wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 10:25 am GMT

PDB ID	:	6I84
EMDB ID	:	EMD-4429
Title	:	Structure of transcribing RNA polymerase II-nucleosome complex
Authors	:	Farnung, L.; Vos, S.M.; Cramer, P.
Deposited on	:	2018-11-19
Resolution	:	4.40 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 (i) 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 (i)) were used in the production of this report:

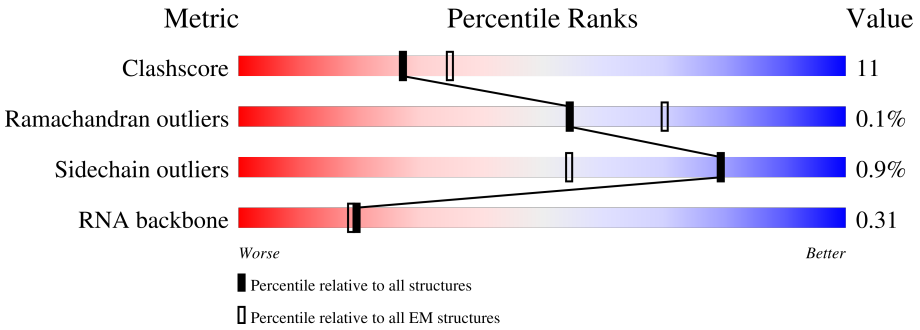
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 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
RNA backbone	4643	859

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	M	136	21% 48% 24% 29%
1	S	136	37% 54% 17% 29%
2	Q	130	60% 55% 24% 21%
2	V	130	55% 58% 22% 19%
3	T	169	15% 62% 35%
4	N	160	11% 66% 31%
5	O	103	26% 47% 32% 19%

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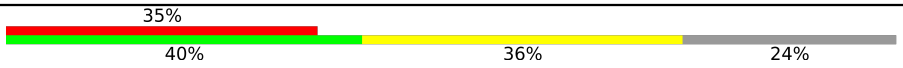
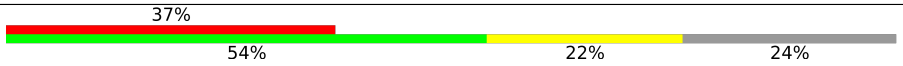
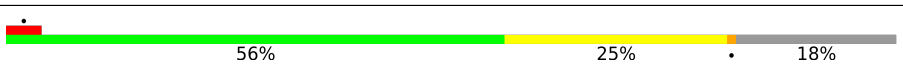
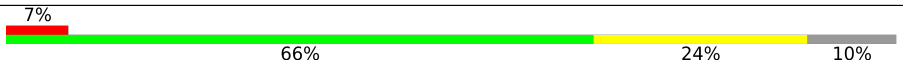
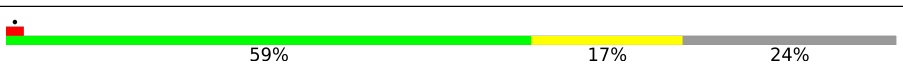
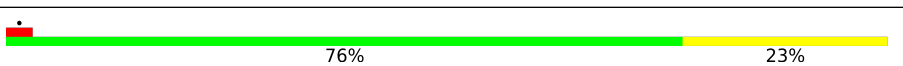
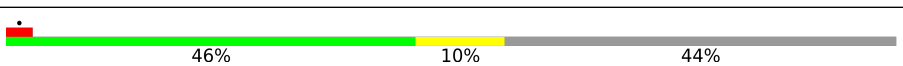
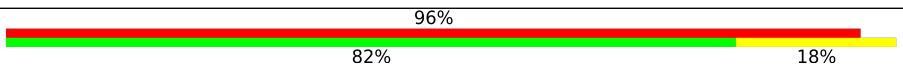
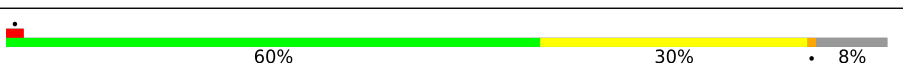
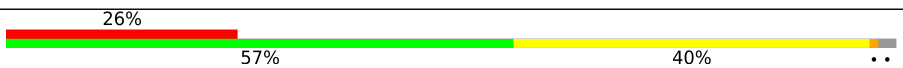
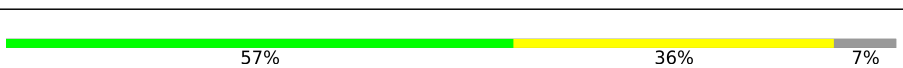
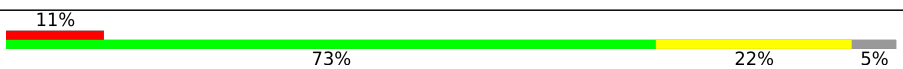
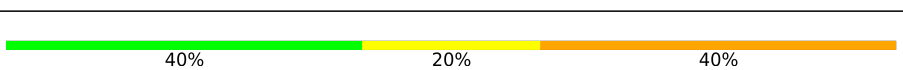
Mol	Chain	Length	Quality of chain
5	U	103	
6	R	123	
6	W	123	
7	A	1733	
8	B	1224	
9	C	348	
10	D	221	
11	E	215	
12	F	155	
13	G	171	
14	H	146	
15	I	122	
16	J	70	
17	K	120	
18	L	70	
19	P	10	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 43988 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	97	Total	C	N	O	S	0	0
			802	506	155	138	3		
1	S	97	Total	C	N	O	S	0	0
			801	504	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	102	ALA	GLY	conflict	UNP P84233
S	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	103	Total	C	N	O	0	0
			795	501	155	139		
2	V	105	Total	C	N	O	0	0
			809	510	158	141		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	99	ARG	GLY	conflict	UNP P06897
Q	123	SER	ALA	conflict	UNP P06897
V	99	ARG	GLY	conflict	UNP P06897
V	123	SER	ALA	conflict	UNP P06897

- Molecule 3 is a DNA chain called DNA (170-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	169	Total	C	N	O	P	0	0
			3453	1641	639	1005	168		

- Molecule 4 is a DNA chain called DNA (158-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	158	Total	C	N	O	P	0	0
			3248	1543	596	952	157		

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
5	U	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	95	Total	C	N	O	S	0	0
			745	469	134	140	2		
6	W	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	0	MET	-	initiating methionine	UNP P02281
R	29	THR	SER	conflict	UNP P02281
W	0	MET	-	initiating methionine	UNP P02281
W	29	THR	SER	conflict	UNP P02281

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1416	Total	C	N	O	S	0	0
			11143	7021	1949	2111	62		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	1104	Total	C	N	O	S	0	0
			8779	5560	1537	1627	55		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-29	MET	-	initiating methionine	UNP P16370
C	-28	GLY	-	expression tag	UNP P16370
C	-27	SER	-	expression tag	UNP P16370
C	-26	HIS	-	expression tag	UNP P16370
C	-25	HIS	-	expression tag	UNP P16370
C	-24	HIS	-	expression tag	UNP P16370
C	-23	HIS	-	expression tag	UNP P16370
C	-22	HIS	-	expression tag	UNP P16370
C	-21	HIS	-	expression tag	UNP P16370
C	-20	SER	-	expression tag	UNP P16370
C	-19	ASN	-	expression tag	UNP P16370
C	-18	SER	-	expression tag	UNP P16370
C	-17	GLY	-	expression tag	UNP P16370
C	-16	LEU	-	expression tag	UNP P16370
C	-15	ASN	-	expression tag	UNP P16370
C	-14	ASP	-	expression tag	UNP P16370
C	-13	ILE	-	expression tag	UNP P16370
C	-12	PHE	-	expression tag	UNP P16370
C	-11	GLU	-	expression tag	UNP P16370
C	-10	ALA	-	expression tag	UNP P16370
C	-9	GLN	-	expression tag	UNP P16370
C	-8	LYS	-	expression tag	UNP P16370
C	-7	ILE	-	expression tag	UNP P16370
C	-6	GLU	-	expression tag	UNP P16370
C	-5	TRP	-	expression tag	UNP P16370
C	-4	HIS	-	expression tag	UNP P16370
C	-3	GLU	-	expression tag	UNP P16370
C	-2	ASP	-	expression tag	UNP P16370
C	-1	THR	-	expression tag	UNP P16370
C	0	GLY	-	expression tag	UNP P16370

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	178	Total	C	N	O	S	0	0
			1434	887	257	288	2		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	134	Total	C	N	O	S	0	0
			1076	677	182	213	4		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	114	Total	C	N	O	S	0	0
			919	590	156	171	2		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 19 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	10	Total	C	N	O	P	0	0
			210	94	35	71	10		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	

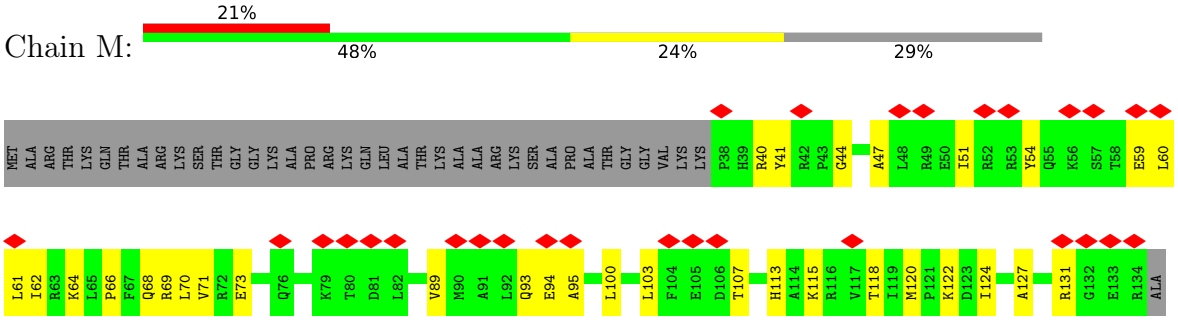
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

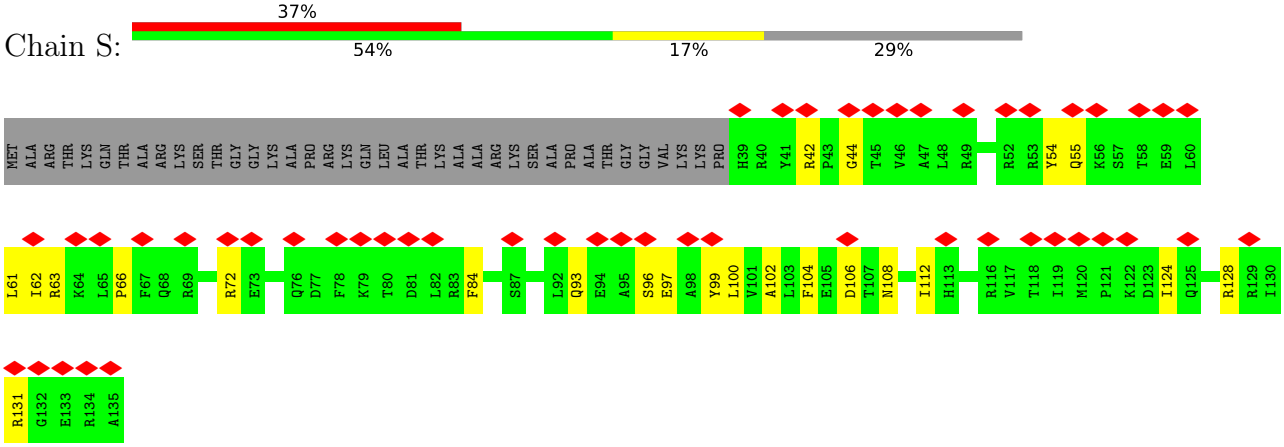
3 Residue-property plots (i)

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.

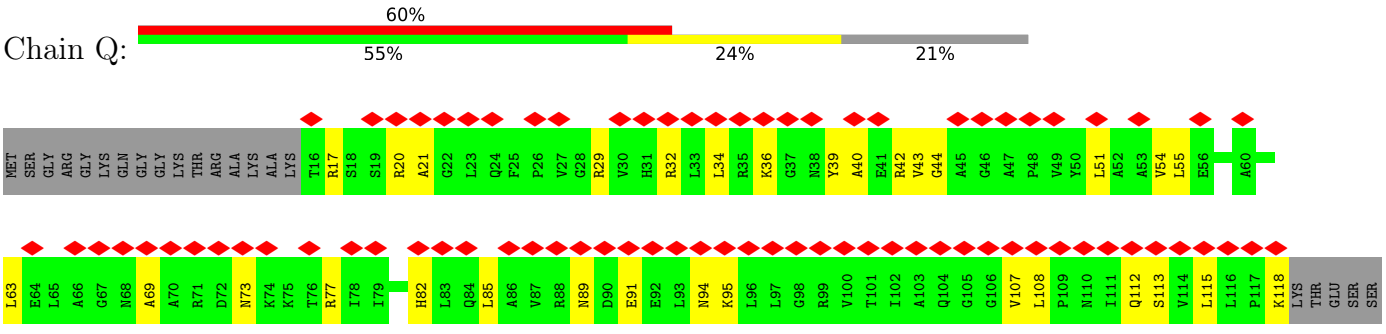
• Molecule 1: Histone H3.2



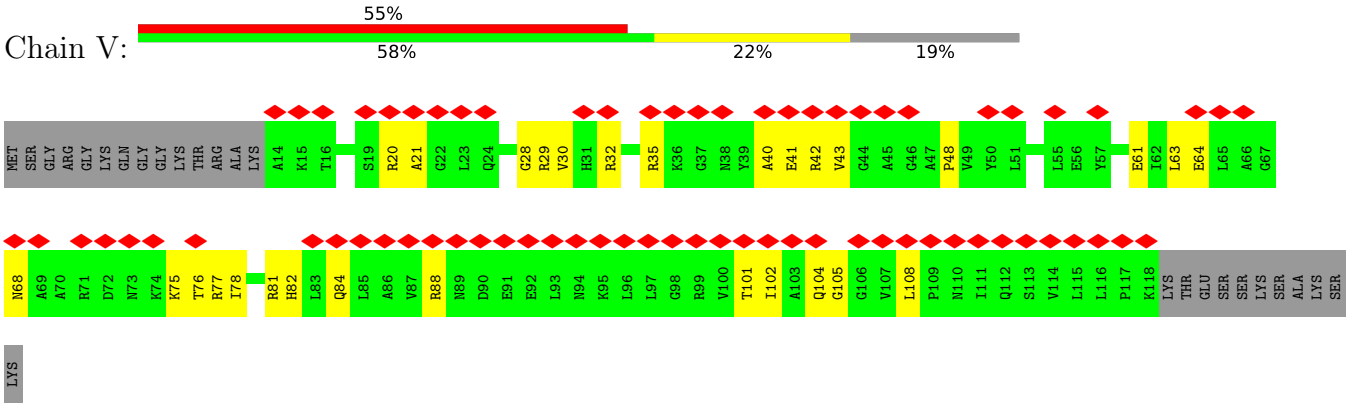
• Molecule 1: Histone H3.2



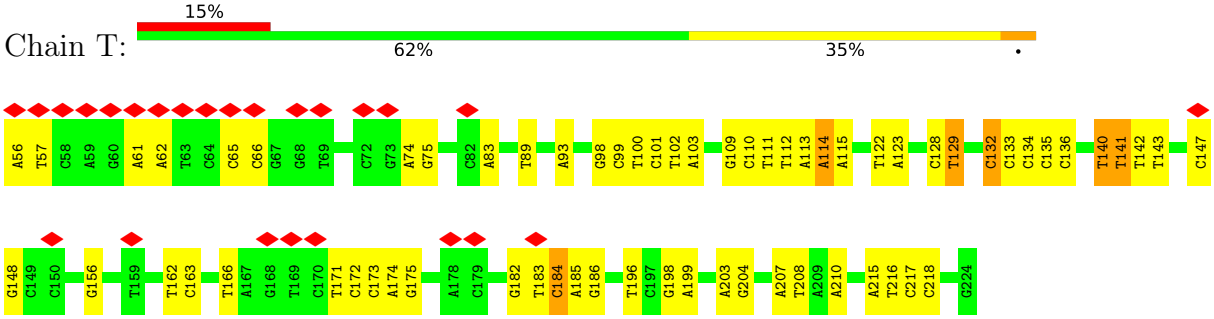
• Molecule 2: Histone H2A type 1



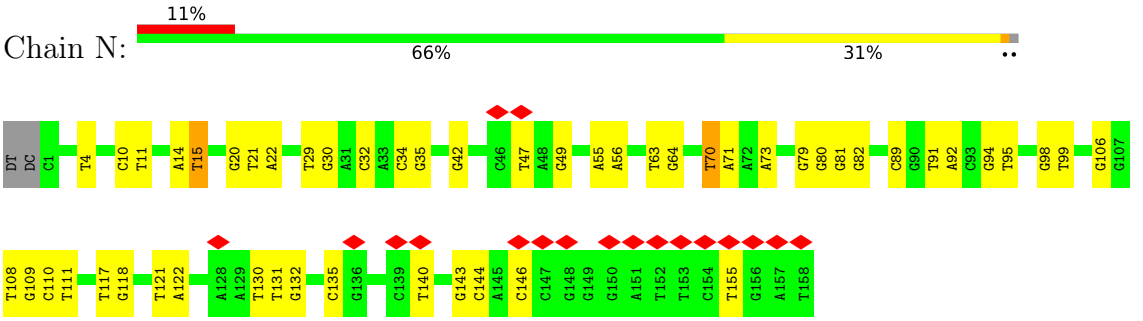
• Molecule 2: Histone H2A type 1



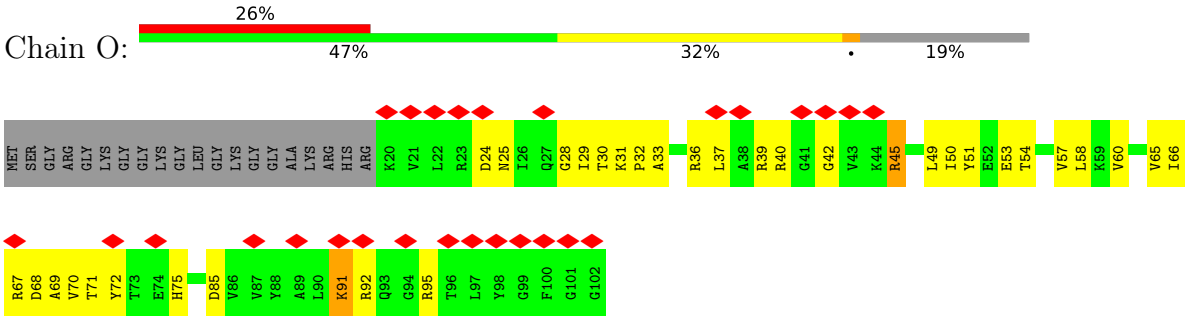
• Molecule 3: DNA (170-MER)



• Molecule 4: DNA (158-MER)

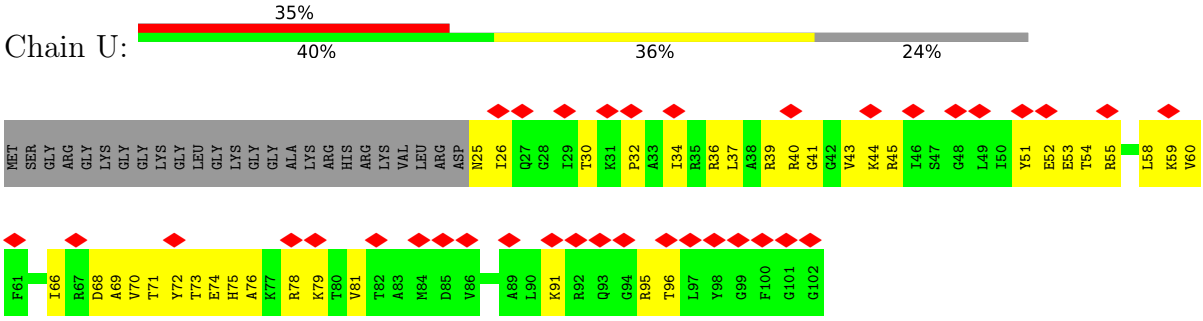


• Molecule 5: Histone H4



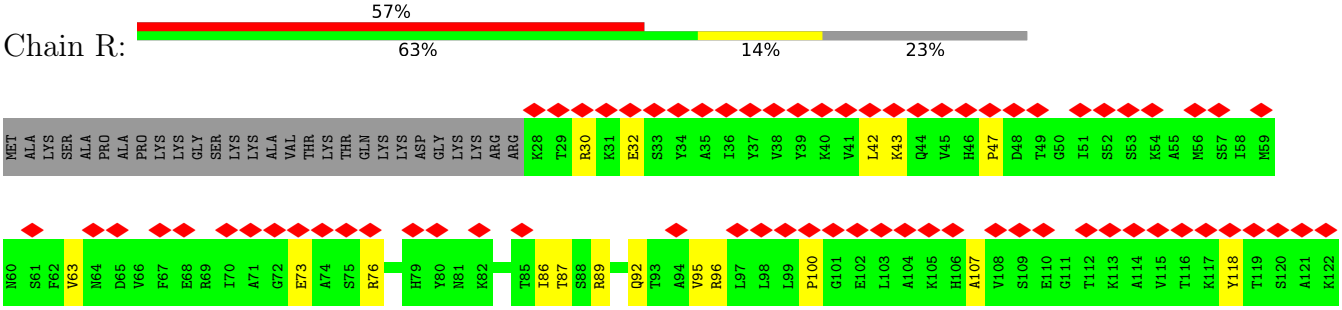
• Molecule 5: Histone H4

Chain U:



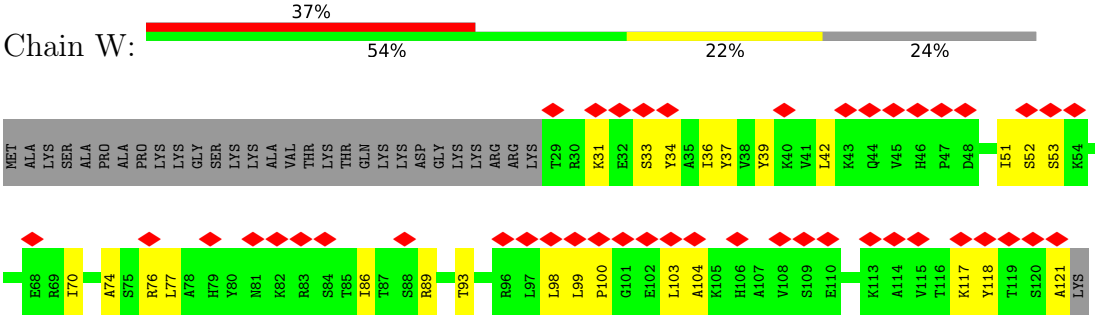
• Molecule 6: Histone H2B 1.1

Chain R:



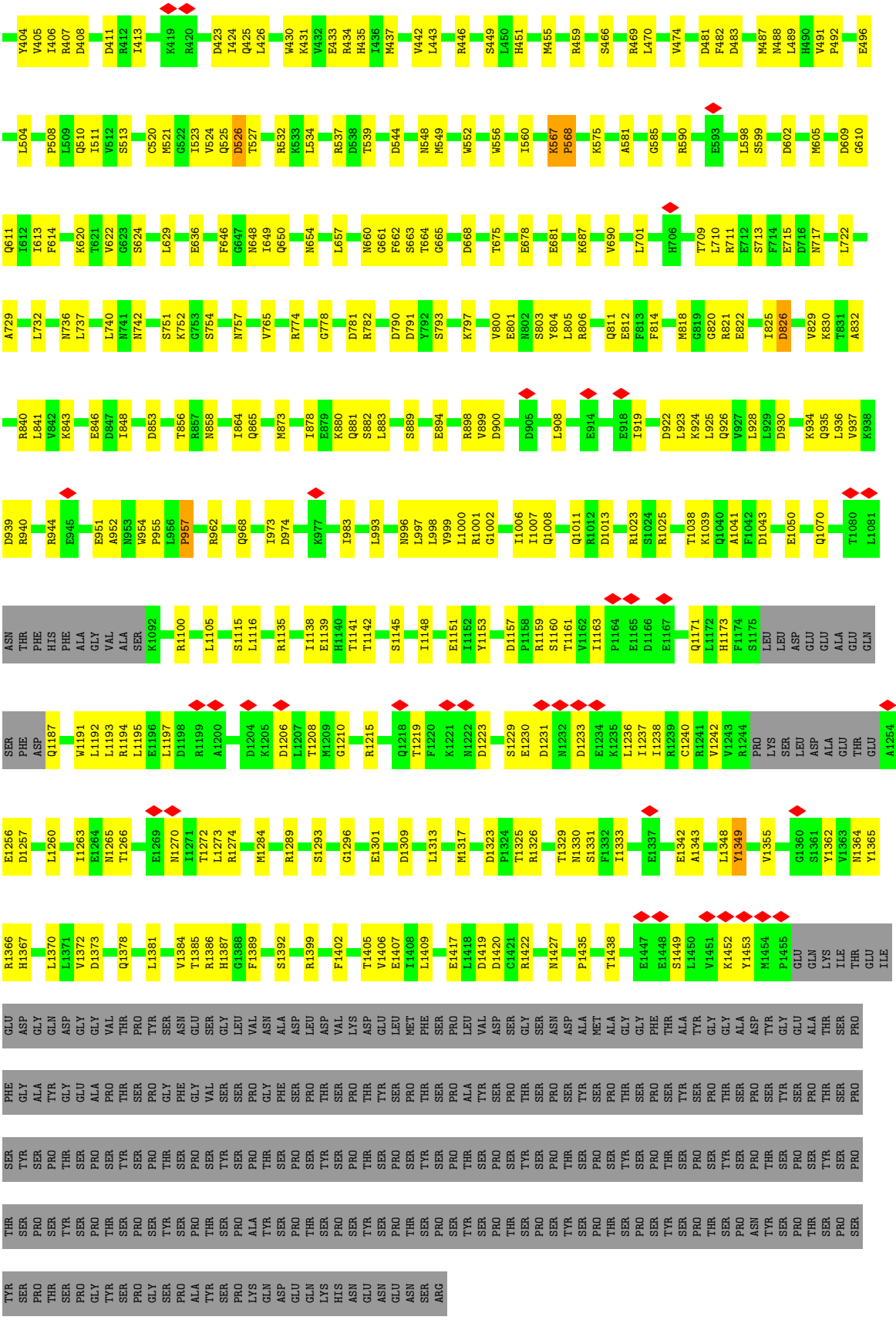
• Molecule 6: Histone H2B 1.1

Chain W:



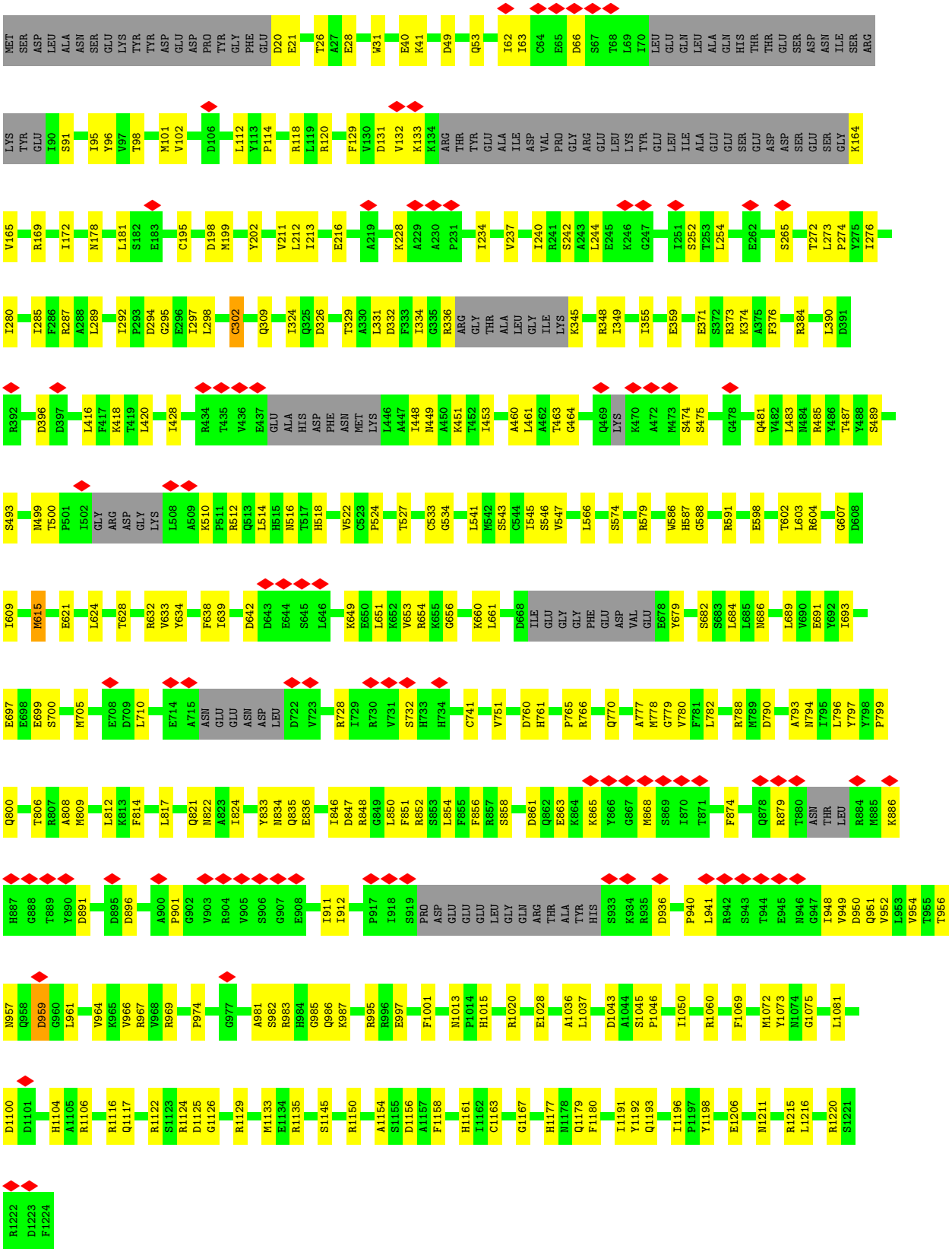
• Molecule 7: DNA-directed RNA polymerase II subunit RPB1

Chain A:



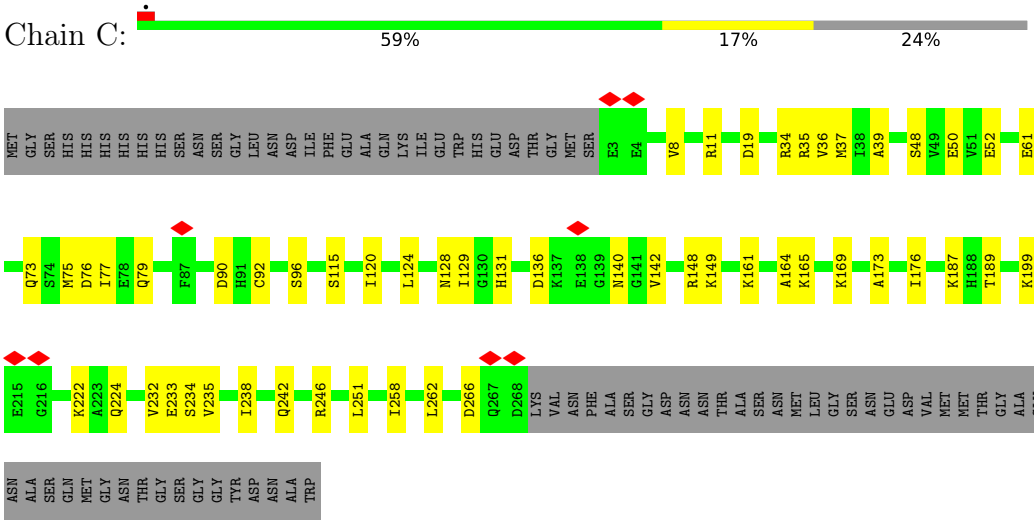
• Molecule 8: DNA-directed RNA polymerase II subunit RPB2

Chain B:



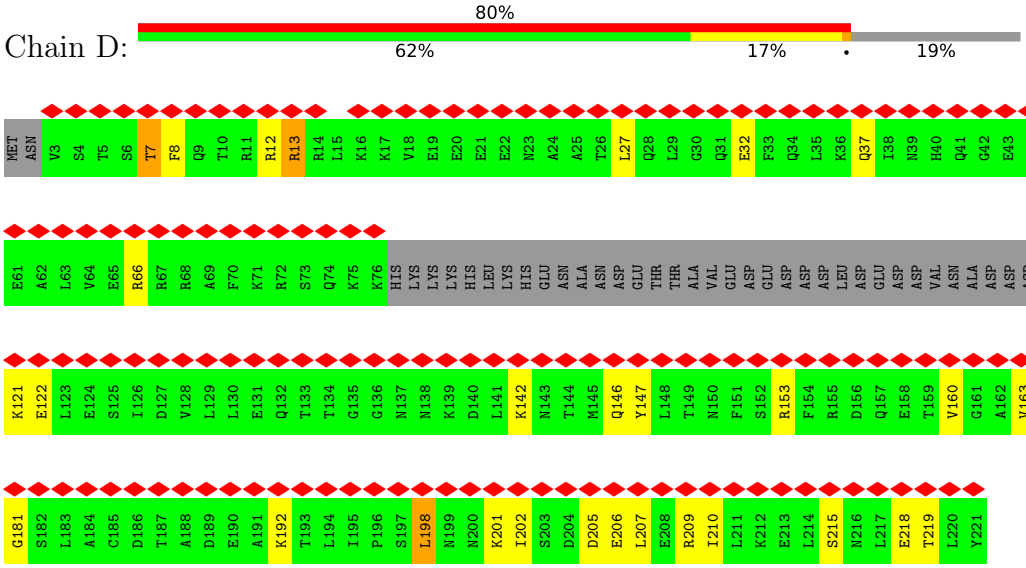
- Molecule 9: DNA-directed RNA polymerase II subunit RPB3

Chain C:



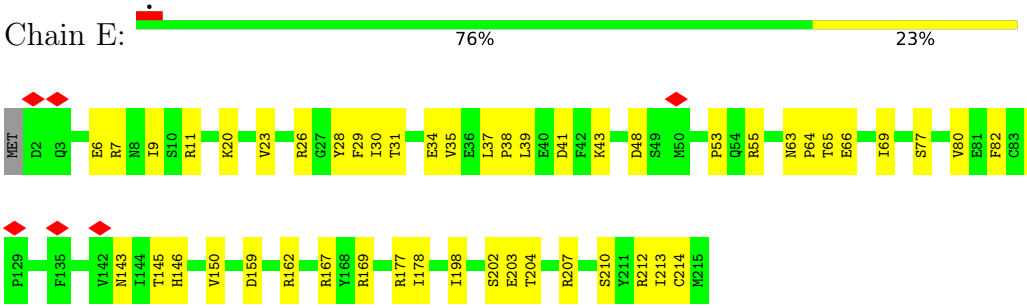
• Molecule 10: DNA-directed RNA polymerase II subunit RPB4

Chain D:



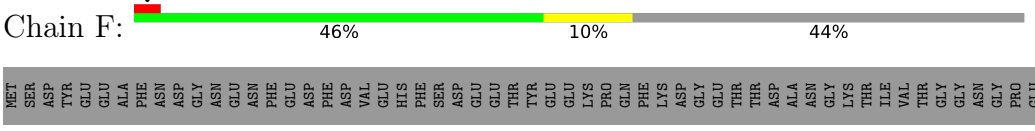
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC1

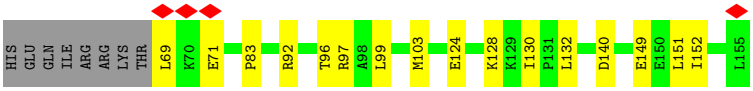
Chain E:



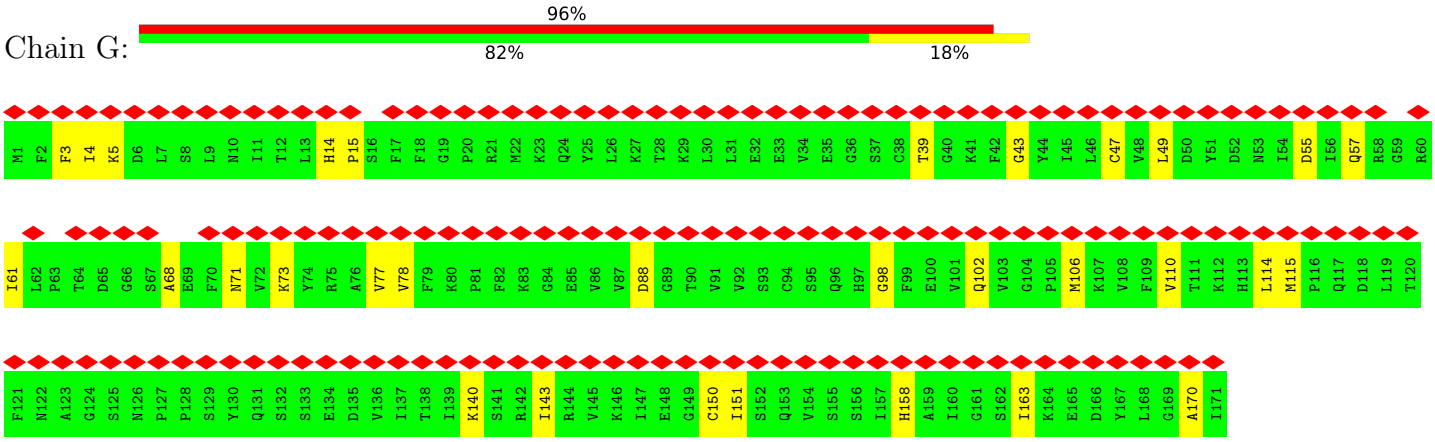
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

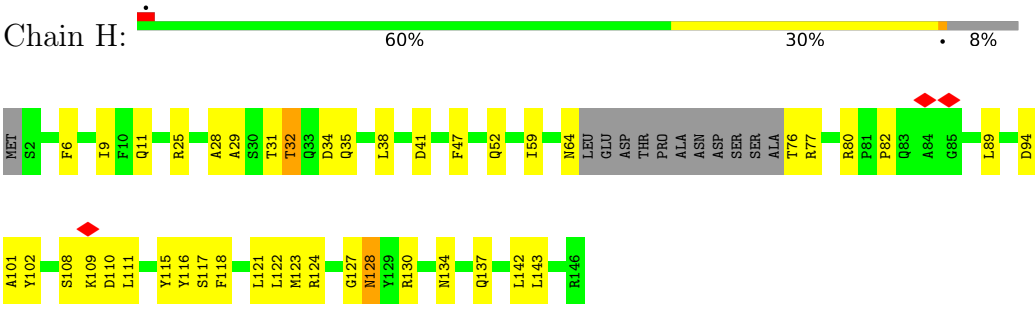




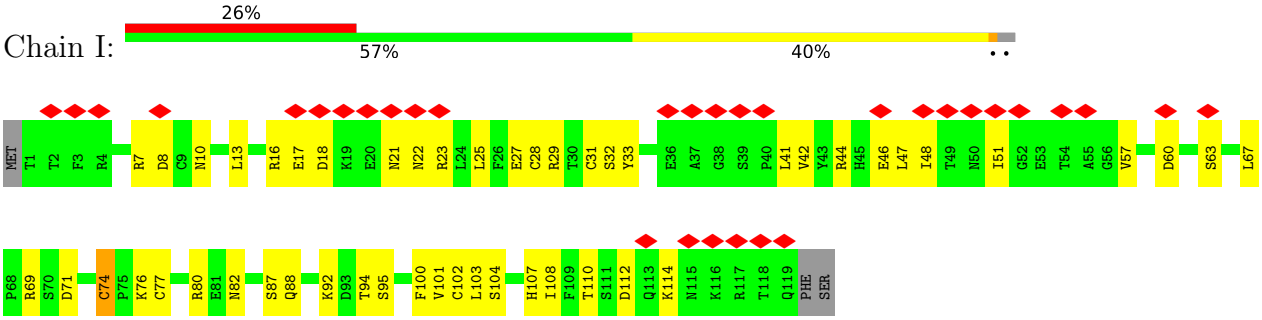
• Molecule 13: DNA-directed RNA polymerase II subunit RPB7



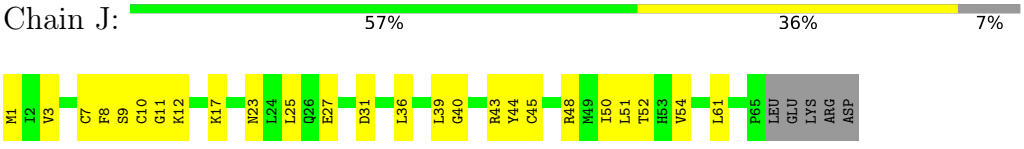
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 15: DNA-directed RNA polymerase II subunit RPB9

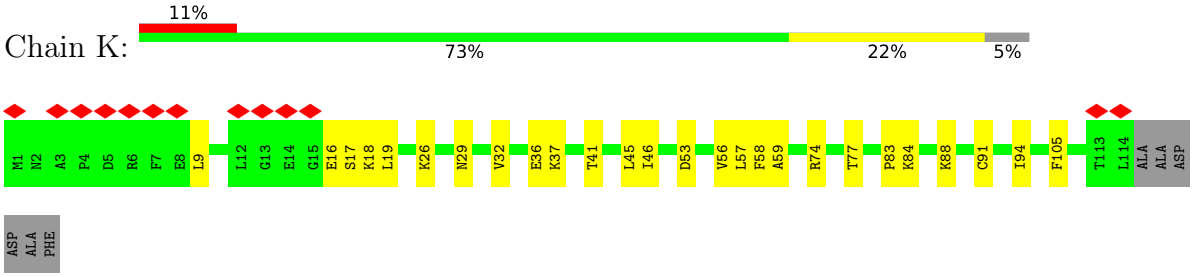


• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5



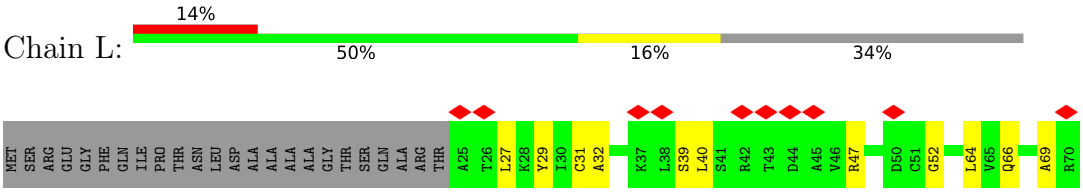
• Molecule 17: DNA-directed RNA polymerase II subunit RPB11

Chain K:



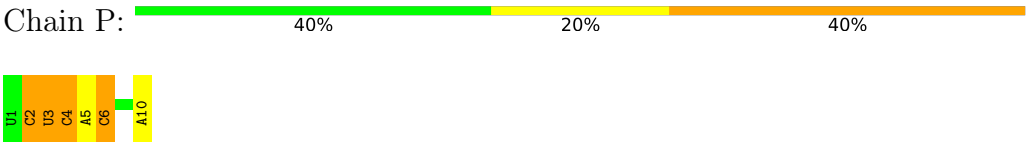
• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



• Molecule 19: RNA

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49703	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 ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.007	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0173	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	M	0.33	0/814	0.54	0/1092
1	S	0.32	0/812	0.57	0/1088
2	Q	0.31	0/805	0.60	1/1088 (0.1%)
2	V	0.31	0/819	0.54	0/1106
3	T	0.86	0/3874	1.11	11/5974 (0.2%)
4	N	0.81	0/3644	1.09	8/5627 (0.1%)
5	O	0.32	0/669	0.59	0/894
5	U	0.32	0/626	0.62	0/837
6	R	0.30	0/756	0.52	0/1015
6	W	0.32	0/737	0.55	0/993
7	A	0.45	1/11342 (0.0%)	0.66	2/15337 (0.0%)
8	B	0.43	0/8949	0.63	2/12065 (0.0%)
9	C	0.42	0/2133	0.59	0/2891
10	D	0.31	0/1444	0.69	2/1935 (0.1%)
11	E	0.44	0/1788	0.58	0/2406
12	F	0.49	0/717	0.60	0/967
13	G	0.32	0/1368	0.57	0/1844
14	H	0.48	0/1094	0.67	0/1481
15	I	0.40	0/989	0.60	1/1331 (0.1%)
16	J	0.51	0/541	0.62	0/727
17	K	0.43	0/937	0.59	0/1265
18	L	0.31	0/365	0.73	1/485 (0.2%)
19	P	0.84	0/233	1.59	5/360 (1.4%)
All	All	0.51	1/45456 (0.0%)	0.74	33/62808 (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
7	A	0	5
8	B	0	3
14	H	0	3
16	J	0	2
18	L	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1349	TYR	CD1-CE1	-5.07	1.31	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	826	ASP	CB-CG-OD1	9.05	126.45	118.30
10	D	27	LEU	CA-CB-CG	8.35	134.49	115.30
4	N	106	DG	O4'-C1'-N9	8.25	113.78	108.00
3	T	140	DT	O4'-C1'-N1	6.84	112.79	108.00
3	T	141	DT	O4'-C1'-N1	6.53	112.57	108.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	524	VAL	Peptide
7	A	55	ASP	Peptide
7	A	567	LYS	Peptide
7	A	92	HIS	Peptide
7	A	957	PRO	Peptide

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	M	802	0	841	28	0
1	S	801	0	838	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	795	0	846	33	0
2	V	809	0	864	28	0
3	T	3453	0	1897	45	0
4	N	3248	0	1780	40	0
5	O	662	0	709	33	0
5	U	619	0	659	35	0
6	R	745	0	773	18	0
6	W	726	0	747	22	0
7	A	11143	0	11219	311	0
8	B	8779	0	8811	209	0
9	C	2095	0	2052	49	0
10	D	1434	0	1460	26	0
11	E	1752	0	1776	34	0
12	F	705	0	731	13	0
13	G	1340	0	1357	24	0
14	H	1076	0	1046	30	0
15	I	971	0	932	38	0
16	J	532	0	544	19	0
17	K	919	0	929	25	0
18	L	363	0	389	7	0
19	P	210	0	107	4	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
All	All	43988	0	41307	905	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 11.

The worst 5 of 905 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)
8:B:298:LEU:O	8:B:302:CYS:HB3	1.61	1.00
7:A:1256:GLU:O	7:A:1260:LEU:HB2	1.88	0.73
7:A:91:PHE:H	7:A:297:GLN:HE22	1.36	0.72
15:I:13:LEU:HA	15:I:27:GLU:O	1.88	0.72
5:U:71:THR:O	5:U:74:GLU:HB2	1.91	0.71

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	M	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
1	S	95/136 (70%)	91 (96%)	4 (4%)	0	100	100
2	Q	101/130 (78%)	89 (88%)	12 (12%)	0	100	100
2	V	103/130 (79%)	95 (92%)	8 (8%)	0	100	100
5	O	81/103 (79%)	77 (95%)	4 (5%)	0	100	100
5	U	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
6	R	93/123 (76%)	89 (96%)	4 (4%)	0	100	100
6	W	91/123 (74%)	85 (93%)	6 (7%)	0	100	100
7	A	1406/1733 (81%)	1236 (88%)	168 (12%)	2 (0%)	51	85
8	B	1084/1224 (89%)	935 (86%)	149 (14%)	0	100	100
9	C	264/348 (76%)	229 (87%)	35 (13%)	0	100	100
10	D	174/221 (79%)	152 (87%)	21 (12%)	1 (1%)	25	65
11	E	212/215 (99%)	194 (92%)	18 (8%)	0	100	100
12	F	85/155 (55%)	76 (89%)	9 (11%)	0	100	100
13	G	169/171 (99%)	149 (88%)	20 (12%)	0	100	100
14	H	130/146 (89%)	106 (82%)	24 (18%)	0	100	100
15	I	117/122 (96%)	92 (79%)	25 (21%)	0	100	100
16	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
17	K	112/120 (93%)	100 (89%)	12 (11%)	0	100	100
18	L	44/70 (63%)	32 (73%)	12 (27%)	0	100	100
All	All	4595/5579 (82%)	4051 (88%)	541 (12%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	D	8	PHE
7	A	1242	VAL
7	A	568	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	M	85/111 (77%)	85 (100%)	0	100 100
1	S	84/111 (76%)	84 (100%)	0	100 100
2	Q	82/102 (80%)	82 (100%)	0	100 100
2	V	83/102 (81%)	83 (100%)	0	100 100
5	O	68/79 (86%)	64 (94%)	4 (6%)	19 47
5	U	63/79 (80%)	62 (98%)	1 (2%)	62 79
6	R	81/103 (79%)	80 (99%)	1 (1%)	71 84
6	W	79/103 (77%)	78 (99%)	1 (1%)	69 82
7	A	1239/1520 (82%)	1226 (99%)	13 (1%)	76 86
8	B	958/1061 (90%)	953 (100%)	5 (0%)	88 93
9	C	234/300 (78%)	232 (99%)	2 (1%)	78 88
10	D	160/200 (80%)	156 (98%)	4 (2%)	47 68
11	E	196/197 (100%)	195 (100%)	1 (0%)	88 93
12	F	77/137 (56%)	77 (100%)	0	100 100
13	G	152/152 (100%)	152 (100%)	0	100 100
14	H	118/128 (92%)	115 (98%)	3 (2%)	47 68
15	I	113/116 (97%)	112 (99%)	1 (1%)	78 88
16	J	60/65 (92%)	58 (97%)	2 (3%)	38 61
17	K	99/102 (97%)	99 (100%)	0	100 100
18	L	40/57 (70%)	40 (100%)	0	100 100
All	All	4071/4825 (84%)	4033 (99%)	38 (1%)	79 88

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	D	13	ARG
15	I	74	CYS
10	D	198	LEU
14	H	32	THR
16	J	45	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	1140	HIS
15	I	21	ASN
8	B	484	ASN
14	H	134	ASN
17	K	52	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	P	9/10 (90%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	P	2	C
19	P	6	C
19	P	10	A

There are no RNA pucker outliers to report.

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)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

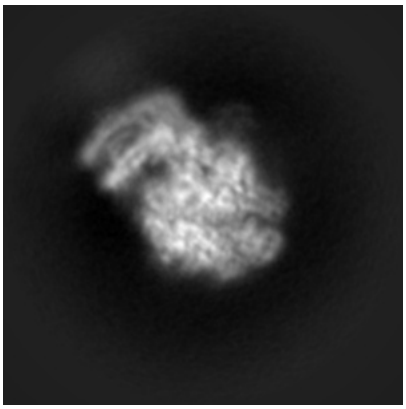
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4429. These allow visual inspection of the internal detail of the map and identification of artifacts.

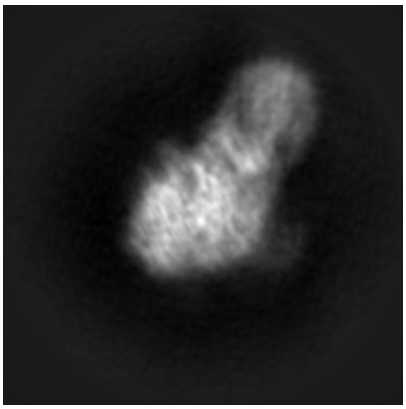
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

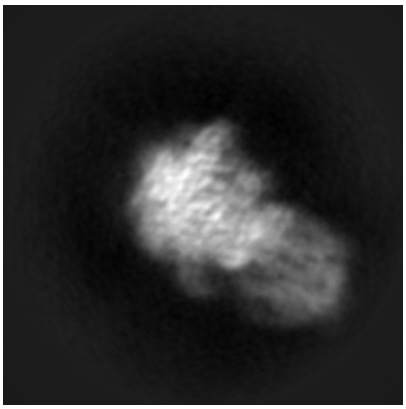
6.1.1 Primary map



X

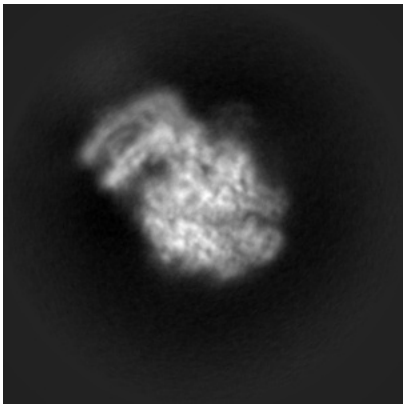


Y

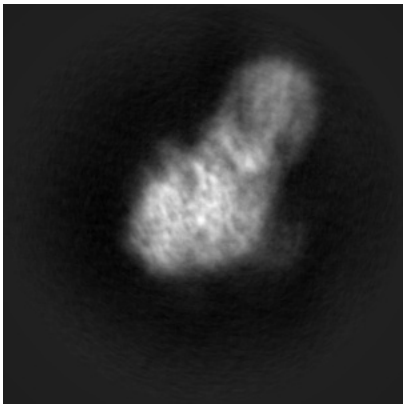


Z

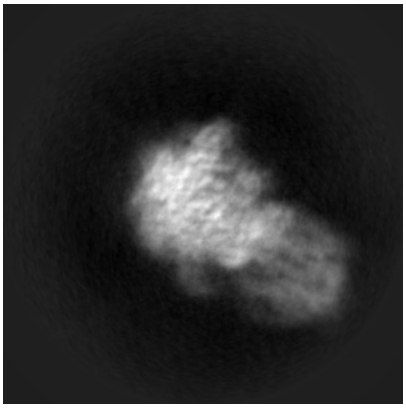
6.1.2 Raw map



X



Y

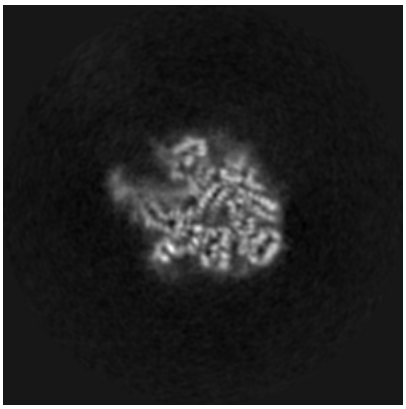


Z

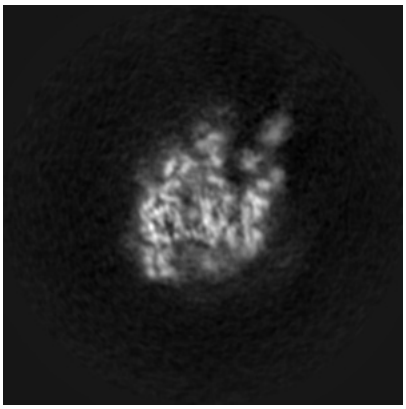
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

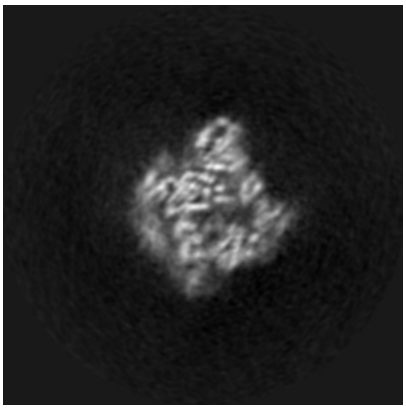
6.2.1 Primary map



X Index: 160

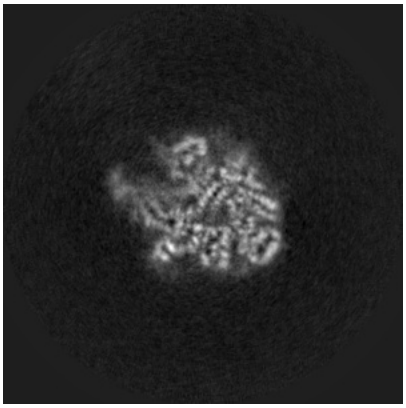


Y Index: 160

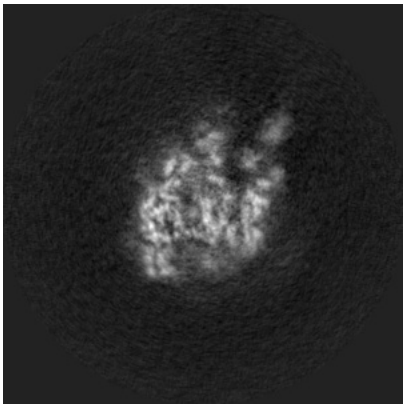


Z Index: 160

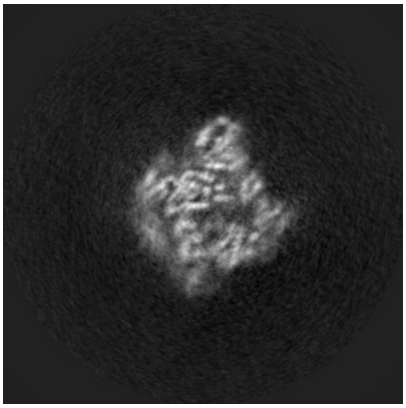
6.2.2 Raw map



X Index: 160



Y Index: 160

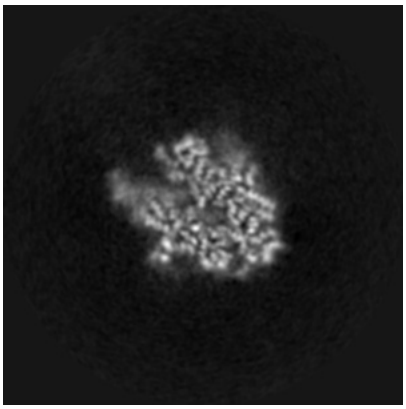


Z Index: 160

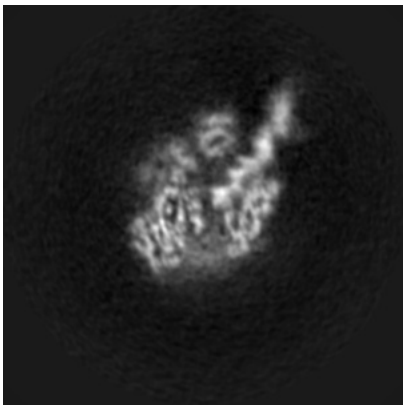
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

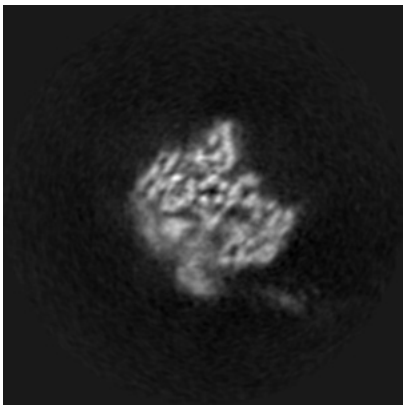
6.3.1 Primary map



X Index: 157

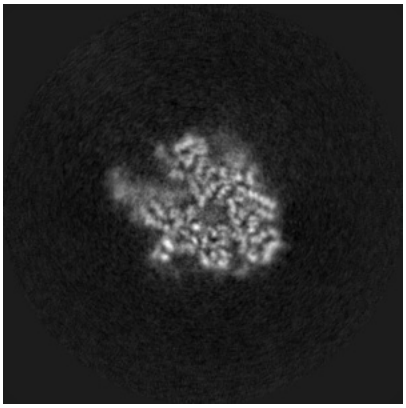


Y Index: 150

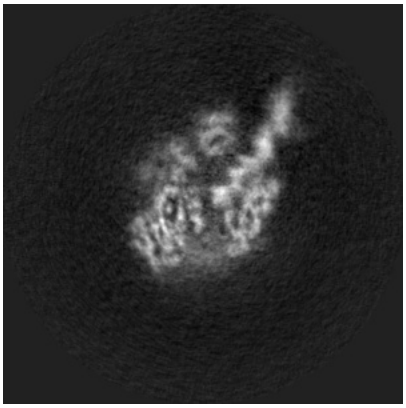


Z Index: 168

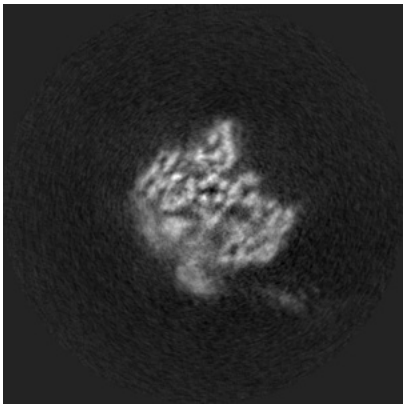
6.3.2 Raw map



X Index: 158



Y Index: 150

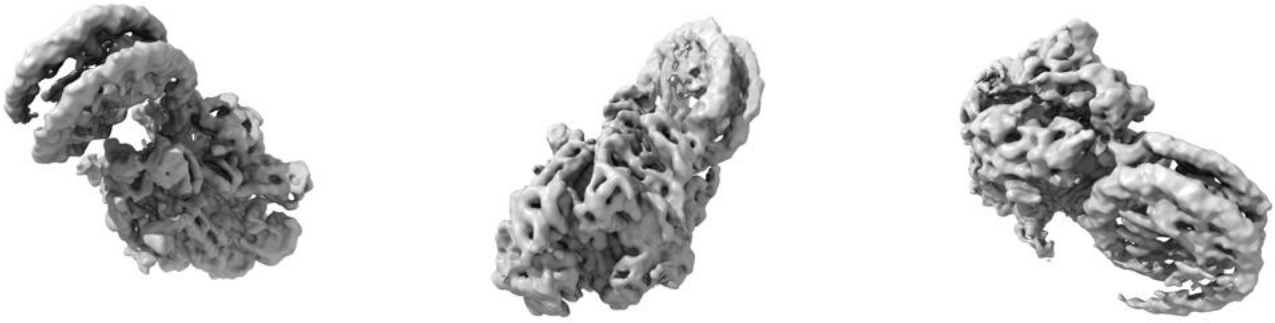


Z Index: 168

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 0.0173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

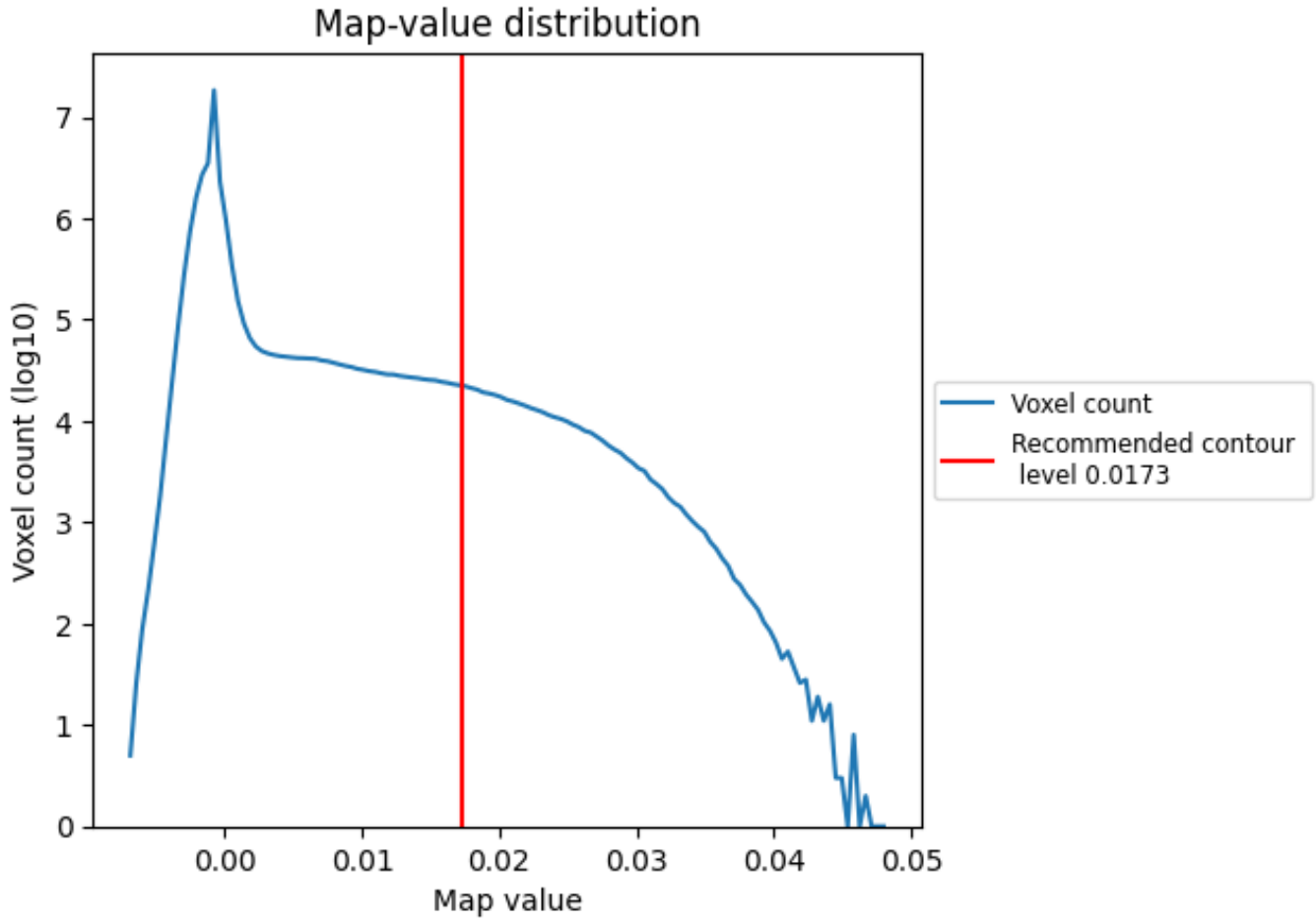
6.5 Mask visualisation (i)

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

7 Map analysis

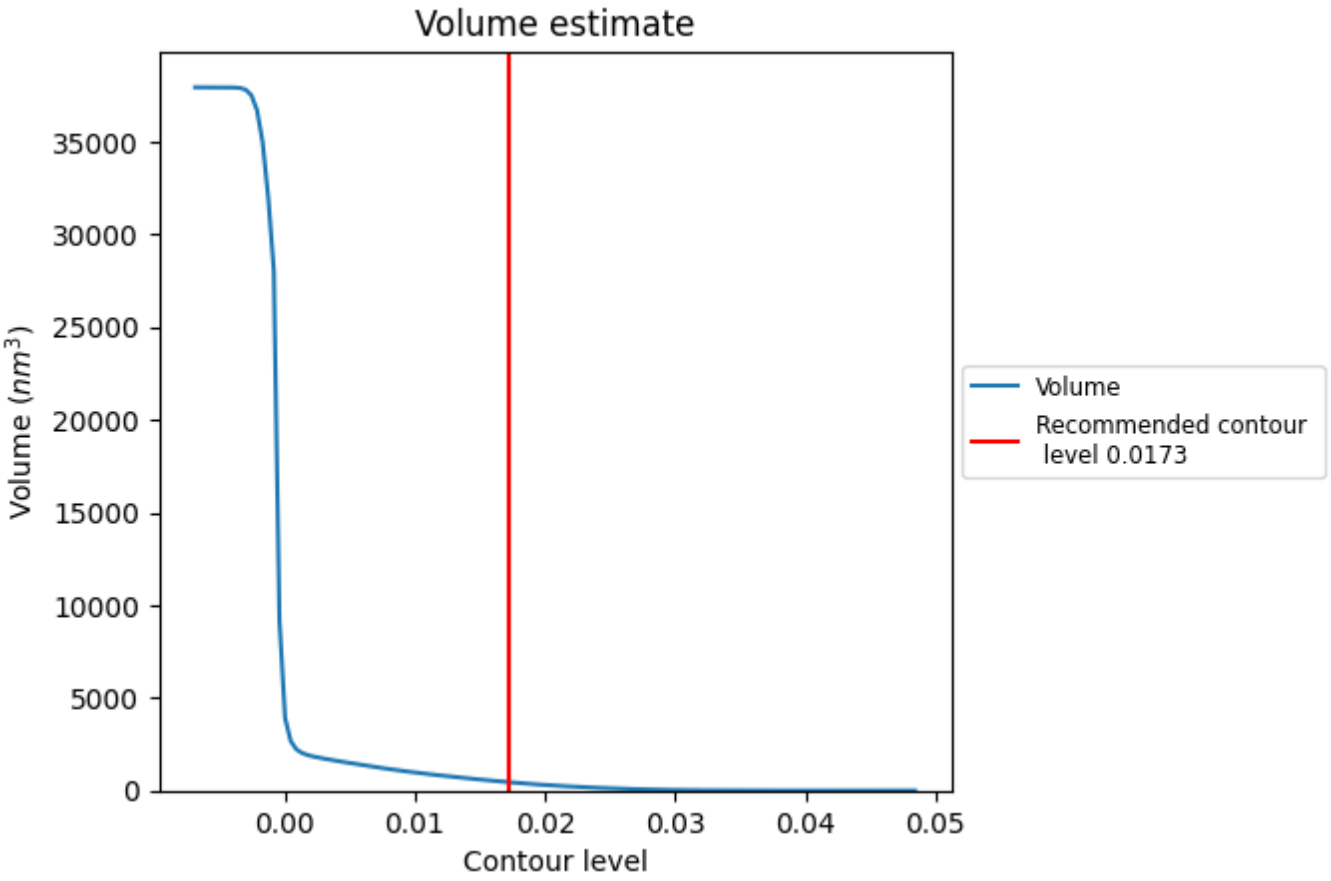
This section contains the results of statistical analysis of the map.

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.

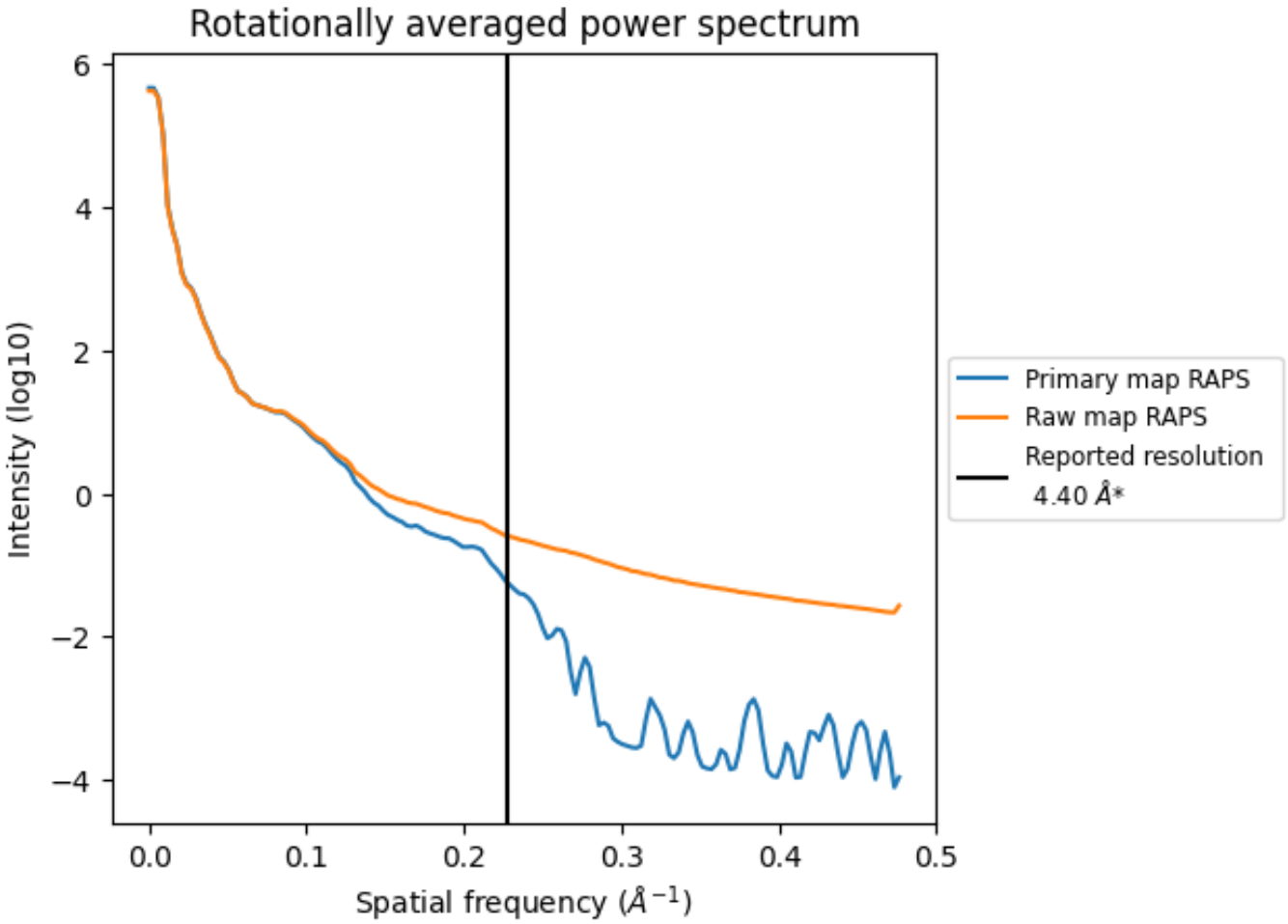
7.2 Volume estimate



The volume at the recommended contour level is 448 nm^3; this corresponds to an approximate mass of 404 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)

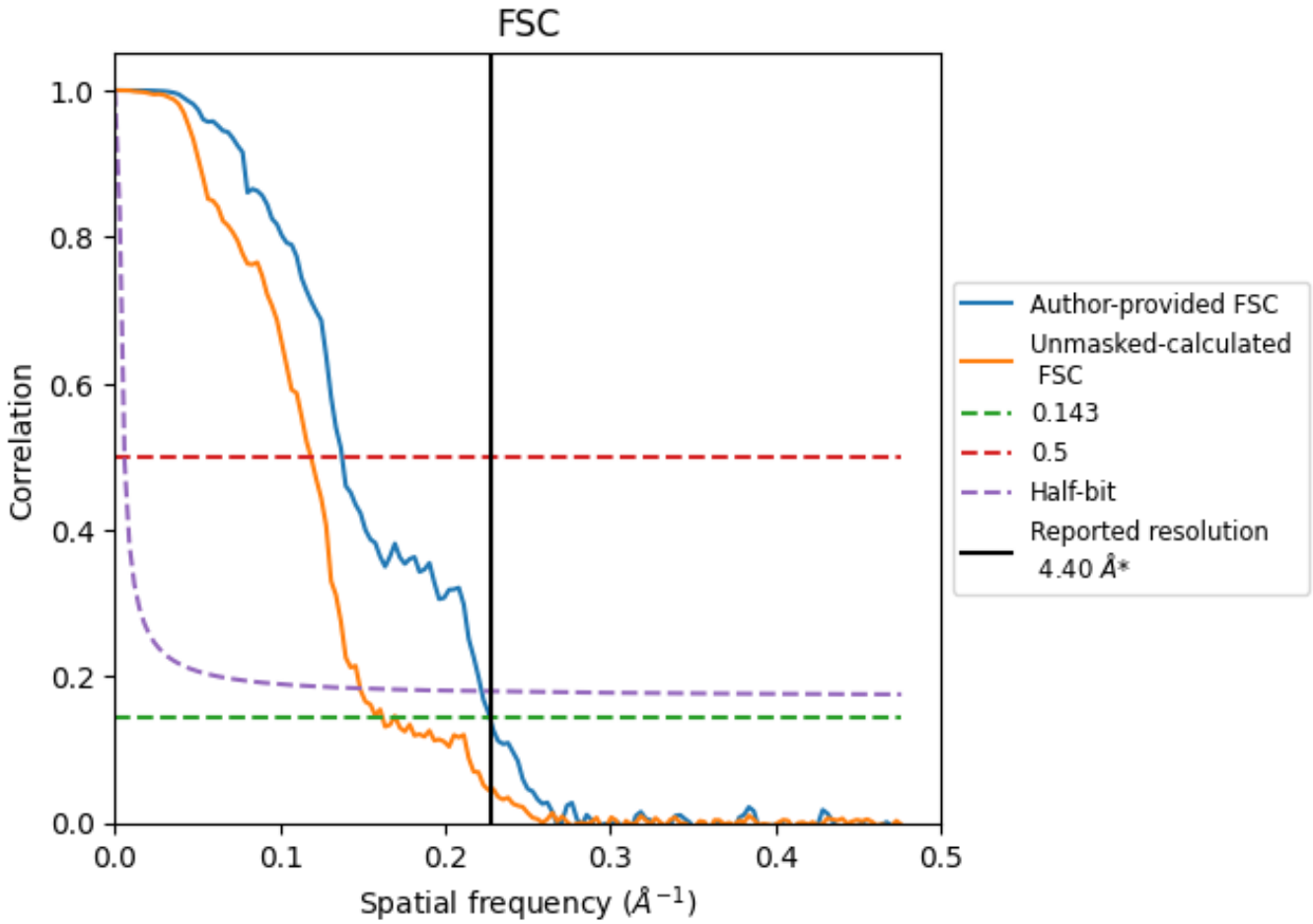


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

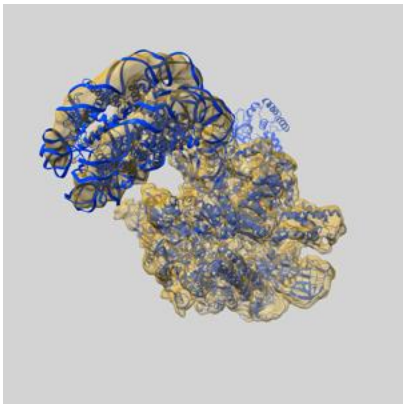
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	7.27	4.50
Unmasked-calculated*	6.17	8.42	6.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.17 differs from the reported value 4.4 by more than 10 %

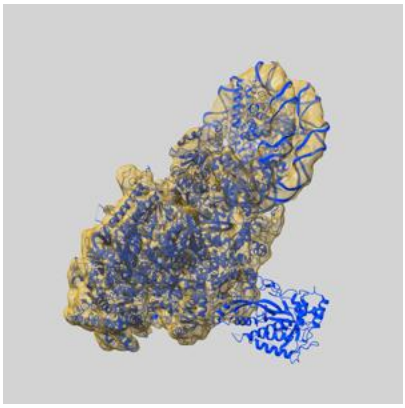
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4429 and PDB model 6I84. Per-residue inclusion information can be found in section 3 on page 9.

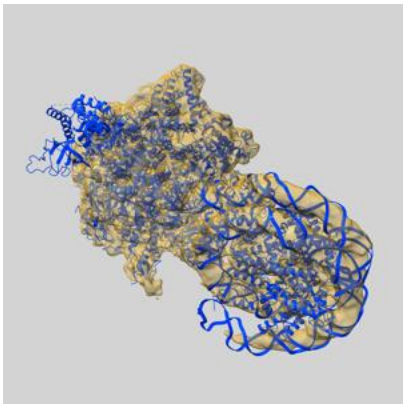
9.1 Map-model overlay



X



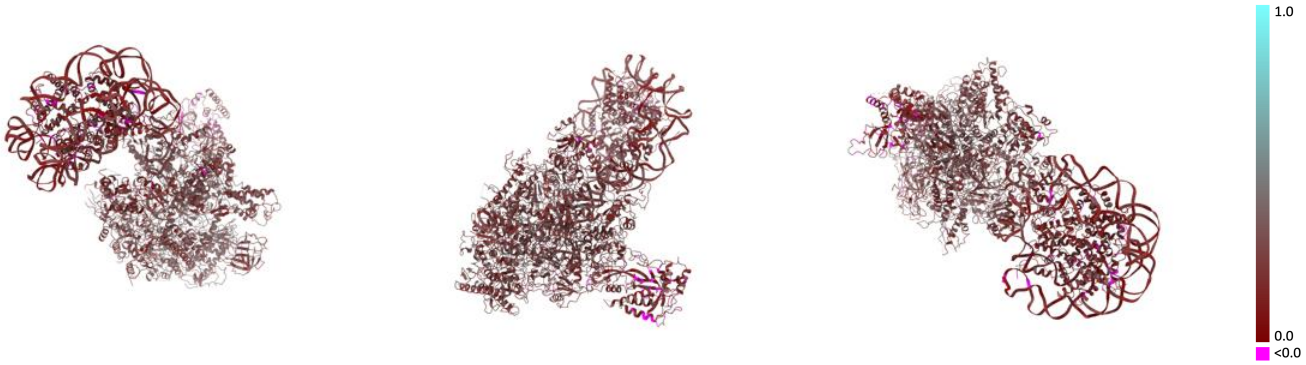
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0173 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.

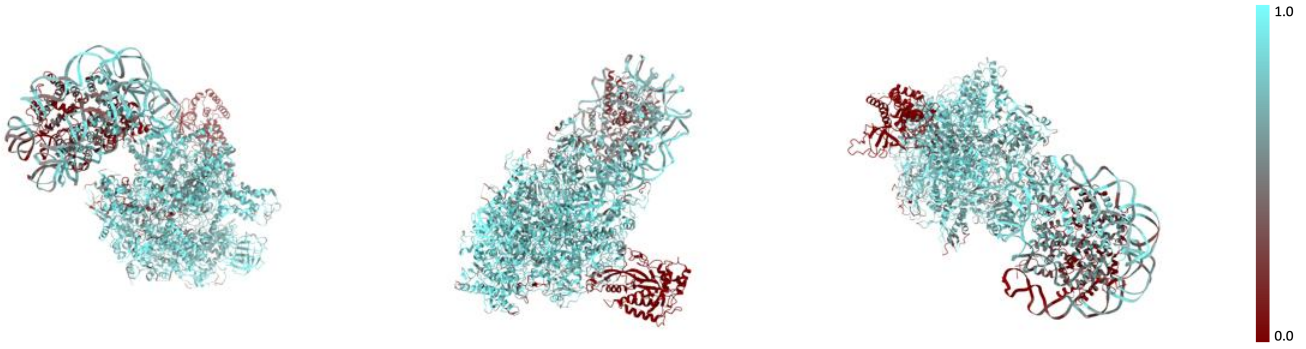
9.2 Q-score mapped to coordinate model



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.

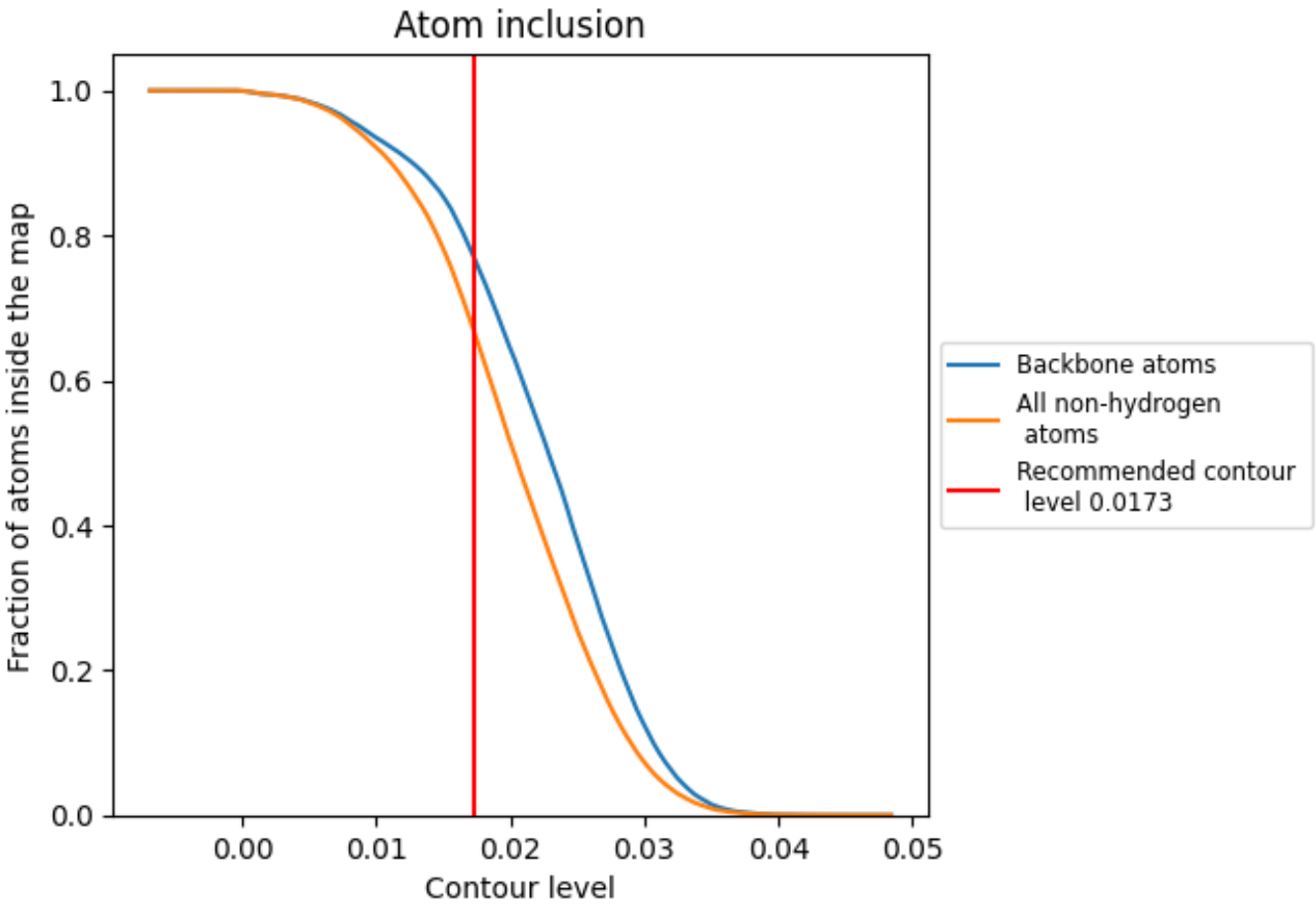
9.3 Atom inclusion mapped to coordinate model



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 (0.0173).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.0173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6682	0.2410
A	0.8031	0.2710
B	0.7686	0.2690
C	0.8414	0.2950
D	0.0057	0.1900
E	0.7718	0.2680
F	0.8151	0.2830
G	0.0416	0.1780
H	0.8454	0.2530
I	0.6533	0.2220
J	0.8665	0.2670
K	0.7506	0.2530
L	0.6980	0.2560
M	0.5577	0.1910
N	0.6709	0.1880
O	0.5110	0.1870
P	0.9524	0.2780
Q	0.2065	0.1930
R	0.2541	0.1780
S	0.4130	0.1880
T	0.6748	0.1950
U	0.4084	0.1790
V	0.3023	0.1940
W	0.4076	0.1880