



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 12:02 PM JST

PDB ID : 6A5O
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 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:

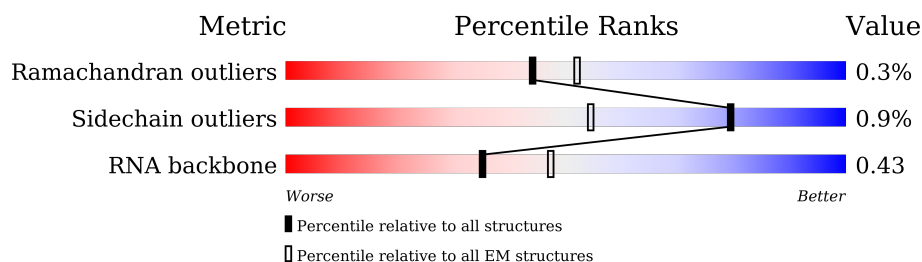
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 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)
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	<div> <div>46%</div> <div>80%</div> <div>19%</div> </div>
2	B	1227	<div> <div>51%</div> <div>93%</div> <div>5%</div> </div>
3	C	304	<div> <div>34%</div> <div>84%</div> <div>13%</div> </div>
4	D	186	<div> <div>84%</div> <div>81%</div> <div>16%</div> </div>
5	E	214	<div> <div>39%</div> <div>97%</div> <div>.</div> </div>
6	F	155	<div> <div>22%</div> <div>54%</div> <div>46%</div> </div>
7	G	171	<div> <div>98%</div> <div>98%</div> <div>.</div> </div>
8	H	145	<div> <div>43%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
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 (three-letter code: 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

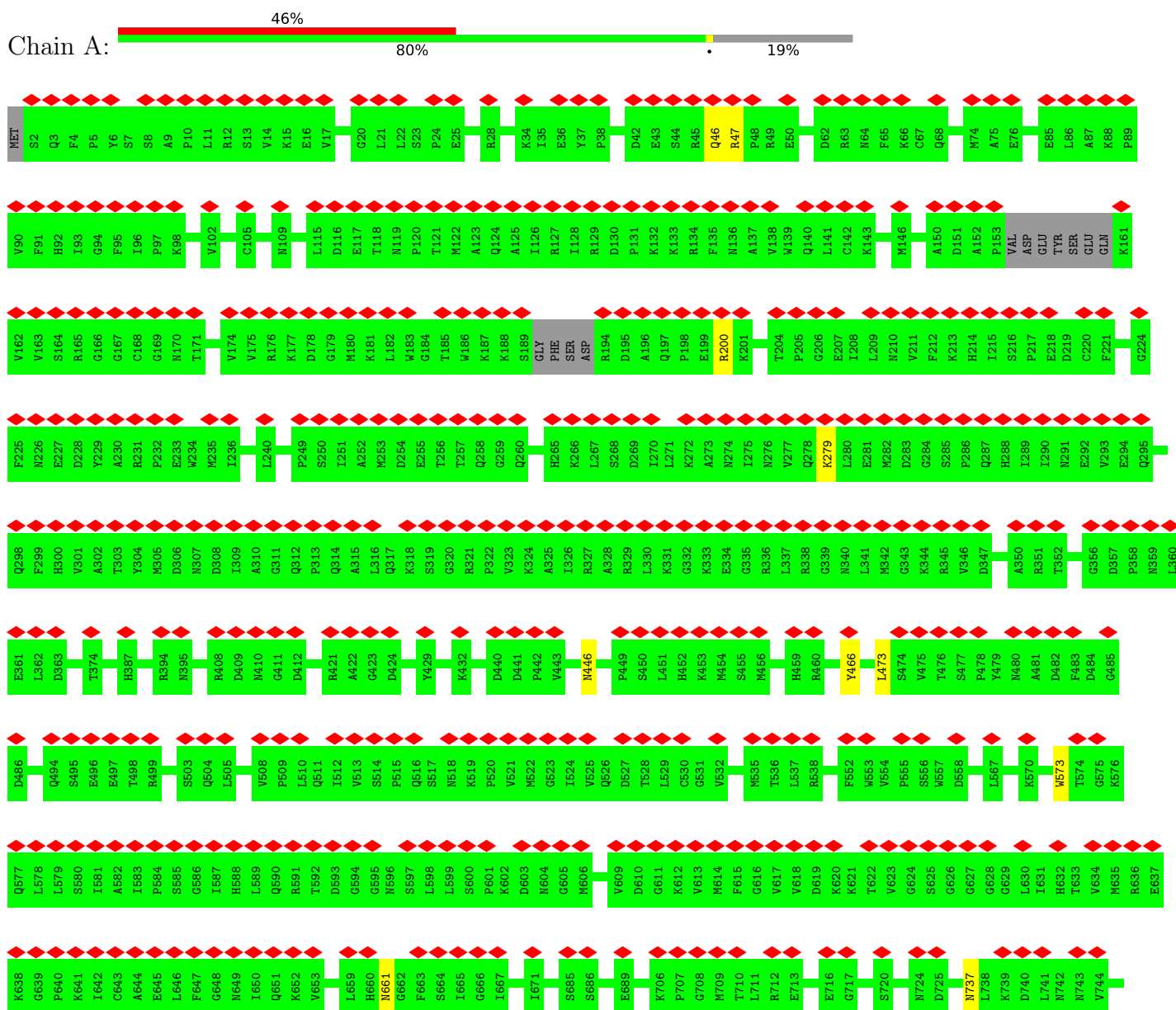
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

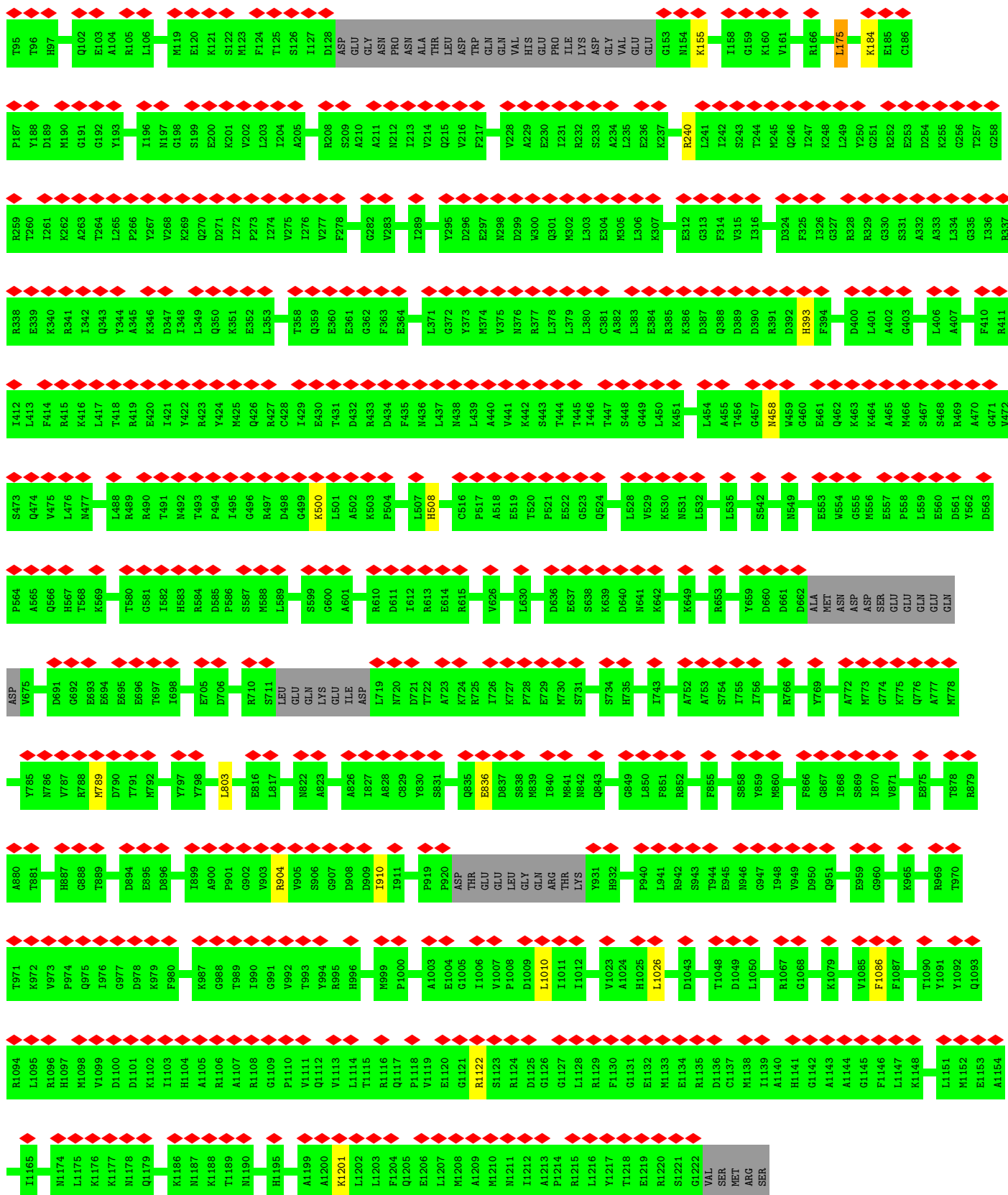
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total 1	Mg 1	0

3 Residue-property plots

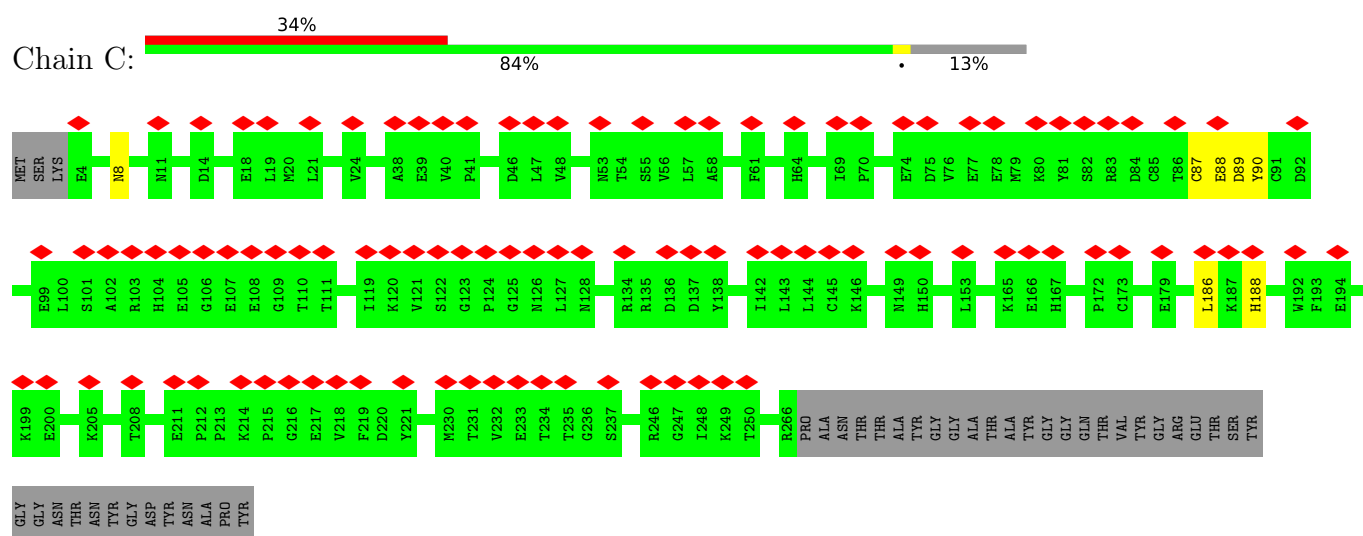
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

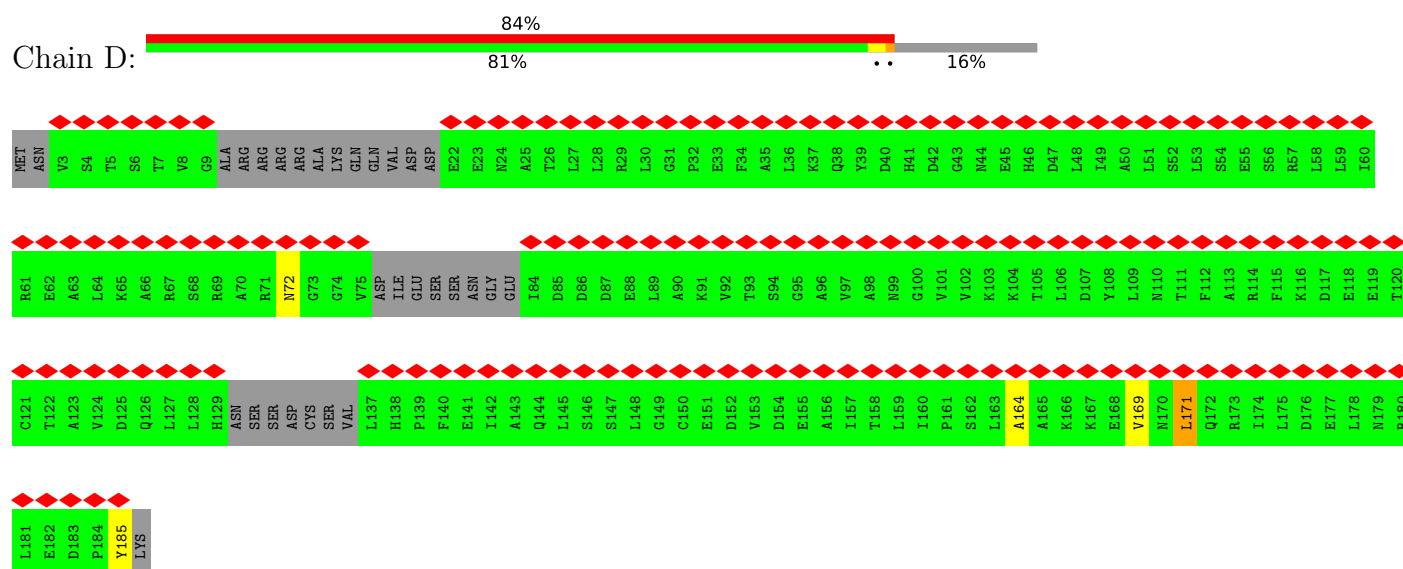




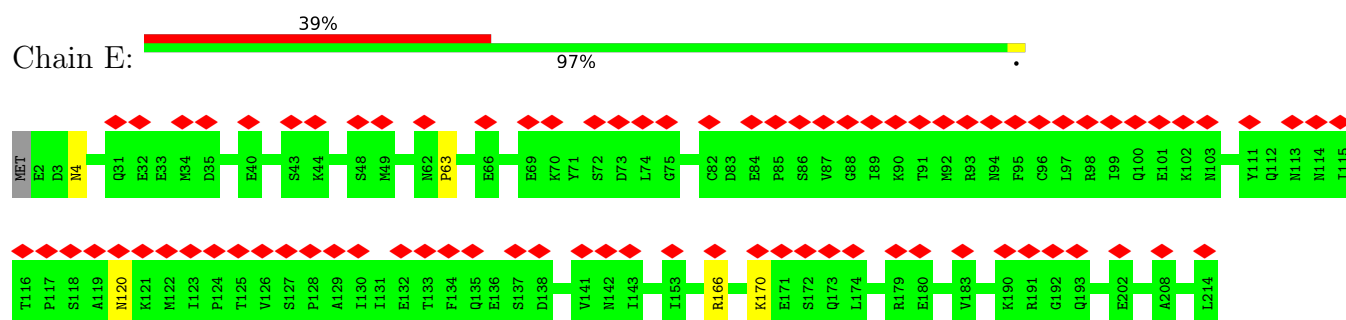
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core



• Molecule 4: RNA polymerase II subunit B32

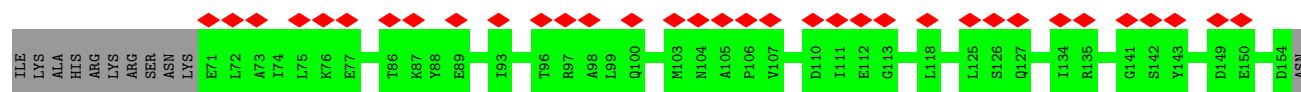


• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

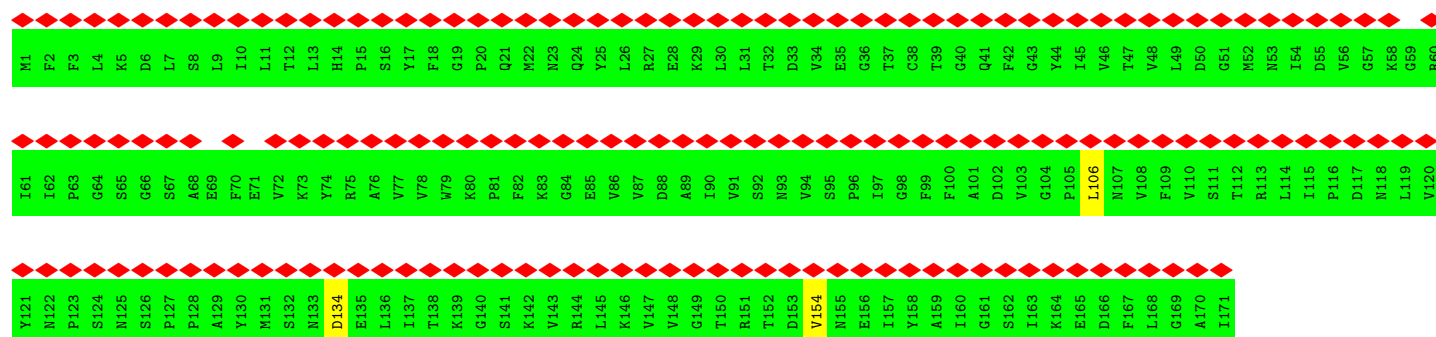


• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

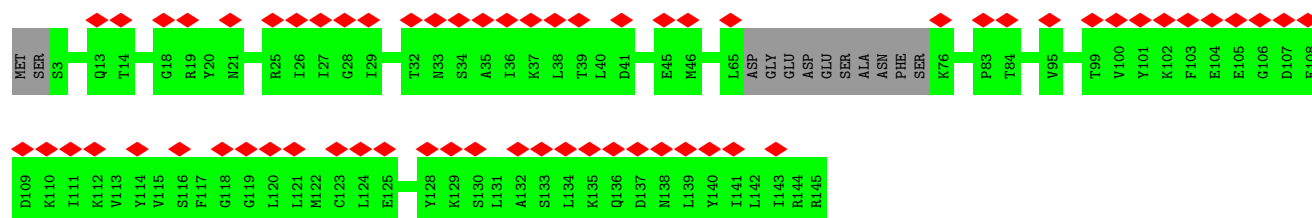
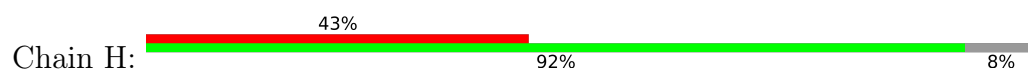




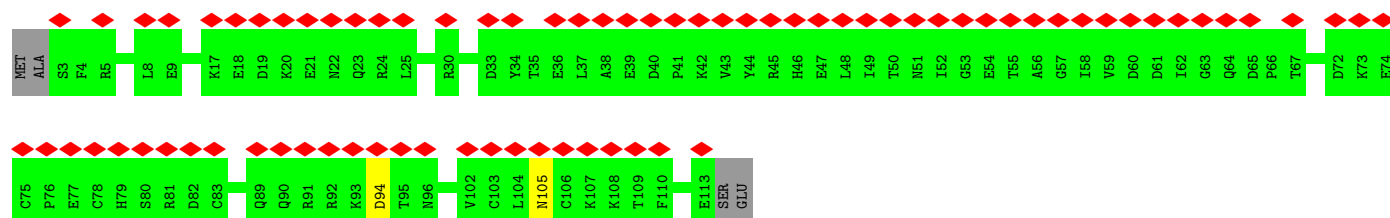
- Molecule 7: RNA polymerase II subunit



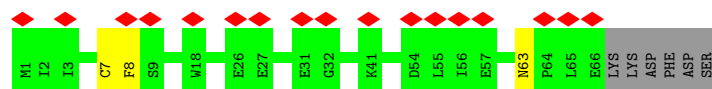
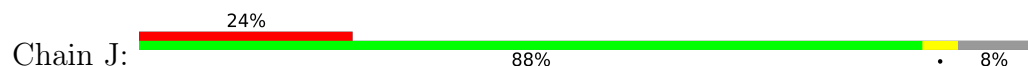
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase subunit

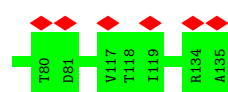
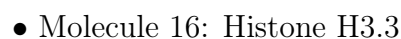


- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

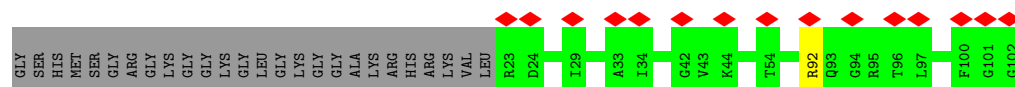


- Molecule 11: RNA polymerase II subunit B12.5

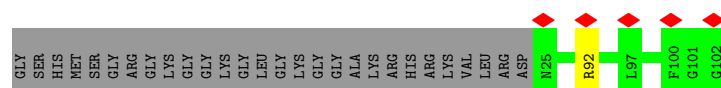




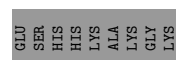
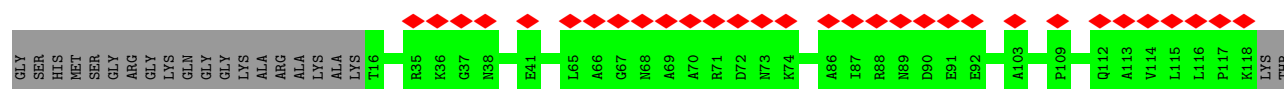
- Molecule 17: Histone H4



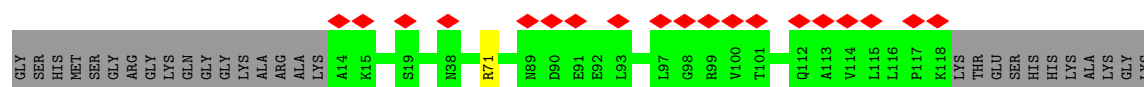
- Molecule 17: Histone H4



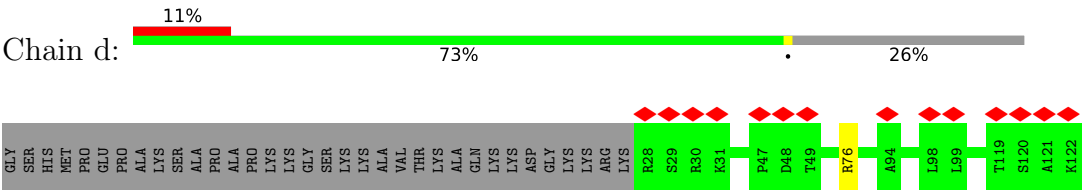
- Molecule 18: Histone H2A type 1-B/E



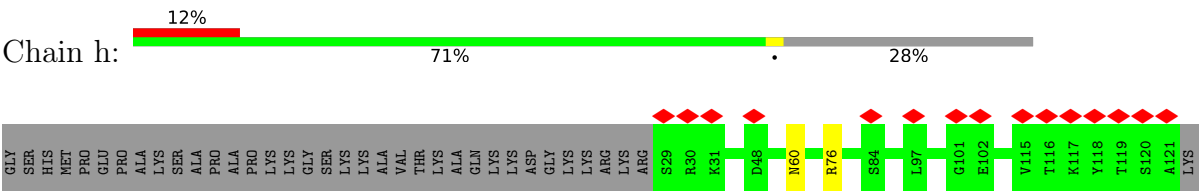
- Molecule 18: Histone H2A type 1-B/E



● 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 (\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: 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	0.62	1/11299 (0.0%)	0.73	3/15266 (0.0%)
2	B	0.65	1/9441 (0.0%)	0.76	2/12732 (0.0%)
3	C	0.66	0/2139	0.76	1/2895 (0.0%)
4	D	0.29	0/1221	0.52	0/1648
5	E	0.59	0/1772	0.66	0/2385
6	F	0.58	0/687	0.64	0/931
7	G	0.33	0/1353	0.61	0/1837
8	H	0.61	0/1069	0.67	0/1444
9	I	0.42	0/934	0.70	0/1257
10	J	0.89	1/554 (0.2%)	0.82	0/742
11	K	0.56	0/953	0.66	0/1291
12	L	0.60	0/365	0.71	0/484
13	P	1.20	3/257 (1.2%)	1.40	2/398 (0.5%)
14	T	0.91	14/4083 (0.3%)	1.32	43/6289 (0.7%)
15	N	0.78	13/3889 (0.3%)	1.35	46/6007 (0.8%)
16	a	0.34	0/809	0.53	0/1085
16	e	0.38	0/807	0.52	0/1081
17	b	0.38	0/645	0.57	0/862
17	f	0.40	0/626	0.56	0/837
18	c	0.35	0/806	0.51	0/1089
18	g	0.35	0/820	0.52	0/1107
19	d	0.38	0/757	0.54	0/1015
19	h	0.38	0/736	0.55	0/990
All	All	0.64	33/46022 (0.1%)	0.86	97/63672 (0.2%)

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	89	DA	C1'-N9	-12.43	1.29	1.47
14	T	88	DA	C1'-N9	-10.08	1.33	1.47
14	T	-72	DA	O5'-C5'	9.22	1.65	1.42
14	T	70	DG	C1'-N9	-7.41	1.36	1.47
15	N	-69	DG	C1'-N9	-6.89	1.37	1.47
14	T	93	DA	C1'-N9	-6.75	1.37	1.47
14	T	96	DA	C1'-N9	-6.40	1.38	1.47
14	T	97	DA	C1'-N9	-6.35	1.38	1.47
1	A	573	TRP	CB-CG	-6.04	1.39	1.50
13	P	1	U	C1'-N1	5.98	1.57	1.48
14	T	91	DA	C1'-N9	-5.93	1.39	1.47
14	T	81	DC	C1'-N1	5.87	1.56	1.49
2	B	789	MET	CA-CB	-5.83	1.41	1.53
15	N	-62	DT	C1'-N1	5.81	1.56	1.49
13	P	2	G	C1'-N9	-5.74	1.38	1.46
14	T	87	DA	C3'-O3'	-5.56	1.36	1.44
15	N	-41	DT	C1'-N1	5.50	1.56	1.49
10	J	7	CYS	CB-SG	-5.41	1.73	1.81
13	P	3	G	C1'-N9	-5.36	1.39	1.46
15	N	-97	DT	C1'-N1	5.30	1.56	1.49
15	N	-53	DT	C1'-N1	5.28	1.56	1.49
14	T	55	DA	C1'-N9	-5.27	1.39	1.47
15	N	-98	DT	C1'-N1	5.22	1.56	1.49
15	N	-96	DT	C1'-N1	5.19	1.56	1.49
15	N	-104	DT	C1'-N1	5.18	1.55	1.49
14	T	101	DC	C1'-N1	5.17	1.55	1.49
15	N	-103	DT	C1'-N1	5.17	1.55	1.49
15	N	-100	DT	C1'-N1	5.16	1.55	1.49
15	N	-60	DT	C1'-N1	5.11	1.55	1.49
15	N	-43	DT	C1'-N1	5.11	1.55	1.49
14	T	62	DA	C1'-N9	-5.10	1.40	1.47
15	N	-105	DC	C1'-N1	5.09	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	99	DC	C1'-N1	5.06	1.55	1.49

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	20	DG	O3'-P-O5'	-12.00	81.20	104.00
15	N	20	DG	OP2-P-O3'	-10.01	83.17	105.20
15	N	14	DT	O4'-C1'-N1	8.62	114.03	108.00
15	N	21	DG	O4'-C1'-N9	8.39	113.88	108.00
15	N	34	DC	P-O3'-C3'	7.98	129.28	119.70
15	N	64	DG	P-O3'-C3'	7.88	129.16	119.70
15	N	5	DT	O4'-C1'-N1	7.81	113.47	108.00
14	T	-53	DG	P-O3'-C3'	7.57	128.78	119.70
14	T	-47	DT	O4'-C1'-N1	7.55	113.29	108.00
14	T	-31	DA	O4'-C1'-N9	7.22	113.05	108.00
14	T	-21	DC	O4'-C1'-N1	7.21	113.05	108.00
15	N	-23	DT	O4'-C1'-N1	7.17	113.02	108.00
15	N	-35	DG	O4'-C1'-N9	-7.09	103.03	108.00
15	N	63	DG	P-O3'-C3'	7.03	128.14	119.70
15	N	-38	DT	P-O3'-C3'	6.95	128.03	119.70
15	N	23	DG	O4'-C1'-N9	6.90	112.83	108.00
15	N	54	DT	P-O3'-C3'	6.90	127.98	119.70
15	N	-63	DT	O4'-C1'-N1	6.88	112.81	108.00
14	T	43	DA	P-O3'-C3'	6.86	127.93	119.70
15	N	21	DG	P-O3'-C3'	6.85	127.92	119.70
14	T	42	DC	P-O3'-C3'	6.75	127.80	119.70
14	T	-51	DC	P-O3'-C3'	6.73	127.77	119.70
15	N	-33	DG	P-O3'-C3'	6.71	127.75	119.70
14	T	23	DA	P-O3'-C3'	6.69	127.73	119.70
13	P	2	G	C4-N9-C1'	6.68	135.18	126.50
2	B	1026	LEU	CA-CB-CG	-6.65	100.02	115.30
14	T	-12	DC	P-O3'-C3'	6.63	127.66	119.70
15	N	-21	DG	P-O3'-C3'	6.53	127.54	119.70
14	T	-13	DA	P-O3'-C3'	6.53	127.53	119.70
15	N	-54	DC	P-O3'-C3'	6.50	127.50	119.70
14	T	-63	DC	P-O3'-C3'	6.50	127.50	119.70
15	N	42	DA	P-O3'-C3'	6.44	127.43	119.70
14	T	16	DA	O4'-C1'-N9	6.40	112.48	108.00
15	N	30	DC	O4'-C1'-N1	6.39	112.48	108.00
15	N	-51	DG	P-O3'-C3'	6.37	127.35	119.70
14	T	58	DG	O4'-C1'-N9	-6.35	103.56	108.00
15	N	21	DG	O5'-P-OP2	6.28	118.23	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	20	DG	P-O3'-C3'	6.24	127.19	119.70
14	T	38	DA	P-O3'-C3'	6.18	127.12	119.70
14	T	22	DC	O4'-C1'-N1	6.16	112.31	108.00
15	N	20	DG	C3'-C2'-C1'	-6.13	95.14	102.50
14	T	12	DT	O4'-C1'-N1	6.04	112.23	108.00
14	T	-15	DA	O4'-C1'-N9	6.02	112.22	108.00
14	T	-29	DC	P-O3'-C3'	6.00	126.89	119.70
14	T	-30	DG	P-O3'-C3'	5.99	126.89	119.70
15	N	20	DG	OP1-P-O3'	-5.98	92.05	105.20
14	T	30	DT	P-O3'-C3'	5.90	126.78	119.70
15	N	9	DT	N3-C2-O2	-5.84	118.80	122.30
14	T	-70	DC	O4'-C1'-N1	5.83	112.08	108.00
1	A	279	LYS	CB-CA-C	5.77	121.94	110.40
14	T	90	DC	O4'-C4'-C3'	-5.76	102.19	104.50
14	T	94	DC	O4'-C1'-N1	5.74	112.02	108.00
15	N	-25	DC	O4'-C1'-N1	5.74	112.01	108.00
15	N	-63	DT	C1'-O4'-C4'	-5.73	104.37	110.10
14	T	-60	DG	O4'-C1'-N9	5.71	112.00	108.00
14	T	-43	DT	P-O3'-C3'	5.71	126.55	119.70
15	N	-58	DC	P-O3'-C3'	5.70	126.54	119.70
14	T	-38	DC	P-O3'-C3'	5.65	126.48	119.70
14	T	41	DA	O4'-C1'-N9	5.64	111.94	108.00
14	T	54	DG	P-O3'-C3'	5.63	126.45	119.70
1	A	977	ARG	CA-CB-CG	5.63	125.78	113.40
14	T	-2	DC	O4'-C1'-N1	5.55	111.89	108.00
13	P	2	G	C8-N9-C1'	-5.55	119.78	127.00
15	N	21	DG	C1'-O4'-C4'	-5.50	104.60	110.10
14	T	-34	DG	C3'-C2'-C1'	-5.47	95.94	102.50
14	T	-4	DC	P-O3'-C3'	5.46	126.26	119.70
14	T	32	DA	O4'-C1'-N9	5.45	111.81	108.00
14	T	1	DT	O4'-C1'-N1	5.41	111.79	108.00
15	N	-21	DG	C1'-O4'-C4'	-5.41	104.69	110.10
15	N	40	DC	P-O3'-C3'	5.41	126.19	119.70
15	N	-53	DT	O4'-C1'-N1	5.35	111.75	108.00
15	N	-53	DT	P-O3'-C3'	5.34	126.11	119.70
15	N	-48	DC	O4'-C1'-N1	5.34	111.74	108.00
15	N	27	DG	C1'-O4'-C4'	-5.34	104.76	110.10
15	N	29	DG	O4'-C1'-N9	5.30	111.71	108.00
15	N	43	DA	P-O3'-C3'	5.29	126.05	119.70
15	N	-17	DT	P-O3'-C3'	5.27	126.02	119.70
14	T	-47	DT	C1'-O4'-C4'	-5.26	104.84	110.10
15	N	-50	DT	O4'-C1'-N1	5.24	111.67	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	87	DA	O4'-C4'-C3'	-5.24	102.41	104.50
3	C	186	LEU	CA-CB-CG	-5.22	103.29	115.30
15	N	-36	DG	P-O3'-C3'	5.21	125.96	119.70
2	B	803	LEU	CA-CB-CG	-5.20	103.34	115.30
14	T	27	DG	O4'-C1'-N9	5.19	111.63	108.00
14	T	-40	DG	O4'-C1'-N9	5.18	111.62	108.00
14	T	70	DG	C4'-C3'-C2'	-5.17	98.44	103.10
15	N	21	DG	OP1-P-OP2	5.14	127.31	119.60
14	T	-2	DC	C1'-O4'-C4'	-5.09	105.01	110.10
15	N	6	DA	C3'-C2'-C1'	-5.07	96.41	102.50
15	N	-20	DC	O4'-C1'-N1	5.07	111.55	108.00
15	N	-32	DT	O4'-C1'-N1	5.06	111.54	108.00
15	N	1	DC	O4'-C1'-N1	5.06	111.54	108.00
14	T	4	DC	P-O3'-C3'	5.05	125.76	119.70
1	A	473	LEU	CA-CB-CG	-5.05	103.69	115.30
14	T	16	DA	C1'-O4'-C4'	-5.05	105.05	110.10
14	T	-1	DG	P-O3'-C3'	5.02	125.73	119.70
14	T	-32	DC	O4'-C1'-N1	5.02	111.52	108.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1108	ASN	Peptide
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
1	A	975	LEU	Peptide
1	A	977	ARG	Peptide
2	B	1086	PHE	Peptide
2	B	175	LEU	Peptide
2	B	393	HIS	Peptide
2	B	458	ASN	Peptide
2	B	508	HIS	Peptide
2	B	64	HIS	Peptide
2	B	836	GLU	Peptide
2	B	910	ILE	Peptide
3	C	87	CYS	Peptide
3	C	88	GLU	Peptide
3	C	89	ASP	Peptide

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Mol	Chain	Res	Type	Group
5	E	170	LYS	Peptide
5	E	63	PRO	Peptide
9	I	94	ASP	Peptide
10	J	63	ASN	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	1396/1743 (80%)	1252 (90%)	142 (10%)	2 (0%)	51	86
2	B	1151/1227 (94%)	1018 (88%)	131 (11%)	2 (0%)	47	81
3	C	261/304 (86%)	231 (88%)	29 (11%)	1 (0%)	34	72
4	D	148/186 (80%)	136 (92%)	9 (6%)	3 (2%)	7	38
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%)	13	50
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%)	4	26
16	e	95/139 (68%)	90 (95%)	5 (5%)	0	100	100
17	b	78/106 (74%)	75 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
19	h	91/129 (70%)	88 (97%)	3 (3%)	0	100	100
All	All	4606/5536 (83%)	4163 (90%)	430 (9%)	13 (0%)	44	77

All (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
4	D	164	ALA
16	a	39	HIS
2	B	155	LYS
16	a	40	ARG
2	B	175	LEU
3	C	90	TYR
1	A	47	ARG
1	A	959	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	1223/1528 (80%)	1217 (100%)	6 (0%)	88	93
2	B	1016/1077 (94%)	1009 (99%)	7 (1%)	84	90
3	C	236/264 (89%)	234 (99%)	2 (1%)	81	89
4	D	133/160 (83%)	130 (98%)	3 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	80
6	F	75/137 (55%)	75 (100%)	0	100	100
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%)	59 (98%)	1 (2%)	60	78
11	K	104/109 (95%)	103 (99%)	1 (1%)	76	86
12	L	38/56 (68%)	36 (95%)	2 (5%)	22	47
16	a	83/112 (74%)	82 (99%)	1 (1%)	71	83
16	e	82/112 (73%)	81 (99%)	1 (1%)	71	83
17	b	65/81 (80%)	64 (98%)	1 (2%)	65	80
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%)	80 (99%)	1 (1%)	71	83
19	h	79/107 (74%)	77 (98%)	2 (2%)	47	68
All	All	4073/4785 (85%)	4038 (99%)	35 (1%)	79	87

All (35) 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
1	A	805	TYR
1	A	1403	CYS
2	B	184	LYS
2	B	240	ARG
2	B	500	LYS
2	B	904	ARG
2	B	1010	LEU
2	B	1122	ARG
2	B	1201	LYS
3	C	8	ASN
3	C	188	HIS

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Mol	Chain	Res	Type
4	D	72	ASN
4	D	171	LEU
4	D	185	TYR
5	E	4	ASN
5	E	120	ASN
5	E	166	ARG
7	G	106	LEU
9	I	105	ASN
10	J	8	PHE
11	K	19	LEU
12	L	51	LYS
12	L	62	ARG
16	a	108	ASN
17	b	92	ARG
19	d	76	ARG
16	e	53	ARG
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 (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	278	GLN
1	A	291	ASN
1	A	298	GLN
1	A	317	GLN
1	A	446	ASN
1	A	516	GLN
1	A	590	GLN
1	A	632	HIS
1	A	651	GLN
1	A	661	ASN
1	A	743	ASN
1	A	787	HIS
1	A	927	GLN
1	A	931	ASN
1	A	968	ASN
1	A	1013	GLN
1	A	1072	GLN

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Mol	Chain	Res	Type
2	B	72	ASN
2	B	426	GLN
2	B	524	GLN
2	B	549	ASN
2	B	641	ASN
2	B	761	HIS
2	B	794	ASN
2	B	996	HIS
2	B	1025	HIS
2	B	1093	GLN
3	C	8	ASN
5	E	4	ASN
5	E	112	GLN
5	E	120	ASN
9	I	105	ASN
10	J	63	ASN
11	K	2	ASN
11	K	44	ASN
11	K	110	ASN
16	a	68	GLN
19	d	81	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 [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.

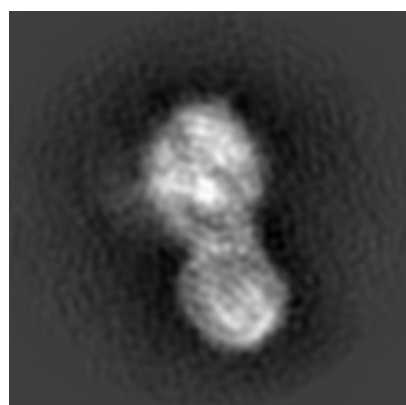
6 Map visualisation [i](#)

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

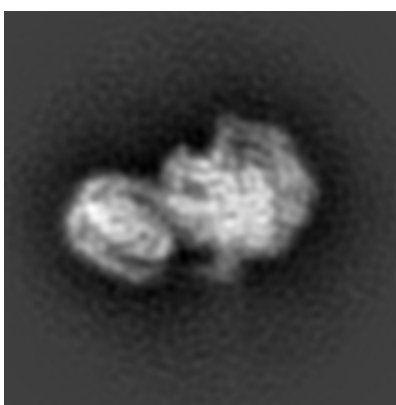
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

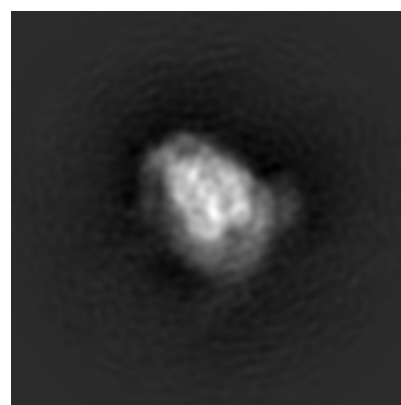
6.1.1 Primary map



X



Y

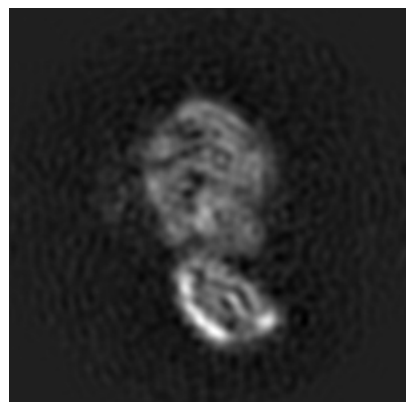


Z

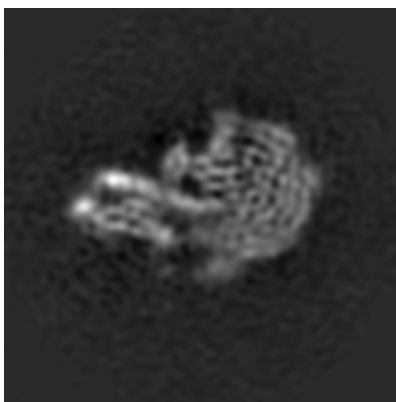
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

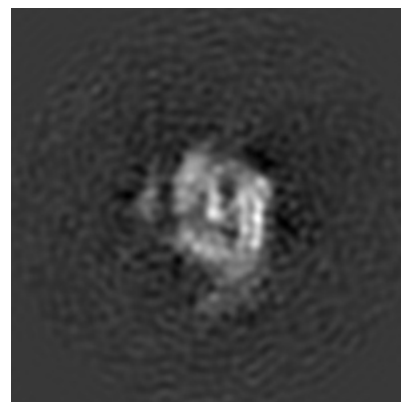
6.2.1 Primary map



X Index: 120



Y Index: 120

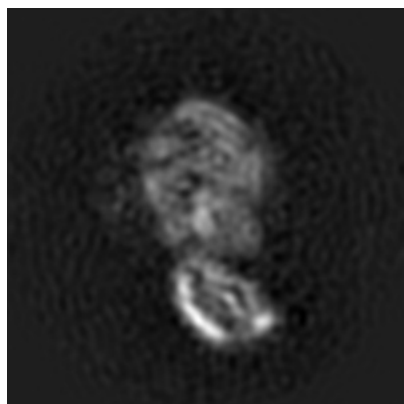


Z Index: 120

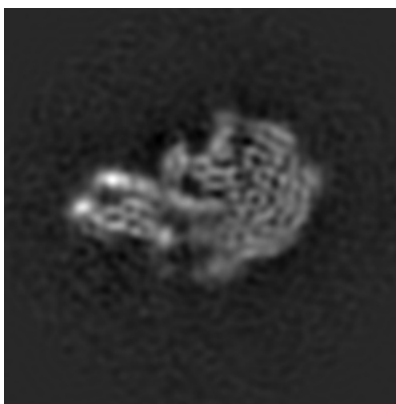
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

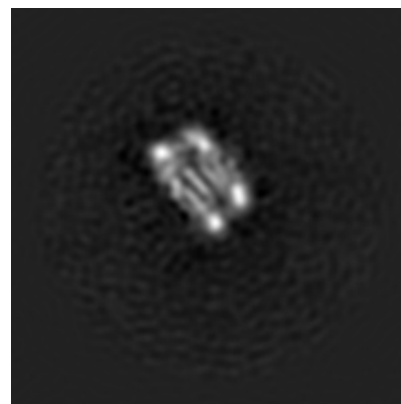
6.3.1 Primary map



X Index: 121



Y Index: 121



Z Index: 57

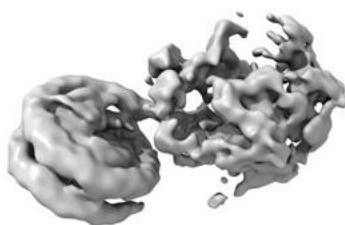
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

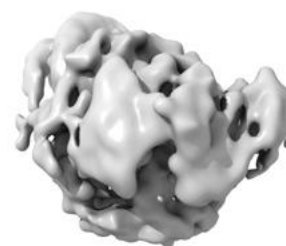
6.4.1 Primary map



X



Y



Z

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

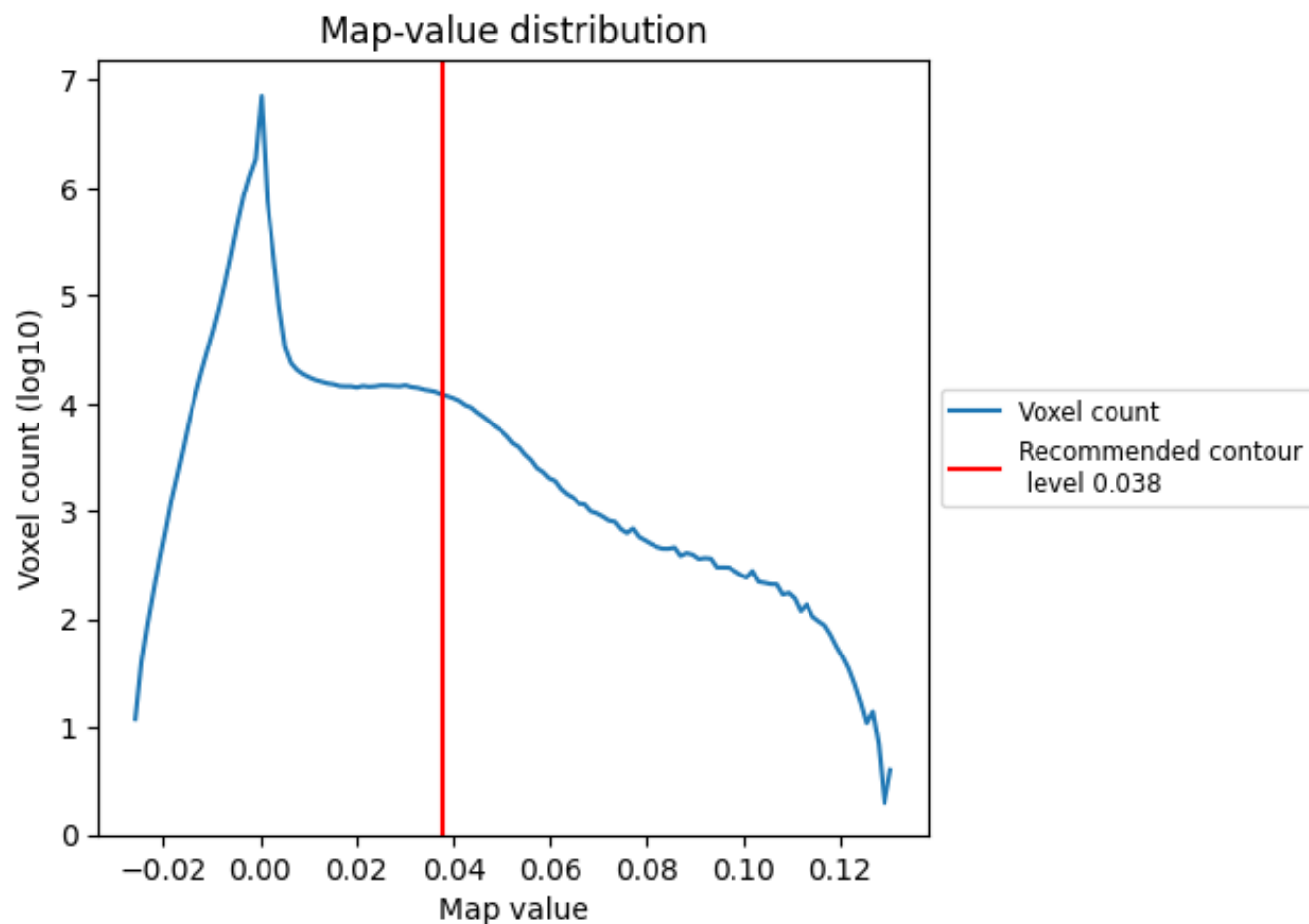
6.5 Mask visualisation

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

7 Map analysis [i](#)

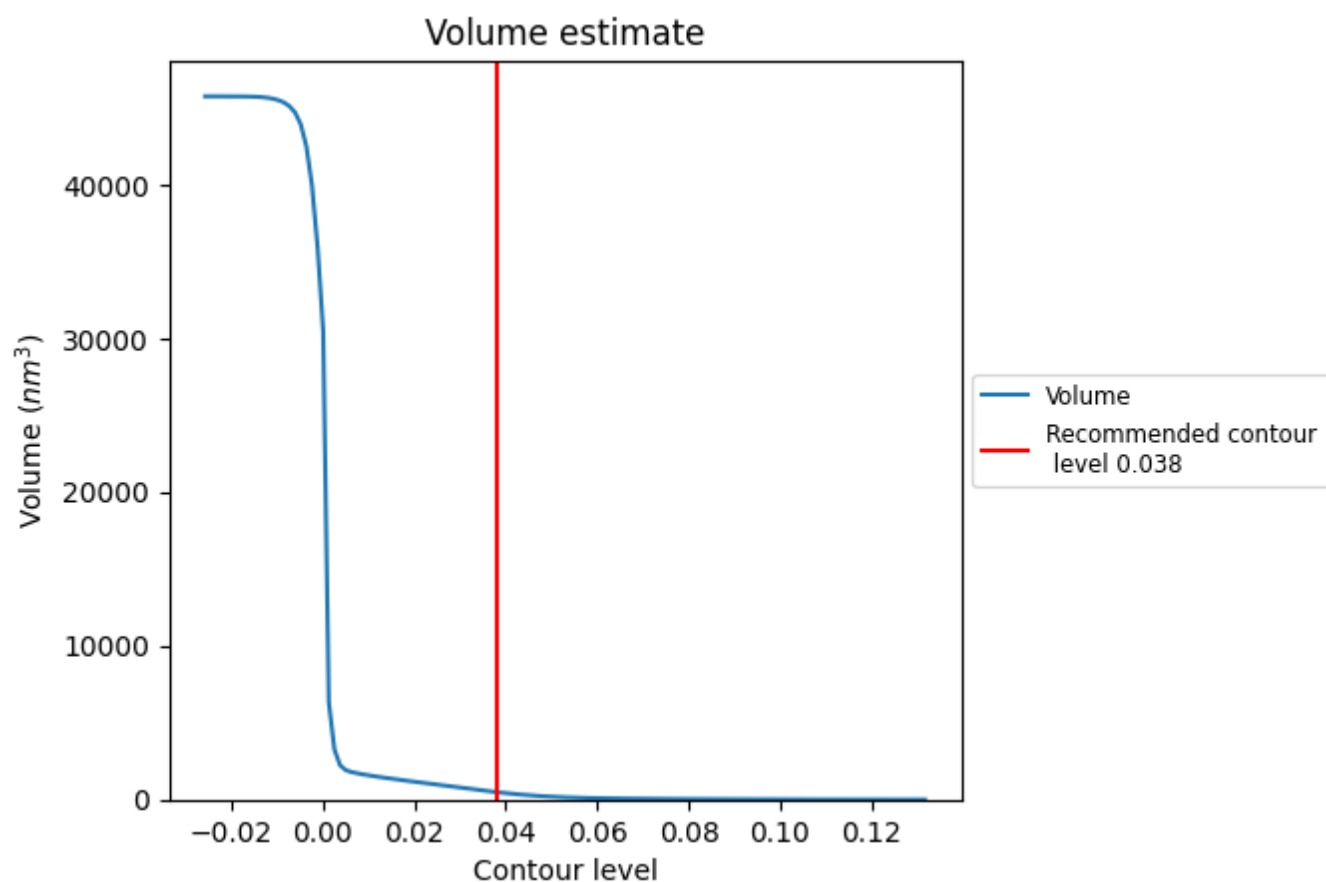
This section contains the results of statistical analysis of the map.

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.

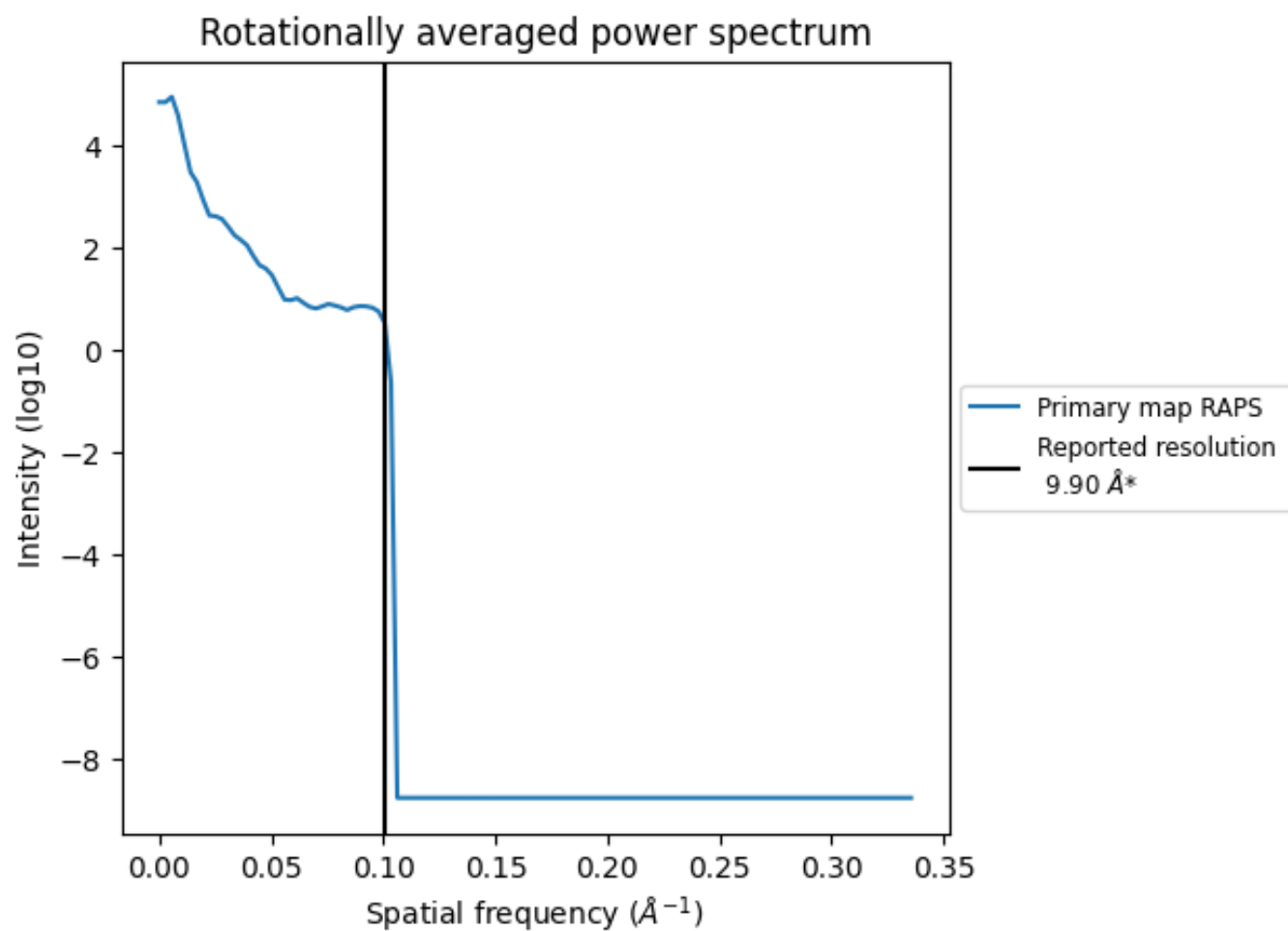
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

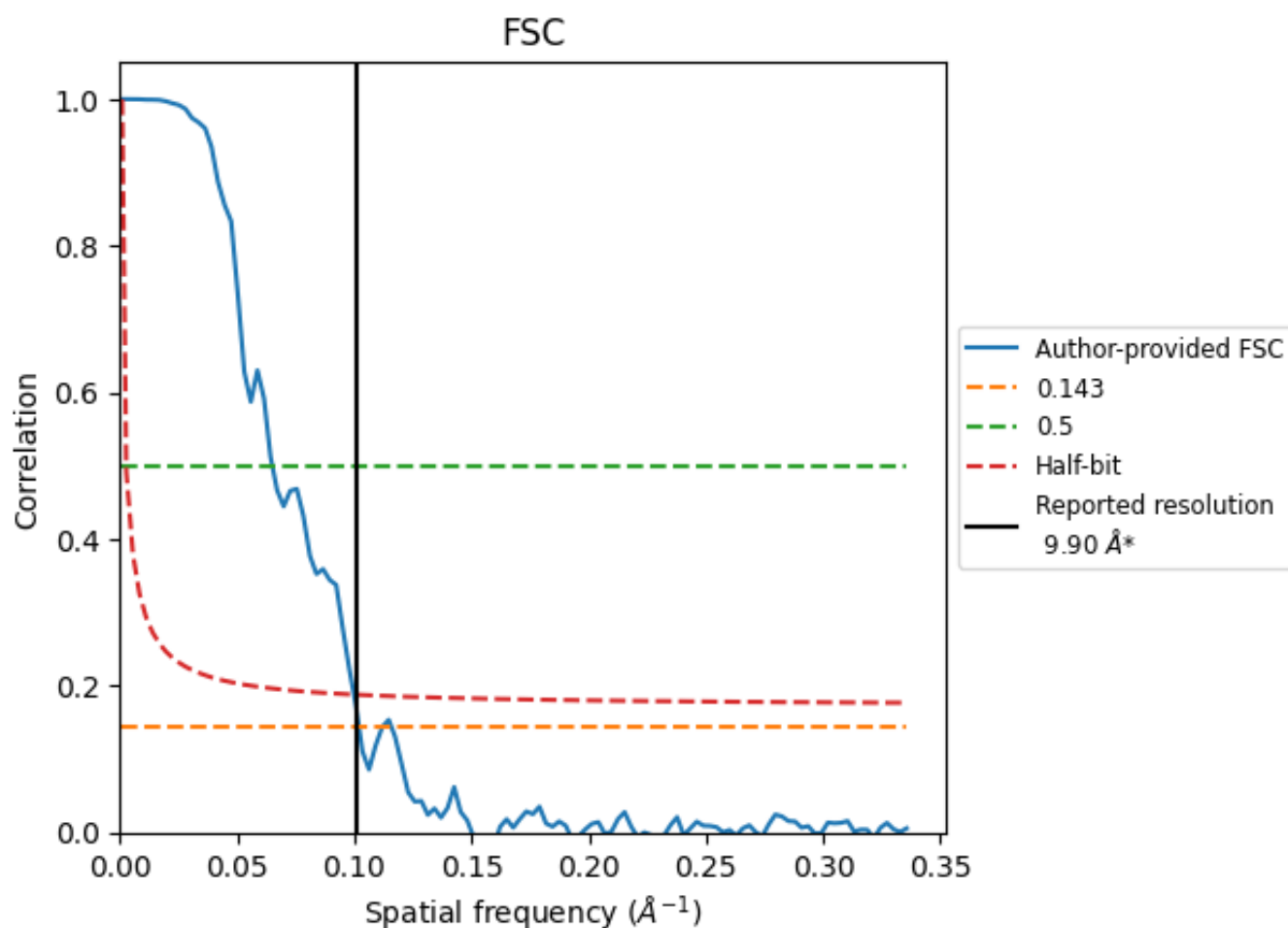


*Reported resolution corresponds to spatial frequency of 0.101 Å⁻¹

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 0.101 \AA^{-1}

8.2 Resolution estimates [i](#)

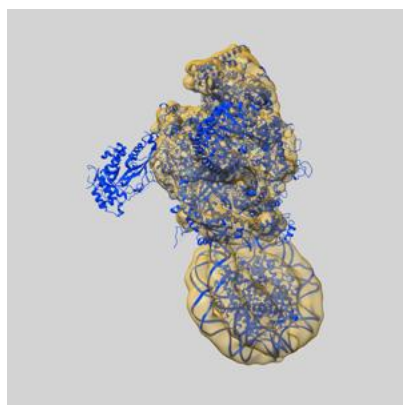
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.90	-	-
Author-provided FSC curve	9.80	15.38	10.02
Unmasked-calculated*	-	-	-

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

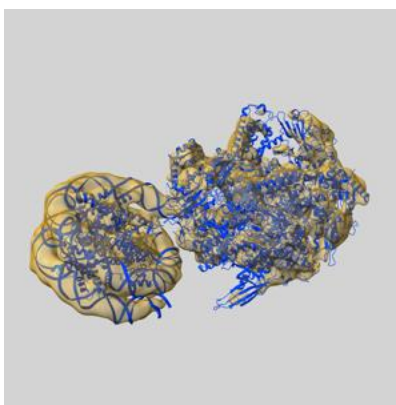
9 Map-model fit [i](#)

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](#).

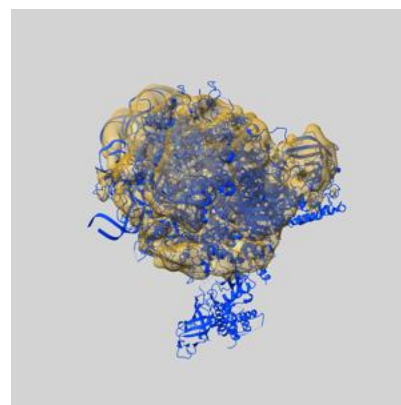
9.1 Map-model overlay [i](#)



X



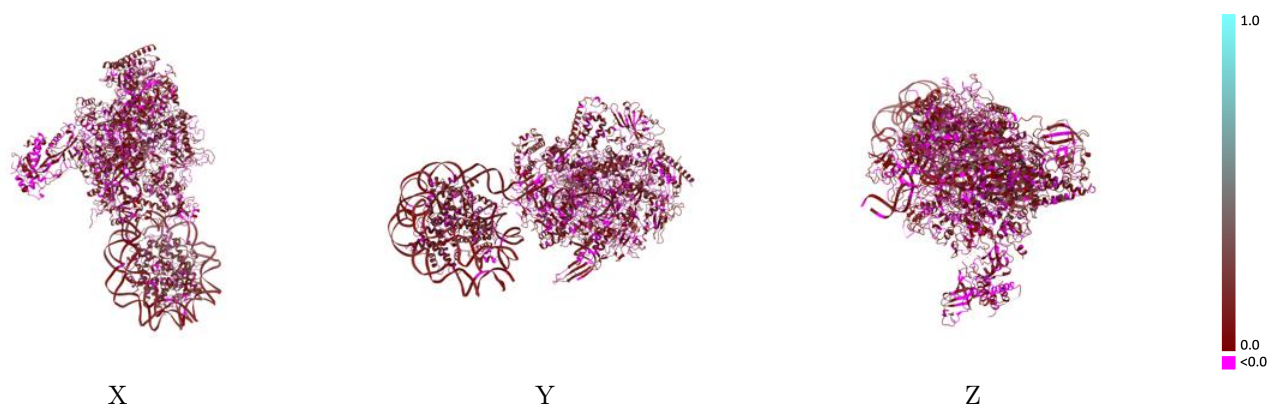
Y



Z

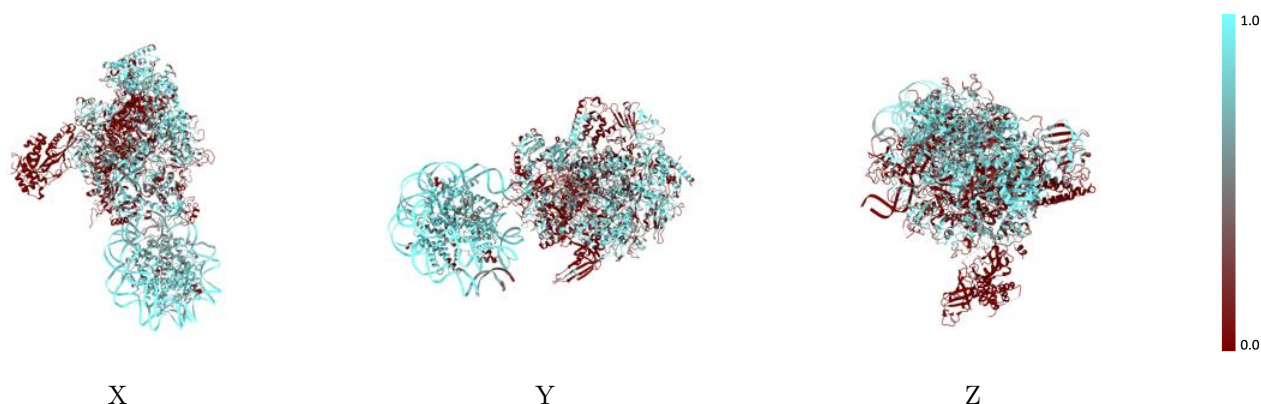
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



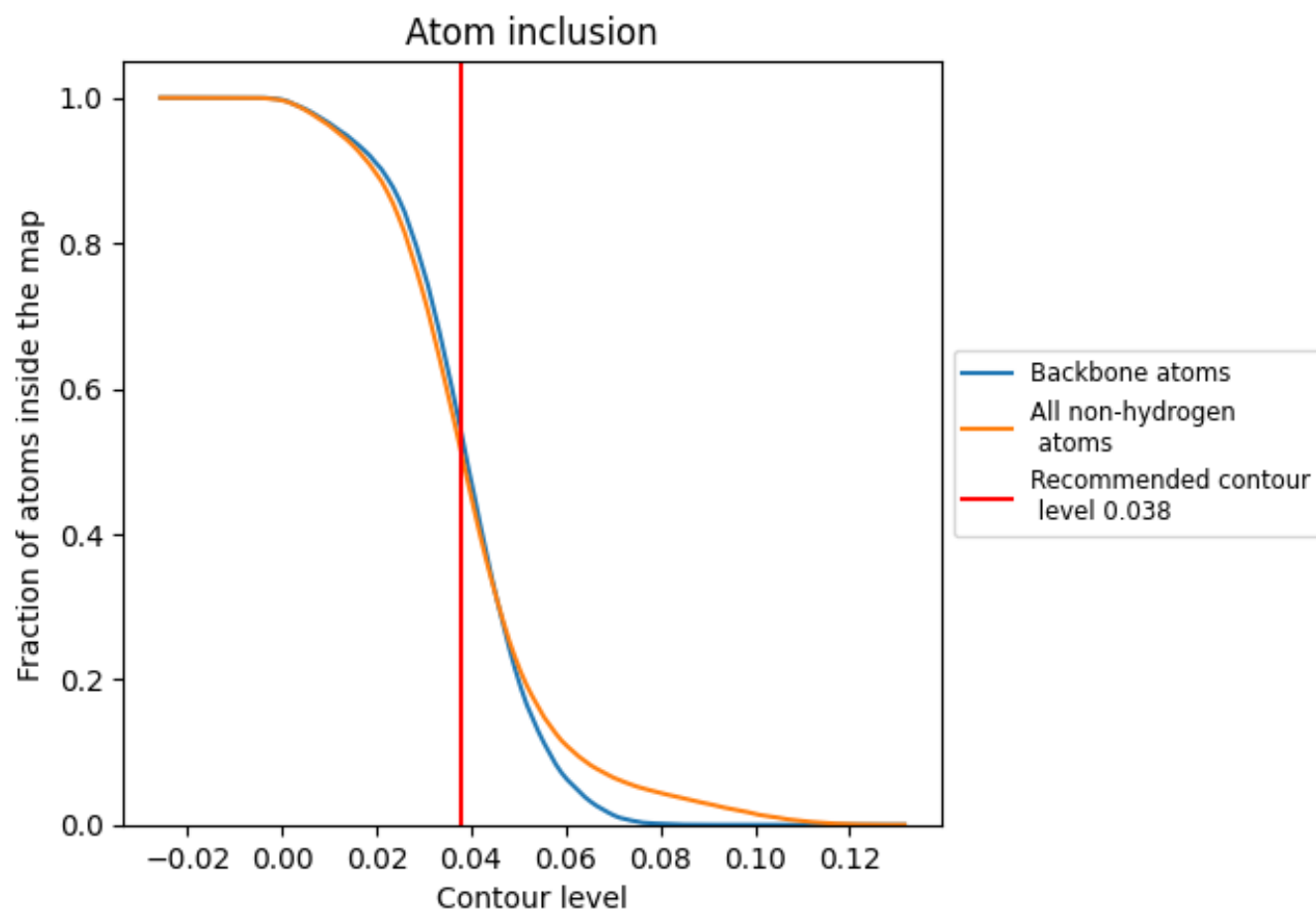
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.038).

















































9.4 Atom inclusion [i](#)



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	 0.5087	 0.0830
A	 0.3905	 0.0820
B	 0.4188	 0.0620
C	 0.5414	 0.0840
D	 0.0000	 0.0120
E	 0.5511	 0.1060
F	 0.5319	 0.0800
G	 0.0184	 0.0260
H	 0.4507	 0.0940
I	 0.2902	 0.0360
J	 0.6528	 0.0990
K	 0.5836	 0.0980
L	 0.2816	 0.0700
N	 0.8021	 0.1110
P	 0.6681	 0.1590
T	 0.7940	 0.1170
a	 0.7245	 0.1020
b	 0.7271	 0.0830
c	 0.6291	 0.0890
d	 0.7882	 0.1220
e	 0.7216	 0.1120
f	 0.7866	 0.0930
g	 0.7427	 0.0930
h	 0.7641	 0.1340

