



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 12:06 PM UTC

PDB ID : 2E2J / pdb_00002e2j
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with GMPCPP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

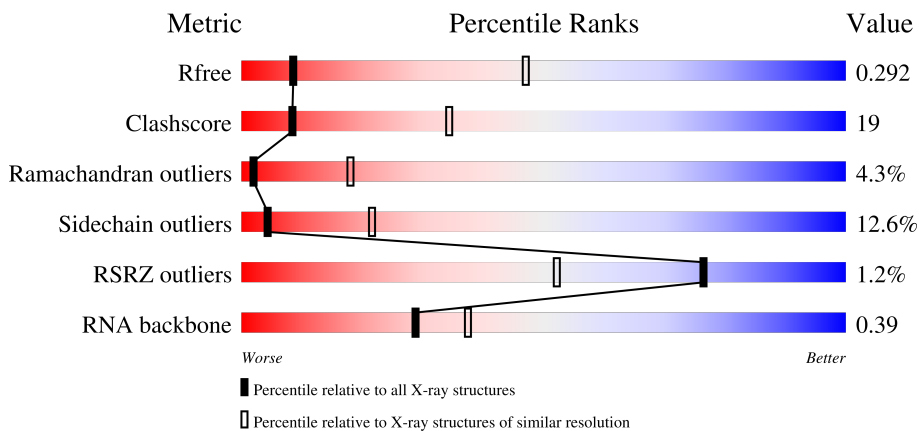
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	R	9	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">11% 67% 11% 11% 11%</p>
2	T	27	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">4% 70% 30%</p>
3	N	13	<div style="display: flex; align-items: center;"> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">92% 8%</p>
4	A	1733	<div style="display: flex; align-items: center;"> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 48% 26% 6% 20%</p>

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Mol	Chain	Length	Quality of chain
5	B	1224	<p>%</p> <p>50% 33% 7% • 10%</p>
6	C	318	<p>50% 28% 5% 16%</p>
7	E	215	<p>2%</p> <p>63% 32% •</p>
8	F	155	<p>32% 20% • 45%</p>
9	H	146	<p>3%</p> <p>49% 36% 6% • 9%</p>
10	I	122	<p>2%</p> <p>60% 30% 7% •</p>
11	J	70	<p>51% 31% 9% • 7%</p>
12	K	120	<p>51% 39% 5% 5%</p>
13	L	70	<p>4%</p> <p>34% 24% 6% • 34%</p>

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29206 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 RNA chain called 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	9	199	88	40	62	9	0	0	0

- Molecule 2 is a DNA chain called 27-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	27	546	261	102	157	26	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	N	13	266	127	44	82	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1395	10969	6917	1923	2068	61	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1105	8782	5560	1537	1630	55	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	267	2101	1320	349	419	13	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	214	1752	1111	309	321	11	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	86	696	445	118	130	3	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	133	1068	673	180	211	4	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	I	119	971	596	179	186	10	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

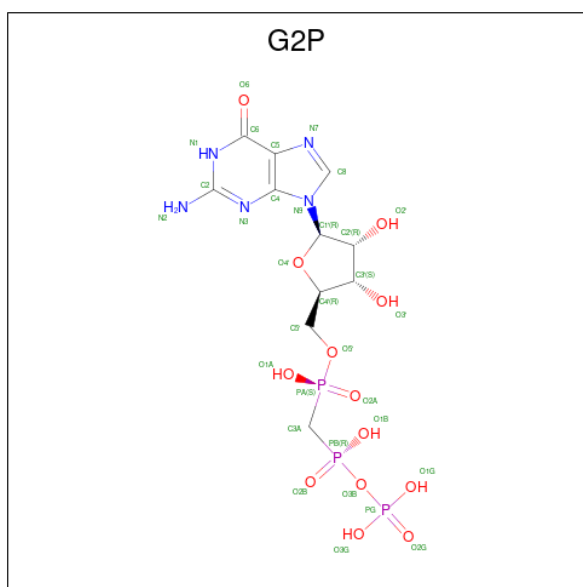
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	114	919	590	156	171	2	0	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

tide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	46	363	224	72	63	4	0	0	0

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	T	1	32	11	5	13	3	0	0

- Molecule 15 is ZINC ION (CCD ID: 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		

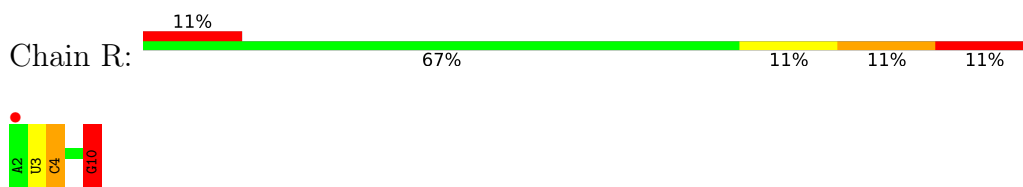
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total 2	Mg 2	0	0

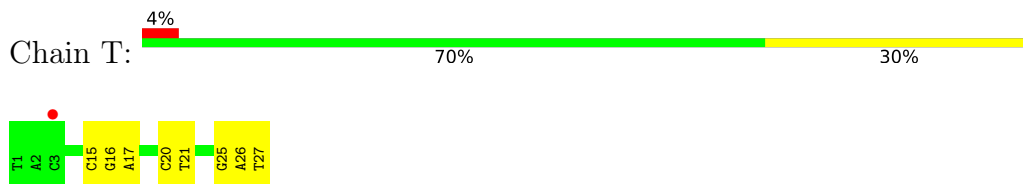
3 Residue-property plots [i](#)

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.

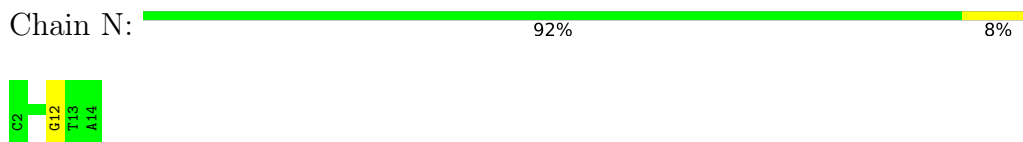
- Molecule 1: 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'



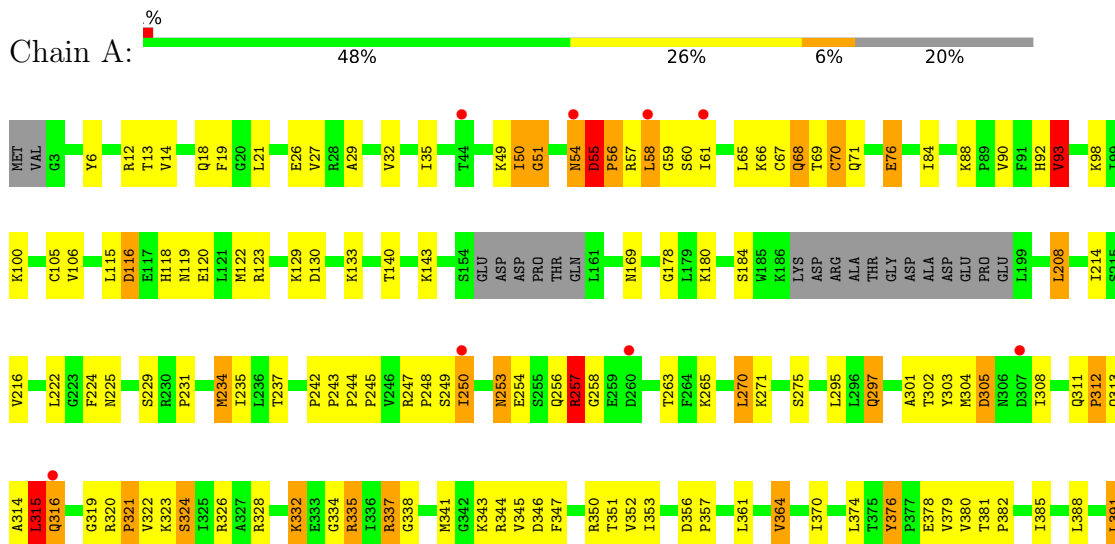
- Molecule 2: 27-MER DNA template strand



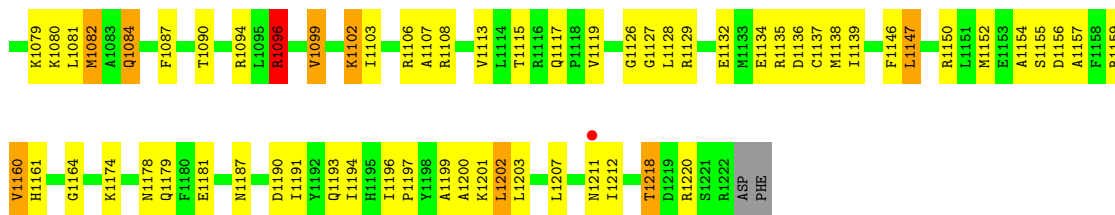
- Molecule 3: 5'-D(P*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*A)-3'



- Molecule 4: DNA-directed RNA polymerase II largest subunit

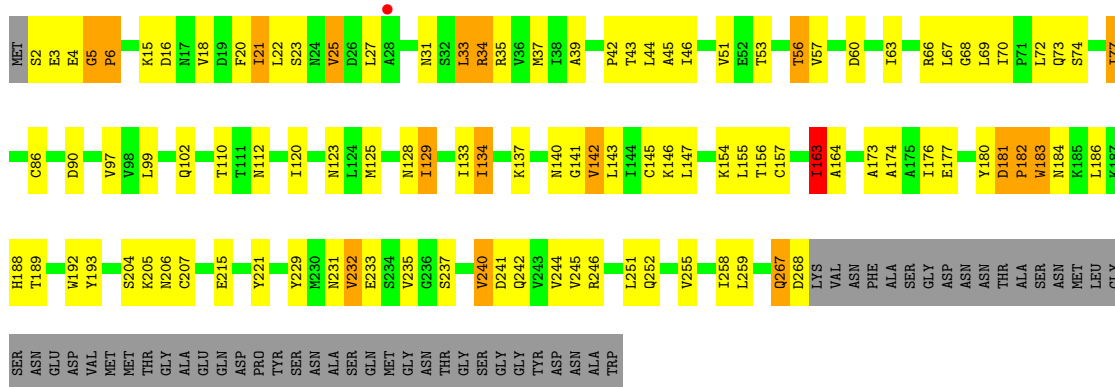


V392	H399	P400	G401	A402	K403	Y404	R407	D408	S409	I413	D414	L415	R416	Y417	S418	K419	I424	Y428	G429	W430	R434	H435	I436	M437	L443	R446	Q447	P448	S449	L450	H451	K452	M453	S454	M455	M456	A457	T463	P464	Y465	S466	T467	R468	R469	L470	M471	L472	T475	S476				
P477	F482	D483	G484	D485	E486	M487	E496	T497	R498	L501	S502	Q503	L504	S505	A506	V507	P508	L509	Q510	L511	V512	S513	K518	P519	G520	M521	G522	L523	T527	L528	I531	T535	L536	R537	D538	L543	D544	V546	M549	L550	T560	P561	R562	L470	P563	A564	I565	M648	K567				
P568	S573	G574	D575	Q576	L577	L578	S579	V580	R583	L588	Q589	R590	L591	D592	E593	T596	L597	L598	Q510	L511	P600	K601	M605	D609	G610	Q611	L612	F613	F614	V617	E618	K619	T621	V622	G623	S624	S625	M626	G628	V632	V633	T634	P642	S915	L645	F646	G647	M648	I649				
Q650	K651	V652	V656	L657	L658	H659	H660	F662	P663	L666	G667	D668	D672	T675	E678	T679	T680	E681	T682	L683	K689	M700	L701	L702	T709	L710	R711	A725	G730	L732	L733	V735	N736	L737	L740	N741	N742	K743	K744	Q745	M746	S754	F755	I756	N757	I758							
A759	Q760	A763	C764	W765	Q766	R774	R775	F778	F779	P785	S793	F794	E795	K797	V800	N801	N802	S803	R806	T809	P810	Q811	E812	F813	F814	F815	H816	A817	G820	T821	L824	I825	A828	W829	R830	T831	T834	I837	Q838	R839	R840	R843	I844	L845									
E846	D847	I848	Y852	D853	H854	T855	T856	R857	S859	L860	I864	I867	E870	D871	G872	H873	D874	A875	I878	K880	T885	R886	G888	S889	A892	F893	R896	Y897	R898	W899	Q900	L901	L902	T907	D909	P910	S911	L912	L913	E914	R915	S917	E918	I919	L920								
G921	D922	L923	K924	L925	Q926	V927	L928	L929	L936	R940	K941	F942	L943	D949	W954	P955	L956	P957	V958	N959	I960	R961	I964	Q969	H972	S979	D980	L981	T982	I986	L993	N996	M1004	I1006	D1009	P1010	V1015	L1016	F1018	C1019	C1020	S915	L1021	L1022	R1025								
T1028	R1029	R1030	V1031	E1034	Y1035	R1036	K1039	L1054	Y1058	H1059	E1062	S1063	V1064	G1065	L1067	T1077	L1081	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ASP	ALA	K1092	K1093	V1094	T1095	G1097	V1098	P1099	R1100	L1101	L1105	L1106	N1107	M1110	L1116	T1117	V1118	Y1119	L1120								
E1129	I1134	R1135	I1138	E1139	H1140	T1141	V1142	V1146	Y1154	D1155	R1159	S1160	T1161	V1162	I1163	H1173	L1176	LEU	ASP	GLU	GLU	ALA	ALA	GLN	PHE	ASP	Q1187	Q1188	S1189	M1190	M1191	L1192	L1193	D1198	M1202	D1206	M1209	V1212	K1221	M1222	D1223	L1236	I1237	I1238									
R1239	C1240	R1241	V1242	V1243	ARG	P90	LYS	LEU	ASP	ALA	GLU	THR	A1254	M1259	K1262	I1263	E1264	M1267	N1270	L1273	R1274	G1275	V1276	E1277	N1278	I1279	E1280	R1281	V1282	D1288	V1291	T1295	V1299	V1305	L1306	E1307	T1308	V1311	N1312	L1313	S1314	E1315	V1316	V1319	P1320								
G1321	I1322	D1323	P1324	R1325	R1326	L1327	Y1328	T1329	F1332	I1333	D1334	I1335	V1338	L1339	G1340	I1341	G1344	R1345	L1348	Y1349	K1350	E1351	T1356	T1357	S1361	M1364	Y1365	R1366	L1370	L1371	V1372	D1373	M1374	T1376	T1377	Q1378	G1379	V1384	T1385	G1388	F1389	M1390	L1391	S1392	M1393	T1394	G1395	L1396	L1397				
M1398	R1399	C1400	S1401	F1402	E1403	E1404	T1405	V1406	L1409	F1410	A1416	E1417	L1418	V1424	S1425	V1428	I1429	Q1432	M1433	A1434	P1435	I1436	G1437	T1438	G1439	A1440	F1441	I1445	ASP	GLU	GLU	LEU	VAL	LEU	VAL	ILE	THR	GLU	ILE	PHE	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	VAL				
THR	PRO	TYR	GLY	ASN	GLU	SER	GLY	LEU	VAL	ASN	ALA	LEU	ASP	VAL	LYS	ASP	GLU	PRO	LEU	VAL	ASP	SER	GLY	ASN	ASN	ASP	ALA	ASP	GLY	GLY	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL			
THR	SER	PRO	THR	SER	PRO	THR	SER	THR	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
TYR	SER	PRO	THR	SER	PRO	THR	SER	THR	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
SER	PRO	SER	TYR	SER	PRO	THR	SER	THR	PRO	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR



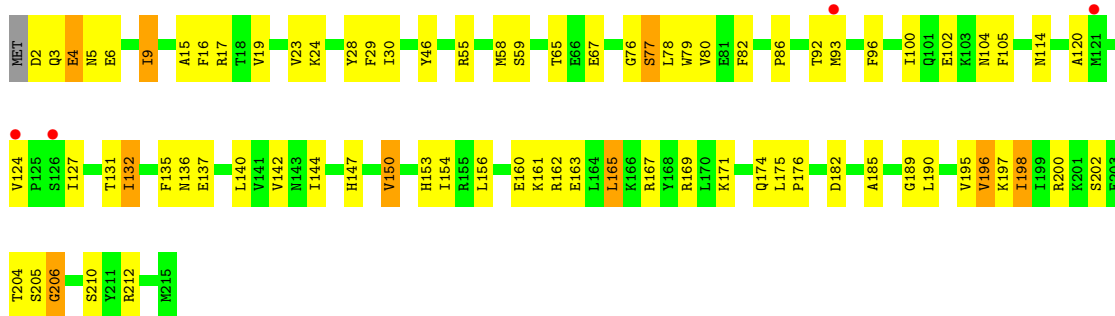
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 50% 28% 5% 16%



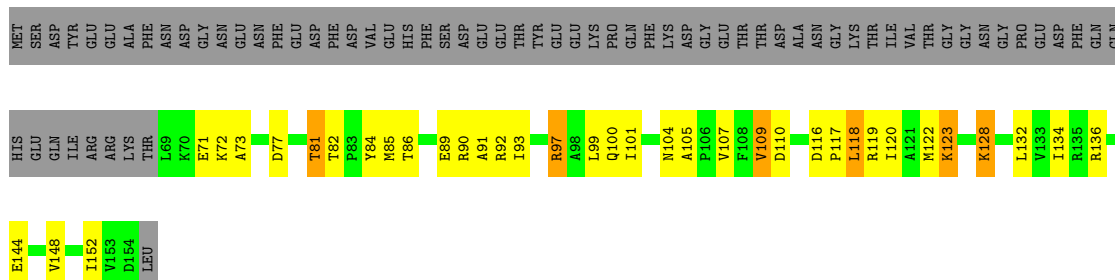
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 2% 63% 32%

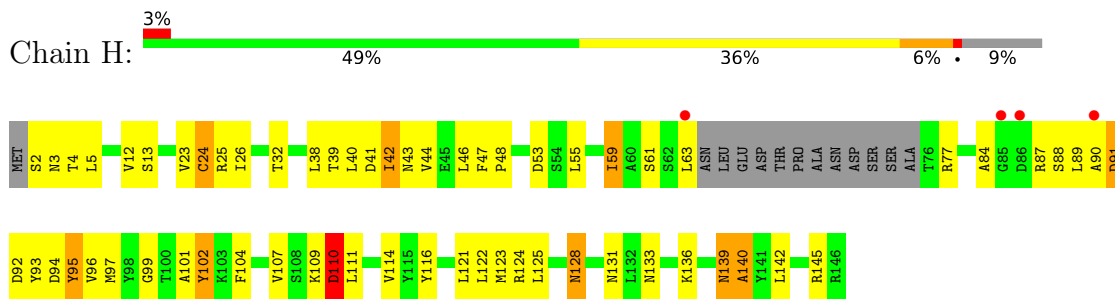


• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

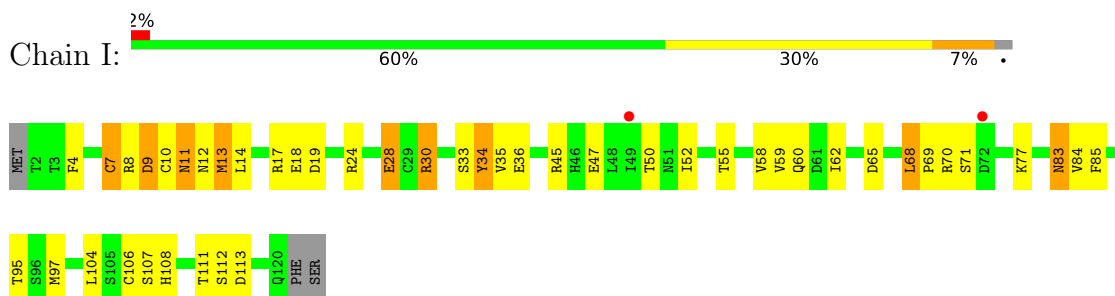
Chain F: 32% 20% 45%



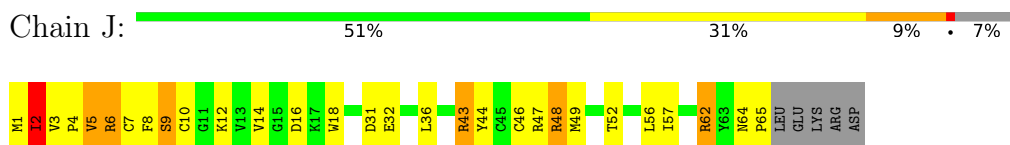
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



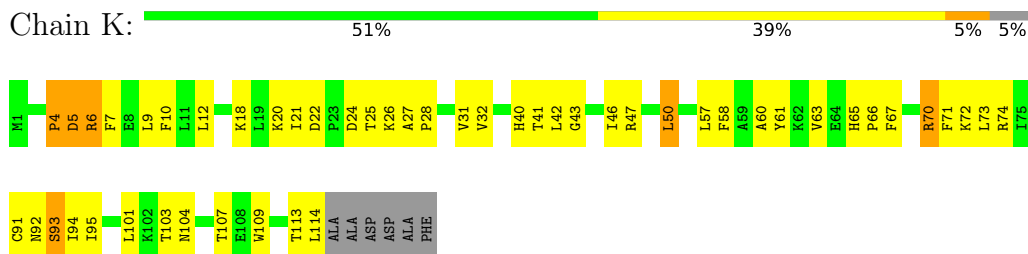
- Molecule 10: DNA-directed RNA polymerase II subunit 9



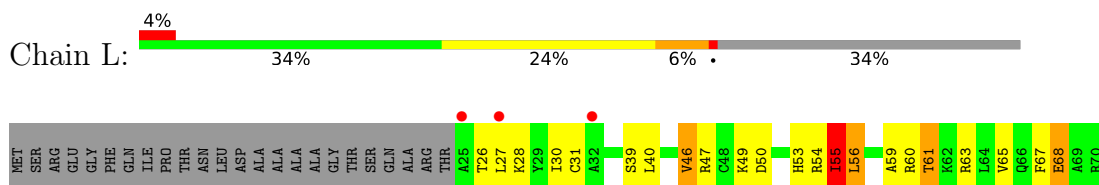
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.14Å 222.02Å 194.65Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-3.50) 94.6 (50.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.306 0.242 , 0.292	Depositor DCC
R_{free} test set	2511 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	101.1	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29206	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: ZN, MG, G2P

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	R	0.70	0/223	1.26	1/345 (0.3%)
2	T	0.41	0/612	1.07	2/941 (0.2%)
3	N	0.37	0/296	1.08	2/453 (0.4%)
4	A	0.75	1/11163 (0.0%)	1.02	23/15091 (0.2%)
5	B	0.78	1/8952 (0.0%)	1.02	20/12071 (0.2%)
6	C	0.73	0/2139	0.99	3/2899 (0.1%)
7	E	0.68	0/1788	0.93	2/2406 (0.1%)
8	F	0.67	0/708	0.91	0/956
9	H	0.69	0/1086	0.95	4/1470 (0.3%)
10	I	0.79	0/989	0.96	2/1331 (0.2%)
11	J	0.78	0/541	0.98	0/727
12	K	0.74	0/937	0.99	0/1265
13	L	0.86	0/365	0.98	0/485
All	All	0.75	2/29799 (0.0%)	1.01	59/40440 (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
4	A	0	3
5	B	0	4
6	C	0	1
9	H	1	1
11	J	0	1
All	All	1	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	250	ILE	CA-CB	7.40	1.61	1.54
5	B	882	THR	CA-CB	5.16	1.61	1.53

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	882	THR	N-CA-C	7.97	119.75	111.14
6	C	5	GLY	CA-C-N	7.55	129.28	119.84
6	C	5	GLY	C-N-CA	7.55	129.28	119.84
1	R	10	G	C5'-C4'-C3'	-7.05	105.42	116.00
4	A	513	SER	CA-C-N	6.99	127.58	119.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	H	110	ASP	CA

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1392	SER	Peptide
4	A	257	ARG	Peptide
4	A	258	GLY	Peptide
5	B	293	PRO	Peptide
5	B	478	GLY	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	R	199	0	98	4	0
2	T	546	0	304	5	0
3	N	266	0	149	0	0
4	A	10969	0	11067	437	0
5	B	8782	0	8816	435	0
6	C	2101	0	2056	93	0
7	E	1752	0	1776	50	0
8	F	696	0	720	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	1068	0	1040	52	0
10	I	971	0	927	29	0
11	J	532	0	542	43	0
12	K	919	0	929	41	0
13	L	363	0	386	10	0
14	T	32	0	14	1	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	2	0	0	0	0
All	All	29206	0	28824	1108	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 19.

The worst 5 of 1108 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)
9:H:109:LYS:HB3	9:H:110:ASP:CA	1.54	1.34
9:H:109:LYS:CB	9:H:110:ASP:HA	1.49	1.31
4:A:399:HIS:CB	4:A:400:PRO:HD3	1.65	1.27
5:B:635:ARG:CG	5:B:636:PRO:HD2	1.65	1.24
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.73	1.18

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	
4	A	1383/1733 (80%)	1136 (82%)	182 (13%)	65 (5%)	2	17
5	B	1087/1224 (89%)	918 (84%)	124 (11%)	45 (4%)	2	19
6	C	265/318 (83%)	222 (84%)	34 (13%)	9 (3%)	3	23
7	E	212/215 (99%)	180 (85%)	25 (12%)	7 (3%)	3	23
8	F	84/155 (54%)	73 (87%)	10 (12%)	1 (1%)	10	41
9	H	129/146 (88%)	101 (78%)	23 (18%)	5 (4%)	2	20
10	I	117/122 (96%)	95 (81%)	18 (15%)	4 (3%)	3	23
11	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	3	24
12	K	112/120 (93%)	97 (87%)	11 (10%)	4 (4%)	2	22
13	L	44/70 (63%)	25 (57%)	11 (25%)	8 (18%)	0	1
All	All	3496/4173 (84%)	2903 (83%)	443 (13%)	150 (4%)	2	18

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	55	ASP
4	A	93	VAL
4	A	248	PRO
4	A	321	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	
4	A	1218/1520 (80%)	1060 (87%)	158 (13%)	4	21
5	B	959/1061 (90%)	833 (87%)	126 (13%)	4	20
6	C	235/274 (86%)	212 (90%)	23 (10%)	7	30
7	E	196/197 (100%)	179 (91%)	17 (9%)	9	33
8	F	76/137 (56%)	67 (88%)	9 (12%)	5	23
9	H	117/128 (91%)	104 (89%)	13 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	113/116 (97%)	97 (86%)	16 (14%)	3	18
11	J	60/65 (92%)	52 (87%)	8 (13%)	4	20
12	K	99/102 (97%)	85 (86%)	14 (14%)	3	18
13	L	40/57 (70%)	32 (80%)	8 (20%)	1	7
All	All	3113/3657 (85%)	2721 (87%)	392 (13%)	4	21

5 of 392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	762	ASN
6	C	23	SER
5	B	807	ARG
5	B	973	ILE
6	C	163	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	1117	GLN
7	E	32	GLN
5	B	1178	ASN
6	C	188	HIS
7	E	147	HIS

5.3.3 RNA [i](#)

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

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	C
1	R	10	G

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 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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
14	G2P	T	3000	-	30,34,34	1.08	1 (3%)	46,54,54	1.78	9 (19%)

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
14	G2P	T	3000	-	-	5/19/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	3000	G2P	PB-O3B	2.79	1.61	1.58

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	G2P	C5-C4-N3	-5.32	119.93	128.39
14	T	3000	G2P	C2-N3-C4	4.58	120.19	112.30
14	T	3000	G2P	PB-O3B-PG	-4.16	117.54	132.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	G2P	N9-C4-N3	3.30	132.56	125.95
14	T	3000	G2P	C2-N1-C6	-2.85	119.94	125.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

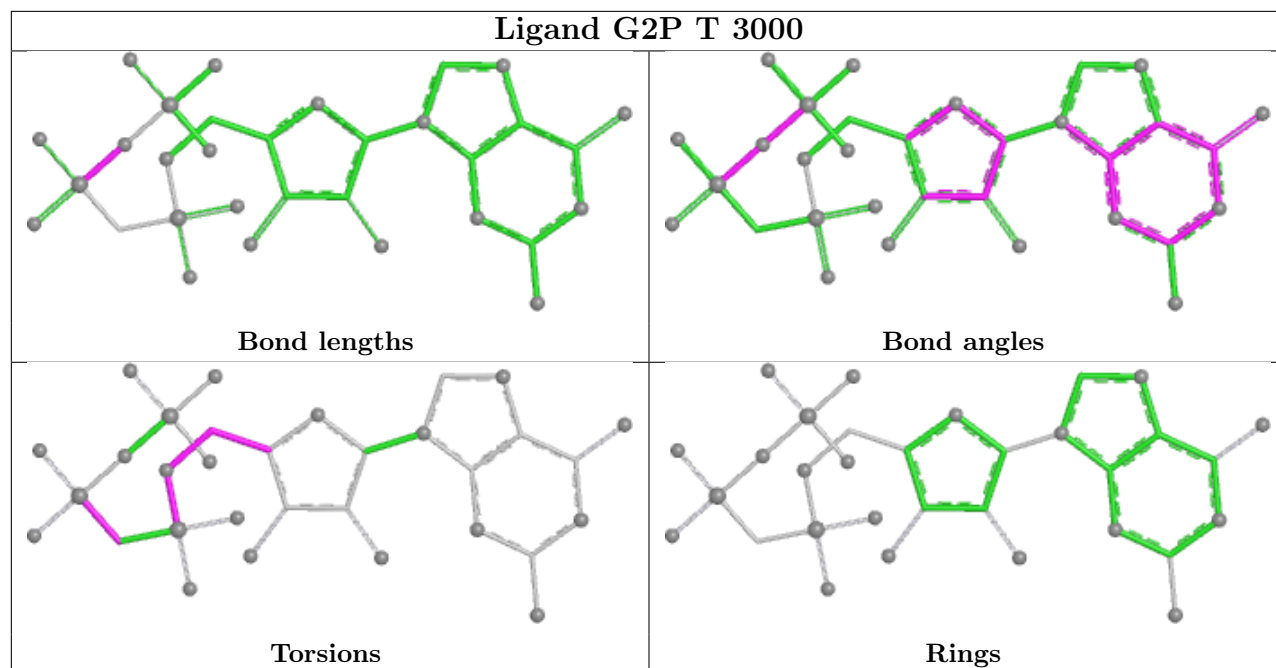
Mol	Chain	Res	Type	Atoms
14	T	3000	G2P	O4'-C4'-C5'-O5'
14	T	3000	G2P	C3'-C4'-C5'-O5'
14	T	3000	G2P	C4'-C5'-O5'-PA
14	T	3000	G2P	PA-C3A-PB-O2B
14	T	3000	G2P	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	3000	G2P	1	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	R	9/9 (100%)	0.46	1 (11%) 10 7	98, 111, 151, 169	0
2	T	27/27 (100%)	0.67	1 (3%) 45 25	100, 203, 234, 238	0
3	N	13/13 (100%)	0.68	0 100 100	197, 219, 252, 258	0
4	A	1395/1733 (80%)	0.00	12 (0%) 81 58	61, 99, 161, 173	0
5	B	1105/1224 (90%)	-0.01	15 (1%) 73 48	64, 94, 139, 155	0
6	C	267/318 (83%)	-0.27	1 (0%) 88 72	74, 89, 122, 144	0
7	E	214/215 (99%)	0.08	4 (1%) 66 41	79, 116, 155, 159	0
8	F	86/155 (55%)	-0.12	0 100 100	75, 105, 145, 156	0
9	H	133/146 (91%)	0.20	4 (3%) 52 30	100, 118, 146, 148	0
10	I	119/122 (97%)	0.09	2 (1%) 69 43	84, 103, 123, 142	0
11	J	65/70 (92%)	-0.33	0 100 100	69, 87, 107, 112	0
12	K	114/120 (95%)	-0.27	0 100 100	73, 95, 112, 115	0
13	L	46/70 (65%)	0.64	3 (6%) 25 15	102, 147, 159, 163	0
All	All	3593/4222 (85%)	-0.01	43 (1%) 76 52	61, 99, 157, 258	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	335	GLY	4.9
4	A	44	THR	3.9
5	B	882	THR	3.9
1	R	2	A	3.8
5	B	883	LEU	3.6

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](#)

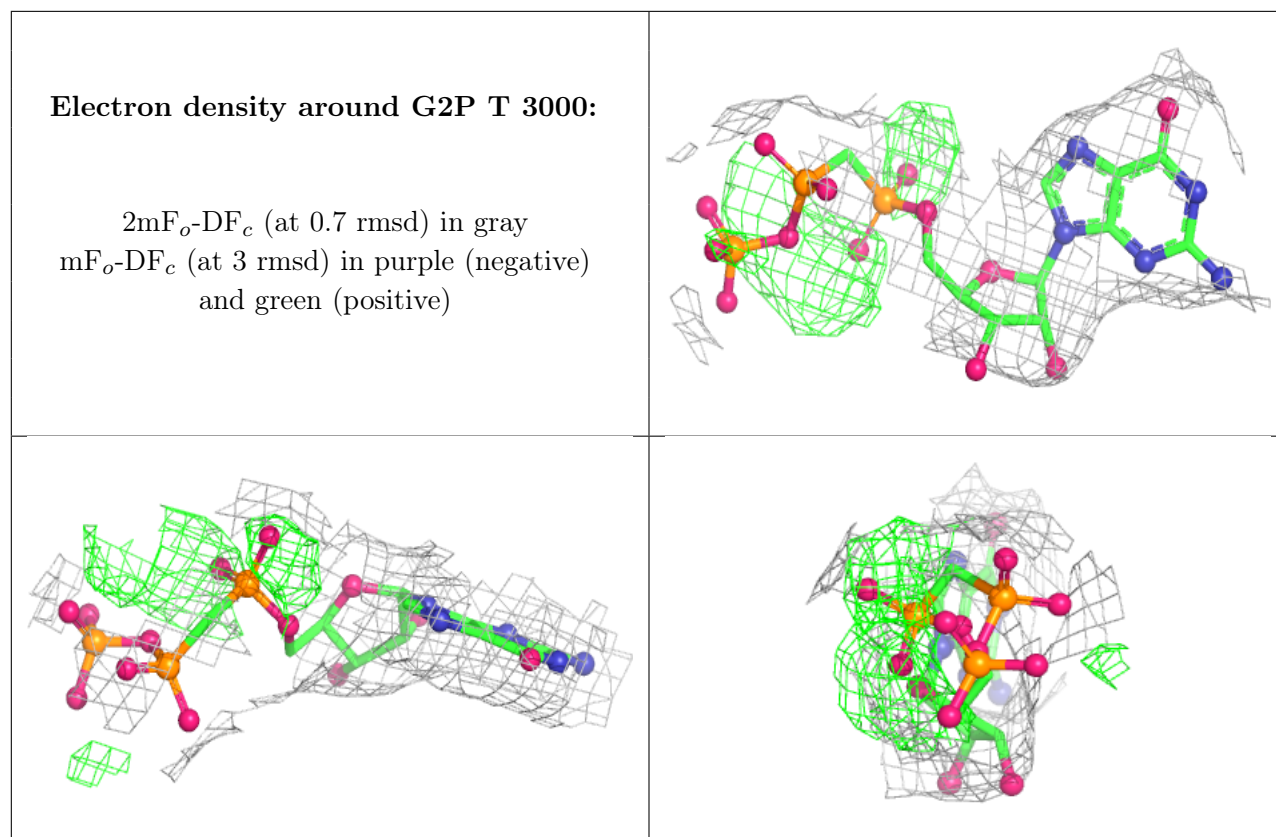
There are no oligosaccharides in this entry.

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
14	G2P	T	3000	32/32	0.85	0.11	125,129,158,158	0
16	MG	A	2002	1/1	0.86	0.22	76,76,76,76	0
15	ZN	A	1734	1/1	0.96	0.09	165,165,165,165	0
16	MG	A	2001	1/1	0.97	0.04	67,67,67,67	0
15	ZN	L	105	1/1	0.98	0.05	146,146,146,146	0
15	ZN	B	1307	1/1	0.99	0.02	138,138,138,138	0
15	ZN	A	1735	1/1	0.99	0.06	153,153,153,153	0
15	ZN	J	101	1/1	1.00	0.02	77,77,77,77	0
15	ZN	C	319	1/1	1.00	0.02	90,90,90,90	0
15	ZN	I	203	1/1	1.00	0.03	101,101,101,101	0
15	ZN	I	204	1/1	1.00	0.02	90,90,90,90	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.