



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Oct 28, 2019 – 12:40 PM EDT

PDB ID : 6A5L
EMDB ID: : EMD-6980
Title : RNA polymerase II elongation complex stalled at SHL(-1) of the nucleosome,
with foreign DNA
Authors : Kujirai, T.; Ehara, H.; Fujino, Y.; Shirouzu, M.; Sekine, S.; Kurumizaka, H.
Deposited on : 2018-06-24
Resolution : 5.60 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

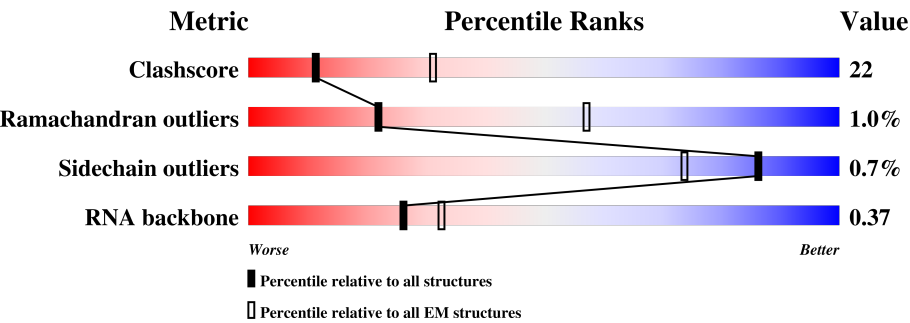
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.60 Å.

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




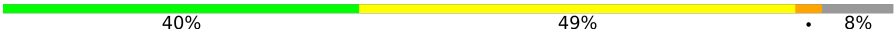

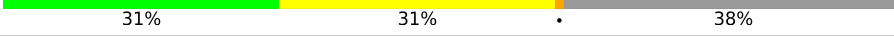
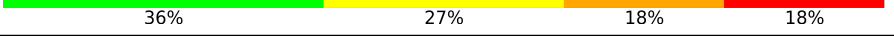
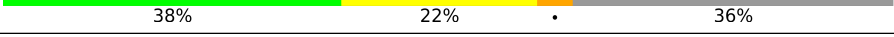
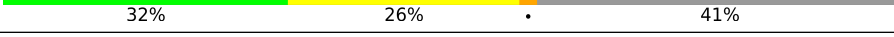

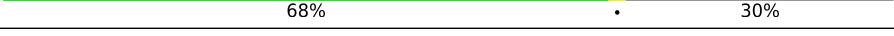

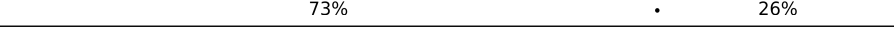
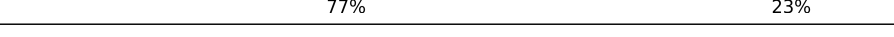

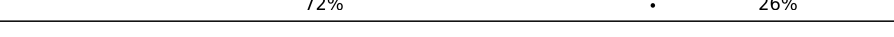



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1743	<div><div>44%</div><div>35%</div><div>•</div><div>19%</div></div>
2	B	1227	<div><div>49%</div><div>44%</div><div>•</div><div>5%</div></div>
3	C	304	<div><div>42%</div><div>44%</div><div></div><div>13%</div></div>
4	D	186	<div><div>52%</div><div>32%</div><div></div><div>16%</div></div>
5	E	214	<div><div>52%</div><div>45%</div><div>•</div><div></div></div>
6	F	155	<div><div>32%</div><div>22%</div><div>•</div><div>46%</div></div>
7	G	171	<div><div>54%</div><div>44%</div><div>•</div><div></div></div>
8	H	145	<div><div>47%</div><div>45%</div><div></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	
20	0	42	
21	1	42	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 44065 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*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*G)-3').

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
16	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
17	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 18 is a protein called Histone H2A 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	91	Total	C	N	O	S	0
			708	447	125	134	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 a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	42	Total	C	N	O	P	0	0
			868	409	182	235	42		

- Molecule 21 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1	42	Total	C	N	O	P	0	0
			854	410	133	269	42		

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

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

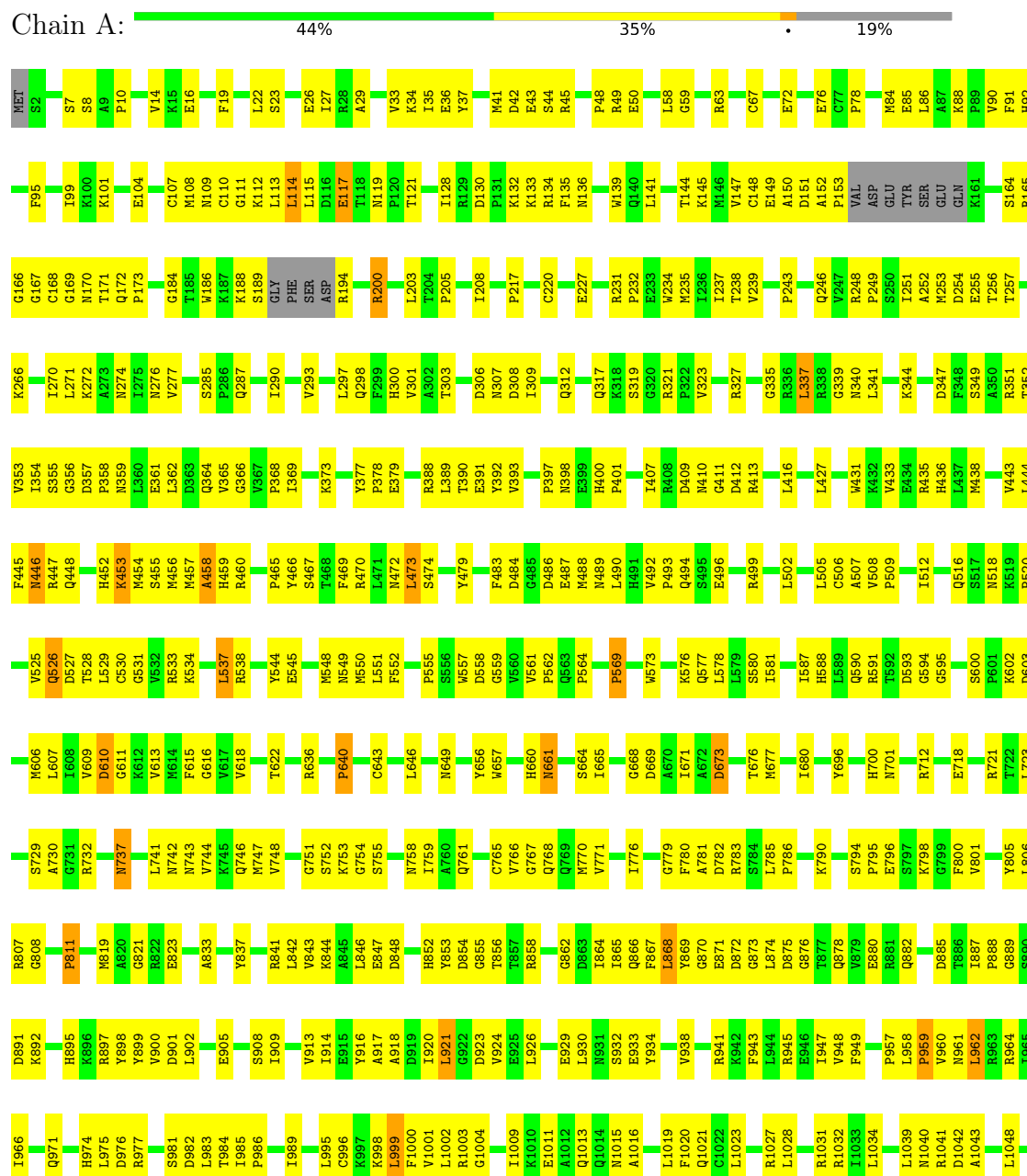
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

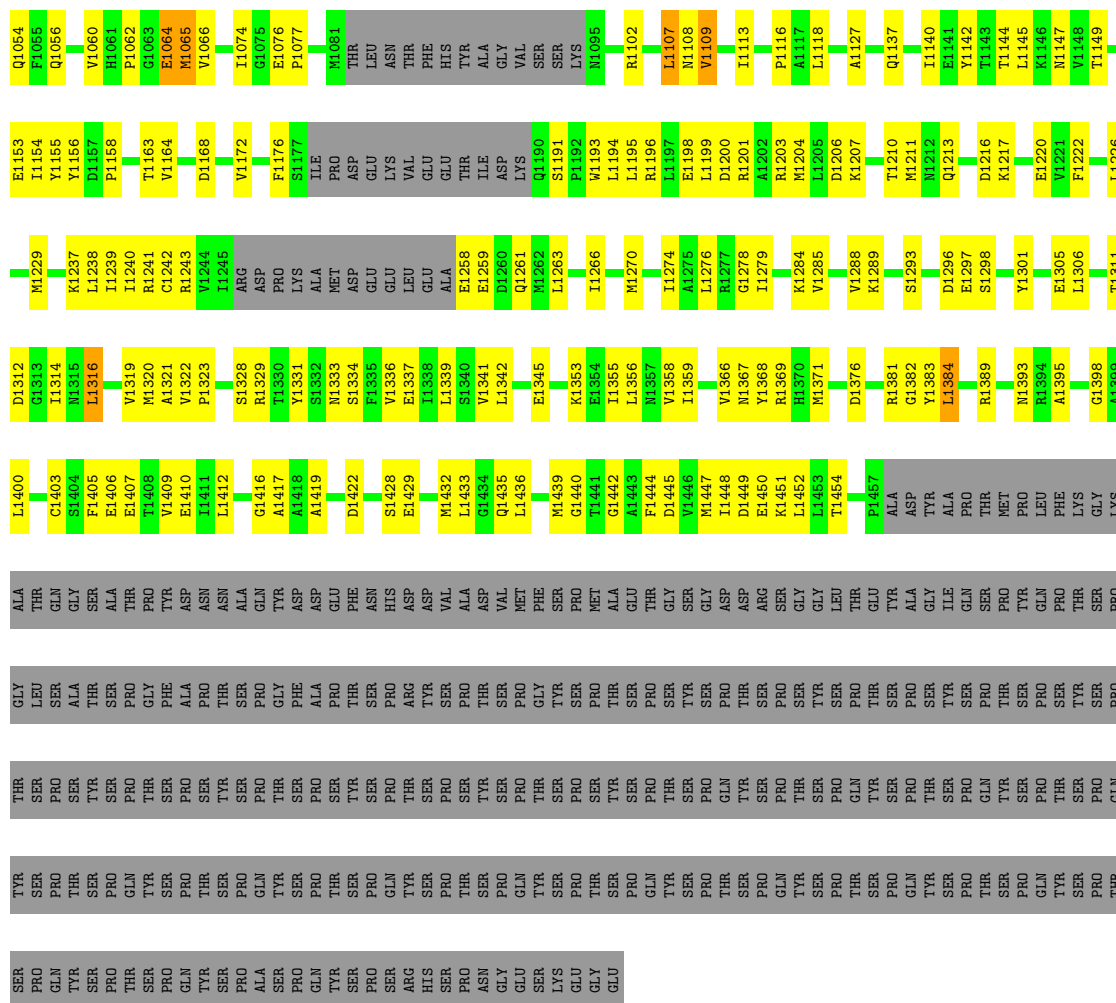
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

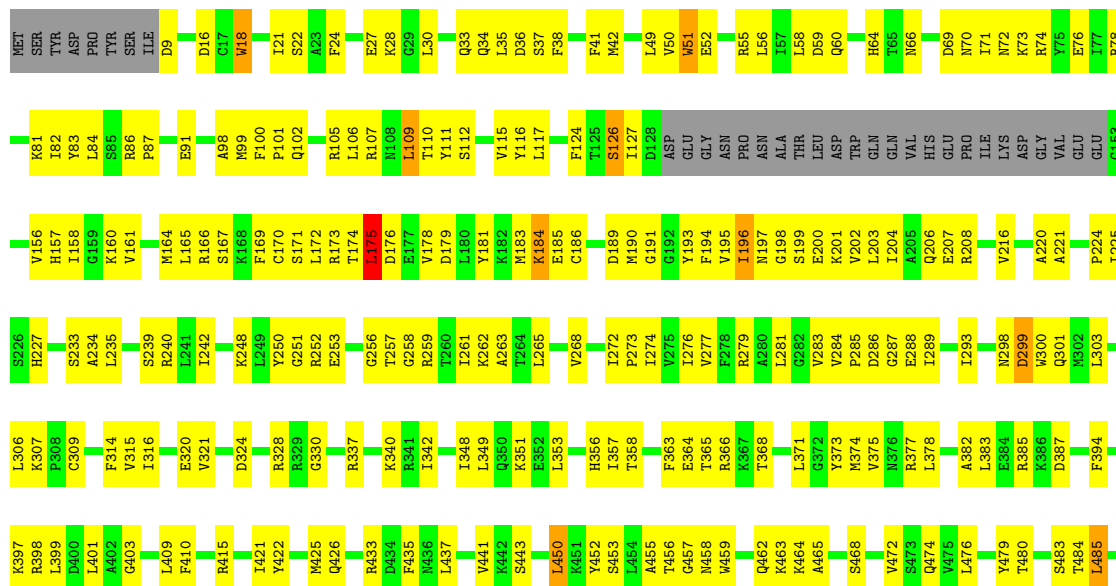
- Molecule 1: DNA-directed RNA polymerase subunit

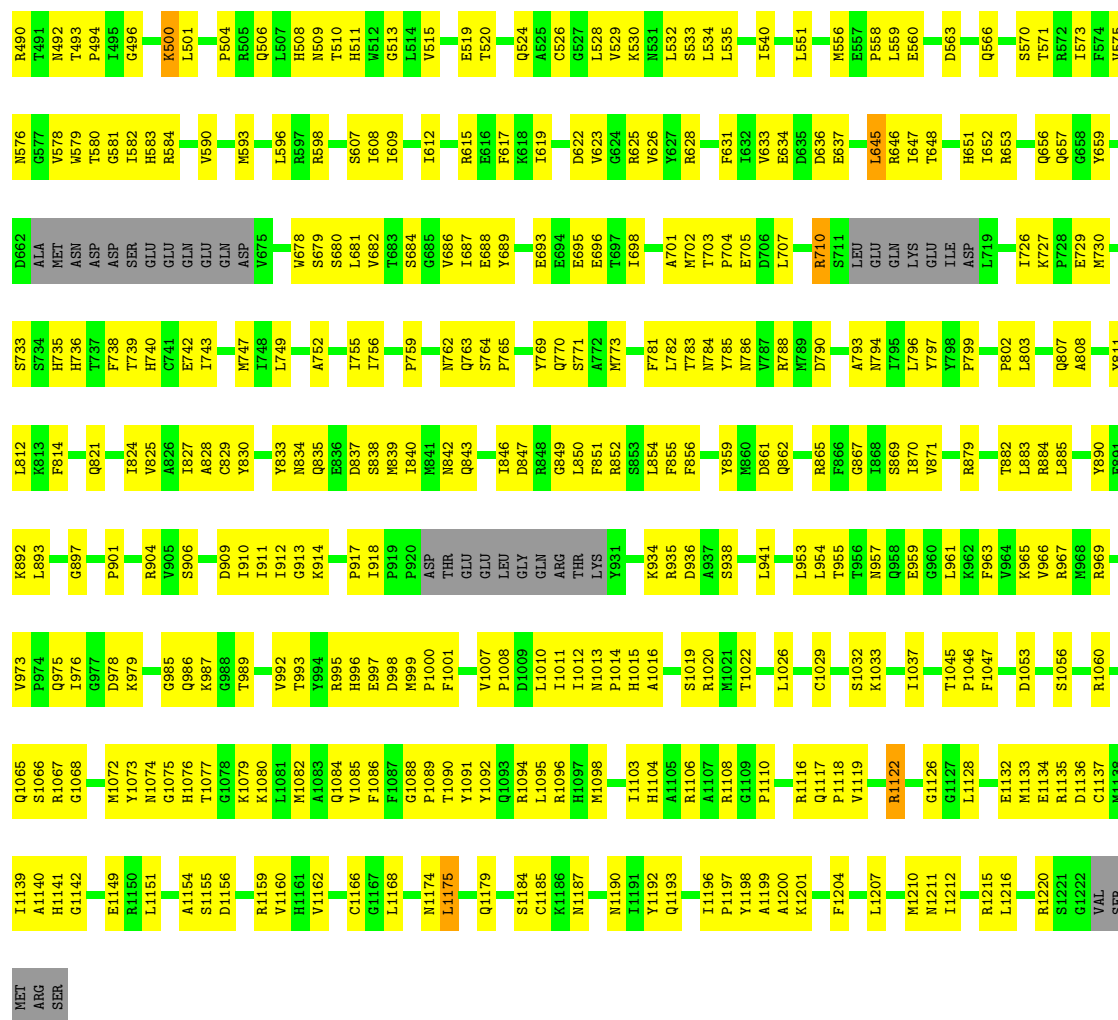




• Molecule 2: DNA-directed RNA polymerase subunit beta

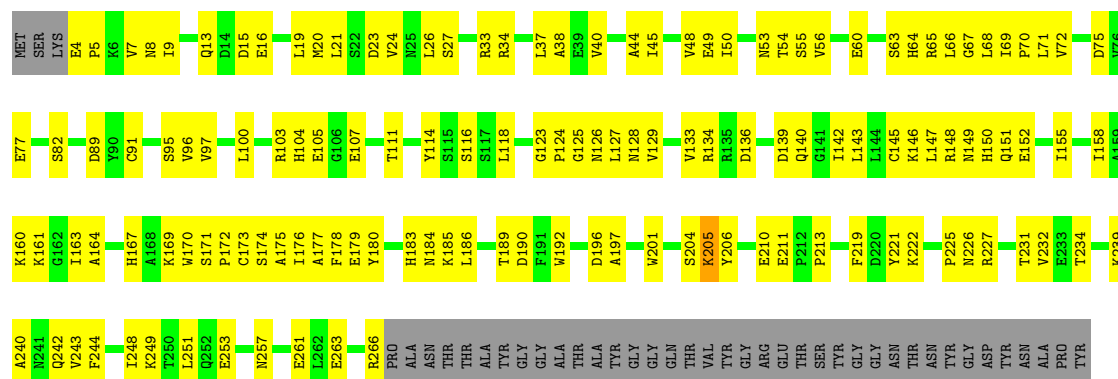
Chain B: 49% 44% • 5%





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

Chain C: 42% 44% 13%



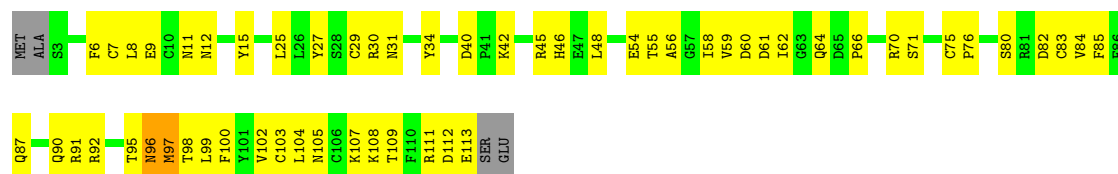
- Molecule 4: RNA polymerase II subunit B32

Chain D: 52% 32% 16%



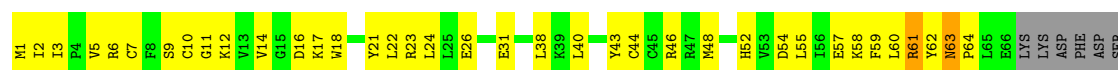
• Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 47% 48% . .



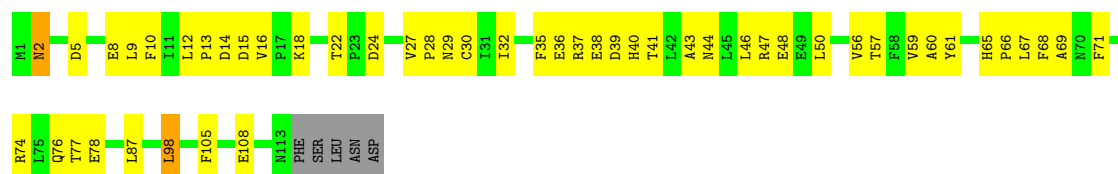
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 40% 49% . 8%



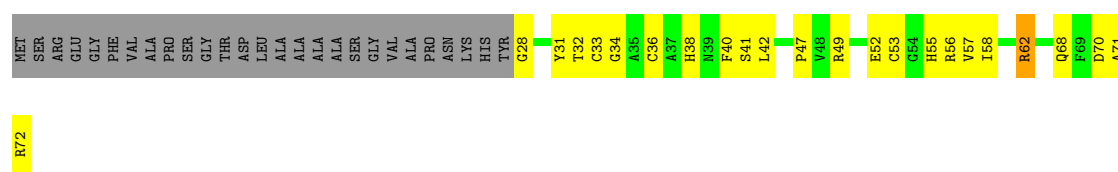
• Molecule 11: RNA polymerase II subunit B12.5

Chain K: 53% 41% . .



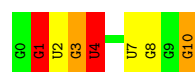
• Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L: 31% 31% . 38%



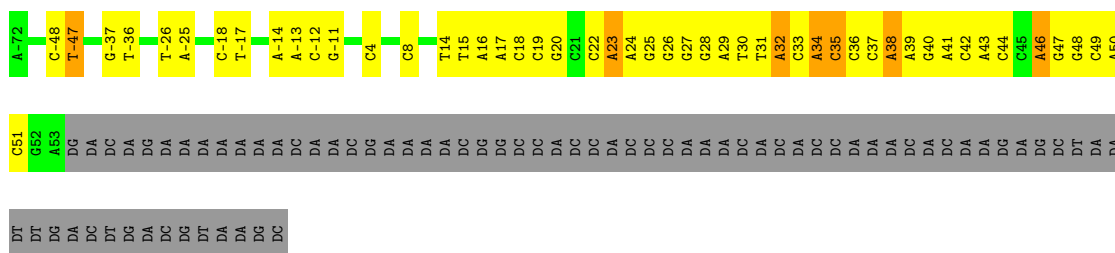
• Molecule 13: RNA (5'-R(P*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*G)-3')

Chain P: 36% 27% 18% 18%

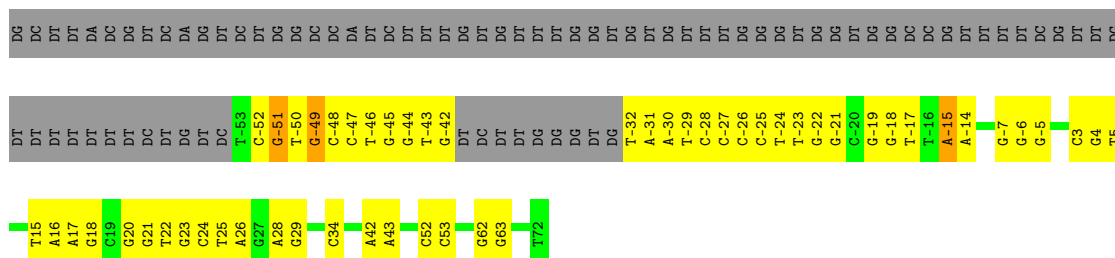
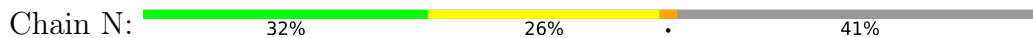


• Molecule 14: DNA (198-MER)

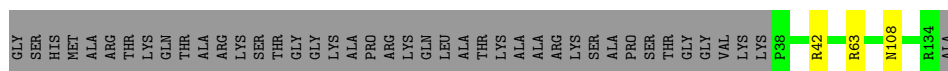
Chain T: 38% 22% . 36%



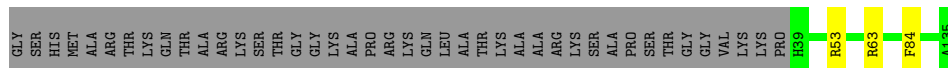
- Molecule 15: DNA (198-MER)



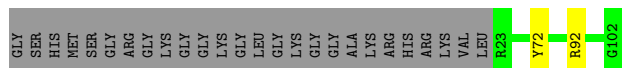
- Molecule 16: Histone H3.3



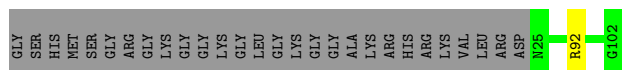
- Molecule 16: Histone H3.3



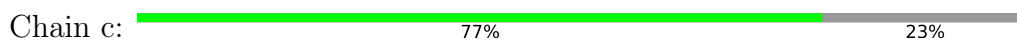
- Molecule 17: Histone H4

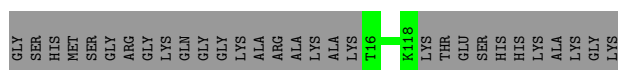


- Molecule 17: Histone H4



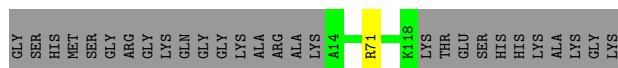
- Molecule 18: Histone H2A type 1-B/E





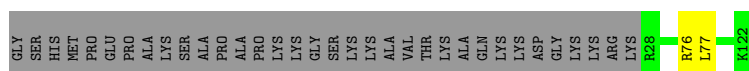
- Molecule 18: Histone H2A type 1-B/E

Chain g: 78% 21%



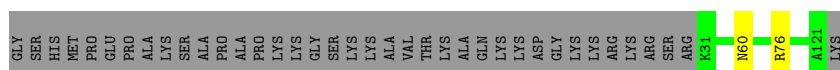
- Molecule 19: Histone H2B type 1-J

Chain d: 72% 26%



- Molecule 19: Histone H2B type 1-J

Chain h: 69% 29%



- Molecule 20: DNA (42-MER)

Chain 0: 76% 24%



- Molecule 21: DNA (42-MER)

Chain 1: 69% 31%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73183	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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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 > 2$	RMSZ	# $ Z > 2$
1	A	0.68	0/11299	0.72	13/15266 (0.1%)
10	J	0.90	0/554	0.80	0/742
11	K	0.68	0/953	0.68	1/1291 (0.1%)
12	L	0.62	0/365	0.66	0/484
13	P	1.19	3/265 (1.1%)	1.28	2/412 (0.5%)
14	T	1.16	9/2880 (0.3%)	1.06	3/4438 (0.1%)
15	N	1.14	5/2701 (0.2%)	1.05	0/4168
16	a	0.42	0/809	0.61	0/1085
16	e	0.45	0/807	0.57	0/1081
17	b	0.44	0/645	0.63	0/862
17	f	0.42	0/626	0.61	0/837
18	c	0.39	0/806	0.58	0/1089
18	g	0.36	0/820	0.55	0/1107
19	d	0.45	0/757	0.56	0/1015
19	h	0.41	0/719	0.57	0/968
2	B	0.75	0/9441	0.75	9/12732 (0.1%)
20	0	0.89	0/980	1.02	1/1509 (0.1%)
21	1	0.88	0/950	1.16	2/1465 (0.1%)
3	C	0.72	0/2139	0.73	1/2895 (0.0%)
4	D	0.31	0/1221	0.53	0/1648
5	E	0.69	0/1772	0.69	0/2385
6	F	0.65	0/687	0.65	0/931
7	G	0.34	0/1353	0.59	1/1837 (0.1%)
8	H	0.77	0/1069	0.69	0/1444
9	I	0.43	0/934	0.58	0/1257
All	All	0.74	17/45552 (0.0%)	0.78	33/62948 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
10	J	0	1
16	a	0	2
16	e	0	1
2	B	0	2
3	C	0	1
4	D	0	1
7	G	0	1
All	All	0	10

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	20	DG	C1'-N9	-8.84	1.34	1.47
14	T	38	DA	C1'-N9	-8.63	1.35	1.47
14	T	17	DA	C1'-N9	-8.44	1.35	1.47
15	N	-15	DA	C1'-N9	-7.85	1.36	1.47
15	N	-51	DG	C1'-N9	-7.77	1.36	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	LEU	CA-CB-CG	-9.82	92.71	115.30
2	B	556	MET	C-N-CA	-8.40	100.71	121.70
2	B	485	LEU	CA-CB-CG	-7.85	97.23	115.30
20	0	52	DG	O4'-C4'-C3'	-7.76	101.34	106.00
14	T	-26	DT	O4'-C4'-C3'	-6.91	101.74	104.50

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	VAL	Peptide
2	B	126	SER	Peptide
2	B	175	LEU	Peptide
3	C	89	ASP	Peptide
4	D	27	LEU	Peptide

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	11095	0	11134	580	0
2	B	9261	0	9266	521	0
3	C	2098	0	2059	119	0
4	D	1210	0	1205	55	0
5	E	1740	0	1754	82	0
6	F	677	0	693	43	0
7	G	1324	0	1342	59	0
8	H	1052	0	1050	54	0
9	I	917	0	868	61	0
10	J	545	0	560	38	0
11	K	932	0	944	50	0
12	L	359	0	360	23	0
13	P	238	0	117	26	0
14	T	2567	0	1409	118	0
15	N	2409	0	1316	104	0
16	a	797	0	835	0	0
16	e	796	0	832	0	0
17	b	638	0	676	0	0
17	f	619	0	659	0	0
18	c	796	0	848	0	0
18	g	810	0	866	0	0
19	d	746	0	771	0	0
19	h	708	0	727	0	0
20	0	868	0	465	6	0
21	1	854	0	482	8	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	I	2	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
23	A	1	0	0	0	0
All	All	44065	0	41238	1724	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 22.

The worst 5 of 1724 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)
14:T:23:DA:H2'	14:T:24:DA:O4'	1.25	1.33
15:N:-51:DG:C2'	15:N:-50:DT:C7	2.23	1.15
15:N:-51:DG:C2'	15:N:-50:DT:H72	1.77	1.11
15:N:-51:DG:H2'	15:N:-50:DT:H72	1.35	1.06
14:T:16:DA:N1	15:N:-15:DA:C2	2.25	1.05

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	1396/1743 (80%)	1139 (82%)	234 (17%)	23 (2%)	11	50
2	B	1151/1227 (94%)	924 (80%)	217 (19%)	10 (1%)	19	61
3	C	261/304 (86%)	207 (79%)	51 (20%)	3 (1%)	16	58
4	D	148/186 (80%)	136 (92%)	12 (8%)	0	100	100
5	E	211/214 (99%)	175 (83%)	32 (15%)	4 (2%)	9	45
6	F	82/155 (53%)	73 (89%)	9 (11%)	0	100	100
7	G	169/171 (99%)	154 (91%)	15 (9%)	0	100	100
8	H	129/145 (89%)	104 (81%)	24 (19%)	1 (1%)	21	65
9	I	109/115 (95%)	88 (81%)	19 (17%)	2 (2%)	9	47
10	J	64/72 (89%)	53 (83%)	10 (16%)	1 (2%)	11	50
11	K	111/118 (94%)	101 (91%)	9 (8%)	1 (1%)	19	61
12	L	43/72 (60%)	31 (72%)	12 (28%)	0	100	100
16	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
16	e	95/139 (68%)	86 (90%)	9 (10%)	0	100	100
17	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
17	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
18	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
19	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
19	h	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	4604/5536 (83%)	3863 (84%)	696 (15%)	45 (1%)	22	59

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	453	LYS
1	A	537	LEU
2	B	257	THR
2	B	1015	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1223/1528 (80%)	1219 (100%)	4 (0%)	93	96
2	B	1016/1077 (94%)	1009 (99%)	7 (1%)	85	93
3	C	236/264 (89%)	235 (100%)	1 (0%)	92	95
4	D	133/160 (83%)	133 (100%)	0	100	100
5	E	196/197 (100%)	193 (98%)	3 (2%)	67	84
6	F	75/137 (55%)	74 (99%)	1 (1%)	71	86
7	G	148/148 (100%)	147 (99%)	1 (1%)	85	93
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	105 (99%)	1 (1%)	81	90
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%)	49	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	a	83/112 (74%)	82 (99%)	1 (1%)	74	87
16	e	82/112 (73%)	80 (98%)	2 (2%)	52	75
17	b	65/81 (80%)	63 (97%)	2 (3%)	43	68
17	f	63/81 (78%)	62 (98%)	1 (2%)	65	83
18	c	82/102 (80%)	82 (100%)	0	100	100
18	g	83/102 (81%)	82 (99%)	1 (1%)	74	87
19	d	81/107 (76%)	79 (98%)	2 (2%)	50	74
19	h	77/107 (72%)	75 (97%)	2 (3%)	49	72
All	All	4071/4785 (85%)	4041 (99%)	30 (1%)	86	93

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	120	ASN
7	G	125	ASN
18	g	71	ARG
6	F	129	LYS
9	I	105	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	462	GLN
3	C	8	ASN
18	g	31	HIS
2	B	736	HIS
4	D	46	HIS

5.3.3 RNA ⓘ

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

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	1	G

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Mol	Chain	Res	Type
13	P	4	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.