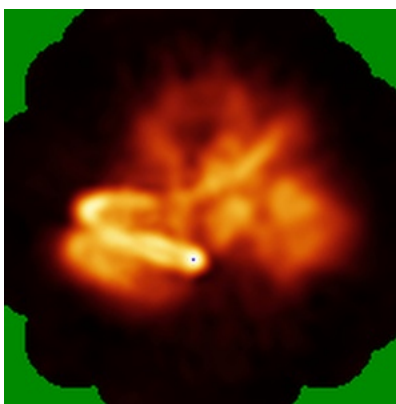
The images above show the largest variance slices of the map in three orthogonal directions.

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

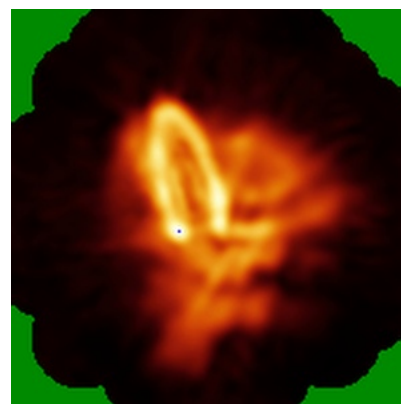
### 6.4.1 Primary map



X



Y

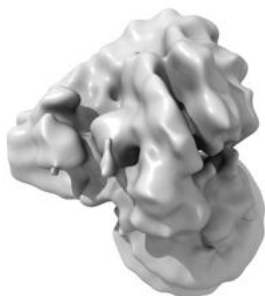


Z

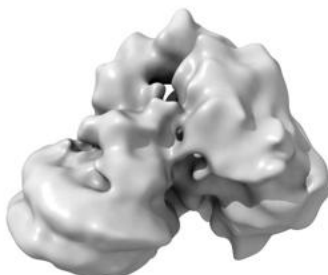
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

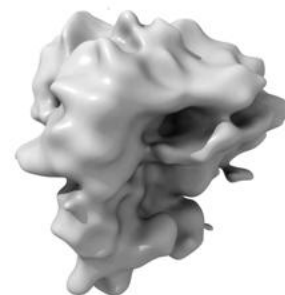
### 6.5.1 Primary map



X



Y



Z

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.

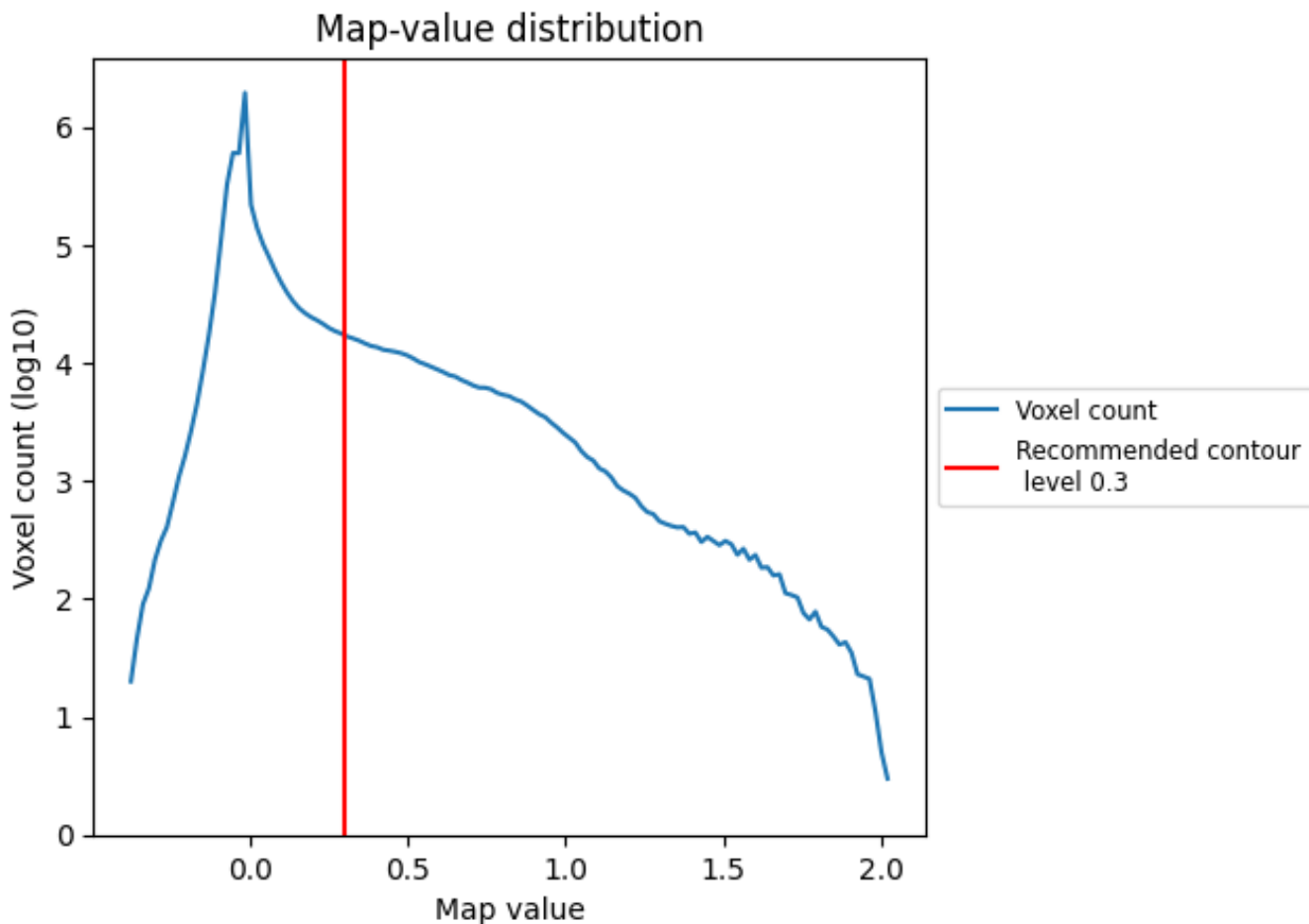
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

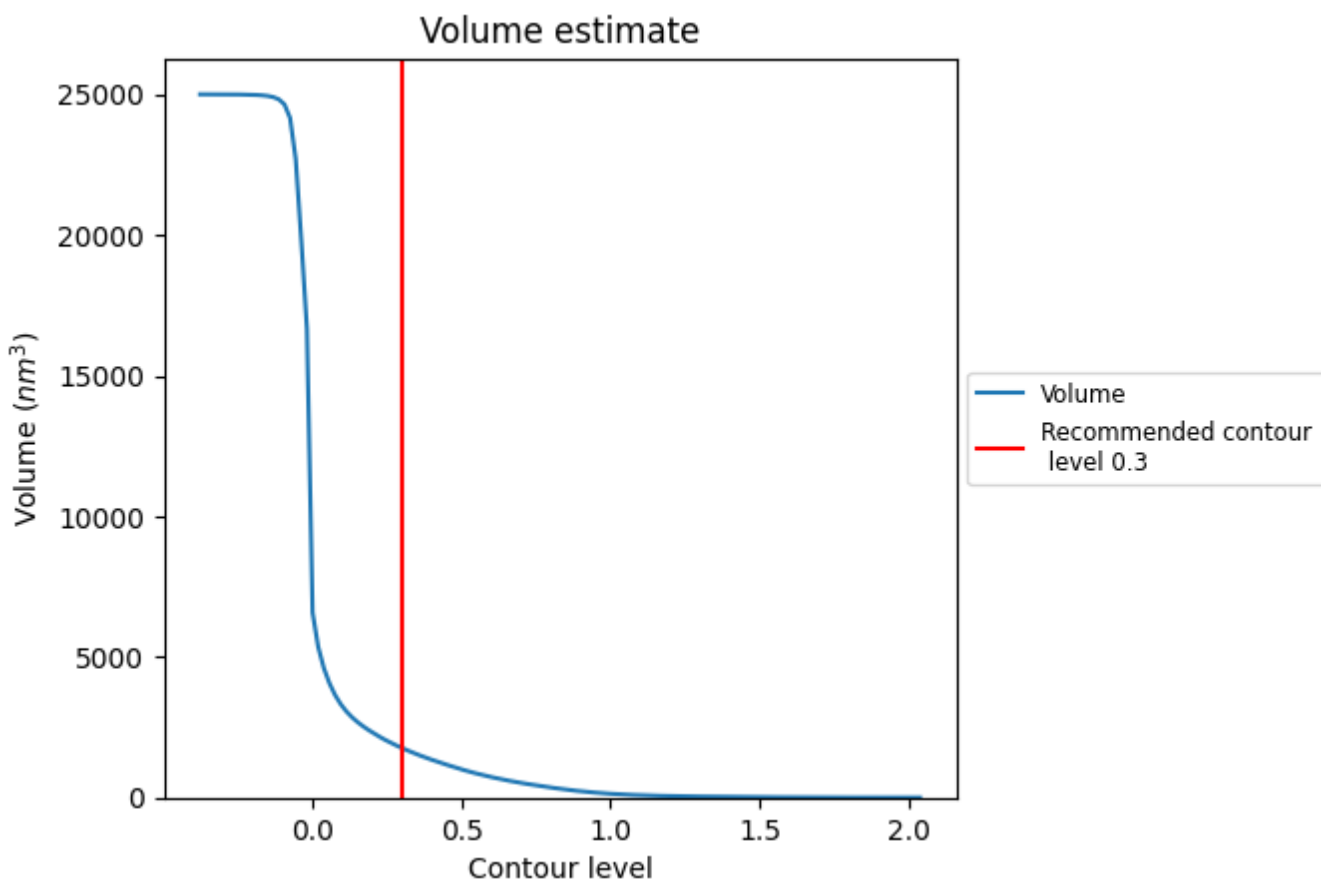
This section contains the results of statistical analysis of the map.

### 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.

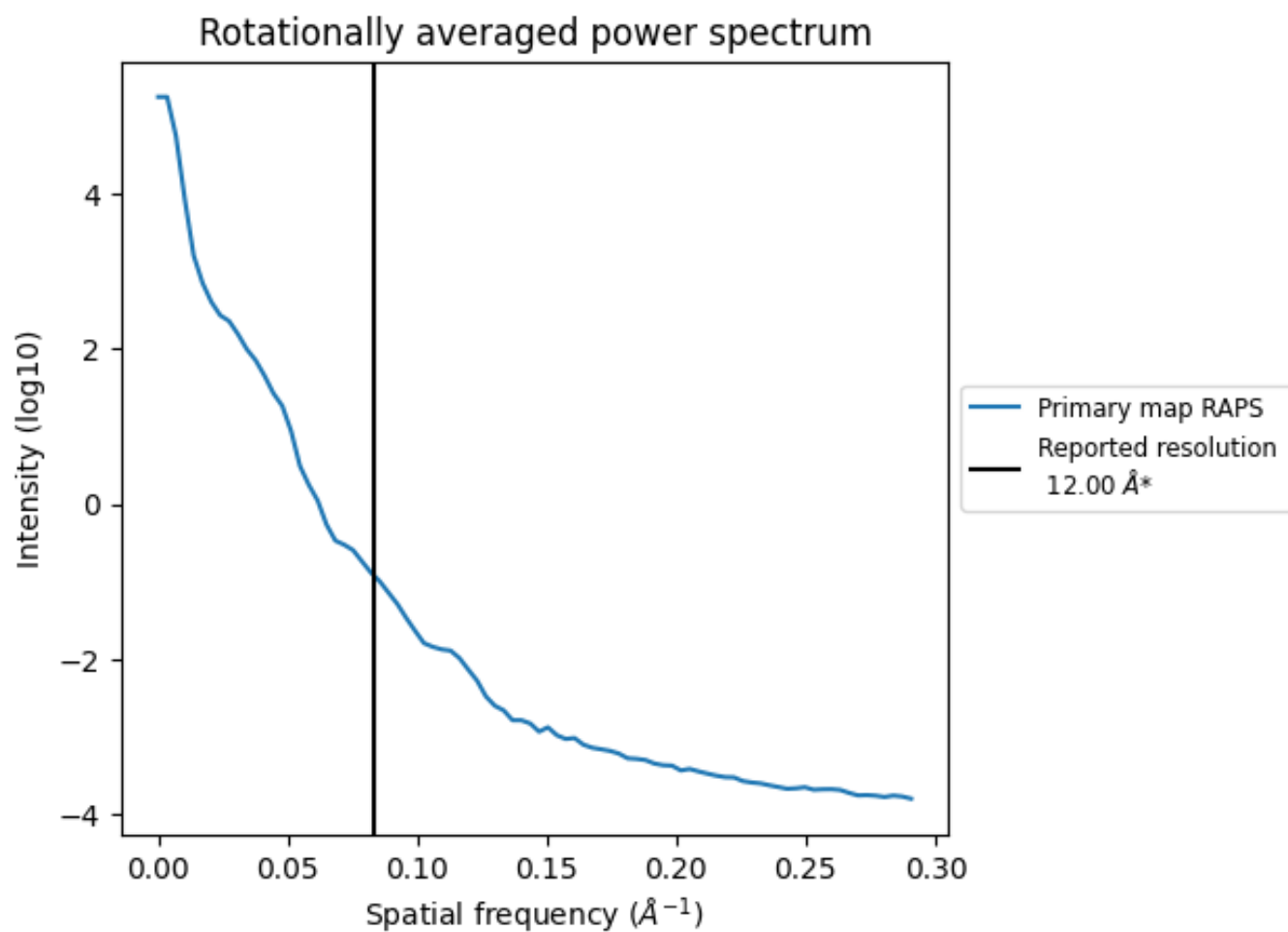
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1765 nm<sup>3</sup>; 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 [i](#)

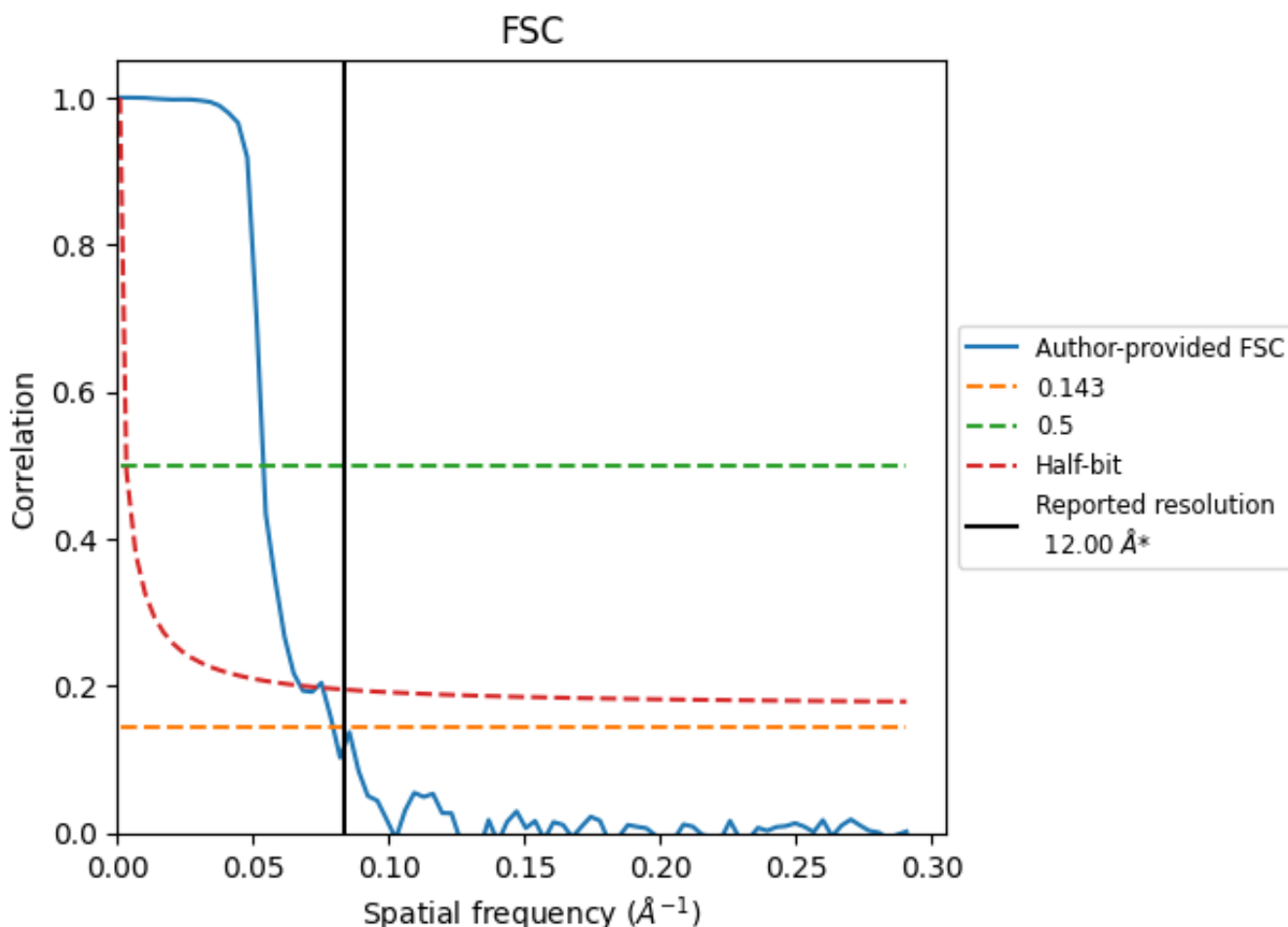


\*Reported resolution corresponds to spatial frequency of 0.083 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

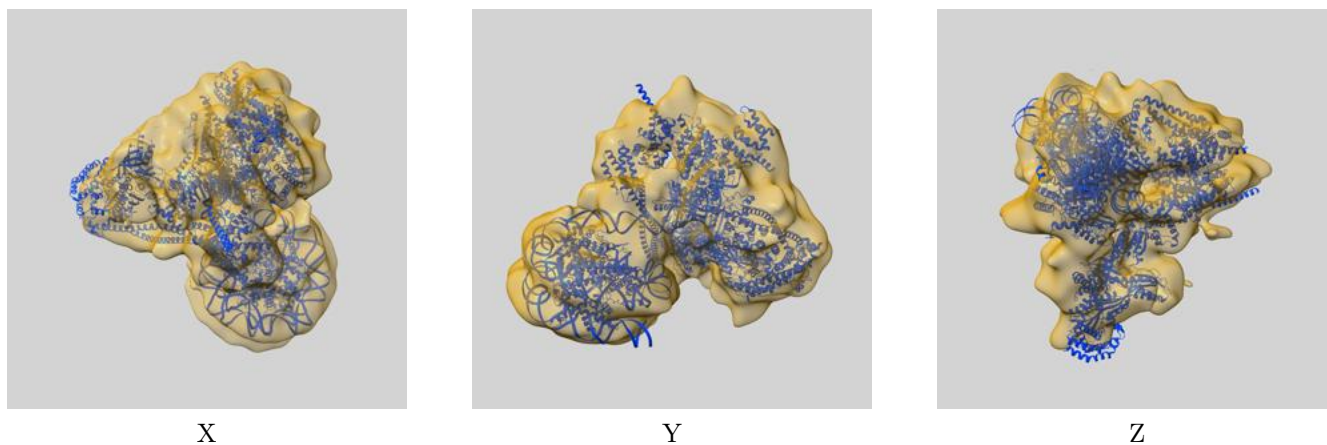
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	12.00	-	-
Author-provided FSC curve	12.58	18.55	14.84
Unmasked-calculated*	-	-	-

\*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.

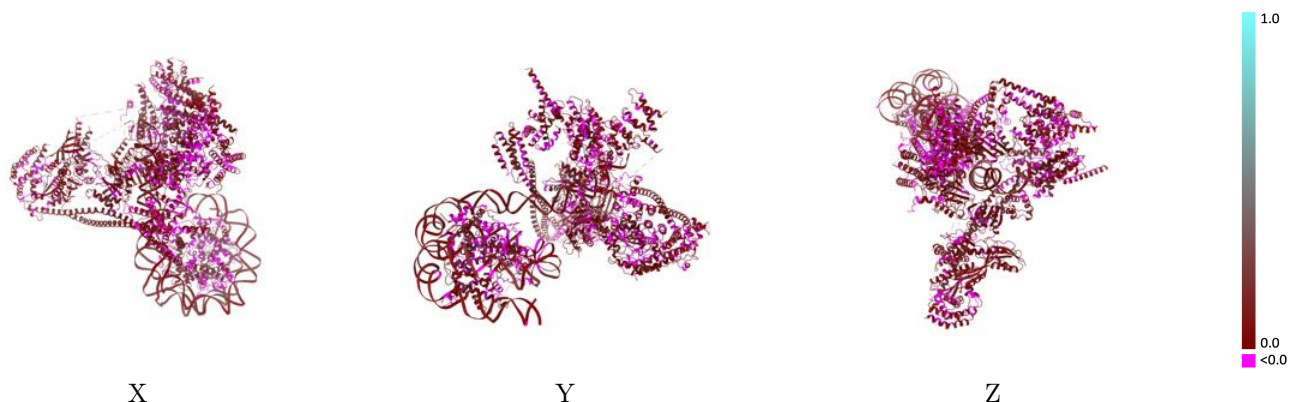
### 9.1 Map-model overlay [i](#)



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.

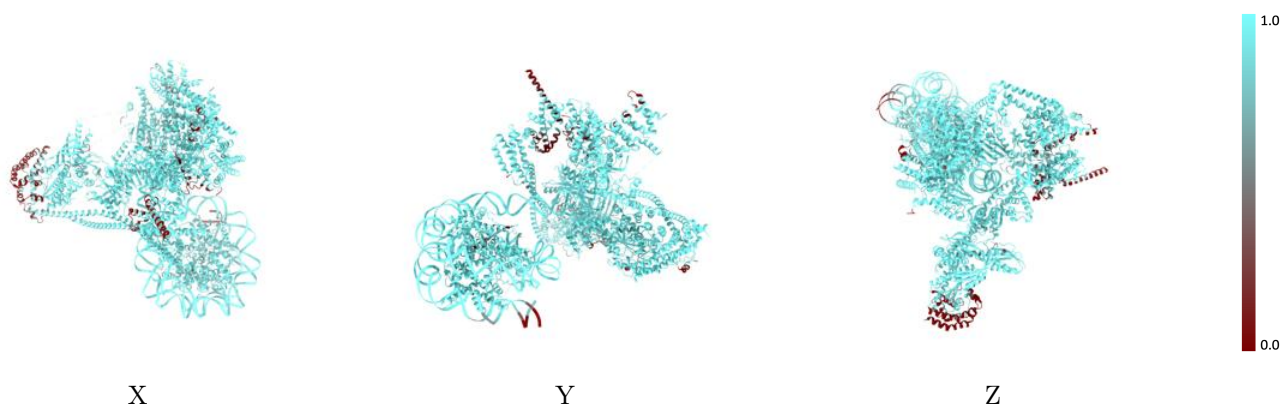


## 9.2 Q-score mapped to coordinate model [i](#)



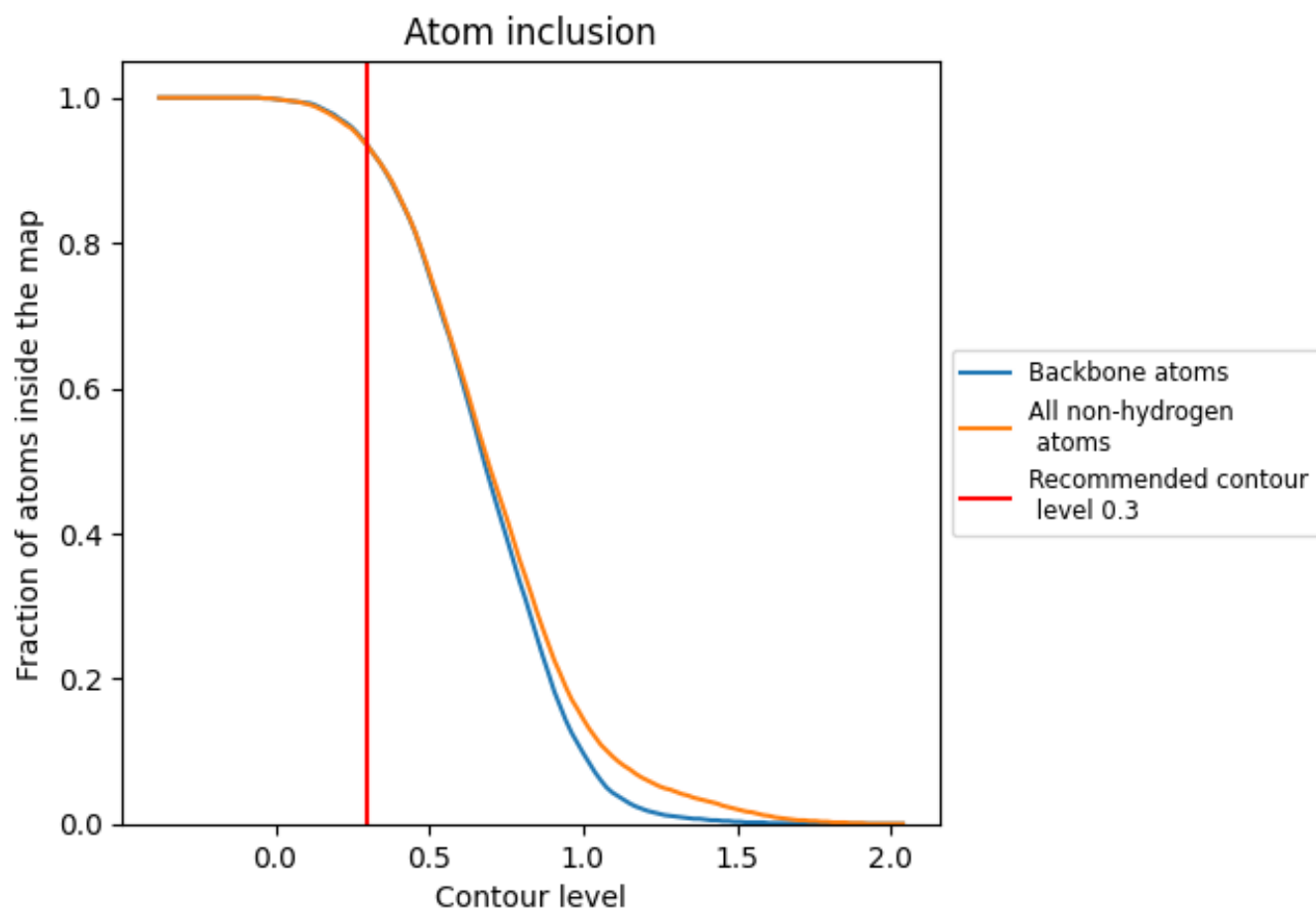
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

