



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:51 PM UTC

PDB ID : 3GTK / pdb_00003gtk
Title : Backtracked RNA polymerase II complex with 18mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.80 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

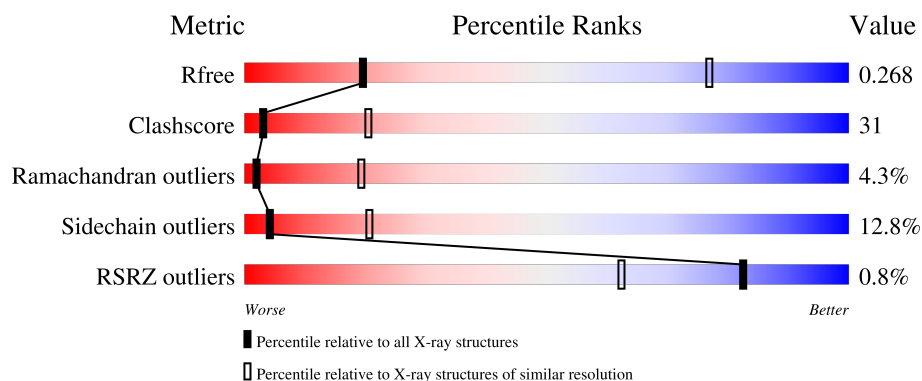
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	18	
12	T	29	
13	N	14	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ZN	A	1734	-	-	X	-
14	ZN	C	319	-	-	X	-
14	ZN	J	101	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1442	Total	C	N	O	S	0	0	0
			11332	7133	1982	2156	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1153	Total	C	N	O	S	0	0	0
			9168	5795	1604	1713	56			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2135	1344	355	423	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1757	1114	310	322	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	136	Total	C	N	O	S	0	0	0
			1087	684	183	215	5			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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 subunit RPABC4.

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

- Molecule 11 is DNA/RNA hybrid called DNA/RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*C)-D(P*AP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	14	Total	C	N	O	P	0	0	0
			284	126	55	90	13			

- Molecule 12 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	29	Total	C	N	O	P	0	0	0
			587	281	109	169	28			

- Molecule 13 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

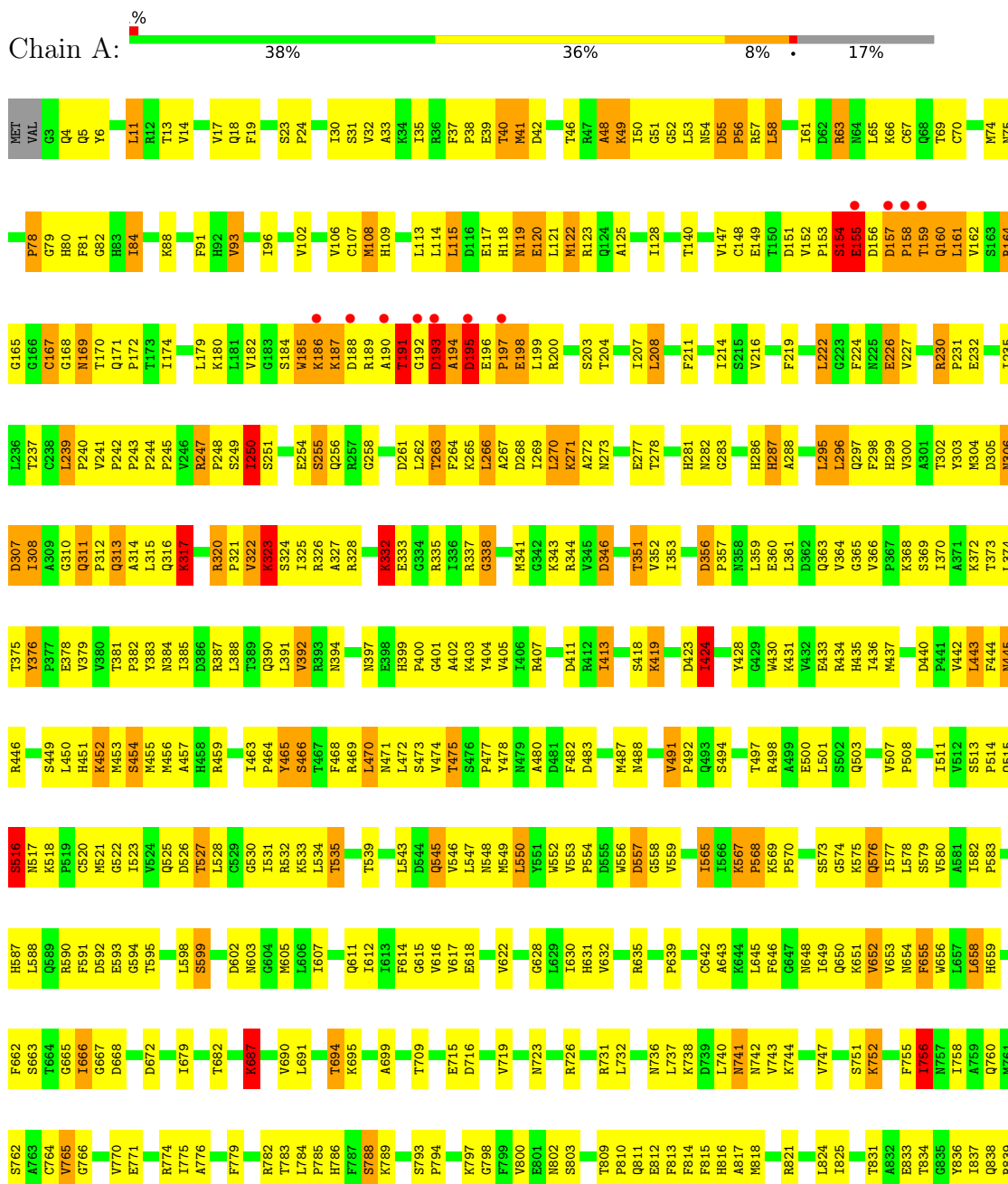
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

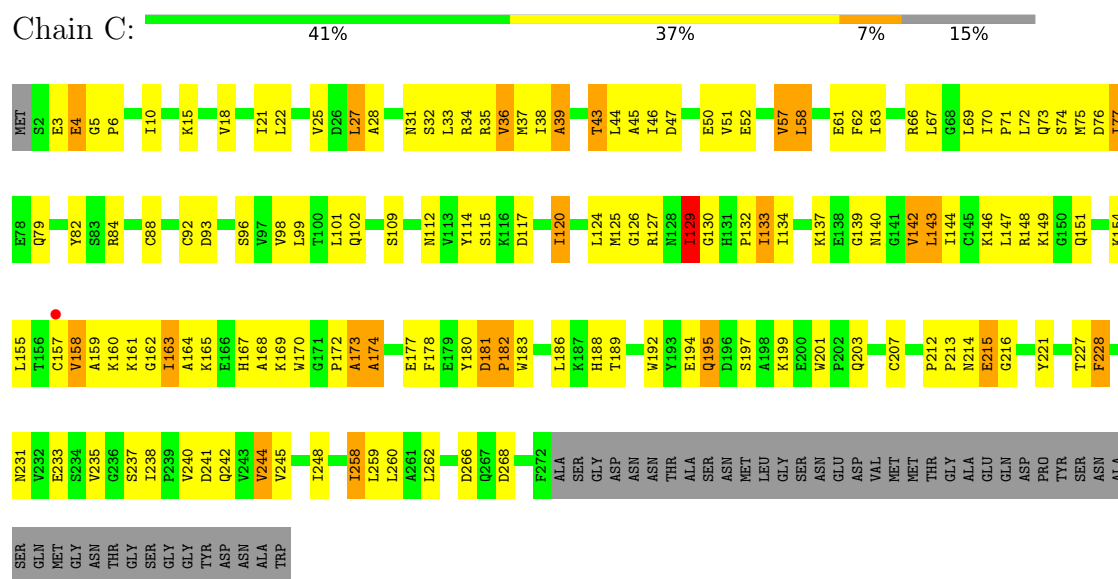
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 subunit RPB1

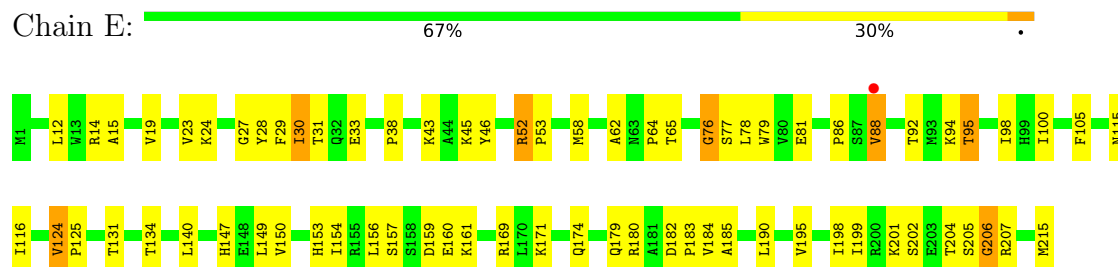


R1215	L1216	Y1217	S145	F146	L147	K148	E149	R150	L151	M152	E153	D156	R159	V160	H161	I162	C163	G164	I165	C166	G167	L168	I172	H173	K174	L175	M176	Q179	F180	E181	M187	K188	L189	D190	Q193	I194	H195	I196	P197	L198	A199	A200	K201	L202	L203	F204	Q205	M208	A209	M210	N211	I212	H213	P214	L215	S218	N221	L222	V223	Q224	V225	S232	S235	H236	E239	L240	R241	S242	L244	K246	Q255	V256	G260	R261	R267	T268	L273	Y275	P274	D276	K277	G280	I281	I282	V283	L284	K285	E286	C287	M289	G290	I291	I292	P293	D294	E296	L298	I301	C302	L305	S208	E209	K210	V211	L212	L213	A214
GLU	LEU	TYR	GLU	GLU	LEU	ILE	ALA	GLU	GLU	SER	GLU	ASP	ASP	SER	GLU	SER	GLY	K154	V165	F166	I167	G168	R169	L170	F171	M173	S176	K177	N178	L181	S182	D188	L189	Y190	K191	L192	K193	E194	C195	M199	G200	I201	Y202	F203	I204	I205	S208	E209	K210	V211	L212	L213	A214																																																						
Q215	S218	N221	L222	V223	Q224	V225	S232	S235	H236	E239	L240	R241	S242	L244	K246	Q255	V256	G260	R261	R267	T268	L273	Y275	P274	D276	K277	G280	I281	I282	V283	L284	K285	E286	C287	M289	G290	I291	I292	P293	D294	E296	L298	I301	C302	L305	S208	E209	K210	V211	L212	L213	A214																																																							
L387	C388	D396	K404	R405	L406	G410	P411	L412	L413	A414	Q415	F417	T419	L420	L428	Y431	M432	Q433	R434	T435	V436	E437	K353	E438	D354	I355	K358	E359	F360	L361	P362	H363	I364	T365	Q366	F370	E371	K374	F377	A462	T463	G464	M465	W466	E468	L386																																																													
Q469	K470	K471	A472	K473	S474	S475	R476	A477	G478	V479	S480	O481	V482	L483	N484	R485	Y486	T487	Y488	S489	S490	T491	L492	L495	R496	R497	T498	L502	GLY	ARG	ASP	GLY	LYS	LEU	A509	R512	Q513	L514	H515	N516	T517	H518	W519	C523	T527	Q530	Q531	L535	V536	K537	L541																																																								
H542	I545	S546	G548	T549	D550	P551	H552	G553	L554	L555	L558	S559	E560	V561	E567	V570	P575	R579	V582	R591	N592	P593	L596	N597	E598	T599	L600	L603	R604	L609	E612	V613	S614	N615	L616	R620	E623	L626	T628	O631	R632	L633	Y634	P636	L637	G638	D642	D643	E644	P645	G647	H648	L651	K652	V653	R654	K655	I658	L661	M662	A663	T664	V676	E677	E678	Y679	T680	S683	L689	V690	E691	Y692	I693	D694	A695	E696	E697	E698	I701	L702	I703	A704	M705	T706	P707	L710	E711	P712	A713	E714																	
A715	N716	E717	E718	N719	D720	L721	D722	V723	R728	L729	R730	T731	H732	S733	H740	T743	H744	P745	S746	M747	L748	L749	T756	P757	F758	P759	D760	H761	N762	R766	N767	T768	Y769	Q770	S771	K775	Q776	A777	M778	G779	V780	F781	L782	T783	Y784	Y785	R788	M789	D790	T791																																																									
M792	A793	N794	I795	L796	Y797	Y798	K801	P802	L803	G804	R805	T806	R807	N808	M809	L812	R815	E816	L817	P818	Q821	N822	V825	A826	I827	C828	Y830	S831	G832	Y833	N834	Q835	E836	D837	S838	M839	I840	M841	N842	Q843	S844	S845	I846	F851	Y856	Y859	H860	Q861	Q862	E863																																																									
K864	K865	S869	I870	T871	E872	T873	F874	E875	K876	Q877	Q878	R879	T880	N881	T882	M885	K886	Y890	D891	L898	I899	P901	V905	S906	V910	I911	I912	G913	K914	T915	T916	P917	I918	S919	PRO	ASP	GLU	GLU	GLU	LEU	GLY	GLN	ARG	THR	ALA	TYR	HIS	K934	S938																																																										
L941	R942	T943	E945	N946	D950	Q951	V952	T955	T956	N957	Q959	L961	K962	F963	V964	K965	V966	R967	V968	R969	T970	T971	K972	P973	P974	Q975	R976	G977	D978	K979	F980	A981	S982	R983	H984	Q985	Q986	K987	G988	T989	I990	G991	I992	T993	Y994	R995	Y996	E997	D998	N999	P1000	F1001	T1002	A1003	E1004																																																				
G1005	I1006	V1007	P1008	D1009	L1010	I1011	I1012	M1013	I1017	P1018	Q1019	R1020	M1021	T1022	V1023	A1024	H1025	L1026	I1027	E1028	C1029	L1030	L1031	S1032	K1033	E1041	G1042	D1043	A1044	S1045	P1046	F1047	T1048	D1049	I1050	T1051	V1052	E1053	G1054	I1055	S1056	Y1064	Q1065	S1066	F1069	E1070	V1071	M1072	Y1073	M1074	T1077	G1078	K1079	K1080																																																					
L1081	M1082	A1083	Q1084	I1085	L1086	F1087	G1088	P1089	T1090	Y1091	Q1092	Q1093	R1094	L1095	R1096	H1097	M1098	V1099	D1100	D1101	K1102	C1103	H1104	A1105	R1106	A1107	L1108	G1109	P1110	M1111	Q1112	L1113	T1115	R1116	Q1117	P1118	V1119	E1120	G1121	L1122	R1123	P1124	D1125	G1126	G1127	L1128	R1129	F1130	G1131	E1132	M1133	E1134	R1135	I1138	A1140	H1141	G1142																																																		
S145	F146	L147	K148	E149	R150	L151	M152	E153	D156	R159	V160	H161	I162	C163	G164	I165	C166	G167	L168	I172	H173	K174	L175	M176	Q179	F180	E181	M187	K188	L189	D190	Q193	I194	H195	I196	P197	L198	A199	A200	K201	L202	L203	F204	Q205	M208	A209	M210	N211	I212	H213	P214																																																								

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

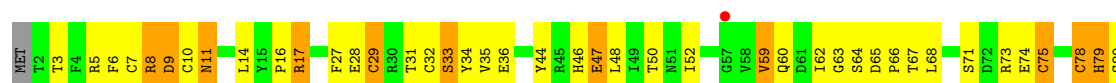
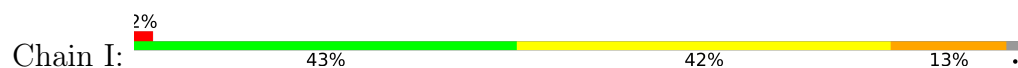


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

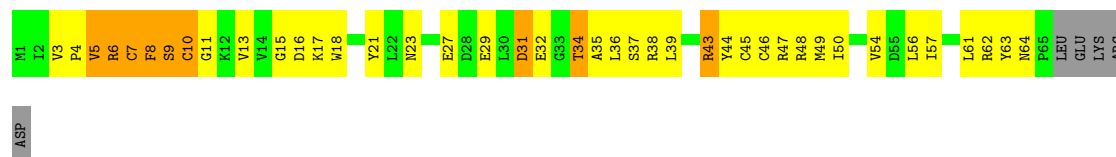




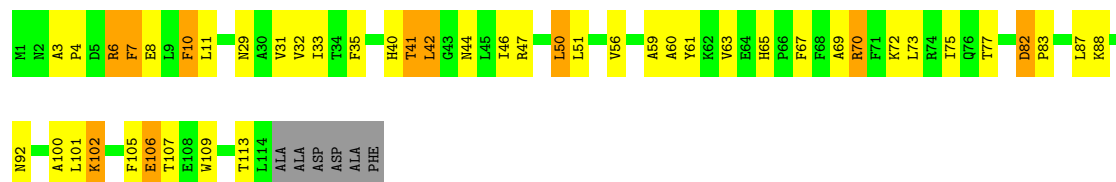
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



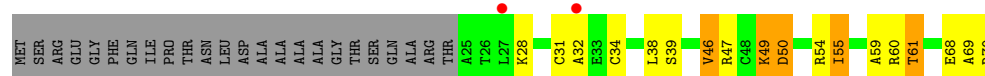
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



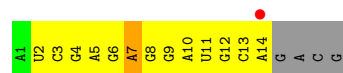
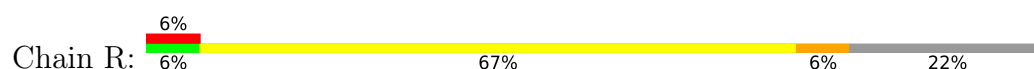
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



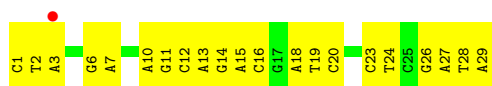
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: DNA/RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*C)-D(P*AP*GP*AP*CP*G)-3')



● Molecule 12: DNA (29-MER)



● Molecule 13: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.45Å 222.29Å 195.09Å 90.00° 101.72° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.80) 97.5 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.278 0.240 , 0.268	Depositor DCC
R_{free} test set	3444 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	116.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 104.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30111	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/11536	1.03	47/15605 (0.3%)
2	B	0.77	1/9348 (0.0%)	1.04	36/12611 (0.3%)
3	C	0.77	0/2174	1.03	8/2946 (0.3%)
4	E	0.63	0/1793	0.92	4/2413 (0.2%)
5	F	0.67	0/696	1.01	5/940 (0.5%)
6	H	0.67	0/1105	0.90	5/1495 (0.3%)
7	I	0.69	0/989	0.95	1/1331 (0.1%)
8	J	0.74	0/541	1.00	0/727
9	K	0.70	0/937	0.98	2/1265 (0.2%)
10	L	0.81	0/365	1.10	1/485 (0.2%)
11	R	0.86	1/318 (0.3%)	1.41	4/496 (0.8%)
12	T	0.47	0/658	1.13	0/1012
13	N	0.63	0/317	1.24	1/488 (0.2%)
All	All	0.72	2/30777 (0.0%)	1.03	114/41814 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	830	TYR	N-CA	5.91	1.53	1.46
11	R	11	U	C1'-N1	5.37	1.56	1.48

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	THR	N-CA-C	10.18	125.85	113.12
3	C	39	ALA	N-CA-C	9.83	122.01	110.41
2	B	344	LYS	N-CA-C	9.50	123.30	112.57
2	B	1156	ASP	N-CA-C	9.44	124.93	113.41
1	A	885	THR	N-CA-C	-9.01	103.39	114.75

There are no chirality outliers.

There are no planarity outliers.

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	11332	0	11391	860	0
2	B	9168	0	9179	649	0
3	C	2135	0	2091	150	0
4	E	1757	0	1781	49	0
5	F	684	0	703	31	0
6	H	1087	0	1062	61	0
7	I	971	0	930	65	0
8	J	532	0	544	50	0
9	K	919	0	929	56	0
10	L	363	0	389	13	0
11	R	284	0	142	18	0
12	T	587	0	327	24	0
13	N	284	0	161	3	0
14	A	2	0	0	2	0
14	B	1	0	0	0	0
14	C	1	0	0	2	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	L	1	0	0	0	0
All	All	30111	0	29629	1866	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 31.

The worst 5 of 1866 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:GLU:HB3	2:B:440:HIS:CD2	1.53	1.43
1:A:1168:GLU:CA	1:A:1171:GLN:HB2	1.51	1.41
1:A:1172:LEU:O	1:A:1174:PHE:N	1.56	1.34
2:B:439:ALA:CB	2:B:440:HIS:HA	1.56	1.29
1:A:1169:ILE:CB	1:A:1170:ILE:HB	1.60	1.29

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	1438/1733 (83%)	1083 (75%)	289 (20%)	66 (5%)	2	18
2	B	1145/1224 (94%)	877 (77%)	219 (19%)	49 (4%)	2	19
3	C	269/318 (85%)	205 (76%)	57 (21%)	7 (3%)	4	27
4	E	213/215 (99%)	180 (84%)	28 (13%)	5 (2%)	5	30
5	F	83/155 (54%)	66 (80%)	13 (16%)	4 (5%)	2	17
6	H	132/146 (90%)	100 (76%)	26 (20%)	6 (4%)	2	18
7	I	117/122 (96%)	82 (70%)	26 (22%)	9 (8%)	1	11
8	J	63/70 (90%)	53 (84%)	6 (10%)	4 (6%)	1	14
9	K	112/120 (93%)	97 (87%)	13 (12%)	2 (2%)	6	33
10	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	2	18
All	All	3616/4173 (87%)	2772 (77%)	690 (19%)	154 (4%)	2	19

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	117	GLU
1	A	120	GLU
1	A	169	ASN
1	A	186	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1258/1520 (83%)	1079 (86%)	179 (14%)	3	17
2	B	1000/1061 (94%)	861 (86%)	139 (14%)	3	18
3	C	238/274 (87%)	208 (87%)	30 (13%)	4	21
4	E	196/197 (100%)	182 (93%)	14 (7%)	13	39
5	F	74/137 (54%)	71 (96%)	3 (4%)	27	51
6	H	119/128 (93%)	110 (92%)	9 (8%)	12	37
7	I	113/116 (97%)	101 (89%)	12 (11%)	6	26
8	J	60/65 (92%)	52 (87%)	8 (13%)	4	19
9	K	99/102 (97%)	88 (89%)	11 (11%)	6	24
10	L	40/57 (70%)	36 (90%)	4 (10%)	7	28
All	All	3197/3657 (87%)	2788 (87%)	409 (13%)	4	21

5 of 409 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	444	MET
2	B	995	ARG
9	K	50	LEU
2	B	470	LYS
2	B	694	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	518	HIS
2	B	878	GLN
7	I	60	GLN
2	B	538	ASN
2	B	762	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1442/1733 (83%)	-0.21	11 (0%) 82 62	77, 132, 243, 401	0
2	B	1153/1224 (94%)	-0.16	9 (0%) 82 62	77, 116, 250, 399	0
3	C	271/318 (85%)	-0.37	1 (0%) 88 74	86, 111, 177, 330	0
4	E	215/215 (100%)	-0.20	1 (0%) 87 71	107, 153, 272, 354	0
5	F	85/155 (54%)	-0.40	0 100 100	107, 129, 169, 217	0
6	H	136/146 (93%)	0.02	2 (1%) 72 50	120, 167, 307, 372	0
7	I	119/122 (97%)	-0.04	2 (1%) 69 47	106, 148, 191, 275	0
8	J	65/70 (92%)	-0.39	0 100 100	83, 101, 151, 176	0
9	K	114/120 (95%)	-0.42	0 100 100	83, 115, 150, 171	0
10	L	46/70 (65%)	0.18	2 (4%) 40 28	102, 161, 254, 269	0
11	R	14/18 (77%)	-0.01	1 (7%) 22 19	106, 130, 215, 216	0
12	T	29/29 (100%)	0.43	1 (3%) 48 33	105, 216, 417, 435	0
13	N	14/14 (100%)	0.53	0 100 100	263, 310, 353, 397	0
All	All	3703/4234 (87%)	-0.19	30 (0%) 82 62	77, 128, 255, 435	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	3.6
1	A	157	ASP	3.4
7	I	57	GLY	3.3
2	B	441	ASP	3.2
11	R	14	DA	3.2

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($\text{\AA}^2$)	Q<0.9
14	ZN	I	204	1/1	0.95	0.08	310,310,310,310	0
14	ZN	A	1734	1/1	0.98	0.03	228,228,228,228	0
14	ZN	A	1735	1/1	0.99	0.07	149,149,149,149	0
14	ZN	J	101	1/1	0.99	0.03	193,193,193,193	0
14	ZN	L	105	1/1	0.99	0.03	131,131,131,131	0
14	ZN	B	1307	1/1	1.00	0.02	157,157,157,157	0
14	ZN	C	319	1/1	1.00	0.02	136,136,136,136	0
14	ZN	I	203	1/1	1.00	0.02	132,132,132,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.