



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:53 PM UTC

PDB ID : 1TWC / pdb_00001twc
Title : RNA polymerase II complexed with GTP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.00 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)
Xtriage (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

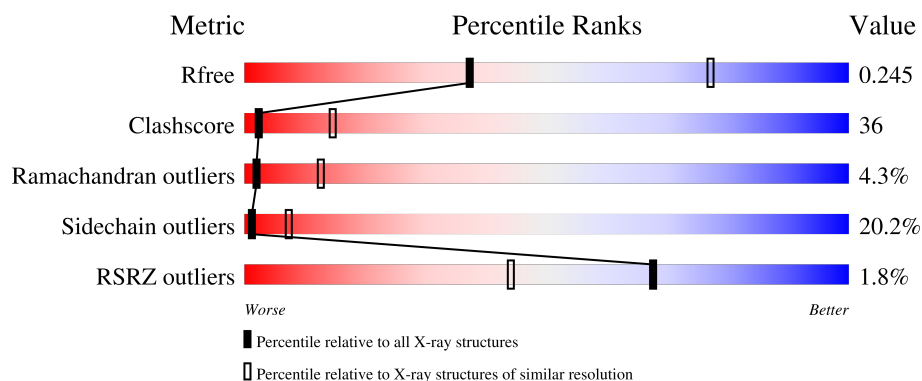
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	
4	E	215	
5	F	155	

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	

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
13	GTP	B	3008	X	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 27772 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 largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1351	Total	C	N	O	S	0	0	0
			10625	6704	1844	2019	58			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1091	Total	C	N	O	S	0	0	0
			8690	5511	1516	1610	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	83	Total	C	N	O	S	0	0	0
			670	428	114	125	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			990	610	181	188	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	64	Total	C	N	O	S	0	0	0
			525	334	92	93	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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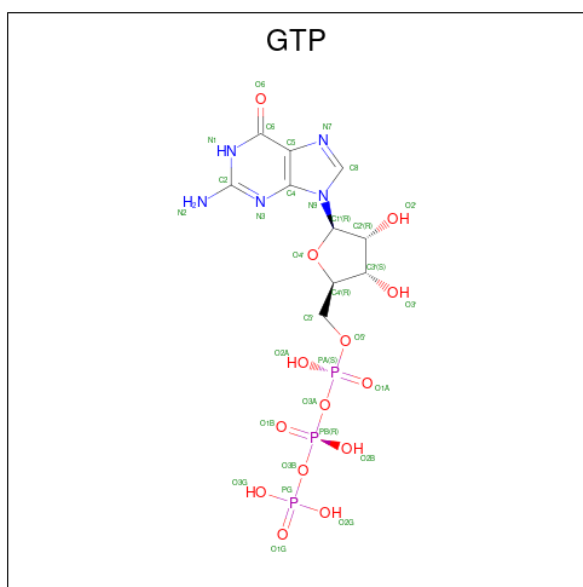
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	1	Total	Zn	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Mn	0	0
			2	2		

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

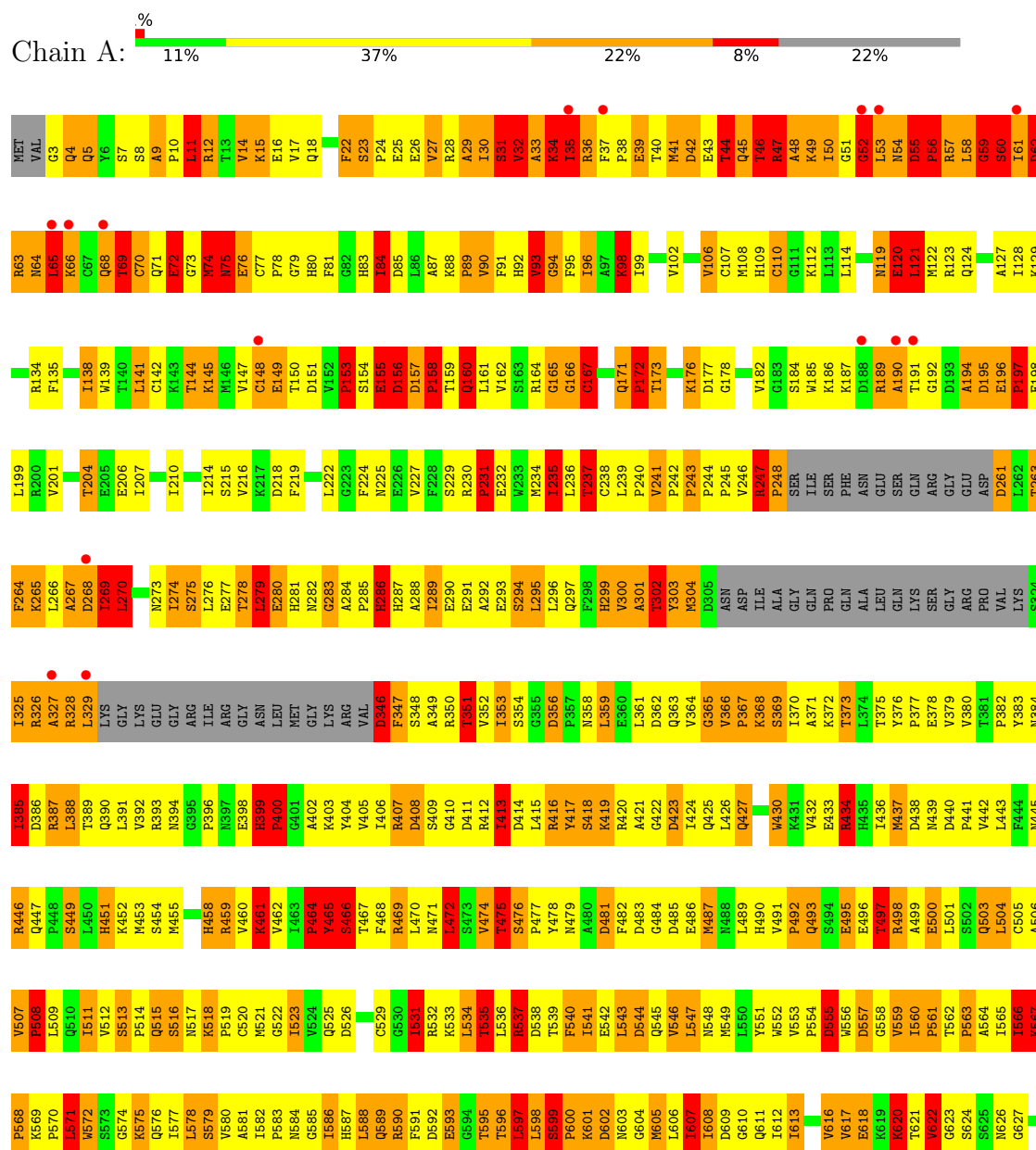
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	11	Total	O	0	0
			11	11		
14	B	11	Total	O	0	0
			11	11		
14	F	1	Total	O	0	0
			1	1		
14	L	1	Total	O	0	0
			1	1		

3 Residue-property plots

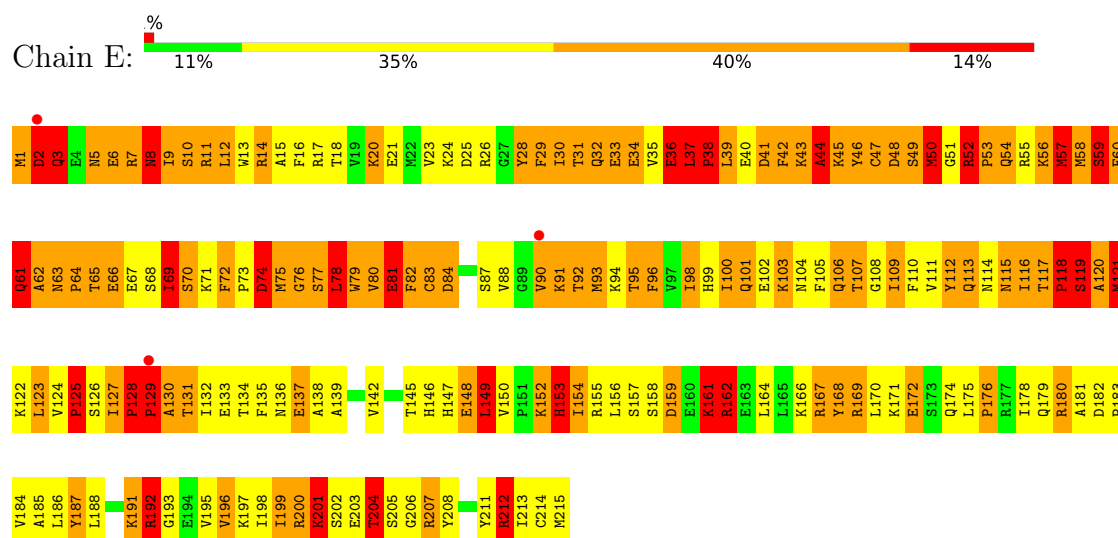
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

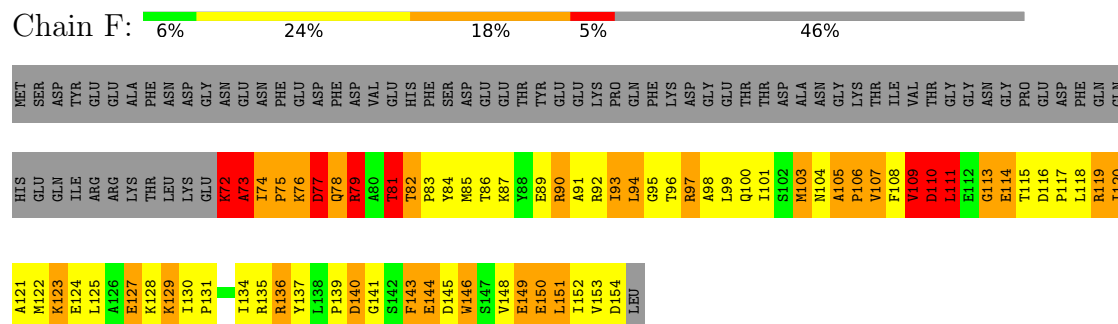


SER	L1418	S1358	T1295	K1235	SER	S1115	L993	Y933	M873	B812	S751	L691	I630
PRO	D1419	D1359	G1296	L1236	L1176	L1116	Q994	K994	D874	F813	K752	D692	H631
GLY	D1420	ASN	E1297	I1237	LEU	T1117	E995	Q995	A875	F814	G753	V693	T634
PHE	C1421	S1361	Y1298	I1238	ASP	Y1118	N996	L936	A876	F815	G754	T694	K635
SER	G1422	Y1362	I1299	G1239	GLU	Y1119	N997	V937	H877	R816	F755	K695	E636
PRO	R1423	Y1363	K1300	G1240	GLU	L1120	L998	K938	H878	A817	F756	K696	E637
THR	V1424	R1241	E1301	R1241	ALA	E1121	V999	D939	E879	M818	T757	A697	G638
SER	S1425	Y1365	P1302	V1242	GLU	F1122	L1000	R940	K880	G819	T758	Q698	G639
PRO	E1426	R1366	E1303	V1243	GLN	G1123	R1001	K941	Q881	G820	A759	A699	P639
THR	N1427	H1367	E1304	ARG	SER	H1124	K1002	F942	S882	R821	Q760	N700	Q640
THR	V1428	H1368	V1305	PRO	PHE	A1125	K1003	L943	L883	M761	Q761	L701	V641
SER	I1429	A1369	L1306	LYS	ASP	A1126	N1004	R944	L884	L824	S762	T702	C642
PRO		Q1187	E1307	SER	GLU	D1127	E1005	E945	T885	R825	A763	T703	A643
THR		Q1188	T1308	LEU	LEU	G1128	I1006	V946	I886	D826	C764	A704	K644
SER		Q1189	D1309	ASP	ASP	E1129	I1007	F947	G887	T827	V765	K705	L645
PRO		P1190	G1310	ALA	ALA	Q1130	Q1008	V948	G888	A828	G766	H706	V652
ALA		W1191	V1311	GLU	GLU	A1131	N1009	D949	S889	V829	Q767	G707	G647
VAL		M1375	N1312	THR	THR	K1132	A1010	Q950	D890	K830	Q768	M708	N648
SER		L1193	L1313	GLU	GLU	G1073	Q1011	E951	A891	T831	S769	T709	I649
PRO		R1194	I1314			E1074	R1012	A952	A892	A832	V770	L710	Q650
THR		L1195	A1315			P1075	D1013	N953	F893	E833	E771	K611	L657
GLY		E1196	S1136			A1076	A1014	N954	E894	T834	G772	E712	V652
SER		E1197	A1137			T1077	V1015	P955	K895	G835	K773	S713	V653
PRO		L1198	I1138			Q1078	T1016	L956	R896	V836	R774	F714	N654
ALA		D1199	E1139			M1079	L1017	P957	Y897	I837	I775	E715	F655
SER		A1200	H1140			T1080	F1018	V958	R898	Q838	A776	D716	M656
PRO		A1201	T1141			ASN	C1019	N959	V899	R840	F777	N717	L657
THR		M1202	T1142			THR	E1020	P960	D900	R840	G778	N718	L658
SER		N1203	L1143			PHE	L1021	R961	L901	L841	F779	V719	H659
PRO		E1264	K1144			ALA	L1022	Q962	L902	V842	V780	R720	N660
THR		K1205	S1145			HIS	R1023	I963	K843	D811	D781	F721	G661
GLY		L1206	P1146			PHE	S1024	I964	T844	R782	L722	F662	F662
ALA		D1207	T1147			ALA	R1025	Q965	D905	L783	R723	M723	S663
THR		M1208	I1148			GLY	L1026	N966	H906	E724	E724	R724	G665
PRO		E1269	A1149			VAL	A1027	A967	T907	D847	F785	A725	G665
SER		M1270	S1150			ALA	T1028	Q968	L908	I848	H786	R726	I666
ASP		Q1211	E1151			SER	R1029	Q969	D909	M849	F787	D727	G667
THR		V1212	I1152			K1092	R1030	T970	P910	V850	S788	K728	D668
GLY		G1213	Y1153			R1093	L1031	F971	S911	H851	K789	A729	T669
ALA		E1214	Y1154			V1094	L1032	H972	L912	Y852	D790	G730	I670
LEU		D1215	D1155			T1095	Q1033	I973	L913	D853	D791	R731	A671
MET		R1216	P1156			S1096	E1034	D974	E914	N854	Y792	L732	D672
ARG		D1217	D1157			G1097	Y1035	H975	S915	T855	S793	A733	G673
CYS		Q1217	P1158			V1098	L1036	T976	G916	T856	F794	E734	P674
SER		K1218	P1159			P1099	L1037	K977	S917	R857	E795	V735	T675
THR		T1219	R1160			R1000	T1038	P978	E918	N858	S796	N736	M676
GLU		F1220	T1161			L1101	K1039	S979	E919	S859	K797	L737	E678
GLN		N1221	V1162			K1102	D980	L860	L920	L860	K738	E678	E678
THR		D1223	I1163			E1103	L981	G921	G921	G861	V800	T739	I679
ASP		L1224	P1164			T1104	V1044	T982	D922	N862		L740	T680
GLY		F1225	E1165			L1105	I1045	N983	L923	V863	N802	M741	E681
PRO		K1285	D1166			M1106	L1046	K984	K924	I864	S803	N742	T682
VAL		Y1287	E1167			V1107	S1047	D985	L925	Q865	N743	M743	I683
THR		D1228	E1168			A1108	N1048	I986	Q926	P866	Y804	K744	A684
SER		S1229	I1169			K1109	V987	V987	V927	I867	L805	R745	E685
PRO		E1230	N1170			N1110	E1050	L988	L928	G807	R806	Q746	E686
THR		D1231	Q1171			M1111	A1051	Q989	L929	G869	L808	M746	A686
ASN		M1232	L1172			T1112	Q1052	V990	D930	E870	T809	V747	K687
GLU		N1233	H1173			T1113	F1053	K991	E931	D871	P810	M748	K688
SER		P1294	PHE			P1114	L1054	D992	E932	G872	Q811	A749	K689
TYR												G750	V690

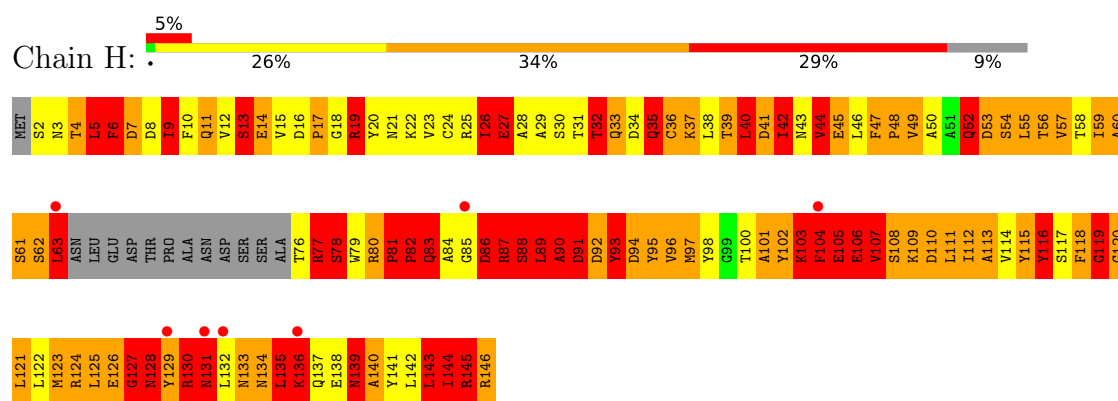




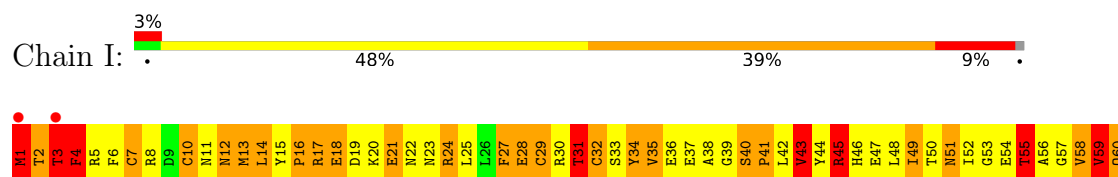
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

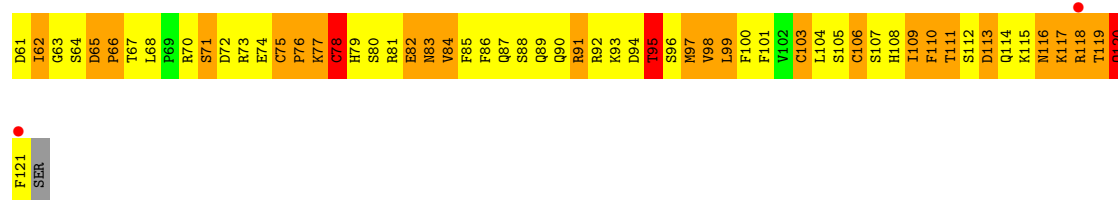


- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

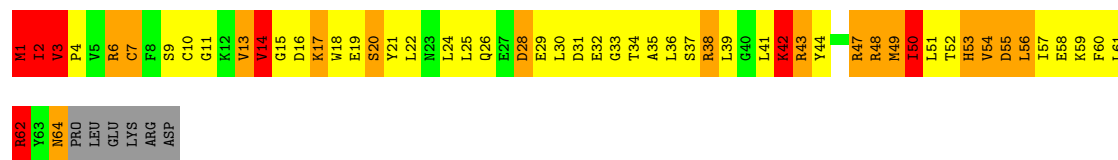
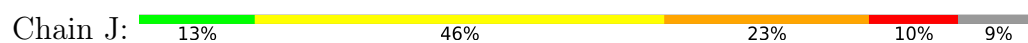


- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

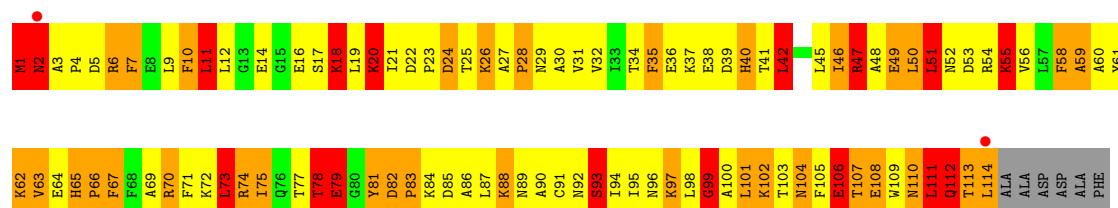




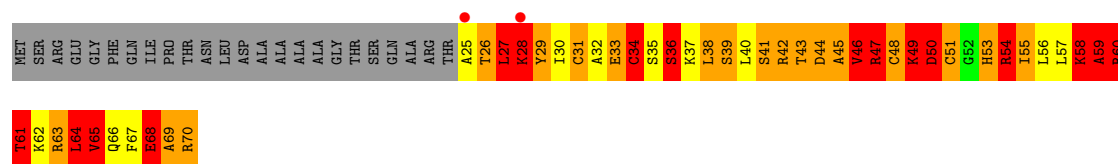
- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.23Å 223.61Å 374.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 89.0 (40.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.255 0.207 , 0.245	Depositor DCC
R_{free} test set	3424 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27772	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GTP, 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	A	3.75	1712/10811 (15.8%)	2.67	938/14626 (6.4%)
2	B	3.92	1505/8860 (17.0%)	2.64	734/11945 (6.1%)
3	C	4.03	377/2133 (17.7%)	2.81	194/2891 (6.7%)
4	E	3.92	285/1796 (15.9%)	2.63	161/2416 (6.7%)
5	F	3.72	111/682 (16.3%)	2.70	55/922 (6.0%)
6	H	3.95	177/1086 (16.3%)	2.66	106/1470 (7.2%)
7	I	4.06	207/1009 (20.5%)	2.80	114/1357 (8.4%)
8	J	3.48	70/533 (13.1%)	2.87	61/715 (8.5%)
9	K	3.75	154/937 (16.4%)	2.77	84/1265 (6.6%)
10	L	4.29	72/366 (19.7%)	2.97	45/485 (9.3%)
All	All	3.86	4670/28213 (16.6%)	2.69	2492/38092 (6.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	28
2	B	0	32
3	C	0	13
4	E	1	7
6	H	0	13
7	I	0	3
9	K	0	2
10	L	0	4
All	All	1	102

The worst 5 of 4670 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	50	MET	SD-CE	36.31	2.70	1.79
2	B	552	MET	SD-CE	30.20	2.55	1.79
2	B	885	MET	SD-CE	30.02	2.54	1.79
1	A	487	MET	SD-CE	-28.01	1.09	1.79
4	E	57	MET	SD-CE	27.29	2.47	1.79

The worst 5 of 2492 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1366	ARG	NE-CZ-NH2	-17.80	103.18	119.20
5	F	81	THR	N-CA-CB	-17.55	86.34	110.38
1	A	61	ILE	N-CA-C	-17.24	91.26	110.05
3	C	34	ARG	NE-CZ-NH2	-16.31	104.53	119.20
2	B	1097	HIS	CB-CG-ND1	-15.75	99.07	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

5 of 102 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	SER	Peptide
1	A	44	THR	Peptide
1	A	60	SER	Peptide
1	A	70	CYS	Peptide
1	A	74	MET	Peptide

5.2 Too-close contacts

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	10625	0	10693	840	0
2	B	8690	0	8713	532	0
3	C	2095	0	2051	145	0
4	E	1760	0	1788	133	0
5	F	670	0	690	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1068	0	1040	163	0
7	I	990	0	949	71	0
8	J	525	0	535	42	0
9	K	919	0	929	67	0
10	L	364	0	386	53	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
13	B	32	0	11	9	0
14	A	11	0	0	3	0
14	B	11	0	0	4	0
14	F	1	0	0	0	0
14	L	1	0	0	1	0
All	All	27772	0	27785	1968	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 36.

The worst 5 of 1968 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:CA	1:A:61:ILE:CB	1.75	1.64
1:A:941:LYS:CD	1:A:941:LYS:CG	1.74	1.64
10:L:61:THR:CB	10:L:61:THR:CG2	1.75	1.64
5:F:72:LYS:CD	5:F:72:LYS:CE	1.76	1.64
1:A:1405:THR:CB	1:A:1405:THR:CA	1.77	1.62

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	1334/1733 (77%)	1196 (90%)	84 (6%)	54 (4%)	2	14
2	B	1071/1224 (88%)	931 (87%)	104 (10%)	36 (3%)	3	17
3	C	264/318 (83%)	225 (85%)	30 (11%)	9 (3%)	3	17
4	E	213/215 (99%)	181 (85%)	20 (9%)	12 (6%)	1	8
5	F	81/155 (52%)	72 (89%)	8 (10%)	1 (1%)	10	40
6	H	129/146 (88%)	89 (69%)	17 (13%)	23 (18%)	0	0
7	I	119/122 (98%)	108 (91%)	10 (8%)	1 (1%)	16	50
8	J	62/70 (89%)	60 (97%)	2 (3%)	0	100	100
9	K	112/120 (93%)	99 (88%)	10 (9%)	3 (3%)	4	22
10	L	44/70 (63%)	25 (57%)	11 (25%)	8 (18%)	0	0
All	All	3429/4173 (82%)	2986 (87%)	296 (9%)	147 (4%)	2	12

5 of 147 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY
1	A	62	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1183/1520 (78%)	966 (82%)	217 (18%)	2	9
2	B	947/1061 (89%)	768 (81%)	179 (19%)	1	9
3	C	234/274 (85%)	190 (81%)	44 (19%)	1	9
4	E	197/197 (100%)	150 (76%)	47 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	73/137 (53%)	62 (85%)	11 (15%)	3	14
6	H	117/128 (91%)	71 (61%)	46 (39%)	0	1
7	I	115/116 (99%)	95 (83%)	20 (17%)	2	10
8	J	59/65 (91%)	46 (78%)	13 (22%)	1	5
9	K	99/102 (97%)	77 (78%)	22 (22%)	1	5
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3064/3657 (84%)	2446 (80%)	618 (20%)	1	7

5 of 618 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	92	THR
8	J	48	ARG
4	E	158	SER
4	E	91	LYS
6	H	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	984	HIS
3	C	184	ASN
2	B	1025	HIS
2	B	1179	GLN
4	E	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
13	GTP	B	3008	12	33,34,34	3.13	9 (27%)	50,54,54	3.27	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GTP	B	3008	12	1/1/7/7	8/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3008	GTP	C1'-N9	11.99	1.81	1.47
13	B	3008	GTP	C4-N9	9.38	1.62	1.38
13	B	3008	GTP	C8-N9	5.36	1.49	1.37
13	B	3008	GTP	C5-N7	-3.52	1.32	1.39
13	B	3008	GTP	C4-N3	3.35	1.41	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	3008	GTP	O4'-C1'-N9	13.53	139.03	108.36
13	B	3008	GTP	C1'-N9-C4	10.95	158.82	126.49
13	B	3008	GTP	C8-N9-C4	-8.03	90.97	106.03
13	B	3008	GTP	C1'-N9-C8	-7.93	104.20	126.73
13	B	3008	GTP	N9-C8-N7	5.49	123.58	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	3008	GTP	C1'

5 of 8 torsion outliers are listed below:

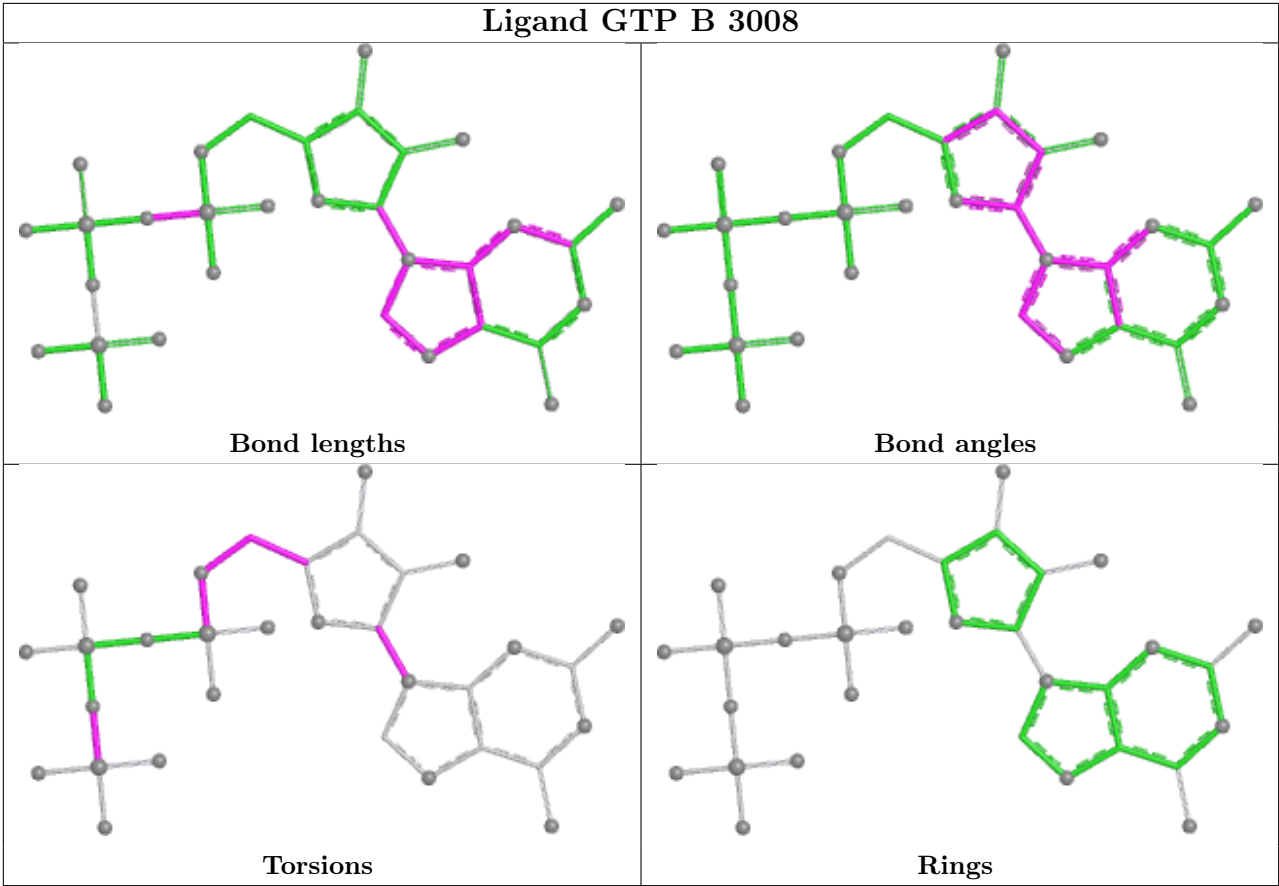
Mol	Chain	Res	Type	Atoms
13	B	3008	GTP	C5'-O5'-PA-O3A
13	B	3008	GTP	O4'-C4'-C5'-O5'
13	B	3008	GTP	C3'-C4'-C5'-O5'
13	B	3008	GTP	PB-O3B-PG-O2G
13	B	3008	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3008	GTP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	366:VAL	C	367:PRO	N	1.20

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1351/1733 (77%)	-0.30	21 (1%) 70 47	20, 46, 110, 159	0
2	B	1091/1224 (89%)	-0.26	22 (2%) 65 41	21, 44, 116, 146	0
3	C	266/318 (83%)	-0.31	0 100 100	29, 50, 79, 131	0
4	E	215/215 (100%)	-0.12	3 (1%) 73 51	23, 60, 108, 138	0
5	F	83/155 (53%)	-0.50	0 100 100	24, 45, 71, 80	0
6	H	133/146 (91%)	0.55	7 (5%) 32 16	56, 88, 128, 135	0
7	I	121/122 (99%)	-0.29	4 (3%) 49 28	30, 50, 81, 111	0
8	J	64/70 (91%)	-0.57	0 100 100	31, 42, 71, 81	0
9	K	114/120 (95%)	-0.28	2 (1%) 67 44	31, 58, 79, 86	0
10	L	46/70 (65%)	0.66	2 (4%) 40 21	49, 95, 122, 125	0
All	All	3484/4173 (83%)	-0.24	61 (1%) 67 44	20, 49, 113, 159	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	4.1
2	B	1110	PRO	4.1
1	A	37	PHE	4.1
2	B	883	LEU	3.9
6	H	132	LEU	3.8

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

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

6.3 Carbohydrates [i](#)

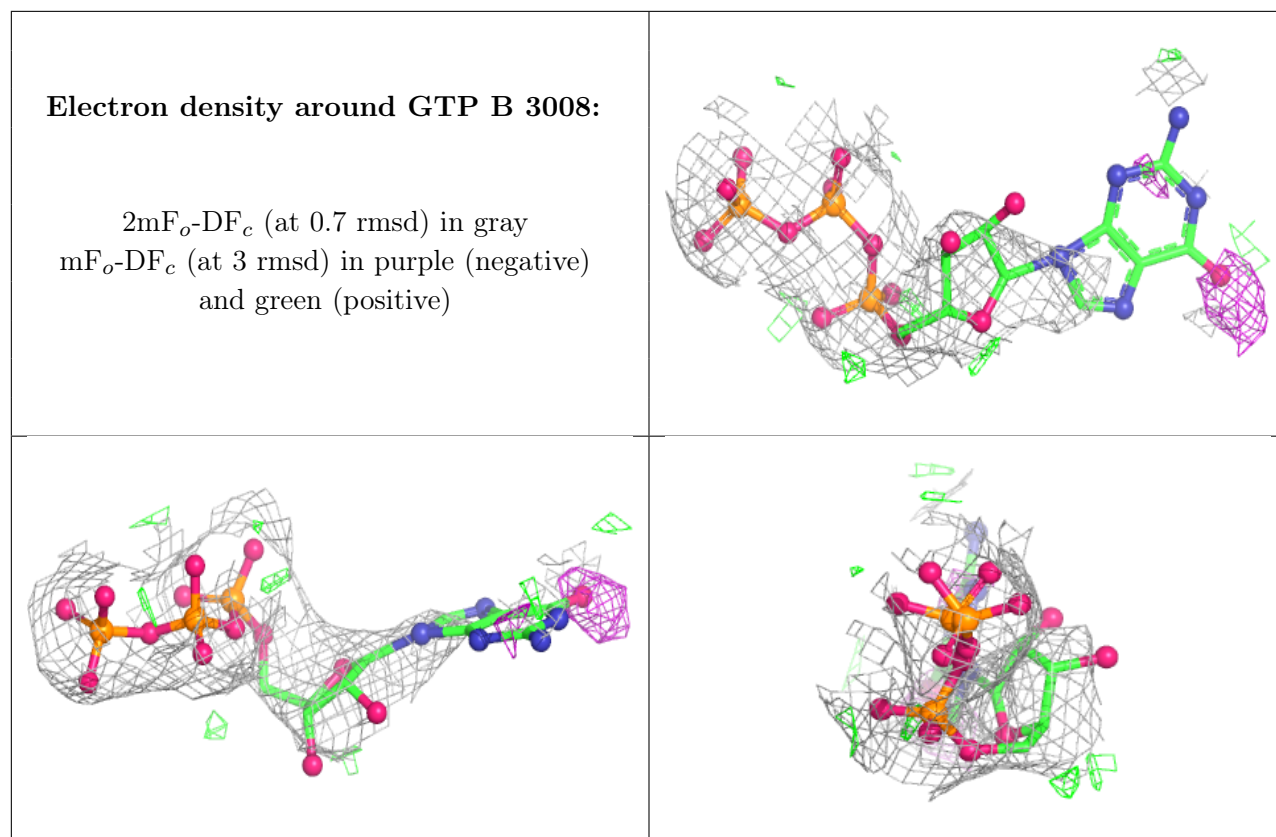
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
13	GTP	B	3008	32/32	0.88	0.14	96,112,119,119	0
12	MN	A	3010	1/1	0.91	0.06	48,48,48,48	0
11	ZN	A	3006	1/1	0.96	0.06	67,67,67,67	0
11	ZN	L	3005	1/1	0.96	0.04	96,96,96,96	0
12	MN	A	3009	1/1	0.98	0.04	36,36,36,36	0
11	ZN	A	3008	1/1	0.99	0.06	91,91,91,91	0
11	ZN	B	3007	1/1	0.99	0.02	64,64,64,64	0
11	ZN	C	3002	1/1	0.99	0.03	53,53,53,53	0
11	ZN	I	3004	1/1	0.99	0.03	80,80,80,80	0
11	ZN	I	3003	1/1	1.00	0.02	59,59,59,59	0
11	ZN	J	3001	1/1	1.00	0.01	47,47,47,47	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.