



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2024 – 10:10 AM EDT

PDB ID : 8U9R
Title : STRUCTURAL BASIS OF TRANSCRIPTION: RNA POLYMERASE II
SUBSTRATE BINDING AND METAL COORDINATION USING A FREE-
ELECTRON LASER
Authors : Arjunan, P.; Calero, G.; Kaplan, C.D.
Deposited on : 2023-09-20
Resolution : 3.34 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

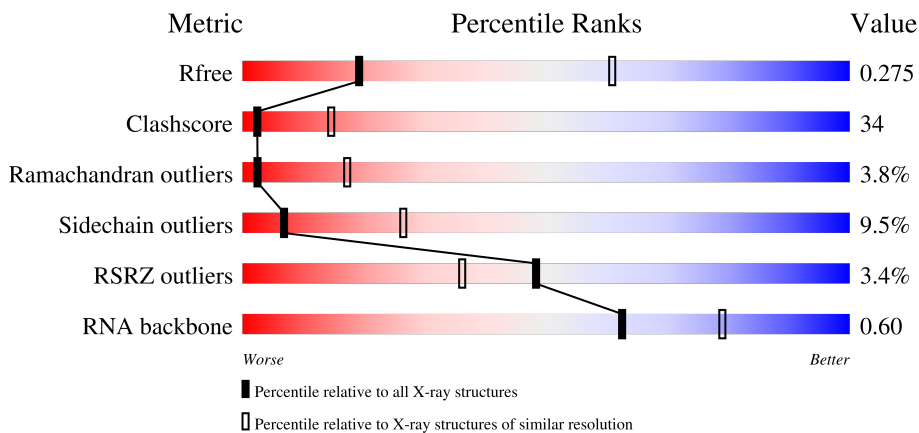
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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.



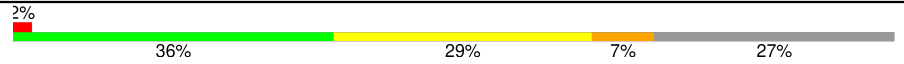
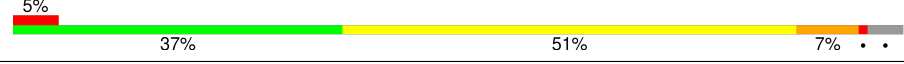
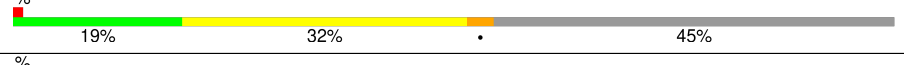

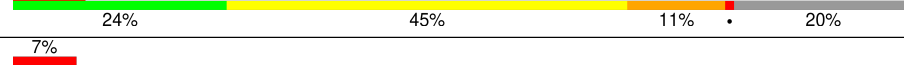
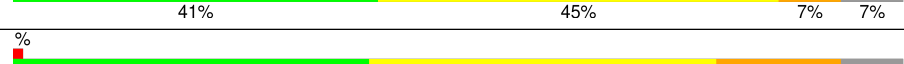

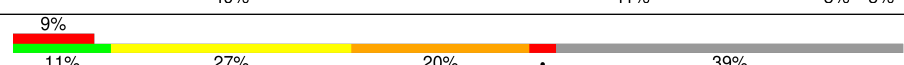
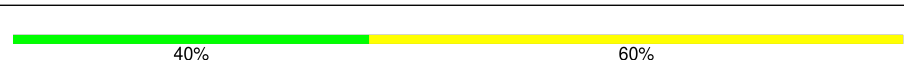
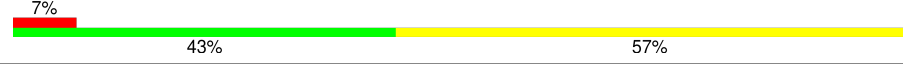
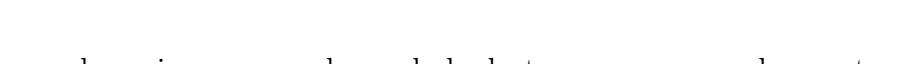
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1325 (3.38-3.30)
Clashscore	180529	1376 (3.38-3.30)
Ramachandran outliers	177936	1376 (3.38-3.30)
Sidechain outliers	177891	1375 (3.38-3.30)
RSRZ outliers	164620	1325 (3.38-3.30)
RNA backbone	3690	1003 (3.70-2.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	10	
14	T	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	ATP	A	1806	-	-	X	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 30677 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1396	10967	6917	1917	2072	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1060	8420	5341	1476	1548	55	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	265	2083	1310	346	414	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	161	1274	790	223	259	2	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	206	1693	1078	298	310	7	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	85	684	437	116	128	3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	171	1340	861	222	249	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	117	951	605	158	184	4	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	113	910	557	166	177	10	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	65	532	339	93	94	6	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	114	919	590	156	171	2	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	43	343	211	69	59	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	R	10	217	98	45	65	9	0	0	0

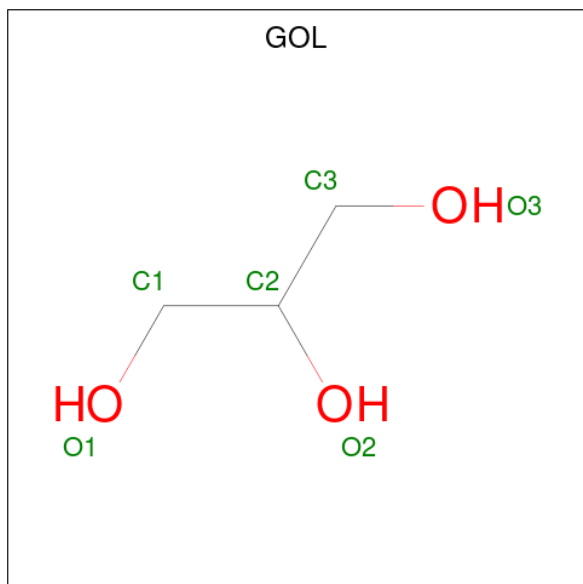
- Molecule 14 is a DNA chain called DNA (5'-D(P*CP*AP*CP*GP*TP*CP*CP*CP*TP*C P*TP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
14	T	14	279	133	47	85	14	0	0	0

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

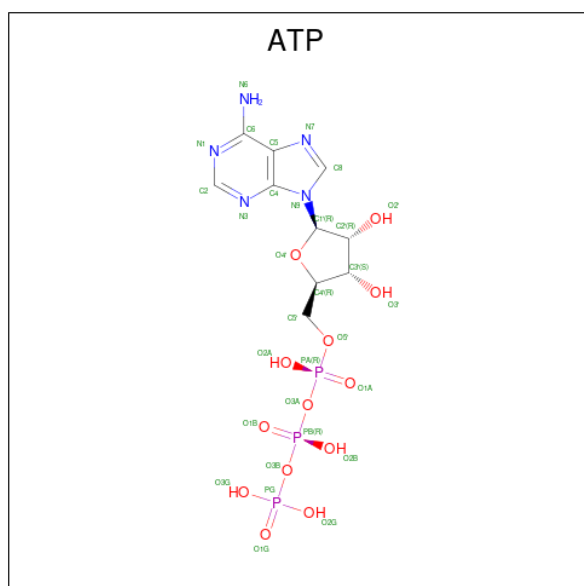


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
16	A	1	6	3	3	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	2	Total Mg 2 2	0	0
17	B	1	Total Mg 1 1	0	0

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C N O P 31 10 5 13 3	0	0

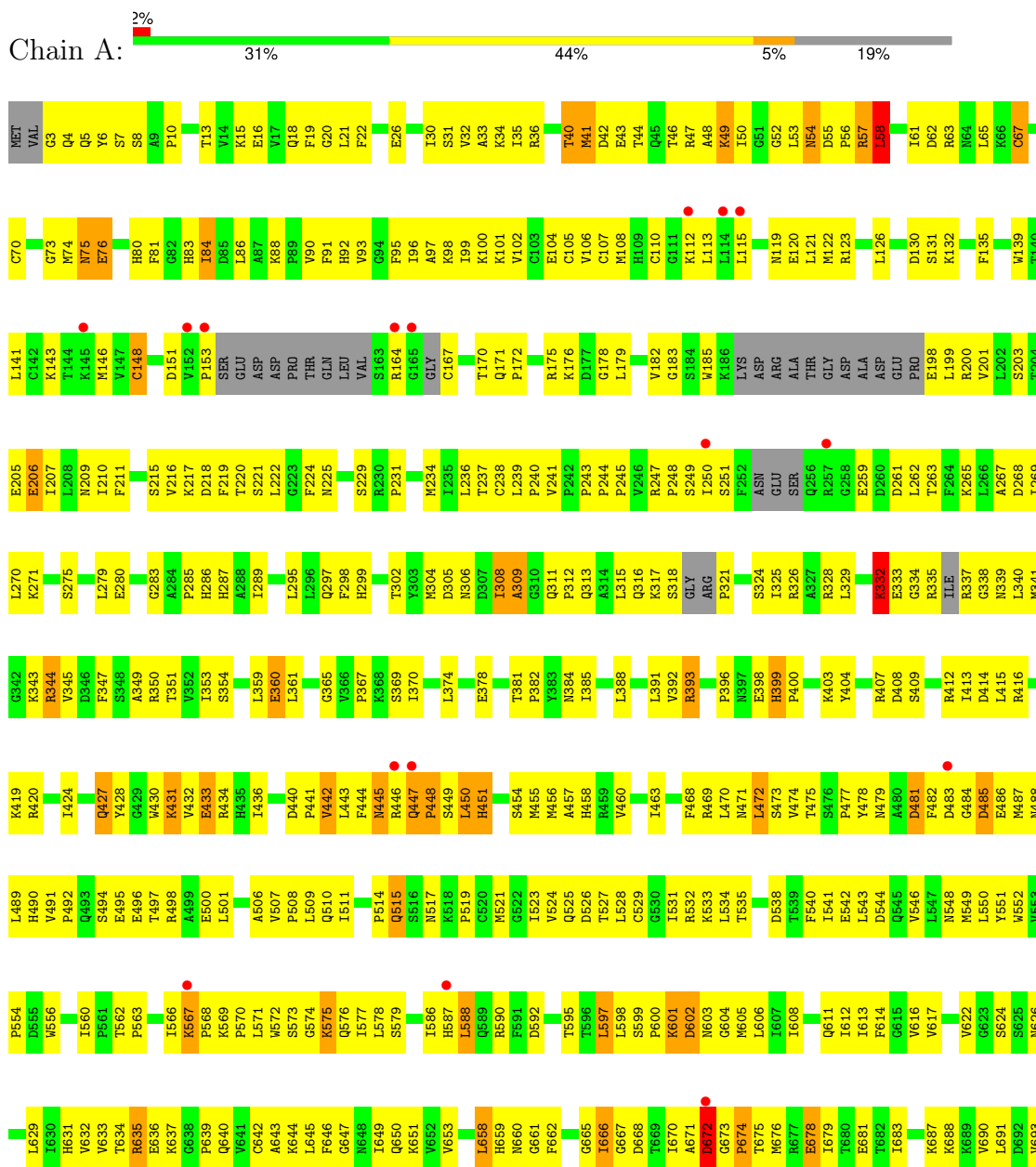
- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	11	Total O 11 11	0	0
19	B	3	Total O 3 3	0	0
19	D	1	Total O 1 1	0	0
19	G	1	Total O 1 1	0	0
19	K	1	Total O 1 1	0	0

3 Residue-property plots [i](#)

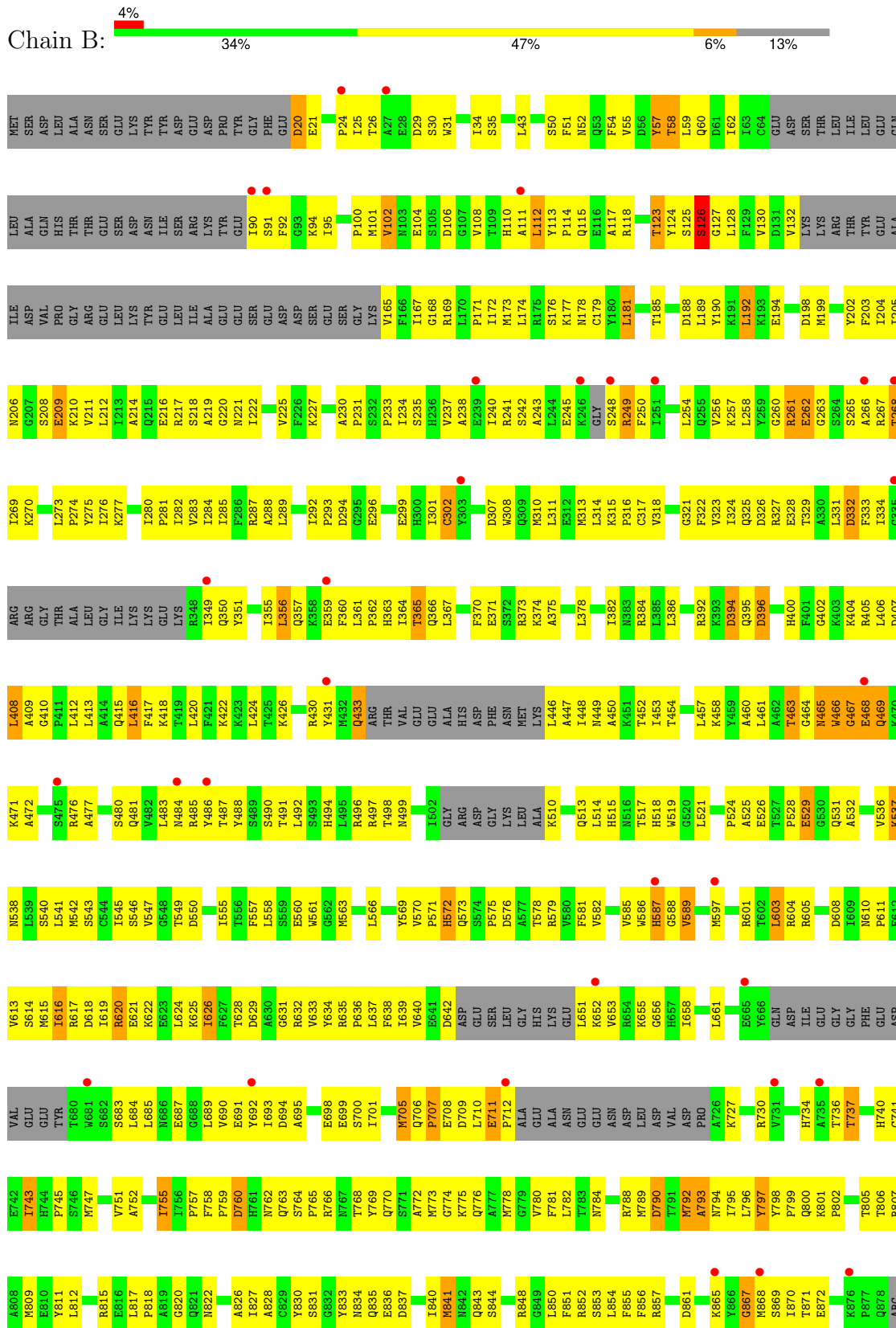
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

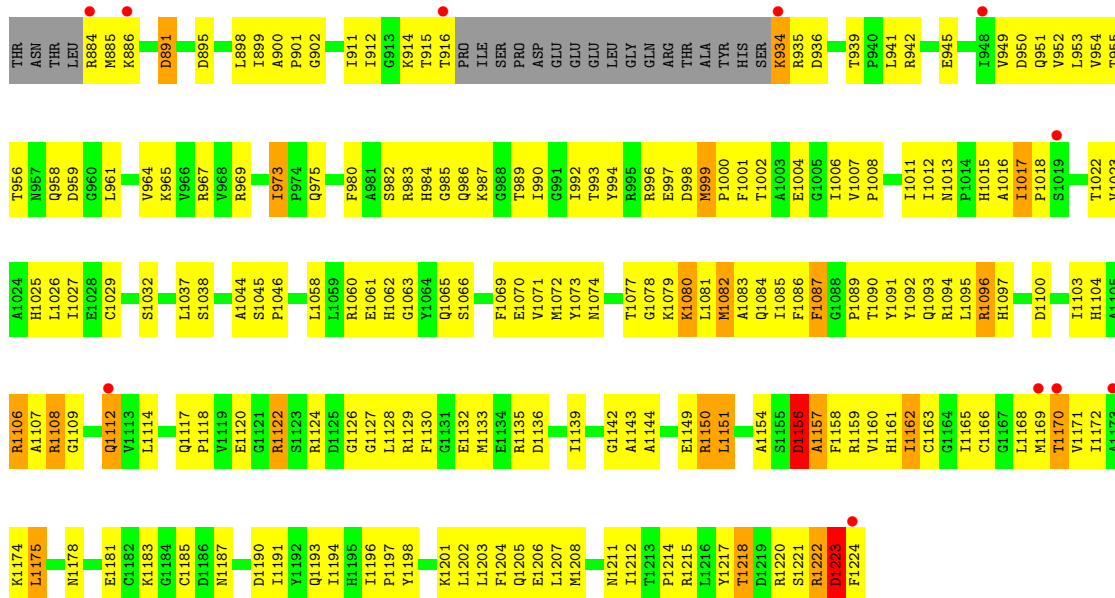
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



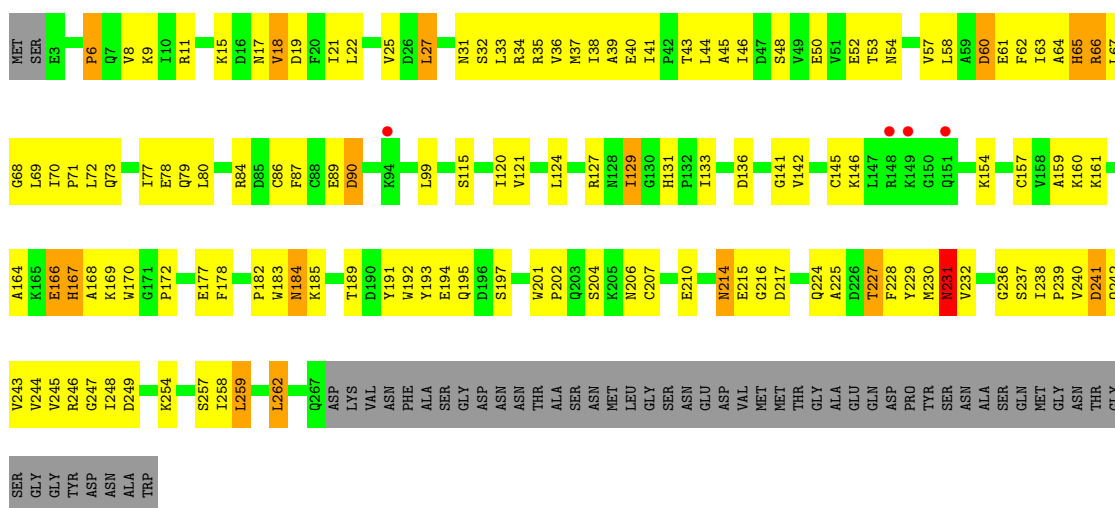
ALA	THR	PRO	PRO	THR	GLU	V1406	L1339	E1264	L1192	E1229	G1063	P985	K830	A759	T694
TYR	PRO	TYR	VAL	GLY	SER	L1409	G1340	M1267	L1193	Q1130	E1062	I986	E833	A695	A695
PRO	PRO	PRO	SER	LEU	GLY	F1410	I1341	L1268	R1194	A1131	M1063	Y987	E883	E696	E696
GLM	ALA	PRO	VAL	VAL	VAL	E1411	E1342	E1269	L1195	L1268	V1064	L988	T834	A697	A697
ASP	SER	THR	GLY	ASN	ASN	R1345	R1345	M1270	L1197	R1135	G1065	G916	G835	G698	G698
GLU	PRO	SER	ALA	ALA	ALA	I1271	I1271	I1271	D1198	I1138	L1067	E918	Y836	A699	A699
GLU	PRO	ASP	ASP	ASP	ASP	T1272	L1348	T1272	A1201	I1139	A1068	I919	Q838	N700	N700
GLM	THR	THR	LEU	LEU	LEU	L1273	Y1349	L1273	M1202	E1139	A1069	L919	Q838	L701	L701
HIS	THR	THR	ASP	ASP	ASP	K1274	I1350	R1274	M1202	H1140	Q1070	G921	R840	L702	L702
ASN	PRO	VAL	VAL	VAL	VAL	G1275	L1351	G1275	D1206	I1141	S1071	D922	R840	T703	T703
ASN	PRO	PRO	LYS	LYS	LYS	V1276	V1352	V1276	D1207	T1142	L1000	L923	Y842	H706	H706
ASN	THR	THR	THR	THR	THR	E1277	V1356	E1277	L1207	L1143	G1073	K924	K843	T709	T709
ASN	THR	SER	GLU	GLU	GLU	M1278	I1356	M1278	V1212	K1144	E1074	L925	A844	L710	L710
ASN	PRO	LEU	LEU	LEU	LEU	I1279	S1357	I1279	S1145	S1145	P1075	Q926	E846	R711	R711
ASN	PRO	MET	MET	MET	MET	E1280	S1358	E1280	I1146	M1004	A1076	Y927	E846	E712	E712
SER	PRO	THR	THR	THR	THR	D1281	D1359	D1281	T1147	E1005	E1005	Q927	D847	E713	E713
SER	PRO	SER	SER	SER	SER	V1282	I1362	V1282	K1217	I1007	I1006	L929	M849	F714	F714
PRO	PRO	PRO	ALA	LEU	LEU	Y1287	Y1363	Y1287	F1220	Q1008	Q1008	D930	V850	E715	E715
TYR	PRO	SER	TYR	VAL	VAL	D1288	M1364	D1288	K1221	E1151	A1090	R938	V850	D716	D716
PRO	PRO	SER	SER	ASP	ASP	L1289	Y1365	L1289	I1152	I1152	F1084	E932	H851	E716	E716
PRO	PRO	PRO	PRO	PRO	PRO	K1290	K1289	K1290	L1224	Y1153	H1085	Y933	Y852	F717	F717
PRO	PRO	PRO	PRO	PRO	PRO	V1291	H1367	V1291	F1225	Y1154	Q1011	K934	Y852	W718	W718
PRO	PRO	SER	THR	THR	THR	P1292	M1368	P1292	V1226	D1155	R1012	Q935	R857	W719	W719
PRO	PRO	ASN	ASN	ASN	ASN	A1369	A1369	A1369	I1227	ASP	G1083	L936	R857	R720	R720
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TYR	PRO	TYR	TYR	ALA	ALA	G1296	L1371	G1296	S1229	ARG	A1091	R938	R864	L722	L722
PRO	PRO	PRO	PRO	PRO	PRO	E1297	L1372	E1297	E1230	SER	S1090	D939	R864	M723	M723
PRO	PRO	PRO	PRO	PRO	PRO	D1300	D1373	D1300	E1230	F1018	K1092	R940	R865	E724	E724
PRO	PRO	PRO	PRO	PRO	PRO	E1301	V1374	E1301	D1231	L1161	K1093	K941	R866	D727	D727
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PRO	PRO	PRO	PRO	PRO	PRO	L1305	L1376	L1305	K1235	I1163	Y1161	V946	R868	A729	A729
PRO	PRO	PRO	PRO	PRO	PRO	L1306	T1377	L1306	D1166	P1164	F1084	A952	R871	G730	G730
PRO	PRO	PRO	PRO	PRO	PRO	E1307	G1379	E1307	I1237	E1167	H1085	A952	R871	R731	R731
PRO	PRO	PRO	PRO	PRO	PRO	G1380	G1380	G1380	I1238	E1168	Y1107	P955	A875	L732	L732
PRO	PRO	PRO	PRO	PRO	PRO	Y1453	S1383	Y1453	R1239	I1169	E1103	V955	I878	A733	A733
ASN	PRO	ASN	ALA	ALA	ALA	M1454	L1384	M1454	C1240	I1170	I1104	V958	E879	N736	N736
TYR	PRO	TYR	TYR	TYR	TYR	GLU	T1385	GLU	R1241	I1170	L1105	N959	S803	L737	L737
TYR	PRO	TYR	TYR	TYR	TYR	GLN	R1386	GLN	V1242	Q1171	M1106	I960	Y804	K738	K738
PRO	PRO	PRO	PRO	PRO	PRO	LYS	H1387	LYS	V1243	HIS	V1107	R961	L808	D739	D739
PRO	PRO	PRO	PRO	PRO	PRO	ILE	G1388	ILE	ARG	PHE	A1108	R962	T885	L740	L740
PRO	PRO	PRO	PRO	PRO	PRO	THR	H1388	THR	LYS	SER	A1108	I963	T886	M741	M741
PRO	PRO	PRO	PRO	PRO	PRO	GLU	R1391	GLU	THR	LEU	M1111	T1037	C887	N742	N742
PRO	PRO	PRO	PRO	PRO	PRO	ILE	S1392	ILE	SER	LEU	K1112	T1038	E888	V743	V743
PRO	PRO	PRO	PRO	PRO	PRO	GLU	T1393	GLU	LEU	ASP	T1113	Q969	F813	K744	K744
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PRO	PRO	PRO	PRO	PRO	PRO	GLN	A1396	GLN	THR	GLU	D1043	I973	Y897	V747	V747
PRO	PRO	PRO	PRO	PRO	PRO	ASP	L1397	ASP	ALA	GLN	L1046	D974	R898	W748	W748
PRO	PRO	PRO	PRO	PRO	PRO	GLY	M1398	GLY	ALA	SER	L1119	H975	V899	A749	A749
PRO	PRO	PRO	PRO	PRO	PRO	GLY	R1399	GLY	ALA	THR	L1120	D974	D900	G750	G750
PRO	PRO	PRO	PRO	PRO	PRO	VAL	C1400	VAL	ALA	PHE	E1121	H975	D900	S751	S751
PRO	PRO	PRO	PRO	PRO	PRO	THR	S1401	THR	ALA	ASP	P1122	S979	L902	K752	K752
PRO	PRO	PRO	PRO	PRO	PRO	THR	F1402	THR	THR	GLU	L1054	S979	I903	G753	G753
PRO	PRO	PRO	PRO	PRO	PRO	TYR	E1403	TYR	THR	GLU	S1056	D980	I903	S754	S754
PRO	PRO	PRO	PRO	PRO	PRO	TYR	E1404	TYR	THR	GLU	S1056	L981	I903	F755	F755
PRO	PRO	PRO	PRO	PRO	PRO	ASN	T1405	ASN	I1263	W1191	Q1128	H1059	H906	W756	W756
PRO	PRO	PRO	PRO	PRO	PRO	ASN	T1405	ASN	I1263	W1191	Q1128	H1059	H906	W756	W756

● Molecule 2: DNA-directed RNA polymerase subunit beta

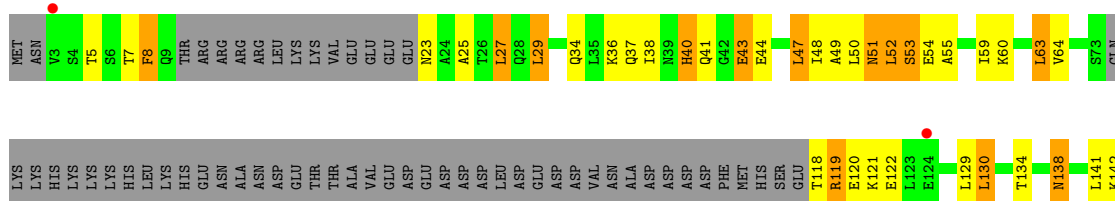


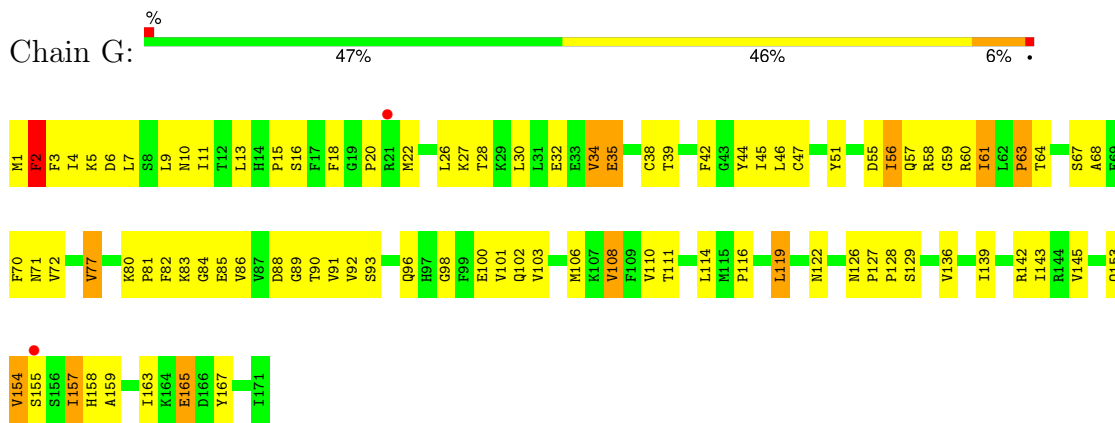
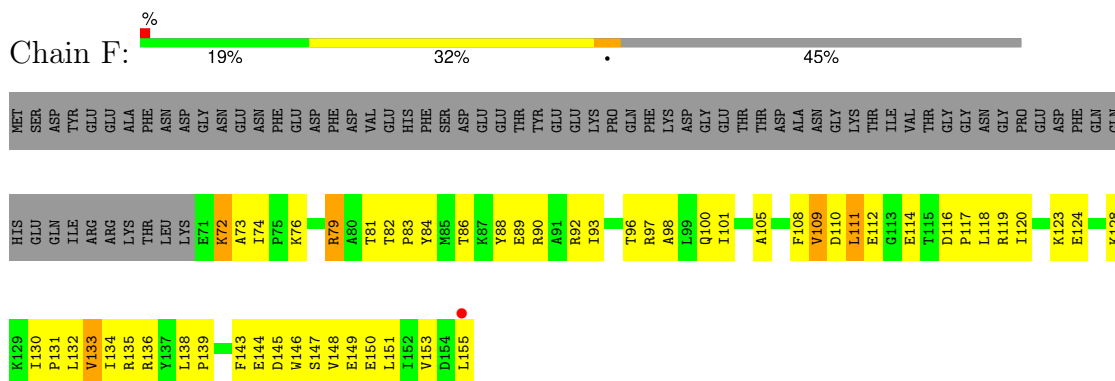
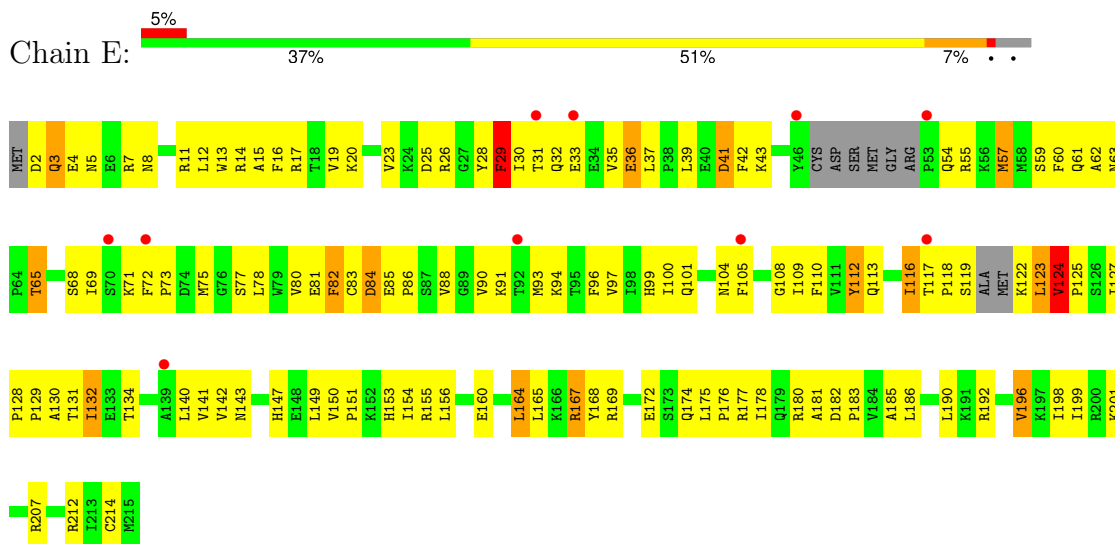
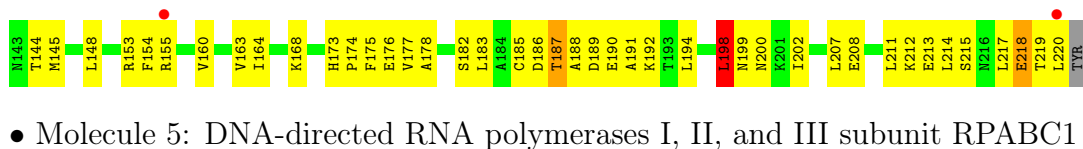


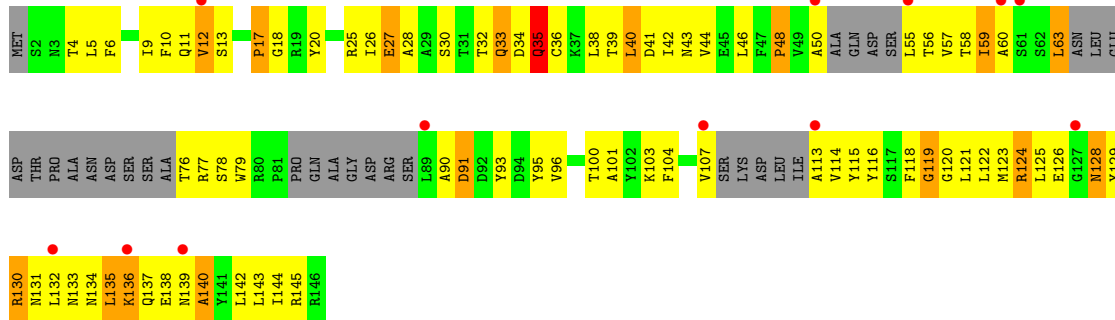
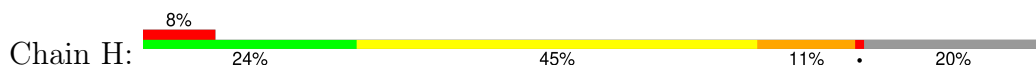
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



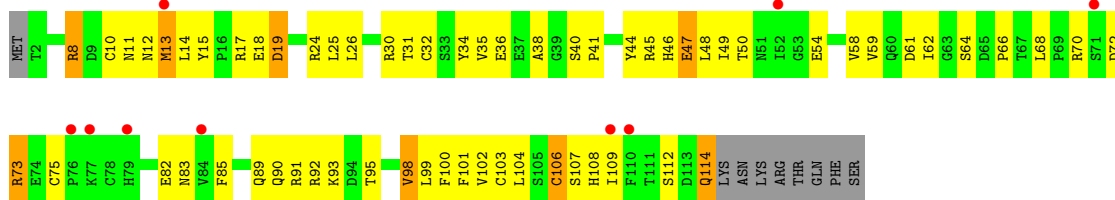
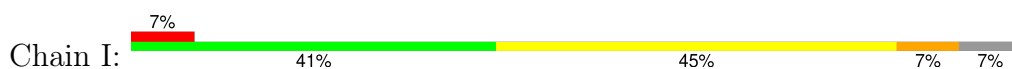
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4







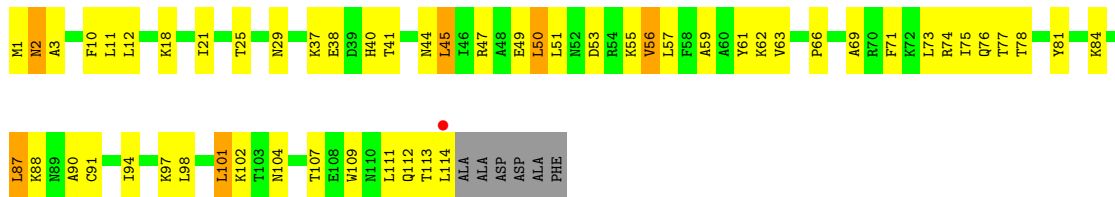
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



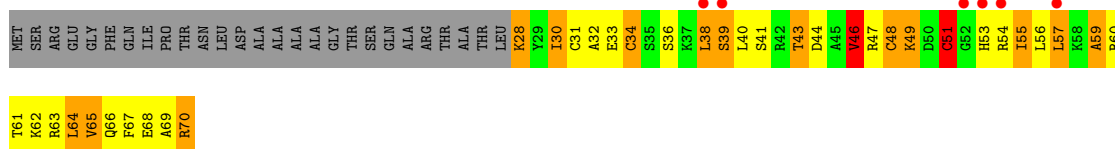
• Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



• Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



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

Chain R:  40% 60%



- Molecule 14: DNA (5'-D(P*CP*AP*CP*GP*TP*CP*CP*CP*TP*CP*TP*CP*GP*A)-3')

Chain T:  7% 43% 57%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	217.19Å 387.44Å 276.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.34 19.97 – 3.34	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.97-3.34) 99.4 (19.97-3.34)	Depositor EDS
R_{merge}	0.60	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.33Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.261 0.267 , 0.275	Depositor DCC
R_{free} test set	8262 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtrriage
Anisotropy	0.341	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.16$	Xtrriage
Estimated twinning fraction	0.146 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.160 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	30677	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, ZN, MG, ATP

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	0.26	0/11158	0.49	0/15080
2	B	0.27	0/8583	0.51	0/11570
3	C	0.27	0/2121	0.46	0/2876
4	D	0.24	0/1282	0.46	0/1723
5	E	0.25	0/1727	0.51	0/2323
6	F	0.26	0/696	0.50	0/940
7	G	0.25	0/1368	0.46	0/1844
8	H	0.24	0/965	0.50	0/1302
9	I	0.24	0/927	0.53	0/1250
10	J	0.27	0/541	0.52	0/727
11	K	0.25	0/937	0.44	0/1265
12	L	0.27	0/345	0.59	0/457
13	R	0.24	0/244	0.77	0/380
14	T	0.65	0/310	0.92	0/474
All	All	0.27	0/31204	0.50	0/42211

There are no bond length outliers.

There are no bond angle outliers.

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	10967	0	11024	910	0
2	B	8420	0	8456	633	0
3	C	2083	0	2036	144	0
4	D	1274	0	1287	82	0
5	E	1693	0	1715	115	0
6	F	684	0	703	60	0
7	G	1340	0	1357	97	0
8	H	951	0	926	96	0
9	I	910	0	857	53	0
10	J	532	0	542	44	0
11	K	919	0	929	48	0
12	L	343	0	363	42	0
13	R	217	0	109	4	0
14	T	279	0	158	11	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	6	0	8	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
18	A	31	0	12	9	0
19	A	11	0	0	0	0
19	B	3	0	0	0	0
19	D	1	0	0	0	0
19	G	1	0	0	2	0
19	K	1	0	0	0	0
All	All	30677	0	30482	2097	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 34.

The worst 5 of 2097 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)
2:B:1160:VAL:HG11	2:B:1169:MET:SD	1.66	1.34
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.14	1.08
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	1.96	1.04
1:A:393:ARG:HH11	1:A:393:ARG:CG	1.72	1.02
2:B:510:LYS:HB2	2:B:513:GLN:HG2	1.42	1.02

There are no symmetry-related clashes.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1376/1733 (79%)	1168 (85%)	166 (12%)	42 (3%)	3	21
2	B	1036/1224 (85%)	854 (82%)	141 (14%)	41 (4%)	2	16
3	C	263/318 (83%)	223 (85%)	29 (11%)	11 (4%)	2	15
4	D	155/221 (70%)	134 (86%)	14 (9%)	7 (4%)	2	14
5	E	200/215 (93%)	178 (89%)	17 (8%)	5 (2%)	4	25
6	F	83/155 (54%)	76 (92%)	5 (6%)	2 (2%)	5	25
7	G	169/171 (99%)	137 (81%)	24 (14%)	8 (5%)	2	13
8	H	107/146 (73%)	80 (75%)	18 (17%)	9 (8%)	0	5
9	I	111/122 (91%)	85 (77%)	24 (22%)	2 (2%)	7	31
10	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	2	13
11	K	112/120 (93%)	96 (86%)	13 (12%)	3 (3%)	4	23
12	L	41/70 (59%)	19 (46%)	15 (37%)	7 (17%)	0	1
All	All	3716/4565 (81%)	3103 (84%)	473 (13%)	140 (4%)	2	17

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	433	GLU
1	A	567	LYS
1	A	672	ASP
1	A	674	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	1213/1520 (80%)	1113 (92%)	100 (8%)	9	32
2	B	917/1061 (86%)	842 (92%)	75 (8%)	9	32
3	C	232/274 (85%)	219 (94%)	13 (6%)	17	46
4	D	143/200 (72%)	128 (90%)	15 (10%)	5	22
5	E	189/197 (96%)	158 (84%)	31 (16%)	2	8
6	F	74/137 (54%)	64 (86%)	10 (14%)	3	14
7	G	152/152 (100%)	137 (90%)	15 (10%)	6	25
8	H	104/128 (81%)	90 (86%)	14 (14%)	3	14
9	I	105/116 (90%)	91 (87%)	14 (13%)	3	14
10	J	60/65 (92%)	51 (85%)	9 (15%)	2	11
11	K	99/102 (97%)	90 (91%)	9 (9%)	7	28
12	L	38/57 (67%)	26 (68%)	12 (32%)	0	1
All	All	3326/4009 (83%)	3009 (90%)	317 (10%)	7	26

5 of 317 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	182	ASP
9	I	114	GLN
6	F	118	LEU
8	H	33	GLN
11	K	87	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	776	GLN
2	B	1062	HIS
2	B	1025	HIS
2	B	1084	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	736	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U
13	R	3	C

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
16	GOL	A	1803	-	5,5,5	1.02	0	5,5,5	1.03	0
18	ATP	A	1806	17	28,33,33	0.81	0	34,52,52	0.97	3 (8%)

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
16	GOL	A	1803	-	-	2/4/4/4	-
18	ATP	A	1806	17	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1806	ATP	O2A-PA-O3A	2.77	114.77	107.27
18	A	1806	ATP	O3A-PA-O1A	-2.42	103.41	110.70
18	A	1806	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1806	ATP	C5'-O5'-PA-O2A
18	A	1806	ATP	C5'-O5'-PA-O3A
18	A	1806	ATP	C3'-C4'-C5'-O5'
18	A	1806	ATP	O4'-C4'-C5'-O5'
16	A	1803	GOL	C1-C2-C3-O3

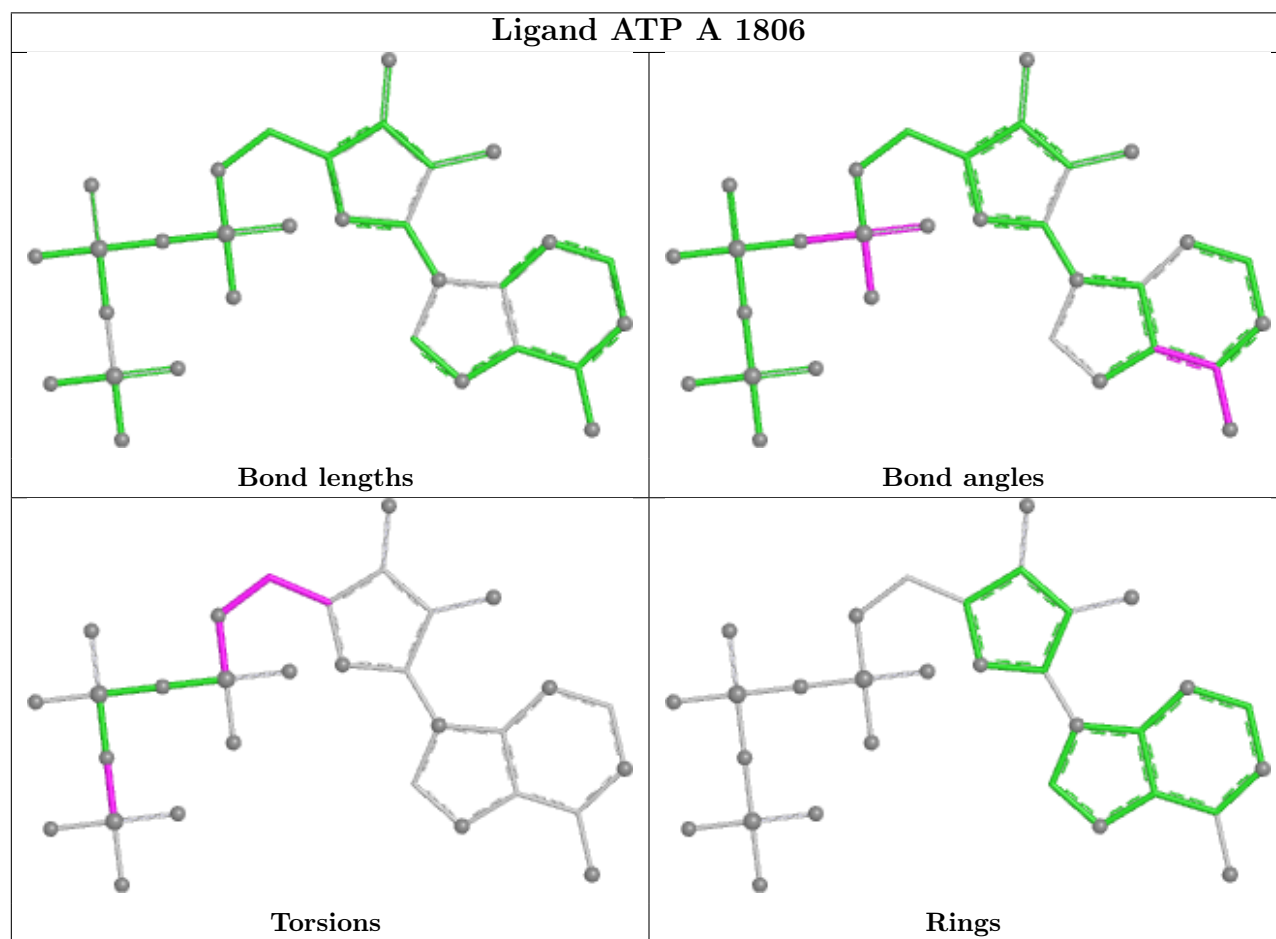
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1806	ATP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1396/1733 (80%)	0.04	34 (2%) 59 46	40, 92, 158, 219	0
2	B	1060/1224 (86%)	0.16	43 (4%) 42 31	30, 99, 165, 276	0
3	C	265/318 (83%)	-0.01	4 (1%) 71 60	60, 98, 143, 188	0
4	D	161/221 (72%)	0.10	4 (2%) 58 45	74, 107, 159, 212	0
5	E	206/215 (95%)	0.38	10 (4%) 36 28	61, 124, 184, 234	0
6	F	85/155 (54%)	-0.29	1 (1%) 76 65	46, 73, 106, 132	0
7	G	171/171 (100%)	-0.12	2 (1%) 76 65	70, 96, 150, 175	0
8	H	117/146 (80%)	0.61	12 (10%) 13 13	95, 135, 180, 221	0
9	I	113/122 (92%)	0.73	9 (7%) 20 18	99, 139, 200, 222	0
10	J	65/70 (92%)	-0.08	1 (1%) 71 60	70, 95, 138, 181	0
11	K	114/120 (95%)	-0.23	1 (0%) 81 71	57, 97, 143, 170	0
12	L	43/70 (61%)	1.03	6 (13%) 7 8	80, 128, 180, 197	0
13	R	10/10 (100%)	0.40	0 100 100	98, 113, 170, 205	0
14	T	14/14 (100%)	0.24	1 (7%) 23 20	86, 106, 203, 205	0
All	All	3820/4589 (83%)	0.11	128 (3%) 48 36	30, 99, 166, 276	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	7.2
9	I	110	PHE	6.1
9	I	76	PRO	5.5
2	B	916	THR	5.3
2	B	246	LYS	5.3

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

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

6.3 Carbohydrates [i](#)

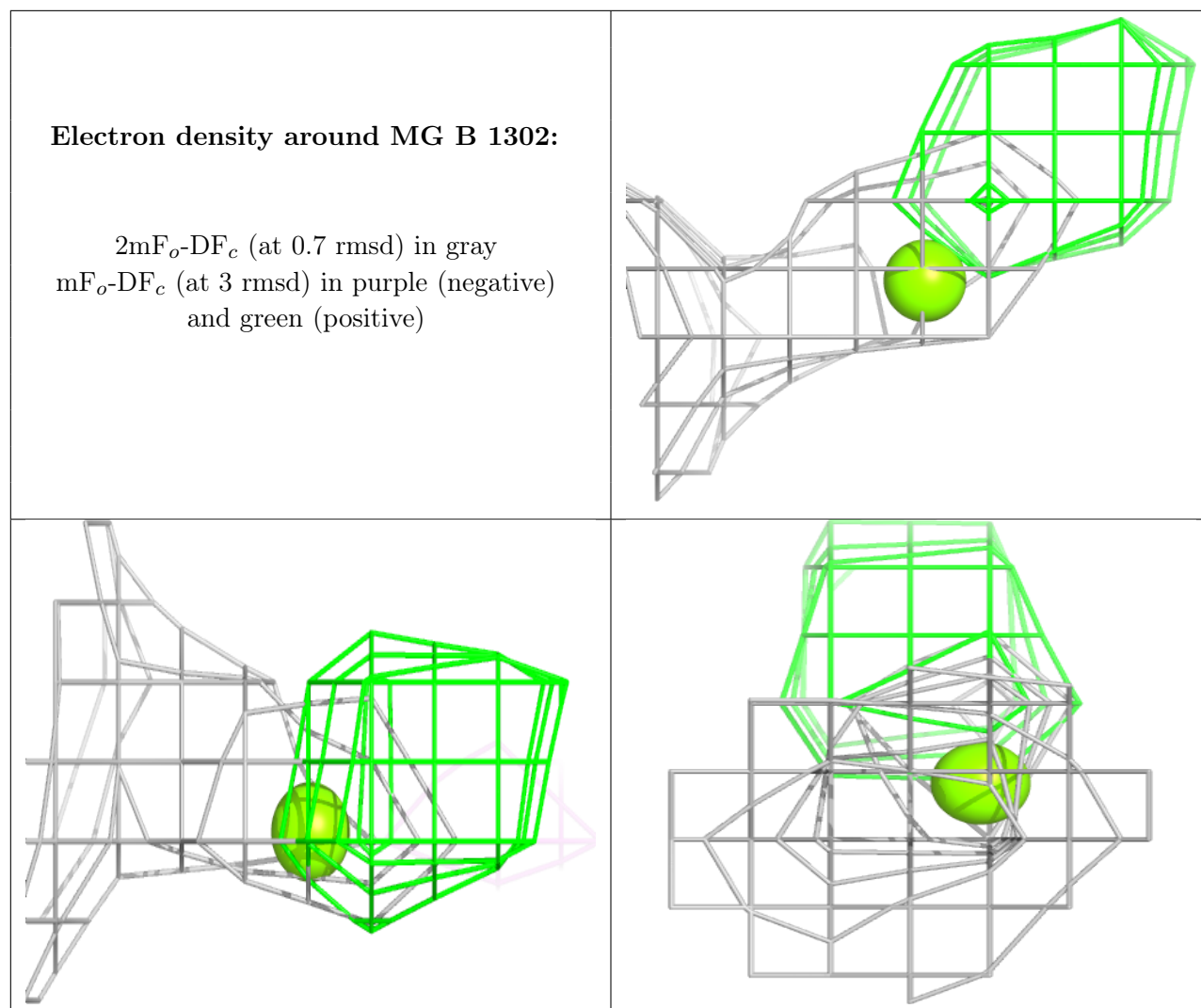
There are no monosaccharides in this entry.

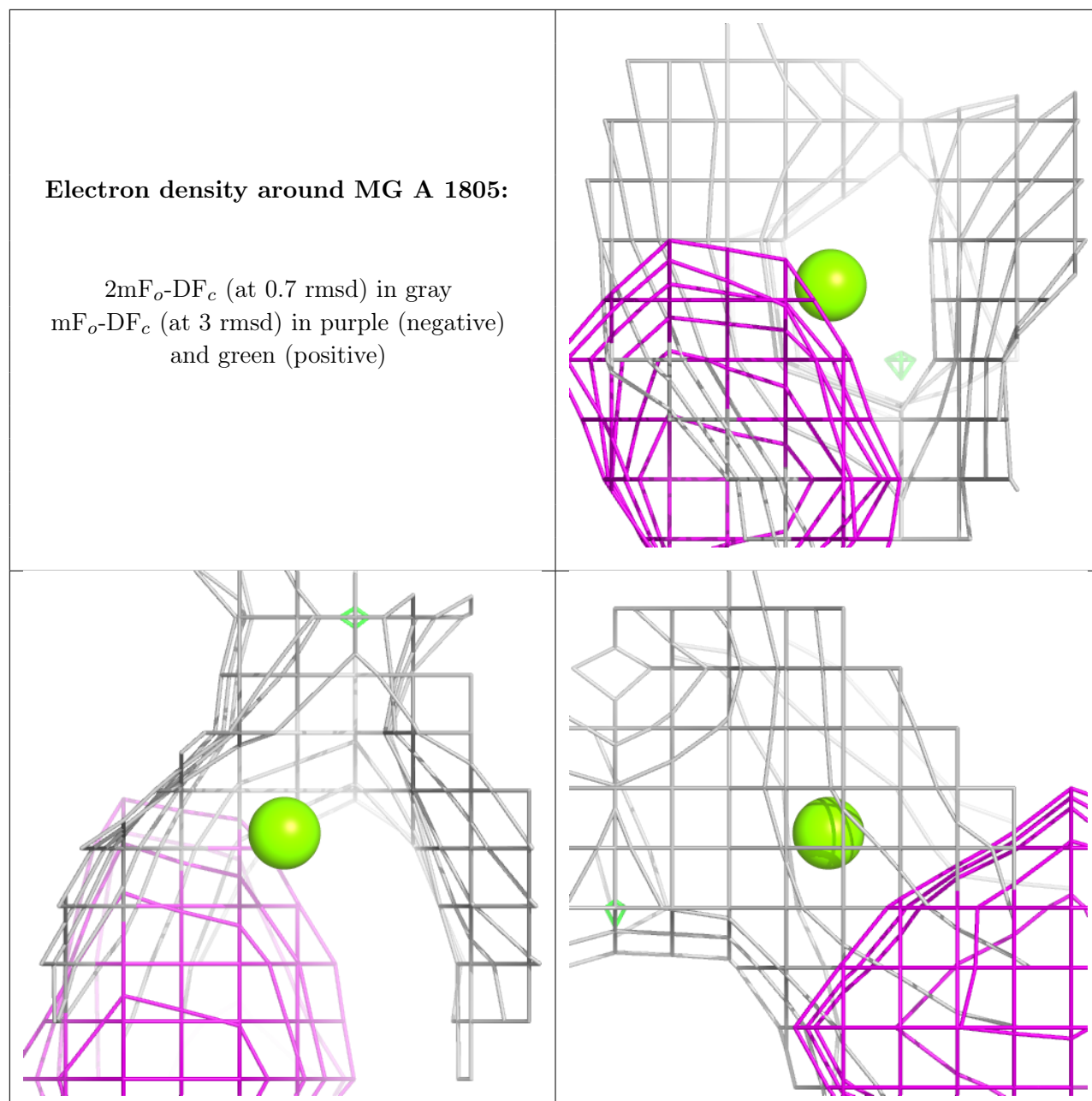
6.4 Ligands [i](#)

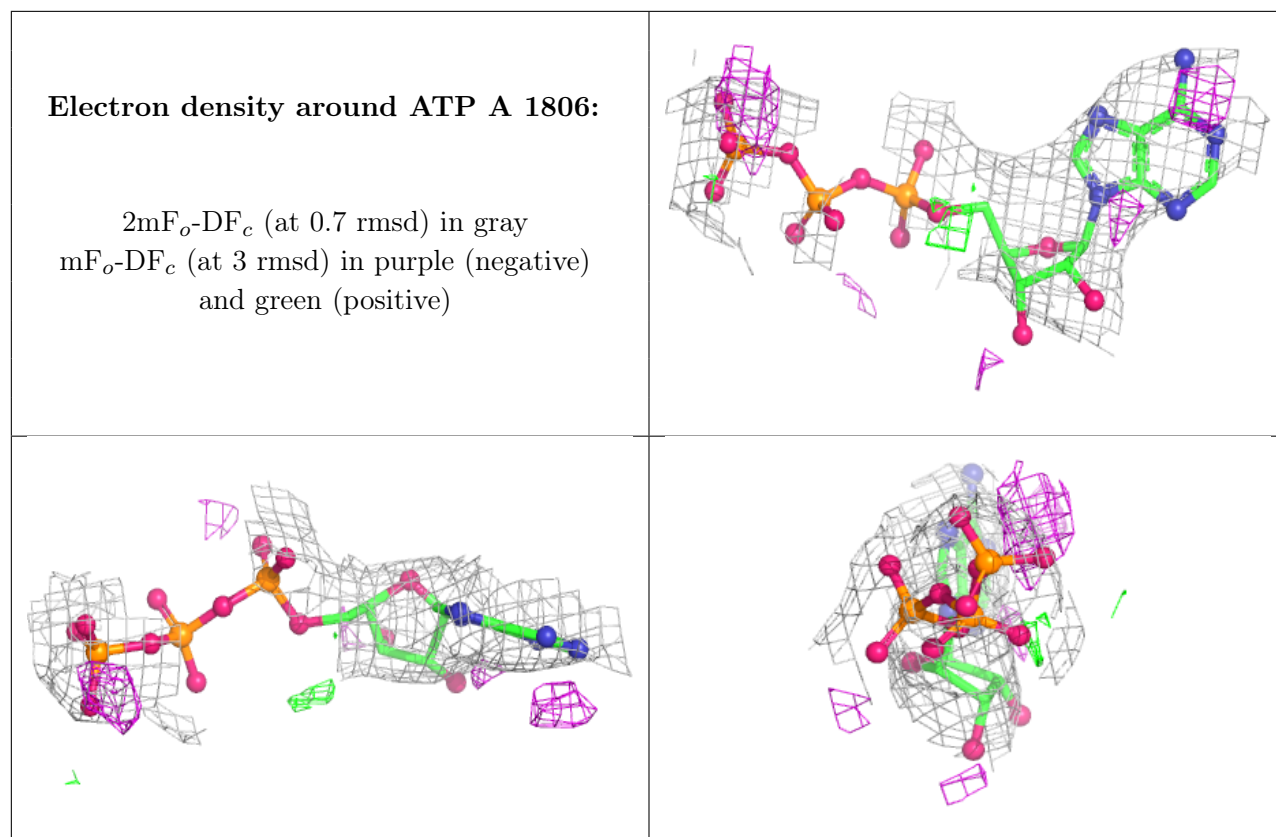
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

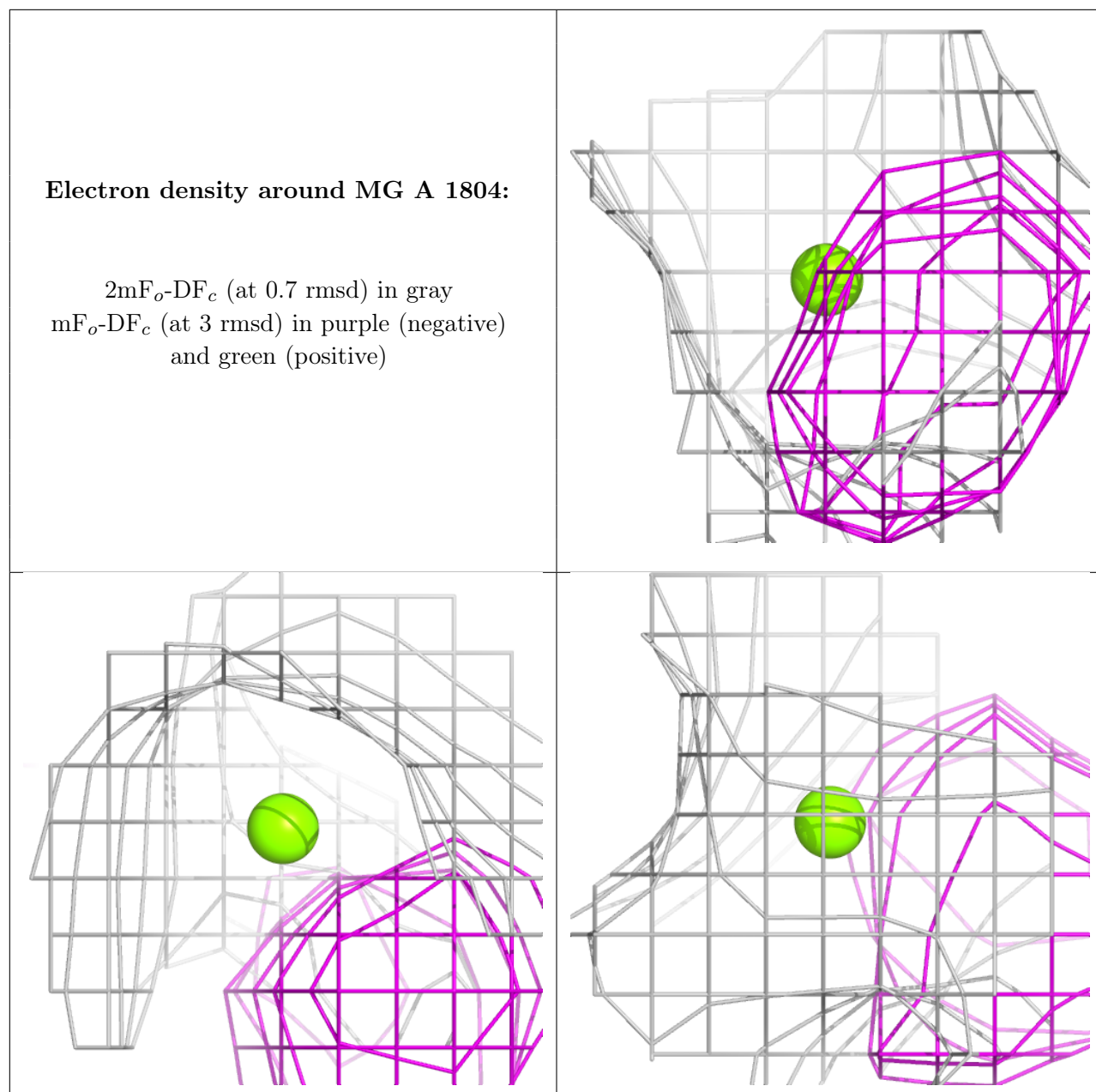
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	ZN	A	1801	1/1	0.79	0.11	213,213,213,213	0
17	MG	B	1302	1/1	0.81	0.76	92,92,92,92	0
17	MG	A	1805	1/1	0.83	0.15	105,105,105,105	0
15	ZN	L	101	1/1	0.90	0.08	173,173,173,173	0
18	ATP	A	1806	31/31	0.92	0.12	112,118,133,155	0
17	MG	A	1804	1/1	0.94	0.10	94,94,94,94	0
16	GOL	A	1803	6/6	0.96	0.14	103,110,116,118	0
15	ZN	A	1802	1/1	0.97	0.03	56,56,56,56	0
15	ZN	I	201	1/1	0.99	0.12	103,103,103,103	0
15	ZN	I	202	1/1	0.99	0.04	181,181,181,181	0
15	ZN	B	1301	1/1	0.99	0.03	61,61,61,61	0
15	ZN	C	401	1/1	0.99	0.04	69,69,69,69	0
15	ZN	J	101	1/1	1.00	0.02	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









6.5 Other polymers [i](#)

There are no such residues in this entry.