



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2026 – 09:56 AM EDT

PDB ID : 8UKQ / pdb_00008ukq
Title : RNA polymerase II elongation complex with Fapy-dG lesion in apo state
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2023-10-15
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

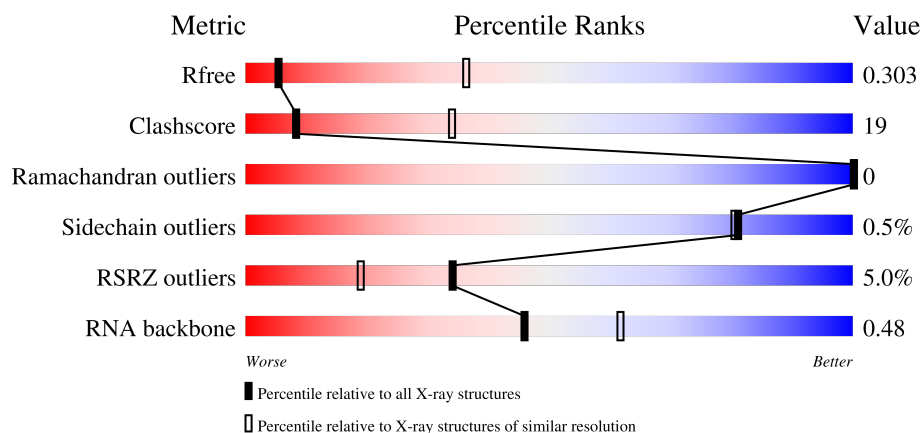
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	R	9	44% 44% 11%
2	T	29	17% 66% 17%
3	N	18	28% 44% 28%
4	A	1733	4% 46% 34% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 28981 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 2 is a DNA chain called tsDNA with FapydG lesion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	24	Total	C	N	O	P	0	0	0
			481	230	76	151	24			

- Molecule 3 is a DNA chain called ntsDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			275	128	61	73	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1126	Total	C	N	O	S	0	0	0
			8874	5616	1555	1650	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- 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

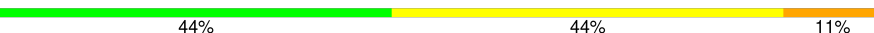
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

3 Residue-property plots

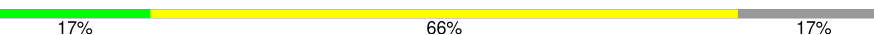
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain R: 

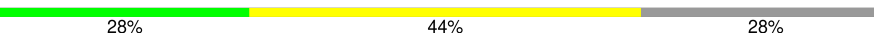


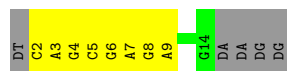
• Molecule 2: tsDNA with FapydG lesion

Chain T: 



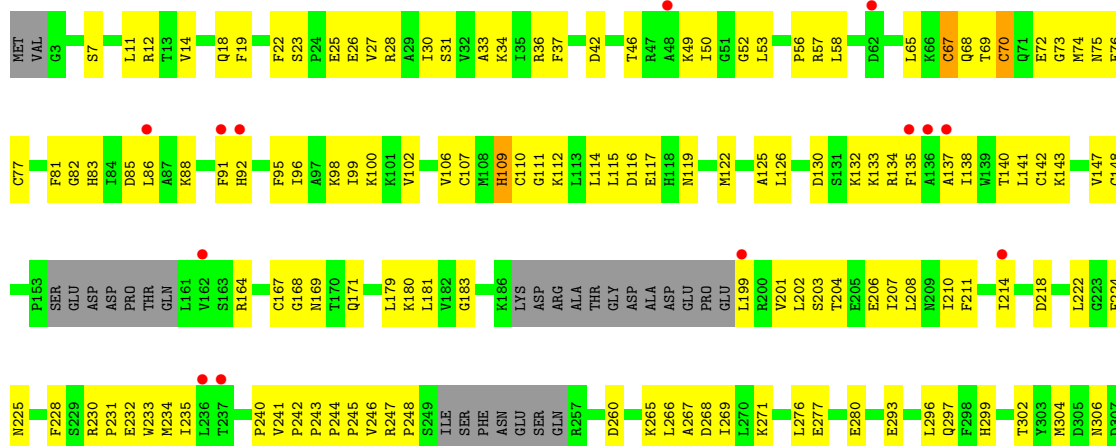
• Molecule 3: ntsDNA

Chain N: 



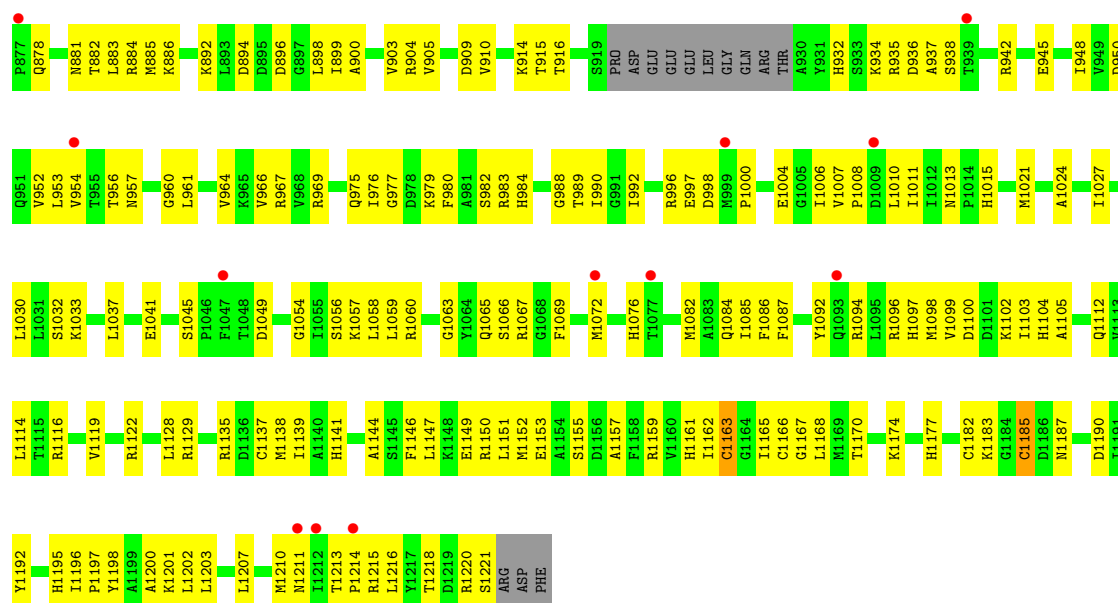
• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A: 

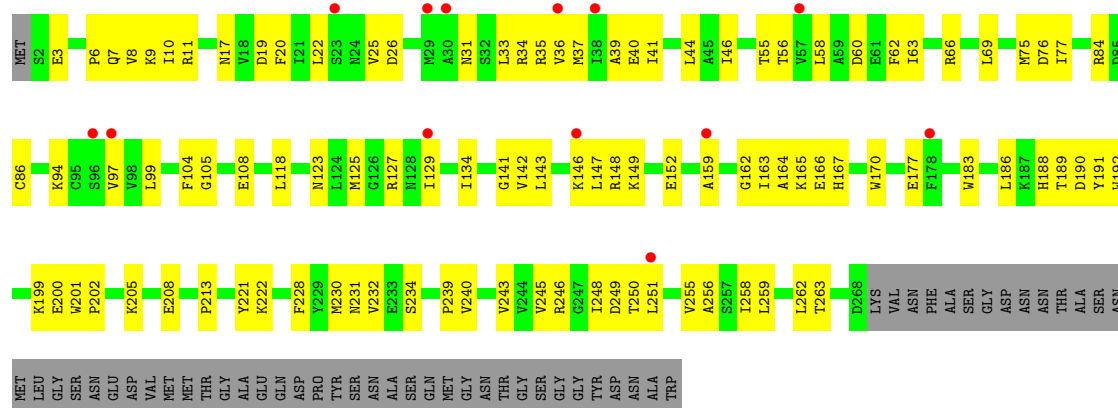


M1444	N1364	R1274	R1199	L1104	R1025	L936	L845	K752	L658	S573	R498	H399	I308
I1445	Y1365	E1277	M1202	L1105	L1026	D939	H851	T756	H659	G574	A499	L415	Q311
D1446	R1366	N1278	M1202	M1111	T1028	D939	T1028	T756	F662	Q575	E500	L415	P312
GLU	H1367	V1282	D1206	P1114	R1029	K941	T856	Q760	T664	L577	A506	R420	Q316
SER	M1283	L1207	L1207	S1115	R1030	F942	R857	M761	G665	S579	V507	D423	R320
LEU	M1284	T1208	T1208	V1118	R1031	L943	R858	W765	I666	T582	P508	D423	R320
VAL	M1285	L1032	L1032	Q1033	R1032	R944	R859	G766	G667	P583	L509	L424	R320
TYR	L1371	Q1033	Q1033	Y1035	Q1034	V946	G861	Q767	T668	P583	V512	L426	K323
MET	V1372	E1129	E1129	E1034	R1036	E951	Q865	R774	I670	H587	S513	V432	K323
PRO	R1288	R1036	R1036	L1037	R1037	E952	Q865	R775	A671	D672	P514	F433	K323
GLU	R1289	L1037	L1037	T1038	T1038	N953	F866	A776	D672	D592	Q515	R434	K326
GLN	L1216	K1132	K1132	K1039	K1039	W954	R867	F777	G673	E593	S516	R436	K327
ILE	K1217	L1134	L1134	R1135	R1135	P955	Y868	G778	P674	G594	N517	H436	K328
THR	Q1218	R1135	R1135	L1136	L1136	L956	G869	F779	T675	T595	K318	V433	K332
GLU	T1219	S1136	S1136	A1137	D1042	P957	E870	W780	M676	T596	P519	M439	K332
ILE	T1220	A1137	A1137	V1044	V1044	I960	G872	D781	R677	L597	C520	V442	K336
GLU	K1221	L1138	L1138	V1045	V1045	R961	R873	R782	E678	K601	G522	V442	K337
ASP	L1224	E1139	E1139	L1046	L1046	R962	D874	T783	I679	M605	W523	L443	G338
GLY	F1225	H1140	H1140	N1047	N1047	I963	A875	P785	I683	L606	D526	R446	N339
GLN	V1226	L1143	L1143	E1049	E1049	I963	A875	H786	I683	L606	D526	P447	L340
ASP	I1227	L1143	L1143	E1050	E1050	I973	H877	H786	A684	I607	T527	P448	G341
GLY	S1229	T1148	T1148	A1051	A1051	D974	R878	K789	K687	I608	L528	P448	K343
GLY	K1235	A1149	A1149	R1055	R1055	H975	E879	D790	K688	I608	C529	H451	K344
VAL	L1236	S1150	S1150	R1055	R1055	I981	K880	P794	L691	Q611	G530	K452	R350
THR	I1237	E1151	E1151	S1056	S1056	L981	Q881	W795	I613	I612	T531	M455	T351
PRO	S1401	E1165	E1165	V1057	V1057	I986	S882	S796	K695	I613	R532	M455	T351
TYR	F1402	D1166	D1166	V1058	V1058	I986	T885	G797	E696	F614	K533	M456	V352
SER	E1403	E1167	E1167	G1061	G1061	V990	T885	G797	A697	V617	L534	A457	I353
ASN	A1404	L1170	L1170	G1065	G1065	V990	D890	F799	Q698	E818	T535	A458	S354
GLU	V1405	Q1171	Q1171	A1069	A1069	L993	R898	W800	Q698	L619	L536	R459	G355
SER	V1406	L1169	L1169	Q1070	Q1070	L993	V899	R801	A704	K619	R537	P464	D356
LEU	V1407	E1176	E1176	S1071	S1071	L993	D900	S803	L710	T621	D538	Y465	E360
LEU	I1408	L1176	L1176	E1074	E1074	L1000	L901	Y804	R711	V622	T539	P464	L361
VAL	A1416	L1176	L1176	E1074	E1074	L1000	L901	R806	L718	G623	L547	Y465	D362
ASN	E1417	L1176	L1176	T1077	T1077	L1004	H906	E812	L722	S625	N548	R469	V364
ASP	L1418	L1176	L1176	L1081	L1081	L1005	T907	F813	D727	N626	N549	L470	G365
ASP	N1330	L1176	L1176	ASN	ASN	E1005	L908	F814	K728	V633	L550	Y471	K368
LEU	S1331	L1176	L1176	THR	THR	I1006	L908	F815	A729	T634	V551	L472	S389
ASP	F1332	L1176	L1176	THR	THR	I1007	P909	R818	C642	R635	W556	V474	I370
VAL	I1333	L1176	L1176	HIS	HIS	A1010	L912	M818	G642	V633	V559	Y478	T375
LYS	D1334	L1176	L1176	PHE	PHE	Q1011	L913	G819	K730	T634	V559	Y478	Y376
ASP	I1335	L1176	L1176	PHE	PHE	Q1011	L913	G819	G731	R635	V559	Y478	Y376
GLU	M1336	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
LEU	E1337	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
MET	V1428	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
PHE	I1429	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
SER	L1430	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
SER	G1431	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
LEU	R1345	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
VAL	R1346	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
VAL	A1434	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
ASP	P1435	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
ASP	A1347	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
SER	L1348	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
GLY	G1437	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
SER	T1438	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
ASN	E1351	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376
ASP	F1441	L1176	L1176	ALA	ALA	A1014	S915	G820	L732	N645	V559	Y478	Y376

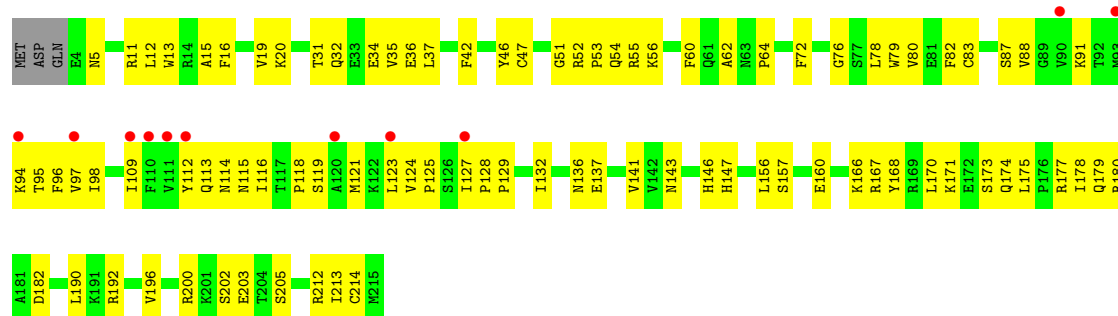




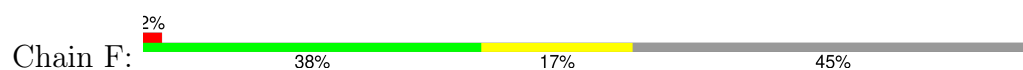
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



MET SER ASP TTR GLU ALA PHE ASN ASP GLY ASN GLU PHE ASP PHE VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU LYS PRO GLN PHE LYS ASP GLY THR THR THR LYS ASN GLY THR ASN GLY ASP PRO GLN

HIS GLU GLN ILE ARG LYS THR L69 K70 E71 I74 T81 T82 P83 Y84 M85 Y88 E89 R90 A91 R92 I93 R97 Q100 M103 V109 D110 L111 D116 R119 K123 E124 L125 L132 R135 R136 P139 E144 V148 V153 D154 LEU

- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



MET S2 F6 D8 V15 Y20 V23 I26 E27 C36 K37 L38 T39 L40 D41 L46 F47 T56 V57 T58 L63 ASN LEU GLU ASP THR PRO ALA ASN SER SER ALA T76 R77 S78 L89 A90 D91 D92 Y93 D94 Y95 V96 M97 Y98 G99 T100 A101

Y102 E105 E106 L111 I112 Y115 Y116 S117 F118 G119 G120 L121 L122 M123 R124 L125 L126 G127 N128 Y129 R130 R131 L135 K136 Q137 L142 L143 I144 R145 R146

- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



MET T2 F6 C7 G10 M11 M12 M13 L14 E18 D19 K20 L26 F27 F28 C29 R30 T31 C32 S33 Y34 V35 E36 E37 S40 P41 L42 R45 R48 I52 G53 E54 Q60 D61 I62 D65 P66 T67 L68 P69 R70 R73 E74 C75 C78 R81 E82

R83 V84 F85 F86 Q87 R97 F100 F101 V102 G103 L104 S105 C106 F110 T111 S112 T119 PHE GLN SER

- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



H1 I2 V3 P4 C7 F8 S9 G15 D16 K17 S20 Y21 L24 D28 E29 L30 G33 T34 A35 L36 S37 R38 L39 G40 L41 Y44 C45 R48 M49 I50 L51 T52 H53 V54 D55 L56 I57 E58 K59 F60 L61 M64 P65 LEU GLU LYS ARG ASP

- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



H1 N2 A3 P4 D5 R6 F7 E8 L9 F10 L11 E14 L19 K20 I21 T25 K26 N29 A30 V31 V32 I33 K37 E38 D39 L42 L46 R47 A48 E49 K55 V56 L57 F58 Y61 H65 P66 F67 F71 K72 L73 R74 I75 Q76 T77 Y81 K84

P85 A86 L87 I94 K97 L98 G99 A100 L101 K102 T103 M104 F105 E108 T113 L114 ALA ALA ASP ASP ALA PHE

- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



MET	SER	ARG	GLU	GLY	PHE	GLN	TLE	PRO	THR	ASN	LEU	ASP	ALA	ALA	ALA	GLY	THR	SER	GLN	ALA	ARG	THR	ALA	THR	LEU	K28	Y29	I30	C31	A32	E33	K37	L38	S39	L40	R47	C48	C51	R54	I55	L56	T61	K62	Q66	F67	R70
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.54Å 223.49Å 191.47Å 90.00° 98.38° 90.00°	Depositor
Resolution (Å)	48.44 – 3.50 48.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.44-3.50) 99.3 (48.44-3.50)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.268 , 0.302 0.268 , 0.303	Depositor DCC
R_{free} test set	2000 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	94.4	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28981	wwPDB-VP
Average B, all atoms (Å ²)	123.0	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, 0.333 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: MG, ZN, WVQ

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	R	0.14	0/218	0.36	0/339
2	T	0.22	0/507	0.50	0/775
3	N	0.20	0/311	0.39	0/479
4	A	0.17	0/11020	0.42	2/14907 (0.0%)
5	B	0.16	0/9046	0.39	0/12210
6	C	0.15	0/2139	0.37	0/2899
7	E	0.16	0/1767	0.39	0/2378
8	F	0.14	0/696	0.36	0/943
9	H	0.20	0/1082	0.50	0/1466
10	I	0.14	0/970	0.41	0/1308
11	J	0.18	0/541	0.44	0/727
12	K	0.17	0/937	0.44	0/1265
13	L	0.16	0/339	0.42	0/450
All	All	0.17	0/29573	0.41	2/40146 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	56	PRO	CA-C-N	5.53	132.10	121.54
4	A	56	PRO	C-N-CA	5.53	132.10	121.54

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	R	194	0	98	6	0
2	T	481	0	262	18	0
3	N	275	0	144	11	0
4	A	10828	0	10876	484	0
5	B	8874	0	8823	365	0
6	C	2101	0	2056	91	0
7	E	1731	0	1758	66	0
8	F	684	0	692	19	0
9	H	1064	0	1029	58	0
10	I	952	0	897	45	0
11	J	532	0	542	31	0
12	K	919	0	929	48	0
13	L	337	0	352	14	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	28981	0	28458	1100	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 19.

The worst 5 of 1100 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)
12:K:30:ALA:HA	12:K:75:ILE:O	1.74	0.88
4:A:613:ILE:HG21	9:H:102:TYR:HB3	1.57	0.85
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.60	0.84
4:A:109:HIS:CE1	4:A:110:CYS:SG	2.71	0.83
4:A:672:ASP:H	4:A:736:ASN:HD21	1.27	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
4	A	1370/1733 (79%)	1341 (98%)	29 (2%)	0	100	100
5	B	1108/1224 (90%)	1088 (98%)	20 (2%)	0	100	100
6	C	265/318 (83%)	263 (99%)	2 (1%)	0	100	100
7	E	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
10	I	116/122 (95%)	114 (98%)	2 (2%)	0	100	100
11	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
12	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3498/4173 (84%)	3429 (98%)	69 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	A	1194/1520 (79%)	1190 (100%)	4 (0%)	86	83
5	B	955/1061 (90%)	952 (100%)	3 (0%)	86	83
6	C	235/274 (86%)	234 (100%)	1 (0%)	84	81
7	E	193/197 (98%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	73/137 (53%)	72 (99%)	1 (1%)	59	71
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	106 (96%)	4 (4%)	31	57
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	70
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	36 (97%)	1 (3%)	39	62
All	All	3072/3657 (84%)	3057 (100%)	15 (0%)	81	80

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C	86	CYS
11	J	7	CYS
8	F	124	GLU
13	L	31	CYS
10	I	32	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	1179	GLN
10	I	60	GLN
5	B	1187	ASN
7	E	115	ASN
12	K	92	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	7/9 (77%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	WVQ	T	19	2	19,24,25	3.62	7 (36%)	18,33,36	1.57	4 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WVQ	T	19	2	-	4/6/40/41	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	WVQ	C5-N7	12.72	1.46	1.28
2	T	19	WVQ	C4-N9	4.83	1.45	1.35
2	T	19	WVQ	C2-N2	4.17	1.45	1.34
2	T	19	WVQ	C6-C5	-3.93	1.36	1.47
2	T	19	WVQ	C6-N1	-3.21	1.32	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	WVQ	N3-C2-N1	-4.25	119.71	126.44
2	T	19	WVQ	C2'-C3'-C4'	2.48	107.83	102.80
2	T	19	WVQ	N2-C2-N3	2.18	120.04	116.57
2	T	19	WVQ	N2-C2-N1	2.04	120.25	117.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	WVQ	O4'-C4'-C5'-O5'
2	T	19	WVQ	C3'-C4'-C5'-O5'
2	T	19	WVQ	C4'-C5'-O5'-P
2	T	19	WVQ	O4'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	R	9/9 (100%)	0.51	0	100	100	104, 120, 189, 222	0
2	T	23/29 (79%)	0.67	0	100	100	107, 185, 252, 281	0
3	N	13/18 (72%)	0.46	0	100	100	203, 228, 274, 280	0
4	A	1384/1733 (79%)	0.44	66 (4%)	35	19	77, 117, 187, 248	0
5	B	1126/1224 (91%)	0.51	59 (5%)	33	19	47, 108, 163, 210	0
6	C	267/318 (83%)	0.46	13 (4%)	35	19	46, 100, 155, 201	0
7	E	212/215 (98%)	0.44	11 (5%)	33	19	88, 137, 215, 274	0
8	F	86/155 (55%)	0.27	3 (3%)	47	26	80, 108, 157, 183	0
9	H	133/146 (91%)	0.37	5 (3%)	44	24	90, 137, 196, 280	0
10	I	118/122 (96%)	0.32	2 (1%)	69	43	93, 133, 178, 231	0
11	J	65/70 (92%)	0.70	9 (13%)	6	5	47, 100, 133, 150	0
12	K	114/120 (95%)	0.33	6 (5%)	32	18	64, 108, 144, 179	0
13	L	43/70 (61%)	0.95	5 (11%)	9	6	94, 170, 235, 272	0
All	All	3593/4229 (84%)	0.46	179 (4%)	34	19	46, 115, 186, 281	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	775	LYS	6.5
5	B	543	SER	6.5
7	E	93	MET	5.8
5	B	779	GLY	5.2
7	E	112	TYR	5.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	WVQ	T	19	23/24	0.83	0.14	140,145,169,176	0

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(Å ²)	Q<0.9
14	ZN	I	202	1/1	0.80	0.10	273,273,273,273	0
14	ZN	L	101	1/1	0.81	0.14	363,363,363,363	0
14	ZN	A	1801	1/1	0.91	0.08	301,301,301,301	0
14	ZN	C	401	1/1	0.96	0.07	120,120,120,120	0
15	MG	A	1803	1/1	0.97	0.05	129,129,129,129	0
14	ZN	B	1301	1/1	0.98	0.04	204,204,204,204	0
14	ZN	J	101	1/1	0.98	0.10	133,133,133,133	0
14	ZN	A	1802	1/1	0.98	0.03	167,167,167,167	0
14	ZN	I	201	1/1	0.98	0.04	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.