



Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 05:33 PM JST

PDB ID : 6A5U
EMDB ID : EMD-6985
Title : RNA polymerase II elongation complex stalled at SHL(-1) of the nucleosome, with foreign DNA, tilt conformation
Authors : Kujirai, T.; Ehara, H.; Fujino, Y.; Shirouzu, M.; Sekine, S.; Kurumizaka, H.
Deposited on : 2018-06-25
Resolution : 7.60 Å(reported)

This is a Full wwPDB EM Validation 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:

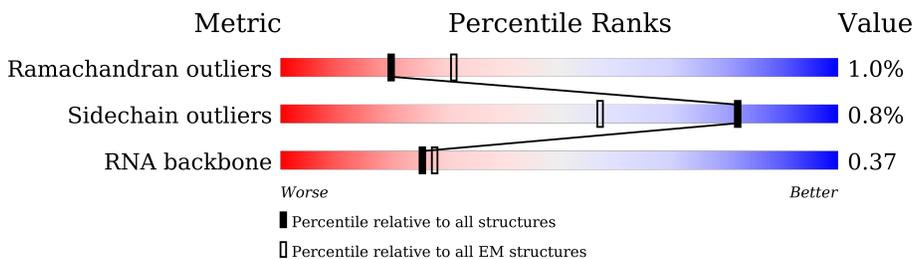
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 7.60 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 $\leq 5\%$. 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	
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	

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Mol	Chain	Length	Quality of chain
9	I	115	66% 94%
10	J	72	19% 89% 8%
11	K	118	25% 94%
12	L	72	19% 61% 38%
13	P	11	9% 64% 18% 18%
14	T	198	19% 60% 36%
15	N	198	6% 58% 41%
16	a	139	29% 68% 30%
16	e	139	15% 68% 30%
17	b	106	29% 74% 25%
17	f	106	11% 73% 26%
18	c	133	19% 77% 23%
18	g	133	47% 78% 21%
19	d	129	19% 72% 26%
19	h	129	28% 69% 29%
20	0	40	25% 98%
21	1	40	28% 95% 5%

2 Entry composition i

There are 23 unique types of molecules in this entry. The entry contains 43983 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	1408	11095	6997	1935	2093	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	1161	9261	5835	1636	1732	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	156	1210	753	210	245	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
			Total	C	N	O	S		
6	F	84	677	429	114	131	3	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
10	J	66	545	349	95	95	6	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	11	Total	C	N	O	P	0	0
			238	105	41	81	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	126	Total	C	N	O	P	0	0
			2567	1217	481	744	125		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	117	Total	C	N	O	P	0	0
			2409	1140	444	708	117		

- 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, 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, Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
19	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 20 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	0	40	824	389	172	223	40	0	0

- Molecule 21 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	1	40	816	392	127	257	40	0	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

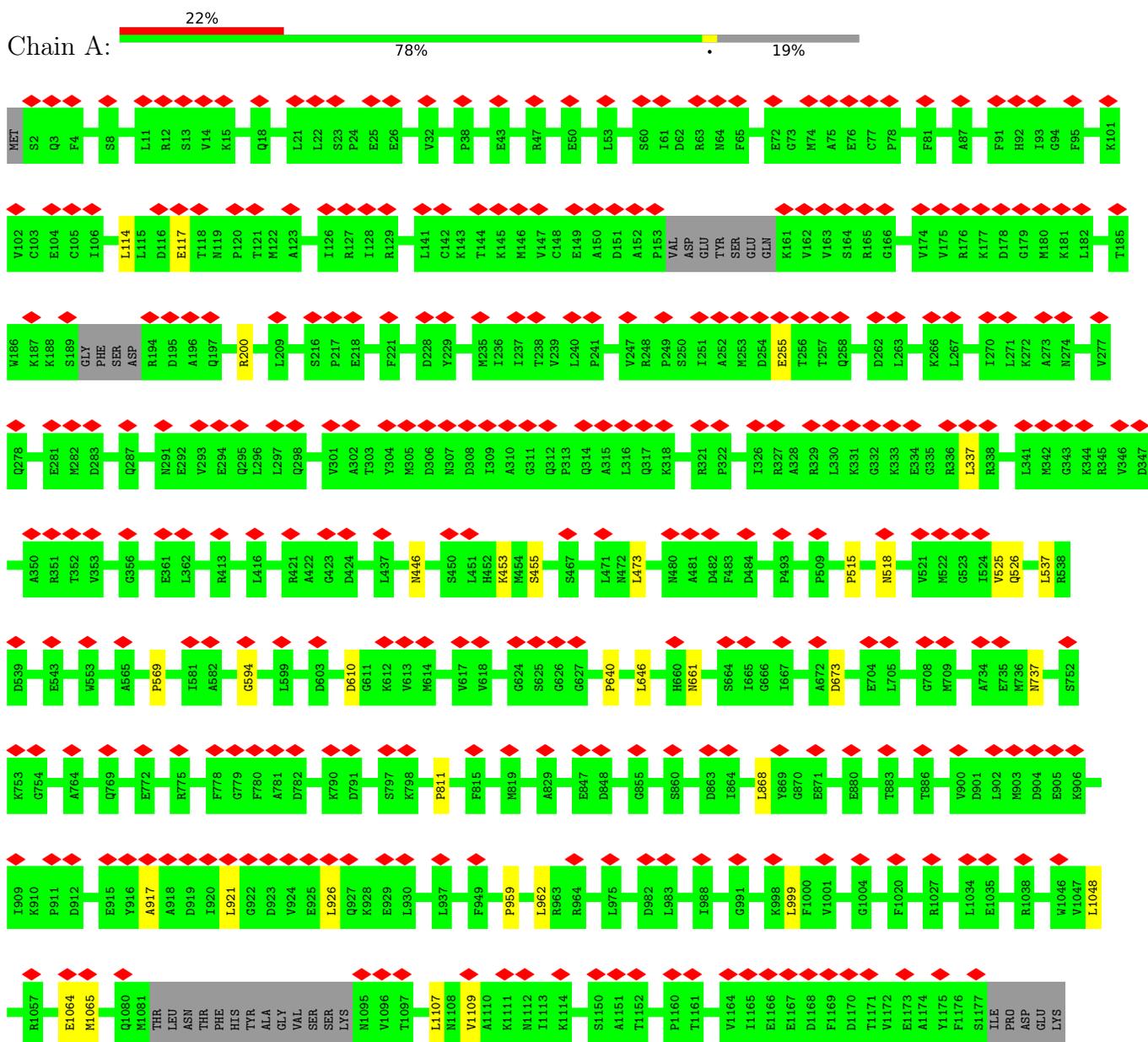
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

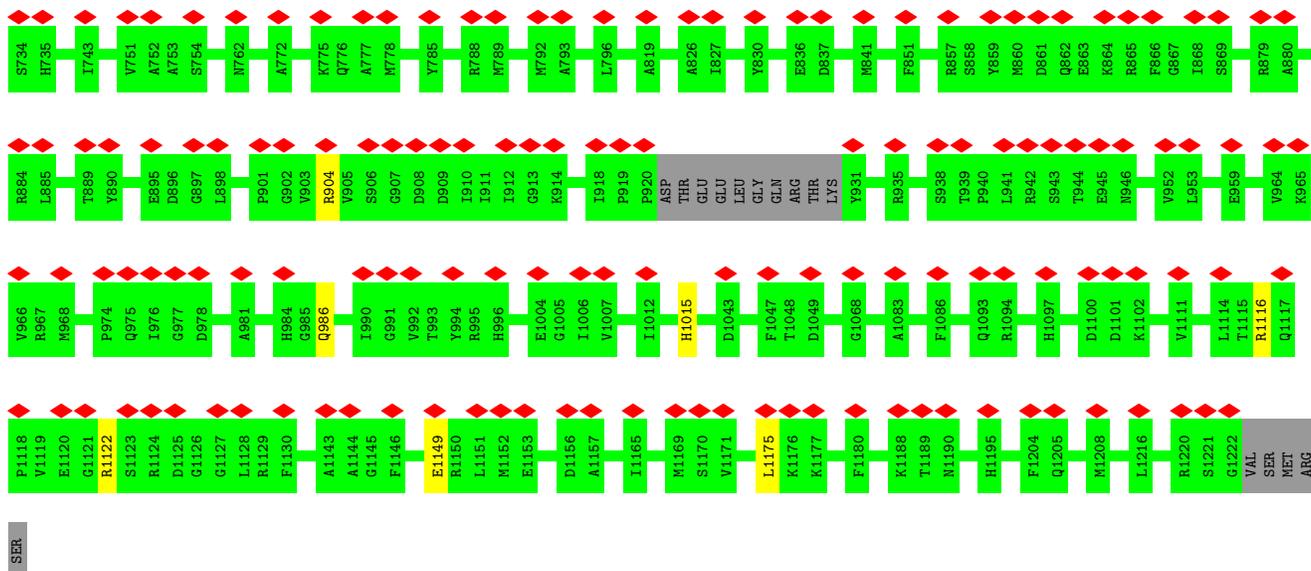
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total 1	Mg 1	0

3 Residue-property plots

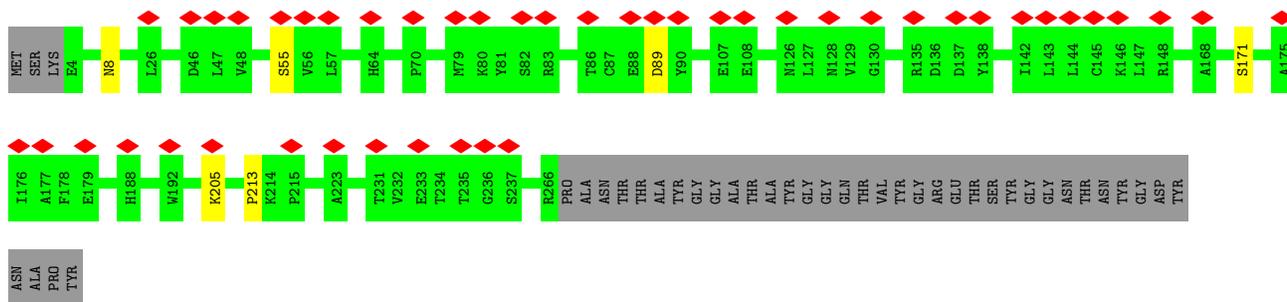
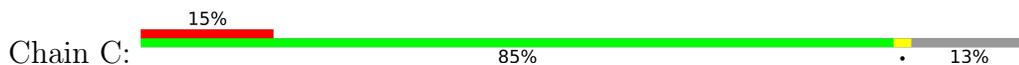
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

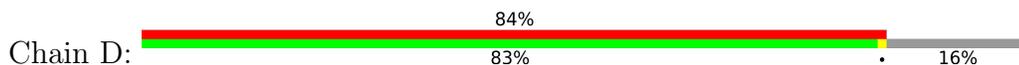




• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

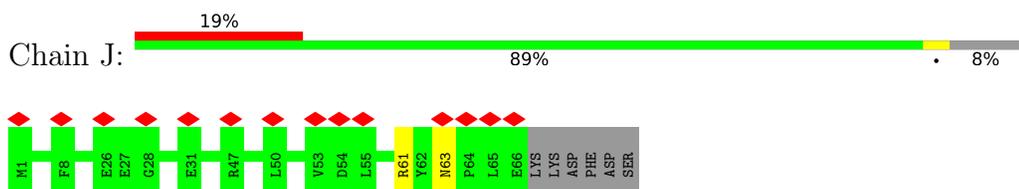


• Molecule 4: RNA polymerase II subunit B32

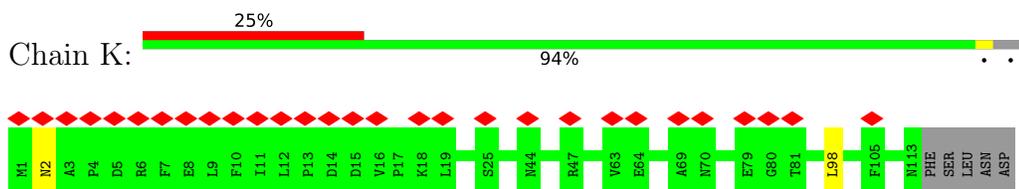


• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

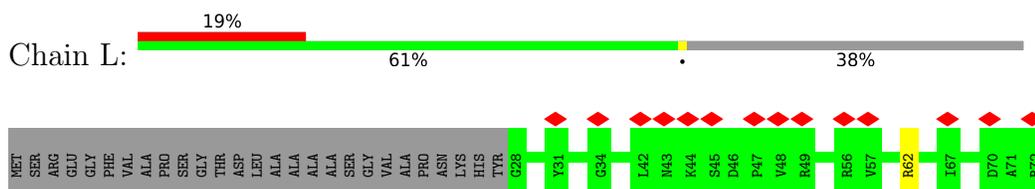
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



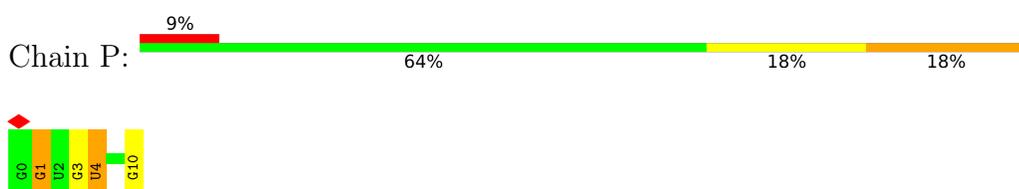
- Molecule 11: RNA polymerase II subunit B12.5



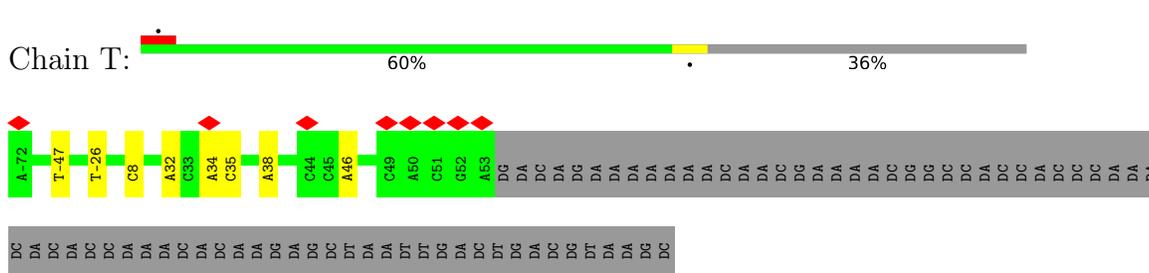
- Molecule 12: RNA polymerase subunit ABC10-alpha



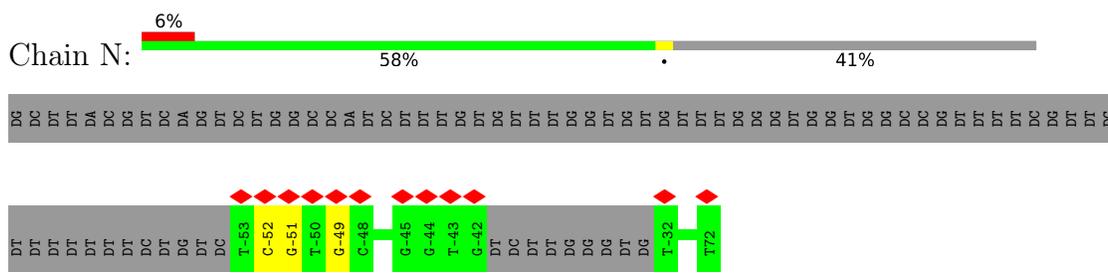
- Molecule 13: RNA (5'-R(P*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*G)-3')



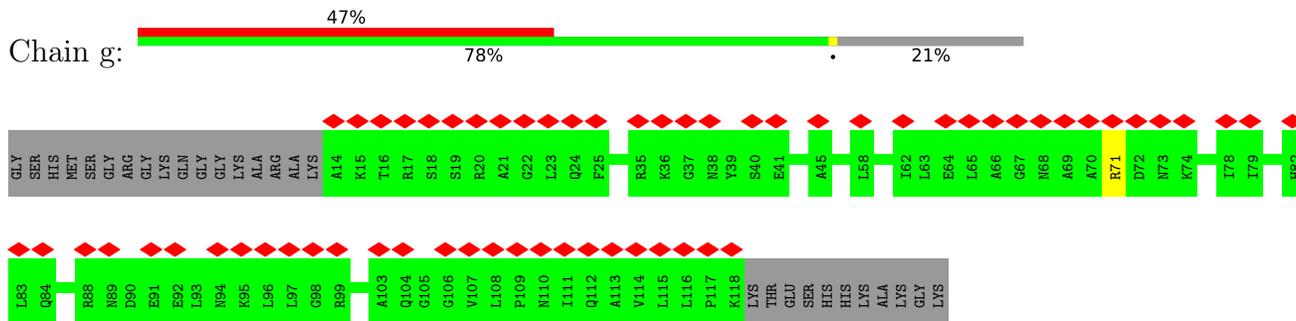
- Molecule 14: DNA (198-MER)



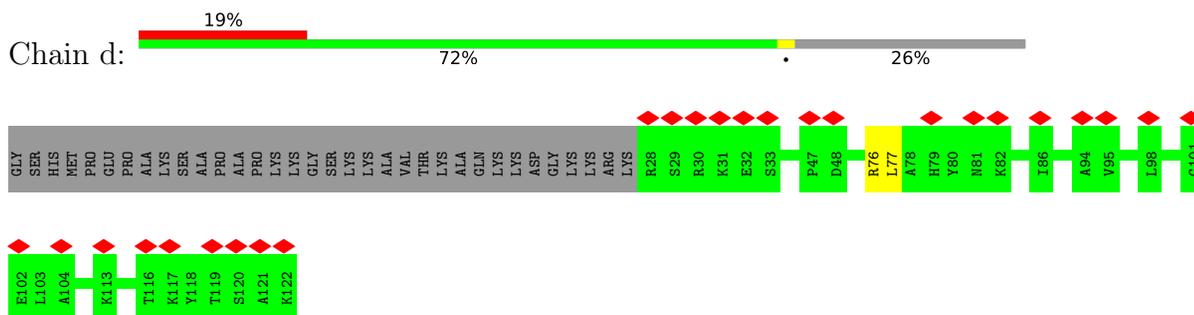
- Molecule 15: DNA (198-MER)



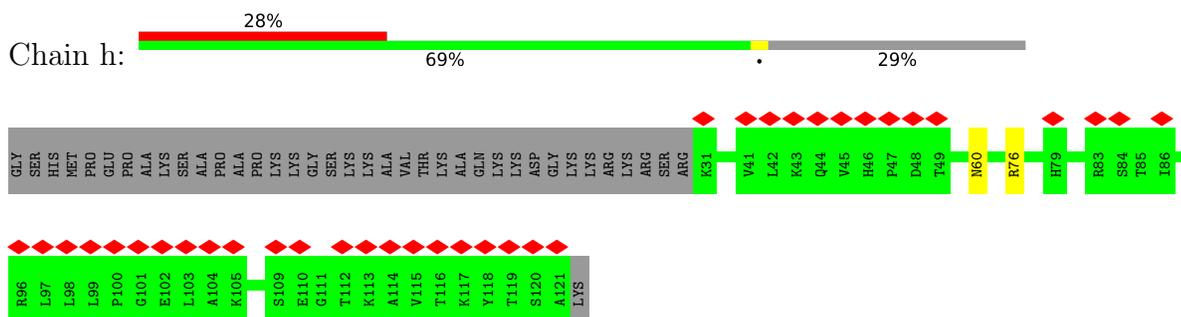
• Molecule 18: Histone H2A, Histone H2A type 1-B/E



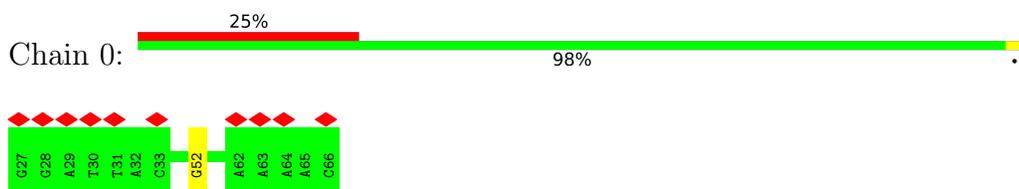
• Molecule 19: Histone H2B, Histone H2B type 1-J



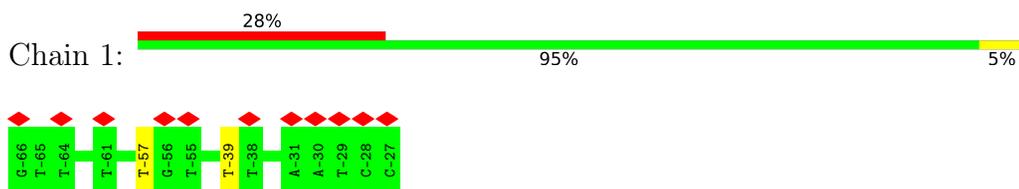
• Molecule 19: Histone H2B, Histone H2B type 1-J



• Molecule 20: DNA (40-MER)



• Molecule 21: DNA (40-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19638	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	0.156	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (\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 (\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: ZN, MG

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	0.68	0/11299	0.72	13/15266 (0.1%)
2	B	0.75	0/9441	0.75	9/12732 (0.1%)
3	C	0.72	0/2139	0.73	1/2895 (0.0%)
4	D	0.31	0/1221	0.53	0/1648
5	E	0.69	0/1772	0.69	0/2385
6	F	0.66	0/687	0.65	0/931
7	G	0.34	0/1353	0.59	1/1837 (0.1%)
8	H	0.77	0/1069	0.69	0/1444
9	I	0.43	0/934	0.58	0/1257
10	J	0.90	0/554	0.80	0/742
11	K	0.68	0/953	0.68	1/1291 (0.1%)
12	L	0.62	0/365	0.66	0/484
13	P	1.19	3/265 (1.1%)	1.28	2/412 (0.5%)
14	T	1.11	6/2880 (0.2%)	1.03	3/4438 (0.1%)
15	N	1.10	3/2701 (0.1%)	1.03	0/4168
16	a	0.42	0/809	0.61	0/1085
16	e	0.46	0/807	0.57	0/1081
17	b	0.44	0/645	0.64	0/862
17	f	0.42	0/626	0.61	0/837
18	c	0.40	0/806	0.58	0/1089
18	g	0.36	0/820	0.55	0/1107
19	d	0.45	0/757	0.56	0/1015
19	h	0.41	0/719	0.56	0/968
20	o	0.89	0/930	1.03	1/1431 (0.1%)
21	l	0.90	0/908	1.18	2/1401 (0.1%)
All	All	0.74	12/45460 (0.0%)	0.77	33/62806 (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	1
2	B	0	2
3	C	0	1
4	D	0	1
7	G	0	1
10	J	0	1
16	a	0	2
16	e	0	1
All	All	0	10

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	38	DA	C1'-N9	-8.65	1.35	1.47
15	N	-51	DG	C1'-N9	-7.74	1.36	1.47
14	T	32	DA	C1'-N9	-7.44	1.36	1.47
15	N	-49	DG	C1'-N9	-6.76	1.37	1.47
13	P	10	G	C1'-N9	-6.69	1.37	1.46
13	P	1	G	C1'-N9	-5.60	1.39	1.46
14	T	34	DA	C3'-O3'	-5.41	1.36	1.44
14	T	46	DA	C1'-N9	-5.39	1.39	1.47
15	N	-52	DC	C1'-N1	5.38	1.56	1.49
14	T	34	DA	C1'-N9	-5.33	1.39	1.47
14	T	35	DC	C3'-O3'	-5.20	1.37	1.44
13	P	3	G	C1'-N9	-5.17	1.39	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	LEU	CA-CB-CG	-9.82	92.72	115.30
2	B	556	MET	C-N-CA	-8.40	100.69	121.70
2	B	485	LEU	CA-CB-CG	-7.86	97.23	115.30
20	0	52	DG	O4'-C4'-C3'	-7.75	101.35	106.00
14	T	-26	DT	O4'-C4'-C3'	-6.86	101.76	104.50
7	G	106	LEU	CA-CB-CG	6.74	130.79	115.30
1	A	1316	LEU	CA-CB-CG	-6.38	100.64	115.30
1	A	926	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	962	LEU	CA-CB-CG	-6.09	101.29	115.30
1	A	646	LEU	CA-CB-CG	-5.98	101.54	115.30
2	B	645	LEU	CB-CG-CD2	-5.95	100.89	111.00
2	B	35	LEU	CA-CB-CG	-5.92	101.69	115.30
2	B	18	TRP	CA-CB-CG	-5.87	102.55	113.70
1	A	1107	LEU	CA-CB-CG	-5.86	101.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	LEU	CA-CB-CG	-5.85	101.84	115.30
11	K	98	LEU	CA-CB-CG	-5.81	101.94	115.30
13	P	4	U	C2-N1-C1'	5.79	124.65	117.70
2	B	450	LEU	CA-CB-CG	-5.75	102.07	115.30
14	T	-47	DT	O4'-C4'-C3'	-5.74	102.20	104.50
13	P	4	U	C6-N1-C1'	-5.67	113.26	121.20
3	C	213	PRO	C-N-CA	-5.66	107.55	121.70
1	A	1048	LEU	CA-CB-CG	-5.61	102.39	115.30
1	A	1412	LEU	CA-CB-CG	-5.59	102.44	115.30
2	B	1175	LEU	CA-CB-CG	-5.59	102.45	115.30
1	A	999	LEU	CA-CB-CG	-5.53	102.59	115.30
2	B	1116	ARG	C-N-CA	-5.52	107.89	121.70
1	A	1339	LEU	CA-CB-CG	-5.46	102.75	115.30
21	1	-57	DT	O4'-C1'-N1	5.37	111.76	108.00
1	A	868	LEU	CA-CB-CG	-5.36	102.98	115.30
1	A	1384	LEU	CA-CB-CG	-5.35	102.99	115.30
14	T	8	DC	O4'-C4'-C3'	-5.26	102.40	104.50
1	A	337	LEU	CA-CB-CG	-5.25	103.24	115.30
21	1	-39	DT	O4'-C4'-C3'	-5.04	102.48	104.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	VAL	Peptide
2	B	126	SER	Peptide
2	B	175	LEU	Peptide
3	C	89	ASP	Peptide
4	D	27	LEU	Peptide
7	G	153	ASP	Peptide
10	J	63	ASN	Peptide
16	a	42	ARG	Peptide
16	a	63	ARG	Peptide
16	e	63	ARG	Peptide

5.2 Too-close contacts

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	1396/1743 (80%)	1139 (82%)	234 (17%)	23 (2%)	9	44
2	B	1151/1227 (94%)	925 (80%)	216 (19%)	10 (1%)	17	57
3	C	261/304 (86%)	207 (79%)	51 (20%)	3 (1%)	14	52
4	D	148/186 (80%)	136 (92%)	12 (8%)	0	100	100
5	E	211/214 (99%)	175 (83%)	32 (15%)	4 (2%)	8	38
6	F	82/155 (53%)	73 (89%)	9 (11%)	0	100	100
7	G	169/171 (99%)	154 (91%)	15 (9%)	0	100	100
8	H	129/145 (89%)	104 (81%)	24 (19%)	1 (1%)	19	60
9	I	109/115 (95%)	88 (81%)	19 (17%)	2 (2%)	8	40
10	J	64/72 (89%)	53 (83%)	10 (16%)	1 (2%)	9	44
11	K	111/118 (94%)	101 (91%)	9 (8%)	1 (1%)	17	57
12	L	43/72 (60%)	31 (72%)	12 (28%)	0	100	100
16	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
16	e	95/139 (68%)	86 (90%)	9 (10%)	0	100	100
17	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
17	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100
18	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
18	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
19	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
19	h	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	4604/5536 (83%)	3864 (84%)	695 (15%)	45 (1%)	20	54

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU

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Mol	Chain	Res	Type
1	A	453	LYS
1	A	537	LEU
2	B	257	THR
2	B	1015	HIS
9	I	96	ASN
10	J	61	ARG
1	A	455	SER
1	A	518	ASN
1	A	1320	MET
2	B	175	LEU
2	B	299	ASP
2	B	458	ASN
2	B	534	LEU
5	E	104	PHE
5	E	171	GLU
8	H	18	GLY
9	I	97	MET
1	A	114	LEU
1	A	673	ASP
1	A	811	PRO
1	A	1064	GLU
1	A	1065	MET
2	B	986	GLN
3	C	55	SER
3	C	205	LYS
5	E	37	SER
1	A	117	GLU
1	A	526	GLN
1	A	594	GLY
1	A	640	PRO
1	A	917	ALA
1	A	921	LEU
2	B	1149	GLU
11	K	2	ASN
1	A	610	ASP
2	B	51	TRP
5	E	182	PRO
1	A	959	PRO
1	A	1109	VAL
3	C	171	SER
2	B	403	GLY
1	A	515	PRO

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Mol	Chain	Res	Type
1	A	1382	GLY
1	A	569	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	A	1223/1528 (80%)	1219 (100%)	4 (0%)	92	95
2	B	1016/1077 (94%)	1009 (99%)	7 (1%)	84	90
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	94
4	D	133/160 (83%)	133 (100%)	0	100	100
5	E	196/197 (100%)	192 (98%)	4 (2%)	55	74
6	F	75/137 (55%)	74 (99%)	1 (1%)	69	81
7	G	148/148 (100%)	147 (99%)	1 (1%)	84	90
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	66
16	a	83/112 (74%)	82 (99%)	1 (1%)	71	83
16	e	82/112 (73%)	80 (98%)	2 (2%)	49	69
17	b	65/81 (80%)	63 (97%)	2 (3%)	40	62
17	f	63/81 (78%)	62 (98%)	1 (2%)	62	79
18	c	82/102 (80%)	82 (100%)	0	100	100
18	g	83/102 (81%)	82 (99%)	1 (1%)	71	83
19	d	81/107 (76%)	79 (98%)	2 (2%)	47	68
19	h	77/107 (72%)	75 (97%)	2 (3%)	46	66
All	All	4071/4785 (85%)	4040 (99%)	31 (1%)	82	89

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	446	ASN
1	A	661	ASN
1	A	737	ASN
2	B	184	LYS
2	B	196	ILE
2	B	240	ARG
2	B	500	LYS
2	B	710	ARG
2	B	904	ARG
2	B	1122	ARG
3	C	8	ASN
5	E	4	ASN
5	E	120	ASN
5	E	166	ARG
5	E	182	PRO
6	F	129	LYS
7	G	125	ASN
9	I	105	ASN
12	L	62	ARG
16	a	108	ASN
17	b	72	TYR
17	b	92	ARG
19	d	76	ARG
19	d	77	LEU
16	e	53	ARG
16	e	84	PHE
17	f	92	ARG
18	g	71	ARG
19	h	60	ASN
19	h	76	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	136	ASN
1	A	172	GLN
1	A	340	ASN
1	A	359	ASN
1	A	364	GLN

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Mol	Chain	Res	Type
1	A	398	ASN
1	A	446	ASN
1	A	494	GLN
1	A	661	ASN
1	A	700	HIS
1	A	787	HIS
1	A	882	GLN
1	A	961	ASN
1	A	1013	GLN
1	A	1015	ASN
1	A	1137	GLN
1	A	1393	ASN
1	A	1435	GLN
2	B	47	GLN
2	B	66	ASN
2	B	108	ASN
2	B	206	GLN
2	B	426	GLN
2	B	462	GLN
2	B	735	HIS
2	B	736	HIS
2	B	986	GLN
2	B	996	HIS
3	C	8	ASN
4	D	46	HIS
4	D	99	ASN
4	D	144	GLN
4	D	179	ASN
5	E	4	ASN
5	E	100	GLN
5	E	112	GLN
7	G	125	ASN
9	I	11	ASN
9	I	46	HIS
9	I	90	GLN
9	I	96	ASN
9	I	105	ASN
11	K	2	ASN
11	K	44	ASN
18	c	89	ASN
19	d	64	ASN
16	e	68	GLN

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Mol	Chain	Res	Type
18	g	31	HIS
18	g	110	ASN
18	g	112	GLN
19	h	46	HIS
19	h	64	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	10/11 (90%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	1	G
13	P	4	U

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.

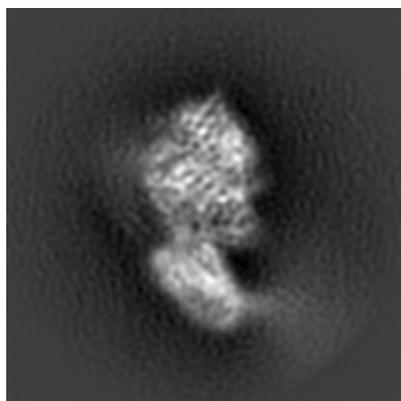
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6985. These allow visual inspection of the internal detail of the map and identification of artifacts.

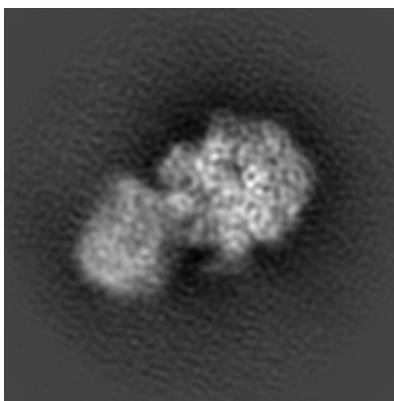
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

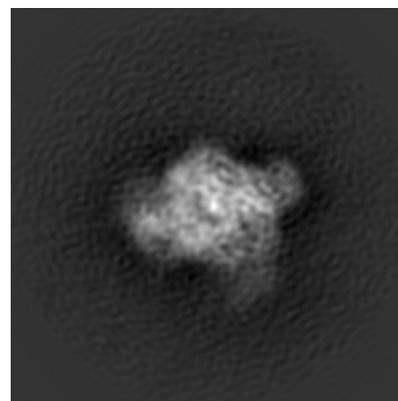
6.1.1 Primary map



X



Y

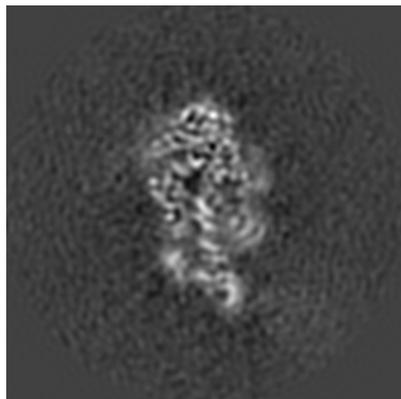


Z

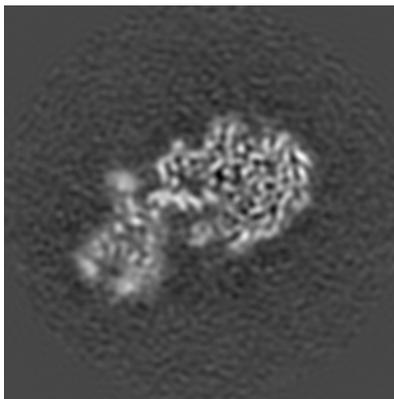
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

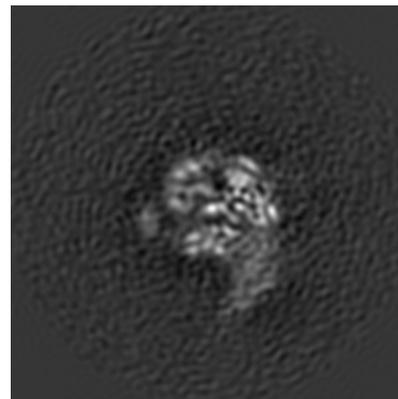
6.2.1 Primary map



X Index: 120



Y Index: 120

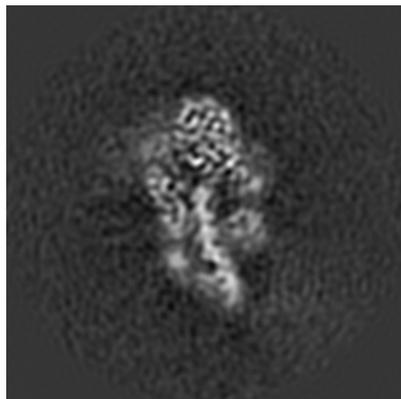


Z Index: 120

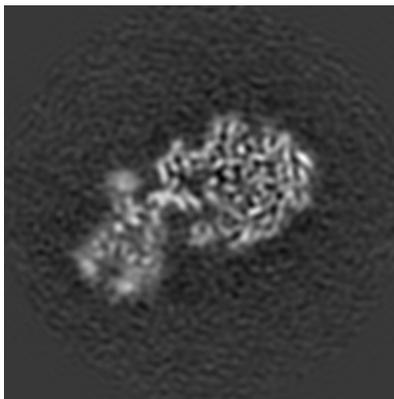
The images above show central slices of the map in three orthogonal directions.

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

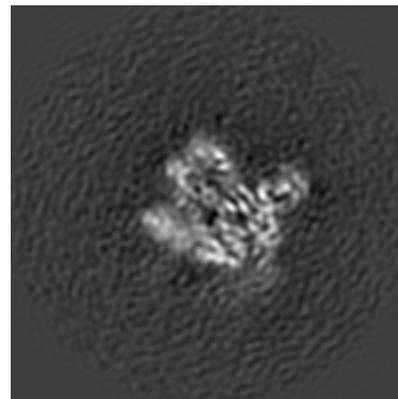
6.3.1 Primary map



X Index: 123



Y Index: 121

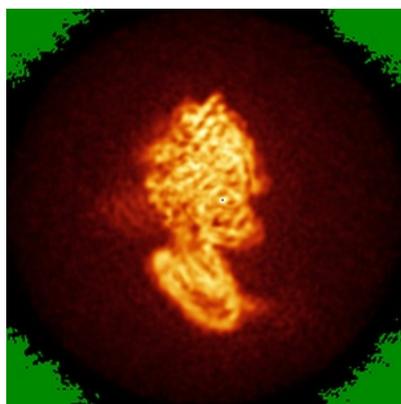


Z Index: 133

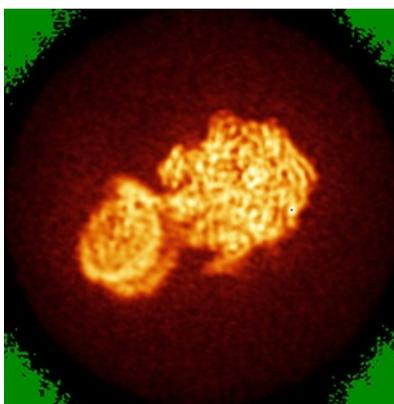
The images above show the largest variance slices of the map in three orthogonal directions.

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

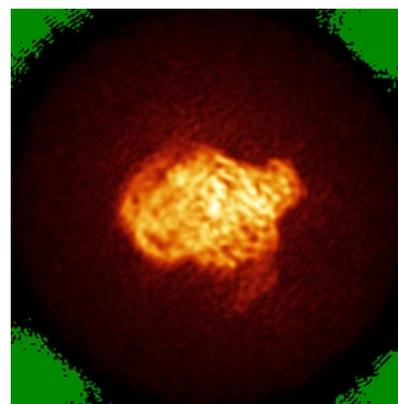
6.4.1 Primary map



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

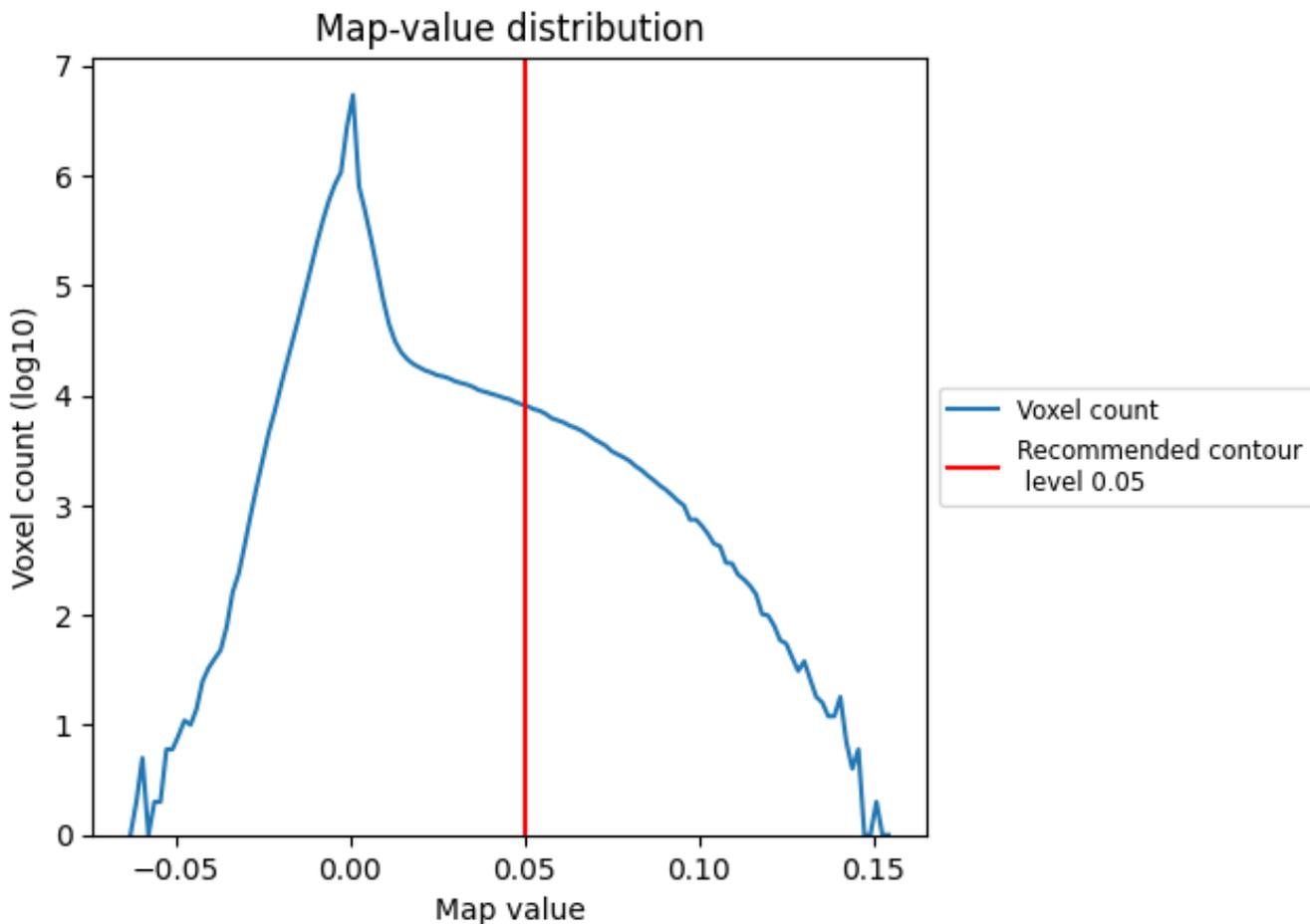
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

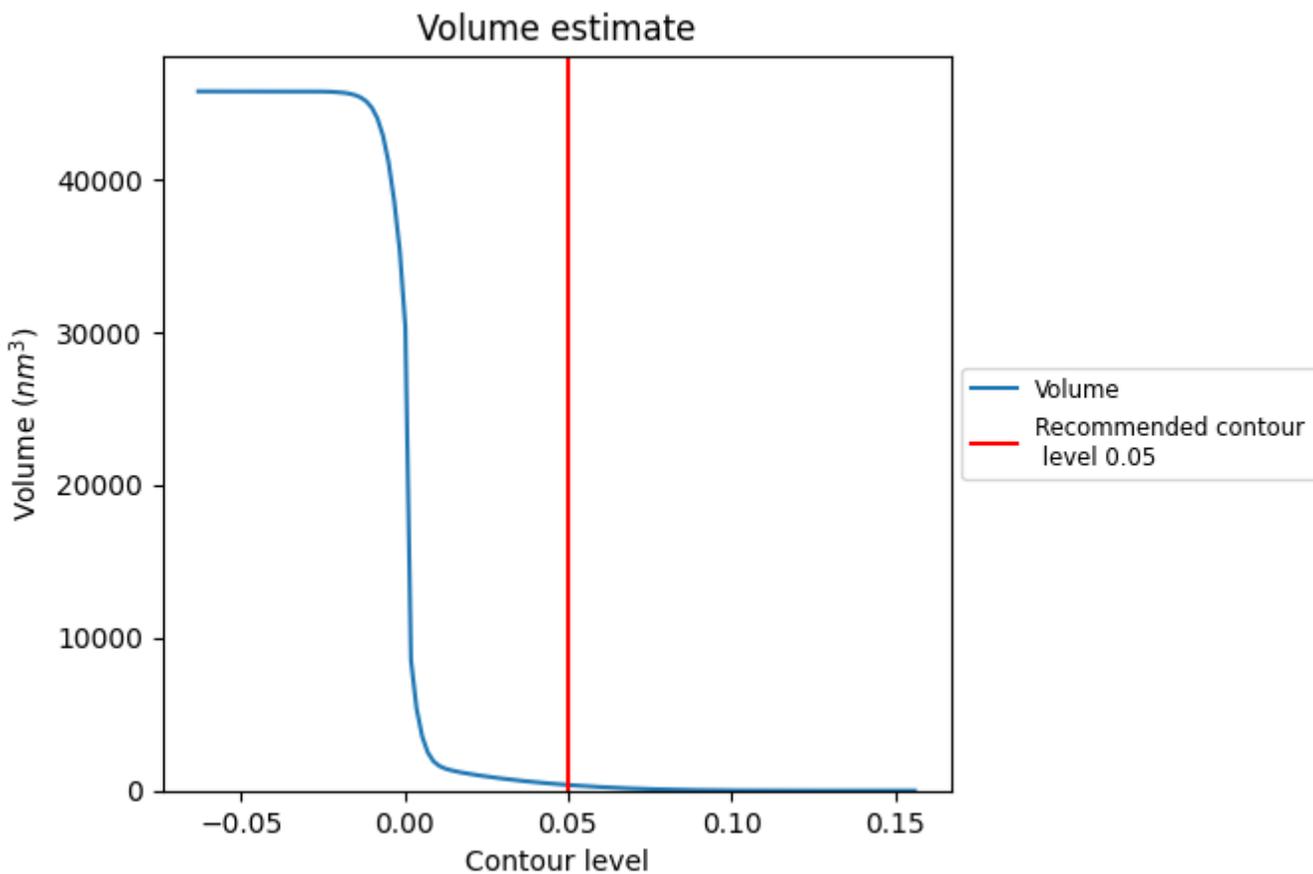
This section contains the results of statistical analysis of the map.

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.

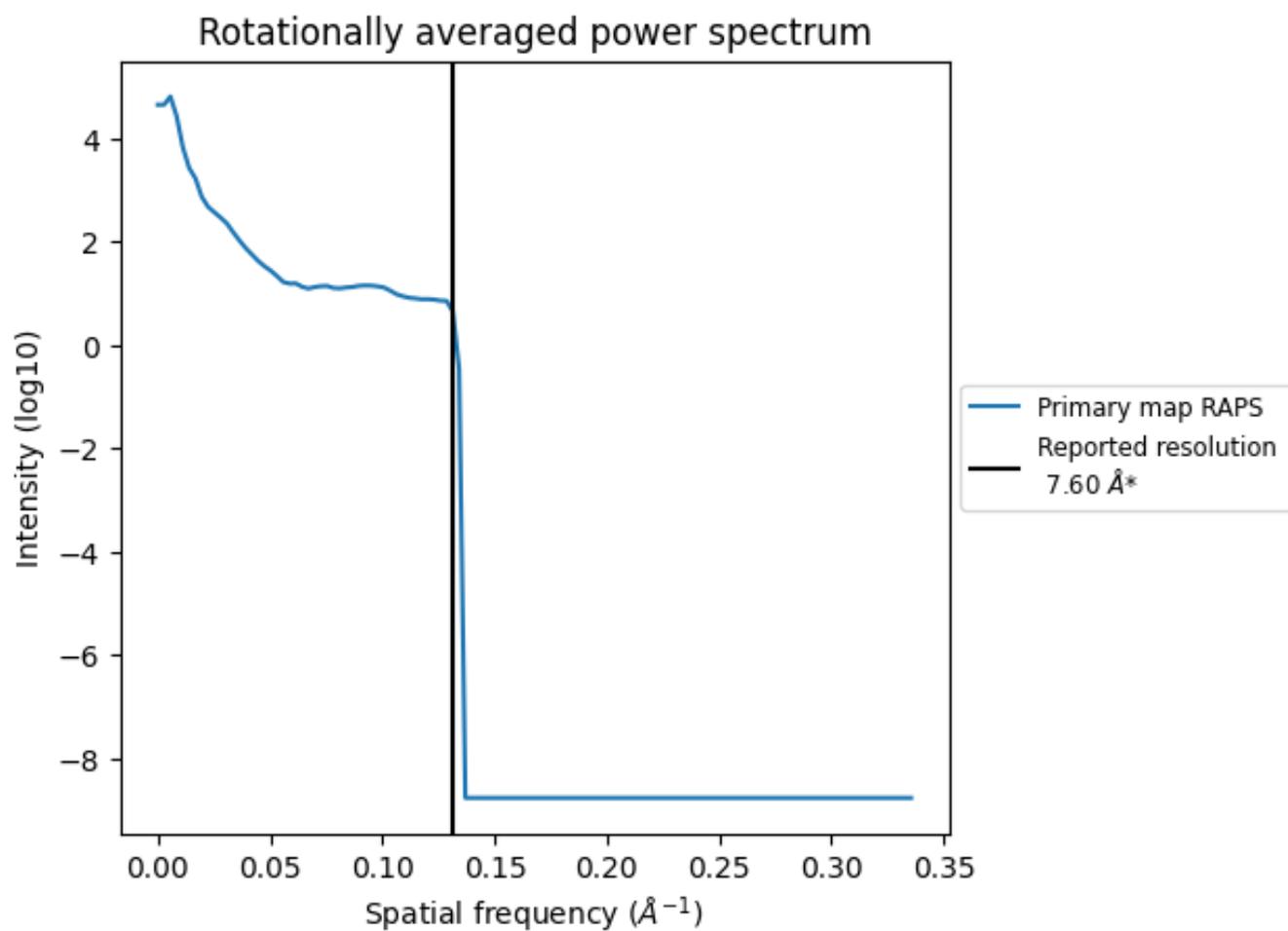
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm³; this corresponds to an approximate mass of 336 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 [\(i\)](#)

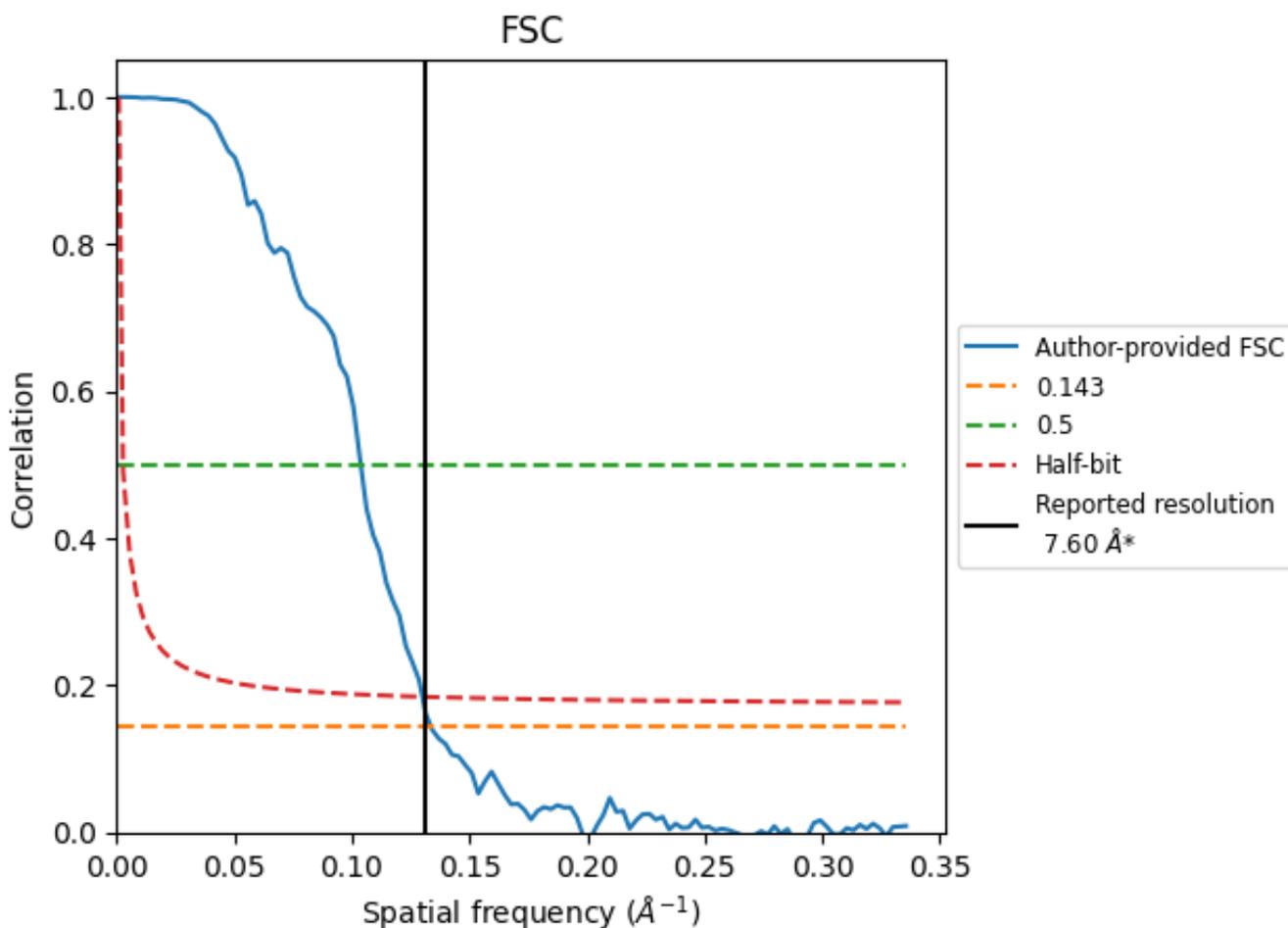


*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

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 0.132 Å⁻¹

8.2 Resolution estimates [i](#)

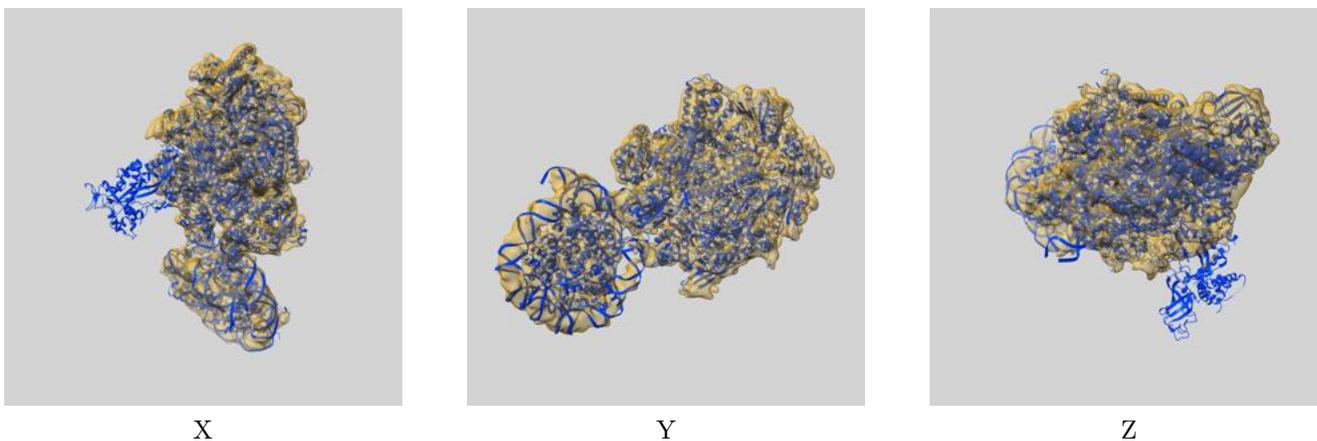
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	7.48	9.63	7.69
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

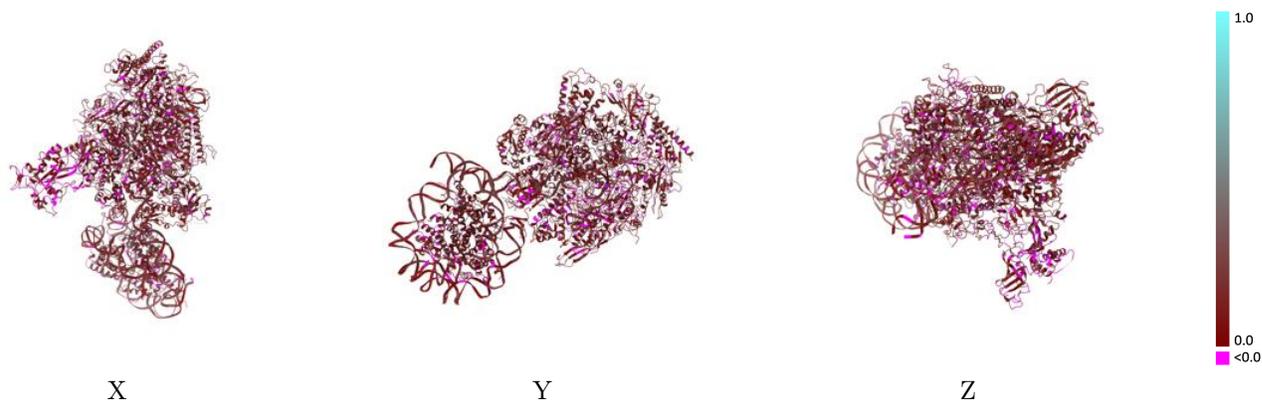
This section contains information regarding the fit between EMDB map EMD-6985 and PDB model 6A5U. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



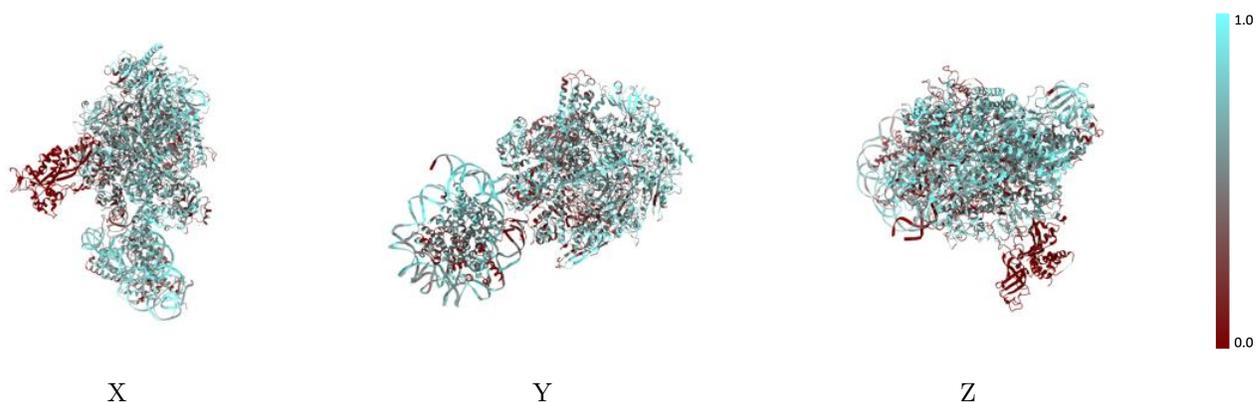
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



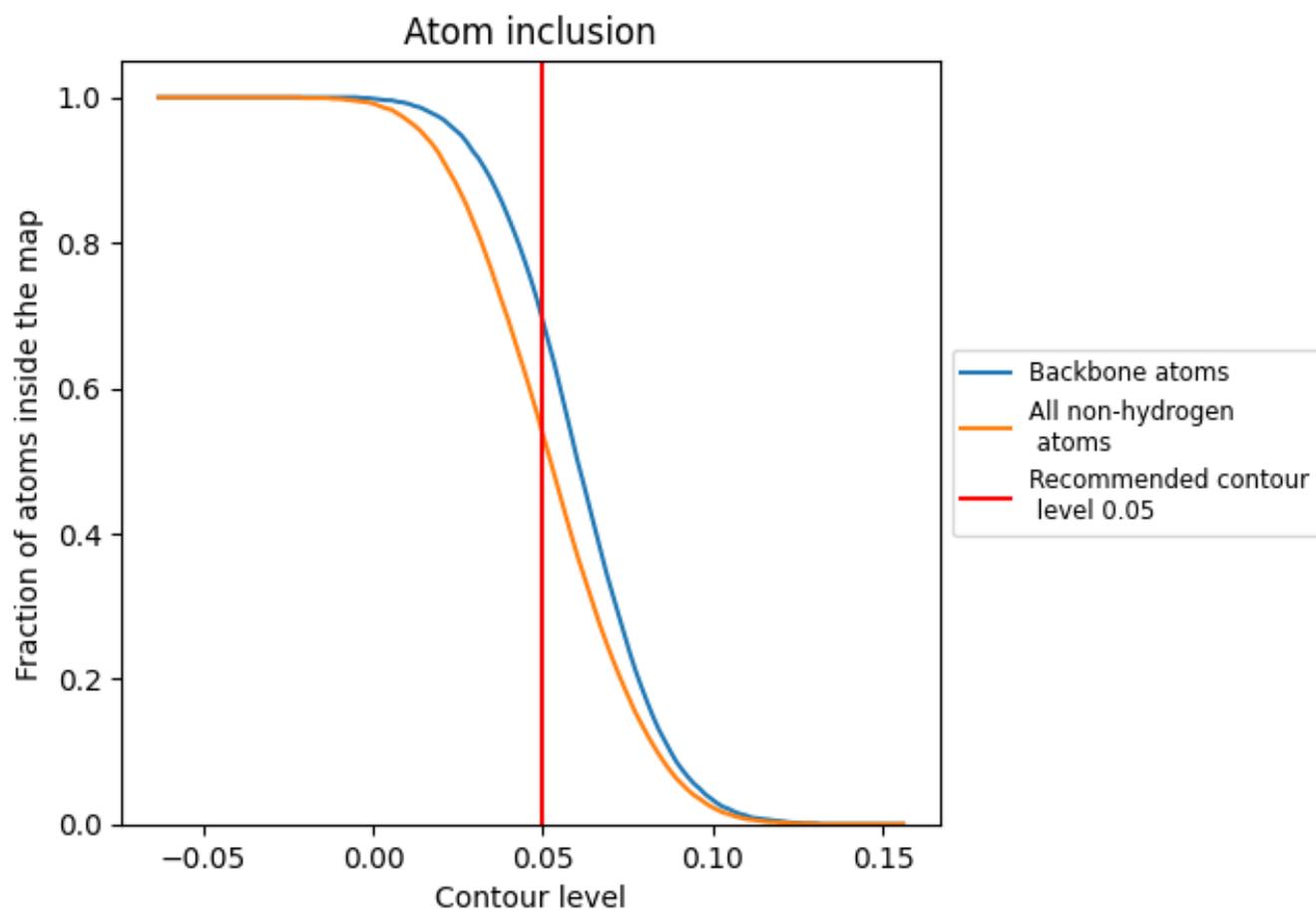
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 54% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5360	 0.1400
0	 0.5420	 0.1100
1	 0.5120	 0.1140
A	 0.5480	 0.1500
B	 0.5250	 0.1350
C	 0.6400	 0.1420
D	 0.0020	 0.0480
E	 0.6680	 0.1670
F	 0.5760	 0.1660
G	 0.0170	 0.0780
H	 0.6920	 0.1670
I	 0.2600	 0.1040
J	 0.6250	 0.1270
K	 0.6030	 0.1360
L	 0.5490	 0.1450
N	 0.7200	 0.1690
P	 0.6850	 0.2090
T	 0.7410	 0.1830
a	 0.4500	 0.1080
b	 0.4980	 0.1160
c	 0.5600	 0.1320
d	 0.5430	 0.1460
e	 0.5950	 0.1450
f	 0.6050	 0.1230
g	 0.3460	 0.0950
h	 0.4560	 0.1320

