wwPDB EM Validation Summary Report

Nov 14, 2022 – 02:42 PM JST

PDB ID	:	6J4Z
EMDB ID	:	EMD-0674
Title	:	RNA polymerase II elongation complex bound with Spt4/5 and foreign DNA, stalled at SHL(-1) of the nucleosome
Authors	:	Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on	:	2019-01-10
Resolution	:	4.10 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:

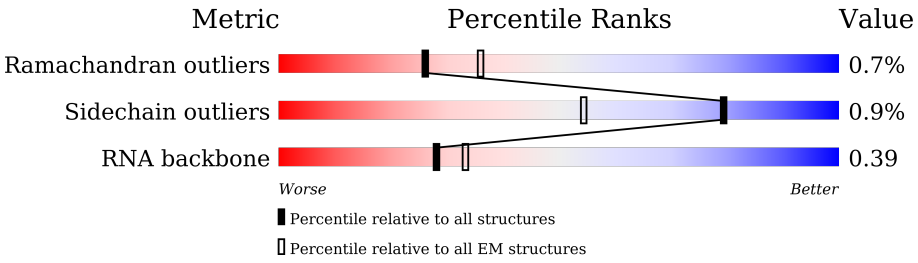
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.10 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)
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	A	1743	8% 80% 19%
2	B	1227	7% 92% 6%
3	C	304	85% 13%
4	D	186	78% 87% 10%
5	E	214	5% 98%
6	F	155	54% 46%
7	G	171	58% 99%
8	H	145	90% 8%

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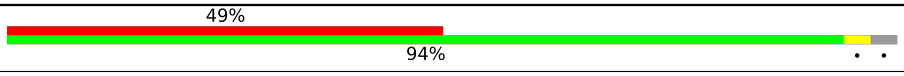
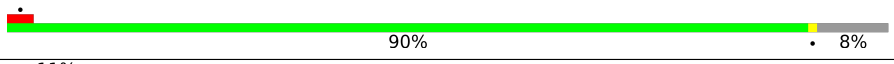
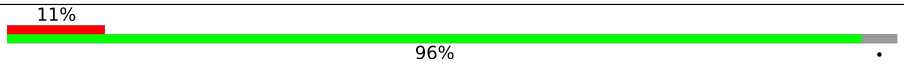
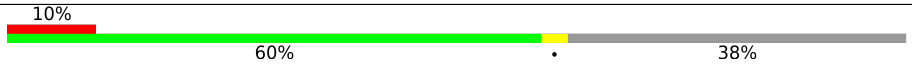
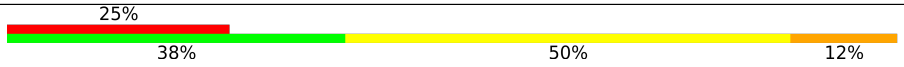
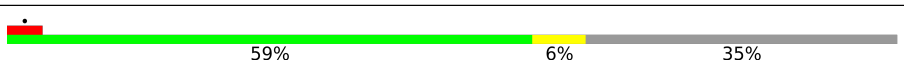
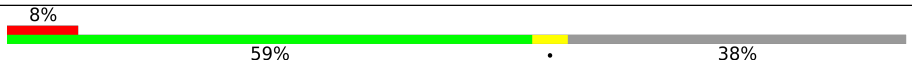
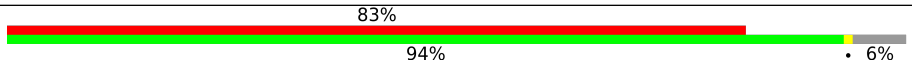
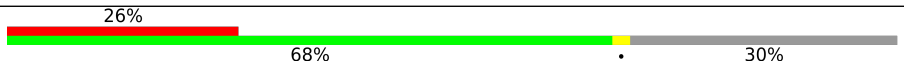
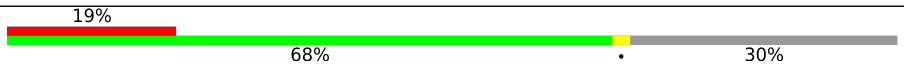
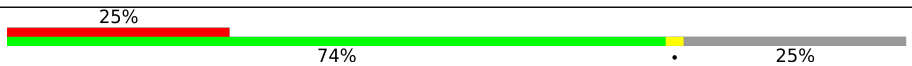
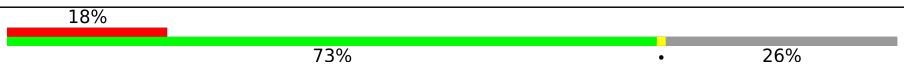
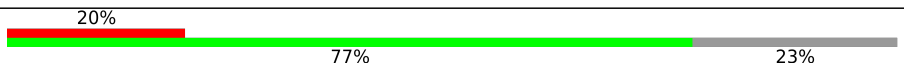
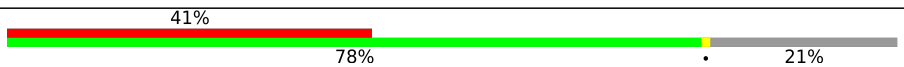
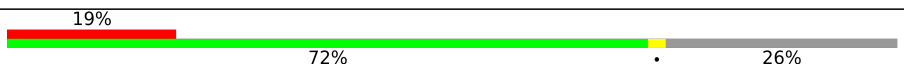
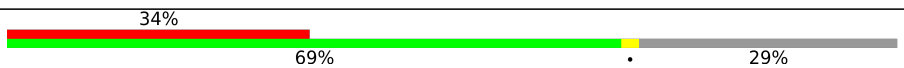
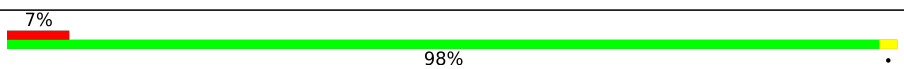
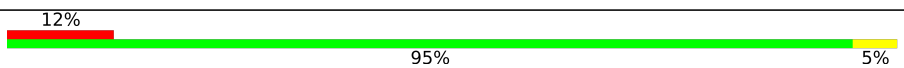
Mol	Chain	Length	Quality of chain
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	16	
14	T	198	
15	N	198	
16	V	108	
17	W	911	
18	a	139	
18	e	139	
19	b	106	
19	f	106	
20	c	133	
20	g	133	
21	d	129	
21	h	129	
22	0	42	
23	1	42	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 47463 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1414	11139	7025	1941	2103	70	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1157	9228	5816	1630	1724	58	0	0

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	263	2098	1319	354	413	12	0	0

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	168	1314	812	237	263	2	0	0

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1740	1094	312	324	10	0	0

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a RNA chain called RNA (5'-R(P*GP*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			341	151	56	118	16		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	128	Total	C	N	O	P	0	0
			2610	1237	491	755	127		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	123	Total	C	N	O	P	0	0
			2527	1198	458	748	123		

- Molecule 16 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	expression tag	UNP C4R0E6

- Molecule 17 is a protein called Spt5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	275	Total	C	N	O	S	0	0
			2226	1425	397	403	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 18 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
18	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 19 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
19	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 20 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	c	103	Total	C	N	O	0	0
			796	502	155	139		
20	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 21 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
21	h	91	Total	C	N	O	S	0	0
			708	447	125	134	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 22 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	42	Total	C	N	O	P	0	0
			868	409	182	235	42		

- Molecule 23 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	42	Total	C	N	O	P	0	0
			854	410	133	269	42		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total Zn 1 1	0
24	C	1	Total Zn 1 1	0
24	I	2	Total Zn 2 2	0
24	J	1	Total Zn 1 1	0
24	L	1	Total Zn 1 1	0
24	V	1	Total Zn 1 1	0

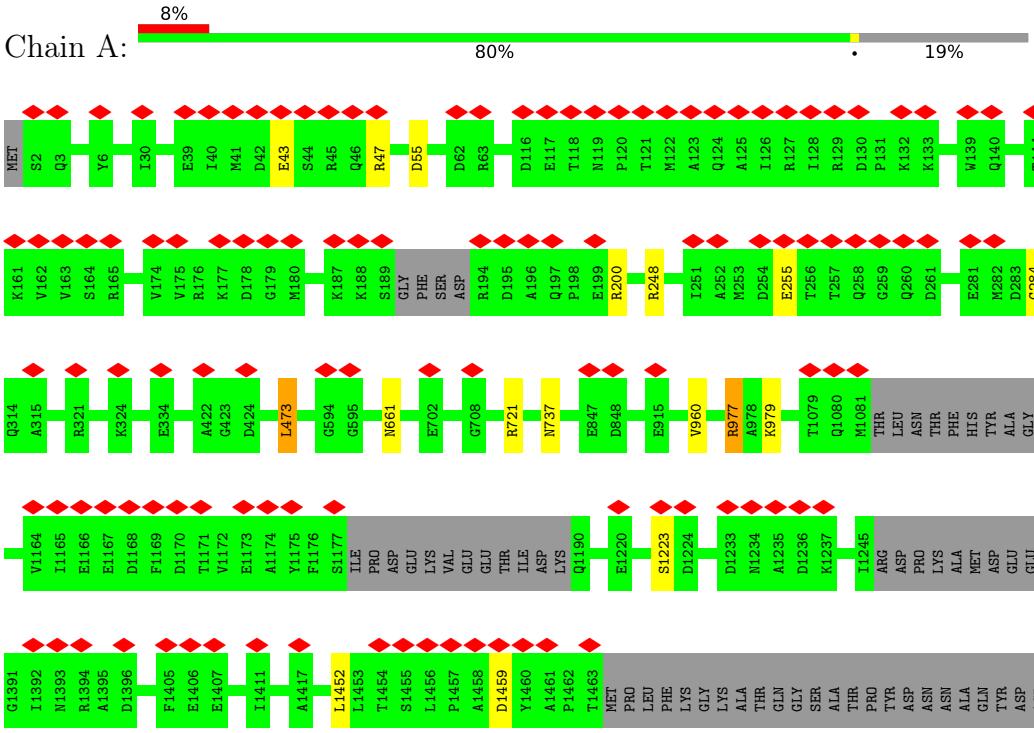
- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots (i)

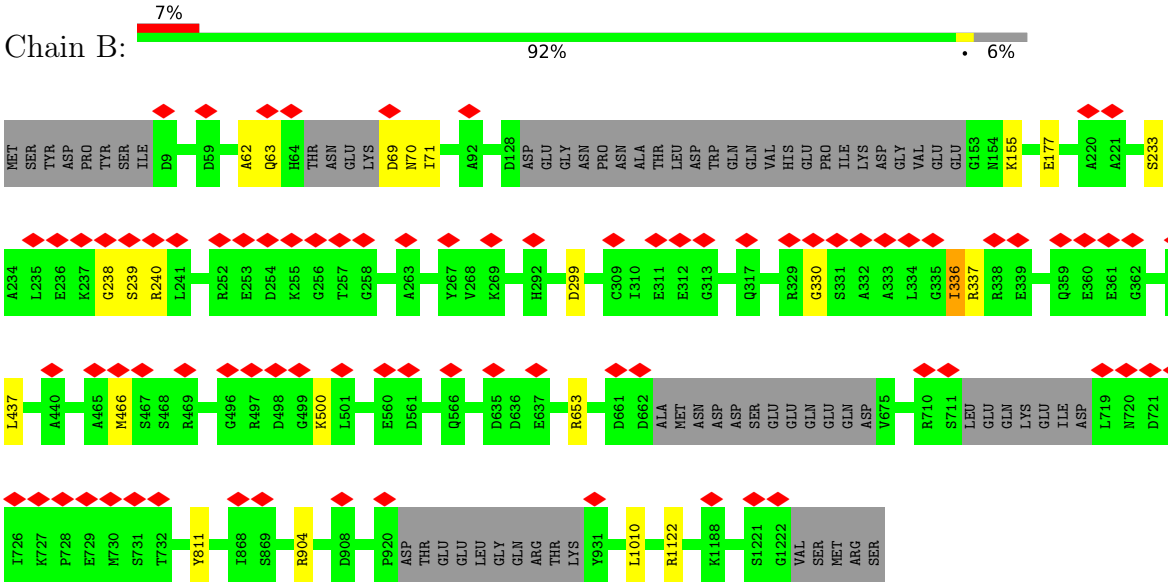
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase subunit



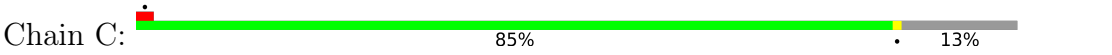
• Molecule 2: DNA-directed RNA polymerase subunit beta

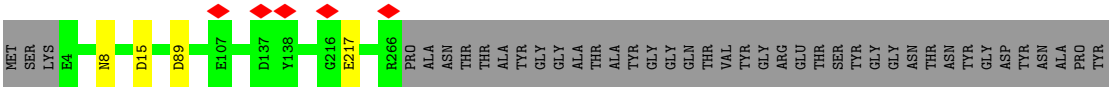
Chain B:



• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

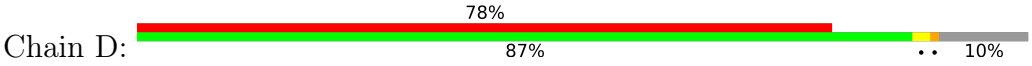
Chain C:

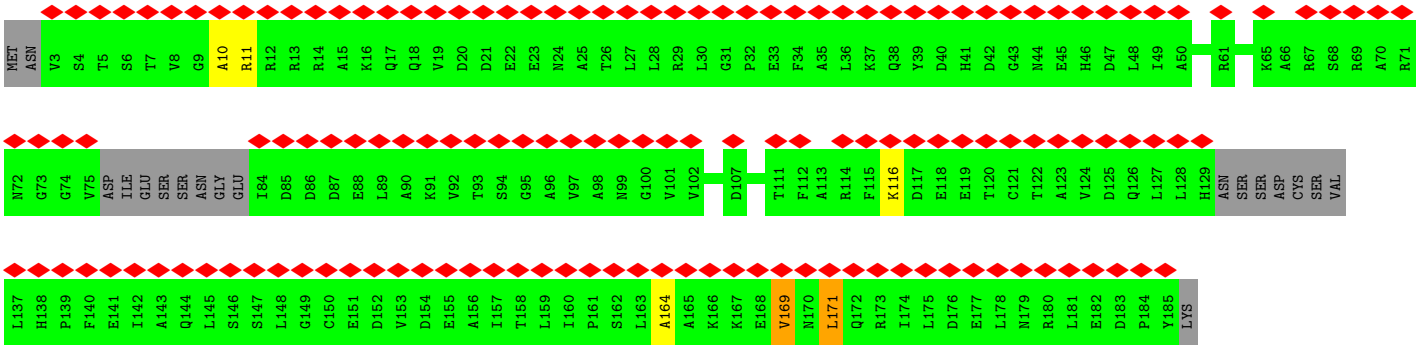




• Molecule 4: RNA polymerase II subunit B32

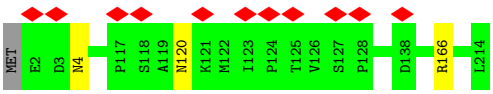
Chain D:





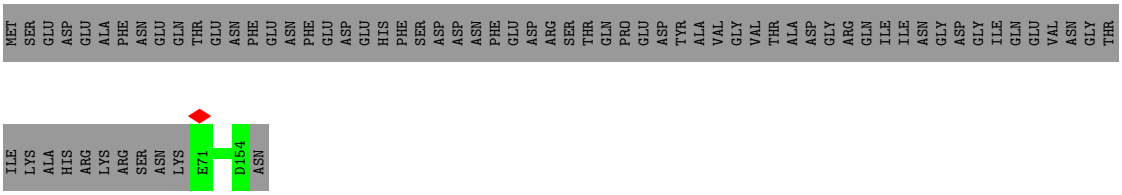
• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

Chain E:



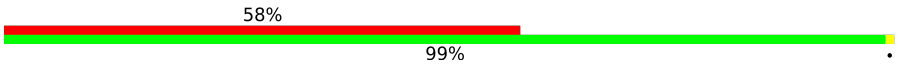
• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

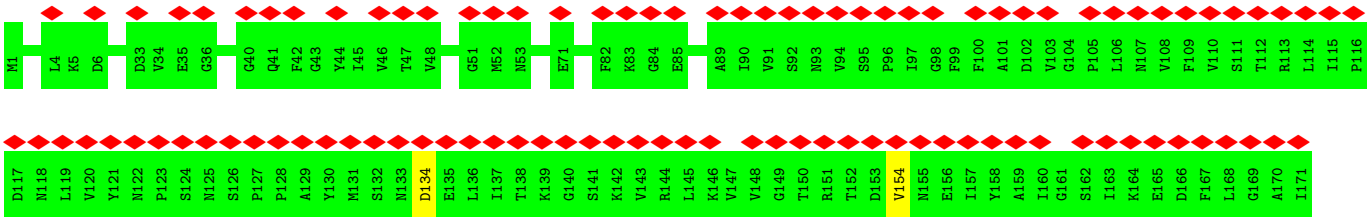
Chain F:



• Molecule 7: RNA polymerase II subunit

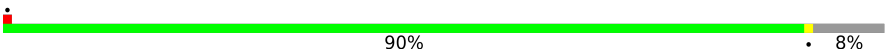
Chain G:

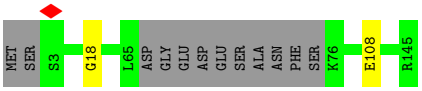




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

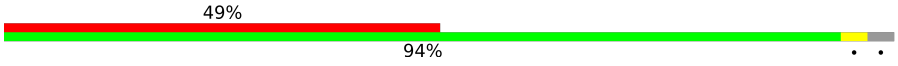
Chain H:

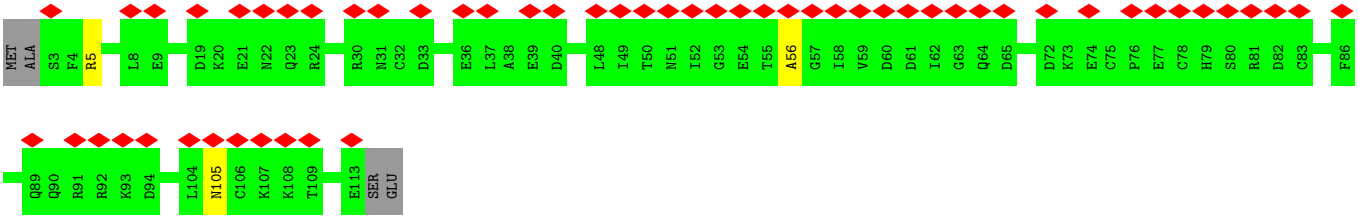




• Molecule 9: DNA-directed RNA polymerase subunit

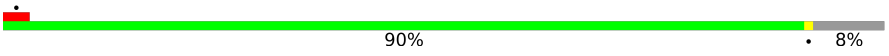
Chain I:

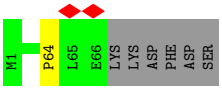




• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

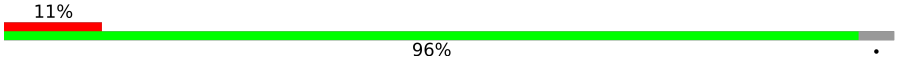
Chain J:

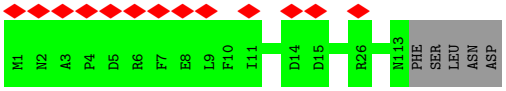




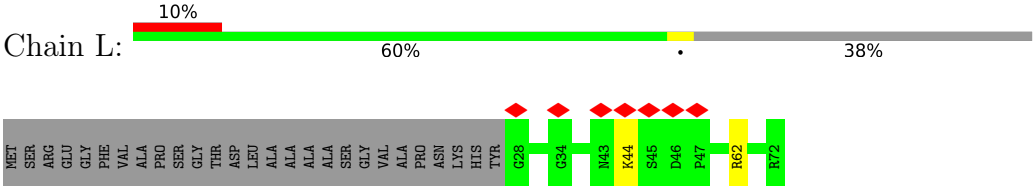
• Molecule 11: RNA polymerase II subunit B12.5

Chain K:



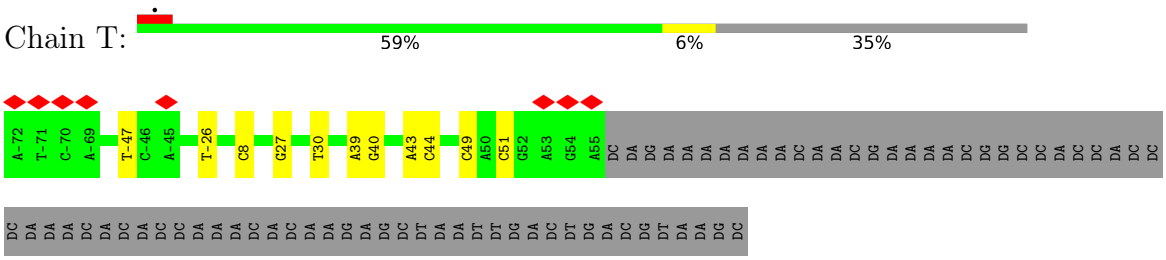


• Molecule 12: RNA polymerase subunit ABC10-alpha



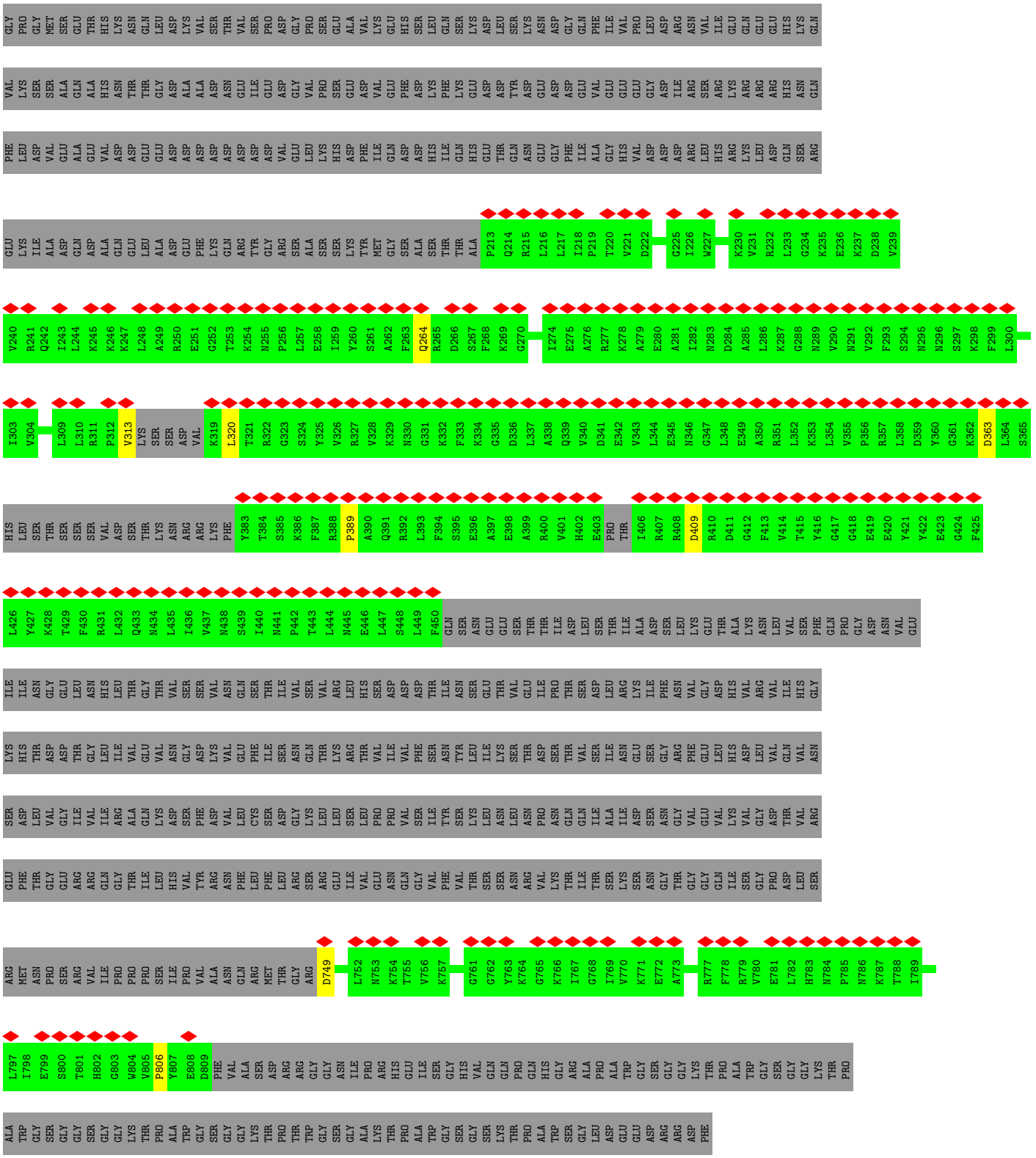
• Molecule 13: RNA (5'-R(P*GP*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP* U)-3')

• Molecule 14: DNA (198-MER)


Chain T:
59%
6%
35%
A-72 T-71 C-70 A-69 T-47 C-46 A-45 T-26 C8 G27 T30 A39 G40 A43 C44 C49 A50 C51 G52 A53 G54 A55
DC DA DG DA DA DA DA DA DA DC DA DA DC DG DA DA DA DC DG DG DC DC DA DC DC DA DC DC DA DC DC DA DA DA DA DC DT DA DA DA DC DT DA DA DA DA DA DA

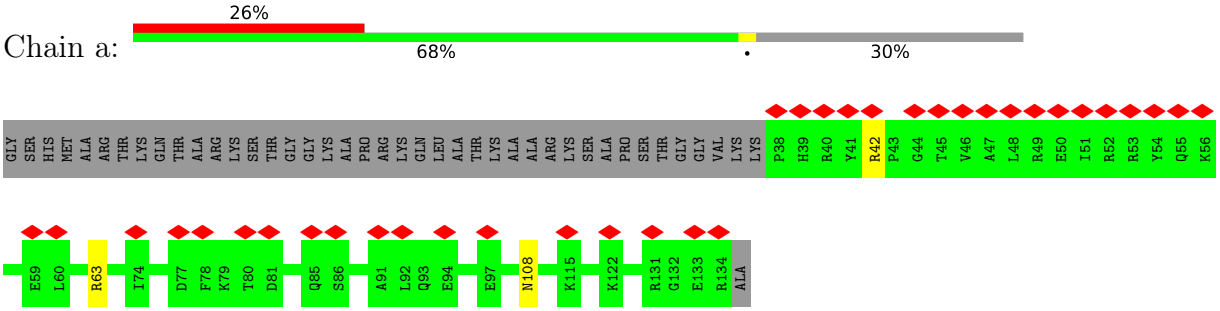
• Molecule 17: Spt5

Chain W:



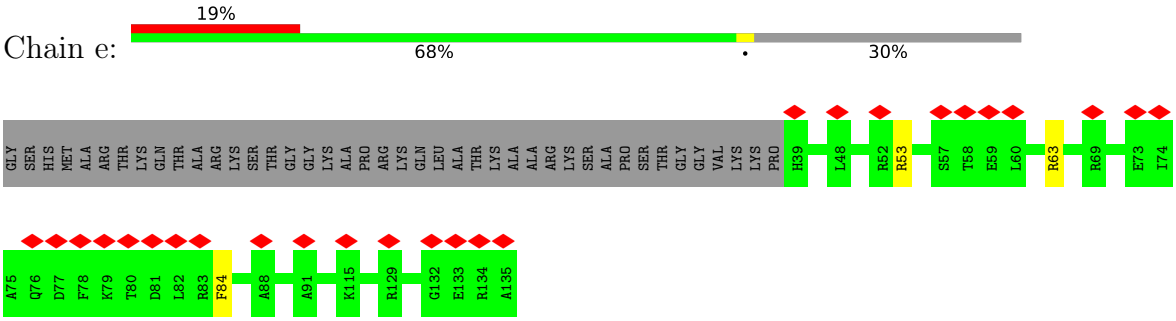
• Molecule 18: Histone H3.3

Chain a:



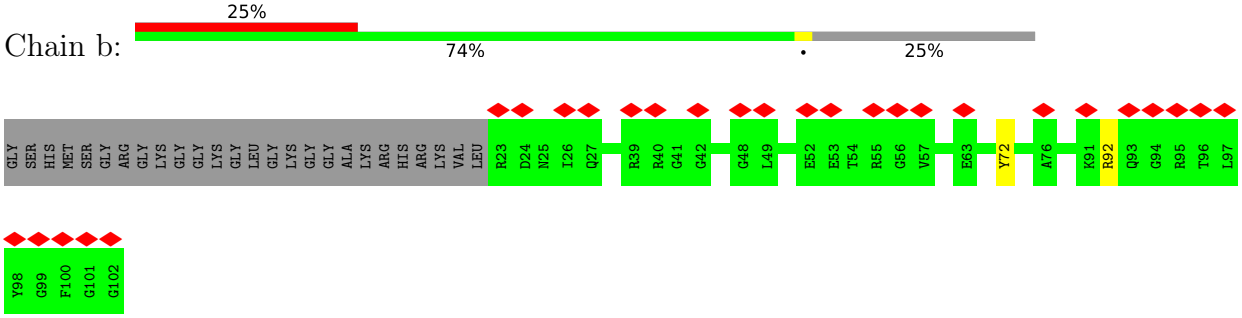
• Molecule 18: Histone H3.3

Chain e:



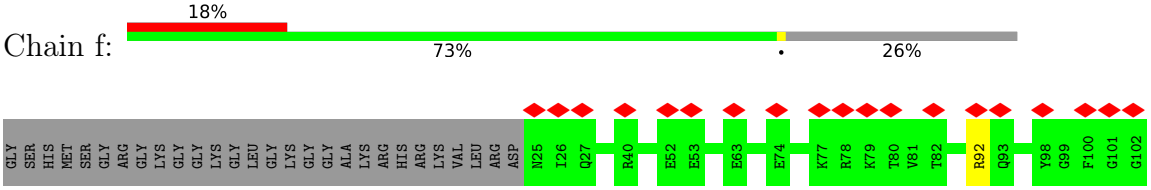
• Molecule 19: Histone H4

Chain b:



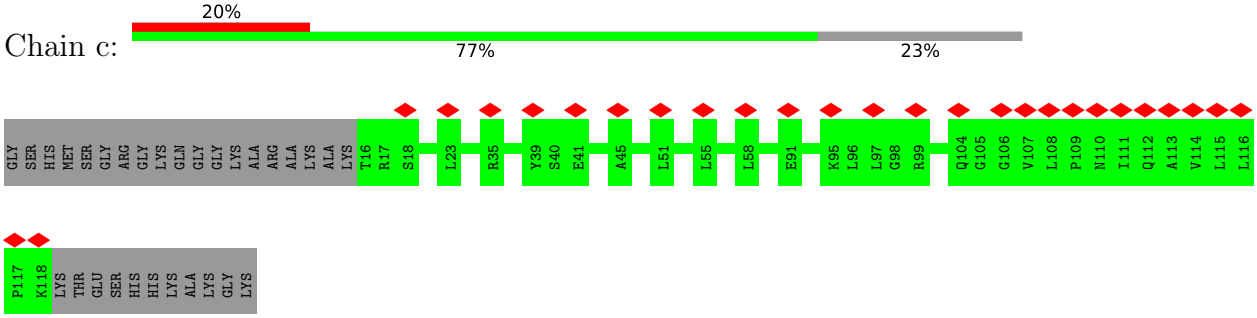
• Molecule 19: Histone H4

Chain f:

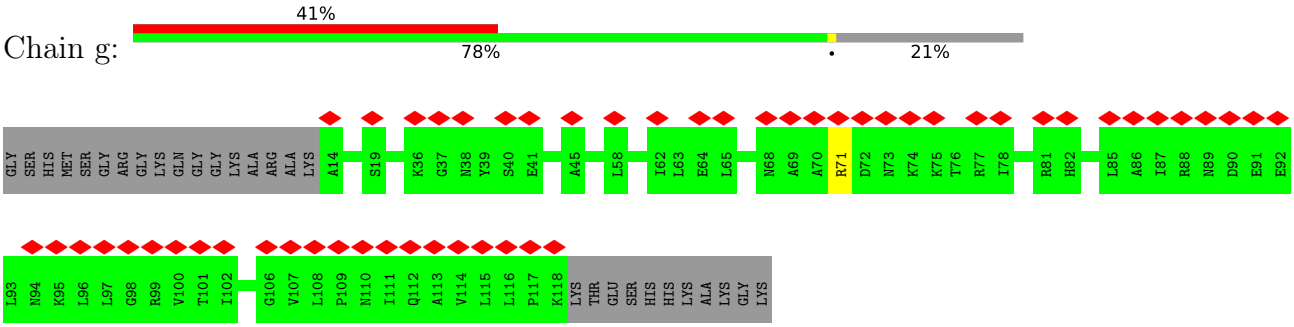


• Molecule 20: Histone H2A type 1-B/E

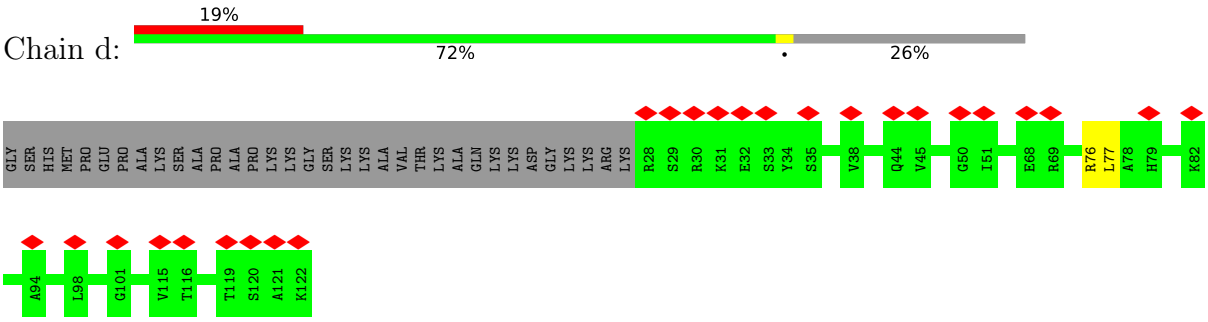
Chain c:



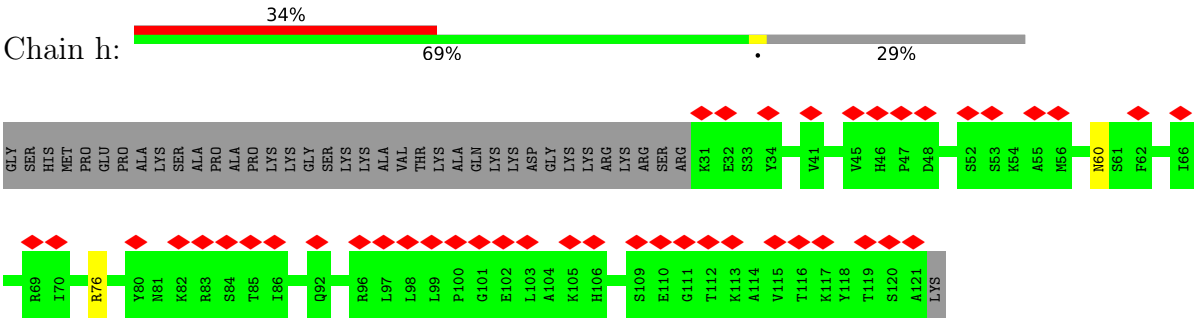
• Molecule 20: Histone H2A type 1-B/E



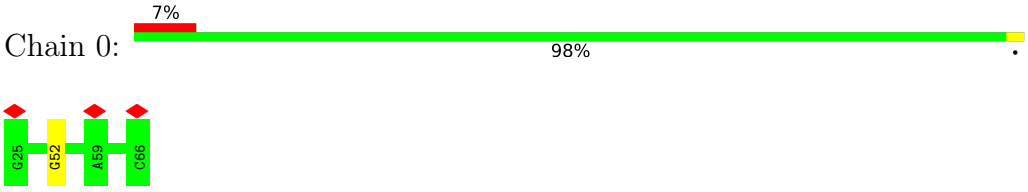
• Molecule 21: Histone H2B type 1-J



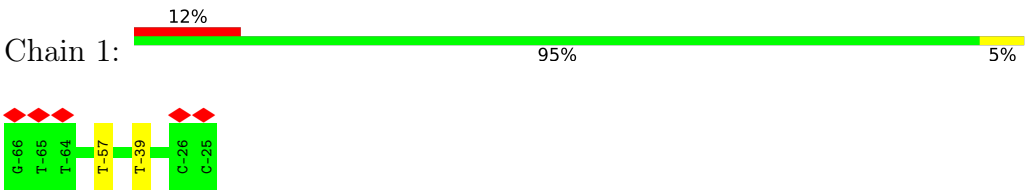
• Molecule 21: Histone H2B type 1-J



• Molecule 22: DNA (42-MER)



• Molecule 23: DNA (42-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50.0	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	0.067	Depositor
Minimum map value	-0.022	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	A	0.44	0/11345	0.67	6/15331 (0.0%)
2	B	0.48	0/9407	0.71	6/12685 (0.0%)
3	C	0.46	0/2139	0.72	1/2895 (0.0%)
4	D	0.32	0/1326	0.68	1/1788 (0.1%)
5	E	0.42	0/1772	0.64	0/2385
6	F	0.45	0/687	0.64	0/931
7	G	0.35	0/1353	0.72	0/1837
8	H	0.42	0/1069	0.67	0/1444
9	I	0.35	0/934	0.80	2/1257 (0.2%)
10	J	0.57	0/554	0.75	0/742
11	K	0.44	0/953	0.65	0/1291
12	L	0.45	0/365	0.76	0/484
13	P	1.18	6/379 (1.6%)	1.27	2/589 (0.3%)
14	T	1.08	8/2929 (0.3%)	1.07	3/4514 (0.1%)
15	N	1.12	7/2831 (0.2%)	1.08	0/4368
16	V	0.46	0/808	0.60	0/1097
17	W	0.40	0/2267	0.68	4/3048 (0.1%)
18	a	0.42	0/809	0.62	0/1085
18	e	0.46	0/807	0.57	0/1081
19	b	0.44	0/645	0.64	0/862
19	f	0.42	0/626	0.61	0/837
20	c	0.40	0/806	0.58	0/1089
20	g	0.36	0/820	0.55	0/1107
21	d	0.45	0/757	0.56	0/1015
21	h	0.41	0/719	0.56	0/968
22	0	0.90	0/980	1.03	1/1509 (0.1%)
23	1	0.89	0/950	1.17	2/1465 (0.1%)
All	All	0.59	21/49037 (0.0%)	0.77	28/67704 (0.0%)

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
2	B	0	1
18	a	0	2
18	e	0	1
All	All	0	4

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	-5	G	C1'-N9	-7.33	1.36	1.46
13	P	-1	G	C1'-N9	-7.31	1.36	1.46
13	P	4	C	C1'-N1	7.27	1.59	1.48
13	P	2	G	C1'-N9	-7.20	1.36	1.46
14	T	27	DG	C1'-N9	-6.67	1.38	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	W	389	PRO	CA-N-CD	-8.54	99.55	111.50
1	A	473	LEU	CA-CB-CG	-8.23	96.37	115.30
22	0	52	DG	O4'-C4'-C3'	-7.77	101.33	106.00
2	B	63	GLN	N-CA-CB	-7.68	96.78	110.60
14	T	-26	DT	O4'-C4'-C3'	-6.93	101.73	104.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	ILE	Mainchain
18	a	42	ARG	Peptide
18	a	63	ARG	Peptide
18	e	63	ARG	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A	1402/1743 (80%)	1345 (96%)	47 (3%)	10 (1%)	22	60
2	B	1145/1227 (93%)	1082 (94%)	55 (5%)	8 (1%)	22	60
3	C	261/304 (86%)	253 (97%)	6 (2%)	2 (1%)	19	58
4	D	162/186 (87%)	149 (92%)	9 (6%)	4 (2%)	5	34
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	13	48
8	H	129/145 (89%)	125 (97%)	2 (2%)	2 (2%)	9	43
9	I	109/115 (95%)	102 (94%)	6 (6%)	1 (1%)	17	54
10	J	64/72 (89%)	61 (95%)	2 (3%)	1 (2%)	9	43
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	0	1 (2%)	6	36
16	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
17	W	265/911 (29%)	246 (93%)	17 (6%)	2 (1%)	19	58
18	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
18	e	95/139 (68%)	86 (90%)	9 (10%)	0	100	100
19	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
19	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100
20	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
20	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
21	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
21	h	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	4983/6555 (76%)	4736 (95%)	214 (4%)	33 (1%)	26	60

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	287	GLN
1	A	960	VAL
1	A	1109	VAL
2	B	155	LYS

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	A	1227/1528 (80%)	1220 (99%)	7 (1%)	86	92
2	B	1012/1077 (94%)	1001 (99%)	11 (1%)	73	84
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	94
4	D	143/160 (89%)	140 (98%)	3 (2%)	53	72
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	79
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	105 (99%)	1 (1%)	78	87
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	46	67
16	V	86/92 (94%)	85 (99%)	1 (1%)	71	83
17	W	241/796 (30%)	239 (99%)	2 (1%)	81	88
18	a	83/112 (74%)	82 (99%)	1 (1%)	71	83
18	e	82/112 (73%)	80 (98%)	2 (2%)	49	69
19	b	65/81 (80%)	63 (97%)	2 (3%)	40	63
19	f	63/81 (78%)	62 (98%)	1 (2%)	62	78
20	c	82/102 (80%)	82 (100%)	0	100	100
20	g	83/102 (81%)	82 (99%)	1 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	d	81/107 (76%)	79 (98%)	2 (2%)	47 68
21	h	77/107 (72%)	75 (97%)	2 (3%)	46 67
All	All	4408/5673 (78%)	4367 (99%)	41 (1%)	79 87

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	W	264	GLN
18	e	53	ARG
17	W	313	VAL
19	b	92	ARG
19	f	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	12	ASN
20	g	110	ASN
17	W	264	GLN
21	h	64	ASN
21	d	64	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/16 (93%)	6 (40%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	C
13	P	-3	C
13	P	-1	G
13	P	0	G
13	P	1	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

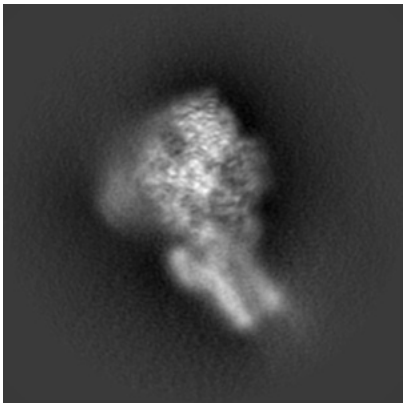
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0674. These allow visual inspection of the internal detail of the map and identification of artifacts.

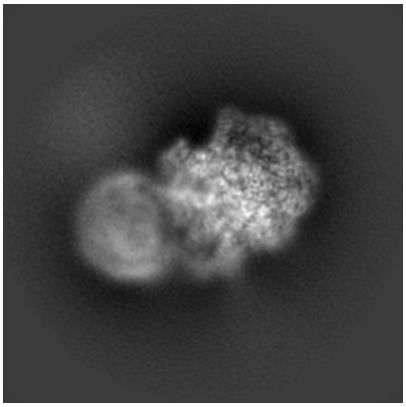
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

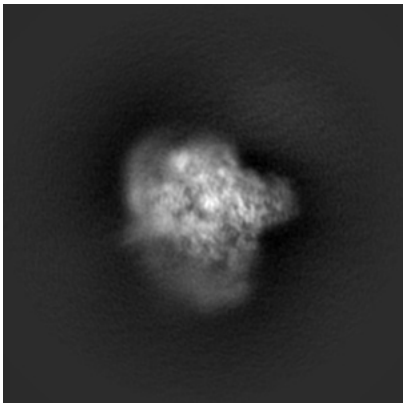
6.1.1 Primary map



X



Y

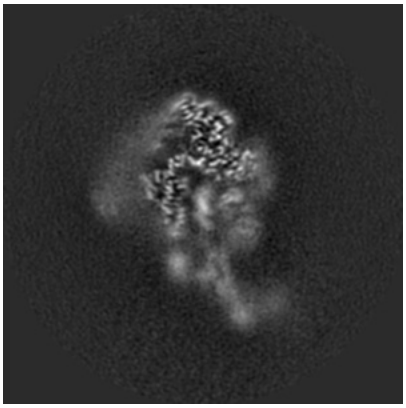


Z

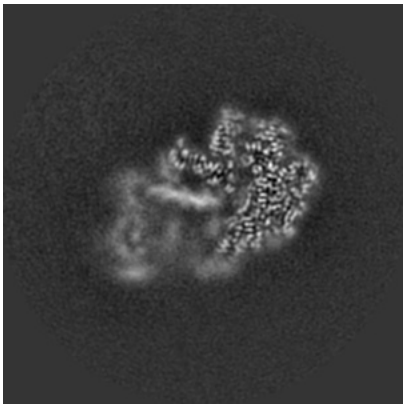
The images above show the map projected in three orthogonal directions.

6.2 Central slices

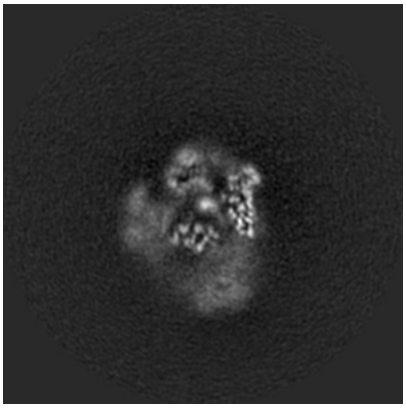
6.2.1 Primary map



X Index: 120



Y Index: 120

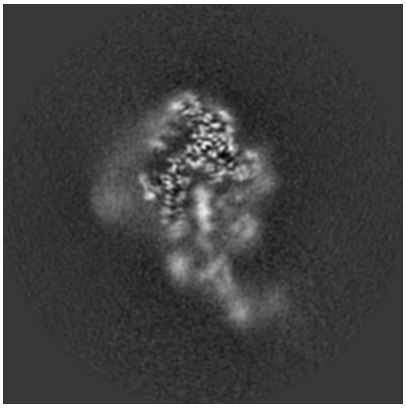


Z Index: 120

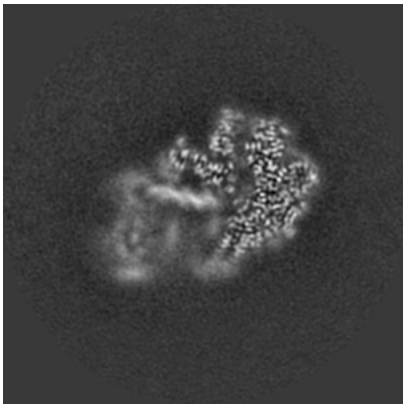
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

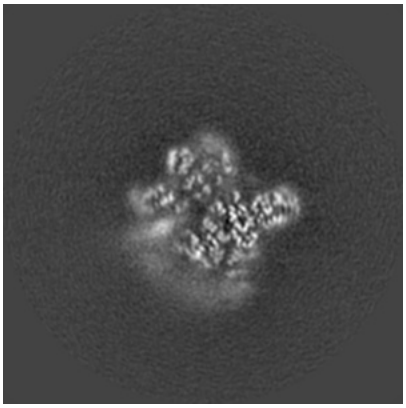
6.3.1 Primary map



X Index: 122



Y Index: 121



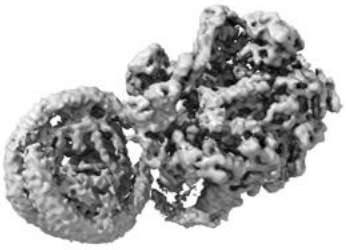
Z Index: 134

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

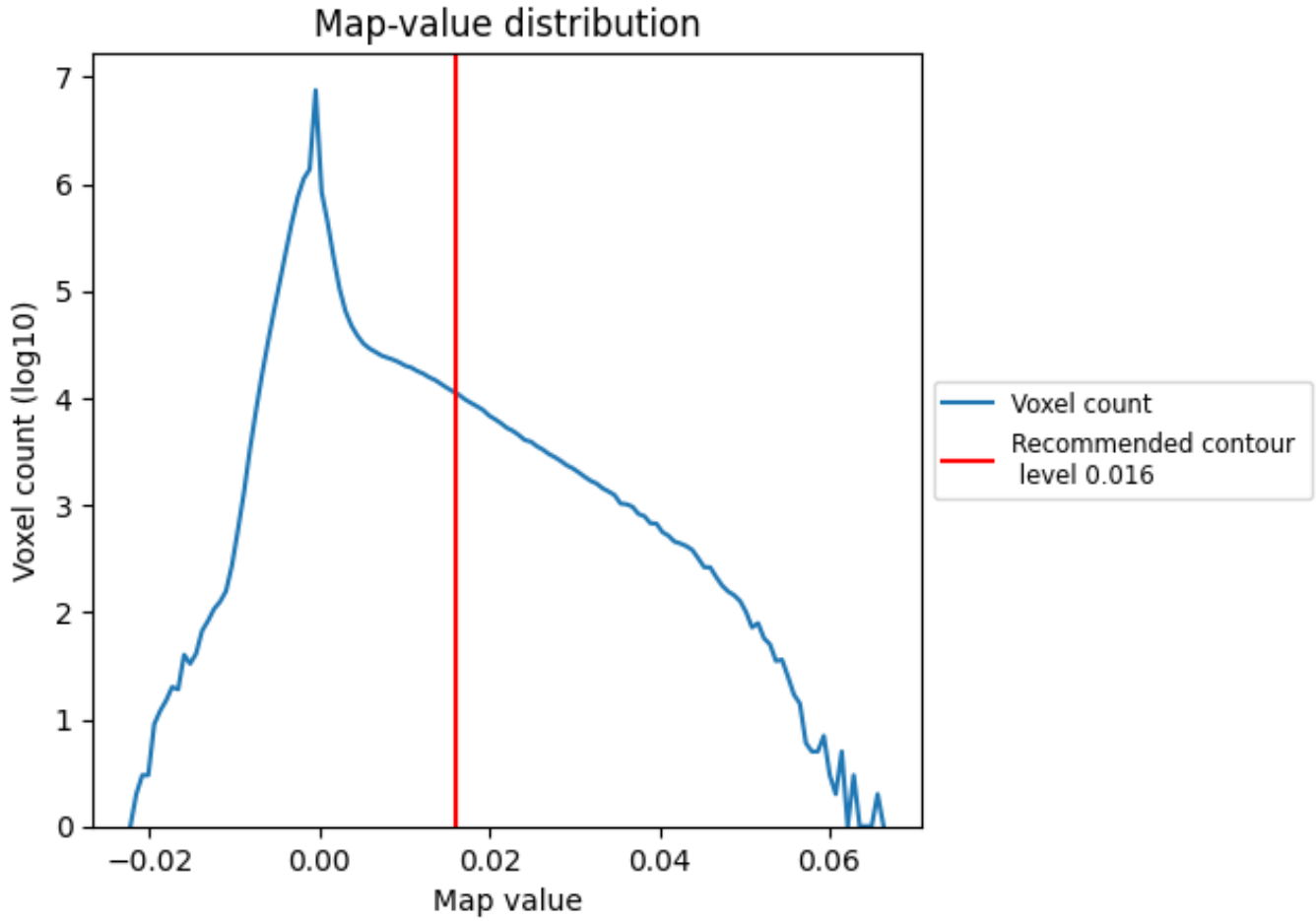
6.5 Mask visualisation (i)

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

7 Map analysis

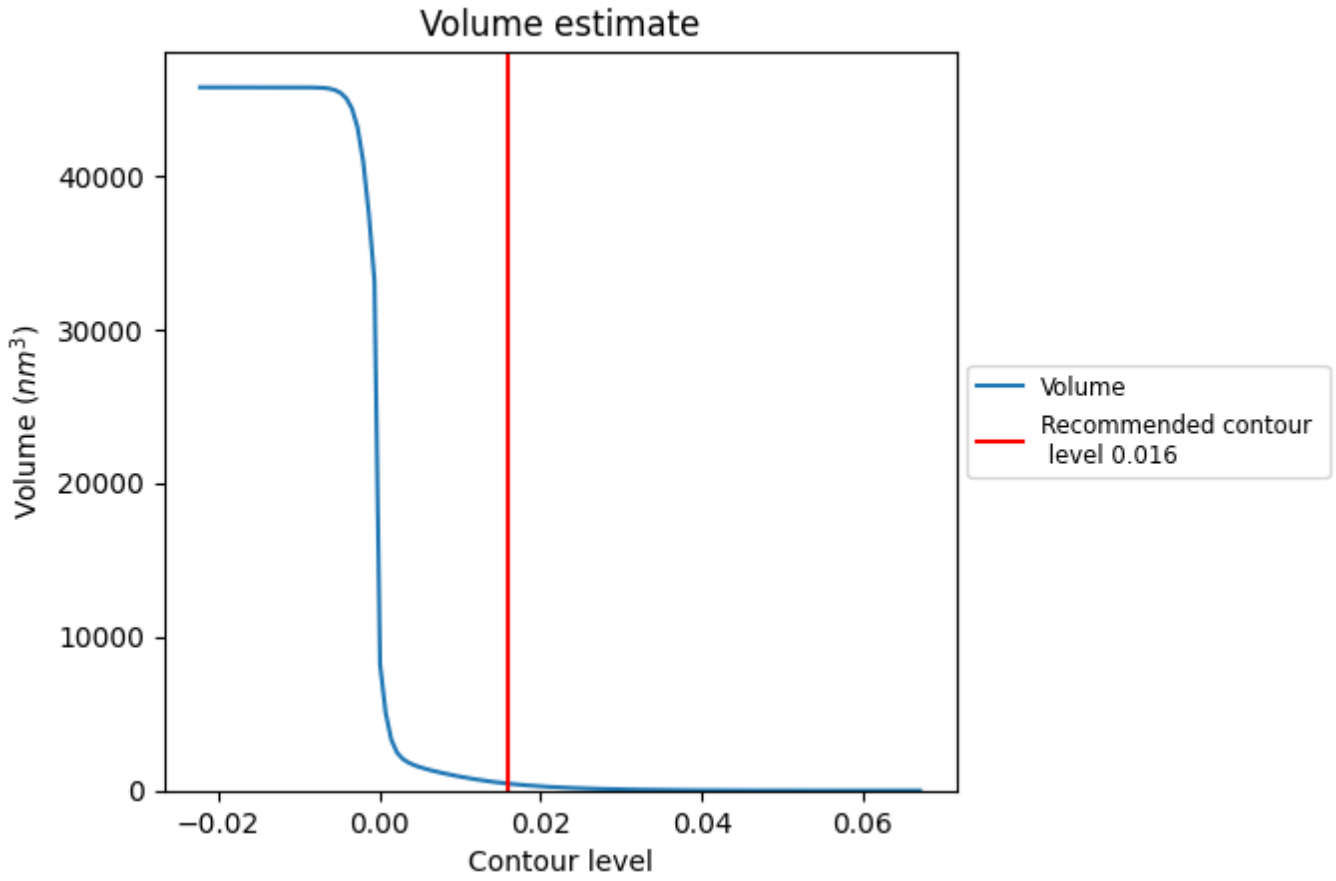
This section contains the results of statistical analysis of the map.

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.

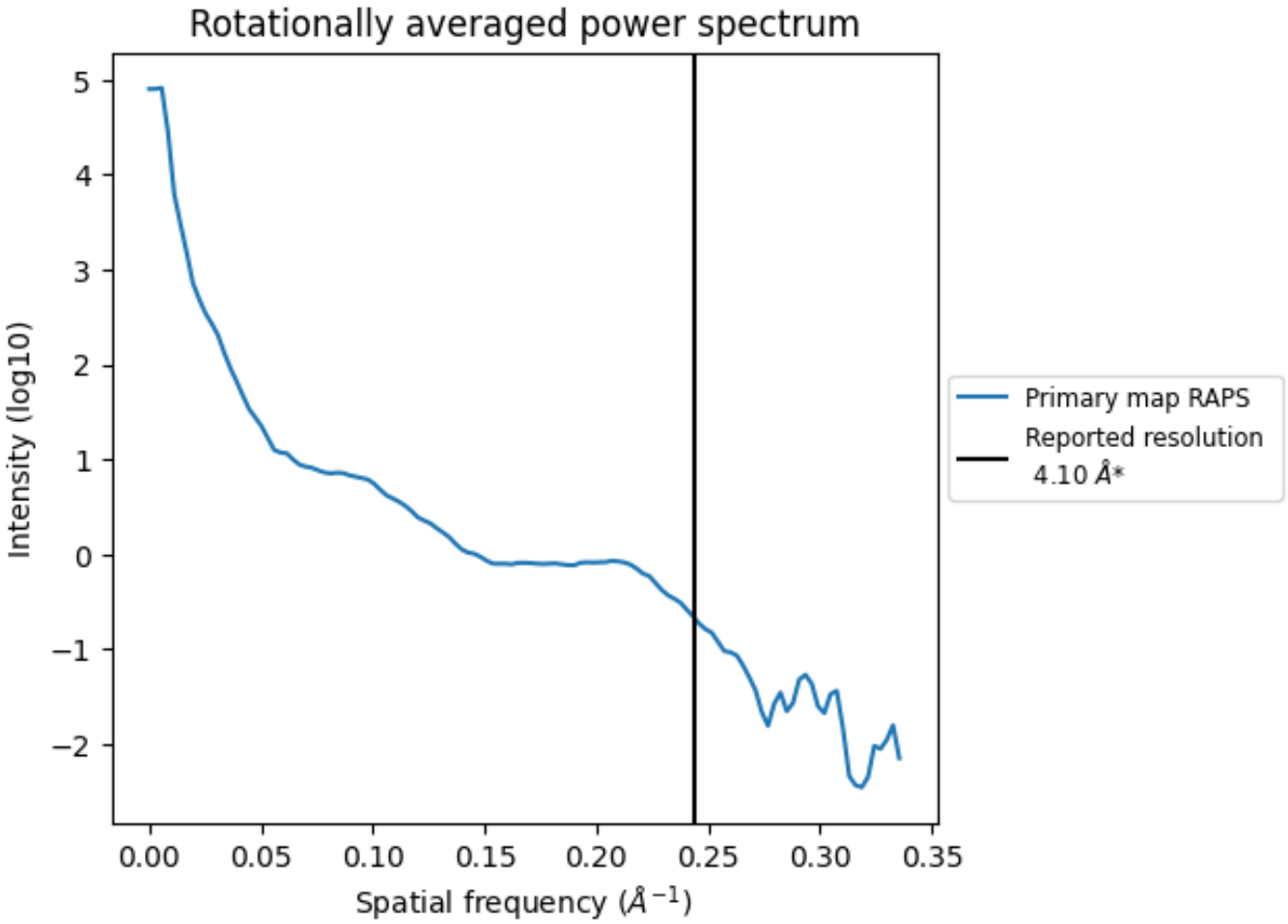
7.2 Volume estimate (i)



The volume at the recommended contour level is 450 nm^3; this corresponds to an approximate mass of 407 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)

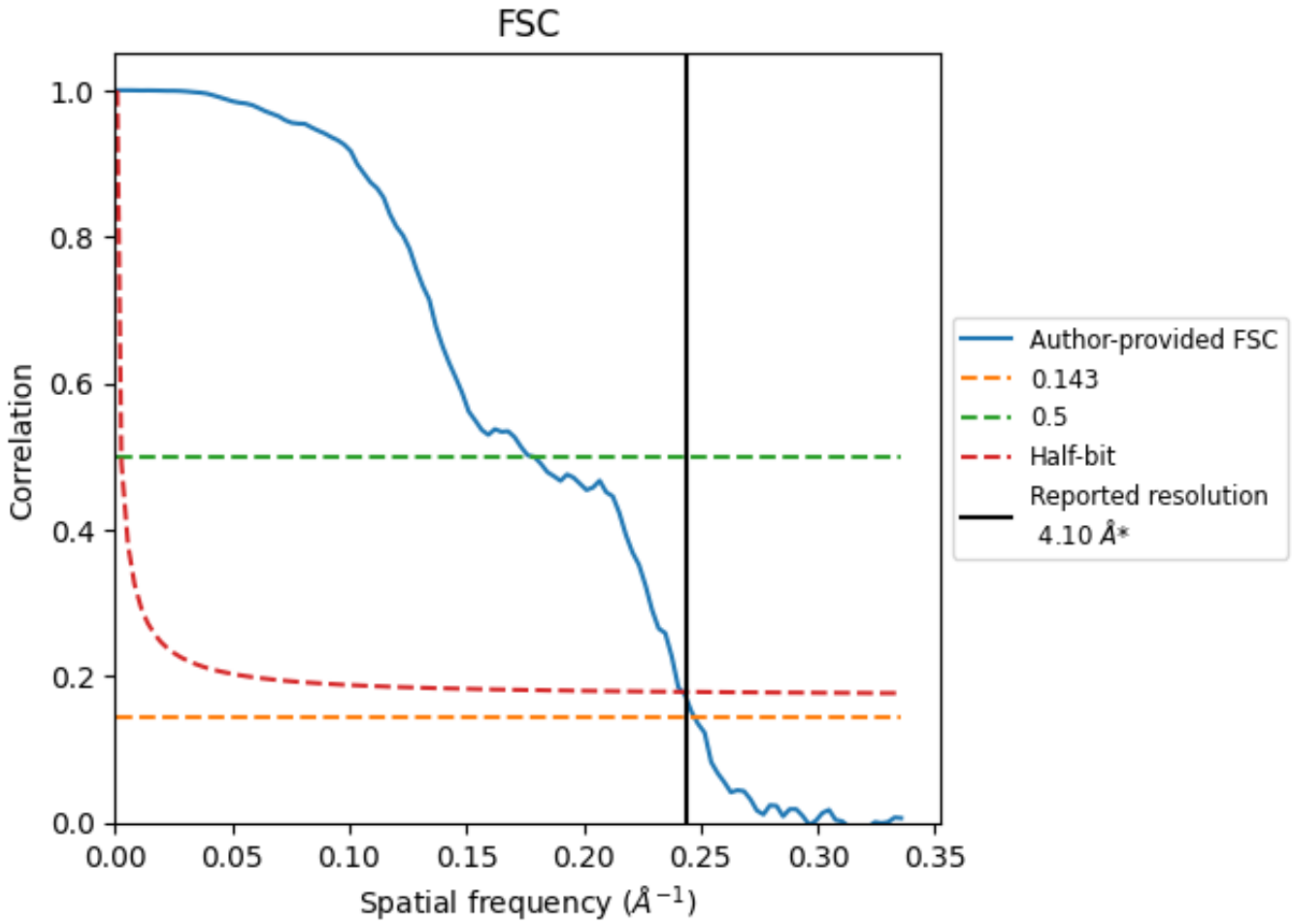


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

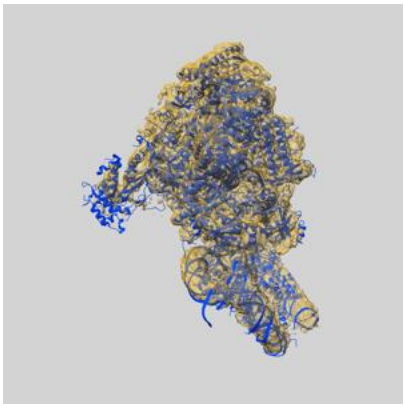
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.04	5.62	4.13
Unmasked-calculated*	-	-	-

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

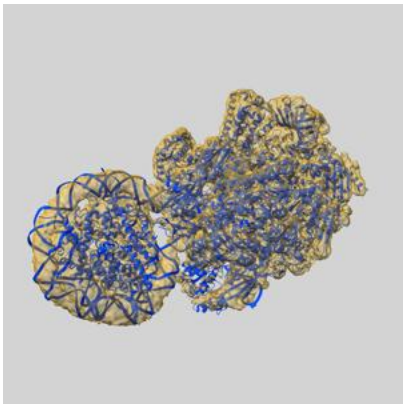
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0674 and PDB model 6J4Z. Per-residue inclusion information can be found in section 3 on page 10.

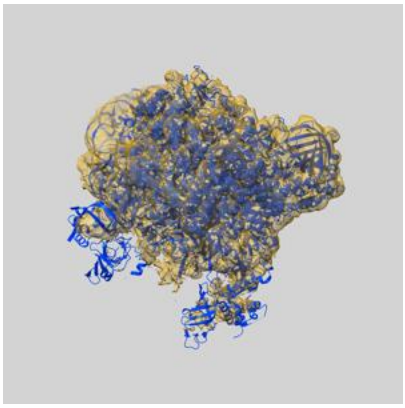
9.1 Map-model overlay



X



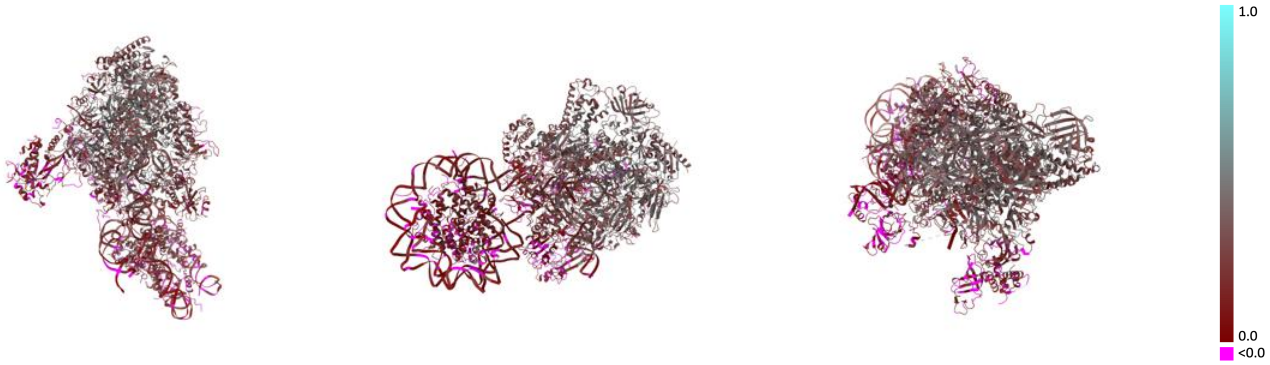
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

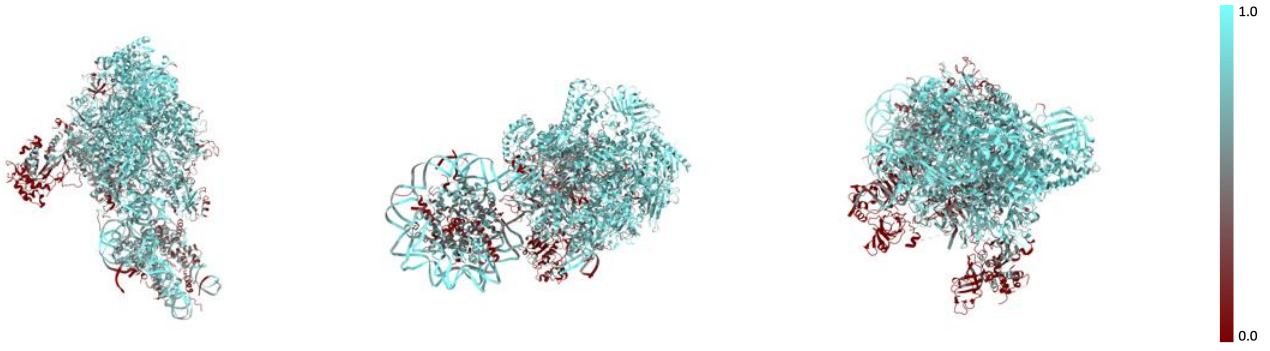
9.2 Q-score mapped to coordinate model



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.

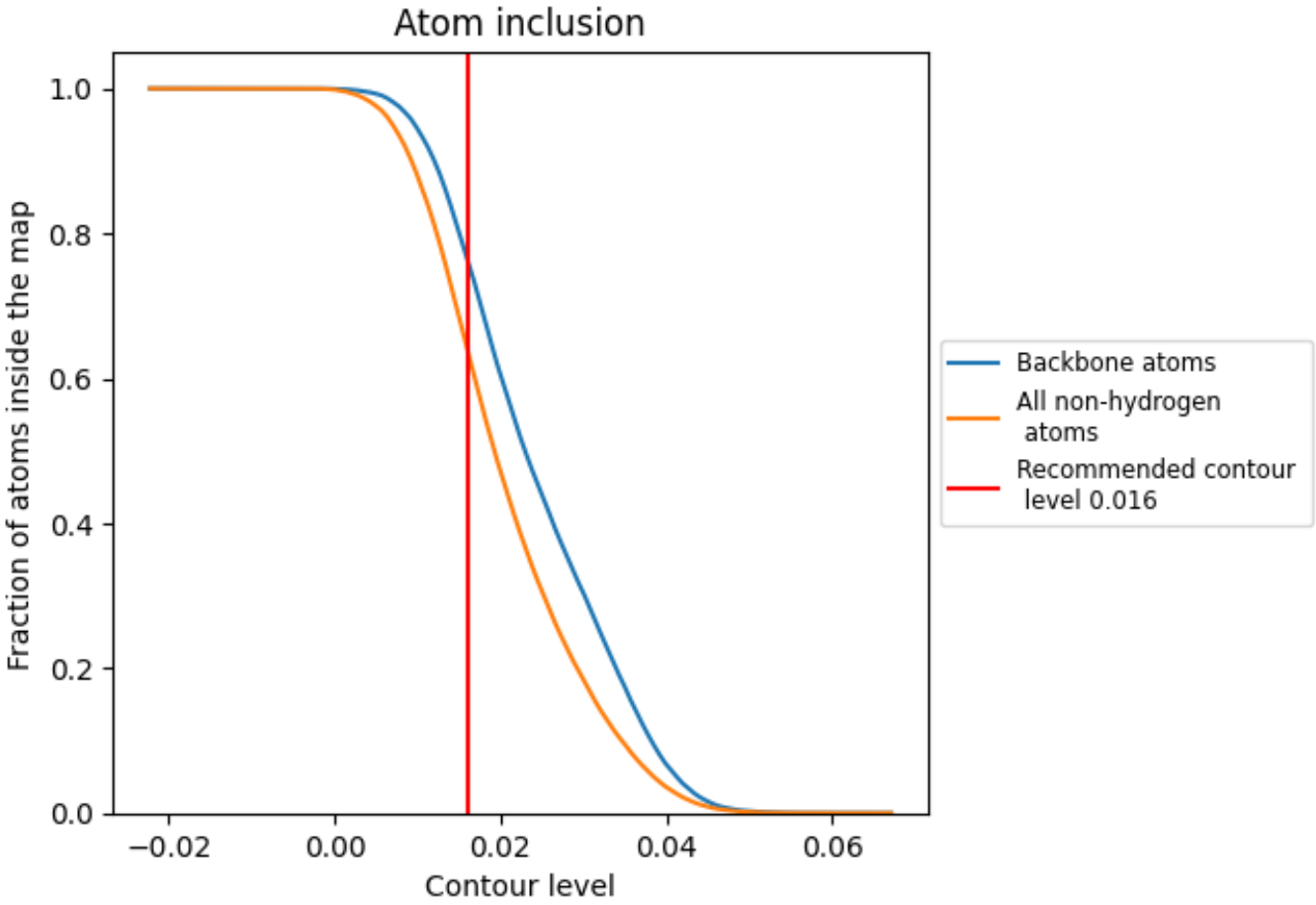
9.3 Atom inclusion mapped to coordinate model



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6402	0.2440
0	0.7074	0.0850
1	0.6874	0.0880
A	0.7182	0.3260
B	0.7391	0.3390
C	0.8211	0.3610
D	0.1058	0.0900
E	0.7844	0.3190
F	0.8009	0.3600
G	0.3129	0.1620
H	0.8607	0.3530
I	0.4007	0.1550
J	0.8208	0.3530
K	0.7749	0.3480
L	0.7098	0.2940
N	0.7056	0.1130
P	0.7478	0.2500
T	0.7398	0.1410
V	0.1378	0.0310
W	0.1438	0.0930
a	0.4869	0.0990
b	0.5261	0.1010
c	0.5863	0.1220
d	0.5585	0.1090
e	0.5621	0.1380
f	0.5832	0.1470
g	0.4102	0.0850
h	0.4329	0.1210