wwPDB EM Validation Summary Report

Dec 10, 2022 – 11:17 am GMT

PDB ID	:	6QLD
EMDB ID	:	EMD-4579
Title	:	Structure of inner kinetochore CCAN-Cenp-A complex
Authors	:	Yan, K.; Yang, J.; Zhang, Z.; McLaughlin, S.H.; Chang, L.; Fasci, D.; Heck, A.J.R.; Barford, D.
Deposited on	:	2019-01-31
Resolution	:	4.15 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:

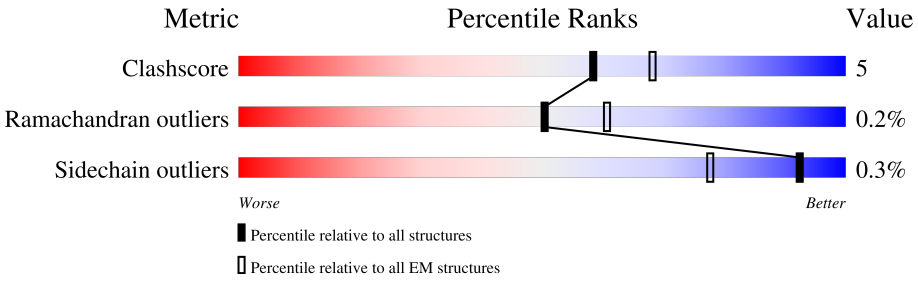
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



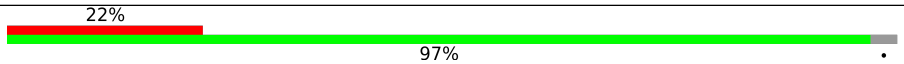
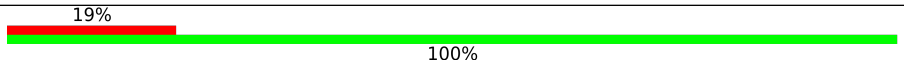
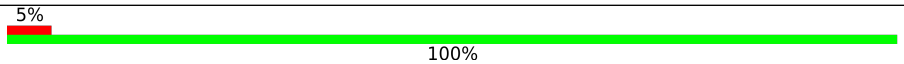
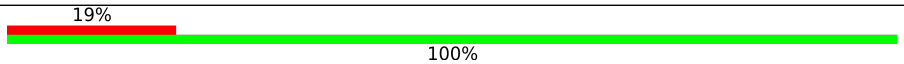
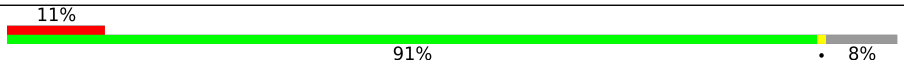
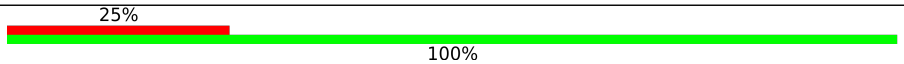
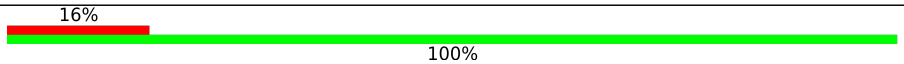
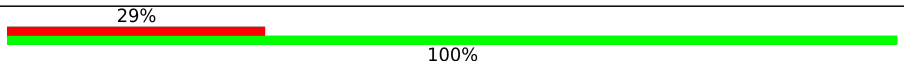
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	C	22	86% 91% 9%
2	G	124	8% 91% 8%
3	H	133	8% 81% 13% 6%
4	I	408	6% 78% 11% 11%
5	J	124	10% 89% 10%
6	K	122	5% 79% 8% 13%
7	L	241	86% 13%
8	N	447	72% 11% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	O	212	
10	P	270	
11	Q	231	
12	U	190	
13	Y	237	
14	Z	151	
15	a	90	
16	b	79	
16	f	79	
17	d	93	
18	e	115	
19	g	105	
20	h	94	
21	i	102	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 29086 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 Inner kinetochore subunit MIF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	22	Total 194	C 127	N 37	O 30	0	0

- Molecule 2 is a DNA chain called DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	124	Total 2524	C 1197	N 459	O 744	P 124	0	0

- Molecule 3 is a protein called Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	125	Total 948	C 607	N 173	O 167	S 1	0	0

- Molecule 4 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	362	Total 2701	C 1761	N 450	O 471	S 19	0	0

- Molecule 5 is a DNA chain called DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	124	Total 2560	C 1209	N 483	O 744	P 124	0	0

- Molecule 6 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	106	Total 774	C 491	N 138	O 142	S 3	0	0

- Molecule 7 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	241	Total	C	N	O	S	0	0
			1937	1242	320	364	11		

- Molecule 8 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	371	Total	C	N	O	S	0	0
			2929	1906	507	504	12		

- Molecule 9 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	205	Total	C	N	O	S	0	0
			1658	1078	271	305	4		

- Molecule 10 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	242	Total	C	N	O	S	0	0
			1865	1208	323	322	12		

- Molecule 11 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	204	Total	C	N	O	S	0	0
			1421	885	261	270	5		

- Molecule 12 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	171	Total	C	N	O	S	0	0
			1229	768	227	231	3		

- Molecule 13 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	223	Total	C	N	O	S	0	0
			1541	965	275	296	5		

- Molecule 14 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	140	Total 995	C 632	N 181	O 181	S 1	0	0

- Molecule 15 is a protein called Histone H3-like centromeric protein CSE4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	87	Total 706	C 450	N 127	O 125	S 4	0	0

- Molecule 16 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	79	Total 625	C 393	N 120	O 112	0	0
16	f	79	Total 627	C 395	N 120	O 112	0	0

- Molecule 17 is a protein called Histone H2B.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	93	Total 719	C 450	N 127	O 141	S 1	0	0

- Molecule 18 is a protein called Histone H3-like centromeric protein CSE4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	106	Total 801	C 507	N 146	O 144	S 4	0	0

- Molecule 19 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	g	105	Total 813	C 511	N 160	O 142	0	0

- Molecule 20 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	94	Total 731	C 459	N 128	O 143	S 1	0	0

- Molecule 21 is a protein called Histone H2A.1.

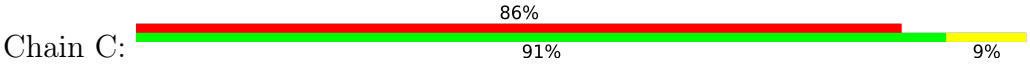
Mol	Chain	Residues	Atoms				AltConf	Trace
21	i	102	Total 788	C 494	N 155	O 139	0	0

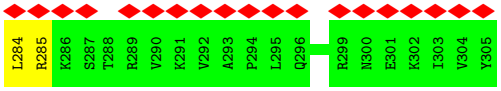
3 Residue-property plots (i)

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: Inner kinetochore subunit MIF2

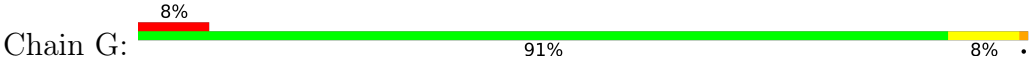
Chain C:

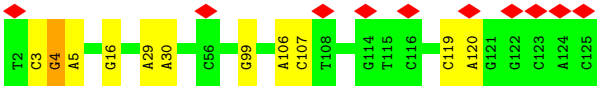




• Molecule 2: DNA (125-MER)

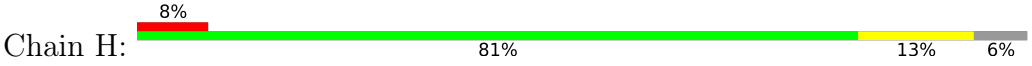
Chain G:

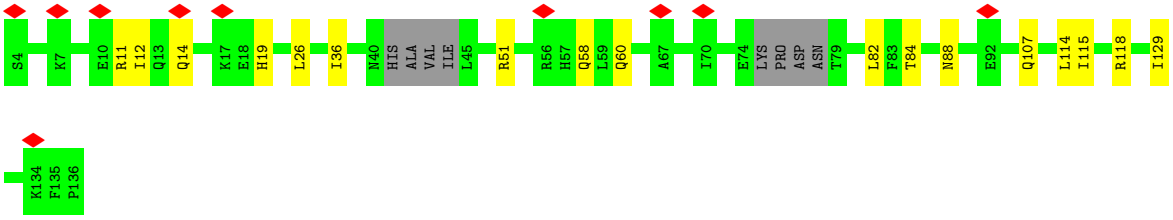




• Molecule 3: Inner kinetochore subunit MCM16

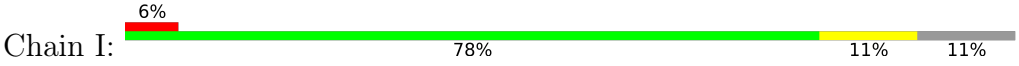
Chain H:

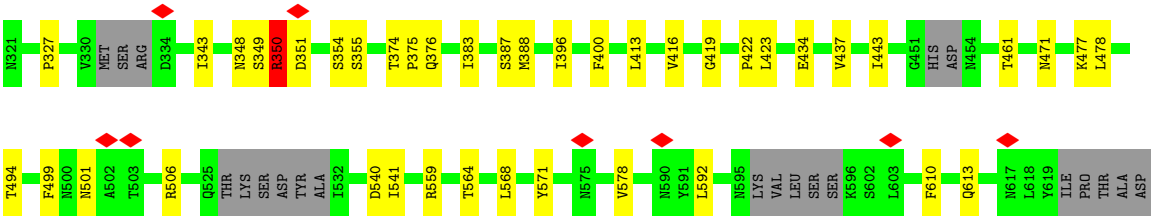


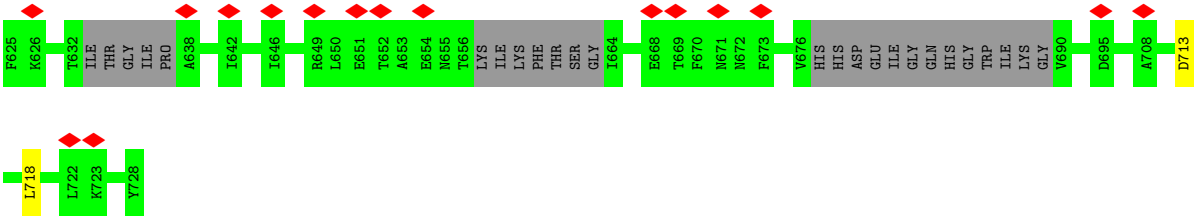


• Molecule 4: Inner kinetochore subunit CTF3

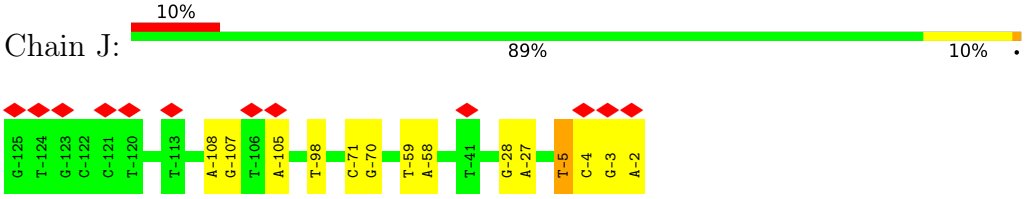
Chain I:



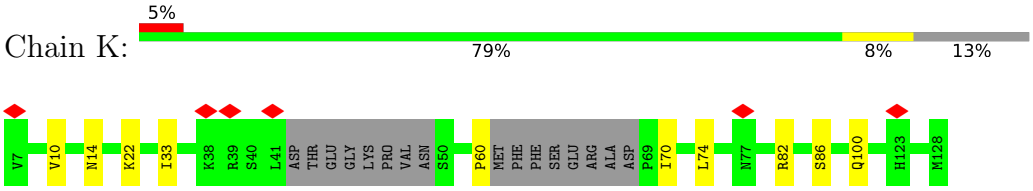




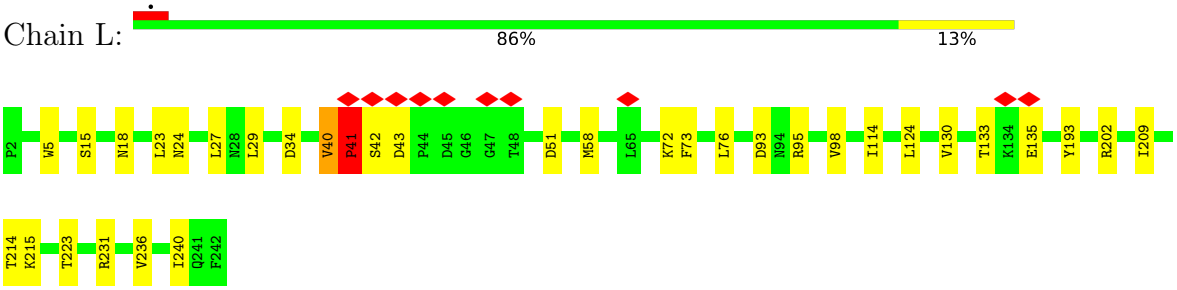
• Molecule 5: DNA (125-MER)



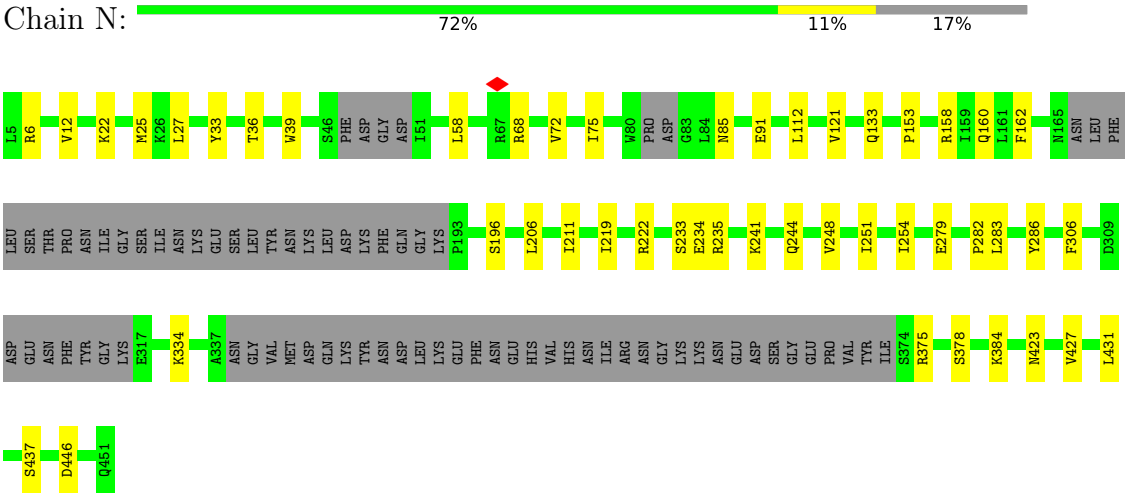
• Molecule 6: Inner kinetochore subunit MCM22



• Molecule 7: Inner kinetochore subunit IML3

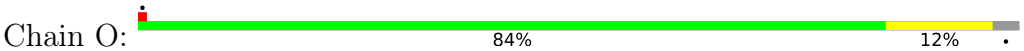


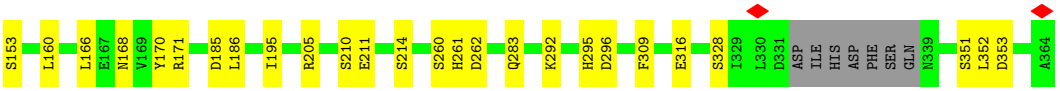
• Molecule 8: Inner kinetochore subunit CHL4



• Molecule 9: Inner kinetochore subunit MCM21

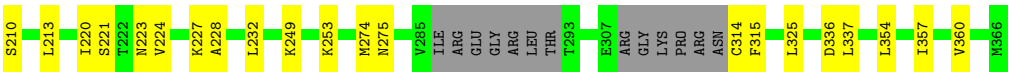
Chain O:





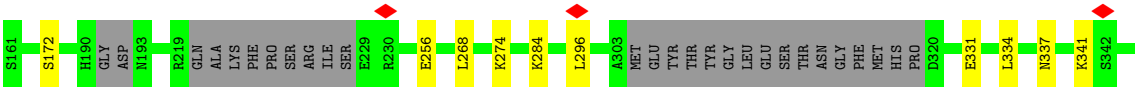
• Molecule 10: Inner kinetochore subunit CTF19

Chain P:



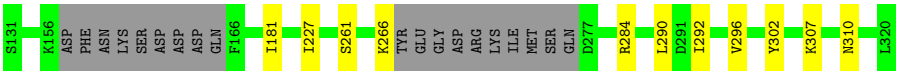
• Molecule 11: Inner kinetochore subunit OKP1

Chain Q:



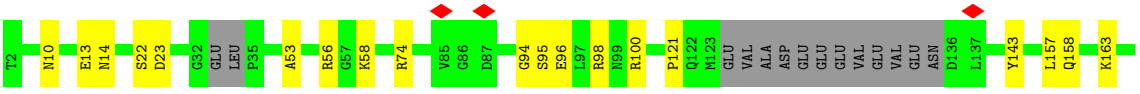
• Molecule 12: Inner kinetochore subunit AME1

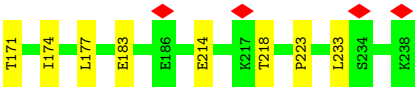
Chain U:



• Molecule 13: Inner kinetochore subunit NKP1

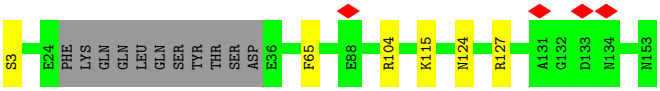
Chain Y:



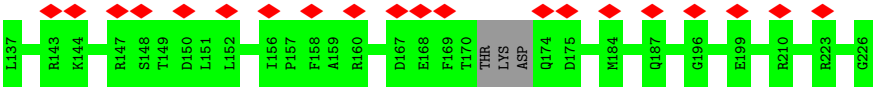


• Molecule 14: Inner kinetochore subunit NKP2

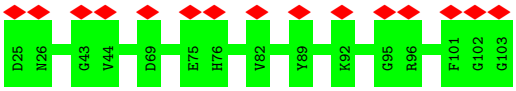
Chain Z:



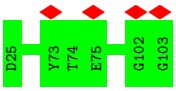
• Molecule 15: Histone H3-like centromeric protein CSE4



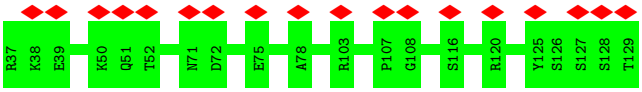
• Molecule 16: Histone H4



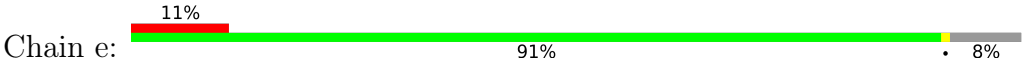
• Molecule 16: Histone H4

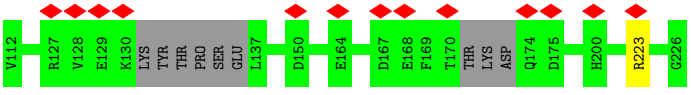


• Molecule 17: Histone H2B.2

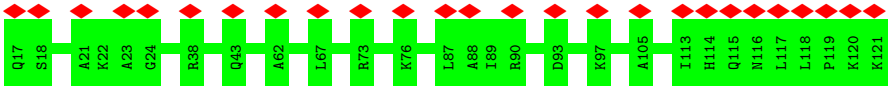


• Molecule 18: Histone H3-like centromeric protein CSE4



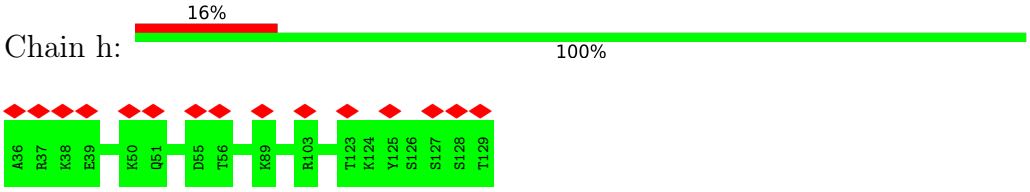


• Molecule 19: Histone H2A.1



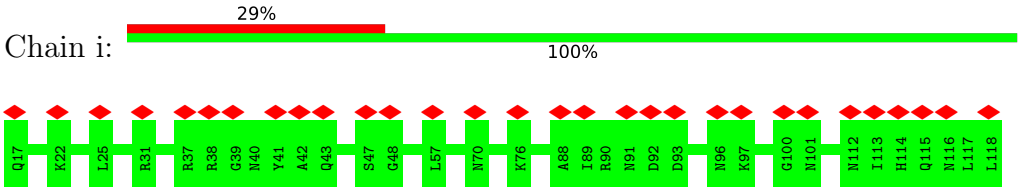
• Molecule 20: Histone H2B.1

Chain h:



• Molecule 21: Histone H2A.1

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145783	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 ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	348.80002, 348.80002, 348.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.26	0/198	0.63	0/266
2	G	0.62	1/2827 (0.0%)	1.00	4/4356 (0.1%)
3	H	0.25	0/956	0.48	1/1291 (0.1%)
4	I	0.30	0/2750	0.57	1/3736 (0.0%)
5	J	0.55	1/2875 (0.0%)	0.95	2/4440 (0.0%)
6	K	0.25	0/780	0.46	1/1055 (0.1%)
7	L	0.30	0/1977	0.51	0/2679
8	N	0.31	0/2994	0.48	0/4046
9	O	0.30	0/1689	0.49	0/2275
10	P	0.28	0/1891	0.50	0/2552
11	Q	0.25	0/1430	0.44	1/1938 (0.1%)
12	U	0.26	0/1236	0.46	0/1676
13	Y	0.27	0/1550	0.53	0/2102
14	Z	0.24	0/1005	0.39	0/1367
15	a	0.24	0/714	0.48	0/958
16	b	0.25	0/632	0.49	0/845
16	f	0.26	0/634	0.48	0/848
17	d	0.26	0/728	0.47	0/980
18	e	0.25	0/808	0.50	0/1088
19	g	0.26	0/824	0.48	0/1113
20	h	0.26	0/741	0.46	0/998
21	i	0.26	0/798	0.52	0/1079
All	All	0.36	2/30037 (0.0%)	0.63	10/41688 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	DG	O3'-P	-12.39	1.46	1.61
5	J	-5	DT	O3'-P	-6.06	1.53	1.61

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	4	DG	OP1-P-O3'	-13.68	75.11	105.20
5	J	-5	DT	P-O3'-C3'	-10.86	106.66	119.70
2	G	4	DG	O3'-P-O5'	8.96	121.03	104.00
4	I	478	LEU	CA-CB-CG	7.33	132.15	115.30
2	G	4	DG	OP2-P-O3'	6.94	120.47	105.20

There are no chirality outliers.

There are no planarity outliers.

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	C	194	0	209	1	0
2	G	2524	0	1390	11	0
3	H	948	0	933	15	0
4	I	2701	0	2573	30	0
5	J	2560	0	1390	10	0
6	K	774	0	748	9	0
7	L	1937	0	1942	25	0
8	N	2929	0	2964	34	0
9	O	1658	0	1665	21	0
10	P	1865	0	1855	28	0
11	Q	1421	0	1237	13	0
12	U	1229	0	1117	12	0
13	Y	1541	0	1425	18	0
14	Z	995	0	911	5	0
15	a	706	0	734	0	0
16	b	625	0	657	0	0
16	f	627	0	664	0	0
17	d	719	0	741	0	0
18	e	801	0	771	0	0
19	g	813	0	860	0	0
20	h	731	0	753	0	0
21	i	788	0	827	0	0
All	All	29086	0	26366	188	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 5.

The worst 5 of 188 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)
7:L:40:VAL:HG23	7:L:51:ASP:OD1	1.75	0.86
7:L:40:VAL:HB	7:L:41:PRO:HD2	1.72	0.70
2:G:16:DG:H5'	8:N:22:LYS:NZ	2.08	0.67
9:O:211:GLU:HB3	9:O:283:GLN:HE22	1.61	0.66
7:L:130:VAL:HG11	7:L:231:ARG:NH1	2.12	0.64

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	C	20/22 (91%)	17 (85%)	3 (15%)	0	100	100
3	H	119/133 (90%)	117 (98%)	2 (2%)	0	100	100
4	I	344/408 (84%)	318 (92%)	24 (7%)	2 (1%)	25	64
6	K	100/122 (82%)	100 (100%)	0	0	100	100
7	L	239/241 (99%)	218 (91%)	19 (8%)	2 (1%)	19	59
8	N	359/447 (80%)	336 (94%)	23 (6%)	0	100	100
9	O	201/212 (95%)	192 (96%)	9 (4%)	0	100	100
10	P	232/270 (86%)	218 (94%)	14 (6%)	0	100	100
11	Q	196/231 (85%)	191 (97%)	5 (3%)	0	100	100
12	U	165/190 (87%)	163 (99%)	2 (1%)	0	100	100
13	Y	217/237 (92%)	199 (92%)	17 (8%)	1 (0%)	29	68
14	Z	136/151 (90%)	134 (98%)	2 (2%)	0	100	100
15	a	83/90 (92%)	77 (93%)	6 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	b	77/79 (98%)	74 (96%)	3 (4%)	0	100 100
16	f	77/79 (98%)	76 (99%)	1 (1%)	0	100 100
17	d	91/93 (98%)	84 (92%)	7 (8%)	0	100 100
18	e	100/115 (87%)	95 (95%)	5 (5%)	0	100 100
19	g	103/105 (98%)	101 (98%)	2 (2%)	0	100 100
20	h	92/94 (98%)	88 (96%)	4 (4%)	0	100 100
21	i	100/102 (98%)	93 (93%)	7 (7%)	0	100 100
All	All	3051/3421 (89%)	2891 (95%)	155 (5%)	5 (0%)	50 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	L	41	PRO
4	I	350	ARG
7	L	42	SER
13	Y	223	PRO
4	I	327	PRO

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	C	21/21 (100%)	21 (100%)	0	100 100
3	H	94/128 (73%)	94 (100%)	0	100 100
4	I	270/380 (71%)	267 (99%)	3 (1%)	73 84
6	K	78/113 (69%)	78 (100%)	0	100 100
7	L	216/217 (100%)	214 (99%)	2 (1%)	78 88
8	N	316/408 (78%)	315 (100%)	1 (0%)	92 95
9	O	185/199 (93%)	185 (100%)	0	100 100
10	P	193/255 (76%)	193 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	Q	120/221 (54%)	119 (99%)	1 (1%)	81 89
12	U	111/181 (61%)	111 (100%)	0	100 100
13	Y	140/218 (64%)	140 (100%)	0	100 100
14	Z	87/141 (62%)	87 (100%)	0	100 100
15	a	74/79 (94%)	74 (100%)	0	100 100
16	b	65/66 (98%)	65 (100%)	0	100 100
16	f	66/66 (100%)	66 (100%)	0	100 100
17	d	80/81 (99%)	80 (100%)	0	100 100
18	e	74/104 (71%)	73 (99%)	1 (1%)	67 80
19	g	84/84 (100%)	84 (100%)	0	100 100
20	h	81/81 (100%)	81 (100%)	0	100 100
21	i	81/81 (100%)	81 (100%)	0	100 100
All	All	2436/3124 (78%)	2428 (100%)	8 (0%)	92 95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	e	223	ARG
11	Q	274	LYS
7	L	41	PRO
7	L	40	VAL
8	N	375	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
14	Z	103	GLN
19	g	91	ASN
14	Z	106	GLN
15	a	187	GLN
21	i	116	ASN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	596:LYS	C	602:SER	N	6.10

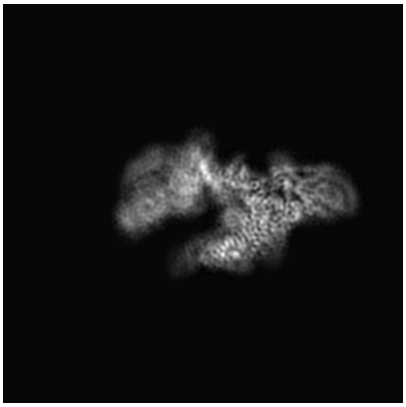
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4579. These allow visual inspection of the internal detail of the map and identification of artifacts.

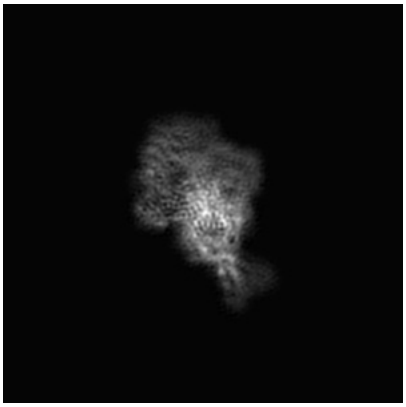
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

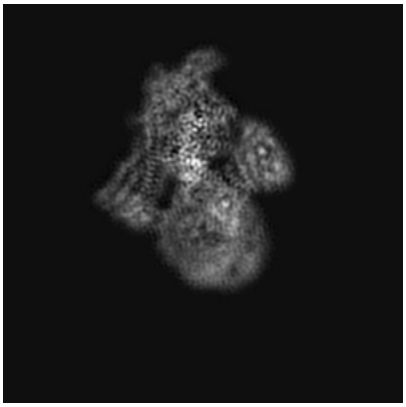
6.1.1 Primary map



X



Y

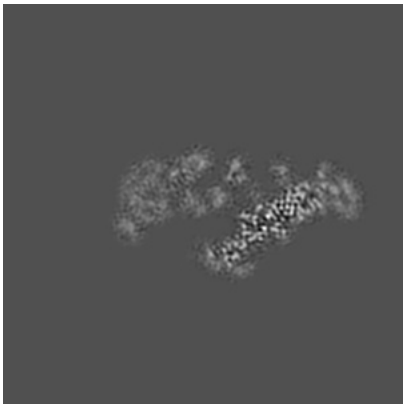


Z

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

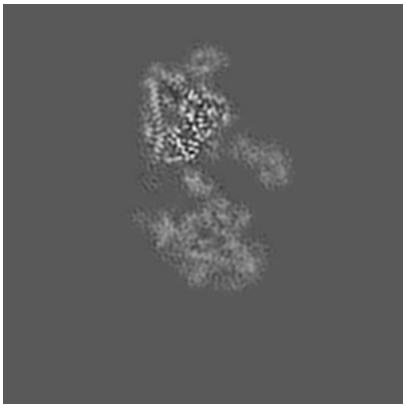
6.2 Central slices

6.2.1 Primary map



X Index: 160

Y Index: 160

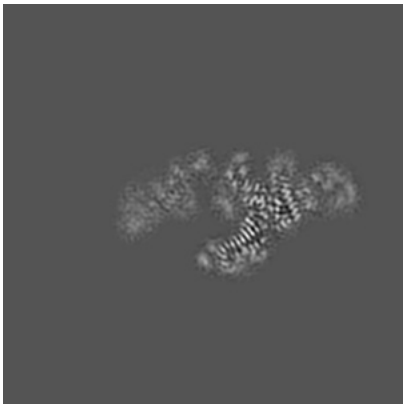


Z Index: 160

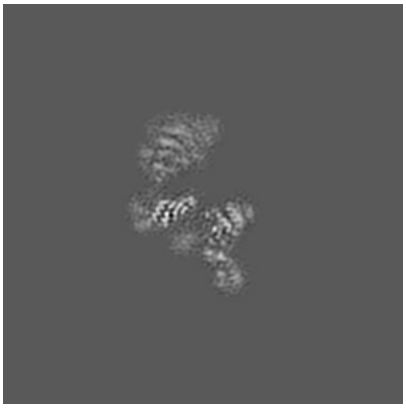
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

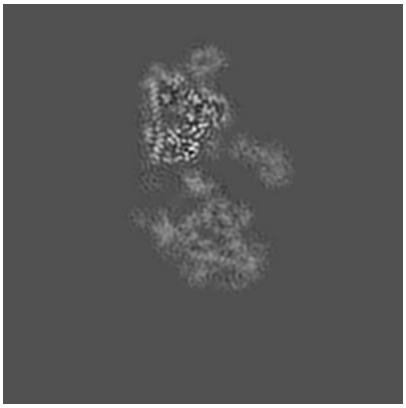
6.3.1 Primary map



X Index: 152



Y Index: 192

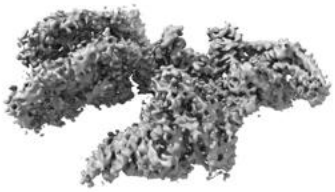


Z Index: 161

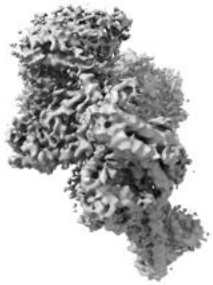
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

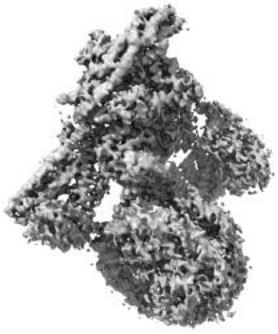
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

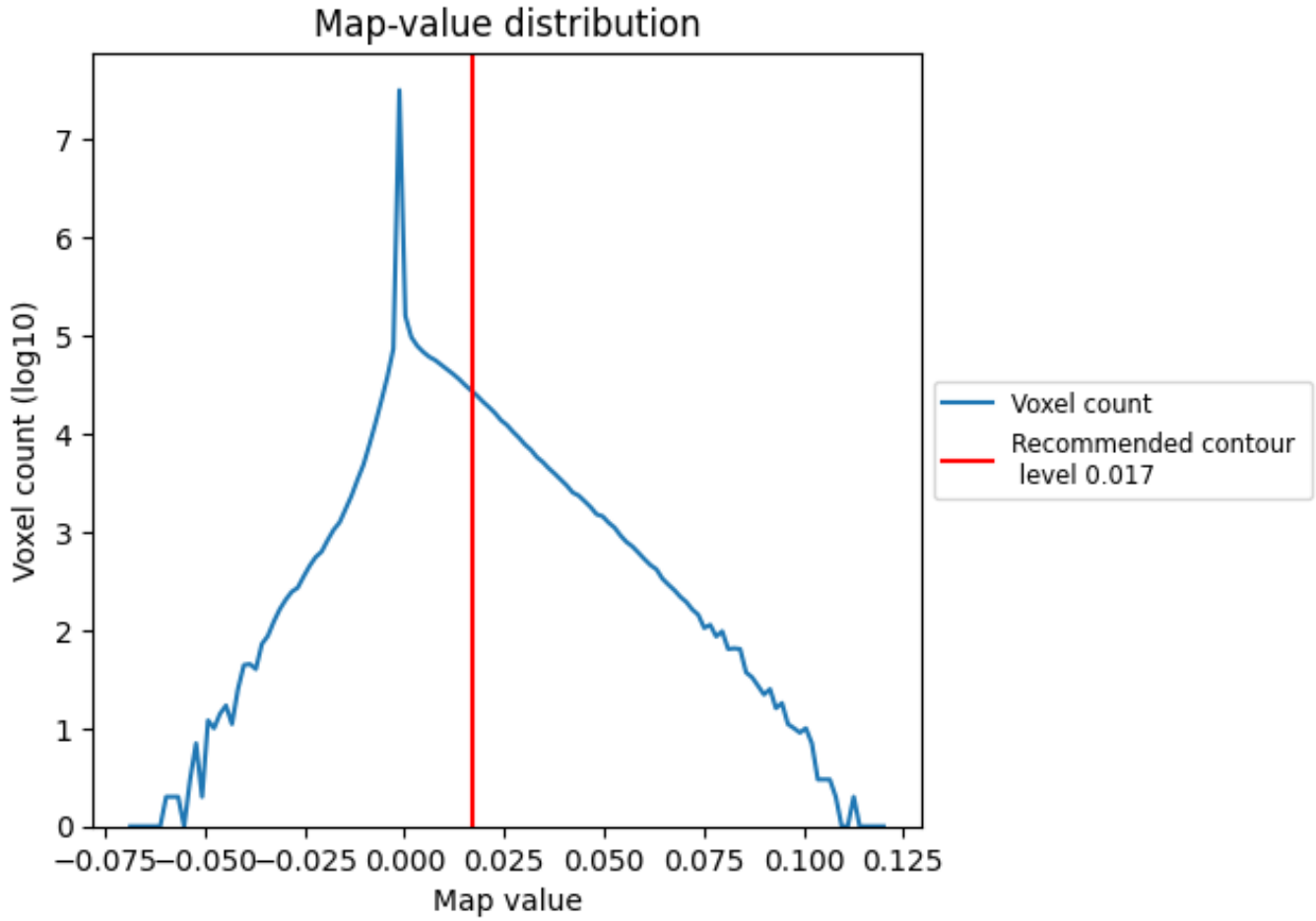
6.5 Mask visualisation (i)

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

7 Map analysis

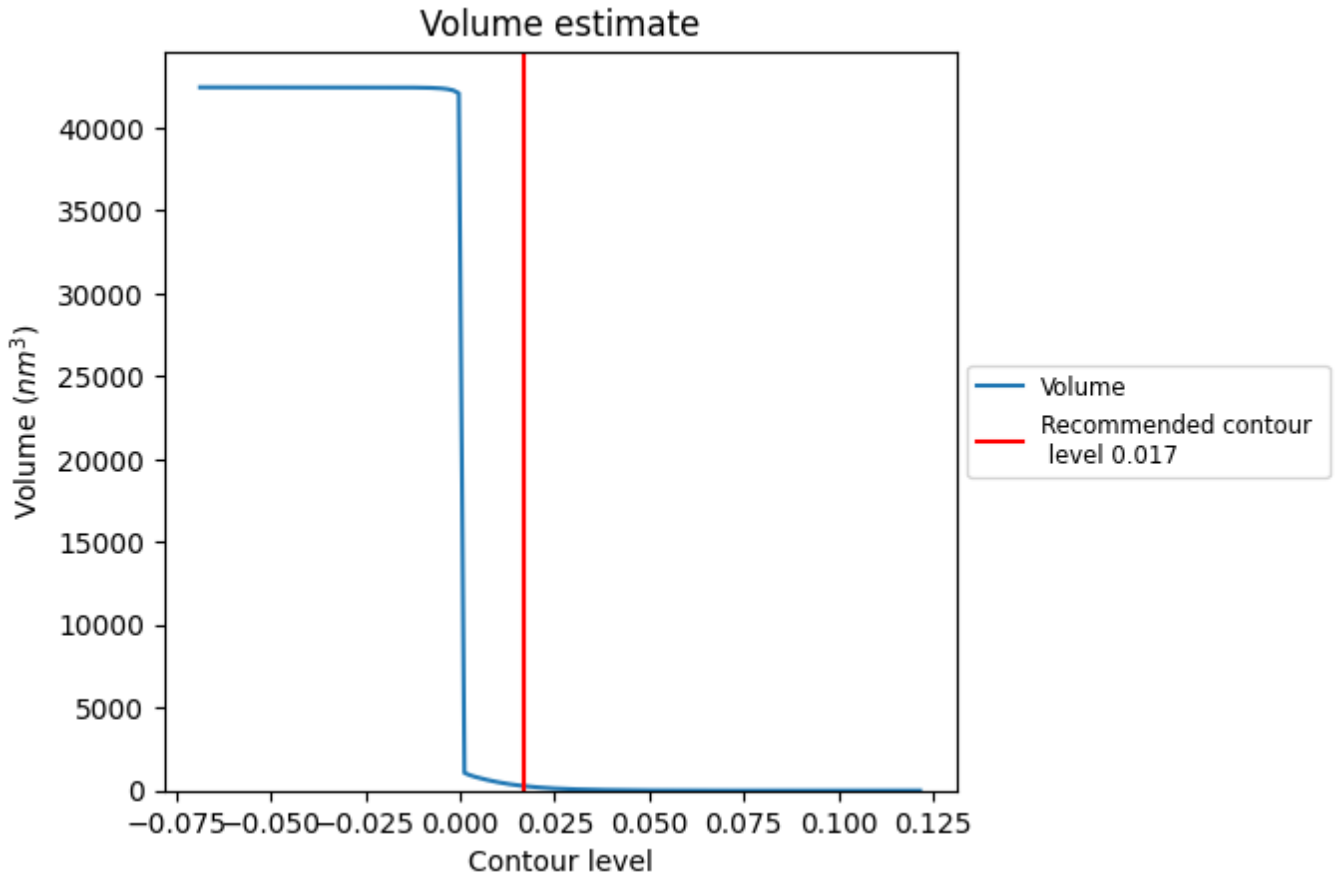
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

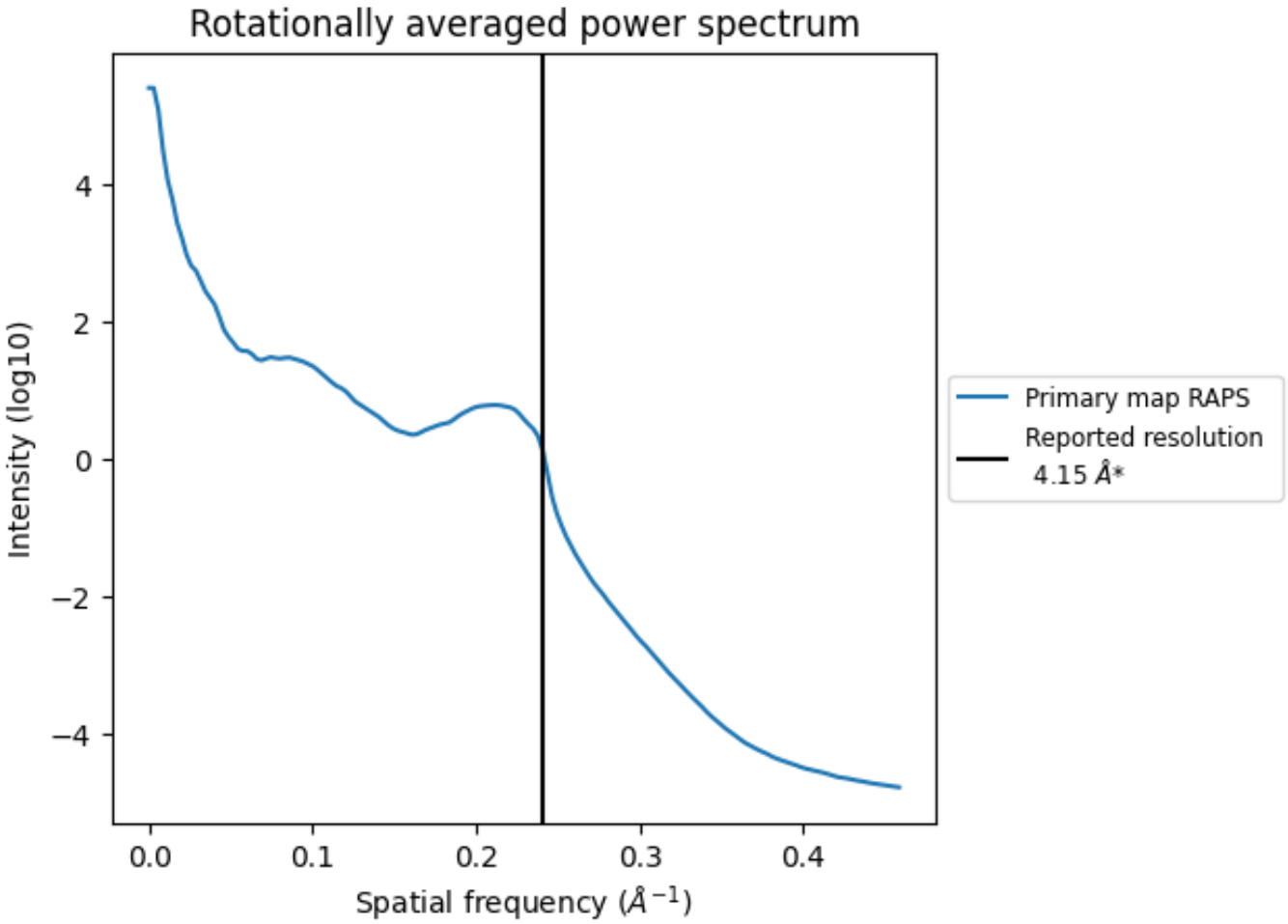
7.2 Volume estimate (i)



The volume at the recommended contour level is 272 nm^3; this corresponds to an approximate mass of 246 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 0.241 Å^{-1}

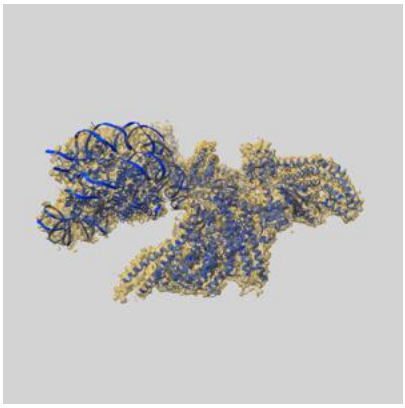
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

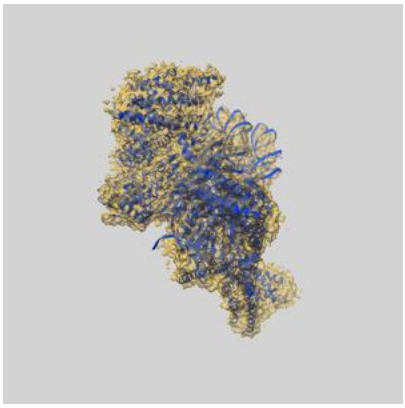
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4579 and PDB model 6QLD. Per-residue inclusion information can be found in section 3 on page 8.

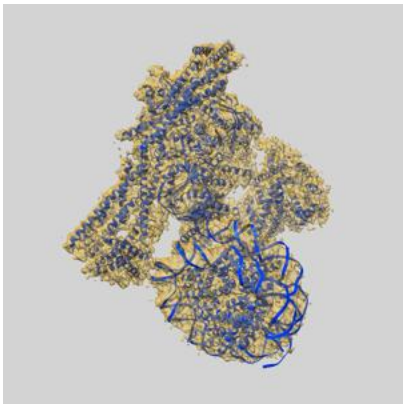
9.1 Map-model overlay



X



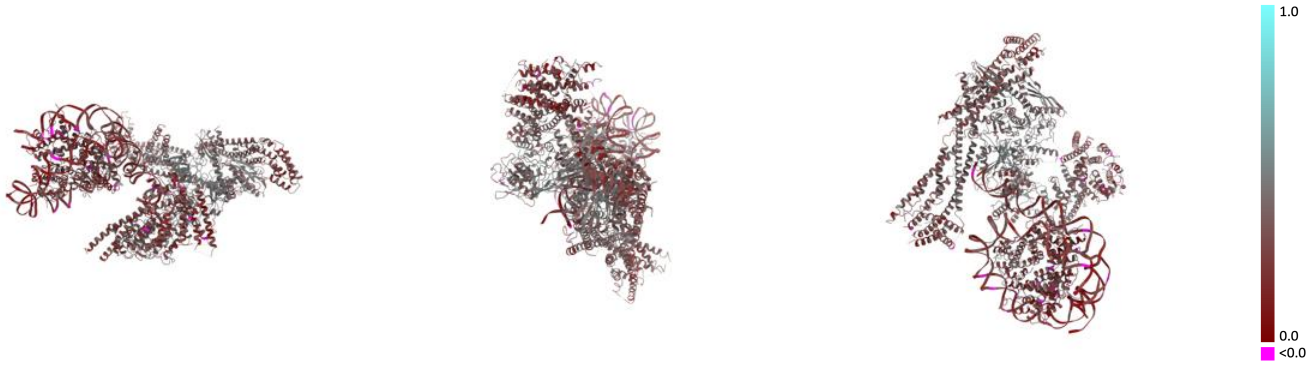
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017 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.

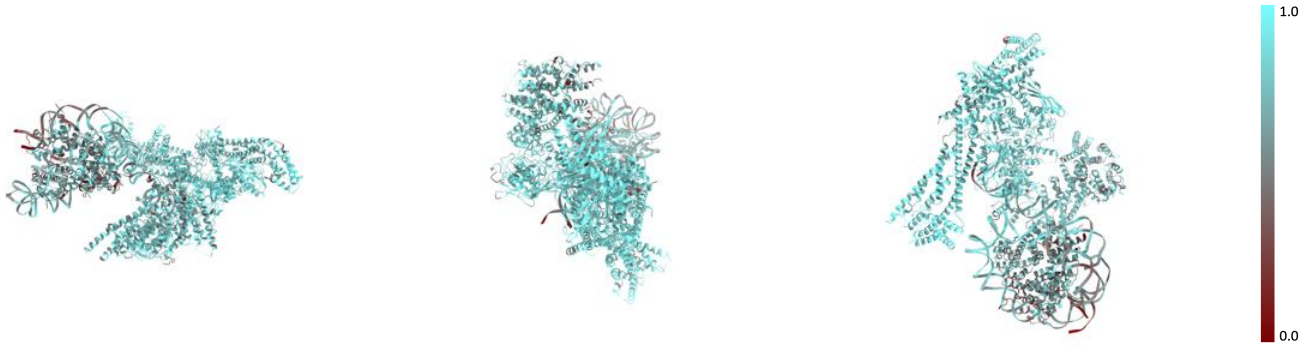
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

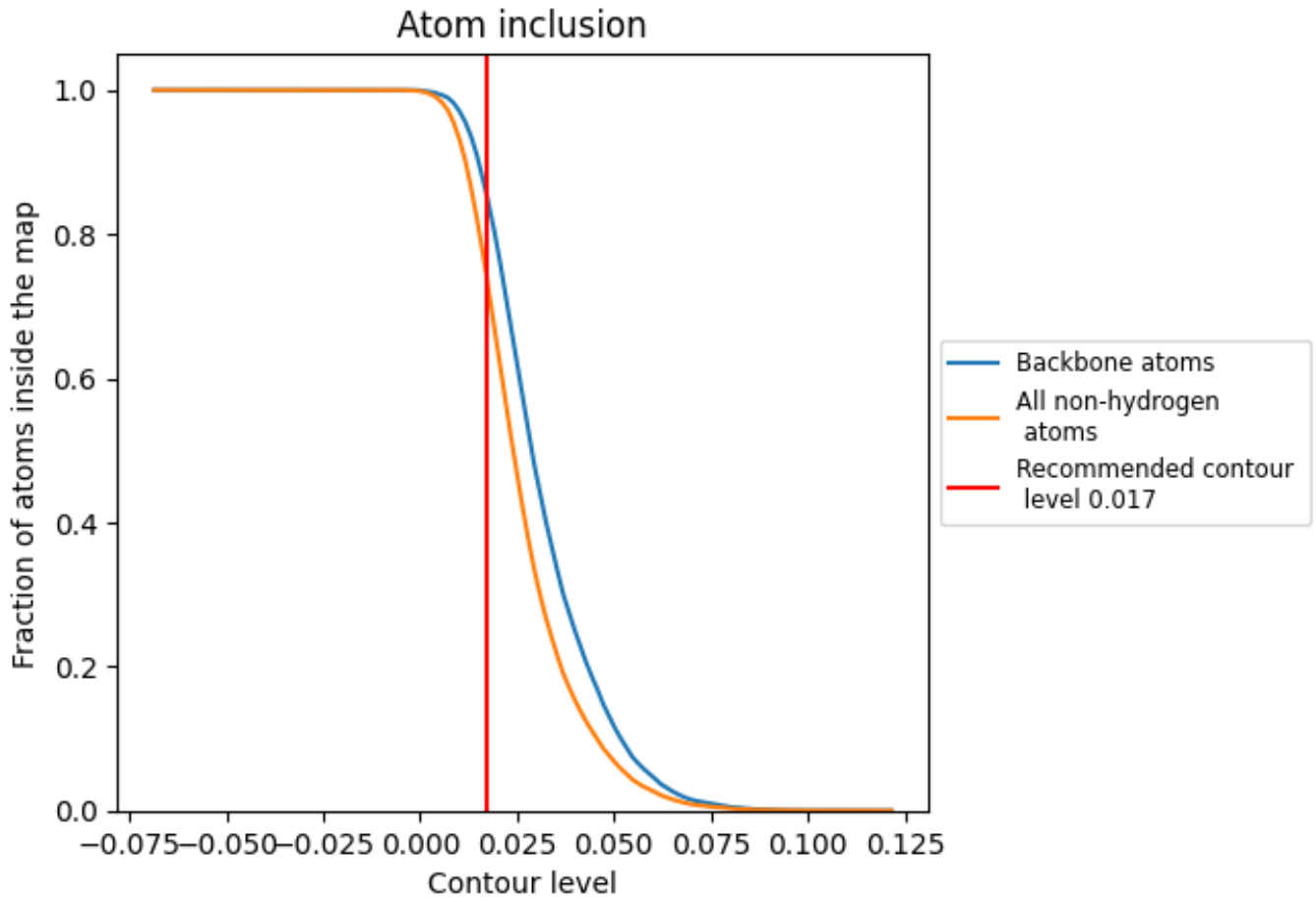
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.017).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7468	0.3280
C	0.1622	0.2560
G	0.6644	0.1990
H	0.7172	0.2860
I	0.7604	0.3230
J	0.6578	0.1970
K	0.7438	0.2900
L	0.8226	0.4110
N	0.8736	0.4470
O	0.8435	0.4370
P	0.8597	0.4230
Q	0.8394	0.3540
U	0.8434	0.3470
Y	0.8190	0.3450
Z	0.8301	0.3210
a	0.5831	0.2720
b	0.6040	0.2810
d	0.6057	0.2890
e	0.6697	0.3430
f	0.7048	0.3390
g	0.5797	0.2780
h	0.6173	0.2790
i	0.5294	0.2880