



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 04:35 PM EST

PDB ID : 6O6C
EMDB ID : EMD-0633
Title : RNA polymerase II elongation complex arrested at a CPD lesion
Authors : Lahiri, I.; Leshziner, A.E.
Deposited on : 2019-03-05
Resolution : 3.10 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:

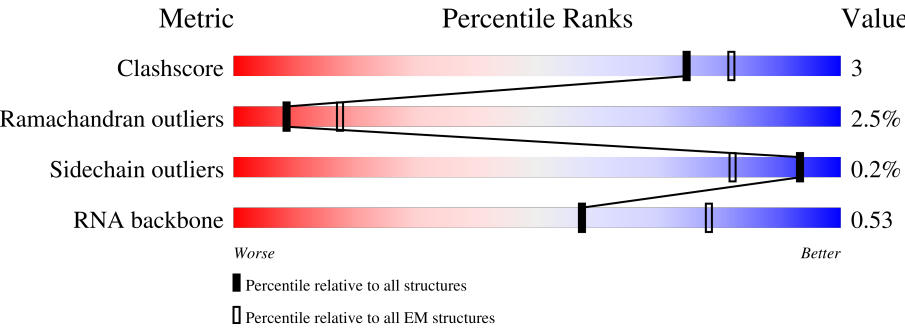
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	1733	
2	B	1224	
3	C	318	
4	D	215	
5	E	155	
6	F	146	
7	G	122	

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Mol	Chain	Length	Quality of chain
8	H	70	 87% 6% 7%
9	I	120	 10% 86% 7% 8%
10	J	70	 34% 56% 10% 34%
11	K	9	 11% 22% 67% 11%
12	L	16	 81% 75% 25%
13	M	27	 48% 37% 59%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 30166 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1446	Total	C	N	O	S	0	0
			11351	7143	1985	2161	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1165	Total	C	N	O	S	0	0
			9284	5865	1620	1743	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	81	Total	C	N	O	S	0	0
			657	419	111	124	3		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	115	Total	C	N	O	S	0	0
			935	576	169	179	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 11 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	9	Total	C	N	O	P	0	0
			198	88	40	61	9		

- Molecule 12 is a DNA chain called DNA (5'-D(P*GP*GP*AP*GP*AP*AP*GP*GP*AP*G P*CP*AP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	16	Total	C	N	O	P	0	0
			340	158	76	90	16		

- Molecule 13 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	27	Total	C	N	O	P	0	0
			555	268	80	179	28		

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	A	2	Total 2	Zn 2	0
14	B	1	Total 1	Zn 1	0
14	C	1	Total 1	Zn 1	0
14	G	2	Total 2	Zn 2	0
14	H	1	Total 1	Zn 1	0
14	J	1	Total 1	Zn 1	0

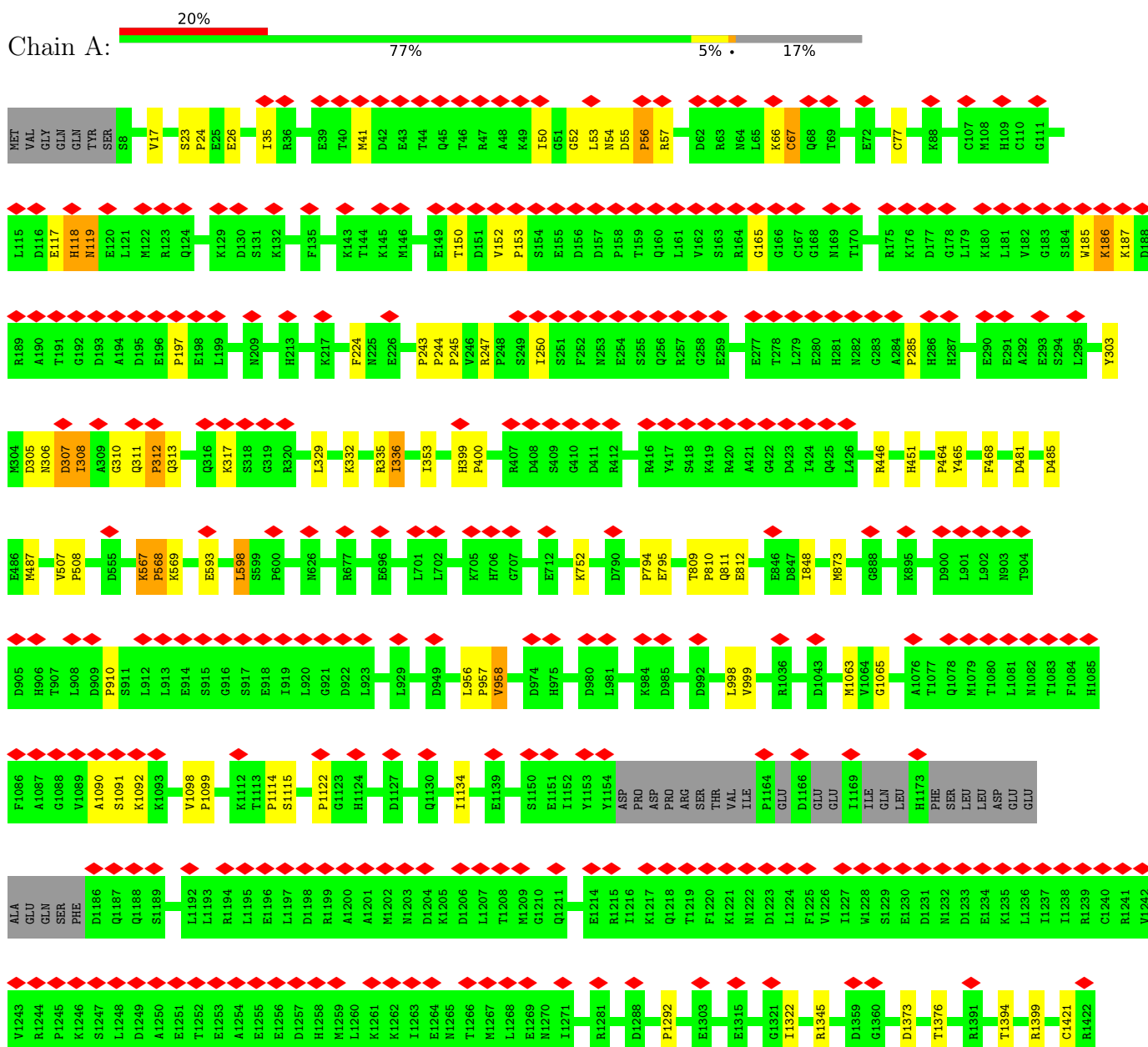
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

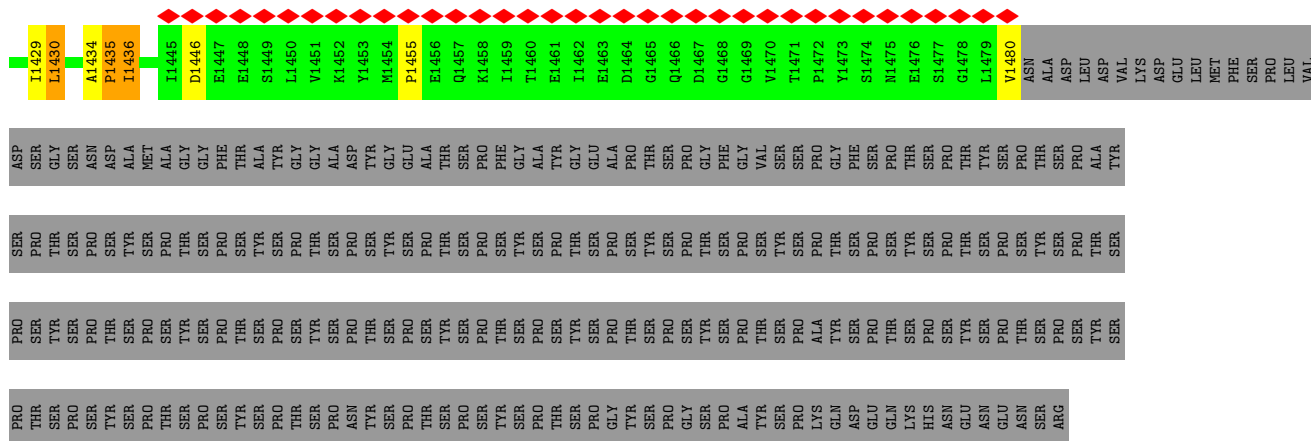
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Mg 1	0

3 Residue-property plots

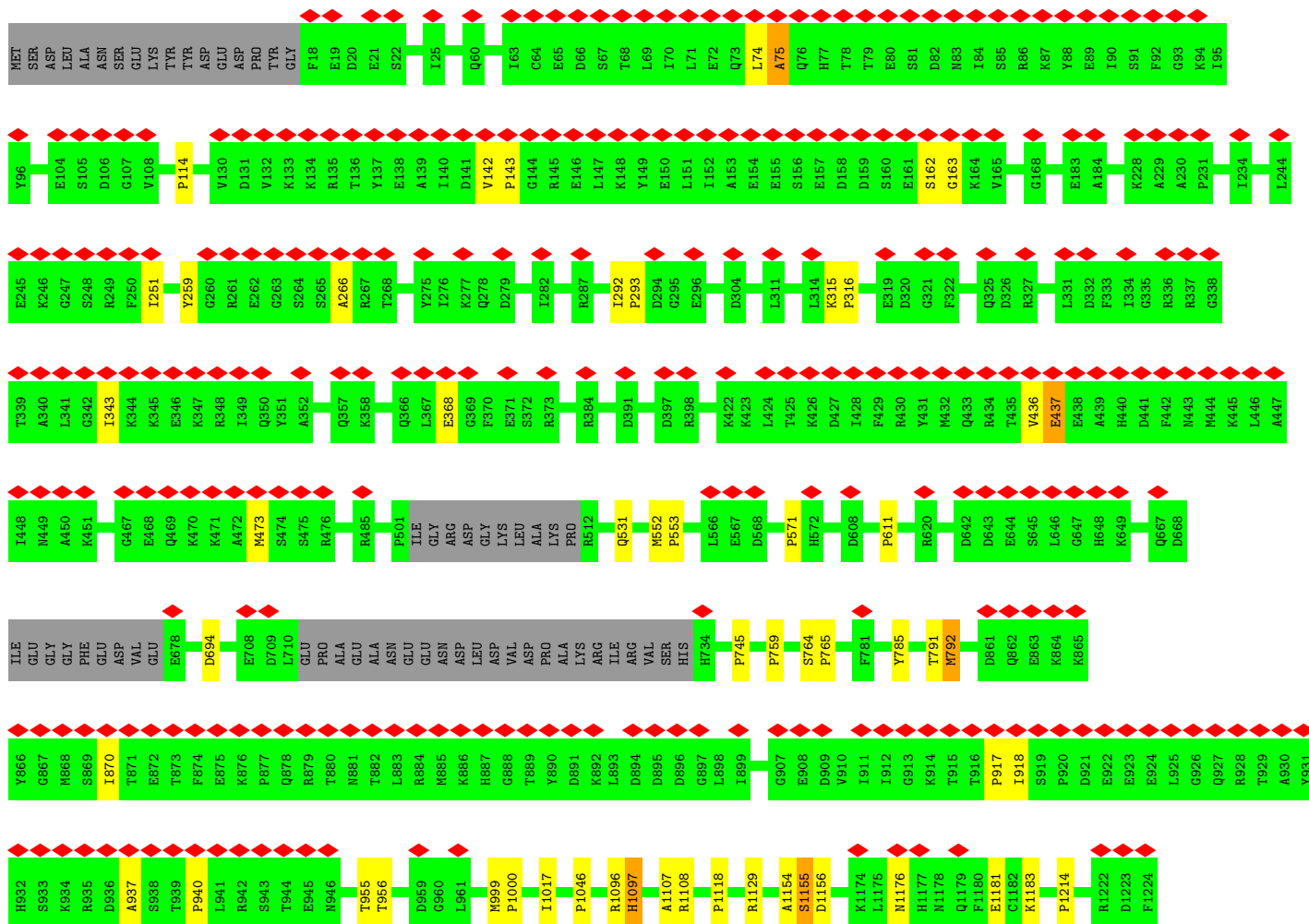
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 II subunit RPB1

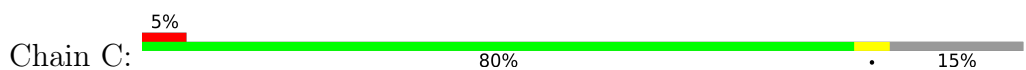


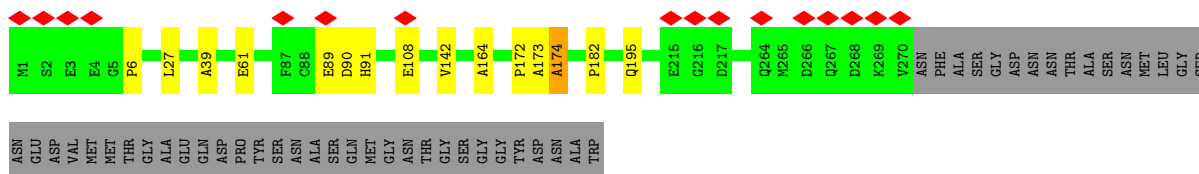


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

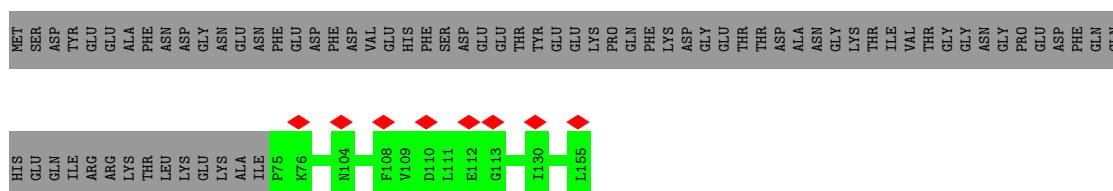




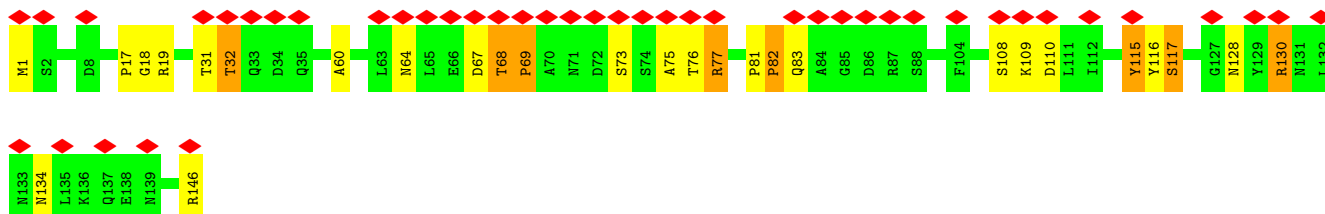
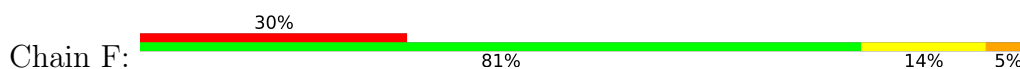
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



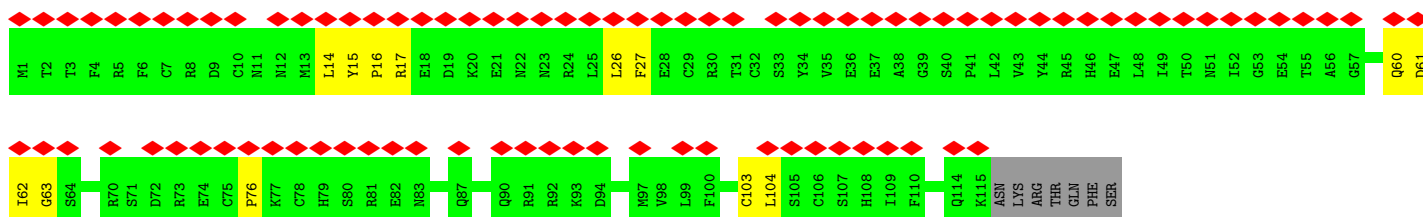
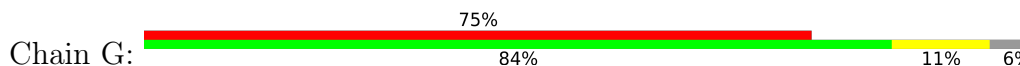
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



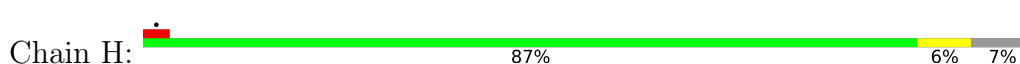
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

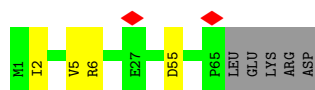


- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

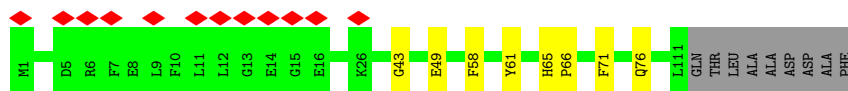
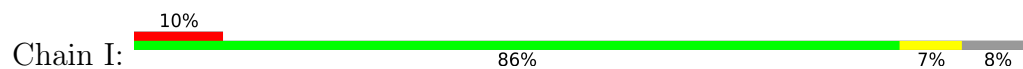


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

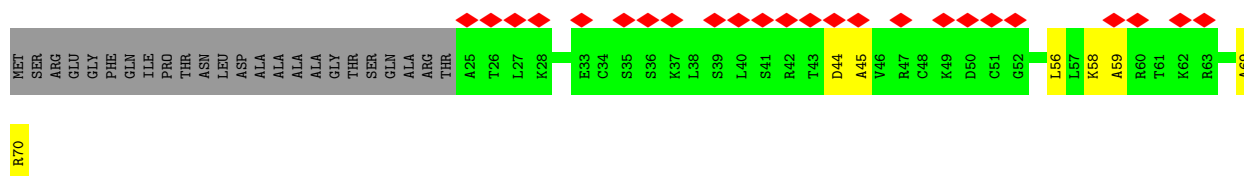




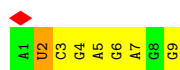
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



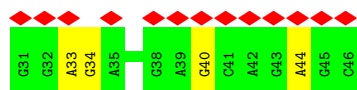
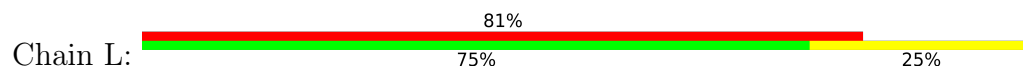
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



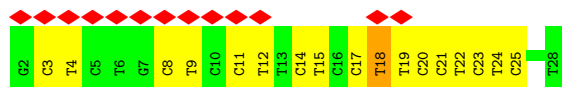
- Molecule 11: RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3')



- Molecule 12: DNA (5'-D(P*GP*GP*AP*GP*AP*AP*GP*GP*AP*GP*CP*AP*GP*AP*GP*C)-3')



- Molecule 13: DNA (27-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61654	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.7	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	0.282	Depositor
Minimum map value	-0.160	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0509	Depositor
Map size (\AA)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	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, TTD, 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	0.72	0/11551	0.53	0/15616
2	B	0.71	0/9467	0.54	0/12768
3	C	0.76	0/2163	0.53	0/2930
4	D	0.76	0/1796	0.54	0/2416
5	E	0.80	0/669	0.53	0/903
6	F	0.70	0/1181	0.64	0/1602
7	G	0.73	0/953	0.52	0/1283
8	H	0.75	0/541	0.57	0/727
9	I	0.75	0/913	0.48	0/1232
10	J	0.65	0/366	0.53	0/485
11	K	0.51	0/222	1.15	2/345 (0.6%)
12	L	0.29	0/385	0.66	0/594
13	M	0.46	0/569	0.86	0/870
All	All	0.72	0/30776	0.56	2/41771 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	K	2	U	C2-N1-C1'	7.14	126.27	117.70
11	K	2	U	C5-C6-N1	5.43	125.41	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11351	0	11405	72	0
2	B	9284	0	9264	29	0
3	C	2125	0	2091	7	0
4	D	1760	0	1788	11	0
5	E	657	0	673	0	0
6	F	1161	0	1124	18	0
7	G	935	0	897	5	0
8	H	532	0	542	2	0
9	I	895	0	903	5	0
10	J	364	0	388	3	0
11	K	198	0	99	3	0
12	L	340	0	177	5	0
13	M	555	0	321	39	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	G	2	0	0	0	0
14	H	1	0	0	0	0
14	J	1	0	0	0	0
15	A	1	0	0	0	0
All	All	30166	0	29672	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:ARG:HE	1:A:1373:ASP:HA	1.15	1.09
13:M:18:TTD:H2'	13:M:18:TTD:H2R1	1.38	1.00
13:M:18:TTD:C2'	13:M:18:TTD:H5R1	1.97	0.93
13:M:18:TTD:H5R1	13:M:18:TTD:C1'	1.99	0.93
13:M:18:TTD:H2R1	13:M:18:TTD:C2'	2.04	0.87
1:A:329:LEU:HD12	1:A:329:LEU:O	1.73	0.87
13:M:18:TTD:H5R1	13:M:18:TTD:H1'	1.60	0.81
1:A:1429:ILE:O	1:A:1429:ILE:HG22	1.80	0.80
13:M:17:DC:H2''	13:M:18:TTD:H5A2	1.64	0.79
13:M:18:TTD:H2'	13:M:18:TTD:H5R1	1.66	0.77
2:B:343:ILE:O	2:B:343:ILE:HG22	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:18:TTD:H1'	13:M:18:TTD:O4R	1.85	0.75
9:I:49:GLU:OE1	9:I:49:GLU:HA	1.87	0.74
1:A:310:GLY:C	1:A:312:PRO:HD2	2.06	0.73
13:M:18:TTD:H2'	13:M:18:TTD:C2R	2.15	0.71
1:A:1345:ARG:HE	1:A:1373:ASP:CA	2.01	0.69
13:M:18:TTD:H1	13:M:18:TTD:PB	2.33	0.68
1:A:308:ILE:HD12	1:A:308:ILE:H	1.58	0.68
1:A:308:ILE:HD12	1:A:308:ILE:N	2.10	0.67
13:M:18:TTD:H1'	13:M:18:TTD:C5R	2.24	0.67
1:A:332:LYS:NZ	13:M:20:DC:OP1	2.29	0.66
1:A:311:GLN:N	1:A:312:PRO:HD2	2.11	0.65
13:M:18:TTD:H1	13:M:18:TTD:O4P	1.96	0.65
13:M:18:TTD:H6	13:M:18:TTD:OP1	1.97	0.65
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.80	0.64
12:L:40:DG:OP2	12:L:40:DG:H8	1.82	0.63
13:M:20:DC:H2'	13:M:21:DC:O4'	1.97	0.63
13:M:17:DC:C2'	13:M:18:TTD:H5A2	2.28	0.63
3:C:108:GLU:OE1	3:C:108:GLU:N	2.29	0.60
6:F:108:SER:O	6:F:110:ASP:N	2.34	0.60
4:D:119:SER:HB3	12:L:44:DA:OP1	2.02	0.59
1:A:1345:ARG:NE	1:A:1373:ASP:HA	2.00	0.59
13:M:18:TTD:H2'	13:M:18:TTD:C5R	2.31	0.59
1:A:332:LYS:CE	13:M:20:DC:OP1	2.51	0.58
1:A:795:GLU:N	1:A:795:GLU:OE1	2.36	0.56
4:D:119:SER:CB	12:L:44:DA:OP1	2.54	0.56
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.07	0.55
4:D:167:ARG:O	4:D:167:ARG:NE	2.36	0.55
2:B:251:ILE:HG22	2:B:251:ILE:O	2.06	0.55
13:M:18:TTD:H5R1	13:M:18:TTD:C3R	2.37	0.54
4:D:167:ARG:NE	4:D:167:ARG:HA	2.21	0.54
1:A:332:LYS:HD2	13:M:20:DC:OP1	2.07	0.54
1:A:1435:PRO:O	1:A:1436:ILE:HB	2.08	0.54
2:B:1129:ARG:NE	13:M:21:DC:OP1	2.34	0.54
1:A:598:LEU:O	1:A:598:LEU:HG	2.07	0.53
2:B:74:LEU:O	2:B:75:ALA:C	2.46	0.53
1:A:247:ARG:O	1:A:247:ARG:HG3	2.08	0.53
1:A:567:LYS:O	1:A:568:PRO:C	2.46	0.53
13:M:21:DC:H2'	13:M:22:DT:C6	2.44	0.53
13:M:19:DT:H2'	13:M:20:DC:O4'	2.09	0.53
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.52
8:H:5:VAL:O	8:H:6:ARG:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:PRO:O	1:A:1436:ILE:CB	2.58	0.52
13:M:11:DC:H2'	13:M:12:DT:C6	2.44	0.52
2:B:343:ILE:O	2:B:343:ILE:CG2	2.56	0.52
2:B:1154:ALA:O	2:B:1155:SER:HB3	2.10	0.51
1:A:306:ASN:O	1:A:307:ASP:HB2	2.11	0.51
13:M:14:DC:H2'	13:M:15:DT:H72	1.92	0.51
1:A:329:LEU:O	1:A:329:LEU:CD1	2.53	0.50
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.74	0.50
3:C:61:GLU:OE1	3:C:61:GLU:N	2.35	0.50
4:D:167:ARG:NE	4:D:167:ARG:CA	2.74	0.50
1:A:1480:VAL:O	1:A:1480:VAL:HG12	2.11	0.50
6:F:82:PRO:O	6:F:83:GLN:HB2	2.11	0.50
6:F:116:TYR:O	6:F:117:SER:CB	2.59	0.50
12:L:40:DG:OP2	12:L:40:DG:H2'	2.13	0.49
2:B:292:ILE:N	2:B:293:PRO:CD	2.76	0.49
4:D:36:GLU:HA	4:D:36:GLU:OE1	2.13	0.49
7:G:26:LEU:C	7:G:26:LEU:HD12	2.33	0.49
1:A:55:ASP:OD1	1:A:55:ASP:C	2.51	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.60	0.49
1:A:335:ARG:O	1:A:336:ILE:C	2.51	0.48
2:B:162:SER:OG	2:B:163:GLY:N	2.46	0.48
6:F:1:MET:SD	6:F:64:ASN:HA	2.53	0.48
2:B:791:THR:O	2:B:792:MET:HB2	2.14	0.48
6:F:116:TYR:O	6:F:117:SER:HB2	2.13	0.48
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.95	0.48
2:B:315:LYS:HB3	2:B:316:PRO:HD3	1.95	0.47
6:F:68:THR:HB	6:F:69:PRO:CD	2.45	0.47
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.54	0.47
6:F:68:THR:HB	6:F:69:PRO:HD3	1.95	0.47
10:J:58:LYS:O	10:J:59:ALA:HB3	2.14	0.47
13:M:3:DC:H2'	13:M:3:DC:OP2	2.14	0.47
13:M:8:DC:H4'	13:M:8:DC:OP1	2.14	0.47
1:A:957:PRO:O	1:A:958:VAL:HB	2.15	0.47
1:A:1429:ILE:O	1:A:1429:ILE:CG2	2.53	0.46
4:D:202:SER:OG	4:D:203:GLU:N	2.49	0.46
13:M:18:TTD:H5R1	13:M:18:TTD:C4R	2.46	0.46
1:A:23:SER:O	1:A:26:GLU:N	2.48	0.46
6:F:31:THR:O	6:F:32:THR:HB	2.15	0.46
6:F:68:THR:CB	6:F:69:PRO:HD3	2.46	0.46
3:C:27:LEU:C	3:C:27:LEU:HD23	2.36	0.46
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:ASP:OD1	2:B:694:ASP:C	2.54	0.46
8:H:55:ASP:OD1	8:H:55:ASP:C	2.55	0.46
13:M:19:DT:OP1	13:M:20:DC:OP2	2.34	0.46
2:B:259:TYR:O	2:B:266:ALA:N	2.50	0.46
2:B:764:SER:HB3	2:B:765:PRO:HD3	1.98	0.46
2:B:918:ILE:O	2:B:918:ILE:HG23	2.16	0.46
9:I:43:GLY:HA3	9:I:71:PHE:CE2	2.50	0.45
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.15	0.45
3:C:173:ALA:O	3:C:174:ALA:HB3	2.17	0.45
10:J:44:ASP:O	10:J:45:ALA:HB3	2.16	0.45
2:B:552:MET:HB3	2:B:553:PRO:HD3	1.99	0.45
6:F:31:THR:O	6:F:32:THR:CB	2.65	0.45
6:F:146:ARG:O	6:F:146:ARG:HG3	2.16	0.45
2:B:436:VAL:O	2:B:437:GLU:HB3	2.17	0.45
3:C:89:GLU:O	3:C:91:HIS:N	2.50	0.45
1:A:464:PRO:O	1:A:465:TYR:HB2	2.17	0.44
6:F:130:ARG:N	6:F:130:ARG:HD3	2.32	0.44
1:A:56:PRO:O	1:A:57:ARG:HB2	2.17	0.44
13:M:17:DC:H2''	13:M:18:TTD:OP1	2.17	0.44
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.99	0.44
1:A:446:ARG:HB2	1:A:487:MET:SD	2.56	0.44
1:A:1394:THR:O	1:A:1399:ARG:NH1	2.49	0.44
2:B:785:TYR:C	2:B:785:TYR:CD1	2.90	0.44
6:F:76:THR:O	6:F:77:ARG:CB	2.66	0.44
6:F:76:THR:O	6:F:77:ARG:HB2	2.17	0.44
1:A:485:ASP:OD1	11:K:9:G:O3'	2.30	0.44
12:L:33:DA:C2'	12:L:34:DG:H5'	2.46	0.44
10:J:69:ALA:O	10:J:70:ARG:C	2.55	0.44
13:M:3:DC:H2''	13:M:4:DT:C5	2.53	0.44
1:A:118:HIS:O	1:A:119:ASN:HB2	2.17	0.44
9:I:58:PHE:HB3	9:I:76:GLN:HB3	2.00	0.44
1:A:507:VAL:HB	1:A:508:PRO:HD3	2.00	0.44
4:D:182:ASP:O	4:D:185:ALA:N	2.51	0.44
1:A:53:LEU:O	1:A:54:ASN:HB2	2.17	0.43
11:K:3:C:H2'	11:K:4:G:C8	2.53	0.43
13:M:22:DT:H2'	13:M:23:DC:C6	2.53	0.43
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.00	0.43
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.00	0.43
1:A:873:MET:SD	1:A:957:PRO:HG3	2.58	0.43
2:B:1154:ALA:O	2:B:1155:SER:CB	2.67	0.43
6:F:17:PRO:O	6:F:19:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:DC:H2''	13:M:12:DT:H5'	2.00	0.43
3:C:89:GLU:OE1	3:C:89:GLU:N	2.49	0.43
13:M:18:TTD:H6	13:M:18:TTD:H2''	1.65	0.43
1:A:1429:ILE:O	1:A:1430:LEU:HB3	2.18	0.43
9:I:61:TYR:CD1	9:I:61:TYR:C	2.92	0.43
1:A:311:GLN:O	1:A:313:GLN:N	2.50	0.42
13:M:18:TTD:H1'	13:M:18:TTD:C4'	2.48	0.42
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.59	0.42
1:A:67:CYS:SG	1:A:77:CYS:SG	3.17	0.42
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.88	0.42
1:A:481:ASP:OD1	1:A:481:ASP:C	2.57	0.42
1:A:1134:ILE:HG21	1:A:1322:ILE:HD11	2.01	0.42
1:A:956:LEU:HB3	1:A:957:PRO:HD2	2.00	0.42
1:A:1429:ILE:O	1:A:1430:LEU:CB	2.67	0.42
7:G:14:LEU:HB3	7:G:27:PHE:HB3	2.00	0.42
1:A:1098:VAL:HB	1:A:1099:PRO:HD3	2.01	0.42
2:B:552:MET:N	2:B:553:PRO:CD	2.82	0.42
1:A:311:GLN:N	1:A:312:PRO:CD	2.80	0.42
4:D:124:VAL:HB	4:D:125:PRO:HD3	2.02	0.42
9:I:65:HIS:HA	9:I:66:PRO:HD2	1.90	0.42
1:A:332:LYS:CD	13:M:20:DC:OP1	2.67	0.42
2:B:955:THR:OG1	2:B:956:THR:N	2.53	0.42
4:D:47:CYS:HA	4:D:53:PRO:HA	2.01	0.42
2:B:870:ILE:O	2:B:870:ILE:HG23	2.18	0.41
4:D:85:GLU:HA	4:D:86:PRO:HD3	1.90	0.41
6:F:67:ASP:O	6:F:69:PRO:HD2	2.20	0.41
7:G:61:ASP:O	7:G:63:GLY:N	2.52	0.41
1:A:811:GLN:OE1	1:A:811:GLN:N	2.49	0.41
2:B:999:MET:HB3	2:B:1000:PRO:HD2	2.03	0.41
7:G:60:GLN:OE1	7:G:60:GLN:N	2.45	0.41
1:A:50:ILE:HB	1:A:53:LEU:O	2.20	0.41
1:A:186:LYS:O	1:A:187:LYS:C	2.58	0.41
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.02	0.41
1:A:117:GLU:O	1:A:119:ASN:N	2.53	0.41
1:A:185:TRP:O	1:A:186:LYS:C	2.59	0.41
1:A:1090:ALA:O	1:A:1092:LYS:N	2.54	0.41
1:A:150:THR:HA	1:A:165:GLY:HA3	2.01	0.41
1:A:507:VAL:N	1:A:508:PRO:CD	2.84	0.41
1:A:1446:ASP:OD1	1:A:1446:ASP:C	2.58	0.41
6:F:75:ALA:O	6:F:76:THR:HB	2.20	0.41
1:A:809:THR:O	1:A:812:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:GLU:OE1	2:B:368:GLU:N	2.47	0.41
1:A:50:ILE:HG22	1:A:52:GLY:H	1.86	0.41
13:M:9:DT:H6	13:M:9:DT:H2'	1.70	0.41
1:A:1345:ARG:HD2	1:A:1376:THR:OG1	2.21	0.40
2:B:142:VAL:O	2:B:142:VAL:HG12	2.21	0.40
7:G:15:TYR:O	7:G:17:ARG:N	2.54	0.40
13:M:24:DT:H2'	13:M:25:DC:C6	2.56	0.40
1:A:305:ASP:OD1	1:A:305:ASP:C	2.59	0.40
1:A:1430:LEU:HD12	1:A:1430:LEU:C	2.42	0.40
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.94	0.40
6:F:115:TYR:OH	6:F:134:ASN:O	2.36	0.40
13:M:21:DC:H2'	13:M:22:DT:H6	1.84	0.40
2:B:315:LYS:N	2:B:316:PRO:CD	2.84	0.40
11:K:5:A:H2'	11:K:6:G:C8	2.56	0.40
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.37	0.40
2:B:1155:SER:O	2:B:1156:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1438/1733 (83%)	1298 (90%)	101 (7%)	39 (3%)	5	25
2	B	1157/1224 (94%)	1057 (91%)	77 (7%)	23 (2%)	7	31
3	C	268/318 (84%)	250 (93%)	11 (4%)	7 (3%)	5	26
4	D	213/215 (99%)	202 (95%)	7 (3%)	4 (2%)	8	33
5	E	79/155 (51%)	73 (92%)	6 (8%)	0	100	100
6	F	144/146 (99%)	114 (79%)	18 (12%)	12 (8%)	1	5
7	G	113/122 (93%)	98 (87%)	10 (9%)	5 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	63/70 (90%)	59 (94%)	3 (5%)	1 (2%)	9	37
9	I	109/120 (91%)	105 (96%)	4 (4%)	0	100	100
10	J	44/70 (63%)	36 (82%)	7 (16%)	1 (2%)	6	28
All	All	3628/4173 (87%)	3292 (91%)	244 (7%)	92 (2%)	9	27

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	197	PRO
1	A	250	ILE
1	A	336	ILE
1	A	567	LYS
1	A	1115	SER
1	A	1430	LEU
1	A	1436	ILE
1	A	1455	PRO
2	B	1046	PRO
2	B	1155	SER
2	B	1214	PRO
3	C	90	ASP
3	C	142	VAL
6	F	32	THR
6	F	68	THR
6	F	69	PRO
6	F	77	ARG
6	F	82	PRO
6	F	109	LYS
6	F	117	SER
7	G	62	ILE
8	H	2	ILE
1	A	41	MET
1	A	118	HIS
1	A	186	LYS
1	A	307	ASP
1	A	400	PRO
1	A	999	VAL
1	A	1091	SER
2	B	75	ALA
2	B	1097	HIS
2	B	1176	ASN

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Mol	Chain	Res	Type
3	C	172	PRO
4	D	125	PRO
6	F	18	GLY
6	F	128	ASN
7	G	16	PRO
7	G	103	CYS
1	A	56	PRO
1	A	66	LYS
1	A	224	PHE
1	A	285	PRO
1	A	312	PRO
1	A	317	LYS
1	A	593	GLU
1	A	752	LYS
1	A	998	LEU
1	A	1114	PRO
2	B	473	MET
2	B	531	GLN
6	F	60	ALA
6	F	73	SER
1	A	67	CYS
1	A	568	PRO
1	A	958	VAL
2	B	611	PRO
2	B	792	MET
2	B	1118	PRO
2	B	1183	LYS
3	C	6	PRO
4	D	183	PRO
7	G	76	PRO
1	A	24	PRO
1	A	35	ILE
1	A	598	LEU
1	A	794	PRO
1	A	810	PRO
1	A	1122	PRO
1	A	1292	PRO
2	B	114	PRO
2	B	437	GLU
2	B	1181	GLU
3	C	174	ALA
3	C	195	GLN

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Mol	Chain	Res	Type
4	D	53	PRO
7	G	104	LEU
10	J	56	LEU
2	B	143	PRO
2	B	571	PRO
2	B	937	ALA
2	B	940	PRO
2	B	1017	ILE
2	B	745	PRO
3	C	182	PRO
4	D	86	PRO
1	A	1435	PRO
1	A	910	PRO
2	B	917	PRO
6	F	81	PRO
1	A	399	HIS
2	B	759	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	1259/1520 (83%)	1256 (100%)	3 (0%)	93	97
2	B	1012/1061 (95%)	1012 (100%)	0	100	100
3	C	238/274 (87%)	238 (100%)	0	100	100
4	D	197/197 (100%)	197 (100%)	0	100	100
5	E	72/137 (53%)	72 (100%)	0	100	100
6	F	128/128 (100%)	126 (98%)	2 (2%)	62	84
7	G	109/116 (94%)	109 (100%)	0	100	100
8	H	60/65 (92%)	60 (100%)	0	100	100
9	I	96/102 (94%)	96 (100%)	0	100	100
10	J	40/57 (70%)	40 (100%)	0	100	100
All	All	3211/3657 (88%)	3206 (100%)	5 (0%)	93	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	TYR
1	A	308	ILE
1	A	451	HIS
6	F	115	TYR
6	F	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	K	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	K	2	U
11	K	7	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	TTD	M	18	13	42,45,46	3.44	20 (47%)	62,74,77	2.33	24 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	TTD	M	18	13	-	12/22/109/110	0/5/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	18	TTD	C2-N3	7.39	1.51	1.38
13	M	18	TTD	C5-C6	-6.98	1.47	1.55
13	M	18	TTD	C2'-C3R	-6.97	1.37	1.52
13	M	18	TTD	C2T-N3T	6.82	1.50	1.38
13	M	18	TTD	C4-N3	6.71	1.48	1.37
13	M	18	TTD	C5T-C6T	-6.69	1.47	1.55
13	M	18	TTD	C2-N1	6.58	1.49	1.36
13	M	18	TTD	C2T-N1T	6.05	1.48	1.36
13	M	18	TTD	C4T-N3T	5.69	1.46	1.37
13	M	18	TTD	PB-O3R	3.89	1.70	1.60
13	M	18	TTD	C3'-C4'	-2.85	1.45	1.53
13	M	18	TTD	C2'-C1'	-2.83	1.44	1.52
13	M	18	TTD	O2T-C2T	-2.71	1.18	1.23
13	M	18	TTD	O4'-C1'	2.49	1.47	1.42
13	M	18	TTD	PB-O5R	2.46	1.69	1.59
13	M	18	TTD	O3R-C3R	2.38	1.52	1.46
13	M	18	TTD	O5'-C5'	-2.29	1.39	1.44
13	M	18	TTD	C6-N1	2.29	1.50	1.46
13	M	18	TTD	O4-C4	-2.28	1.18	1.22
13	M	18	TTD	O4T-C4T	-2.06	1.19	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	18	TTD	O4R-C1R-N1T	7.81	117.91	108.65
13	M	18	TTD	C4T-N3T-C2T	-4.95	119.06	126.67
13	M	18	TTD	C4-N3-C2	-4.87	119.18	126.67
13	M	18	TTD	N3T-C2T-N1T	3.97	120.81	116.69
13	M	18	TTD	C5T-C4T-N3T	3.95	119.50	116.06
13	M	18	TTD	C5-C4-N3	3.88	119.44	116.06
13	M	18	TTD	C3R-C2'-C1'	3.86	110.30	102.91
13	M	18	TTD	N3-C2-N1	3.75	120.59	116.69
13	M	18	TTD	O4-C4-C5	-3.65	119.96	122.88
13	M	18	TTD	O4T-C4T-C5T	-3.12	120.38	122.88
13	M	18	TTD	O2T-C2T-N1T	-2.82	119.11	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	18	TTD	O4P-PB-O5R	2.71	120.35	107.75
13	M	18	TTD	C6T-C5T-C4T	2.67	122.10	114.50
13	M	18	TTD	O4'-C1'-N1	-2.64	105.53	108.65
13	M	18	TTD	O4P-PB-O3R	2.54	116.80	106.78
13	M	18	TTD	O2-C2-N1	-2.45	119.69	123.49
13	M	18	TTD	C6-C5-C4	2.44	121.46	114.50
13	M	18	TTD	C5-C6-N1	2.32	118.86	115.61
13	M	18	TTD	C5'-C4R-C3R	-2.31	109.25	114.53
13	M	18	TTD	C3'-C2R-C1R	-2.27	96.84	102.54
13	M	18	TTD	C4'-O4R-C1R	-2.24	104.03	109.45
13	M	18	TTD	C4R-O4'-C1'	-2.18	104.17	109.45
13	M	18	TTD	C5T-C5-C6	2.16	91.07	88.38
13	M	18	TTD	C5A-C5-C5T	-2.10	110.32	116.39

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	18	TTD	C4R-C5'-O5'-P
13	M	18	TTD	C2'-C3R-O3R-PB
13	M	18	TTD	O4R-C4'-C5R-O5R
13	M	18	TTD	O4'-C1'-N1-C2
13	M	18	TTD	C2'-C1'-N1-C6
13	M	18	TTD	O4'-C1'-N1-C6
13	M	18	TTD	C2R-C1R-N1T-C6T
13	M	18	TTD	C2'-C1'-N1-C2
13	M	18	TTD	C4'-C5R-O5R-PB
13	M	18	TTD	O4R-C1R-N1T-C6T
13	M	18	TTD	O4R-C1R-N1T-C2T
13	M	18	TTD	C2R-C1R-N1T-C2T

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	18	TTD	20	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

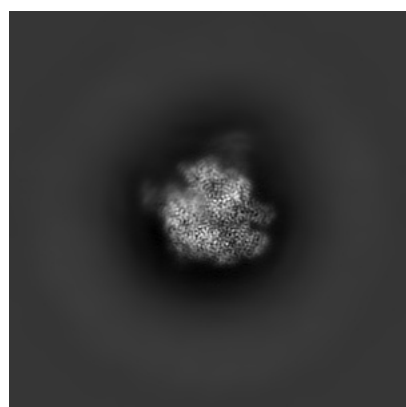
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0633. These allow visual inspection of the internal detail of the map and identification of artifacts.

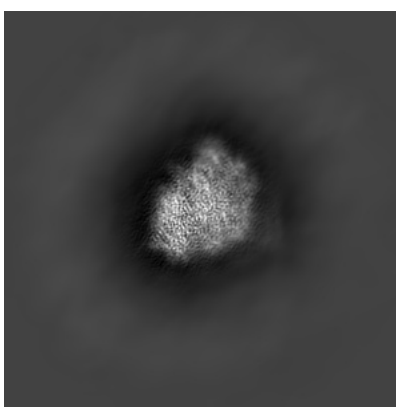
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

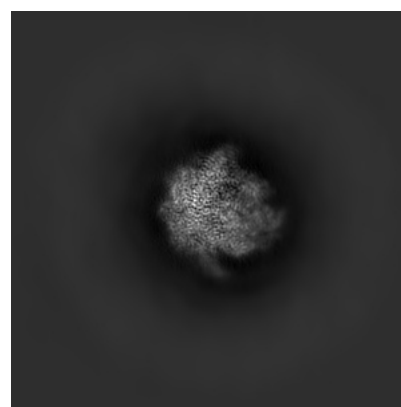
6.1.1 Primary map



X



Y

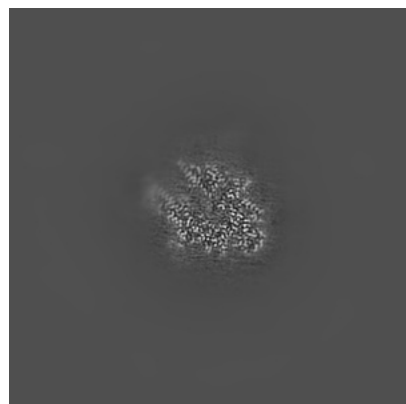


Z

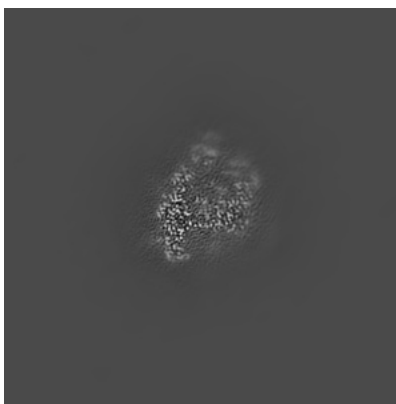
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

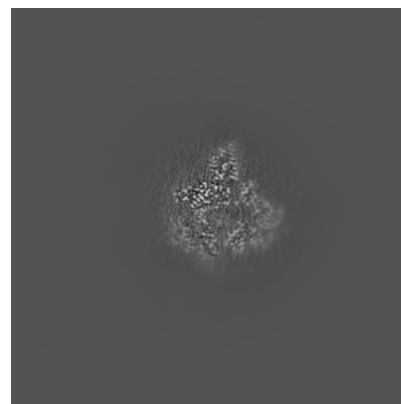
6.2.1 Primary map



X Index: 192



Y Index: 192

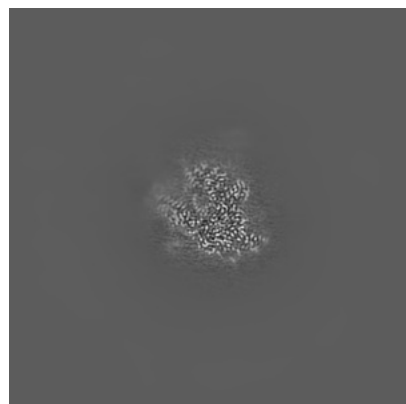


Z Index: 192

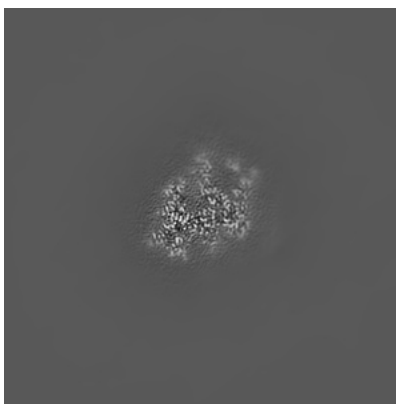
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

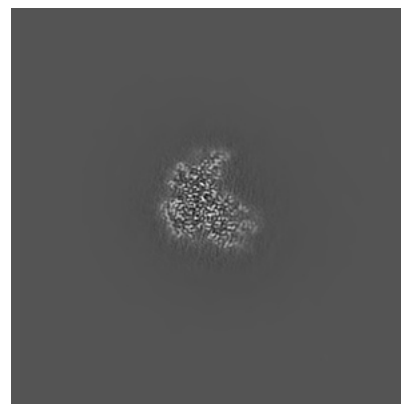
6.3.1 Primary map



X Index: 184



Y Index: 198

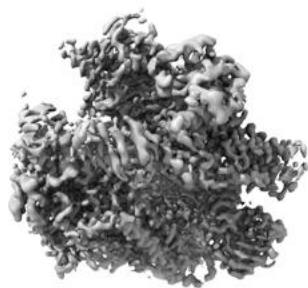


Z Index: 166

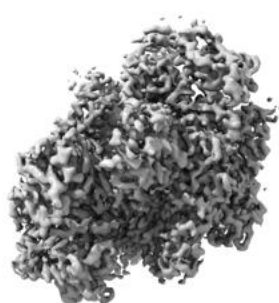
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

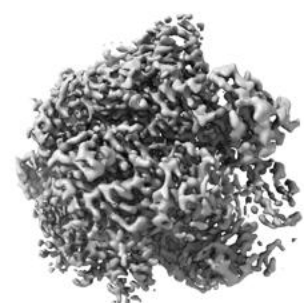
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0509. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

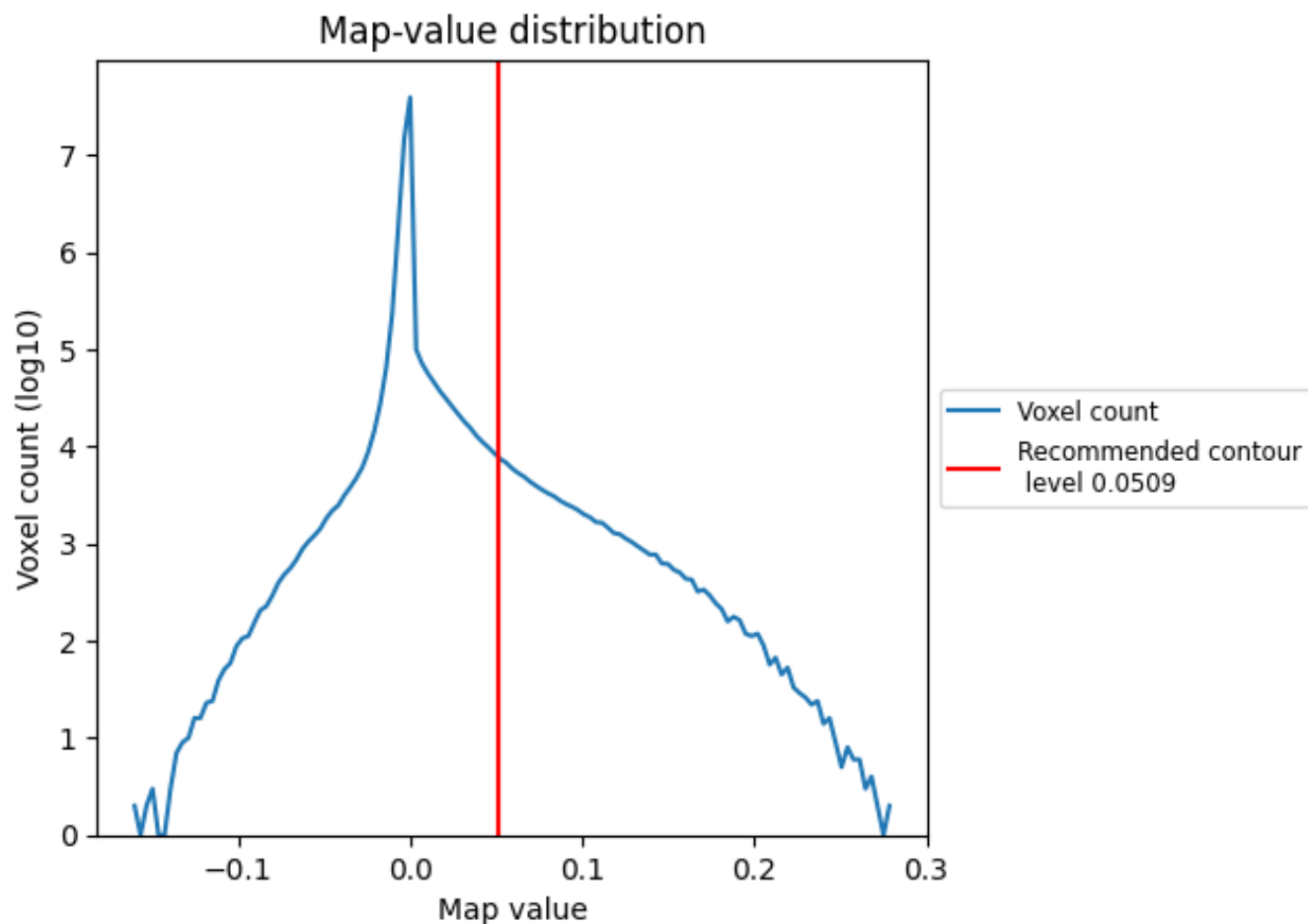
6.5 Mask visualisation

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

7 Map analysis [i](#)

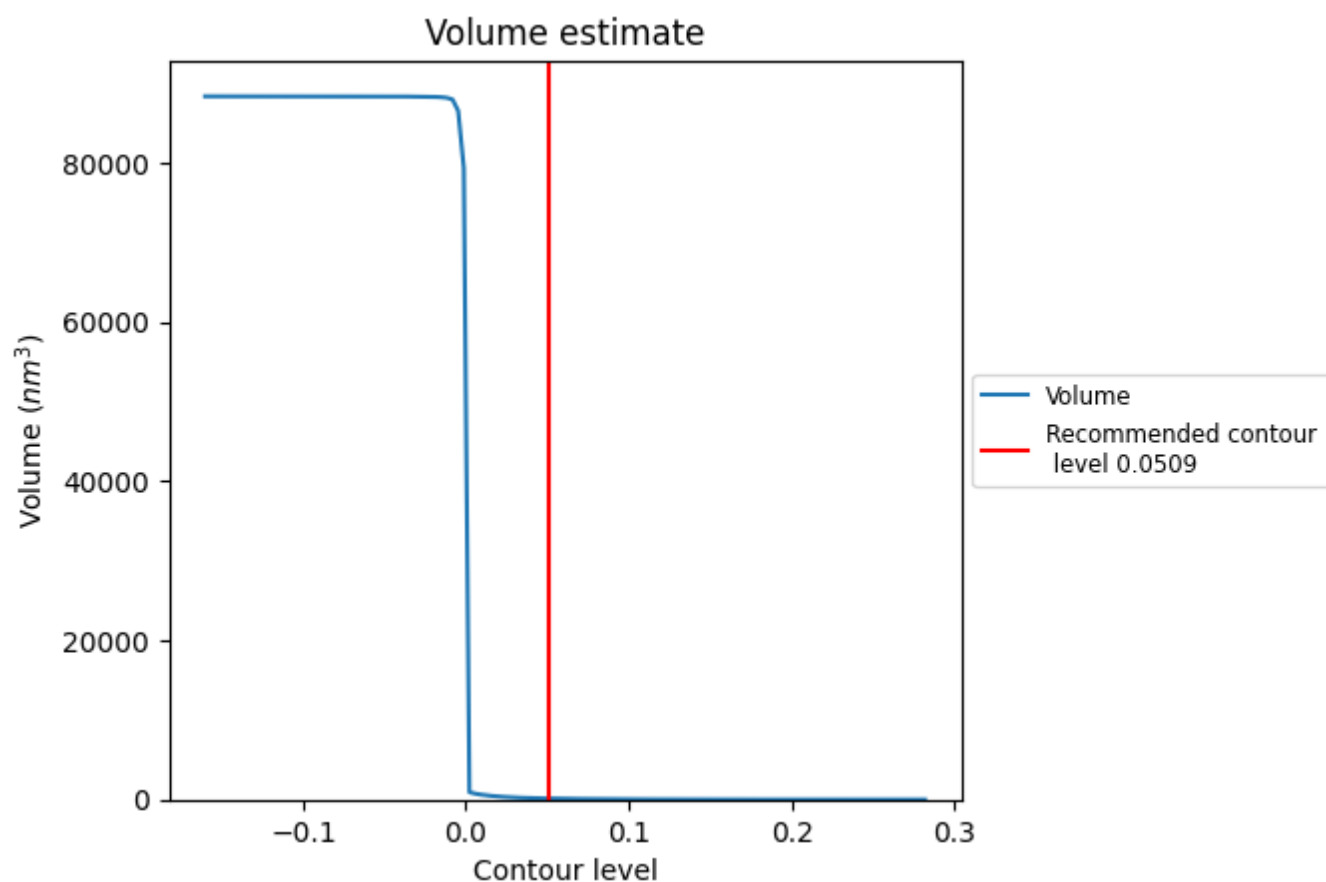
This section contains the results of statistical analysis of the map.

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.

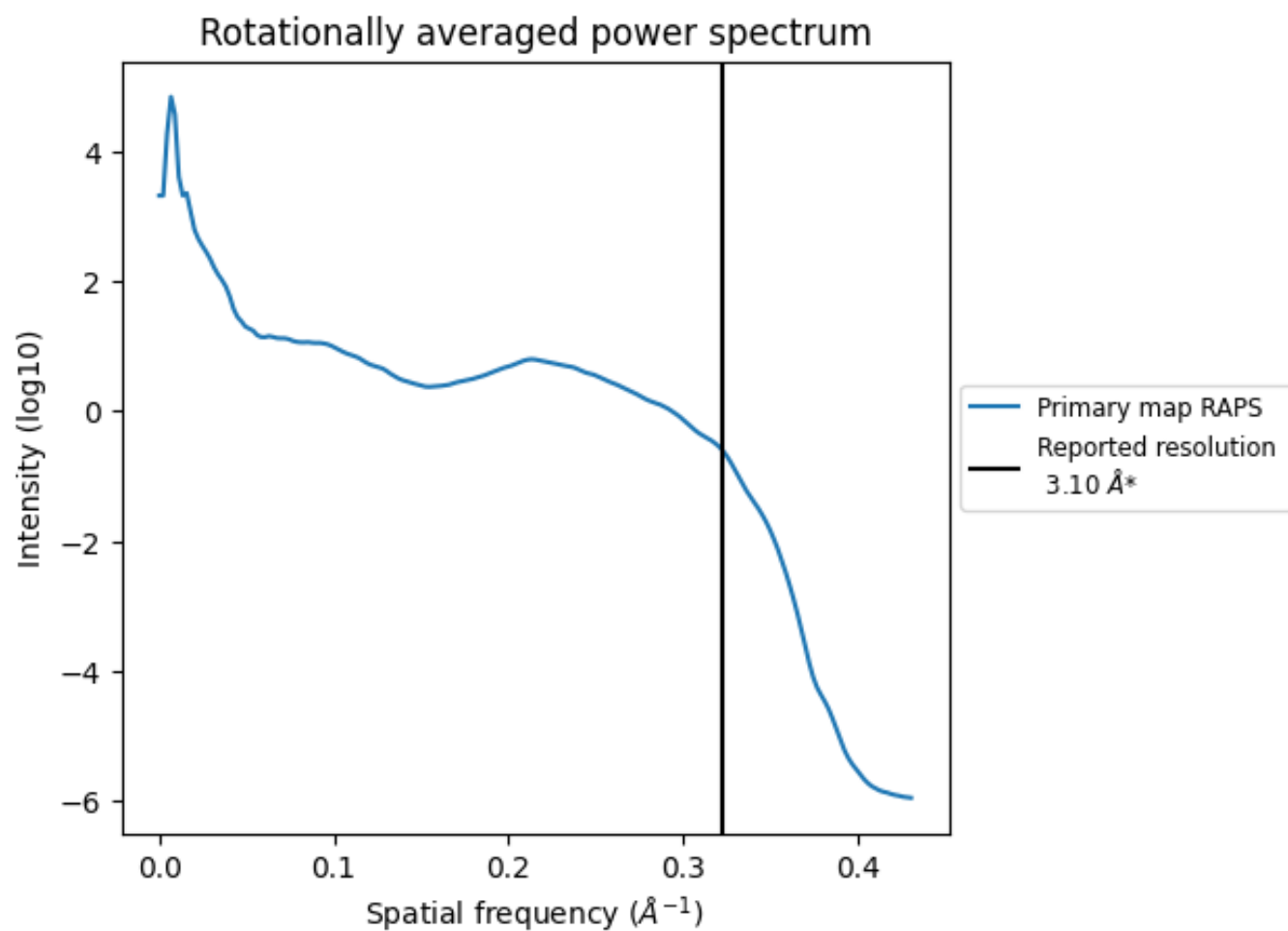
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 0.323 Å⁻¹

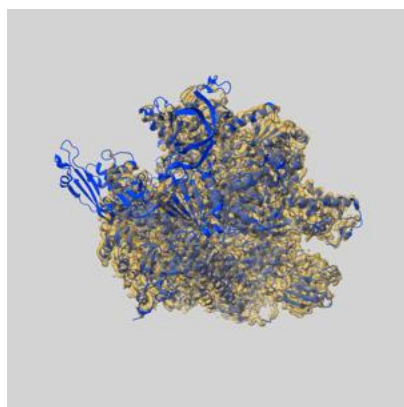
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

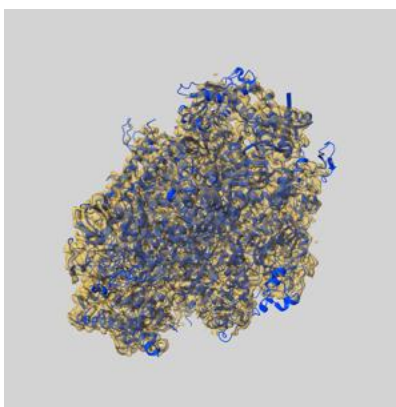
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0633 and PDB model 6O6C. Per-residue inclusion information can be found in section [3](#) on page [7](#).

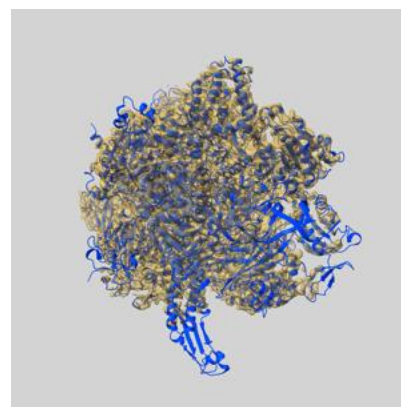
9.1 Map-model overlay [i](#)



X



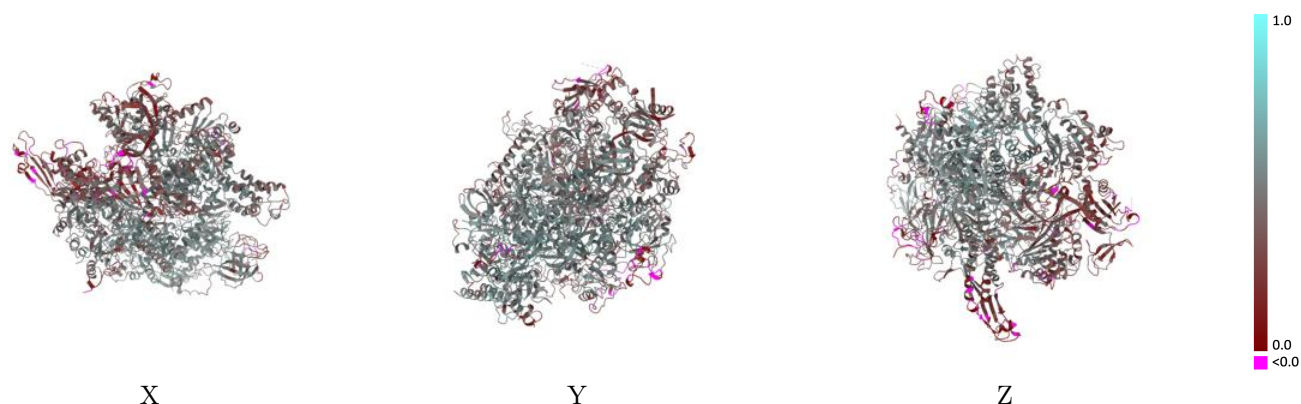
Y



Z

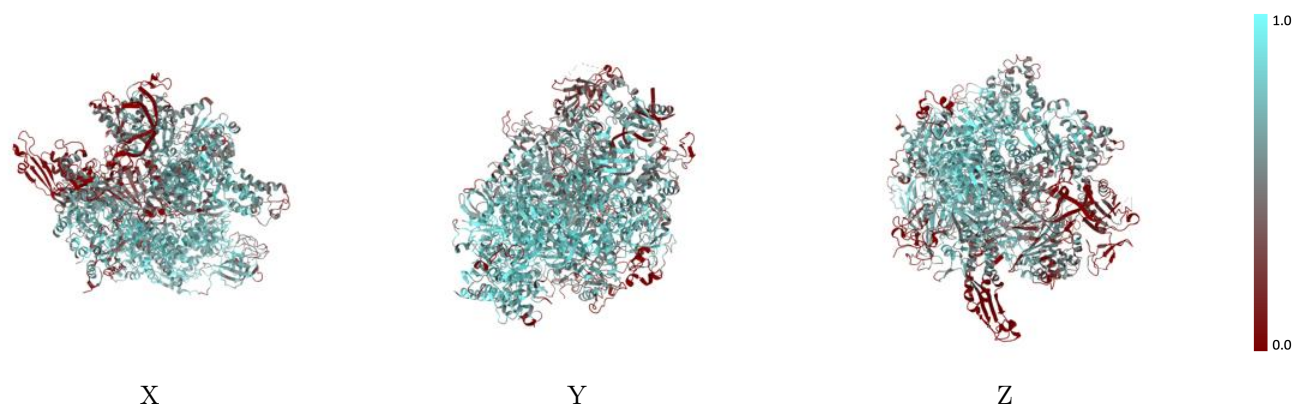
The images above show the 3D surface view of the map at the recommended contour level 0.0509 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



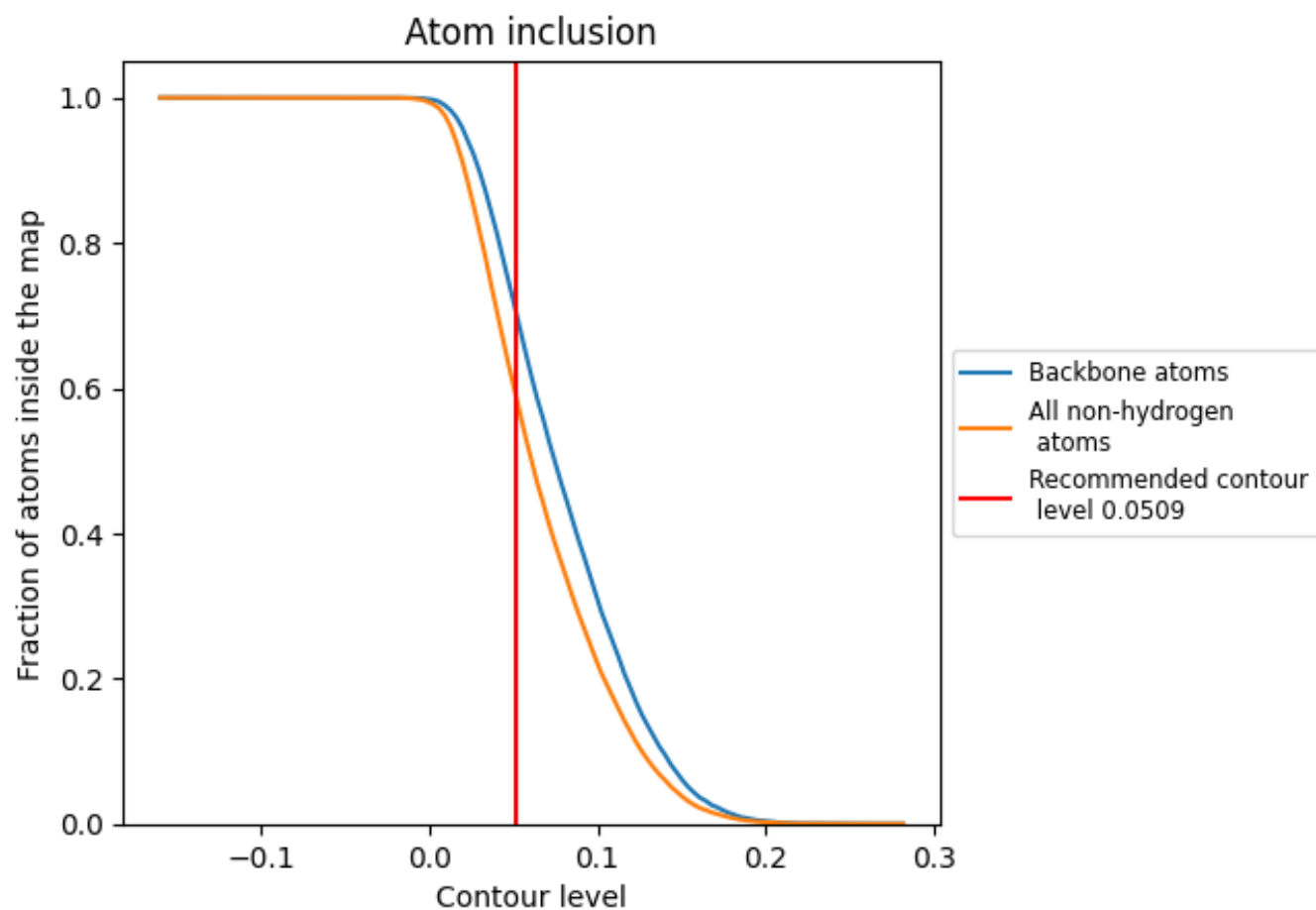
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0509).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 59% 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 (0.0509) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5946	 0.4350
A	 0.6008	 0.4420
B	 0.5946	 0.4300
C	 0.7512	 0.4970
D	 0.6168	 0.4290
E	 0.6886	 0.5040
F	 0.5666	 0.3810
G	 0.2050	 0.3260
H	 0.7911	 0.5110
I	 0.7268	 0.5020
J	 0.3693	 0.3390
K	 0.6919	 0.4690
L	 0.2059	 0.2940
M	 0.3514	 0.3390

