



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2017 – 08:15 PM EDT

PDB ID : 3GTQ
Title : Backtracked RNA polymerase II complex induced by damage
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : unknown
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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

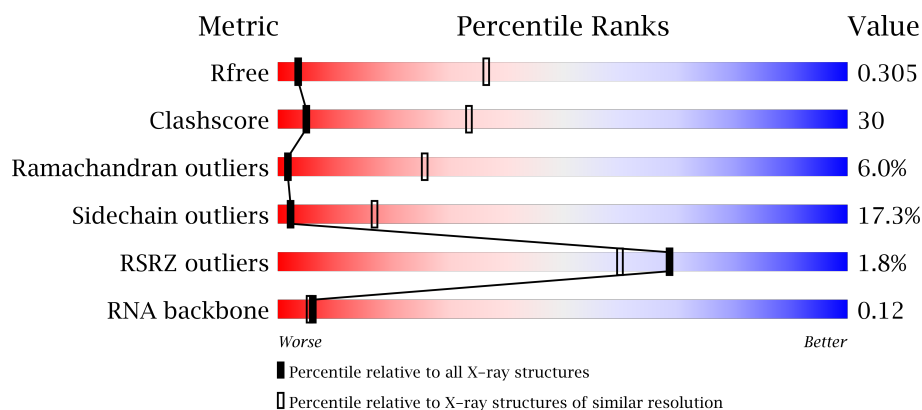
1 Overall quality at a glance

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.



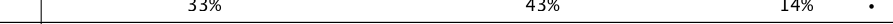

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)
RNA backbone	2435	1016 (4.70-2.90)

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>2%</div> <div> <div>37%</div> <div>33%</div> <div>9%</div> <div>20%</div> </div> </div>
2	B	1224	<div> <div>0%</div> <div> <div>38%</div> <div>42%</div> <div>10%</div> <div>10%</div> </div> </div>
3	C	318	<div> <div>0%</div> <div> <div>35%</div> <div>41%</div> <div>7%</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>3%</div> <div> <div>55%</div> <div>36%</div> <div>8%</div> </div> </div>

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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	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28625 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(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*A P*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	11	Total	C	N	O	P	0	0	0
			243	108	50	74	11			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*CP*AP*TP*AP*AP *CP*CP*AP*CP*AP*GP*GP*CP*TP*CP*CP*TP*CP*TP*CP*CP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	12	Total	C	N	O	P	0	0	0
			234	113	34	75	12			

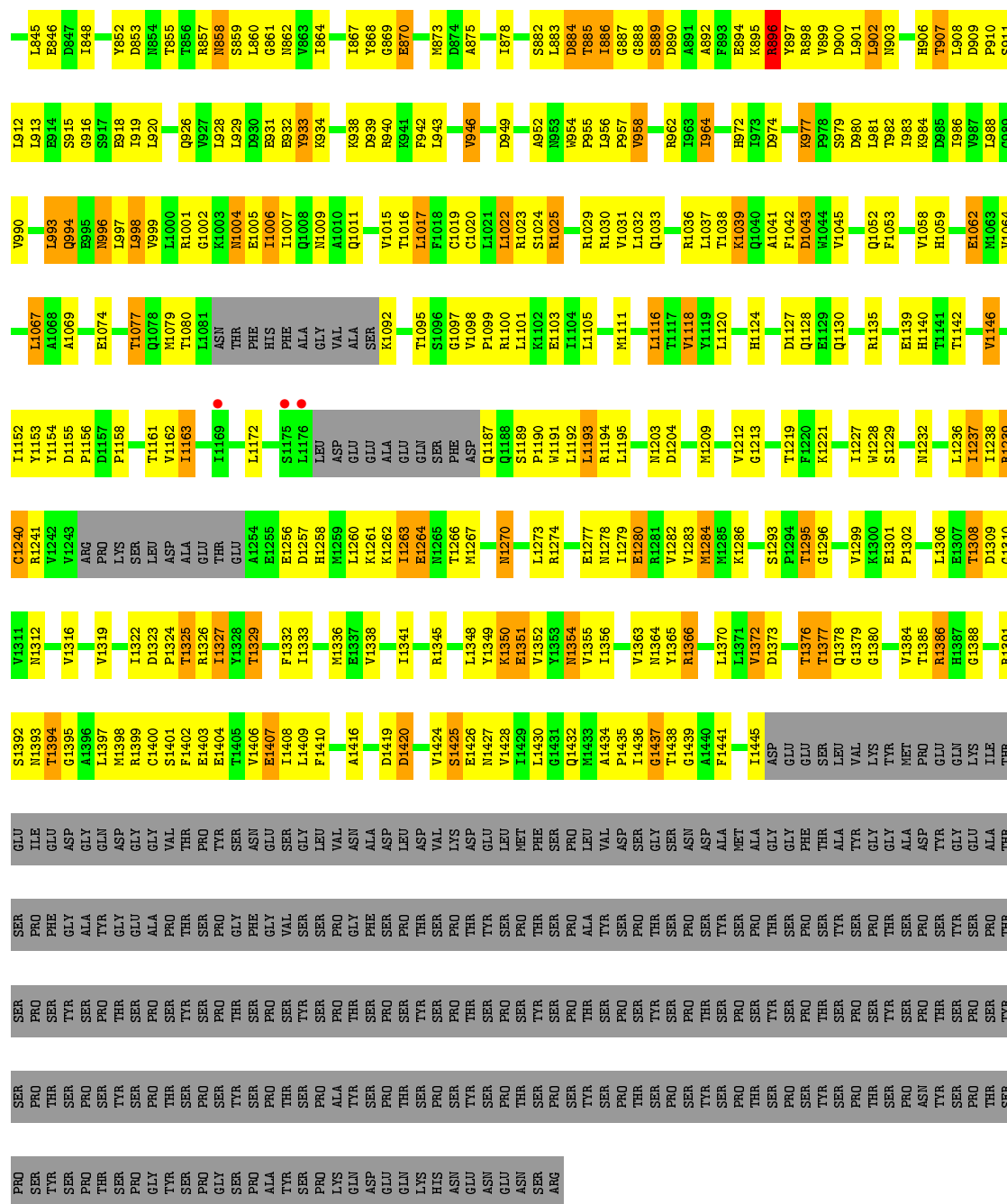
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

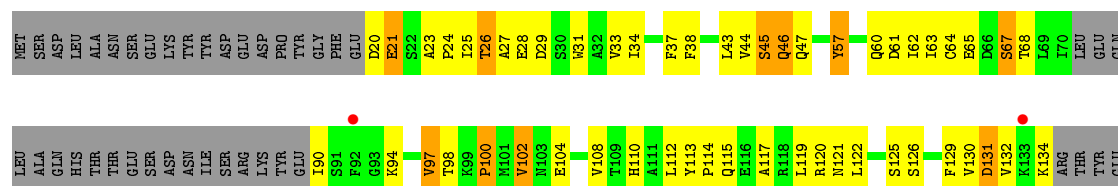
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0



• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

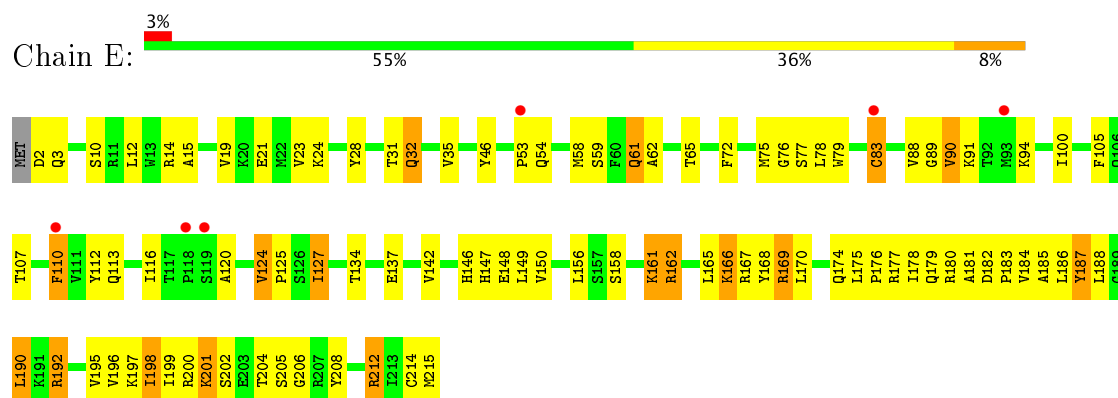


A1157	Q1093	R1020	Q951	H733	GLY	P593	H515	P362	Y275	Y202	ALA
F1158	R1094	M1021	V952	H734	PRE	P593	H516	H963	I276	F203	ILE
R1159	L1095	T1022	L953	A735	GLU	L596	T517	A450	F277	F203	ASP
V1160	R1096	V1023	T954	T736	ASP	M597	H518	T365		I204	VAL
H1162	M1097	A1024	T955	T737	VAL	L600	H519	G369	R287	E209	PRO
H1098	H1098	H1025	T956	T738	GLU	L600	G520	F370	L289	K210	GLY
C1163	V1099	L1026	T957	T739		D608	G521	E371		V211	ARG
G1164	D1100	L1027	Q958	H740	E678	D608	V522	S372	P293	L212	LEU
G1165	D1101	E1028	T959	C741	Y679	L600	C523	K374	D294	I213	LYS
C1166	C1102	G960	L983	H744	W881	I609	T527	A462	G295	Q215	TVR
C1167	I1103	L1030	R834	P745	S682	P611	P528	K375	E296	Q216	GLU
M1168	R1106	S1032	K965	P746	S683	P611	E529	F376	I297	R217	LEU
T1170	A1107	K1033	V966	K747	L684	P612	G530	F377	L298		ILE
V1171	R1108	V1034	T967	I749	L685	S614		L378		S218	ALA
I1172	G1109	A1035	Y968	I750	M686	S614	K537	I301		A219	GLU
A1173	P1110	A1036	R969	I751	G688	I616		C302		I222	GLU
K1174	P1111	L1037	T970	G751	G688	I616	L541	V305		Y223	SER
L1175	V1113	G1051	T971	S754	L689	R617	M542	N306		Q224	ASP
M1176	L1114	S1045	I972	I755	E891	E821	I545	N307		V225	ASP
N1177	T1115	P1046	A900	T756	E892	R622	S546	W308		K228	SER
N1178	R1116	F1047	P901	D760	D693	R623	V547	Q309		A229	SER
Q1179	Q1117	T1048	G902	R766	I693	G634	G549	M310		A230	GLY
	Q1117	Q975	V903		D694	L624	T556	L311		P231	
	P1118	A976	R904	H761	A695	T628	F557	C388			
	I976	I976		N762	E696		L483	C387			
	G977	G977		Q763	E897		M494	I171			
	D978	D978		S764	E698		R485	F322			
	K979	K979		I765	E699		Y486	I172			
	F980	F980		G832	D700		T487	M173			
	A981	A981		R766	L710		Y488	L174			
	Q982	Q982		Y769	E711		S489	L244			
	R983	R983		G834	P712		S490	E245			
	H984	H984		Q835	L782		L492	K246			
	H984	H984		E936	R783		S493	G247			
	Q986	Q986		D837	L784		H494	S248			
	G991	G991		M839	T784		L495	R249			
	I992	I992		Q843	A715		R496	L181			
	T993	T993		S844	ASN		R497	L185			
	T994	T994		D847	GLU			T185			
	R995	R995		R348	GLU			E186			
	D996	D996		G849	ASN			S187			
	E997	E997		L850	ASP			D188			
	D998	D998		F851	LEU			L189			
	F1000	F1000		R852	LEU			Y190			
	T1001	T1001		S853	ASP			K193			
	T1002	T1002		L854	LEU			E194			
	A1003	A1003		R857	D722			C195			
	K934	K934		M860	V723			P196			
	R935	R935		D861	V724			F197			
	D936	D936		Q862	P725			D198			
	P1008	P1008		N794	A726			M199			
	D1009	D1009		L795	K727			G200			
	L1010	L1010		L796	I728			L273			
	I1011	I1011		Y797	I729			P274			
	E945	E945		K864							
	M1012	M1012		K865							
	M1013	M1013		Y866							
	P1014	P1014		S869							
	H1015	H1015									
	F1015	F1015									
	D1156	D1156									

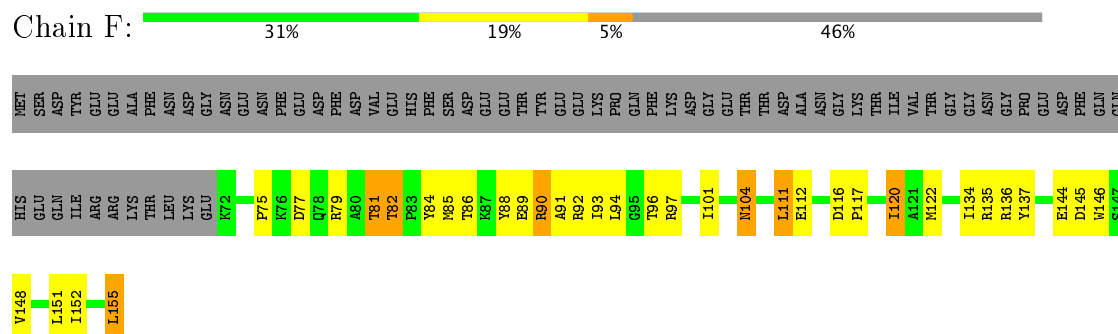
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



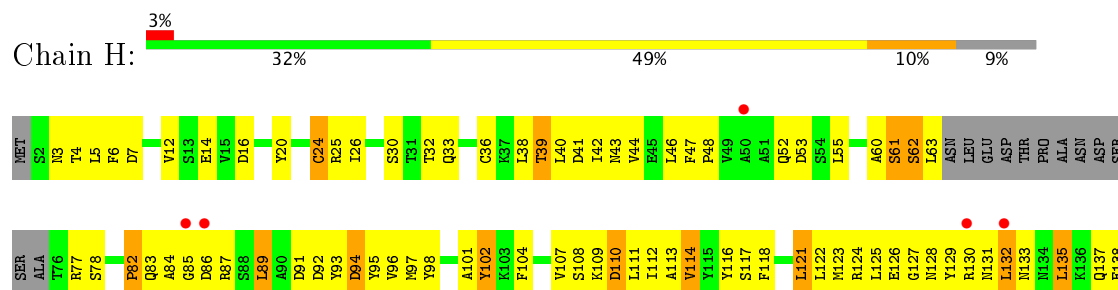
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

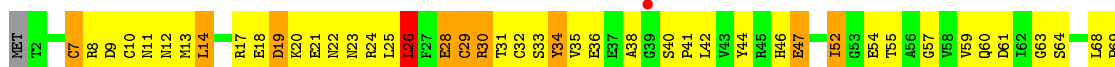


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

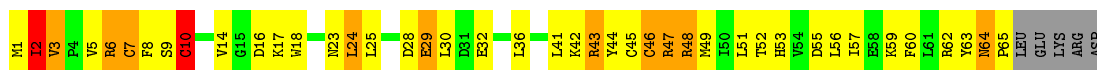
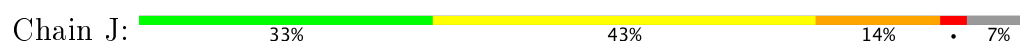




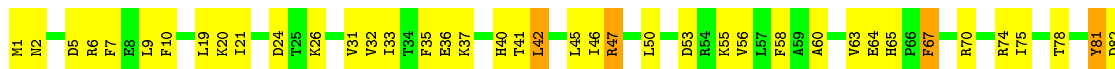
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



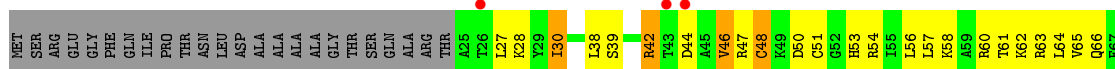
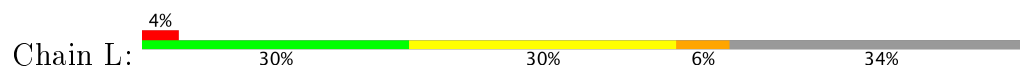
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



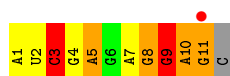
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



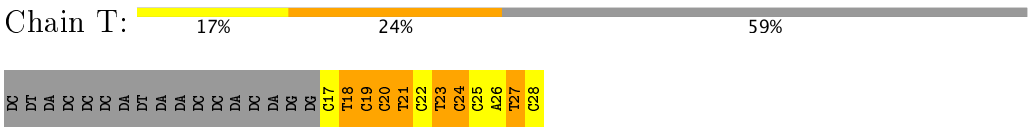
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*CP*AP*TP*AP*AP*CP*CP*AP*CP*AP*G P*GP*CP*TP*CP*CP*TP*CP*TP*CP*CP*AP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.19Å 221.58Å 192.80Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 45.33 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-3.80) 95.5 (45.33-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.271 , 0.335 0.253 , 0.305	Depositor DCC
R_{free} test set	3287 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	98.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.0	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	0.88	EDS
Total number of atoms	28625	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: 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	0.55	0/11163	0.73	1/15091 (0.0%)
2	B	0.59	0/8963	0.74	1/12086 (0.0%)
3	C	0.55	0/2133	0.71	0/2891
4	E	0.50	0/1788	0.68	2/2406 (0.1%)
5	F	0.52	0/691	0.70	0/933
6	H	0.48	0/1086	0.76	1/1470 (0.1%)
7	I	0.57	0/989	0.75	1/1331 (0.1%)
8	J	0.59	0/541	0.86	2/727 (0.3%)
9	K	0.55	0/937	0.68	0/1265
10	L	0.57	0/365	0.80	0/485
11	R	1.00	0/273	1.71	3/425 (0.7%)
12	T	1.09	0/258	2.33	23/393 (5.9%)
All	All	0.57	0/29187	0.78	34/39503 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	21	DT	O4'-C4'-C3'	-10.41	99.76	106.00
12	T	20	DC	OP2-P-O3'	-8.94	85.53	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	T	20	DC	OP1-P-O3'	-8.71	86.03	105.20
12	T	20	DC	O4'-C1'-N1	8.67	114.07	108.00
12	T	19	DC	N3-C2-O2	-8.28	116.11	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1172	LEU	Peptide
1	A	320	ARG	Peptide
2	B	473	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	10969	0	11070	714	0
2	B	8792	0	8823	656	0
3	C	2095	0	2052	142	0
4	E	1752	0	1776	82	0
5	F	679	0	701	31	0
6	H	1068	0	1040	74	0
7	I	971	0	930	57	0
8	J	532	0	544	61	0
9	K	919	0	929	47	0
10	L	363	0	387	19	0
11	R	243	0	121	26	0
12	T	234	0	137	19	0
13	A	2	0	0	1	0
13	B	1	0	0	1	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	1	0
13	L	1	0	0	0	0
All	All	28625	0	28510	1712	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 30.

The worst 5 of 1712 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:704:ALA:HB1	2:B:710:LEU:CD1	1.55	1.34
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.51	1.28
2:B:634:TYR:CE1	2:B:692:TYR:HD1	1.52	1.27
2:B:879:ARG:CB	2:B:880:THR:HA	1.68	1.22
7:I:75:CYS:SG	7:I:78:CYS:HB2	1.82	1.19

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%)	1075 (78%)	218 (16%)	90 (6%)	1	24
2	B	1088/1224 (89%)	849 (78%)	169 (16%)	70 (6%)	1	25
3	C	264/318 (83%)	211 (80%)	39 (15%)	14 (5%)	2	29
4	E	212/215 (99%)	177 (84%)	31 (15%)	4 (2%)	9	50
5	F	82/155 (53%)	73 (89%)	6 (7%)	3 (4%)	4	36
6	H	129/146 (88%)	96 (74%)	20 (16%)	13 (10%)	1	12
7	I	117/122 (96%)	92 (79%)	18 (15%)	7 (6%)	2	26
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	25
9	K	112/120 (93%)	95 (85%)	15 (13%)	2 (2%)	10	50
10	L	44/70 (63%)	32 (73%)	9 (20%)	3 (7%)	1	23
All	All	3494/4173 (84%)	2748 (79%)	536 (15%)	210 (6%)	2	26

5 of 210 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	A	93	VAL
1	A	226	GLU
1	A	253	ASN
1	A	254	GLU

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%)	1008 (83%)	210 (17%)	2	17
2	B	960/1061 (90%)	786 (82%)	174 (18%)	2	15
3	C	234/274 (85%)	189 (81%)	45 (19%)	1	12
4	E	196/197 (100%)	169 (86%)	27 (14%)	4	27
5	F	74/137 (54%)	65 (88%)	9 (12%)	6	30
6	H	117/128 (91%)	101 (86%)	16 (14%)	4	27
7	I	113/116 (97%)	90 (80%)	23 (20%)	1	11
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	11
9	K	99/102 (97%)	86 (87%)	13 (13%)	5	28
10	L	40/57 (70%)	30 (75%)	10 (25%)	1	6
All	All	3111/3657 (85%)	2572 (83%)	539 (17%)	2	17

5 of 539 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	234	ILE
2	B	653	VAL
7	I	91	ARG
2	B	273	LEU
2	B	463	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	515	HIS
2	B	835	GLN
7	I	22	ASN
2	B	518	HIS
2	B	740	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	10/12 (83%)	6 (60%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	3	C
11	R	5	A
11	R	8	G
11	R	9	G
11	R	10	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	1395/1733 (80%)	-0.15	27 (1%) 67 58	61, 90, 153, 177	0
2	B	1106/1224 (90%)	-0.16	18 (1%) 72 63	57, 85, 129, 160	0
3	C	266/318 (83%)	-0.36	2 (0%) 86 79	67, 83, 112, 124	0
4	E	214/215 (99%)	-0.06	6 (2%) 53 43	75, 119, 155, 165	0
5	F	84/155 (54%)	-0.32	0 100 100	72, 95, 115, 119	0
6	H	133/146 (91%)	0.01	5 (3%) 41 33	96, 109, 138, 142	0
7	I	119/122 (97%)	-0.25	1 (0%) 86 79	75, 99, 121, 136	0
8	J	65/70 (92%)	-0.42	0 100 100	66, 79, 99, 106	0
9	K	114/120 (95%)	-0.41	0 100 100	71, 87, 98, 100	0
10	L	46/70 (65%)	0.15	3 (6%) 20 14	93, 144, 156, 157	0
11	R	11/12 (91%)	-0.24	1 (9%) 10 8	65, 94, 118, 135	0
12	T	12/29 (41%)	-0.52	0 100 100	73, 91, 126, 135	0
All	All	3565/4214 (84%)	-0.18	63 (1%) 69 60	57, 90, 146, 177	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	6.0
1	A	1176	LEU	5.6
2	B	1223	ASP	5.0
4	E	118	PRO	4.9
2	B	1222	ARG	4.6

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
13	ZN	B	1307	1/1	0.98	0.14	-1.16	141,141,141,141	0
13	ZN	I	203	1/1	0.98	0.12	-1.37	148,148,148,148	0
13	ZN	A	1735	1/1	0.94	0.05	-1.67	118,118,118,118	0
13	ZN	I	204	1/1	0.99	0.05	-1.72	107,107,107,107	0
13	ZN	J	101	1/1	0.95	0.20	-1.76	187,187,187,187	0
13	ZN	C	319	1/1	0.98	0.05	-1.81	83,83,83,83	0
13	ZN	L	105	1/1	0.93	0.04	-2.08	169,169,169,169	0
13	ZN	A	1734	1/1	0.94	0.04	-2.41	128,128,128,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.