



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:25 PM UTC

PDB ID : 3GTG / pdb_00003gtg
Title : Backtracked RNA polymerase II complex with 12mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.78 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

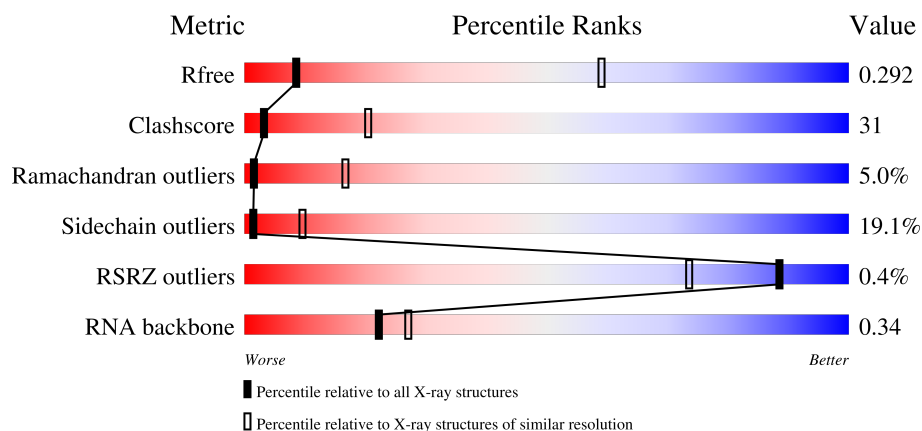
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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.



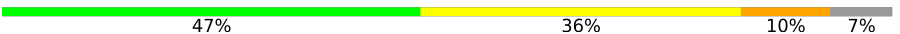
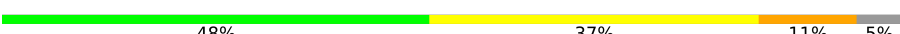
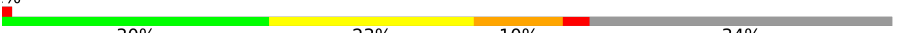
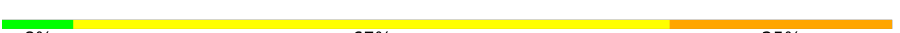
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)
RNA backbone	3983	1002 (4.46-3.10)

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	A	1733	 35% 36% 10% 17%
2	B	1224	 38% 41% 13% 6%
3	C	318	 35% 35% 14% 15%
4	E	215	 61% 33% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	12	
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	B	1307	-	-	X	-
14	ZN	J	101	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 30067 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
			9167	5794	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 a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	12	Total	C	N	O	P	0	0	0
			260	117	52	80	11			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- 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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

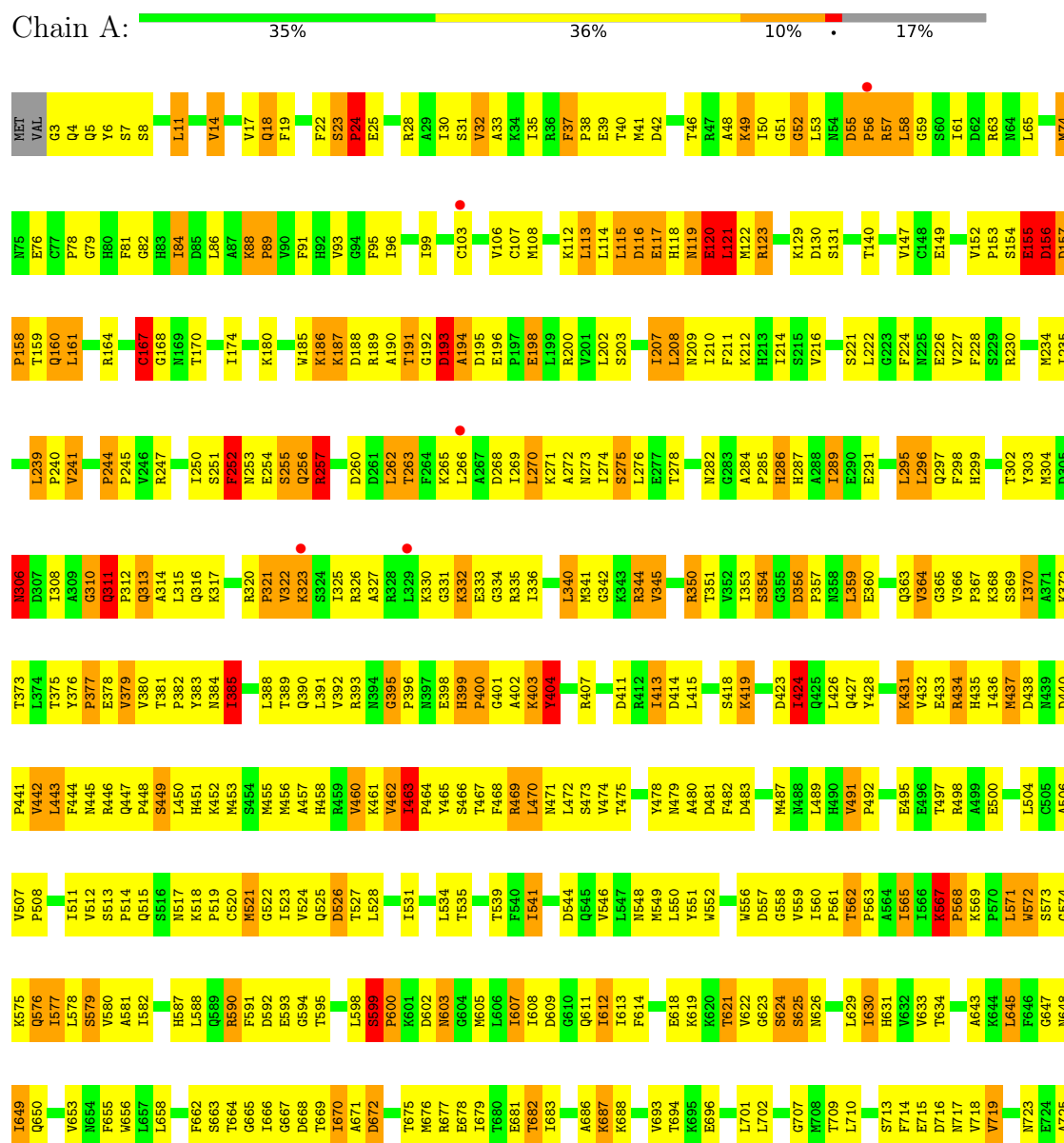
- Molecule 16 is water.

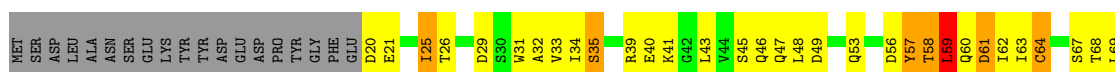
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	1	Total 1	O 1	0	0

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

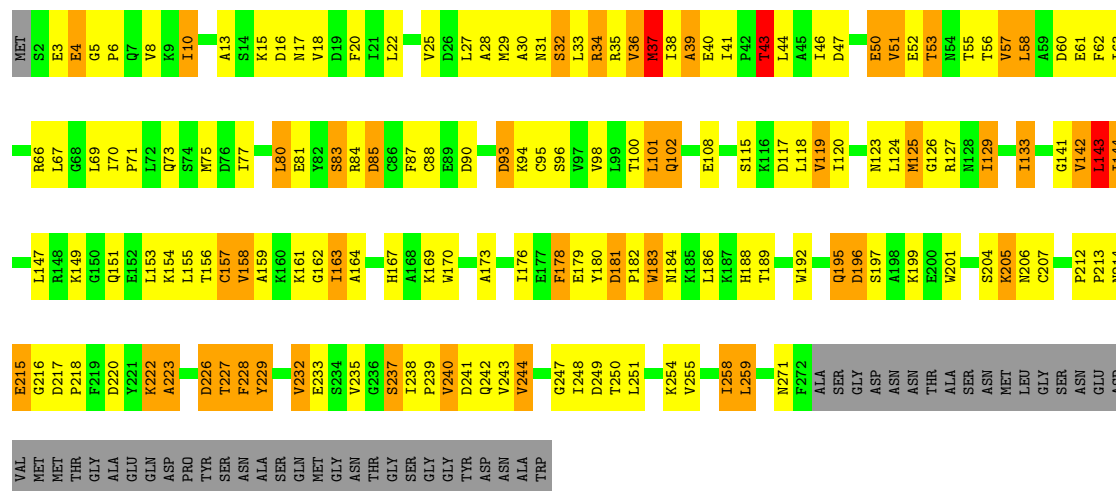
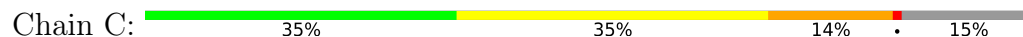




M1098	V1023	L961	K984	A819	A753	V676	L596	V522	Y459	L386	D304	G234	L195	L70
V1099	A1024	K962	D895	G820	S754	V676	M697	C523	A460	L387	V305	V225	Tyr	L71
K1102	H1025	F963		Q821	I755			P524	A462	C389	N306	F226	Leu	E72
H1103	L1026	V964	L898	N822	I756	T680	L600	A525	A462	L461	D307		Leu	Q73
H1104	I1027	K965	L899	A823	F757	S682	T602	E526	G464	D391	V308	A230	Ala	L74
A1105	E1028	V966	A900	R824	P758	S683	L603	T527	G464	D394	Q309	P231	Ala	A75
R1106	C1029	R967	P901	V825	P759	S684	R604	P528	M465	D394	K310	S232	Glu	Q76
L1030	L1030		V905	A826	D760	L884		E529	W466	Q395	L311		Glu	H77
A1107	L1031	T970	S906	R827	H761		I609	E529	W466	D396	E312	V237	Ser	T78
R1108	S1032	I973	S906	A828	Q762	L689		Q531	E468	D397	M313	A238	Glu	T79
K1109	K1033	Q907	Q907	C829	Q763	P690		A532	Q469	E239	L314	E239	Asp	E80
P1110	V1034			Y830	S764	E691	E612	C533	K470	F401	K315	S242	Asp	S85
M1111			V910	S831	S765	Y692	V613		K471	G402	S317	A243	Glu	R86
Q1112	L1037		I911	C832	R766	I693	S614	K537	A472			A243	Ser	S85
V1113	G977		I912	Y833	T767	D694	M615	M538	M473	G403		L244	Glu	R86
S1045	D978	D978	G913	N834	T768	A695	I616	L539	S474	K404	V323	E245	Gly	E89
P1046	K979	K979	K914	Q835	Y769		R617	S540	S475			K246	I90	I90
F1047	F980	F980	T915	Q836			L541	M542	R476		R327	G247	S91	S91
T1048	A981	A981	T916	D837	M773	E698	D618		R477	L408		S248		
D1049	S982	S982	P917	S838	G774	I701	R620	C543	C478	L412	F333	R249	I95	I95
I1050	R983	R983	I918	M839	K775	L702	E621	S544	Y479	L413	I334	F250	Y96	Y96
T1051	H984	H984	S919	I840	Q776	I703	K622	C544	S480	A414	G335	I251		
	G985	G985	PR0	M841	A777	A704	E623	S546	Q481	Q415	R336	S252	K99	K99
G1054	K986	K986	ASP	N842	M778	M705	L624	V547	V482	L416	R337	T253	M173	P100
I1055	Q987	Q987	GLJ	Q843	Q779	Q706	K625	G548	L483	F417		Q255	M101	M101
S1056	G988	G988	GLJ	S844	W780		I626	T549	M484	K418	K344	Q255	V102	V102
K1057	T989	T989	GLJ	S845	F781	D709	F627	P551	Y486	L420	K345	V256		
	I990	I990	GLJ	G849	E711	L710	T628	P551	Y486	L420	K346	V256	V108	V108
R1060	G991	G991	GLN	W843	T784	P712	V633	I554	Y488	K422	K347	G260	L112	L112
Y1064	T993	T993	ARG	R851	Y785		Y634	I555	S489		R348	G261	Y113	Y113
Q1065	Y994	Y994	THR	R852		A715	R635	T556	S490	T426	I349	G262	F183	F183
	R995	R995	ALA	S853	R788	M716	P636	T557	T491	K426	Y351	G263	A184	A184
E1070	R996	R996	TYR	L854	M789	E717	L637	L558	L492	D427	K352	S294	Q115	Q115
E1071	E997	E997	HIS	F855	Q790		F638		S493		K353	R267	E116	E116
M1072	D998	D998		R856	T791	L721	I639	M563	H494	R430	D354	T268	R118	R118
Y1073	N999	N999	K934	R857	Q792	D722	V640				I355		L119	L119
N1074	P1000	P1000			A793		E641	L566	R497	Q433	I356	L273	R120	R120
	F1001	F1001	S938	M860	W794	R728	D642		T496		Q357	P274	M121	M121
T1077	T1002	T1002	T939	D861	I795	I729	D643	Y569	N499	V436		Y275	L122	L122
G1078	A1003	A1003	P940	Q862	L796	R730	E644	V570	T500	E437	L361	I276	Y202	Y202
K1079	E1004	E1004	L941	E863	Y797	V731	S645		P501	E438	P362	F203	F203	F203
L1080	G1005	G1005	R942	K864	Y798	S732	L646	Q573	I502	A439	H363	I283	I204	I204
K1081	I1006	I1006	S943		Q799	H733	G647	S574	GLY	H440	I364	V293		
M1082	V1007	V1007		T871	Q800		H648	P575	ARG	D441	T365	I294	G207	V130
E1083	P1008	P1008	N946	E872	K801	T736	K649	D576	ASP	F442		R287	S208	S208
Q1084	D1009	D1009	G947	T873	P802		E650	A577	GLY	N443	E371	A288	E209	K134
F1085	I1011	I1011	I948	E874	L803				LYS	N444	S372	L289	K210	ARG
F1086	I1012	I1012	P949	E875		T739	V653	V580	LEU	K445	R373	G290	V211	THR
F1087	I1013	I1013	P950		T806	C741	R654	F581	A509	L446			L212	TYR
G1088	N1014	N1014	Q951	Q878	R807	E742	K655	V582		A447			I213	GLU
P1089	P1014	P1014	V952	R879	A808	I743	G656	V583	Q513	F376		P293	ALA	ALA
H1015	H1015	H1015	L953	T880	M809	H744	H657	G584	L514	F377		D294	ILE	ILE
Y1091	Y1091	Y1091	V954	P745	E810	P745	I658	V585	H515			G295	ASP	ASP
I1092	T955	T955	T955	T882	Y811	S746			A450			E216	E216	E216
Q1093	I1018	I1018	T956	L883	L812	T747	M662	V589	N516	K451	Y380	E296	R217	VAL
R1094	S1019	S1019	R957			I748	A653	H590	T517	T453	M381	I297	S218	PRO
L1095	R1020	R1020	Q958	K886	E816		T664	H590	H518	L457	I382		N221	GLY
R1096	M1021	M1021	Q959	L893	P818	V751		M592	W519	L457	N383	I301	R222	ARG
H1097	T1022	T1022	G960			A752	G671		G520		R384	C302	GLU	GLU



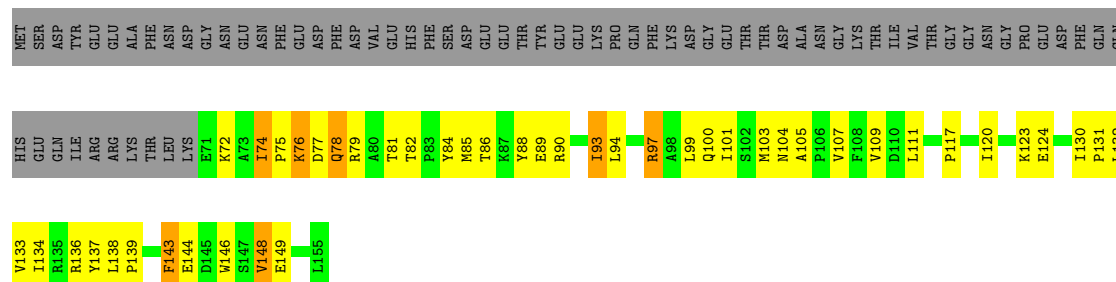
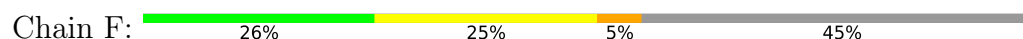
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



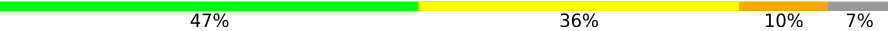
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

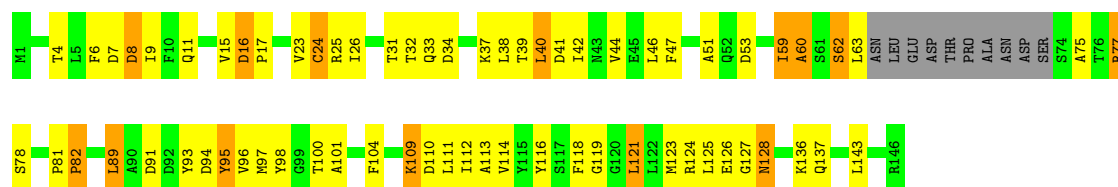


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



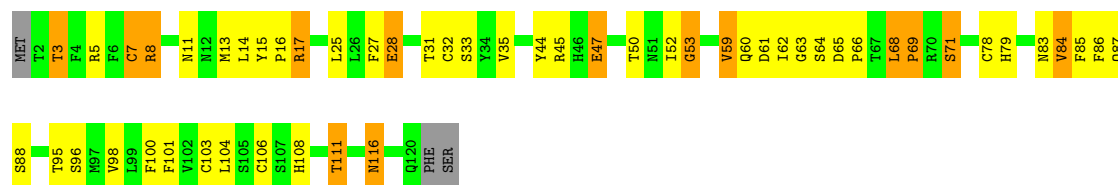
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

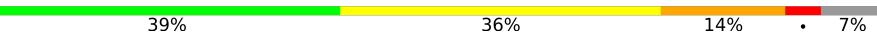


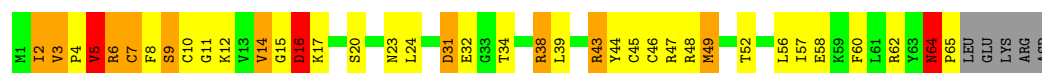
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 

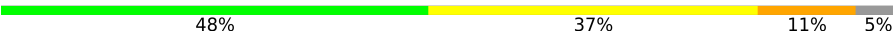


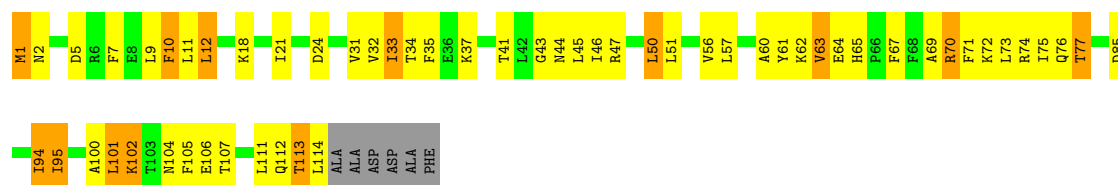
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



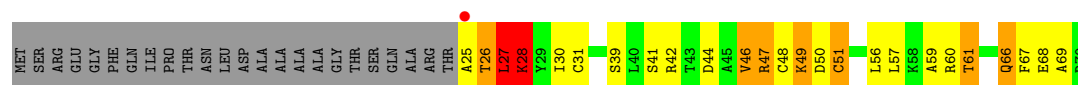
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



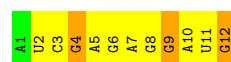
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 

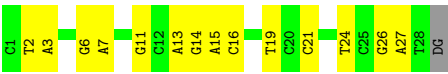


- Molecule 11: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*G)-3')

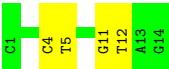
Chain R: 



● Molecule 12: DNA (28-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	170.96Å 223.00Å 195.41Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	50.00 – 3.78 50.00 – 3.78	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-3.78) 95.4 (50.00-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.253 , 0.300 0.254 , 0.292	Depositor DCC
R_{free} test set	3441 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30067	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

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	0.67	1/11536 (0.0%)	1.12	72/15605 (0.5%)
2	B	0.74	0/9347	1.11	47/12609 (0.4%)
3	C	0.76	1/2174 (0.0%)	1.09	5/2946 (0.2%)
4	E	0.60	0/1793	0.93	1/2413 (0.0%)
5	F	0.64	0/696	1.03	5/940 (0.5%)
6	H	0.68	0/1105	1.06	6/1495 (0.4%)
7	I	0.66	0/989	1.07	7/1331 (0.5%)
8	J	0.77	0/541	1.25	8/727 (1.1%)
9	K	0.73	1/937 (0.1%)	1.04	2/1265 (0.2%)
10	L	0.71	0/365	1.14	5/485 (1.0%)
11	R	0.76	0/292	1.13	1/455 (0.2%)
12	T	0.41	0/634	1.01	0/975
13	N	0.35	0/317	0.89	0/488
All	All	0.69	3/30726 (0.0%)	1.09	159/41734 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	VAL	CA-CB	5.65	1.60	1.54
9	K	10	PHE	CA-C	5.23	1.58	1.52
3	C	43	THR	CA-CB	5.11	1.61	1.53

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	885	THR	N-CA-C	16.15	132.25	112.54
2	B	974	PRO	N-CA-C	-14.72	88.18	111.14
1	A	718	VAL	N-CA-C	13.23	122.85	110.42
2	B	296	GLU	N-CA-C	-11.61	99.64	114.04
6	H	59	ILE	CB-CA-C	-11.40	92.45	110.69

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	11392	801	1
2	B	9167	0	9178	677	0
3	C	2135	0	2090	164	1
4	E	1757	0	1781	58	0
5	F	684	0	703	28	0
6	H	1087	0	1062	50	0
7	I	971	0	929	33	0
8	J	532	0	545	57	0
9	K	919	0	929	60	0
10	L	363	0	387	28	0
11	R	260	0	132	21	0
12	T	566	0	316	15	0
13	N	284	0	161	3	0
14	A	2	0	0	3	0
14	B	1	0	0	2	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	R	1	0	0	0	0
All	All	30067	0	29605	1834	1

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 1834 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:399:HIS:CG	1:A:400:PRO:HD3	1.52	1.43
2:B:439:ALA:CB	2:B:440:HIS:HA	1.41	1.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CD2	1:A:400:PRO:HD3	1.62	1.34
1:A:1081:LEU:CD2	1:A:1082:ASN:H	1.47	1.27
2:B:439:ALA:HB3	2:B:440:HIS:CA	1.66	1.24

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:SER:OG	3:C:87:PHE:O[2_555]	2.17	0.03

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%)	1054 (73%)	303 (21%)	81 (6%)	1	15
2	B	1145/1224 (94%)	855 (75%)	231 (20%)	59 (5%)	1	16
3	C	269/318 (85%)	207 (77%)	48 (18%)	14 (5%)	1	16
4	E	213/215 (99%)	175 (82%)	33 (16%)	5 (2%)	5	29
5	F	83/155 (54%)	66 (80%)	14 (17%)	3 (4%)	2	21
6	H	132/146 (90%)	104 (79%)	22 (17%)	6 (4%)	2	18
7	I	117/122 (96%)	84 (72%)	29 (25%)	4 (3%)	3	23
8	J	63/70 (90%)	48 (76%)	12 (19%)	3 (5%)	2	17
9	K	112/120 (93%)	86 (77%)	24 (21%)	2 (2%)	6	32
10	L	44/70 (63%)	31 (70%)	9 (20%)	4 (9%)	0	8
All	All	3616/4173 (87%)	2710 (75%)	725 (20%)	181 (5%)	1	17

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	A	115	LEU
1	A	116	ASP
1	A	117	GLU
1	A	119	ASN

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	1258/1520 (83%)	1004 (80%)	254 (20%)	1	8
2	B	1000/1061 (94%)	800 (80%)	200 (20%)	1	8
3	C	238/274 (87%)	184 (77%)	54 (23%)	1	5
4	E	196/197 (100%)	175 (89%)	21 (11%)	6	25
5	F	74/137 (54%)	61 (82%)	13 (18%)	2	12
6	H	119/128 (93%)	107 (90%)	12 (10%)	7	27
7	I	113/116 (97%)	98 (87%)	15 (13%)	4	19
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	11
9	K	99/102 (97%)	78 (79%)	21 (21%)	1	7
10	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3197/3657 (87%)	2586 (81%)	611 (19%)	1	9

5 of 611 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	THR
8	J	14	VAL
3	C	94	LYS
3	C	37	MET
4	E	157	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	648	HIS
2	B	984	HIS
9	K	44	ASN
2	B	744	HIS
2	B	862	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/12 (91%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	10	A
11	R	12	G

There are no RNA pucker outliers to report.

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 9 ligands modelled in this entry, 9 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%)	-0.11	6 (0%) 88 73	72, 131, 247, 370	0
2	B	1153/1224 (94%)	-0.07	9 (0%) 82 62	71, 114, 240, 374	0
3	C	271/318 (85%)	-0.26	0 100 100	80, 106, 165, 306	0
4	E	215/215 (100%)	-0.13	0 100 100	106, 165, 276, 316	0
5	F	85/155 (54%)	-0.30	0 100 100	107, 137, 170, 200	0
6	H	136/146 (93%)	0.03	0 100 100	126, 169, 276, 299	0
7	I	119/122 (97%)	-0.14	0 100 100	109, 150, 180, 237	0
8	J	65/70 (92%)	-0.33	0 100 100	80, 94, 135, 153	0
9	K	114/120 (95%)	-0.33	0 100 100	83, 112, 136, 139	0
10	L	46/70 (65%)	0.17	1 (2%) 62 43	99, 175, 228, 246	0
11	R	12/12 (100%)	-0.15	0 100 100	104, 119, 182, 208	0
12	T	28/29 (96%)	0.31	0 100 100	102, 222, 413, 422	0
13	N	14/14 (100%)	0.55	0 100 100	270, 329, 352, 379	0
All	All	3700/4228 (87%)	-0.11	16 (0%) 88 73	71, 128, 251, 422	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1211	ASN	3.2
2	B	441	ASP	2.8
2	B	262	GLU	2.6
1	A	266	LEU	2.6
2	B	529	GLU	2.4

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($\text{\AA}^2$)	Q<0.9
14	ZN	J	101	1/1	0.94	0.08	218,218,218,218	0
14	ZN	A	1734	1/1	0.96	0.04	232,232,232,232	0
14	ZN	A	1735	1/1	0.98	0.05	136,136,136,136	0
14	ZN	L	105	1/1	0.98	0.04	155,155,155,155	0
14	ZN	I	204	1/1	0.99	0.02	125,125,125,125	0
14	ZN	B	1307	1/1	0.99	0.03	163,163,163,163	0
14	ZN	I	203	1/1	0.99	0.02	103,103,103,103	0
14	ZN	C	319	1/1	1.00	0.03	118,118,118,118	0
15	MG	A	1736	1/1	1.00	0.02	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.