



Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 06:22 AM JST

PDB ID : 6IR9
EMDB ID : EMD-9713
Title : RNA polymerase II elongation complex bound with Elf1 and Spt4/5, stalled at SHL(-1) of the nucleosome
Authors : Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2018-11-12
Resolution : 3.80 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:

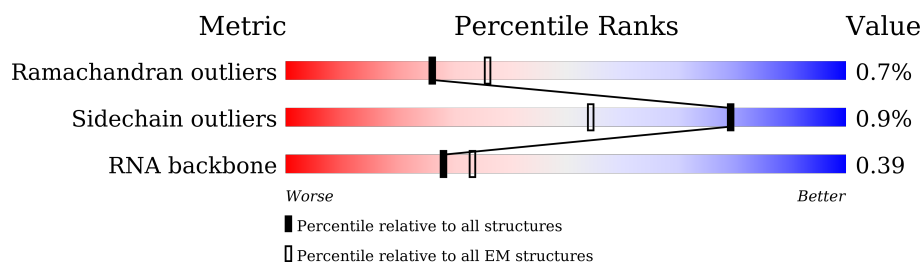
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	
10	J	72	
11	K	118	
12	L	72	
13	P	16	
14	T	198	
15	N	198	
16	M	113	
17	V	108	
18	W	911	
19	a	139	
19	e	139	
20	b	106	
20	f	106	
21	c	133	
21	g	133	
22	d	129	
22	h	129	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 46231 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	1412	Total	C	N	O	S	0	0
			11123	7014	1938	2101	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9228	5816	1630	1724	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	168	Total	C	N	O	S	0	0
			1314	812	237	263	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*GP*CP*CP*UP*GP*GP*UP*GP*UP*C P*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 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called Spt5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	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 19 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
19	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 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
20	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

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

- Molecule 21 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	103	Total	C	N	O	0	0
			796	502	155	139		
21	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 22 is a protein called Histone H2B type 1-J.

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

There are 6 discrepancies between the modelled and reference sequences:

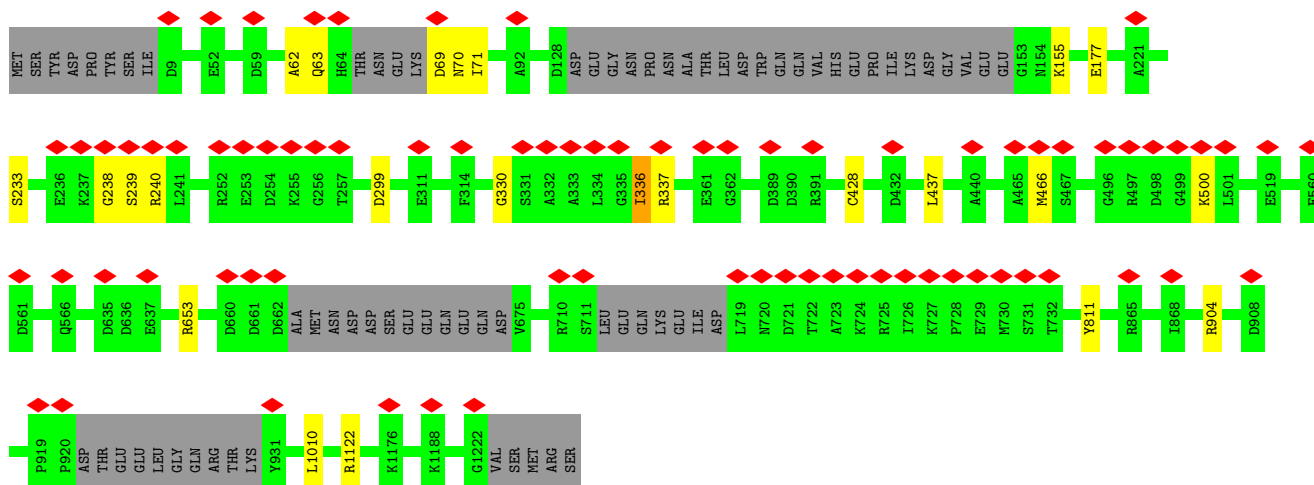
Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

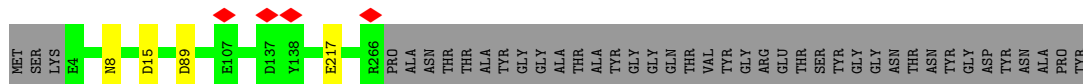
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



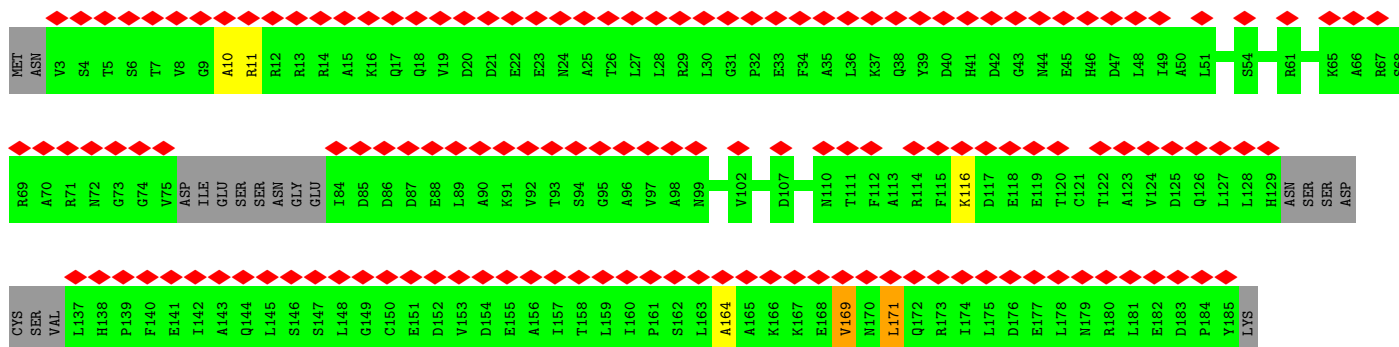
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C: 85% 13%



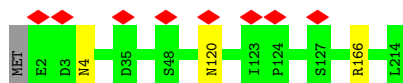
- Molecule 4: RNA polymerase II subunit B32

Chain D: 78% 87% 10%



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

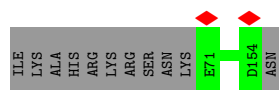
Chain E: 98%



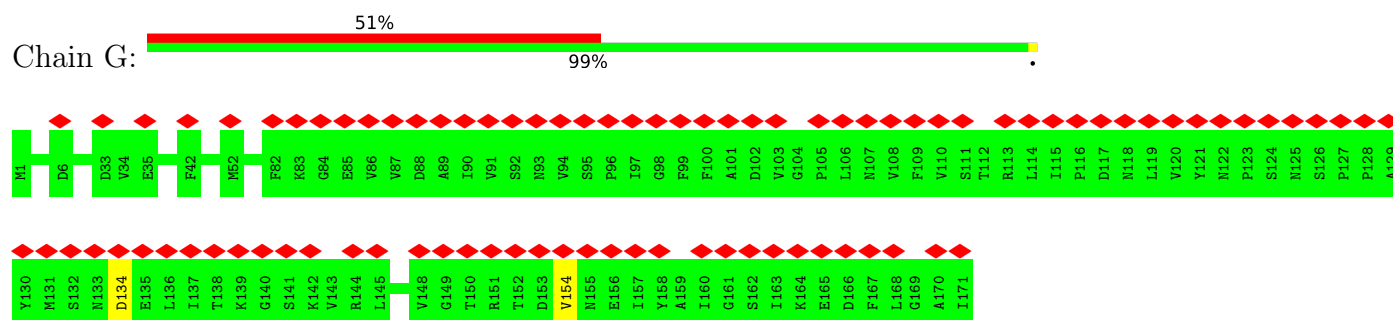
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F: 54% 46%

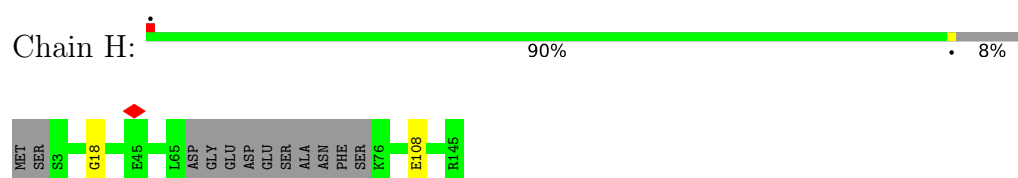




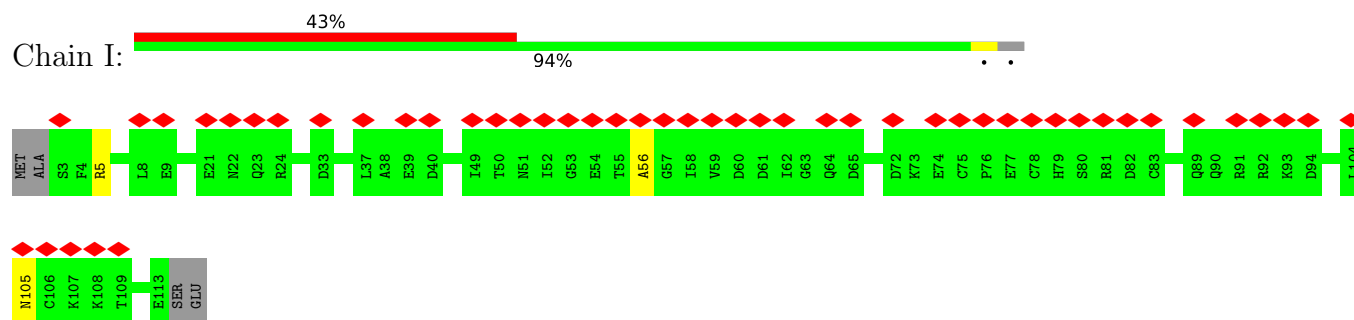
- Molecule 7: RNA polymerase II subunit



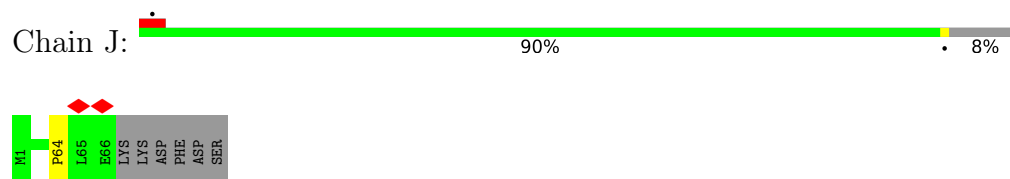
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



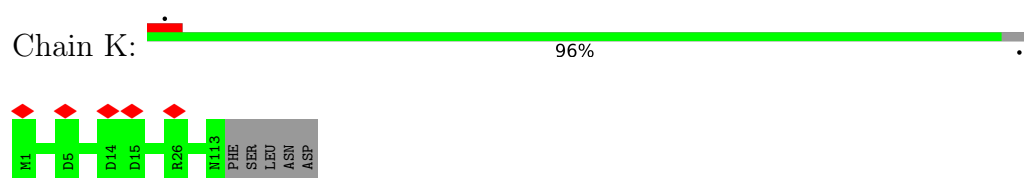
- Molecule 9: DNA-directed RNA polymerase subunit



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



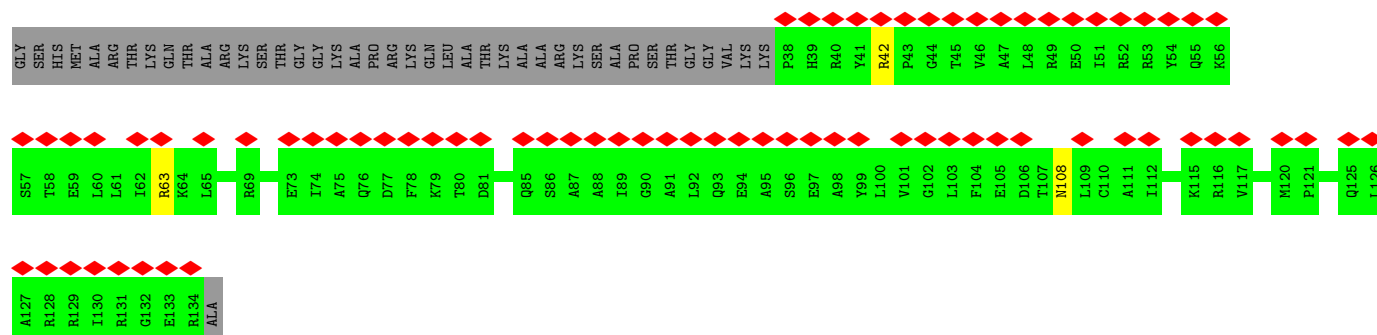
- Molecule 11: RNA polymerase II subunit B12.5



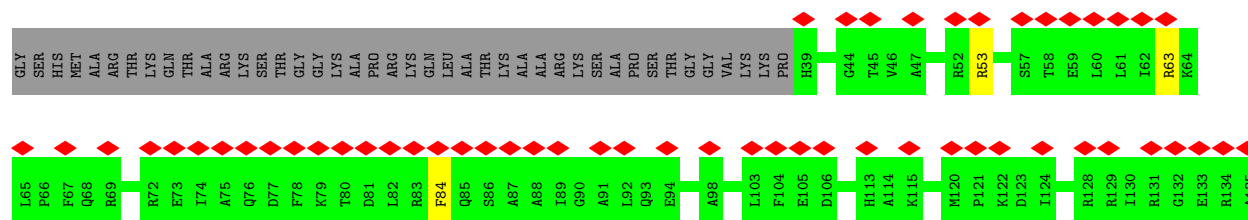
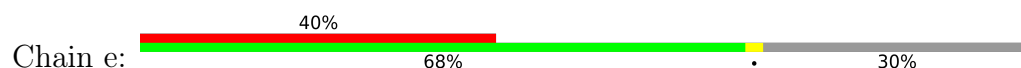
- Molecule 12: RNA polymerase subunit ABC10-alpha



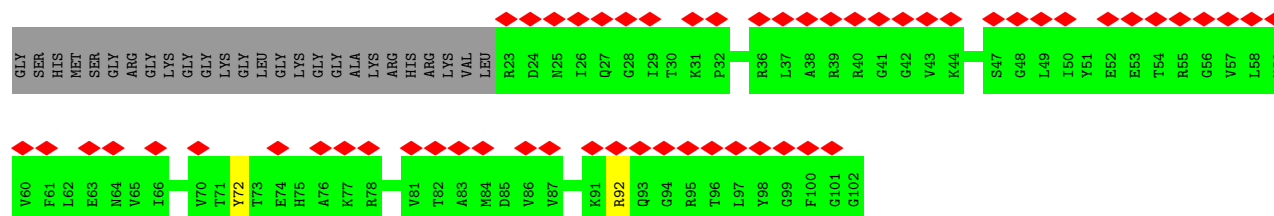
- Molecule 19: Histone H3.3



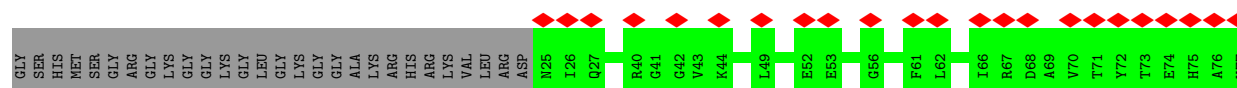
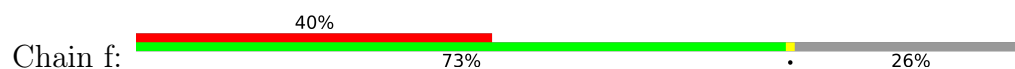
- Molecule 19: Histone H3.3



- Molecule 20: Histone H4

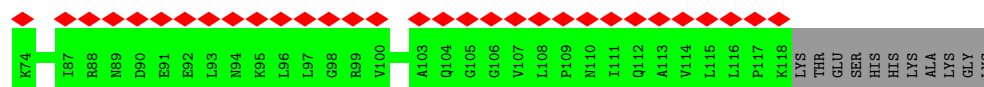
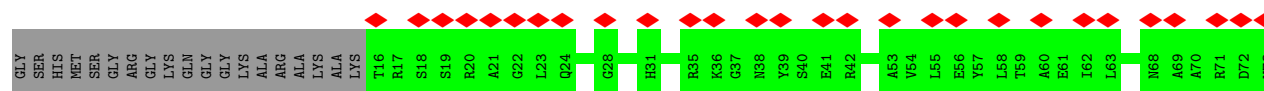
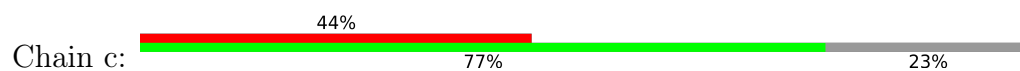


- Molecule 20: Histone H4

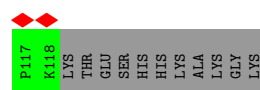
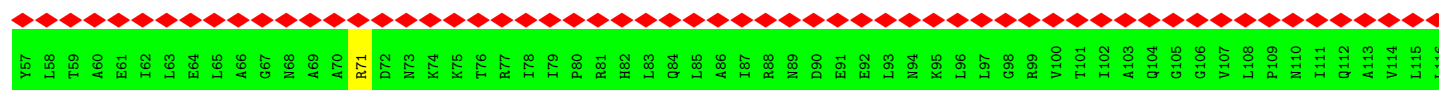
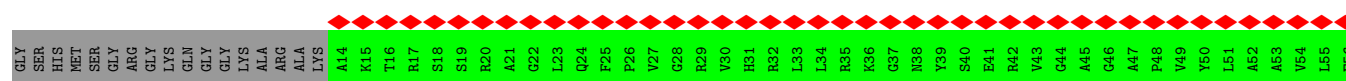
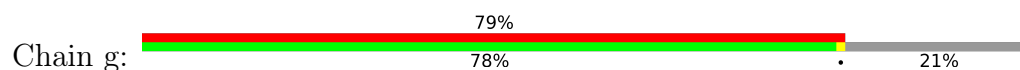




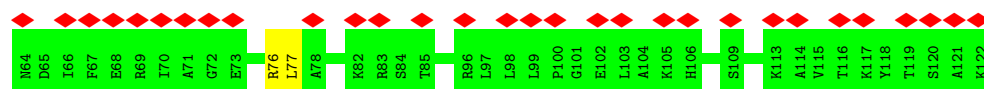
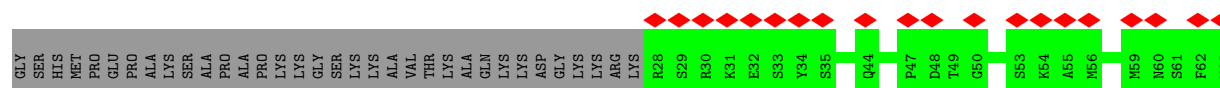
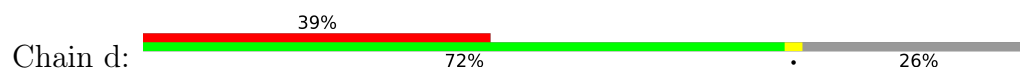
• Molecule 21: Histone H2A type 1-B/E



• Molecule 21: Histone H2A type 1-B/E



• Molecule 22: Histone H2B type 1-J



• Molecule 22: Histone H2B type 1-J



A114	V115	T116	K117	Y118	T119	S120	A121	LYS	K54	A55	M56	G57	I58	M59	N60	S61	F62	V63	N64	D65	I66	F67	E68	R69	I70	A71	G72	E73	A74	S75	R76	L77	A78	H79	Y80	K82	S84	R83	T85	I86	T87	S88	R89	E90	T91	Q92	T93	A94	V95	R96	L97	L98	L99	P100	G101	E102	L103	A104	K105	H106	A107	V108	S109	E110	G111	T112	K113
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96742	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 ($e^-/\text{\AA}^2$)	50.0	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	0.083	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0165	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 ⓘ

5.1 Standard geometry ⓘ

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	0.44	0/11329	0.67	6/15310 (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	0.71	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	1.19	6/379 (1.6%)	1.28	2/589 (0.3%)
14	T	1.11	8/2929 (0.3%)	1.10	3/4514 (0.1%)
15	N	1.13	7/2831 (0.2%)	1.08	0/4368
16	M	0.25	0/513	0.46	0/693
17	V	0.46	0/808	0.60	0/1097
18	W	0.40	0/2267	0.68	4/3048 (0.1%)
19	a	0.42	0/809	0.61	0/1085
19	e	0.54	1/807 (0.1%)	0.55	0/1081
20	b	0.44	0/645	0.64	0/862
20	f	0.42	0/626	0.62	0/837
21	c	0.40	0/806	0.58	0/1089
21	g	0.36	0/820	0.55	0/1107
22	d	0.45	0/757	0.56	0/1015
22	h	0.41	0/719	0.56	0/968
All	All	0.57	22/47604 (0.0%)	0.75	25/65402 (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
19	a	0	2
19	e	0	1
All	All	0	4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	e	84	PHE	C-N	8.54	1.53	1.34
14	T	17	DA	C1'-N9	-8.51	1.35	1.47
15	N	-15	DA	C1'-N9	-7.85	1.36	1.47
13	P	-5	G	C1'-N9	-7.33	1.36	1.46
13	P	2	G	C1'-N9	-7.28	1.36	1.46
13	P	-1	G	C1'-N9	-7.27	1.36	1.46
13	P	4	C	C1'-N1	7.20	1.59	1.48
14	T	40	DG	C1'-N9	-6.61	1.38	1.47
14	T	27	DG	C1'-N9	-6.55	1.38	1.47
14	T	43	DA	C1'-N9	-6.43	1.38	1.47
15	N	-54	DC	C1'-N1	6.27	1.57	1.49
15	N	-52	DC	C1'-N1	6.17	1.57	1.49
13	P	6	U	C1'-N1	5.82	1.57	1.48
15	N	-43	DT	C1'-N1	5.37	1.56	1.49
15	N	-55	DT	C1'-N1	5.26	1.56	1.49
15	N	-50	DT	C1'-N1	5.25	1.56	1.49
14	T	44	DC	C1'-N1	5.24	1.56	1.49
15	N	-47	DC	C1'-N1	5.22	1.56	1.49
13	P	1	U	C1'-N1	5.17	1.56	1.48
14	T	30	DT	C1'-N1	5.09	1.55	1.49
14	T	51	DC	C1'-N1	5.06	1.55	1.49
14	T	39	DA	C3'-O3'	-5.01	1.37	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	389	PRO	CA-N-CD	-8.57	99.50	111.50
1	A	473	LEU	CA-CB-CG	-8.23	96.38	115.30
2	B	63	GLN	N-CA-CB	-7.70	96.75	110.60
2	B	63	GLN	N-CA-C	-6.93	92.28	111.00
14	T	-26	DT	O4'-C4'-C3'	-6.92	101.73	104.50
1	A	721	ARG	NE-CZ-NH1	-6.49	117.06	120.30
18	W	749	ASP	CB-CG-OD1	6.46	124.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	5	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	306	ASP	CB-CG-OD1	5.93	123.63	118.30
2	B	811	TYR	CB-CG-CD1	-5.88	117.47	121.00
13	P	4	C	C2-N1-C1'	5.74	125.11	118.80
1	A	1452	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	336	ILE	CA-CB-CG2	5.69	122.28	110.90
4	D	169	VAL	CA-CB-CG1	5.54	119.20	110.90
14	T	-47	DT	O4'-C4'-C3'	-5.52	102.29	104.50
9	I	5	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	1010	LEU	CA-CB-CG	5.41	127.75	115.30
14	T	8	DC	O4'-C4'-C3'	-5.39	102.34	104.50
2	B	330	GLY	N-CA-C	5.37	126.51	113.10
1	A	55	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	55	ASP	CB-CG-OD2	-5.26	113.56	118.30
13	P	4	C	C6-N1-C1'	-5.21	114.54	120.80
18	W	363	ASP	CB-CG-OD2	5.19	122.97	118.30
18	W	409	ASP	CB-CG-OD2	5.14	122.93	118.30
3	C	15	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	ILE	Mainchain
19	a	42	ARG	Peptide
19	a	63	ARG	Peptide
19	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	1400/1743 (80%)	1343 (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	57
4	D	162/186 (87%)	149 (92%)	9 (6%)	4 (2%)	5	36
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	50
8	H	129/145 (89%)	125 (97%)	2 (2%)	2 (2%)	9	44
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	44
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	0	1 (2%)	6	38
16	M	62/113 (55%)	58 (94%)	4 (6%)	0	100	100
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	265/911 (29%)	246 (93%)	17 (6%)	2 (1%)	19	57
19	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
19	e	95/139 (68%)	87 (92%)	8 (8%)	0	100	100
20	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
20	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100
21	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
21	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
22	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
22	h	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	5043/6668 (76%)	4793 (95%)	217 (4%)	33 (1%)	26	60

All (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

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Mol	Chain	Res	Type
2	B	155	LYS
2	B	239	SER
2	B	337	ARG
3	C	89	ASP
7	G	134	ASP
8	H	108	GLU
12	L	44	LYS
18	W	320	LEU
1	A	284	GLY
1	A	977	ARG
1	A	1223	SER
2	B	62	ALA
2	B	177	GLU
2	B	299	ASP
4	D	169	VAL
4	D	171	LEU
7	G	154	VAL
8	H	18	GLY
1	A	979	LYS
4	D	10	ALA
9	I	56	ALA
1	A	47	ARG
2	B	437	LEU
3	C	217	GLU
4	D	164	ALA
1	A	43	GLU
2	B	238	GLY
10	J	64	PRO
18	W	806	PRO

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	1225/1528 (80%)	1218 (99%)	7 (1%)	86	92
2	B	1012/1077 (94%)	1001 (99%)	11 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	95
4	D	143/160 (89%)	140 (98%)	3 (2%)	53	74
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	81
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	88
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	69
16	M	61/99 (62%)	61 (100%)	0	100	100
17	V	86/92 (94%)	85 (99%)	1 (1%)	71	84
18	W	241/796 (30%)	239 (99%)	2 (1%)	81	89
19	a	83/112 (74%)	82 (99%)	1 (1%)	71	84
19	e	82/112 (73%)	81 (99%)	1 (1%)	71	84
20	b	65/81 (80%)	63 (97%)	2 (3%)	40	65
20	f	63/81 (78%)	62 (98%)	1 (2%)	62	79
21	c	82/102 (80%)	82 (100%)	0	100	100
21	g	83/102 (81%)	82 (99%)	1 (1%)	71	84
22	d	81/107 (76%)	79 (98%)	2 (2%)	47	70
22	h	77/107 (72%)	75 (97%)	2 (3%)	46	69
All	All	4467/5772 (77%)	4427 (99%)	40 (1%)	79	88

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	248	ARG
1	A	473	LEU
1	A	661	ASN
1	A	737	ASN
1	A	977	ARG
1	A	1459	ASP
2	B	69	ASP
2	B	70	ASN

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Mol	Chain	Res	Type
2	B	71	ILE
2	B	233	SER
2	B	240	ARG
2	B	428	CYS
2	B	466	MET
2	B	500	LYS
2	B	653	ARG
2	B	904	ARG
2	B	1122	ARG
3	C	8	ASN
4	D	11	ARG
4	D	116	LYS
4	D	171	LEU
5	E	4	ASN
5	E	120	ASN
5	E	166	ARG
9	I	105	ASN
12	L	62	ARG
17	V	33	ASP
18	W	264	GLN
18	W	313	VAL
19	a	108	ASN
20	b	72	TYR
20	b	92	ARG
22	d	76	ARG
22	d	77	LEU
19	e	53	ARG
20	f	92	ARG
21	g	71	ARG
22	h	60	ASN
22	h	76	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	197	GLN
1	A	651	GLN
1	A	661	ASN
1	A	787	HIS
1	A	1190	GLN
1	A	1435	GLN

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Mol	Chain	Res	Type
2	B	887	HIS
2	B	996	HIS
3	C	8	ASN
3	C	13	GLN
3	C	242	GLN
5	E	4	ASN
5	E	145	HIS
5	E	193	GLN
8	H	13	GLN
9	I	12	ASN
9	I	90	GLN
9	I	105	ASN
18	W	264	GLN
18	W	330	ASN
18	W	339	GLN
18	W	402	HIS
18	W	434	ASN
18	W	784	ASN
21	c	89	ASN
22	d	64	ASN
19	e	68	GLN
19	e	76	GLN
21	g	31	HIS
21	g	110	ASN
21	g	112	GLN
22	h	64	ASN

5.3.3 RNA ⓘ

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

All (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
13	P	3	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 11 ligands modelled in this entry, 11 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.

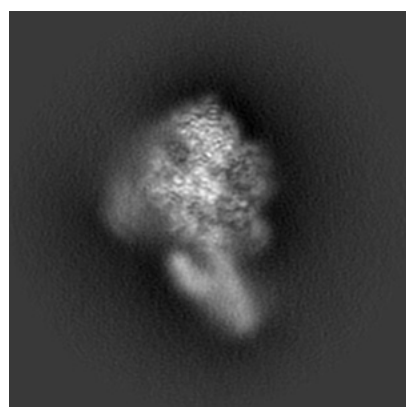
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9713. These allow visual inspection of the internal detail of the map and identification of artifacts.

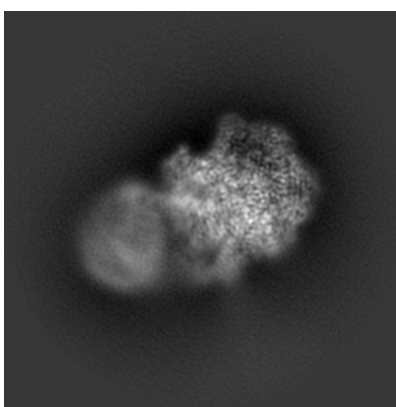
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

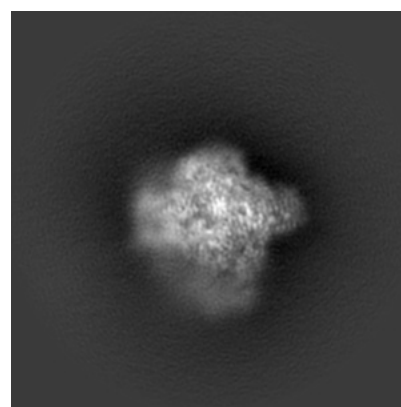
6.1.1 Primary map



X



Y

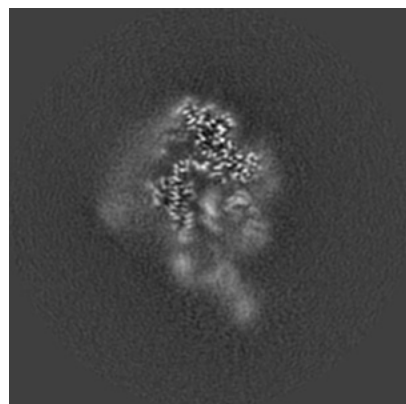


Z

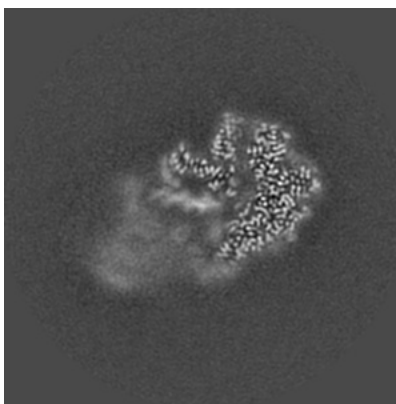
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

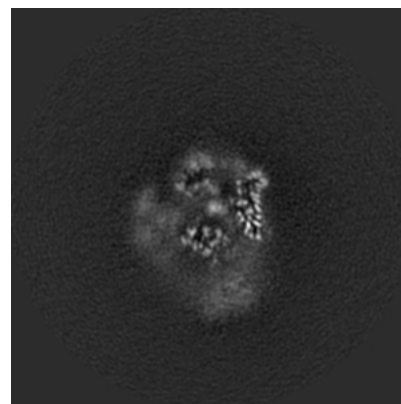
6.2.1 Primary map



X Index: 120



Y Index: 120

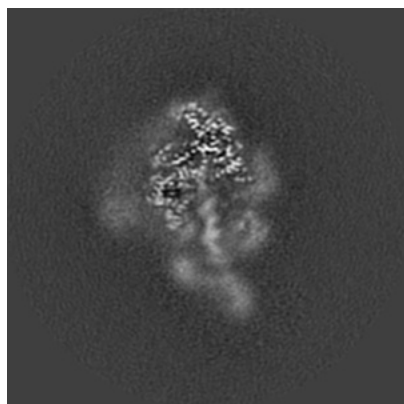


Z Index: 120

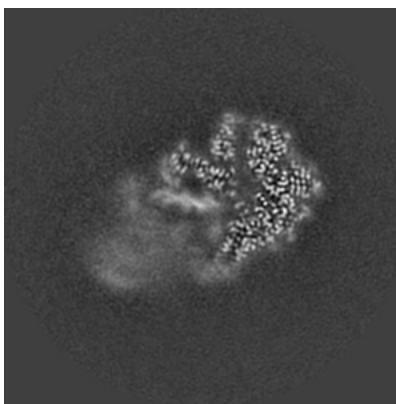
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

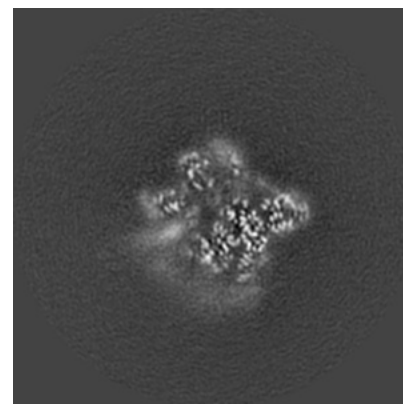
6.3.1 Primary map



X Index: 125



Y Index: 121



Z Index: 133

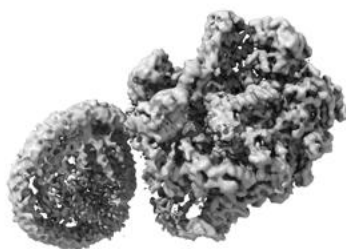
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

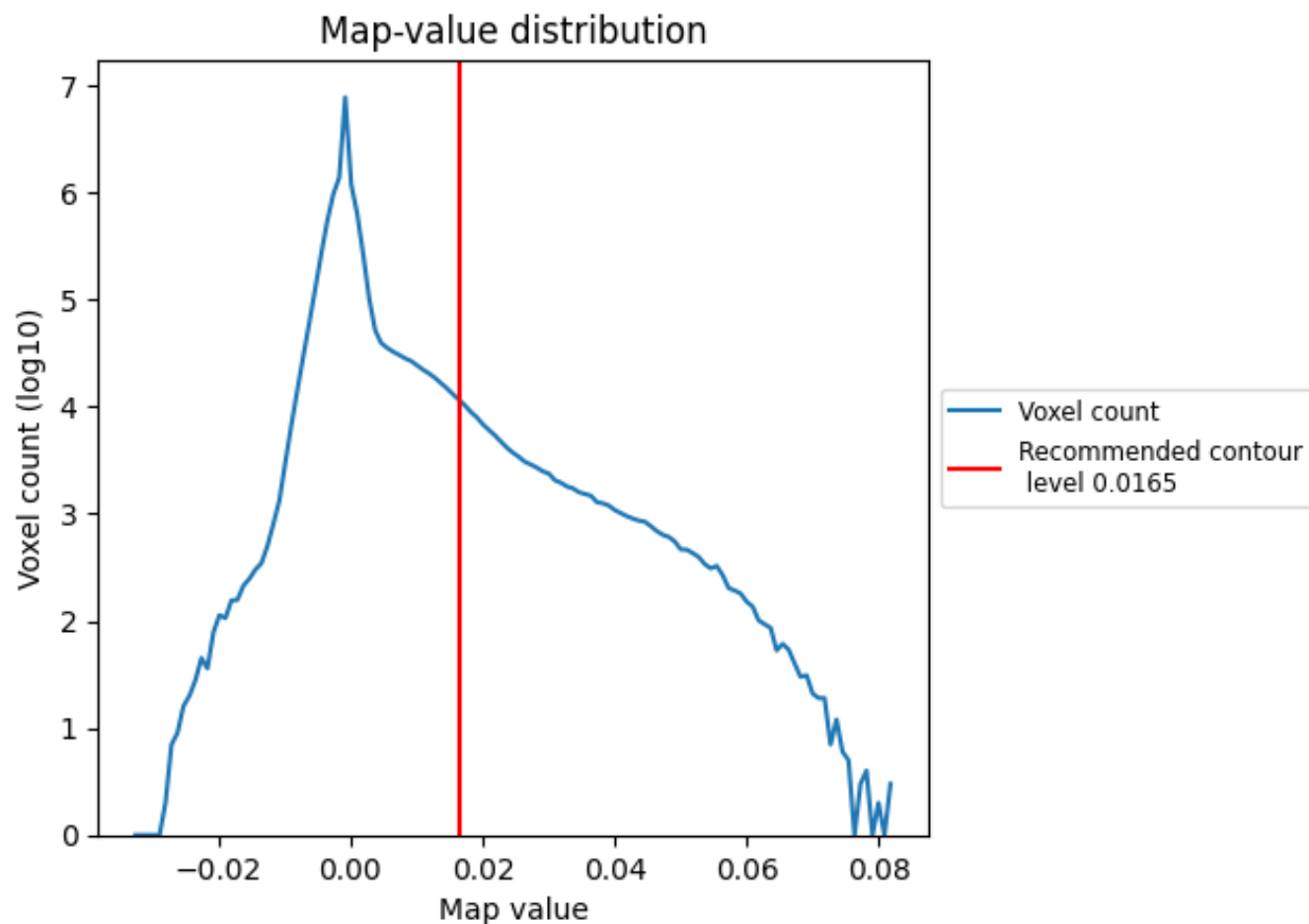
6.5 Mask visualisation

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

7 Map analysis [i](#)

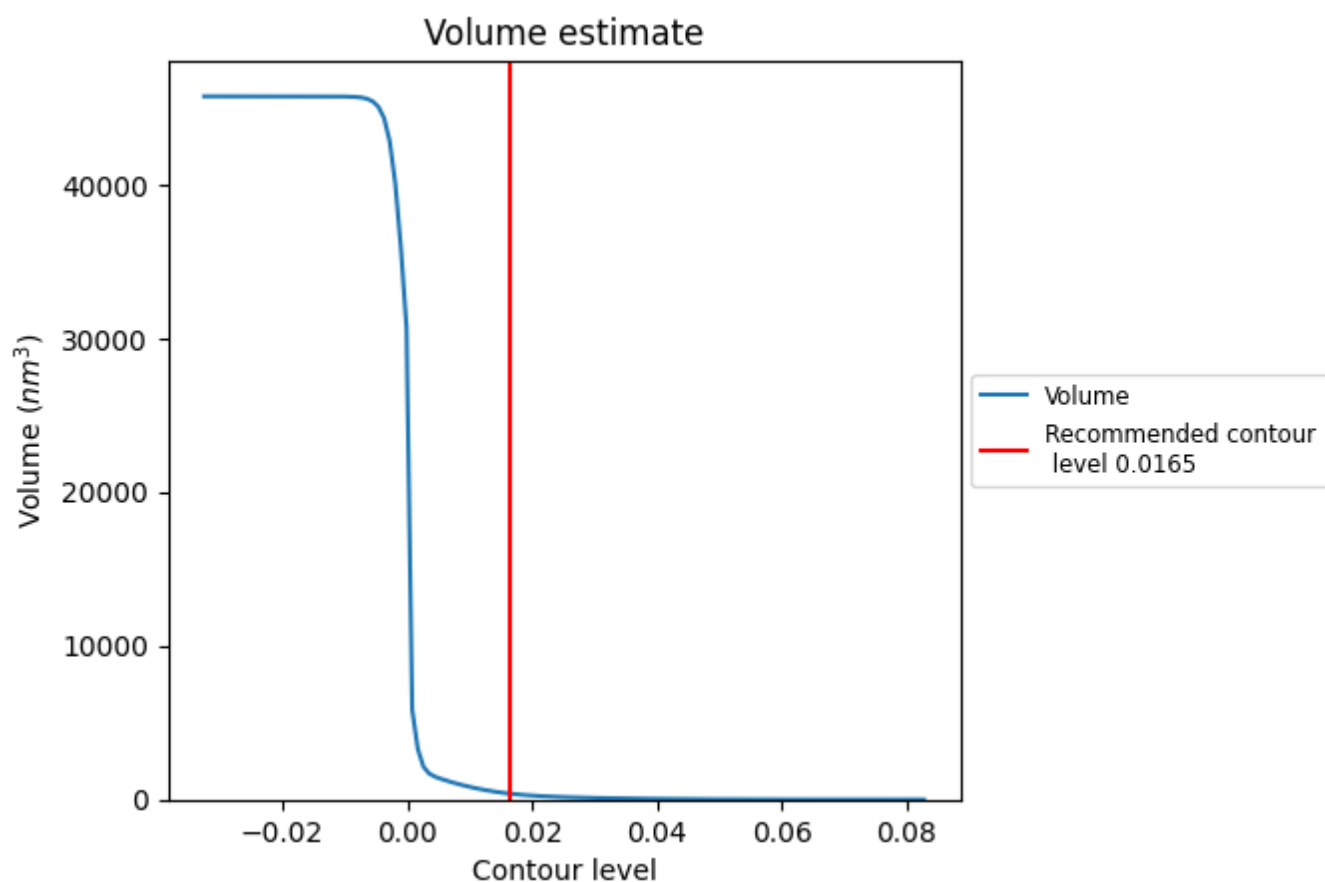
This section contains the results of statistical analysis of the map.

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.

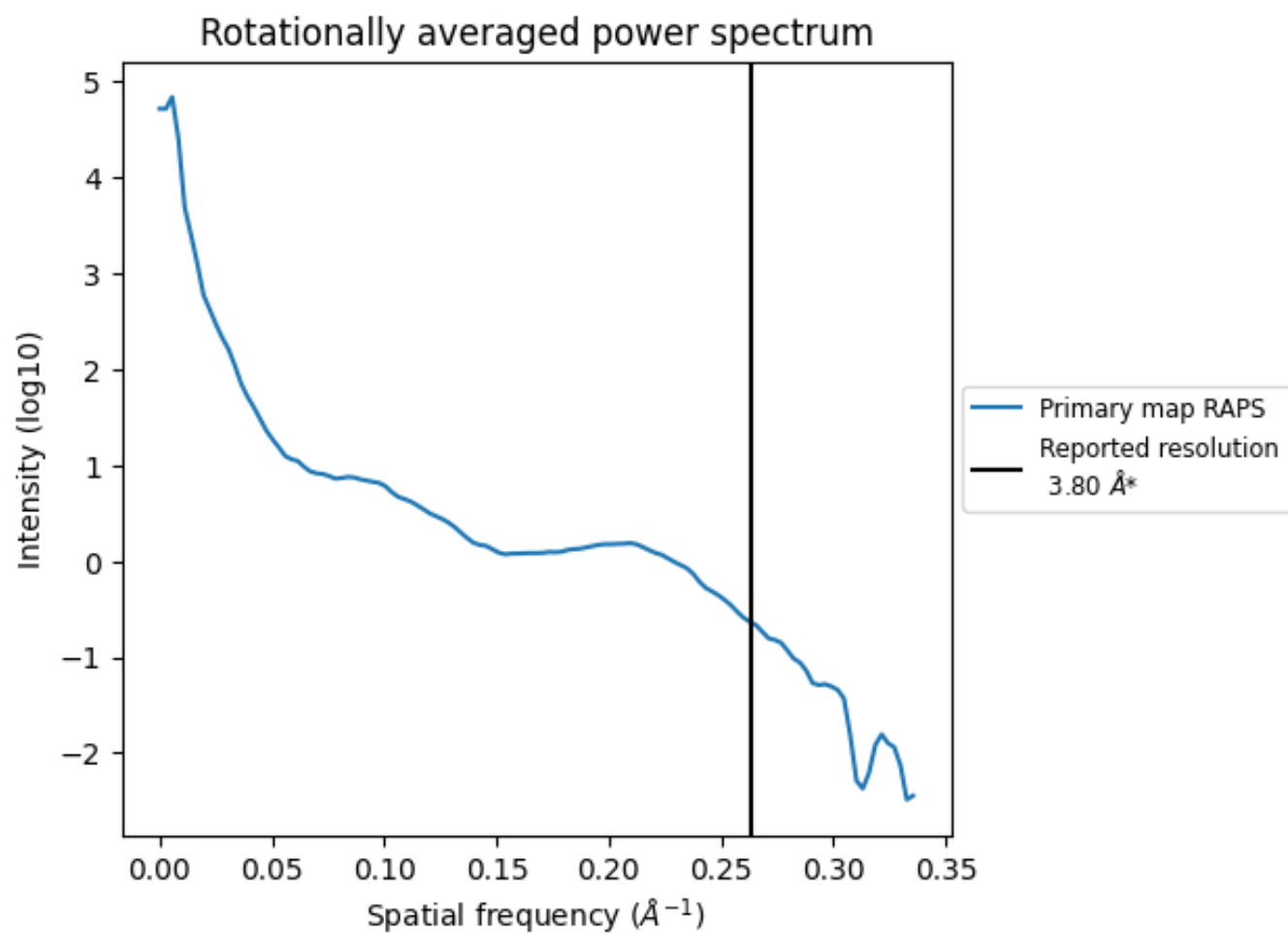
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 381 nm³; this corresponds to an approximate mass of 344 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 ⓘ

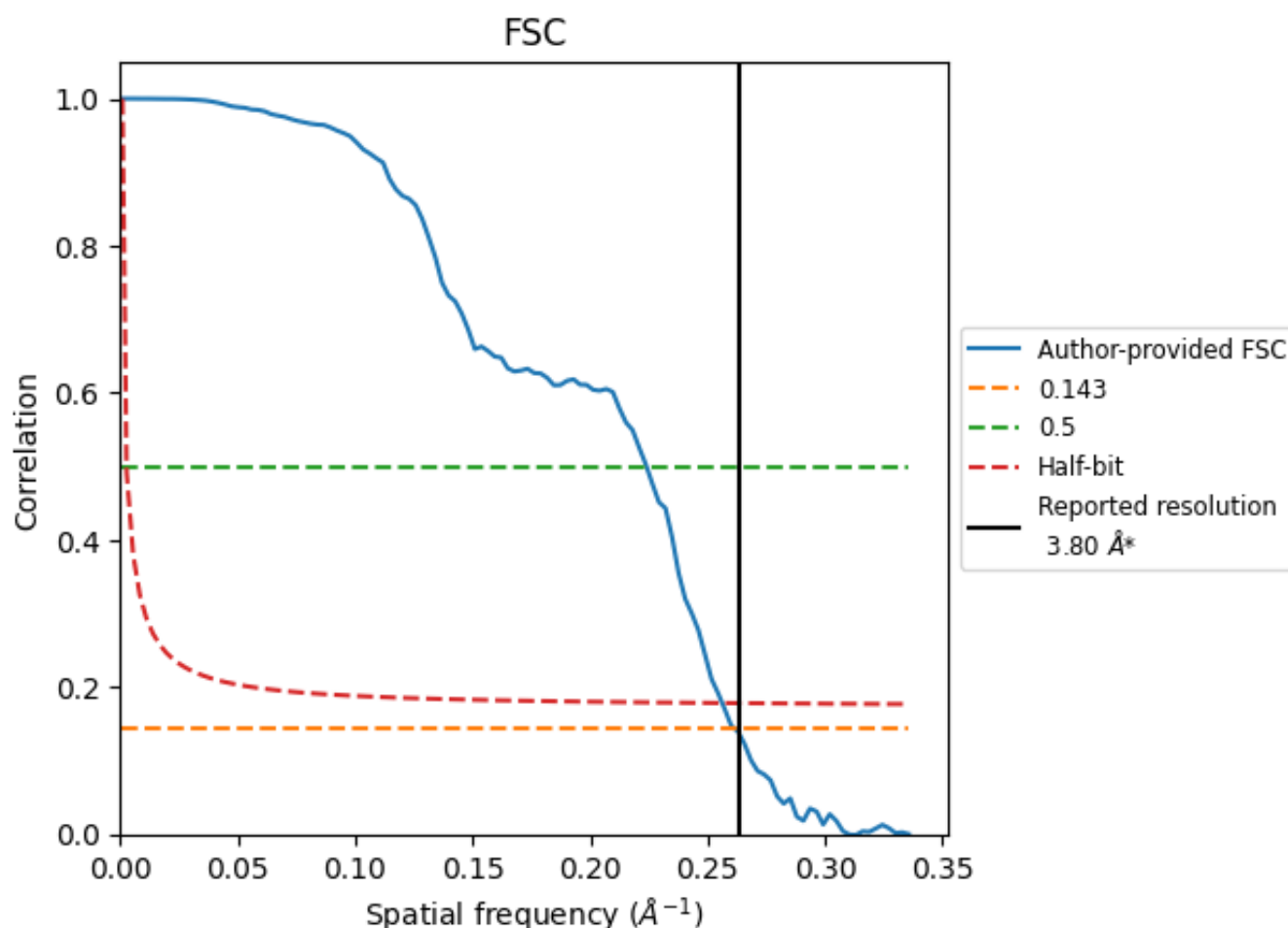


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

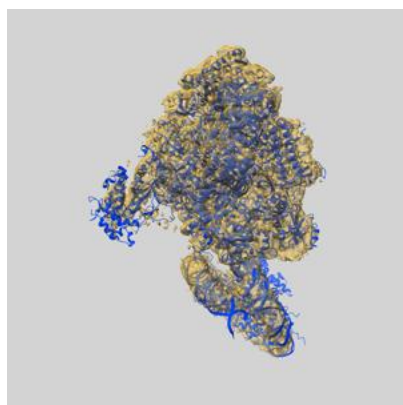
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.46	3.90
Unmasked-calculated*	-	-	-

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

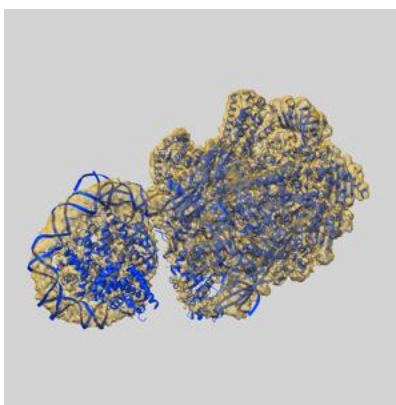
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9713 and PDB model 6IR9. Per-residue inclusion information can be found in section 3 on page 10.

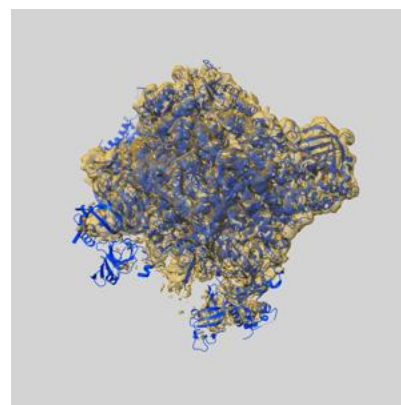
9.1 Map-model overlay [i](#)



X



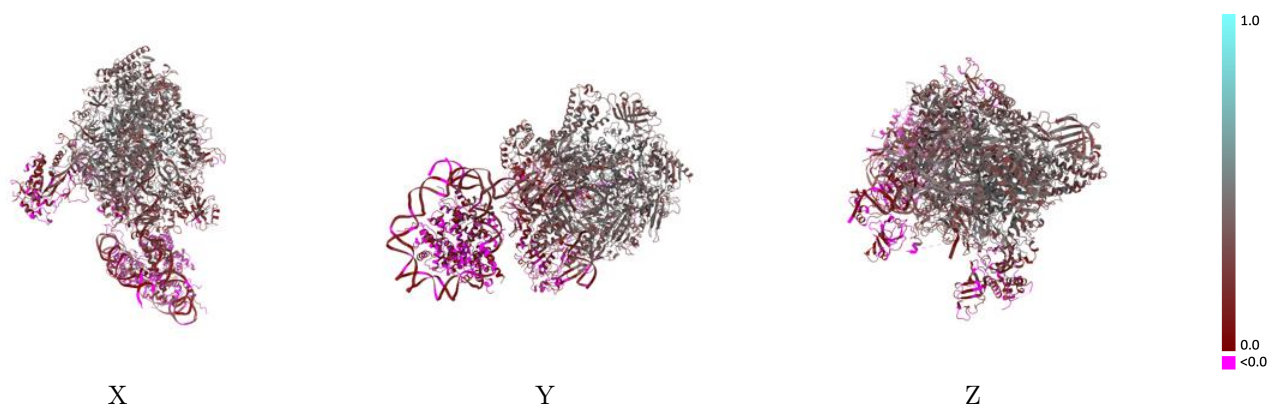
Y



Z

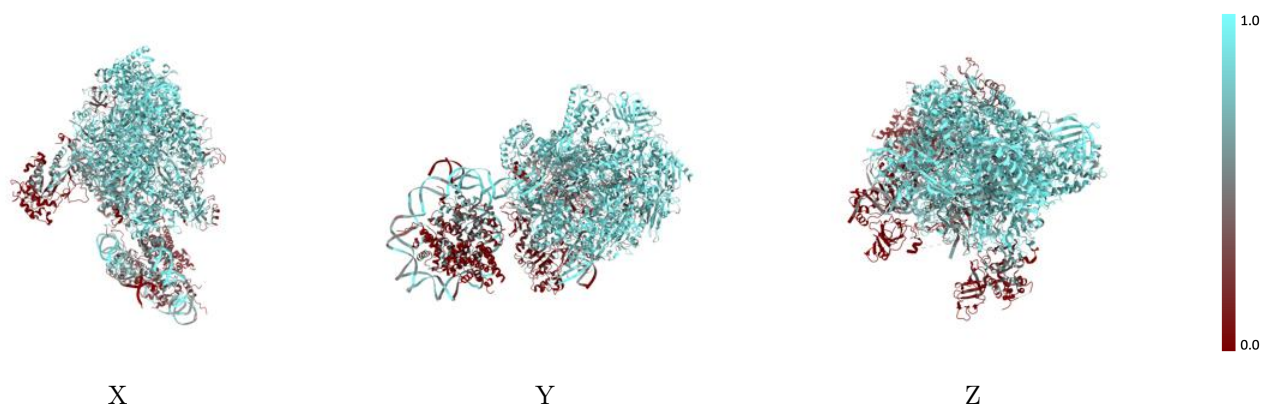
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



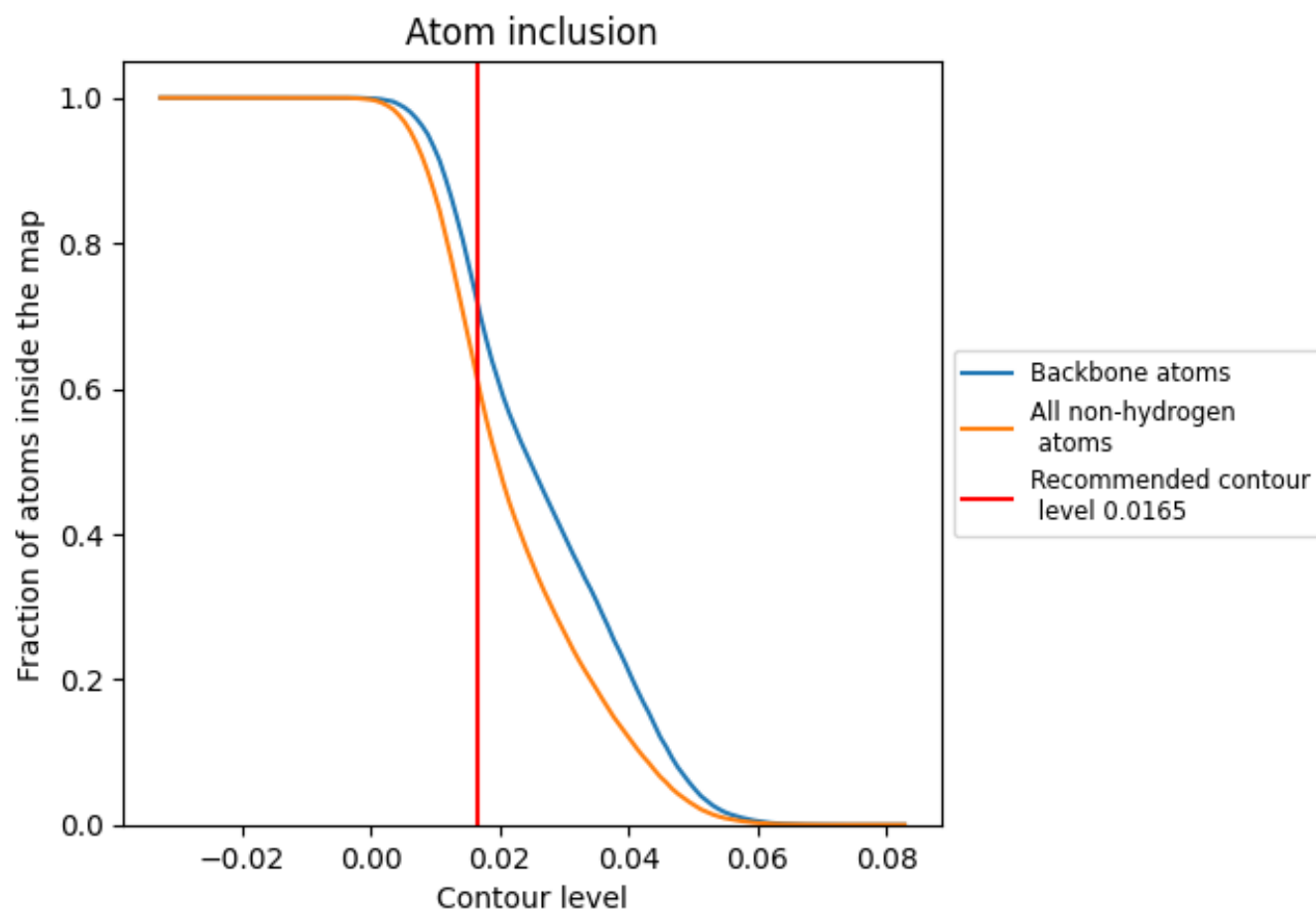
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0165).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6136	 0.2640
A	 0.7479	 0.3660
B	 0.7693	 0.3780
C	 0.8216	 0.3750
D	 0.1237	 0.1010
E	 0.8004	 0.3330
F	 0.8313	 0.4070
G	 0.3758	 0.1900
H	 0.8433	 0.3560
I	 0.4665	 0.1900
J	 0.8151	 0.3800
K	 0.8153	 0.3840
L	 0.7356	 0.3070
M	 0.1548	 0.1530
N	 0.6391	 0.1010
P	 0.7654	 0.2790
T	 0.6973	 0.1350
V	 0.1430	 0.0420
W	 0.1714	 0.1080
a	 0.2324	 0.0510
b	 0.2925	 0.0400
c	 0.3722	 0.0590
d	 0.4058	 0.0490
e	 0.3647	 0.0950
f	 0.3849	 0.1030
g	 0.0051	 0.0000
h	 0.0245	 0.0400

