



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:01 AM GMT

PDB ID : 3GTO
Title : Backtracked RNA polymerase II complex with 15mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 4.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

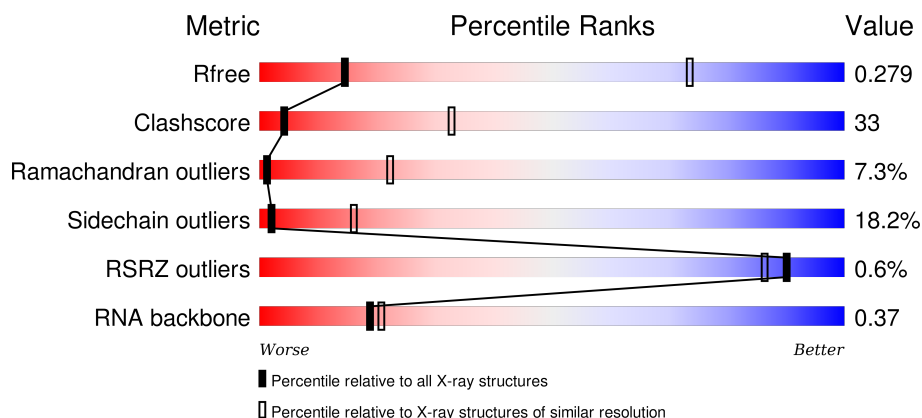
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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.



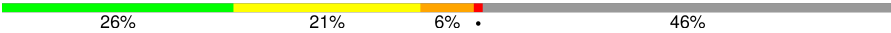
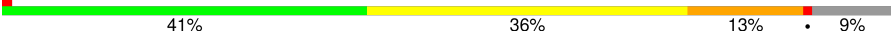

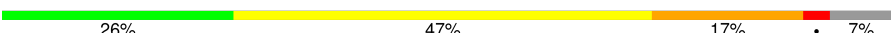


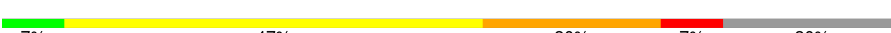


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div> <div></div> <div>32%</div> <div>35%</div> <div>12%</div> <div>•</div> <div>20%</div> </div> </div>
2	B	1224	<div> <div>36%</div> <div>42%</div> <div>11%</div> <div>•</div> <div>10%</div> </div>
3	C	318	<div> <div>34%</div> <div>39%</div> <div>9%</div> <div>•</div> <div>16%</div> </div>
4	E	215	<div> <div>47%</div> <div>40%</div> <div>10%</div> <div>•</div> </div>

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	15	
12	T	28	
13	N	14	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 29259 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	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

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

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 subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	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	84	Total	C	N	O	S	0	0	0
			679	434	115	127	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	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 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*GP*CP*AP*C)-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 (three-letter code: ZN) (formula: Zn).

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

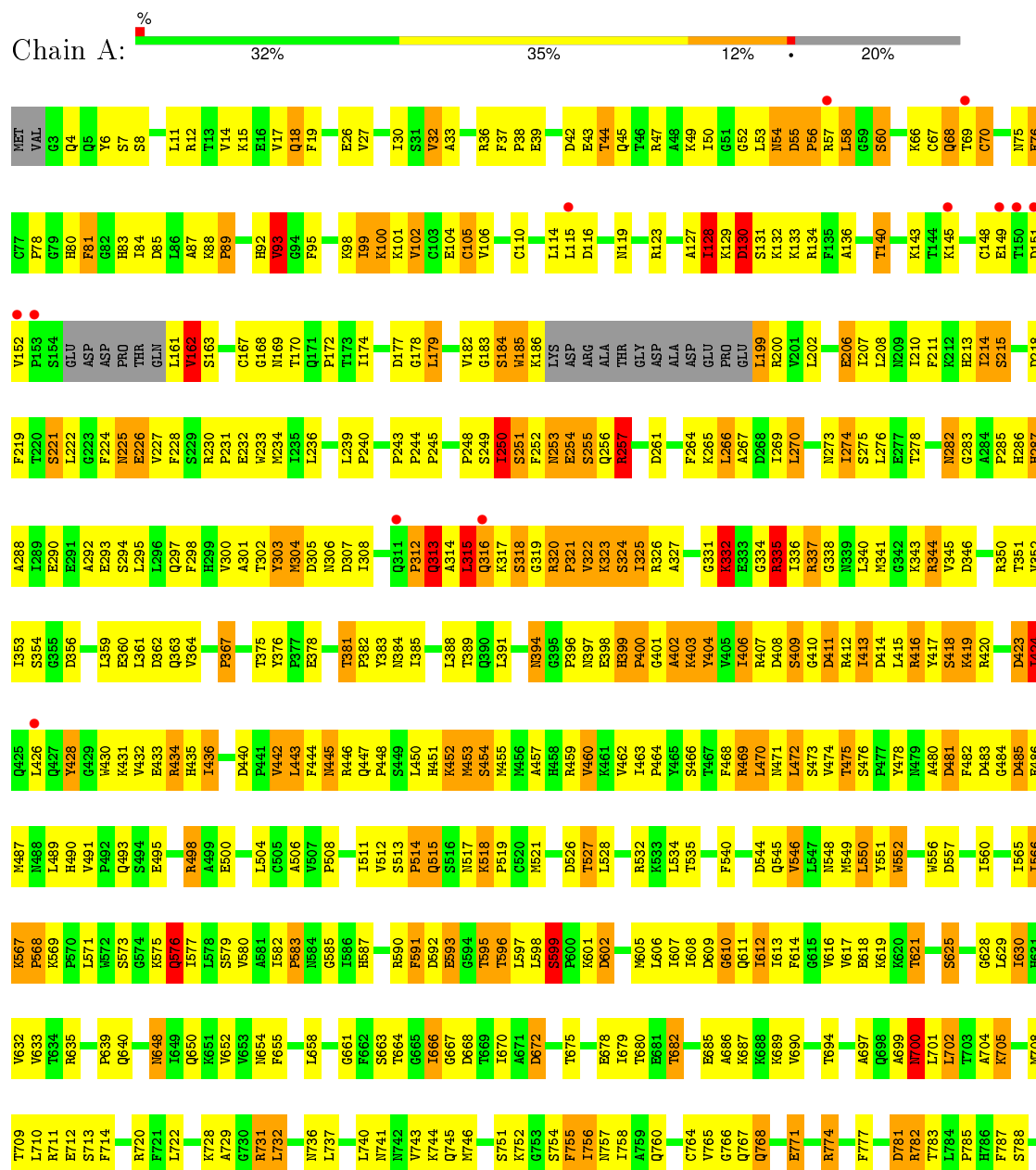
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



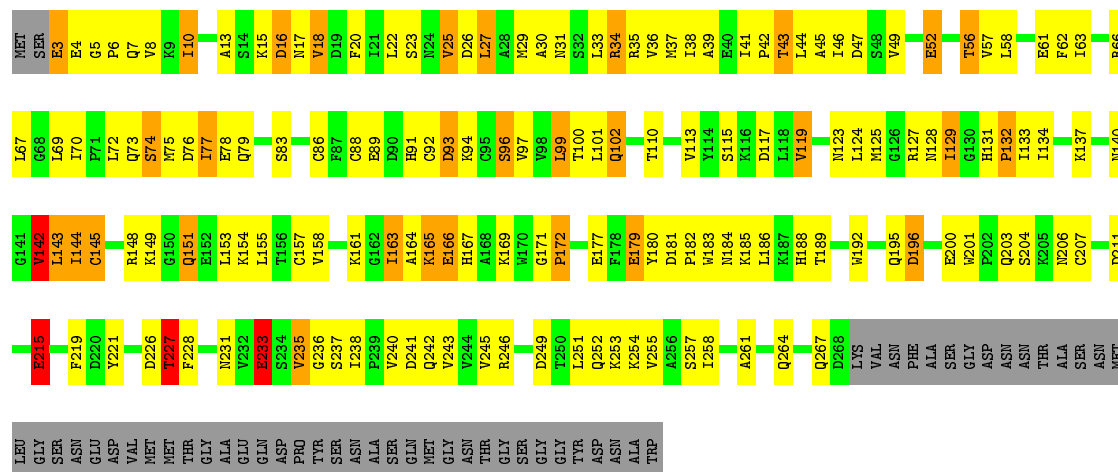


E1134	E1061	G991	GLU	R848	T783	D642	Y569	R497	M432	R363	I291	I204	TYR	GLU
R1136	H1062	I992	GLU	G849	M784	D643	W570	T498	Q433	I364	I292	I205	GLN	GLN
D1137		T993	LEU	F851		E644			R434	T365	P293	M206	ALA	ALA
M1138	Q1065	Y994	GLY	R852	R788		Q573	P501	T435	Q366	D294	M205	ASP	GLN
I1139	S1066	R995	GLN	R853	M789	G647	P574	I502	T436	L367	S208	E209	VAL	HIS
A1140	G1068	R996	ARG	R854	T791	H648	P576	ARG	E437	E296	K210	V211	PRO	THR
H1141	F1069	D997	THR	F855	M792	G649	A577	ASP	GLU	G369	I297		GLY	THR
G1142	E1070	M999	ALA	F856	A793	E650		ASP	ALA	F370			ARG	GLU
A1143		R999	ALA	R857	A794	L651	F581	GLY	HIS	E371	C302	L212	LEU	ASP
S1145	Y1073	F1001	HIS	S858	T795	K652	V582	LEU	ASP	R373	W308	M221	LEU	LEU
G1074	M1075	T1002	ASP	R859	T796	K654			PHE	K374	Q309	I222	LYS	ASN
H1076	H1076	A1003	ASP	M660	T797	R655	V586	ASN	MET	A375	M310	V225	THR	ILE
T1077		R935	R935	D861	Y798	I658	M586	Q513	LYS	F376	L311		GLU	SER
K1078	G1078	A937	D936	Q862	P799		H587	L514	L446	F377	E312		LEU	ARG
K1079	K1079	A937	R937	E863	T729	I658	G588	H515	A447	L378	M312	A229	LEU	ILE
K1080	P1008	V1007	S938	K864	W731	L661	V589	N516	T448	G379	K314	A230	ALA	ALA
L1081	P1008	P1008	P1008	K865	T732	Y666	H590	H518	H449	L385	L315	P231	GLU	GLU
M1082	L1010	D1009	L941	Y866	H733	Q867	R591	H519	K450	Q381	P316		GLU	T90
A1083	I1011	R942	R942	G867	H734	Q868	M592	W519	K451	I382	E319	S235	SER	S91
Q1084	I1012	T944	T944	R868	T736	IIE	P593	G519	L452	R384	D320	H236	ASP	F92
D1156	M1013	E945	E945	L870	T737	GLU	A594	L521	T453	L386	G321	S242	ASP	ASP
A1157	P1014	T871	T871	T872	F738	GLY	R595	V522	T454	L387	L385		GLY	GLU
F1087	H1015	E872	Q851	E872	T739	GLY	L596		L457	L387	V323	L244	SER	T98
G1088	A1016	V952	V952	T873	H740	PHE	E598	T527	K458	L388	I324	E245	SER	K99
P1089	I1017	L953	L953	F874	C741	GLU	T599	P528	K459	A399	G325	G247	GLY	P100
T1090	P1018	V954	V954	E875	E742	ASP	L600		A460	L390	D326	K246	GLY	M101
Y1091	S1019	T955	T955	K876	I743	VAL	T609	Q831	L461	D391	R327	G247	F165	V102
Y1092	R1020	R977	R977	P877	H744	GLU	N610	G534	L462	R392	R328	R249	I167	N103
Q1093	M1021	M957	Q878	Q878	P745		P611	L539	T463	K393	T329	E250	E104	E104
R1094	T1022	Q958	R879	R879	S746		D608	S540		D394	A330		S105	S105
L1095	V1023	T880	R881	R881	T747	W681	T609	V536	W466	R398	L331	V256	R168	L106
R1096	A1024	G960	P818	P818	I748	S882	N610	N338	Q487	R399	D332	K257	R169	E107
H1097	H1025	L961	A819	T882		L684		L539	E488	R400	I334	Y259	P171	V108
M1098	L1026	K965	G820	L883	V751		P612	S540	K471		G345	G260	L174	T109
V1099	I1027	R884	Q821	R884	I755	L889	E621	L541	A472	K404	ARG	R261	R175	L112
	E1028	V966	N822	N885		V690	V613		M473	R405	ARG		S176	Y113
	C1029	R957	A823	K886	F758	E691	S614	S543	S474		GLY	S264	K177	P114
	L1030	V969	I824			Y692				L408	THR	S265	N178	Q115
	K1033	R969	V825	D891	N762	D694	E621	V547	S475	L412	ALA	A266	C179	E116
	A1036	K972	A826	D895	T763	A695	E622	G548	R476	L413	LEU	R267	Y180	A117
	G1039	I973	A828		S764	E696	K625	T549	A477		ILE	T268	L181	L118
	P1046	P974	C829	C829	R766	E697	K626	D650	C478	L416	GLY		S182	L119
	F1047	Q975	S831	S831		E698	I626	P651	V479	L417	LYS	L273	R120	R120
	Q1047	I976	G832	G832	Y769	E699	F627	M552	Q481	F417	K345	L273	S187	N121
		G977	G832	G832		S700	T628	P553	V482	K418	D188	P274	D188	L122
		D978	Q835	Q835	A772	I701	G631	I554	L483	T419	K347	Y275	L189	L123
	I1050	D978	E836	E836		L702		I555	M484	L420	R348	I276	Y190	Y124
	T1051	R979			R773	L703	R632		R485		Y351	K277		S125
	V1052	F980	M839	M839	Q774	Y703	V634	E560	A486	K423	E194	Q278	E194	S126
	E1053	A981	I840	I840	R775	A704	V634	W561	T487	L424	C195		G127	G127
	G1054	S982	Q913	Q913	Q776	M705	R635	G562	Y488	T425	D354	V283	L128	F129
	I1055	R983	G913	G913	A777	Q706	P636	N563	S489	K426	I355	I284	M198	V130
	S1056	R984	K914	K914	M778	P707	L637	E564	S490	D427	L356	I285	M199	V130
	K1057	G985	S844	S844	G779	E708	F638	P665	T491	I428	Q357	F286	G200	
		Q986	S845	S845	Y780	D709	I639	L566	H494	F429	L361	A288	G201	K134
			P190	P190	F781	L710	V640	E567		R430			ARG	ARG
			ASP	ASP	L782	E711	B541	D568		Y431	P362		F203	THR



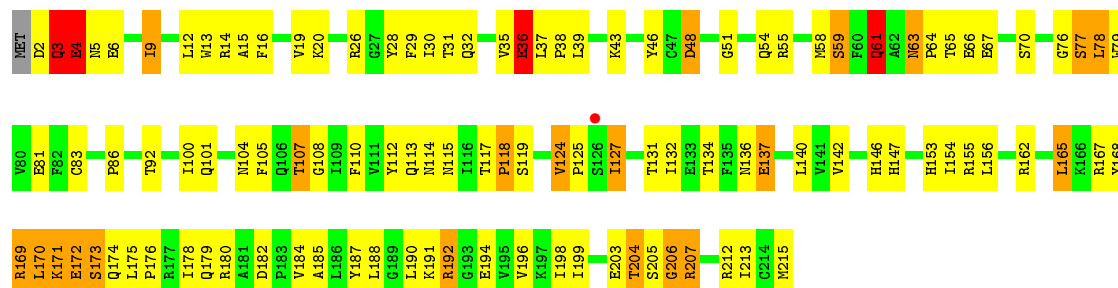
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 34% 39% 9% 16%



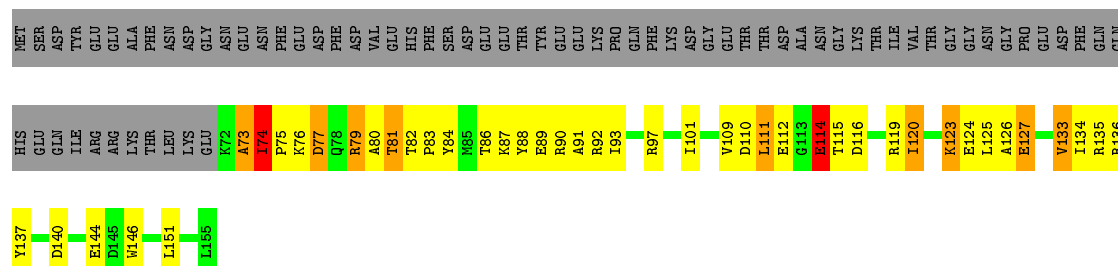
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 47% 40% 10%



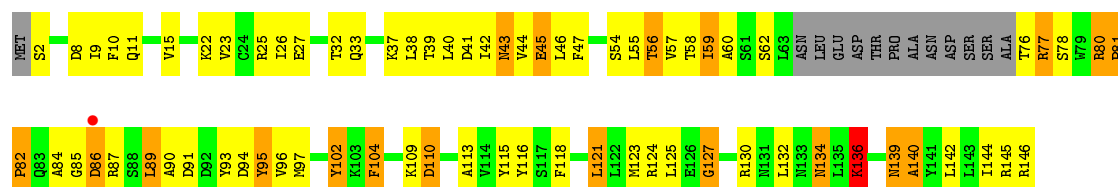
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 26% 21% 6% 46%



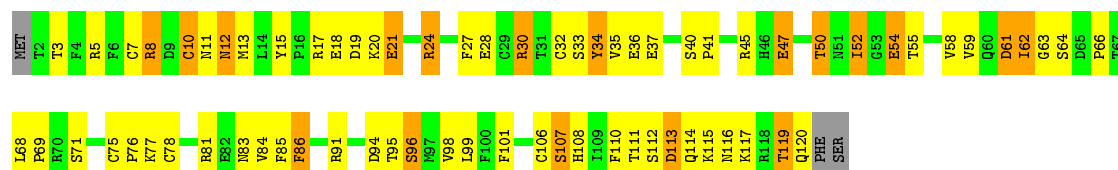
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 41% 36% 13% 9%



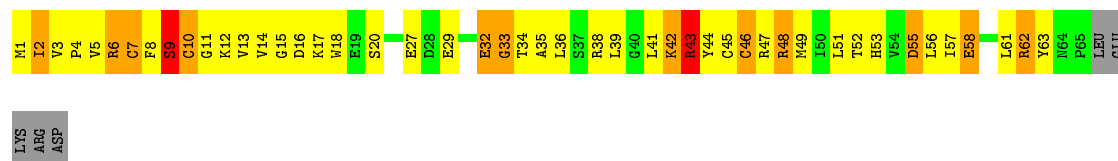
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 39% 43% 15%



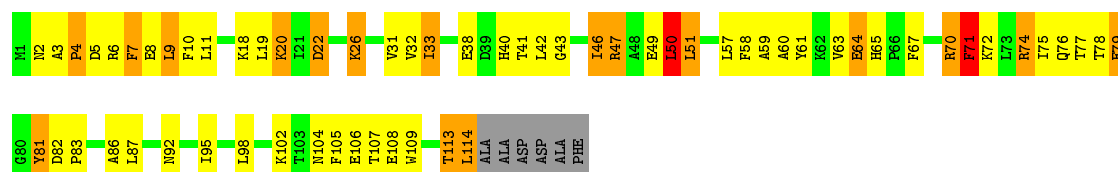
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 26% 47% 17% 7%



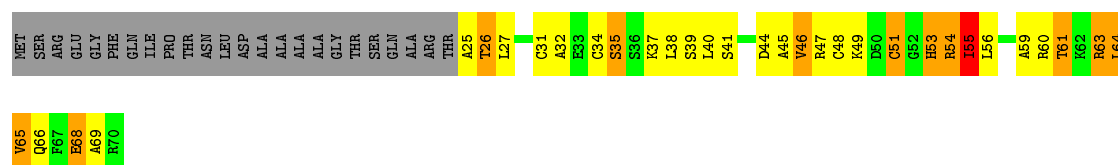
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 43% 37% 14% 5%



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

Chain L: 20% 29% 16% 34%



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

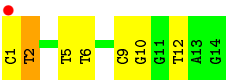
Chain R: 7% 47% 20% 7% 20%



● 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	170.85Å 222.80Å 194.98Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 49.45 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-4.00) 93.6 (49.45-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.269 , 0.290 0.264 , 0.279	Depositor DCC
R_{free} test set	2847 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 56200 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29259	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	1.02	43/11163 (0.4%)	0.81	10/15091 (0.1%)
2	B	1.13	48/8963 (0.5%)	0.88	19/12086 (0.2%)
3	C	1.16	11/2133 (0.5%)	0.84	0/2891
4	E	1.12	9/1788 (0.5%)	0.80	3/2406 (0.1%)
5	F	1.14	3/691 (0.4%)	0.87	0/933
6	H	1.01	3/1086 (0.3%)	0.84	0/1470
7	I	1.26	9/989 (0.9%)	0.95	5/1331 (0.4%)
8	J	1.28	9/541 (1.7%)	0.97	3/727 (0.4%)
9	K	1.08	3/937 (0.3%)	0.80	1/1265 (0.1%)
10	L	1.09	0/365	0.93	0/485
11	R	1.25	1/292 (0.3%)	1.79	5/455 (1.1%)
12	T	1.39	1/634 (0.2%)	1.90	22/975 (2.3%)
13	N	1.83	8/317 (2.5%)	1.67	6/488 (1.2%)
All	All	1.11	148/29899 (0.5%)	0.91	74/40603 (0.2%)

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
3	C	0	1
6	H	0	1
7	I	0	1
All	All	0	3

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	574	SER	CB-OG	12.89	1.59	1.42
4	E	137	GLU	CD-OE1	11.71	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	54	GLU	CD-OE1	11.17	1.38	1.25
1	A	1426	GLU	CD-OE1	10.61	1.37	1.25
2	B	598	GLU	CD-OE2	10.45	1.37	1.25

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	O4'-C4'-C3'	-10.87	99.48	106.00
1	A	1173	HIS	N-CA-C	9.95	137.86	111.00
1	A	1172	LEU	N-CA-C	9.54	136.75	111.00
12	T	16	DC	O4'-C1'-N1	8.87	114.21	108.00
12	T	27	DA	O4'-C4'-C3'	-8.83	100.70	106.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	172	PRO	Peptide
6	H	136	LYS	Peptide
7	I	77	LYS	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	10969	0	11071	924	0
2	B	8792	0	8824	632	0
3	C	2095	0	2052	131	0
4	E	1752	0	1776	91	0
5	F	679	0	701	45	0
6	H	1068	0	1040	64	0
7	I	971	0	928	46	0
8	J	532	0	544	65	0
9	K	919	0	929	64	0
10	L	363	0	387	21	0
11	R	260	0	132	15	0
12	T	566	0	316	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	284	0	161	5	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	1	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	1	0
15	A	1	0	0	0	0
All	All	29259	0	28861	1940	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 33.

The worst 5 of 1940 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	1.44	1.48
1:A:315:LEU:HB2	1:A:316:GLN:C	1.39	1.43
1:A:315:LEU:HB2	1:A:316:GLN:CA	1.51	1.38
1:A:256:GLN:CA	1:A:257:ARG:HB3	1.59	1.30
1:A:1111:MET:CG	1:A:1114:PRO:HG3	1.64	1.27

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	1383/1733 (80%)	1038 (75%)	233 (17%)	112 (8%)	1	19
2	B	1088/1224 (89%)	822 (76%)	188 (17%)	78 (7%)	1	23
3	C	264/318 (83%)	209 (79%)	48 (18%)	7 (3%)	6	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	212/215 (99%)	162 (76%)	39 (18%)	11 (5%)	2	31
5	F	82/155 (53%)	65 (79%)	13 (16%)	4 (5%)	3	32
6	H	129/146 (88%)	97 (75%)	21 (16%)	11 (8%)	1	17
7	I	117/122 (96%)	83 (71%)	25 (21%)	9 (8%)	1	20
8	J	63/70 (90%)	45 (71%)	14 (22%)	4 (6%)	2	27
9	K	112/120 (93%)	89 (80%)	16 (14%)	7 (6%)	2	27
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0	1
All	All	3494/4173 (84%)	2634 (75%)	606 (17%)	254 (7%)	1	22

5 of 254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	54	ASN
1	A	55	ASP
1	A	56	PRO
1	A	93	VAL

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	1218/1520 (80%)	987 (81%)	231 (19%)	2	14
2	B	960/1061 (90%)	790 (82%)	170 (18%)	2	18
3	C	234/274 (85%)	188 (80%)	46 (20%)	1	13
4	E	196/197 (100%)	164 (84%)	32 (16%)	3	22
5	F	74/137 (54%)	63 (85%)	11 (15%)	4	26
6	H	117/128 (91%)	97 (83%)	20 (17%)	2	19
7	I	113/116 (97%)	95 (84%)	18 (16%)	3	23
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	13
9	K	99/102 (97%)	81 (82%)	18 (18%)	2	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	L	40/57 (70%)	31 (78%)	9 (22%)	1 9
All	All	3111/3657 (85%)	2544 (82%)	567 (18%)	2 16

5 of 567 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	264	SER
2	B	751	VAL
7	I	83	ASN
2	B	354	ASP
2	B	487	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	465	ASN
2	B	822	ASN
7	I	83	ASN
2	B	515	HIS
2	B	657	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/15 (73%)	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	1395/1733 (80%)	-0.34	13 (0%) 85 80	76, 116, 186, 214	0
2	B	1106/1224 (90%)	-0.37	3 (0%) 94 92	72, 109, 156, 180	0
3	C	266/318 (83%)	-0.50	0 100 100	83, 106, 145, 154	0
4	E	214/215 (99%)	-0.41	1 (0%) 91 88	104, 151, 192, 196	0
5	F	84/155 (54%)	-0.47	0 100 100	99, 123, 142, 147	0
6	H	133/146 (91%)	-0.21	1 (0%) 87 82	123, 143, 165, 167	0
7	I	119/122 (97%)	-0.43	0 100 100	113, 132, 150, 160	0
8	J	65/70 (92%)	-0.62	0 100 100	77, 94, 126, 131	0
9	K	114/120 (95%)	-0.45	0 100 100	87, 108, 124, 131	0
10	L	46/70 (65%)	-0.22	0 100 100	100, 161, 179, 181	0
11	R	12/15 (80%)	0.19	0 100 100	100, 128, 185, 192	0
12	T	28/28 (100%)	0.10	1 (3%) 46 36	102, 210, 322, 325	0
13	N	14/14 (100%)	0.48	1 (7%) 19 13	287, 311, 317, 318	0
All	All	3596/4230 (85%)	-0.37	20 (0%) 90 86	72, 116, 181, 325	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	5.2
1	A	1176	LEU	4.3
1	A	150	THR	3.9
1	A	153	PRO	3.2
12	T	3	DA	3.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
14	ZN	C	319	1/1	1.00	0.05	-1.34	97,97,97,97	0
14	ZN	A	1735	1/1	0.97	0.07	-1.39	155,155,155,155	0
14	ZN	I	203	1/1	0.99	0.05	-1.44	123,123,123,123	0
14	ZN	B	1307	1/1	0.99	0.07	-1.51	158,158,158,158	0
14	ZN	I	204	1/1	0.99	0.05	-1.58	131,131,131,131	0
15	MG	A	1736	1/1	0.80	0.15	-1.85	92,92,92,92	0
14	ZN	A	1734	1/1	0.90	0.05	-2.28	212,212,212,212	0
14	ZN	J	101	1/1	0.99	0.12	-2.38	93,93,93,93	0
14	ZN	L	105	1/1	0.98	0.05	-	169,169,169,169	0

6.5 Other polymers [i](#)

There are no such residues in this entry.