



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 05:24 AM UTC

PDB ID : 2E2H / pdb_00002e2h
Title : RNA polymerase II elongation complex at 5 mM Mg²⁺ with GTP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.95 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

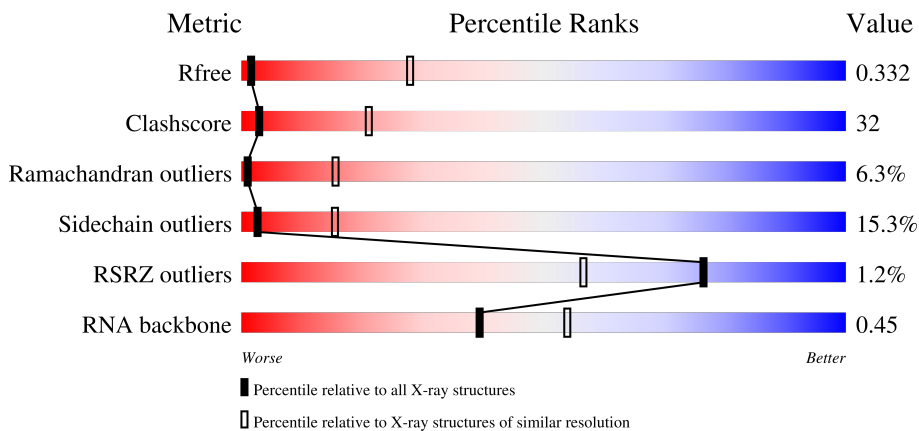
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)
RNA backbone	3983	1016 (4.80-3.10)

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	10	 20% 80%
2	T	28	 50% 46%
3	N	14	 7% 86% 14%
4	A	1733	 39% 30% 10% 19%

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Mol	Chain	Length	Quality of chain
5	B	1224	<p>%</p> <p>47% 34% 8% • 10%</p>
6	C	318	<p>51% 29% • 16%</p>
7	E	215	<p>2%</p> <p>54% 29% 6% • 10%</p>
8	F	155	<p>%</p> <p>30% 17% 6% 46%</p>
9	H	146	<p>%</p> <p>43% 28% 7% 13% 9%</p>
10	I	122	<p>2%</p> <p>37% 32% 19% 10% •</p>
11	J	70	<p>50% 34% 9% 7%</p>
12	K	120	<p>68% 22% • • 5%</p>
13	L	70	<p>4%</p> <p>33% 24% 6% • 34%</p>

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29003 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(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	10	216	98	45	64	9	0	0	0

- Molecule 2 is a DNA chain called 28-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	28	564	270	102	165	27	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	N	14	284	137	49	85	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	1398	10984	6930	1924	2069	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	1096	8701	5508	1518	1620	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	266	2095	1317	348	417	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	193	1594	1016	283	287	8	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	83	670	428	114	125	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.

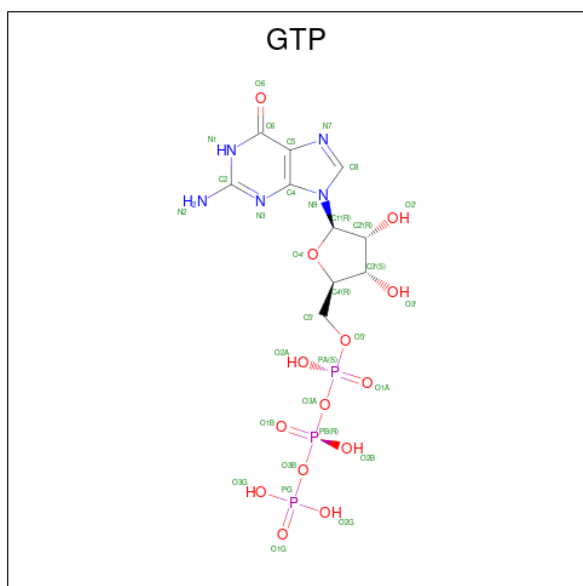
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	114	919	590	156	171	2	0	0	0

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

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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 GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	T	1	32	10	5	14	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.

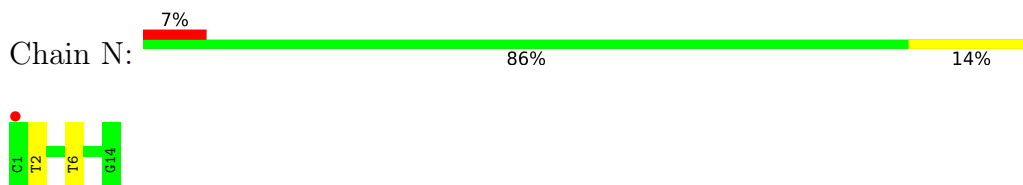
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'



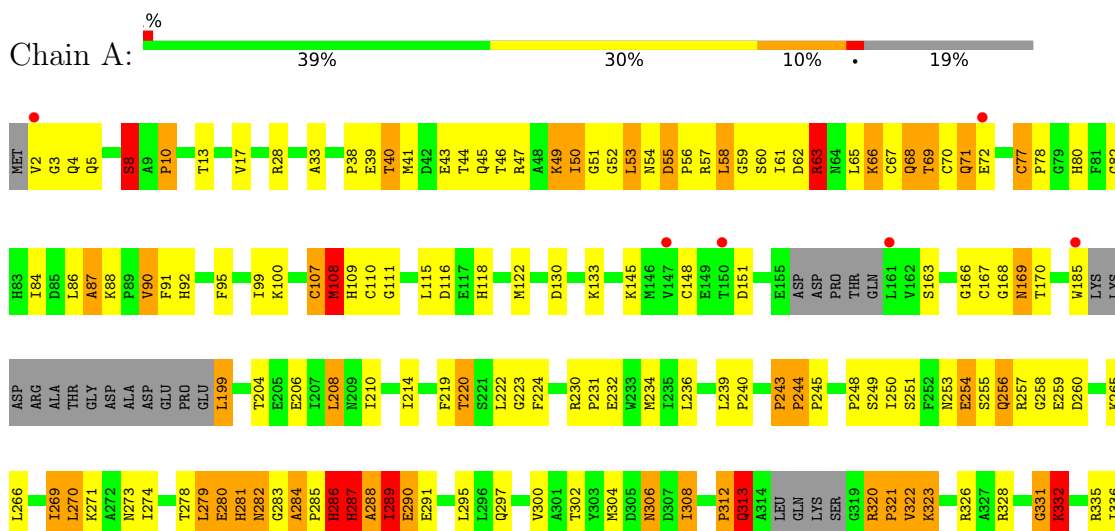
- Molecule 2: 28-MER DNA template strand



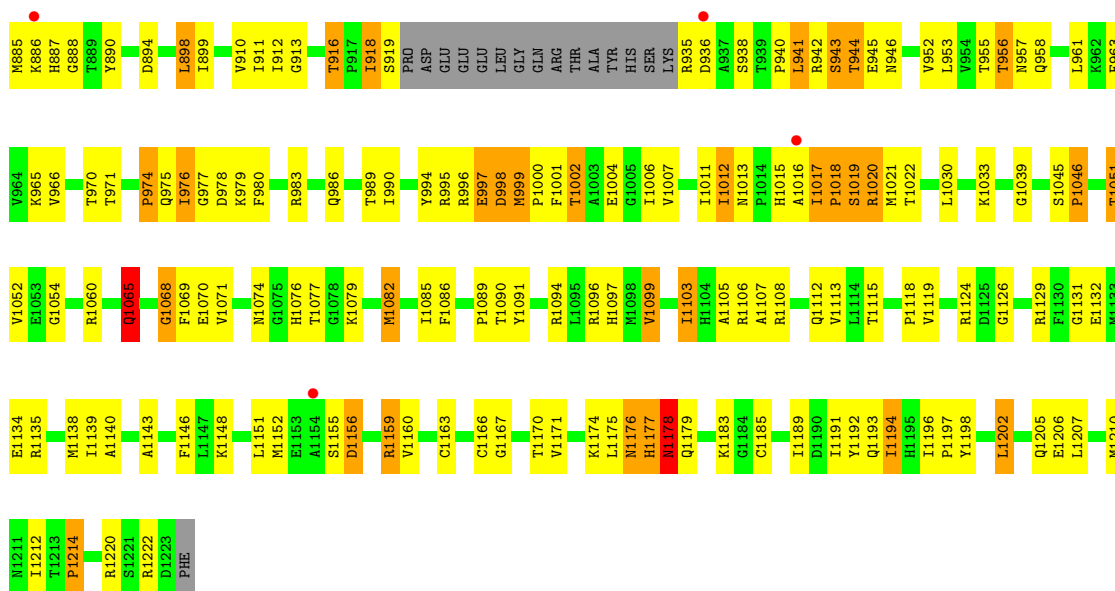
- Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'



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

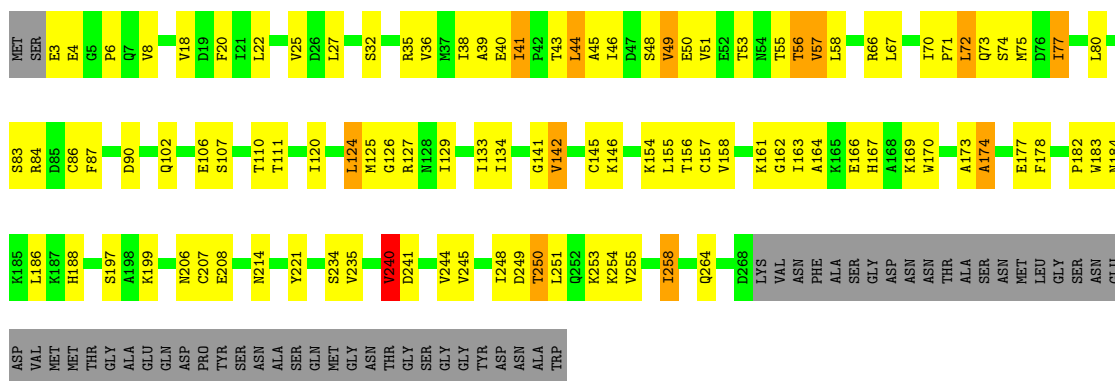


VAL	V1372	L1273	R1199	E1129	P1060	K984	L901	A817	K738	S663	R590	A506	D423	R337
LYS	T1376	R1274	A1200	Q1130	G1061	D985	L902	M618	D739	S666	F591	L509	I424	G338
THR	N1278	N1278	A1201	L1133	M1063	D986	N903	G819	N741	I667	T595	L509	N359	N359
MET	Q1378	N1278	M1203	L1133	M1063	D987	N903	G820	N741	I667	T595	L509	L340	L340
PRO	Q1378	R1281	D1206	T1141	V1064	D988	T907	R821	N742	D668	T596	S513	M341	M341
GLU	T1385	V1282	L1207	T1142	V1066	D989	L909	E822	N743	D669	L597	S513	Y428	Y428
GLN	G1388	V1283	L1207	L1143	L1067	D990	P910	D826	K744	I670	L598	Q515	W430	W430
ILE	F1389	M1284	L1208	V1146	A1068	D992	S911	T827	Q745	P674	P690	M517	R434	R434
THR	M1390	D1288	M1209	V1147	A1069	D993	L912	A828	N748	T675	K601	H435	H435	H435
ILE	R1391	Q1211	Q1211	Q1070	A1070	L993	L913	V829	S751	E678	D602	I523	R350	R350
GLU	S1293	S1293	Q1211	E1151	S1071	N996	E914	R830	S751	E678	G604	Q525	T351	T351
ASP	P1294	P1294	G1213	L1152	G1073	L997	S915	E833	S754	T680	G605	D526	V352	V352
GLY	T1295	T1295	R1214	Y1154	P1075	L998	L920	G835	F755	E681	L606	T527	I353	I353
ASP	M1398	L1306	L1219	D1156	A1076	L1000	G921	R836	N757	I683	L607	L528	S354	S354
GLN	S1401	L1307	T1219	D1157	T1077	L1000	G921	I837	N757	I683	L608	L528	D356	D356
VAL	V1406	D1389	D1223	P1165	M1078	E1005	D922	R840	V765	A686	G610	I531	P448	P448
THR	E1407	G1310	L1224	R1159	M1080	M1009	L925	L841	Q766	K687	G611	L534	S449	S449
PRO	N1408	F1225	L1224	S1160	L1081	M1009	Q926	L841	Q767	K687	I612	T535	L450	L450
TYR	L1409	N1312	V1226	T1161	M1082	Q1011	Q926	V842	Q768	V690	G615	R537	R451	R451
SER	F1410	L1313	M1227	V1162	T1083	Q1011	L929	K843	S769	V693	G615	R537	M453	M453
ASN	F1410	S1314	W1228	L1163	T1083	V1015	D930	A844	V770	V693	V616	D538	S454	S454
GLU	A1414	E1315	D1231	P1164	H1085	T1016	L930	E846	R774	E686	V617	F540	M455	M455
SER	S1415	M1317	ASN	E1166	F1086	L1017	Y933	D847	I775	A697	E618	I541	A457	A457
GLY	A1416	G1318	ASP	E1166	A1087	F1018	L936	R855	I775	A697	V622	I541	R372	R372
LEU	A1417	ASP	ASP	E1168	G1088	C1019	L936	R855	F777	A699	V622	I541	K373	K373
VAL	L1418	L1319	GLU	E1168	V1089	C1020	V937	Y852	G778	A699	G623	L543	H458	H458
ASN	L1419	L1322	LYS	T1170	A1090	L1021	K938	R853	G778	N700	G624	L543	R459	R459
ALA	D1420	I1322	L1236	T1170	S1091	L1022	D939	R854	V780	L702	S625	Q545	V460	V460
ASP	C1421	D1323	L1237	Q1171	K1092	L1022	D939	R854	V780	L702	S625	Q545	K461	K461
LEU	V1424	P1324	L1237	Q1171	K1092	L1022	D939	R854	V780	L702	S625	Q545	V462	V462
ASP	V1424	P1324	L1237	Q1171	K1092	L1022	D939	R854	V780	L702	S625	Q545	V462	V462
LYS	V1425	F1174	C1240	S1175	S1095	R1030	V946	R855	P785	L702	S625	Q545	V462	V462
ASP	E1426	F1174	V1242	L1176	G1097	V1031	F947	R855	P785	L702	S625	Q545	V462	V462
GLU	N1427	F1332	V1243	LEU	V1098	L1032	G861	R860	K789	I709	E636	I560	R469	R469
LEU	V1428	I1333	ARG	ASP	P1099	Q1033	N862	N862	D790	L710	K637	I560	R469	R469
MET	L1430	I1333	PRO	GLU	R1100	E1034	V863	V863	D790	L710	K637	I560	R469	R469
PHE	L1430	I1333	LYS	GLU	R1100	E1034	V863	V863	D790	L710	K637	I560	R469	R469
SER	G1431	M1336	LYS	GLU	L1101	Y1035	W954	P955	S793	E712	P639	I566	V474	V474
LEU	G1340	G1340	SER	ALA	L1104	T1038	P955	I867	P794	S713	P640	K567	P477	P477
LEU	R1345	R1345	ASP	GLN	L1106	T1038	L956	I868	P794	S713	P640	K567	Y478	Y478
VAL	P1435	Y1345	ALA	SER	M1106	A1041	P957	G869	F799	D716	S573	S573	F482	F482
ASP	P1435	Y1345	ALA	PHE	V1107	A1041	V958	E801	Y800	N717	L645	L645	D483	D483
SER	I1436	I1356	THR	ASP	A1108	V1045	N959	N802	N802	V718	F646	F646	Y404	Y404
GLY	G1437	A1357	GLU	Q1187	K1109	V1045	I960	M873	N802	V718	G647	Q576	D485	D485
SER	T1438	S1358	GLU	O1188	K1109	V1045	I960	M873	N802	V718	G647	Q576	D485	D485
ASN	G1439	D1359	ASP	S1189	M1048	N1048	Q869	A875	L805	F721	K651	L578	E486	E486
ASP	A1440	K1261	ALA	P1190	K1112	I1049	Q869	A875	L805	F721	K651	L578	E486	E486
ALA	F1441	K1262	ALA	W1191	T1113	E1050	T970	I878	L808	N723	V652	S579	M488	M488
ALA	F1441	K1262	ALA	W1191	T1113	E1050	T970	I878	L808	N723	V652	S579	M488	M488
MET	I1263	I1263	I1263	I1192	S1115	F1053	F971	I886	P810	E724	V653	I582	E495	E495
ALA	N1364	L1193	L1193	L1193	L1116	L1054	H972	I886	P810	E724	V653	I582	E495	E495
GLY	Y1365	R1194	R1194	R1194	T1117	R1055	I973	I886	P810	E724	V653	I582	E495	E495
GLY	R1366	T1266	T1266	L1195	T1117	R1055	I973	I886	P810	E724	V653	I582	E495	E495
THR	GLU	M1267	M1267	L1195	V1118	S1056	H975	R897	F813	R731	L658	H587	A499	A499
PHE	GLU	E1196	E1196	E1196	T976	R898	H975	R897	F813	R731	L658	H587	A499	A499
THR	LEU	L1197	L1197	L1197	T976	R898	H975	R897	F813	R731	L658	H587	A499	A499
ALA	LEU	D1197	D1197	D1197	K977	V1058	F815	R899	F814	N736	N660	L588	Q503	Q503
ALA	LEU	D1197	D1197	D1197	K977	V1058	F815	R899	F814	N736	N660	L588	Q503	Q503
ALA	LEU	D1197	D1197	D1197	K977	V1058	F815	R899	F814	N736	N660	L588	Q503	Q503
ALA	LEU	D1197	D1197	D1197	K977	V1058	F815	R899	F814	N736	N660	L588	Q503	Q503



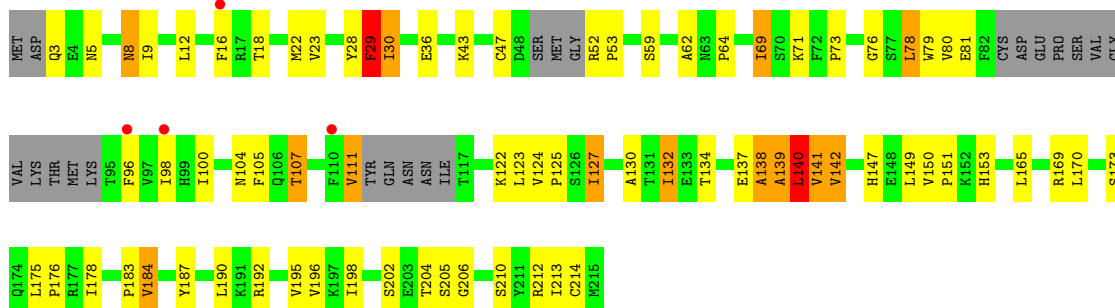
- Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 51% 29% 16%

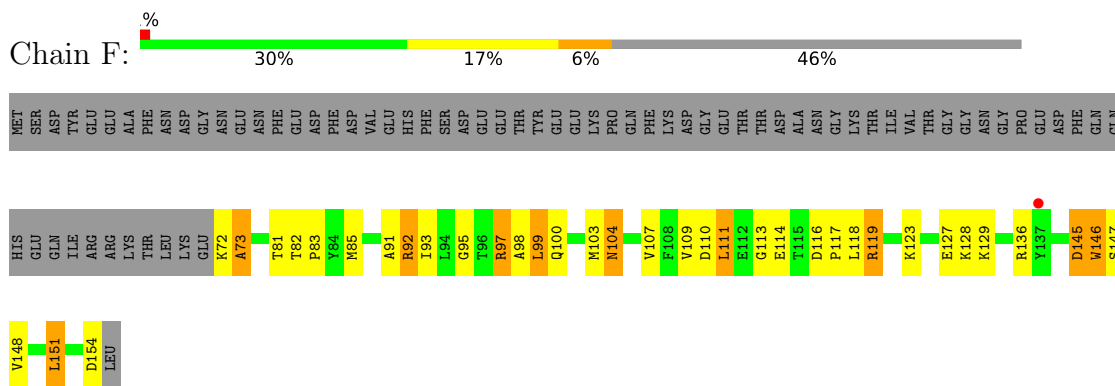


- Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

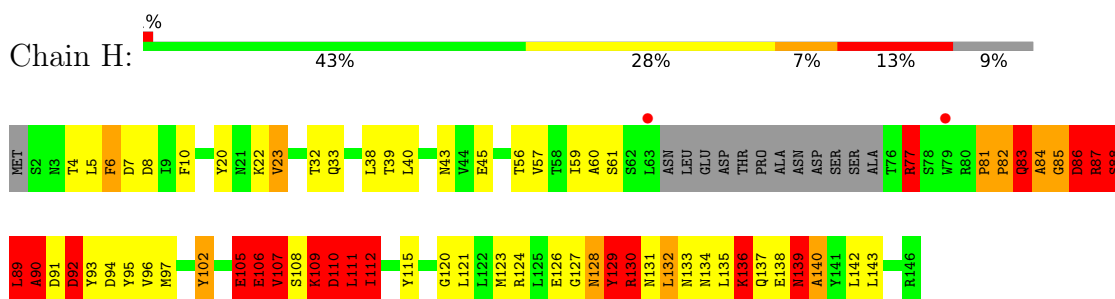
Chain E: 2% 54% 29% 6% 10%



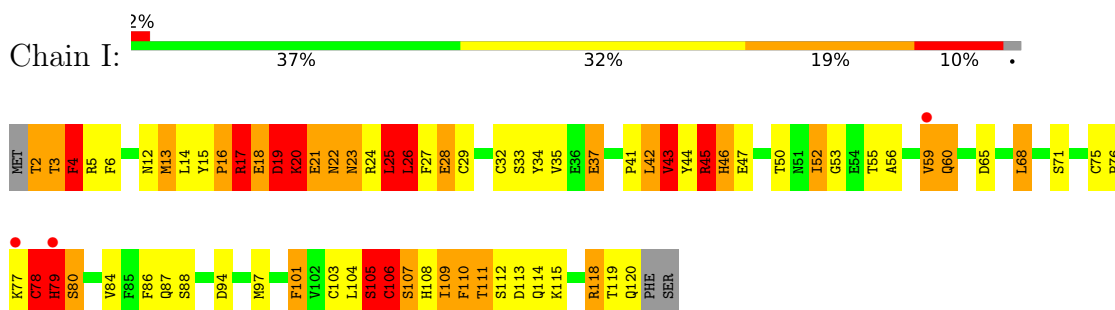
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



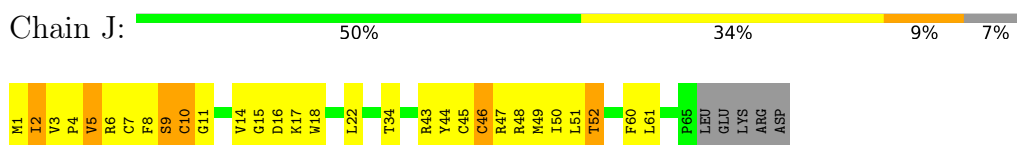
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



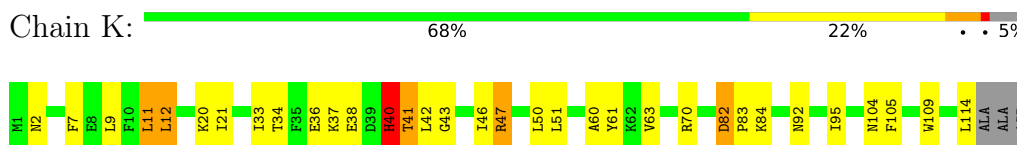
- Molecule 10: DNA-directed RNA polymerase II subunit 9



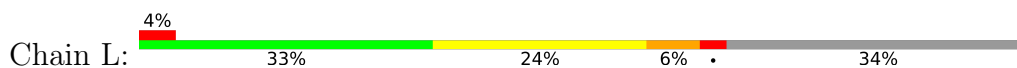
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

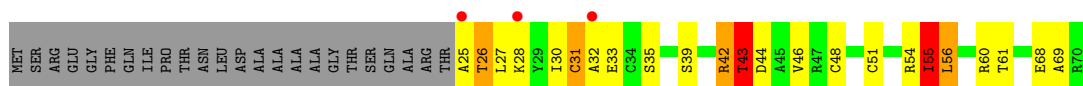


- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- 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	171.11Å 222.00Å 195.16Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	45.08 – 3.95 45.08 – 3.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.08-3.95) 97.7 (45.08-3.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 4.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.290 , 0.368 0.270 , 0.332	Depositor DCC
R_{free} test set	3078 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	115.3	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29003	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GTP, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	R	0.49	0/243	0.86	0/378
2	T	0.34	0/631	0.87	1/970 (0.1%)
3	N	0.30	0/317	0.81	0/488
4	A	0.56	0/11180	0.90	18/15117 (0.1%)
5	B	0.57	0/8866	0.88	8/11956 (0.1%)
6	C	0.54	0/2133	0.88	2/2891 (0.1%)
7	E	0.57	0/1625	0.87	2/2182 (0.1%)
8	F	0.54	0/682	0.82	0/922
9	H	0.61	0/1086	0.83	1/1470 (0.1%)
10	I	0.58	0/989	0.86	4/1331 (0.3%)
11	J	0.45	0/541	0.85	0/727
12	K	0.54	0/937	0.92	2/1265 (0.2%)
13	L	0.51	0/365	0.81	0/485
All	All	0.55	0/29595	0.88	38/40182 (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	42
5	B	0	26
7	E	0	2
9	H	0	14
10	I	0	15
12	K	0	1
13	L	0	2
All	All	0	102

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	452	LYS	N-CA-C	-6.75	105.33	113.97
4	A	243	PRO	CA-C-N	6.72	127.30	120.38
4	A	243	PRO	C-N-CA	6.72	127.30	120.38
4	A	244	PRO	N-CA-C	6.68	118.85	110.70
12	K	82	ASP	CA-C-N	6.61	126.38	119.05

There are no chirality outliers.

5 of 102 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	107	CYS	Peptide
4	A	108	MET	Peptide
4	A	166	GLY	Peptide
4	A	256	GLN	Peptide
4	A	8	SER	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	216	0	109	10	0
2	T	564	0	316	13	0
3	N	284	0	161	2	0
4	A	10984	0	11070	896	0
5	B	8701	0	8729	537	0
6	C	2095	0	2051	72	0
7	E	1594	0	1622	60	0
8	F	670	0	690	33	0
9	H	1068	0	1040	132	0
10	I	971	0	930	128	0
11	J	532	0	543	32	0
12	K	919	0	929	25	0
13	L	363	0	387	26	0
14	T	32	0	12	4	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	29003	0	28589	1861	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 32.

The worst 5 of 1861 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)
4:A:289:ILE:CG2	4:A:290:GLU:HB3	1.38	1.50
11:J:43:ARG:HG3	11:J:46:CYS:SG	1.49	1.49
4:A:1191:TRP:CA	4:A:1192:LEU:HB2	1.35	1.48
4:A:973:ILE:CG2	4:A:974:ASP:HA	1.43	1.46
4:A:287:HIS:HA	4:A:289:ILE:CB	1.46	1.45

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	1384/1733 (80%)	1048 (76%)	236 (17%)	100 (7%)	1	13
5	B	1074/1224 (88%)	863 (80%)	152 (14%)	59 (6%)	1	17
6	C	264/318 (83%)	220 (83%)	37 (14%)	7 (3%)	4	28
7	E	185/215 (86%)	149 (80%)	29 (16%)	7 (4%)	2	22
8	F	81/155 (52%)	67 (83%)	8 (10%)	6 (7%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	129/146 (88%)	86 (67%)	25 (19%)	18 (14%)	0	3
10	I	117/122 (96%)	70 (60%)	33 (28%)	14 (12%)	0	4
11	J	63/70 (90%)	52 (82%)	8 (13%)	3 (5%)	2	19
12	K	112/120 (93%)	99 (88%)	13 (12%)	0	100	100
13	L	44/70 (63%)	28 (64%)	11 (25%)	5 (11%)	0	5
All	All	3453/4173 (83%)	2682 (78%)	552 (16%)	219 (6%)	1	15

5 of 219 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	63	ARG
4	A	66	LYS
4	A	108	MET
4	A	169	ASN

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%)	1023 (84%)	195 (16%)	2	14
5	B	951/1061 (90%)	810 (85%)	141 (15%)	3	16
6	C	234/274 (85%)	208 (89%)	26 (11%)	6	23
7	E	177/197 (90%)	154 (87%)	23 (13%)	4	19
8	F	73/137 (53%)	63 (86%)	10 (14%)	3	17
9	H	117/128 (91%)	93 (80%)	24 (20%)	1	8
10	I	113/116 (97%)	83 (74%)	30 (26%)	0	4
11	J	60/65 (92%)	53 (88%)	7 (12%)	5	21
12	K	99/102 (97%)	89 (90%)	10 (10%)	7	26
13	L	40/57 (70%)	34 (85%)	6 (15%)	3	16
All	All	3082/3657 (84%)	2610 (85%)	472 (15%)	3	15

5 of 472 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	346	GLU
10	I	104	LEU
5	B	861	ASP
10	I	78	CYS
9	H	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	842	ASN
7	E	61	GLN
5	B	986	GLN
5	B	1211	ASN
9	H	33	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	0	0

There are no RNA backbone outliers to report.

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	GTP	T	3000	16	33,34,34	0.91	2 (6%)	50,54,54	1.58	7 (14%)

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	GTP	T	3000	16	-	9/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	3000	GTP	C2-N3	2.61	1.39	1.33
14	T	3000	GTP	PA-O3A	2.03	1.61	1.59

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	GTP	C5-C4-N3	-5.43	119.75	128.39
14	T	3000	GTP	C2-N3-C4	4.38	119.85	112.30
14	T	3000	GTP	N9-C4-N3	3.35	132.66	125.95
14	T	3000	GTP	C2-N1-C6	-3.17	119.37	125.11
14	T	3000	GTP	C5-C6-N1	2.47	119.55	113.25

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

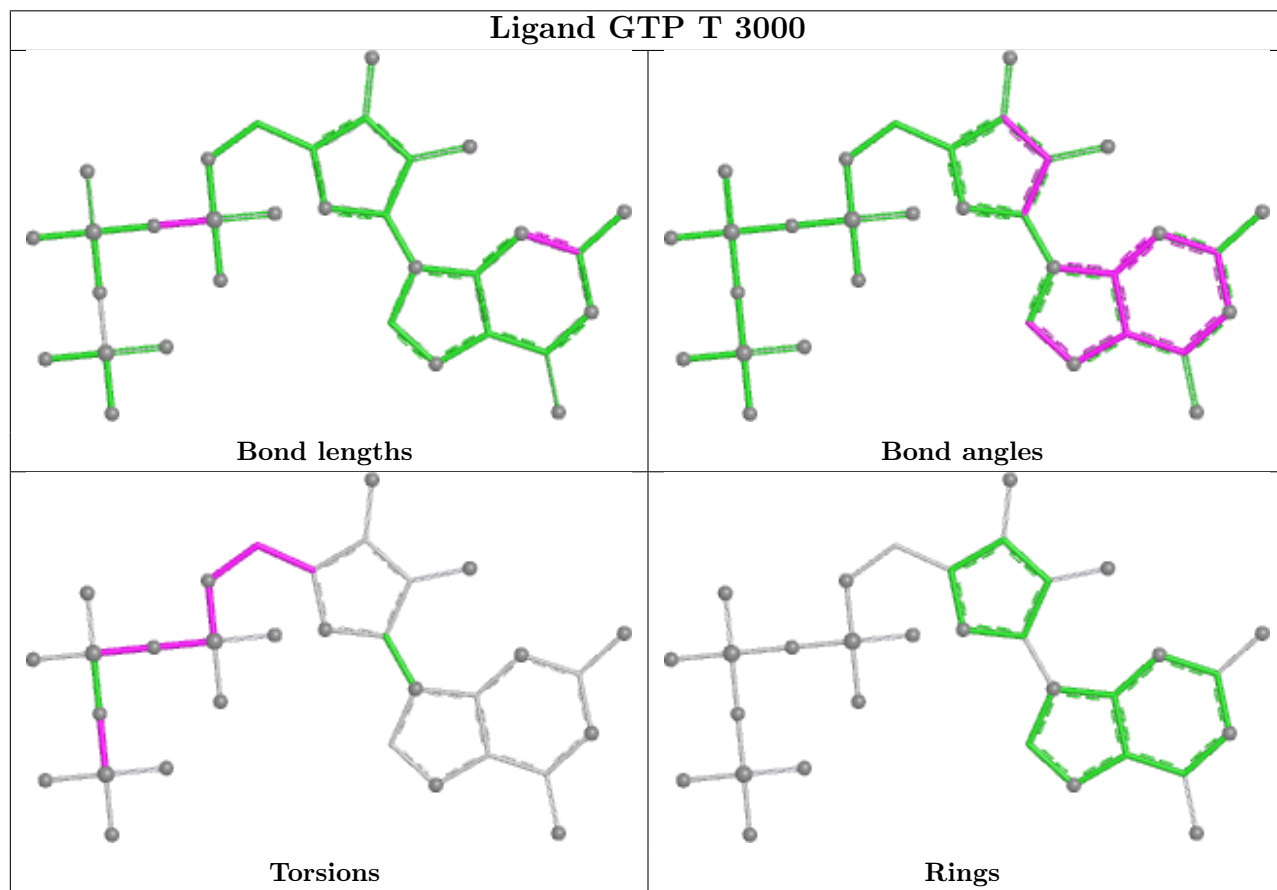
Mol	Chain	Res	Type	Atoms
14	T	3000	GTP	PB-O3B-PG-O2G
14	T	3000	GTP	PB-O3B-PG-O3G
14	T	3000	GTP	C5'-O5'-PA-O3A
14	T	3000	GTP	C5'-O5'-PA-O1A
14	T	3000	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	3000	GTP	4	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

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	10/10 (100%)	-0.14	0 100 100	88, 113, 158, 169	0
2	T	28/28 (100%)	0.27	0 100 100	88, 190, 261, 264	0
3	N	14/14 (100%)	0.60	1 (7%) 22 20	251, 259, 268, 269	0
4	A	1398/1733 (80%)	0.07	12 (0%) 81 62	76, 118, 174, 192	0
5	B	1096/1224 (89%)	0.11	16 (1%) 72 51	86, 115, 155, 171	0
6	C	266/318 (83%)	-0.17	0 100 100	93, 115, 146, 151	0
7	E	193/215 (89%)	0.05	4 (2%) 63 45	94, 131, 165, 172	0
8	F	83/155 (53%)	0.08	1 (1%) 76 56	106, 123, 135, 139	0
9	H	133/146 (91%)	0.17	2 (1%) 72 51	118, 140, 172, 175	0
10	I	119/122 (97%)	0.49	3 (2%) 58 41	131, 150, 166, 169	0
11	J	65/70 (92%)	-0.08	0 100 100	101, 113, 134, 138	0
12	K	114/120 (95%)	-0.24	0 100 100	98, 116, 132, 132	0
13	L	46/70 (65%)	0.60	3 (6%) 25 22	134, 176, 186, 188	0
All	All	3565/4225 (84%)	0.08	42 (1%) 76 56	76, 119, 170, 269	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	388	CYS	3.8
5	B	335	GLY	3.7
7	E	110	PHE	3.7
13	L	32	ALA	3.6
13	L	25	ALA	3.4

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](#)

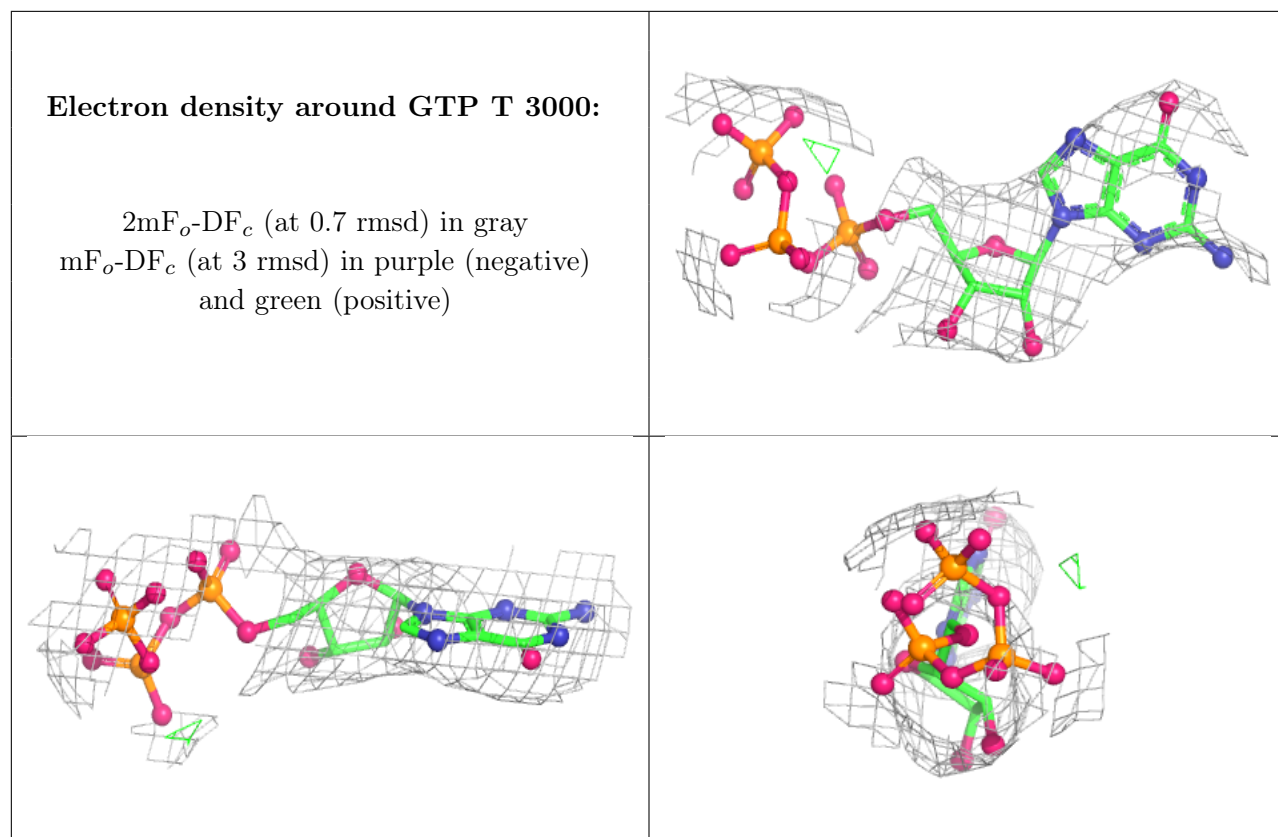
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
16	MG	A	2002	1/1	0.92	0.08	100,100,100,100	0
15	ZN	I	204	1/1	0.93	0.12	164,164,164,164	0
14	GTP	T	3000	32/32	0.95	0.09	105,109,114,114	0
15	ZN	L	105	1/1	0.95	0.05	175,175,175,175	0
15	ZN	B	1307	1/1	0.95	0.05	149,149,149,149	0
16	MG	A	2001	1/1	0.96	0.08	96,96,96,96	0
15	ZN	A	1734	1/1	0.96	0.06	178,178,178,178	0
15	ZN	A	1735	1/1	0.97	0.04	170,170,170,170	0
15	ZN	I	203	1/1	0.97	0.09	133,133,133,133	0
15	ZN	J	101	1/1	0.98	0.04	106,106,106,106	0
15	ZN	C	319	1/1	1.00	0.02	112,112,112,112	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.