



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:35 PM UTC

PDB ID : 6A5O / pdb_00006a5o
EMDB ID : EMD-6981
Title : RNA polymerase II elongation complex stalled at SHL(-6) of the nucleosome
Authors : Kujirai, T.; Ehara, H.; Fujino, Y.; Shirouzu, M.; Sekine, S.; Kurumizaka, H.
Deposited on : 2018-06-25
Resolution : 9.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

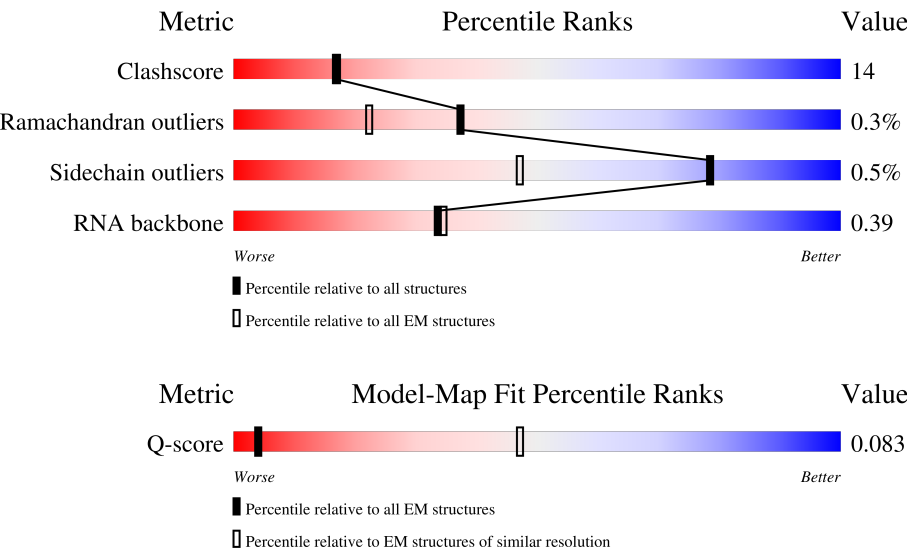
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 9.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	149 (9.40 - 10.40)

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

Mol	Chain	Length	Quality of chain
1	A	1743	
2	B	1227	
3	C	304	

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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	11	
14	T	198	
15	N	198	
16	a	139	
16	e	139	
17	b	106	
17	f	106	
18	c	133	
18	g	133	
19	d	129	
19	h	129	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 44485 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
1	A	1408	Total	C	N	O	S	0	0
			11095	6997	1935	2093	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1161	Total	C	N	O	S	0	0
			9261	5835	1636	1732	58		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	156	Total	C	N	O	S	0	0
			1210	753	210	245	2		

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

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

- 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*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*P*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	11	Total	C	N	O	P	0	0
			232	103	34	84	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	178	Total	C	N	O	P	0	0
			3631	1720	707	1027	177		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	169	Total	C	N	O	P	0	0
			3476	1653	606	1048	169		

- Molecule 16 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
16	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 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
17	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 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	103	Total	C	N	O	0	0
			796	502	155	139		
18	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 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	d	95	Total	C	N	O	S	0
			746	468	136	140	2	0
19	h	93	Total	C	N	O	S	0
			725	456	130	137	2	0

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 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

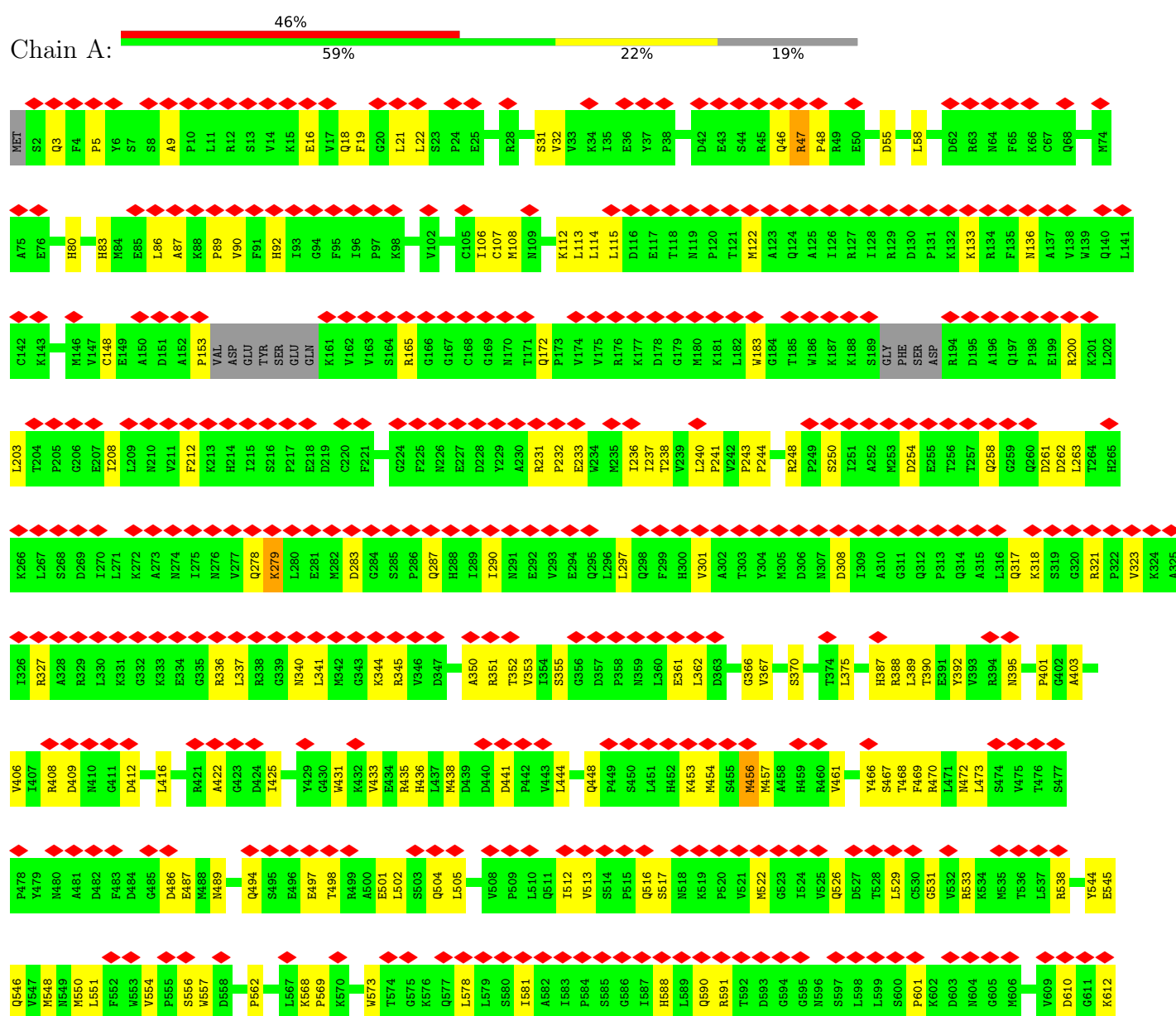
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

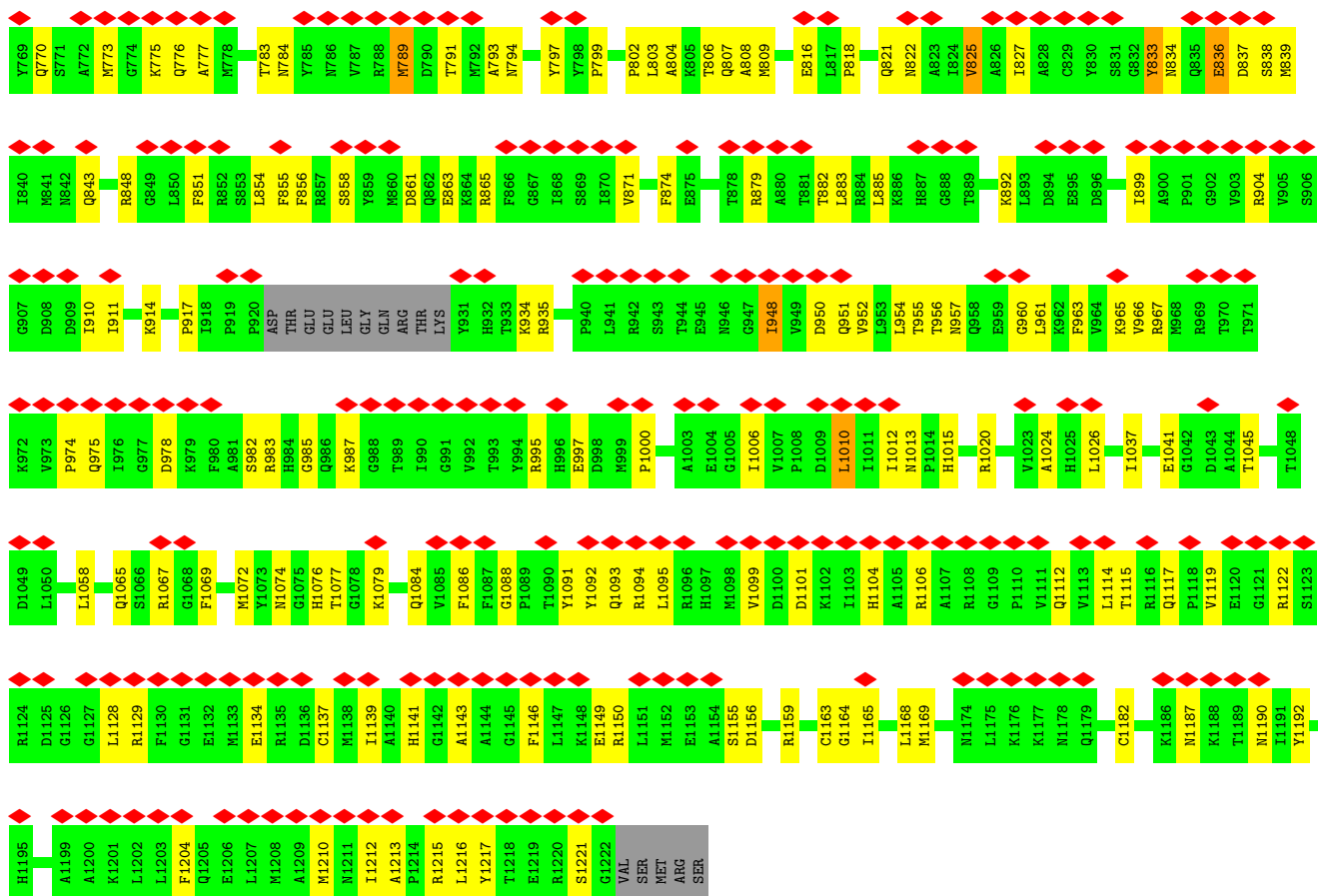
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

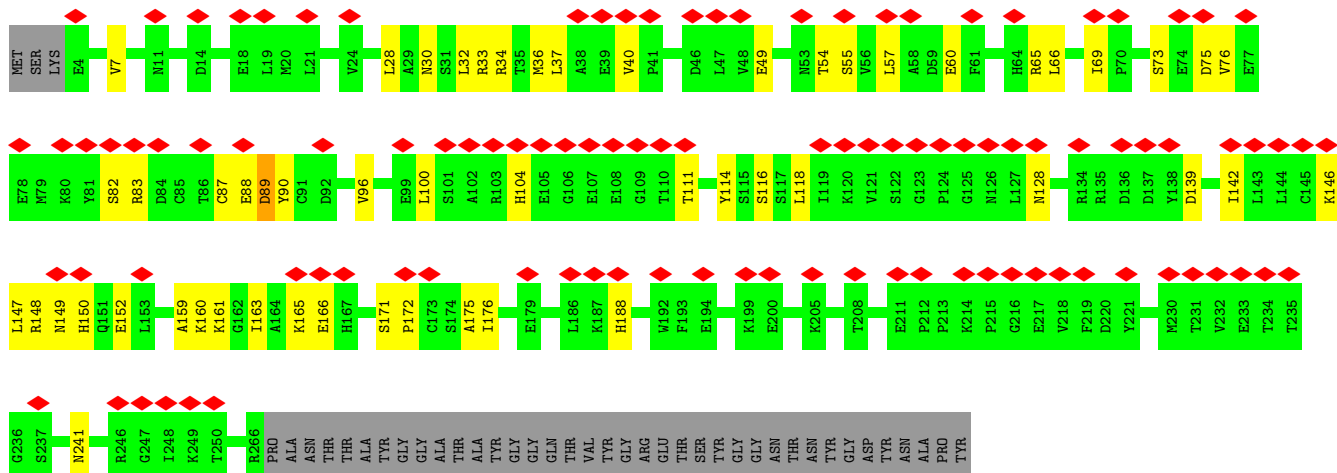
• Molecule 1: DNA-directed RNA polymerase subunit



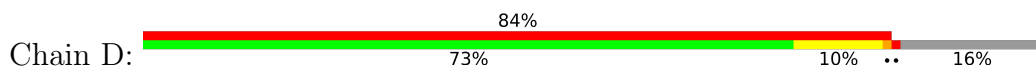
SER	VAL	L1433	M1371	I1266	ASP	A1117	F1055	G991	I920	A945	C765	I680	V613
PRO	ALA	G1434	A1372	E1267	LYS	L1118	Q1056	V992	L921	L846	V766	I680	M614
THR	ASP	Q1435	L1373	A1268	THR	T1119	R1067	R993	G922	E947	Q767	A683	F615
PRO	VAL	L1436	L1374	M1269	THR	Y1121	S1068	D994	D923	D948	Q768	I684	G616
GLY	PHE	A1437	V1377	M1270	THR	L1122	L1060	L995	V924	I949	M770	S686	V617
THR	SER	P1438	M1378	L1271	THR	D1123	H1061	C996	E925	M950	V771	S686	V618
PRO	PRO	A1439	M1378	D1272	THR	R1124	H1062	K997	L926	T857	E772	K688	D619
THR	ALA	G1440	R1381	L1273	THR	E1125	E1063	K998	Q927	R858	G773	E689	K620
PRO	THR	Y1441	Y1382	R1277	THR	I1126	E1064	L999	K928	N859	K774	E689	K621
SER	GLY	G1442	L1384	I1278	THR	A1127	M1065	F1000	E929	R775	I776	Y696	V623
THR	SER	A1443	A1201	L1128	THR	D1129	V1066	V1001	L930	I776	A777	K697	G624
SER	SER	V1446	A1202	L1280	THR	K1132	G1067	L1002	N931	A777	F778	H700	S625
PRO	ASP	M1447	A1203	P1280	THR	Y1133	V1068	R1003	S932	E702	E778	E702	G626
THR	ASP	T1448	M1204	I1281	THR	L1144	I1069	G1004	E933	I864	A781	E702	G627
PRO	SER	D1449	L1205	S1283	THR	T1145	A1071	E1005	E935	I865	D782	E702	G628
SER	GLY	E1450	D1206	K1284	THR	K1146	Q1072	N1006	Y934	R866	F867	K706	G629
THR	GLY	K1451	L1209	V1285	THR	N1147	I1073	E1007	E936	F867	R783	K706	L630
PRO	LEU	L1452	L1210	M1287	THR	V1148	I1074	L1008	L937	L868	K790	M709	L631
THR	THR	L1453	M1211	V1288	THR	T1149	G1075	I1009	Y939	D872	F793	L710	H632
SER	TYR	T1454	D1216	E1297	THR	A1151	P1077	Q1013	K942	G873	S794	L711	T633
PRO	ALA	S1455	D1216	E1297	THR	A1151	P1077	Q1014	K942	L874	P795	R712	V634
SER	GLY	L1456	E1220	L1309	THR	T1152	T1078	S1018	F943	D875	E796	E713	M635
THR	ILE	P1457	E1220	L1309	THR	E1153	Q1080	L1019	L944	G876	S797	E713	R636
SER	GLN	A1457	D1224	T1311	THR	I1154	M1081	F1020	E946	T877	K798	E716	E637
PRO	SER	ALA	D1224	T1311	THR	Y1155	THR	Q1021	Q878	Q878	E802	G717	K638
THR	THR	TYR	D1224	T1311	THR	Y1155	THR	C1022	L958	Y879	E802	G717	P640
PRO	GLN	ALA	D1224	T1311	THR	Y1155	THR	L1023	P959	E880	Y806	S720	G639
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	V1024	V960	R881	P640	R721	K641
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	R1025	N961	Q882	L806	N724	I642
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	A1026	L962	T883	R907	N724	I642
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	R1027	R963	I884	P811	D725	C643
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	L1028	R964	D885	A726	A726	A644
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	A1029	I965	T886	R227	R227	E645
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	T1030	I966	I887	F816	A730	L646
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	R1031	Q967	P888	H817	A730	L646
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	R1032	N968	A818	A734	A734	G648
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	I1033	A969	M819	N649	N649	I650
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	L1034	Q970	H822	I650	N737	Q651
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	E1035	Q971	E923	K739	L738	K652
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	E1036	I972	G824	D740	D740	K652
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	F1037	F973	L825	L741	N742	L741
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	R1038	H974	I826	N743	N743	N743
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	L1039	L975	V830	V744	V744	N743
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	M1040	D976	K906	K331	A750	L659
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	R1041	R977	N907	T832	A750	H660
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	D1042	A978	S908	T832	A750	H660
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	A1043	K979	I909	T832	A750	H660
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	F1044	A980	K910	T832	A750	H660
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	E1045	S981	P911	T832	A750	H660
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	M1046	D982	Q839	T832	A750	H660
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	V1047	L983	R940	T832	A750	H660
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	L1048	T984	R841	T832	A750	H660
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	G1049	I985	L942	T832	A750	H660
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	T1050	P986	V943	T832	A750	H660
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	I1051	E987	Y916	T832	A750	H660
THR	THR	ALA	D1224	T1311	THR	Y1155	THR	E1052	E988	A917	T832	A750	H660
PRO	THR	ALA	D1224	T1311	THR	Y1155	THR	A1053	I989	A918	T832	A750	H660
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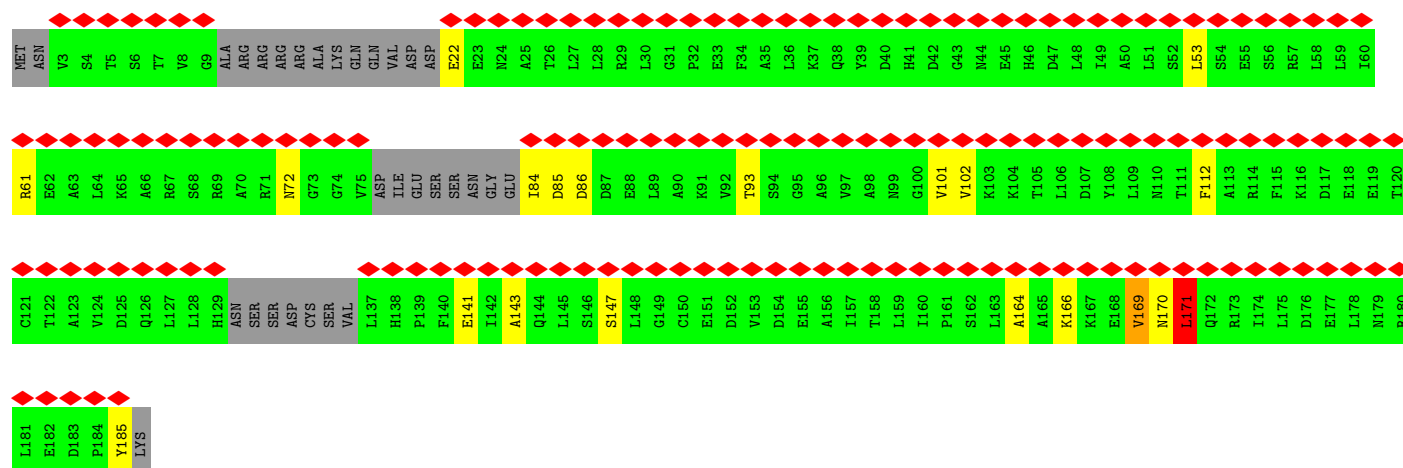


• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

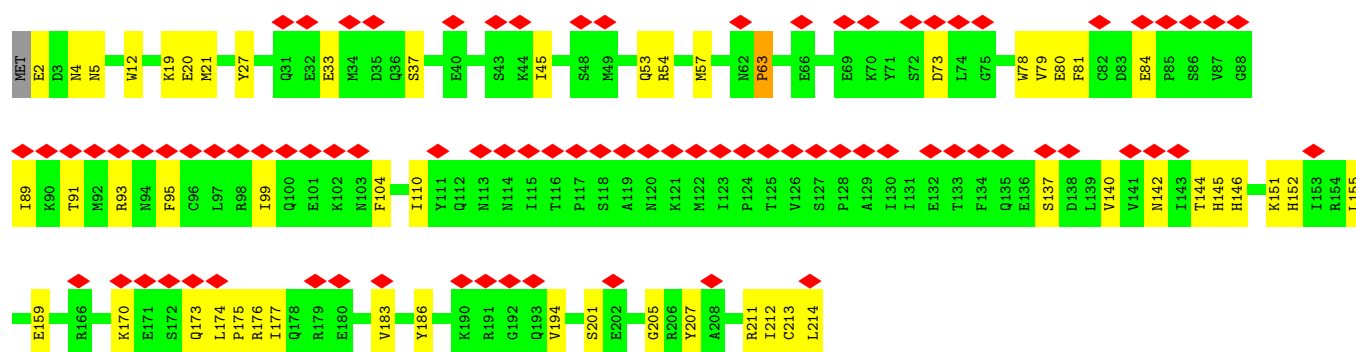
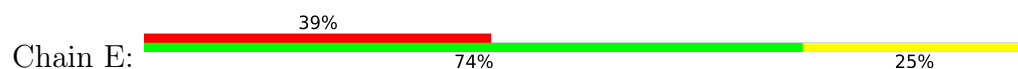


• Molecule 4: RNA polymerase II subunit B32

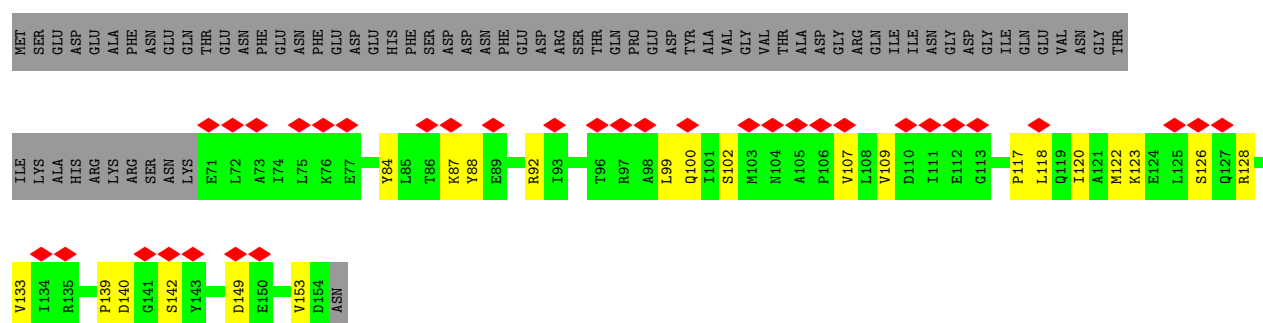
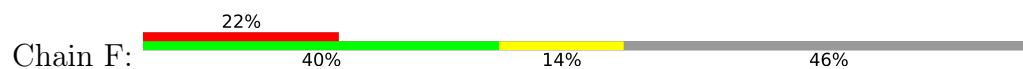




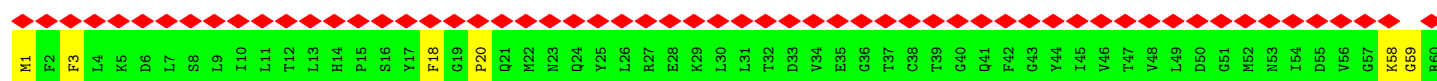
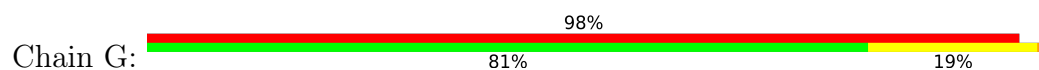
- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

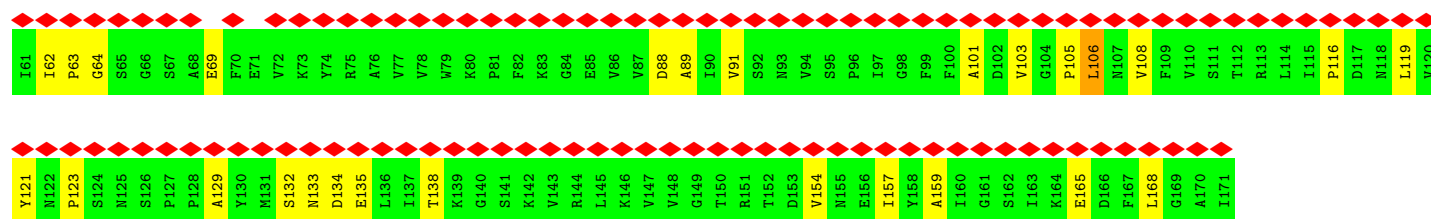


- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

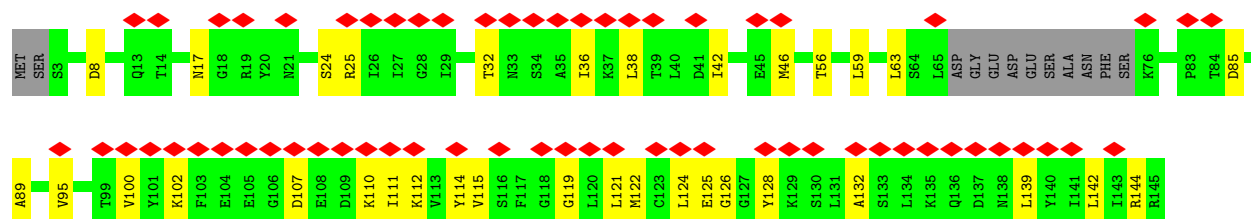
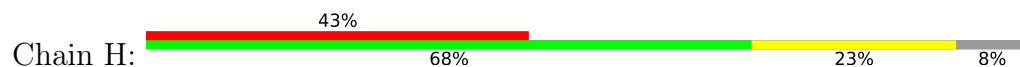


- Molecule 7: RNA polymerase II subunit

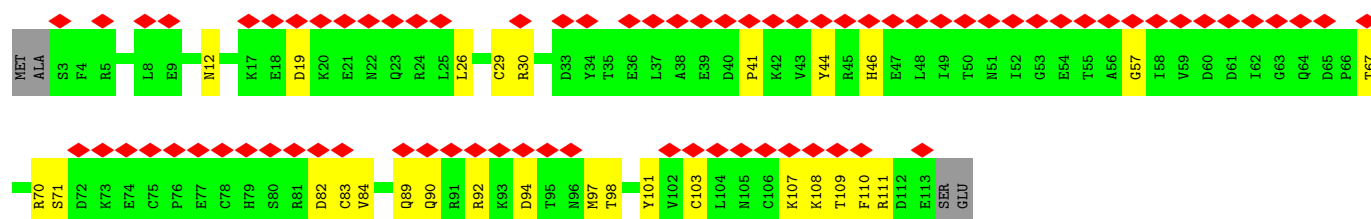
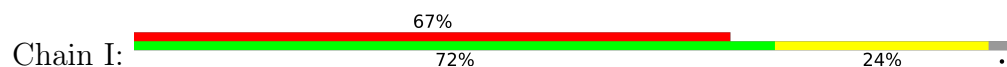




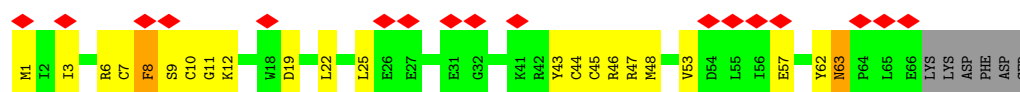
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



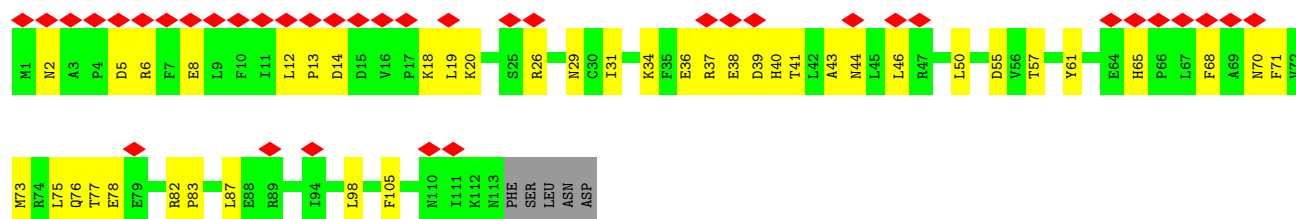
• Molecule 9: DNA-directed RNA polymerase subunit



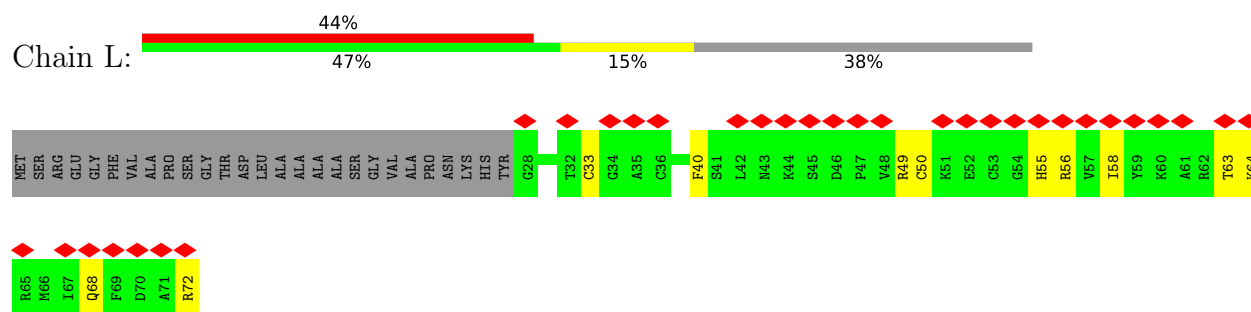
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



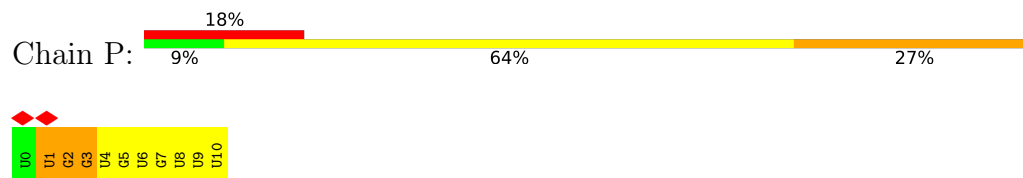
• Molecule 11: RNA polymerase II subunit B12.5



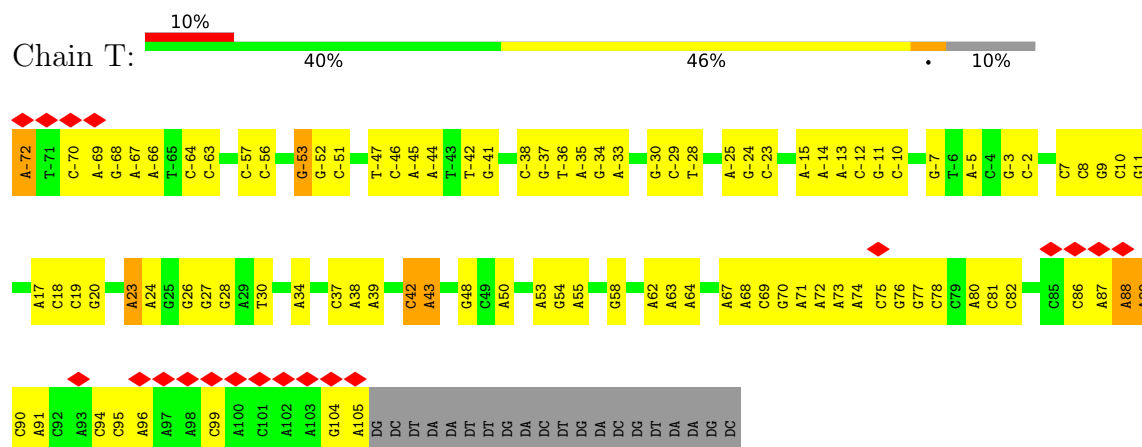
• Molecule 12: RNA polymerase subunit ABC10-alpha



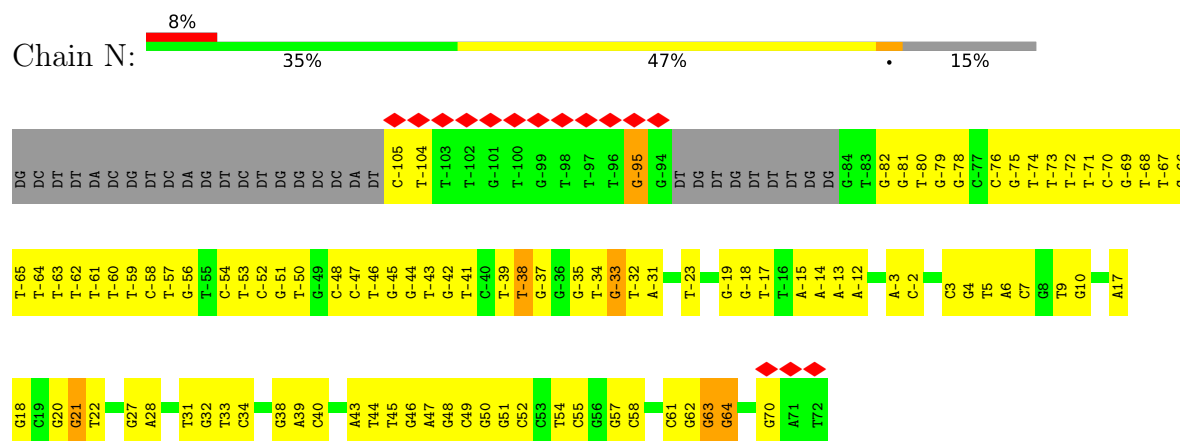
- Molecule 13: RNA (5'-R(P*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*C)-3')



- Molecule 14: DNA (198-MER)

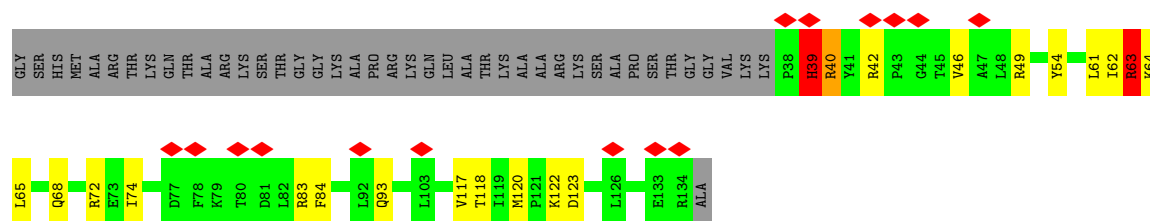


- Molecule 15: DNA (198-MER)

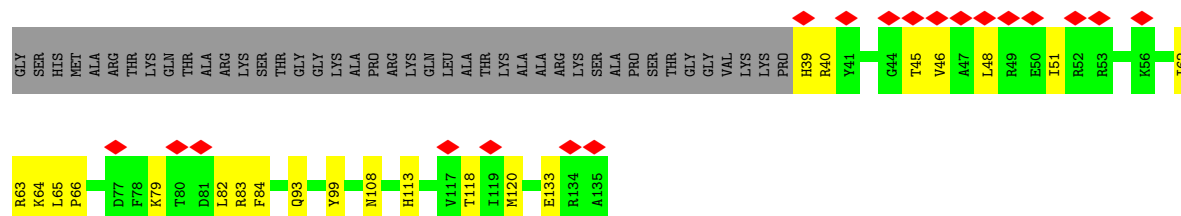


- Molecule 16: Histone H3.3

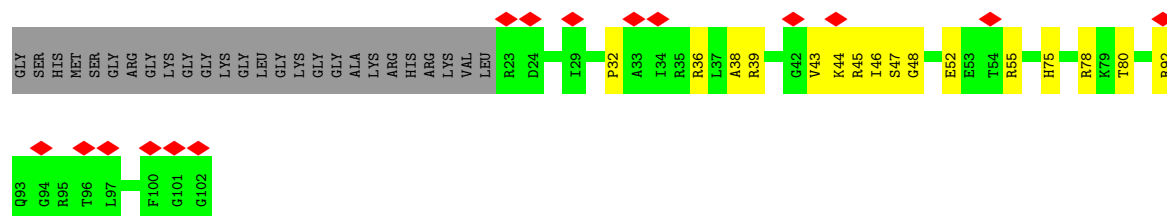




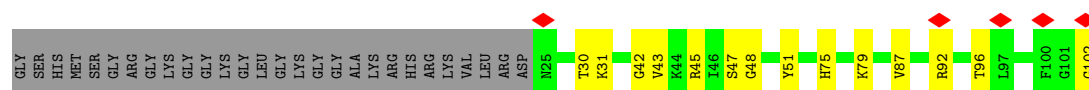
• Molecule 16: Histone H3.3



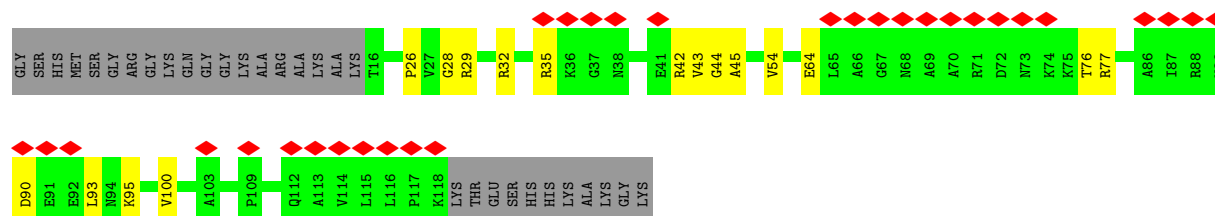
• Molecule 17: Histone H4



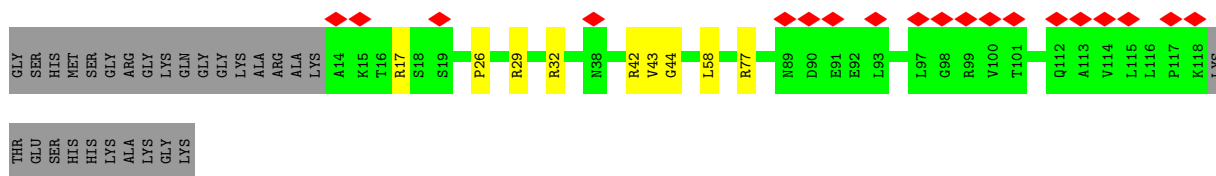
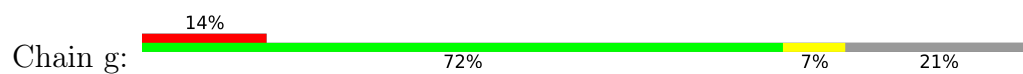
• Molecule 17: Histone H4



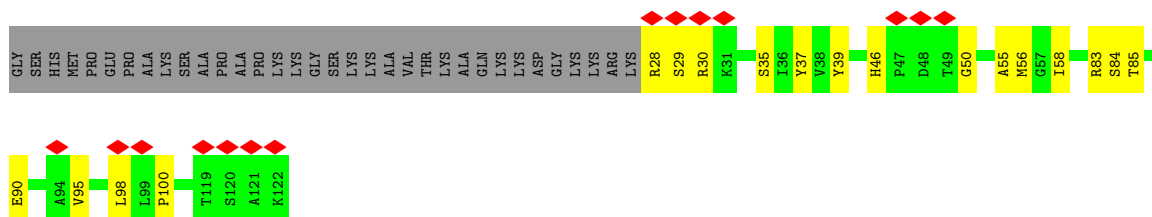
• Molecule 18: Histone H2A type 1-B/E



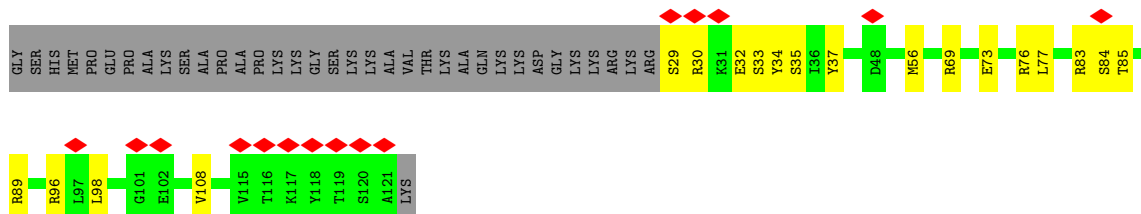
• Molecule 18: Histone H2A type 1-B/E



- Molecule 19: Histone H2B type 1-J



- Molecule 19: Histone H2B type 1-J



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12692	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 ($e^-/\text{\AA}^2$)	50	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	0.132	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.038	Depositor
Map size ($\text{\AA}$)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.61	1/11299 (0.0%)	0.85	9/15266 (0.1%)
2	B	0.64	1/9441 (0.0%)	0.90	6/12732 (0.0%)
3	C	0.65	0/2139	0.90	2/2895 (0.1%)
4	D	0.22	0/1221	0.51	0/1648
5	E	0.57	0/1772	0.79	1/2385 (0.0%)
6	F	0.54	0/687	0.75	0/931
7	G	0.25	0/1353	0.61	2/1837 (0.1%)
8	H	0.58	0/1069	0.79	0/1444
9	I	0.40	0/934	0.83	0/1257
10	J	0.75	0/554	0.98	0/742
11	K	0.53	0/953	0.77	0/1291
12	L	0.52	0/365	0.86	0/484
13	P	1.02	3/257 (1.2%)	0.61	0/398
14	T	0.45	3/4083 (0.1%)	0.88	5/6289 (0.1%)
15	N	0.34	0/3889	0.96	11/6007 (0.2%)
16	a	0.30	0/809	0.58	0/1085
16	e	0.33	0/807	0.58	0/1081
17	b	0.32	0/645	0.61	0/862
17	f	0.33	0/626	0.61	0/837
18	c	0.31	0/806	0.55	0/1089
18	g	0.29	0/820	0.54	0/1107
19	d	0.30	0/757	0.54	0/1015
19	h	0.31	0/736	0.54	0/990
All	All	0.54	8/46022 (0.0%)	0.83	36/63672 (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
1	A	0	8
2	B	0	8
3	C	0	3
5	E	0	2
9	I	0	1
10	J	0	1
All	All	0	23

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	89	DA	C1'-N9	-8.30	1.29	1.46
2	B	789	MET	CA-CB	-8.06	1.41	1.53
14	T	-72	DA	O5'-C5'	7.52	1.65	1.42
14	T	88	DA	C1'-N9	-6.66	1.33	1.46
13	P	1	U	C1'-N1	6.18	1.57	1.48

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	20	DG	O3'-P-O5'	-15.20	81.20	104.00
15	N	20	DG	OP2-P-O3'	-8.28	83.17	108.00
1	A	504	GLN	CA-C-N	-6.37	111.96	122.79
1	A	504	GLN	C-N-CA	-6.37	111.96	122.79
2	B	256	GLY	CA-C-N	6.08	129.24	120.79

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	GLN	Peptide
1	A	466	TYR	Peptide
1	A	846	LEU	Peptide
1	A	920	ILE	Peptide
1	A	959	PRO	Peptide

5.2 Too-close contacts

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	A	11095	0	11132	284	0
2	B	9261	0	9265	261	0
3	C	2098	0	2060	36	0
4	D	1210	0	1205	17	0
5	E	1740	0	1754	31	0
6	F	677	0	693	17	0
7	G	1324	0	1342	29	0
8	H	1052	0	1050	22	0
9	I	917	0	870	19	0
10	J	545	0	561	24	0
11	K	932	0	944	35	0
12	L	359	0	359	8	0
13	P	232	0	114	15	0
14	T	3631	0	1981	265	0
15	N	3476	0	1916	227	0
16	a	797	0	835	61	0
16	e	796	0	832	40	0
17	b	638	0	676	20	0
17	f	619	0	659	12	0
18	c	796	0	848	47	0
18	g	810	0	866	50	0
19	d	746	0	771	40	0
19	h	725	0	745	39	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	44485	0	41478	1186	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 14.

The worst 5 of 1186 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)
15:N:-66:DG:H2''	15:N:-65:DT:C5'	1.29	1.61
15:N:-45:DG:H3'	18:g:32:ARG:NH1	1.25	1.47
14:T:-72:DA:O5'	14:T:-72:DA:C5'	1.65	1.44
15:N:-66:DG:C2'	15:N:-65:DT:H5'	1.49	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:-13:DA:C5'	16:a:63:ARG:HH22	1.35	1.39

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	A	1396/1743 (80%)	1252 (90%)	142 (10%)	2 (0%)	48	83
2	B	1151/1227 (94%)	1018 (88%)	131 (11%)	2 (0%)	43	78
3	C	261/304 (86%)	231 (88%)	29 (11%)	1 (0%)	30	67
4	D	148/186 (80%)	136 (92%)	9 (6%)	3 (2%)	6	31
5	E	211/214 (99%)	195 (92%)	16 (8%)	0	100	100
6	F	82/155 (53%)	73 (89%)	9 (11%)	0	100	100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	10	44
8	H	129/145 (89%)	113 (88%)	16 (12%)	0	100	100
9	I	109/115 (95%)	94 (86%)	15 (14%)	0	100	100
10	J	64/72 (89%)	57 (89%)	7 (11%)	0	100	100
11	K	111/118 (94%)	100 (90%)	11 (10%)	0	100	100
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
16	a	95/139 (68%)	89 (94%)	3 (3%)	3 (3%)	3	21
16	e	95/139 (68%)	90 (95%)	5 (5%)	0	100	100
17	b	78/106 (74%)	75 (96%)	3 (4%)	0	100	100
17	f	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
18	c	101/133 (76%)	95 (94%)	6 (6%)	0	100	100
18	g	103/133 (77%)	97 (94%)	6 (6%)	0	100	100
19	d	93/129 (72%)	89 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	h	91/129 (70%)	88 (97%)	3 (3%)	0	100	100
All	All	4606/5536 (83%)	4163 (90%)	430 (9%)	13 (0%)	37	72

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	171	LEU
7	G	134	ASP
4	D	169	VAL
7	G	154	VAL
16	a	63	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1223/1528 (80%)	1219 (100%)	4 (0%)	86	86
2	B	1016/1077 (94%)	1011 (100%)	5 (0%)	81	83
3	C	236/264 (89%)	235 (100%)	1 (0%)	84	84
4	D	133/160 (83%)	130 (98%)	3 (2%)	44	64
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	147 (99%)	1 (1%)	76	81
8	H	120/130 (92%)	119 (99%)	1 (1%)	73	80
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	59 (98%)	1 (2%)	53	69
11	K	104/109 (95%)	103 (99%)	1 (1%)	68	78
12	L	38/56 (68%)	38 (100%)	0	100	100
16	a	83/112 (74%)	80 (96%)	3 (4%)	31	52
16	e	82/112 (73%)	82 (100%)	0	100	100
17	b	65/81 (80%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	f	63/81 (78%)	63 (100%)	0	100	100
18	c	82/102 (80%)	82 (100%)	0	100	100
18	g	83/102 (81%)	83 (100%)	0	100	100
19	d	81/107 (76%)	81 (100%)	0	100	100
19	h	79/107 (74%)	79 (100%)	0	100	100
All	All	4073/4785 (85%)	4053 (100%)	20 (0%)	78	83

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	42	ILE
16	a	39	HIS
16	a	74	ILE
16	a	63	ARG
2	B	948	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	761	HIS
18	c	24	GLN
3	C	8	ASN
17	b	27	GLN
11	K	2	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

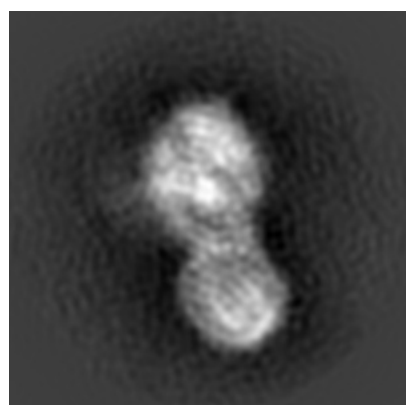
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6981. These allow visual inspection of the internal detail of the map and identification of artifacts.

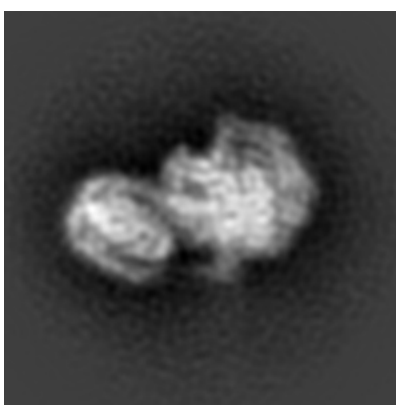
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

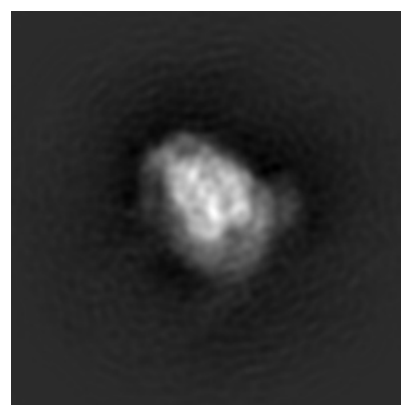
6.1.1 Primary map



X



Y

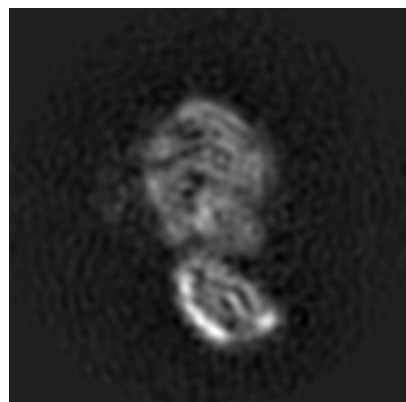


Z

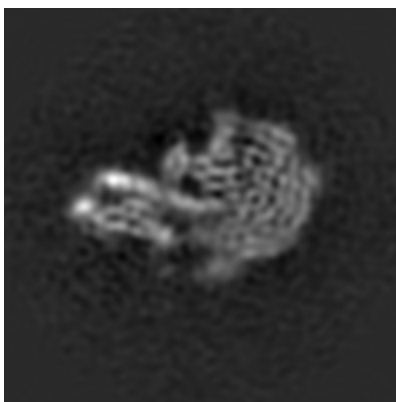
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

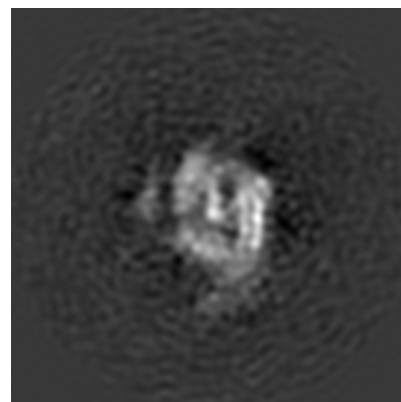
6.2.1 Primary map



X Index: 120



Y Index: 120

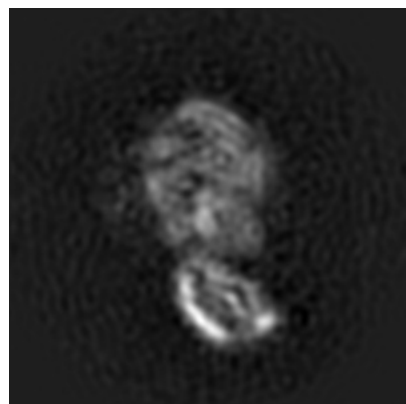


Z Index: 120

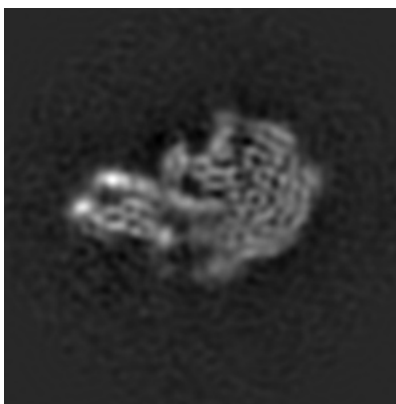
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

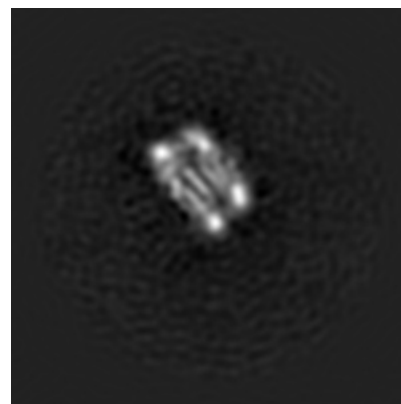
6.3.1 Primary map



X Index: 121



Y Index: 121

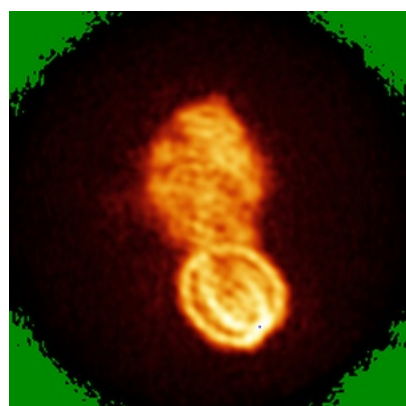


Z Index: 57

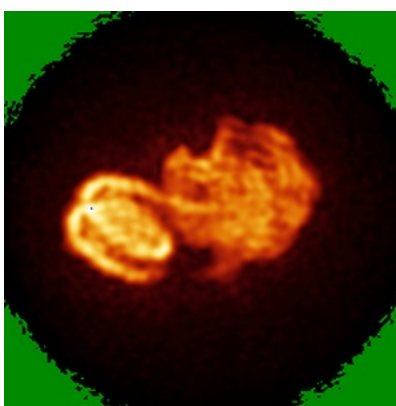
The images above show the largest variance slices of the map in three orthogonal directions.

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

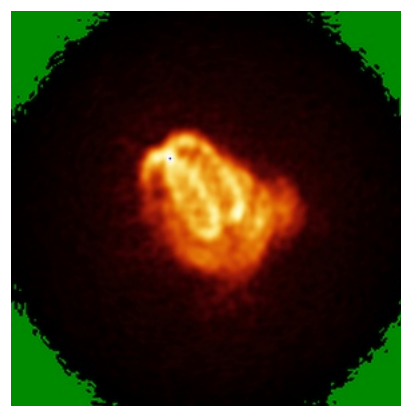
6.4.1 Primary map



X



Y

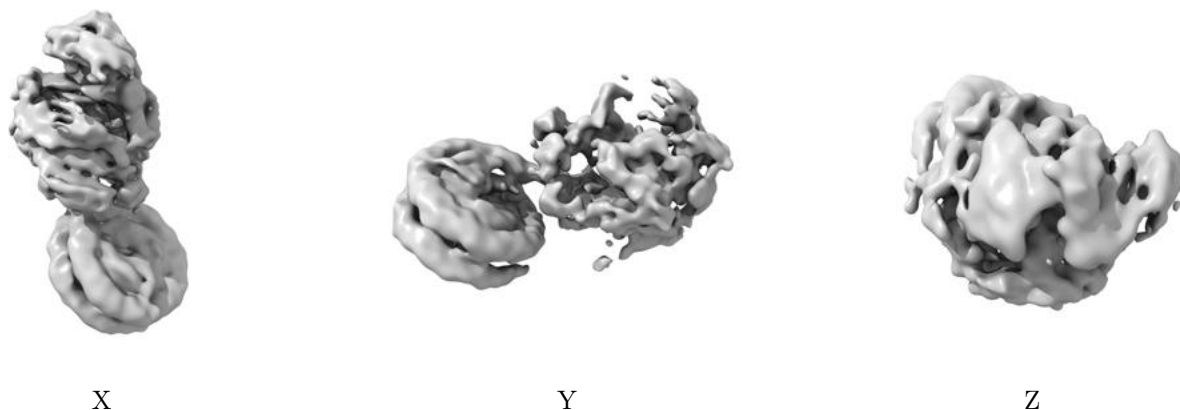


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

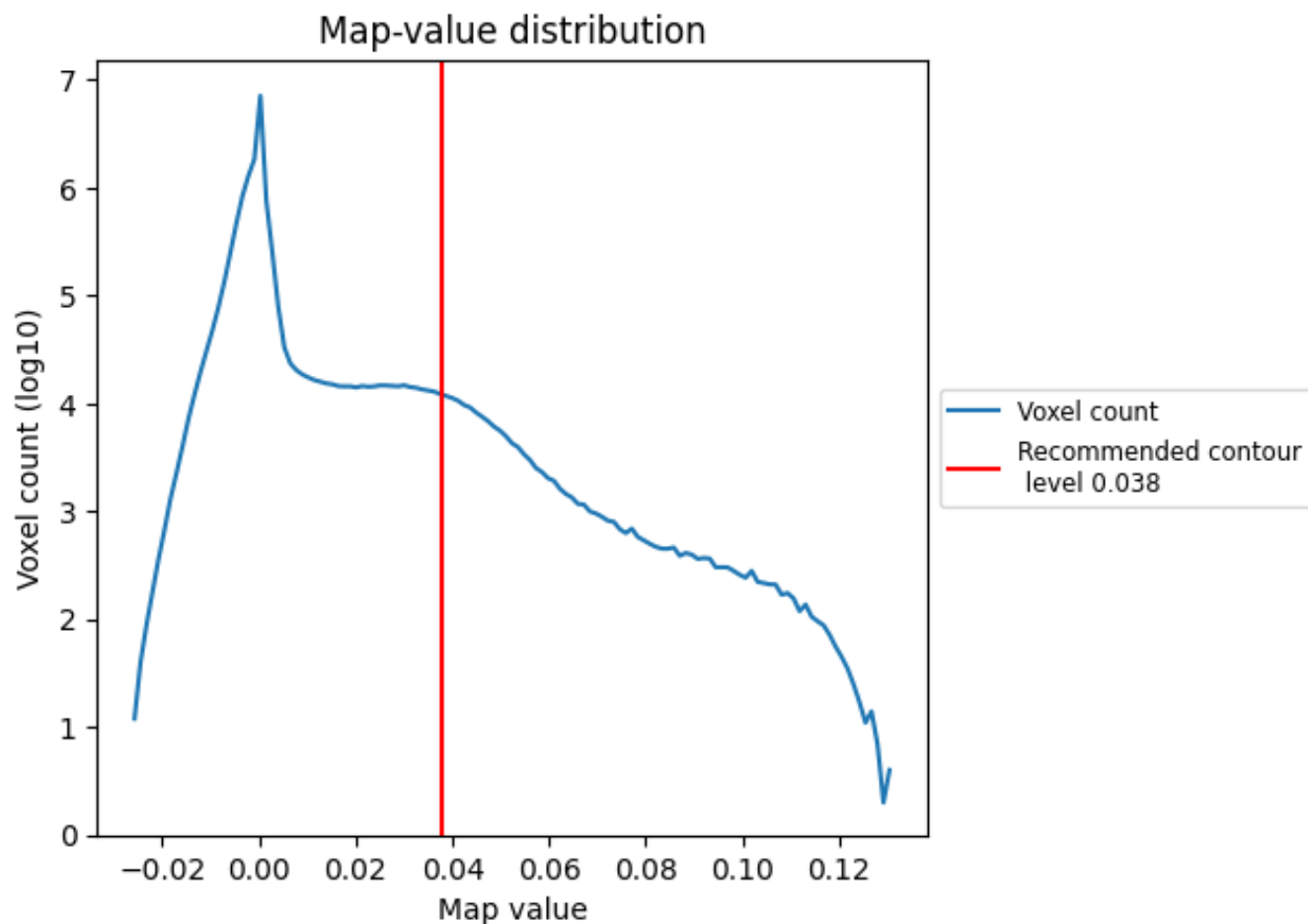
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

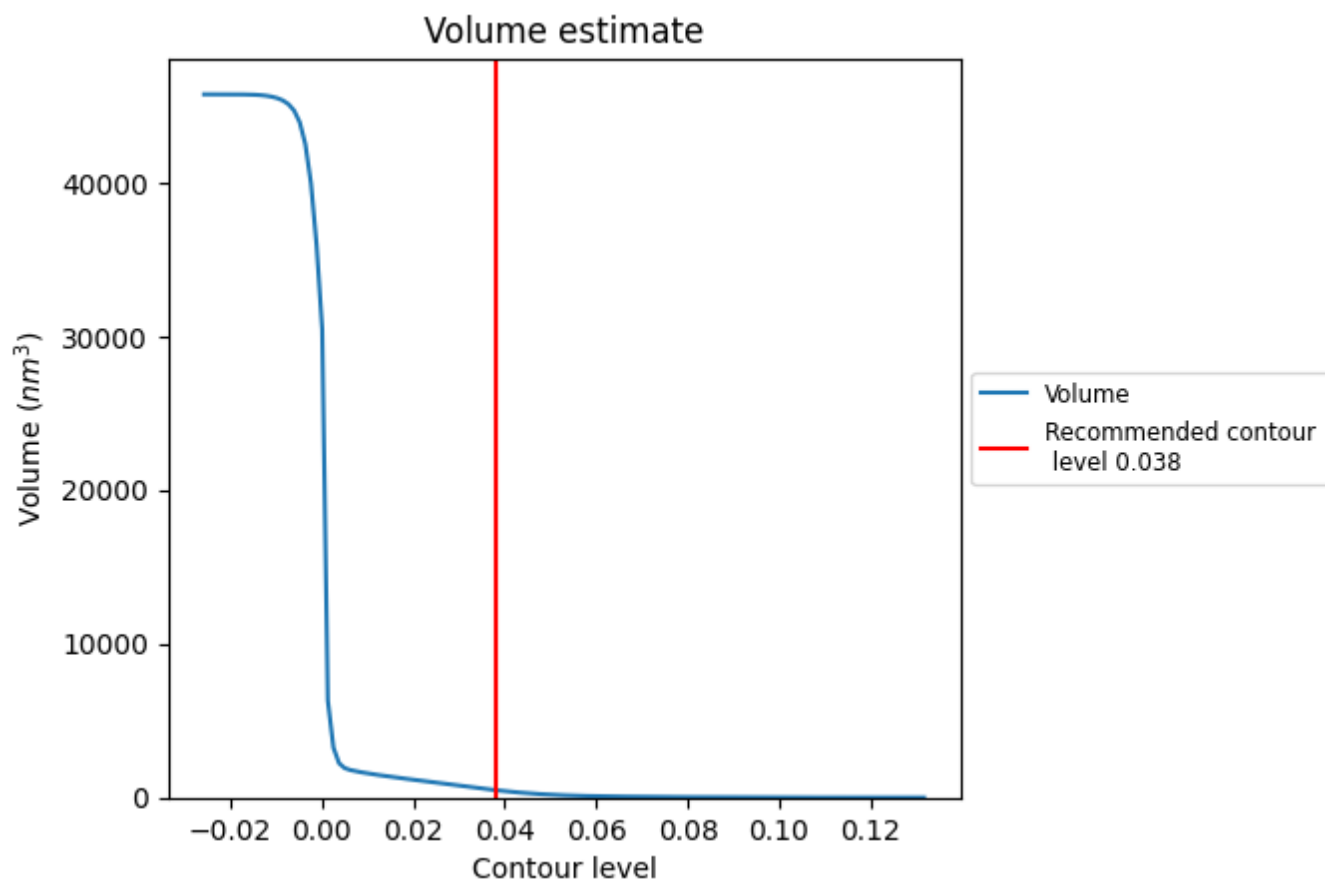
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

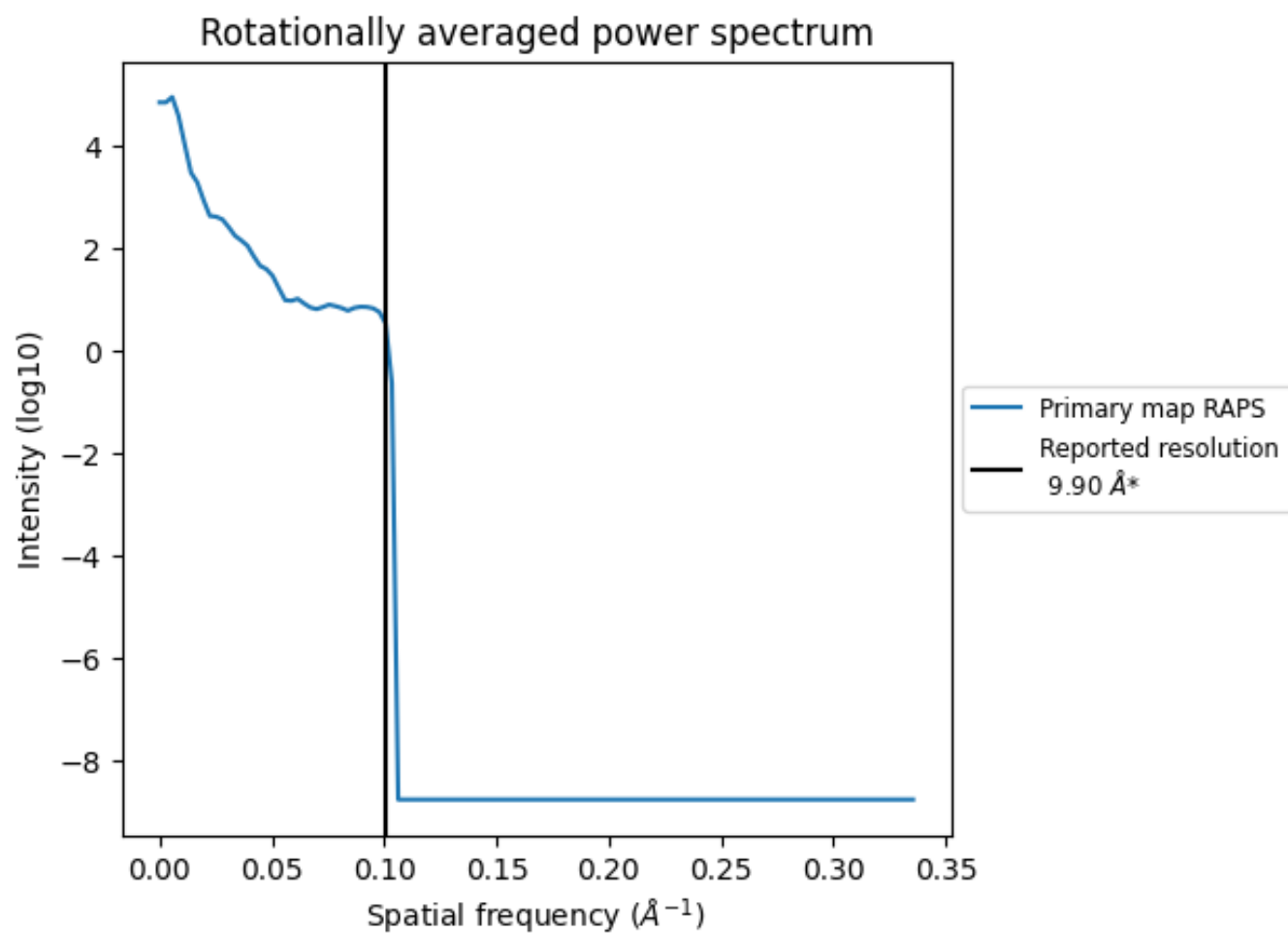
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm³; this corresponds to an approximate mass of 436 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

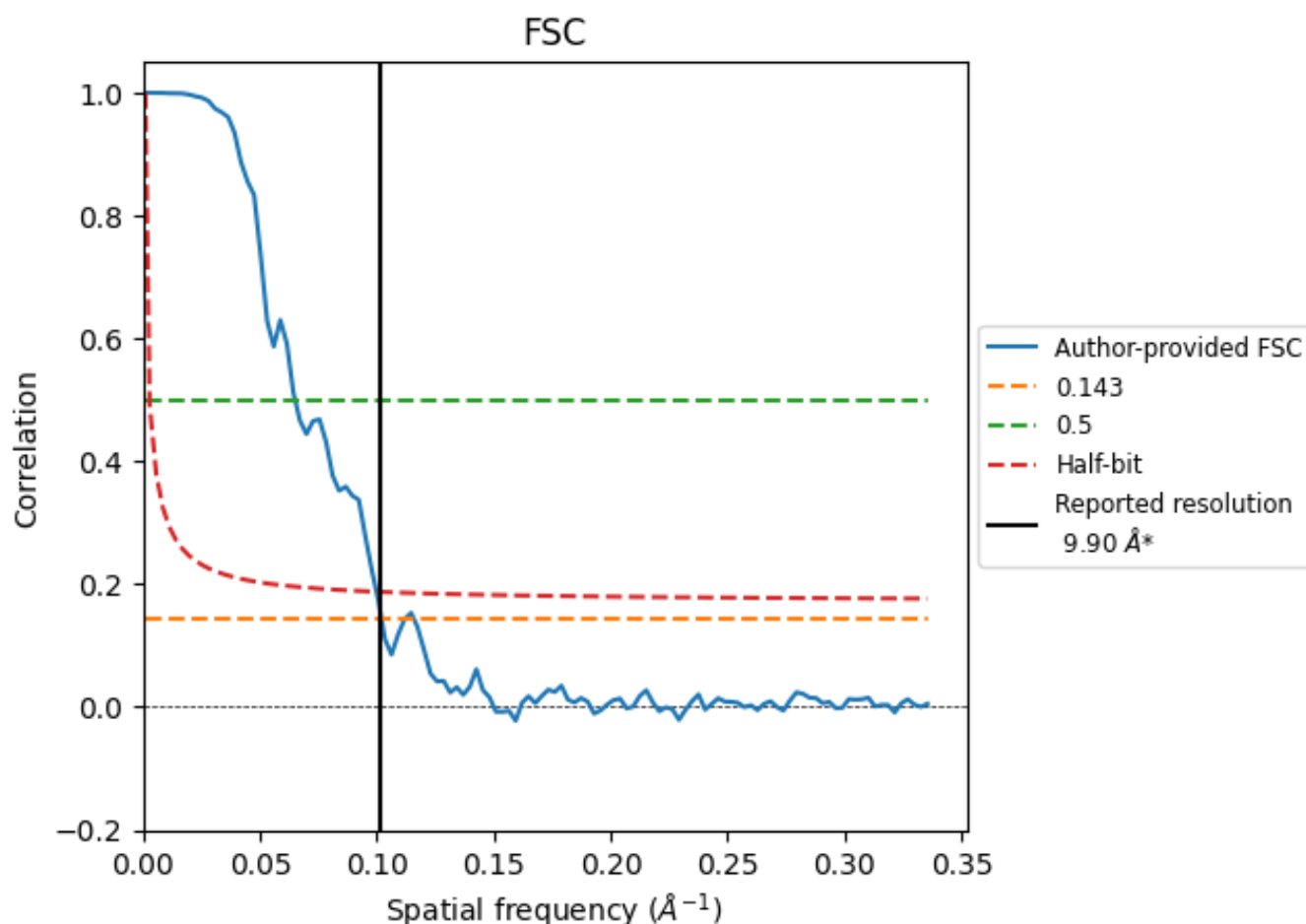


*Reported resolution corresponds to spatial frequency of 0.101 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.101 Å⁻¹

8.2 Resolution estimates [i](#)

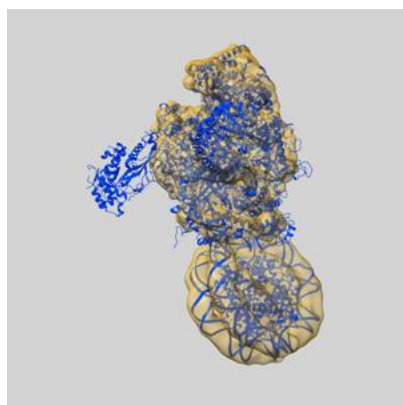
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.90	-	-
Author-provided FSC curve	9.80	15.38	10.02
Unmasked-calculated*	-	-	-

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

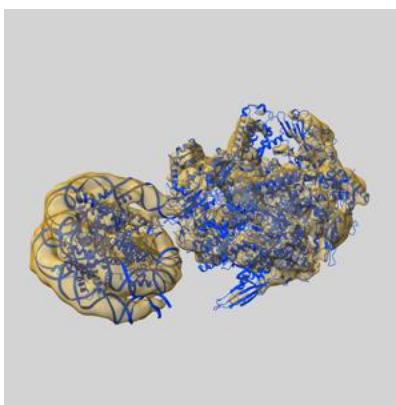
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6981 and PDB model 6A5O. Per-residue inclusion information can be found in section [3](#) on page [9](#).

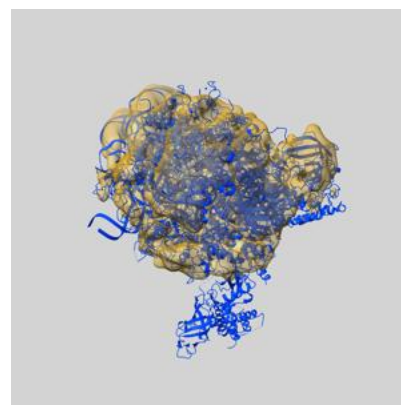
9.1 Map-model overlay [i](#)



X



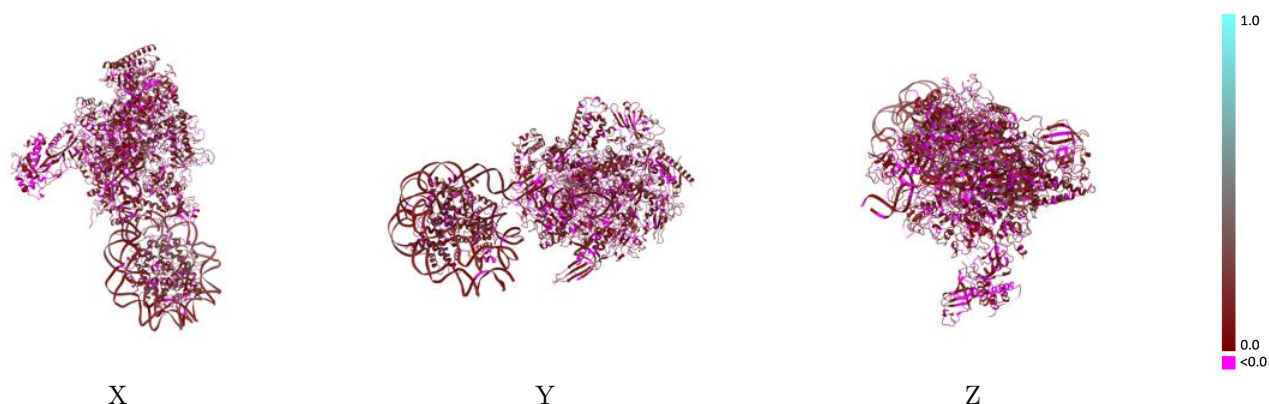
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

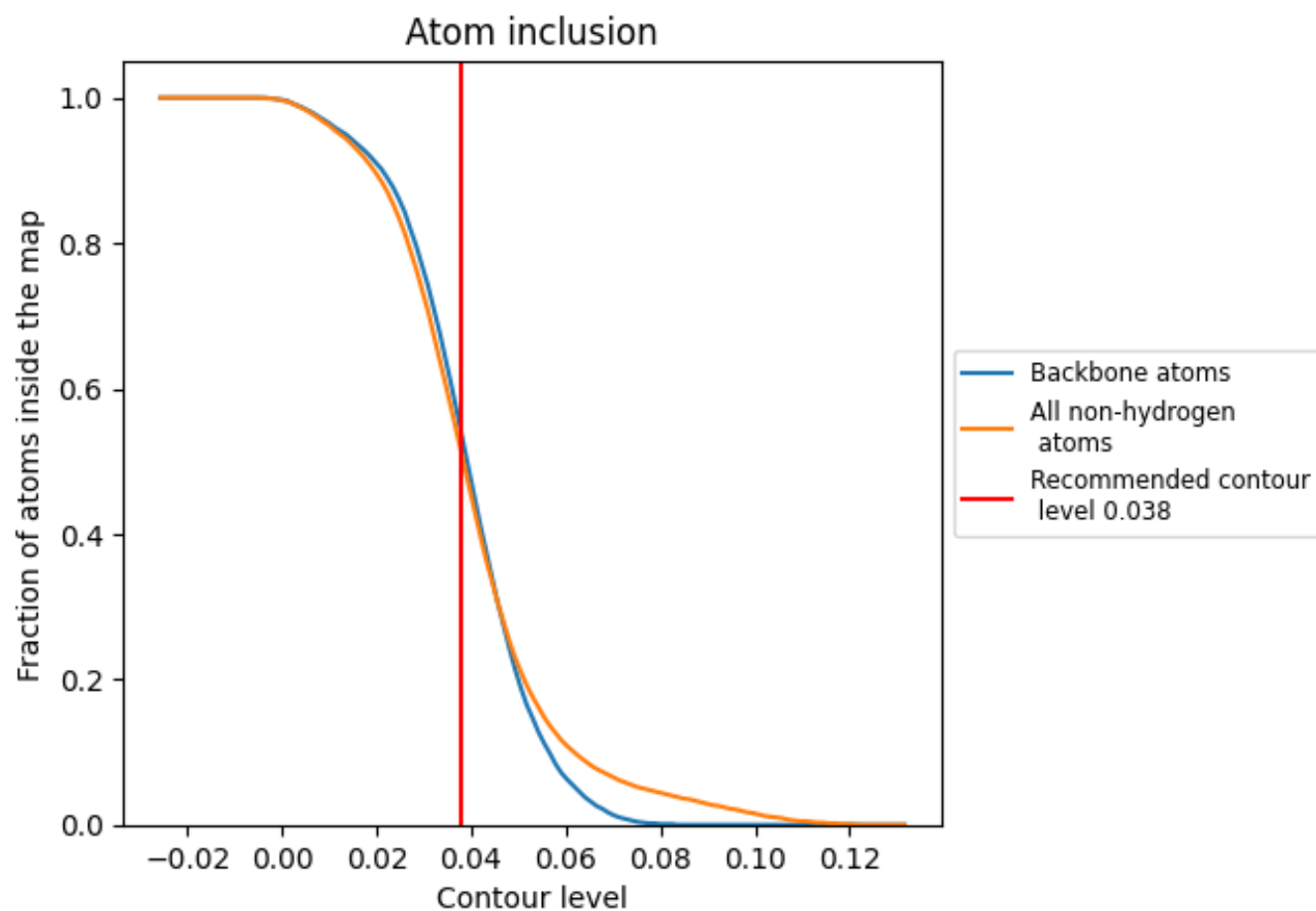


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 54% of all backbone atoms, 51% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5090	 0.0830
A	 0.3910	 0.0820
B	 0.4190	 0.0620
C	 0.5410	 0.0840
D	 0.0000	 0.0120
E	 0.5510	 0.1060
F	 0.5320	 0.0800
G	 0.0180	 0.0260
H	 0.4510	 0.0940
I	 0.2900	 0.0360
J	 0.6530	 0.0990
K	 0.5840	 0.0980
L	 0.2820	 0.0700
N	 0.8020	 0.1110
P	 0.6680	 0.1590
T	 0.7940	 0.1170
a	 0.7250	 0.1020
b	 0.7270	 0.0830
c	 0.6290	 0.0890
d	 0.7880	 0.1220
e	 0.7220	 0.1120
f	 0.7870	 0.0930
g	 0.7430	 0.0930
h	 0.7640	 0.1340

