



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:36 AM UTC

PDB ID : 2B63 / pdb\_00002b63  
Title : Complete RNA Polymerase II-RNA inhibitor complex  
Authors : Kettenberger, H.; Eisenfuehr, A.; Brueckner, F.; Theis, M.; Famulok, M.; Cramer, P.  
Deposited on : 2005-09-30  
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](mailto: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>.

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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

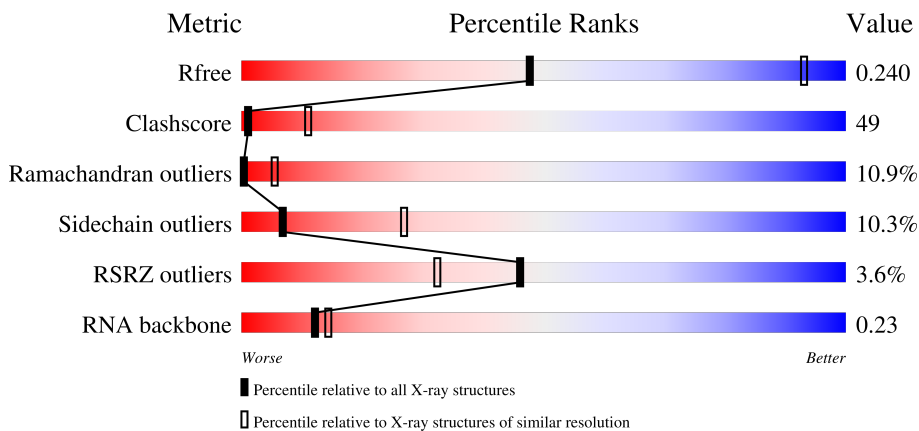
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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  $\geq 3$ , 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	31	
2	A	1733	
3	B	1224	
4	C	318	

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
5	D	221	
6	E	215	
7	F	155	
8	G	171	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 31731 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 31-MER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
1	R	31	666	4	296	119	217	30	88	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	1416	11140	7021	1946	2111	62	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	1112	8836	5594	1548	1639	55	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	266	2095	1317	348	417	13	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	177	1356	840	241	273	2	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	214	1752	1111	309	321	11	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	F	84	679	434	115	127	3	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	G	171	1340	861	222	249	8	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	133	1068	673	180	211	4	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	115	924	593	157	172	2	0	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

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

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

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

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

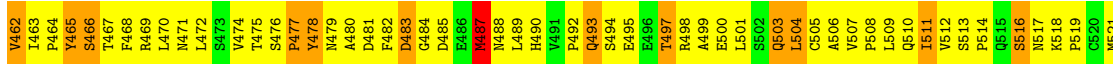
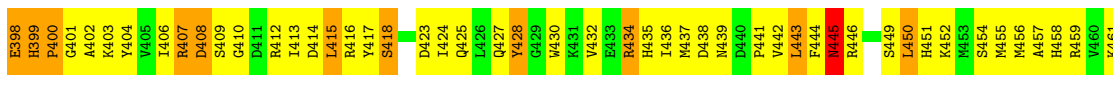
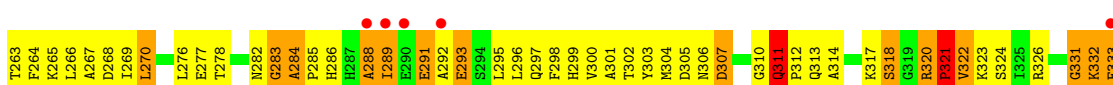
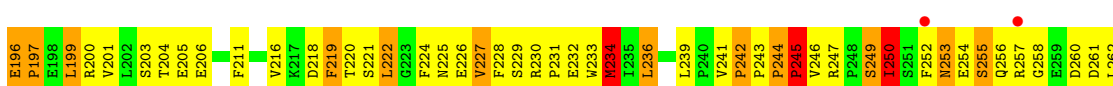
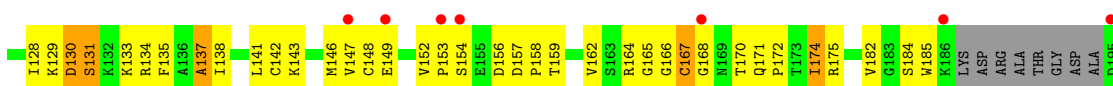
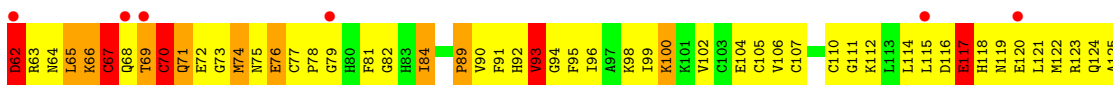
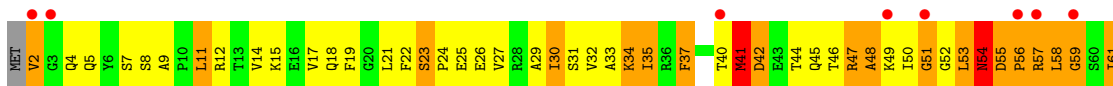
### 3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 31-MER



- Molecule 2: DNA-directed RNA polymerase II largest subunit

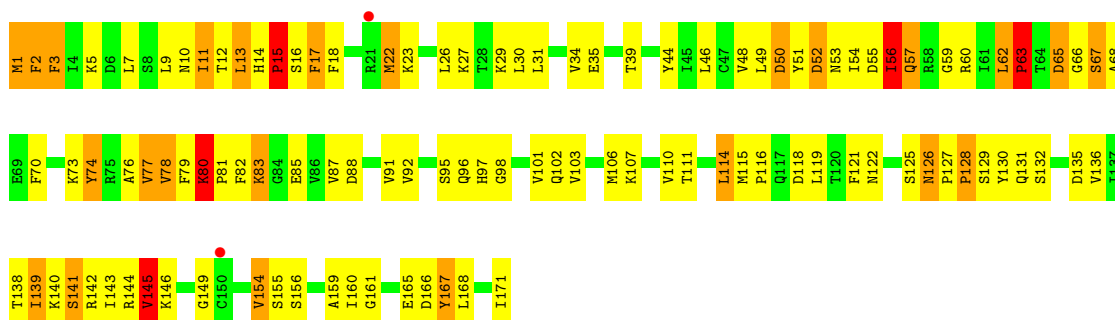


LEU	I1429	H1367	K1300	L1236	I1163	K1092	A1027	T809	L740	L658	H587	G522
MET	L1430	M1368	E1301	I1237	D1166	K1093	A1028	P810	N741	L658	L588	I523
PHE	L1431	A1369	E1302	I1238	D1166	V1094	T1028	Q811	N742	L658	Q589	Q524
SER	Q1432	L1370	E1303	R1239	D1166	T1095	R1029	Q812	N743	S663	R590	Q525
PRO	M1433	L1371	V1304	R1240	I1170	S1096	R1030	F813	N744	T664	F591	D526
LEU	A1434	V1372	V1305	R1241	I1170	G1097	V1031	F814	N745	G665	F592	T527
VAL	P1435	D1373	L1306	V1242	H1173	V1098	L1032	F815	N746	I666	D528	L528
ASP	I1436	V1374	E1307	V1243	H1173	P1099	Q1033	H816	N747	G667	T595	G529
SER	G1437	M1375	T1308	ARG	L1176	R1100	E1034	R817	N748	D688	T596	G530
GLY	T1438	T1376	D1309	PRO	ASP	L1101	Y1035	M818	G751	T675	L597	R531
SER	G1439	T1377	LYS	LEU	LEU	K1102	R1036	R821	K752	M676	L598	R532
ASN	A1440	Q1378	SER	SER	GLU	M1106	L1037	G822	G753	P600	K533	K533
ASP	F1441	Q1379	LEU	LEU	ALA	V1107	K1038	G823	S754	K601	L534	L534
ALA	D1442	G1380	ASP	ASP	ALA	V1107	K1039	G823	S754	K601	T535	T535
MET	V1443	L1381	ALA	ALA	GLN	M1111	Q1040	R896	F755	N602	L536	L536
GLY	M1444	V1384	GLN	GLU	GLN	M1111	Q1041	R896	F755	N602	L536	L536
GLY	I1445	T1385	GLU	GLU	GLN	K1112	D1042	I625	T756	G604	D538	D538
GLY	D1446	R1386	THR	THR	SER	T1113	F1043	R898	N757	I683	G604	G604
PHE	E1447	H1387	PHE	PHE	PHE	P1114	V1044	R899	N758	I684	M605	T539
THR	E1448	H1387	ASP	ASP	ASP	S1115	V1044	D900	A828	E685	L606	F540
ALA	S1449	G1388	Q1187	Q1187	Q1187	L1116	L1045	L901	G766	A686	L607	I541
ALA	L1450	F1389	S1189	S1189	S1189	L1116	L1046	L902	N761	V690	L608	E542
GLY	V1451	N1390	P1190	P1190	P1190	V1118	S1047	N903	S762	D609	L543	L543
GLY	L1452	R1391	V1191	V1191	V1191	I1119	N1048	A832	C764	G610	D544	D544
ALA	M1454	S1392	L1192	L1192	L1192	L1120	E1060	E833	V765	Q611	Q545	Q545
ASP	F1455	N1393	L1193	K1261	L1193	E1121	E1060	G835	G766	L612	V546	V546
TYR	G1456	T1394	R1194	K1262	R1194	P1122	V1057	Y836	Q767	L613	L547	L547
GLY	L1457	G1395	L1195	L1263	L1195	P1122	V1058	Y837	Q768	G615	M548	M548
GLY	L1458	A1396	L1196	L1264	L1196	A1124	H1059	R908	Q768	G615	L550	L550
ALA	I1459	L1397	E1196	E1264	E1196	H1125	P1060	Q838	R774	V616	L551	L551
THR	T1460	M1398	D1198	N1265	L1197	A1126	G1061	R840	I775	E618	W552	W552
SER	L1461	H1399	L1198	M1267	D1198	D1127	E1062	L841	A776	K619	V553	V553
PRO	L1462	C1400	A1201	M1268	A1201	Q1128	M1063	V842	F779	K620	P554	P554
PHE	L1463	S1401	M1202	L1268	M1202	Q1128	V1064	K843	R779	L621	I560	I560
GLY	L1464	F1402	K1205	I1271	K1205	Q1130	A1068	L944	R782	F714	P561	P561
ALA	L1465	E1403	D1206	T1272	D1206	K1132	A1068	L945	T783	E715	T562	T562
TYR	L1466	E1404	L1207	L1273	L1207	L1133	A1069	E846	L784	D716	P563	P563
GLY	L1467	T1405	T1208	R1274	T1208	L1134	Q1070	D847	F785	R717	A564	A564
GLY	L1468	V1406	T1208	G1275	T1208	R1135	S1071	M849	H786	V718	I565	I565
ALA	L1469	L1410	M1209	G1276	M1209	G1136	I1072	V826	V719	L629	L629	L629
PRO	L1470	F1411	Q1210	N1278	Q1210	S1136	G1073	V927	R720	I630	I630	I630
THR	L1471	F1411	Q1211	E1278	Q1211	E1139	L1074	H851	K789	H631	H631	H631
PRO	L1472	A1412	V1212	I1279	V1212	E1139	P1075	Y852	D790	V632	V632	V632
GLY	L1473	G1413	G1213	E1280	G1213	E1139	A1076	D853	D791	V633	V633	V633
PHE	L1474	A1414	E1214	R1281	E1214	T1142	A1076	M854	R723	E636	E636	E636
ASN	L1475	A1414	R1215	V1282	R1215	L1143	T1077	T855	E724	E724	E724	E724
GLY	L1476	S1415	I1216	V1283	I1216	K1144	Q1008	T856	A725	A725	A725	A725
VAL	L1477	A1416	K1217	M1284	K1217	S1145	M1079	R857	S796	R726	P639	P639
SER	L1478	F1417	Q1218	M1284	Q1218	V1146	A1010	N858	K797	D727	Q640	Q640
SER	L1479	L1418	T1219	R1289	T1219	T1147	T1080	S859	G798	K728	L645	L645
PRO	L1480	D1419	F1220	R1289	F1220	I1148	L1081	L860	F799	A729	L645	L645
GLY	L1481	V1291	K1221	K1290	K1221	A1149	ASN	L860	V800	G730	F646	F646
ASN	L1482	P1292	M1222	P1292	M1222	S1150	THR	G861	V800	G730	F646	F646
PHE	L1483	L1293	I1223	L1293	I1223	H1151	PHE	N862	E801	R731	G647	G647
ASP	L1484	G1294	L1224	L1294	L1224	H1152	HIS	R940	N802	R731	G647	G647
PRO	L1485	T1295	F1225	L1295	F1225	I1152	ALA	K941	H802	L732	L578	L578
THR	L1486	G1296	V1226	L1296	V1226	D1155	GLY	F942	S803	A733	S579	S579
SER	L1487	M1364	V1227	L1296	V1227	L1021	ALA	L943	H804	E734	V500	V500
PRO	L1488	E1426	W1227	L1296	W1227	L1021	GLY	I867	L805	E734	Q650	Q650
THR	L1489	M1427	W1228	L1298	W1228	L1022	VAL	Y868	R806	L737	K651	K651
GLY	L1490	R1366	L1228	L1298	L1228	L1161	ALA	G869	G807	K738	V652	V652
TYR	L1491	R1366	L1228	L1299	L1228	V1162	SER	E870	L808	D739	N654	N654

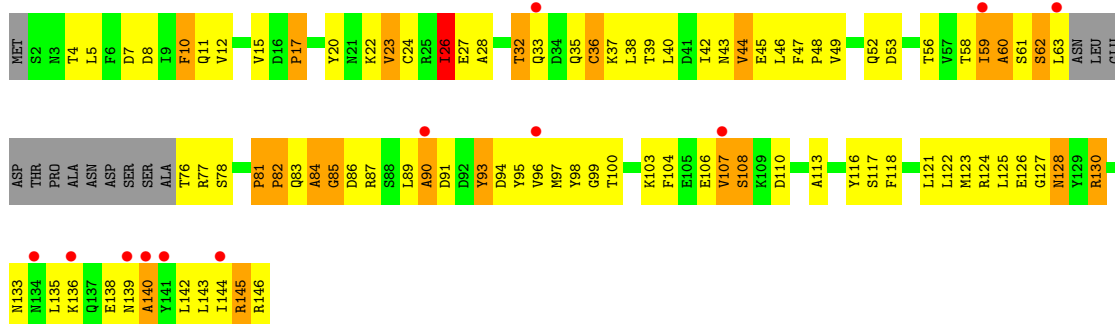




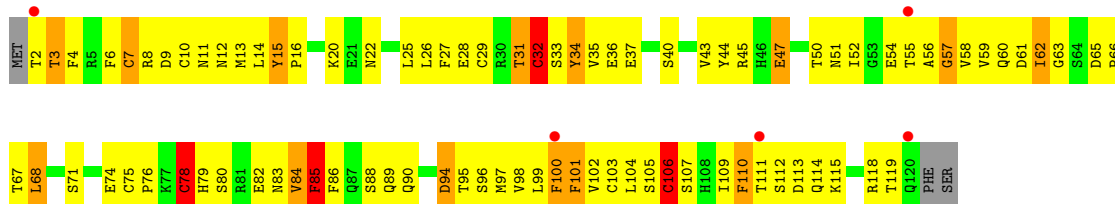




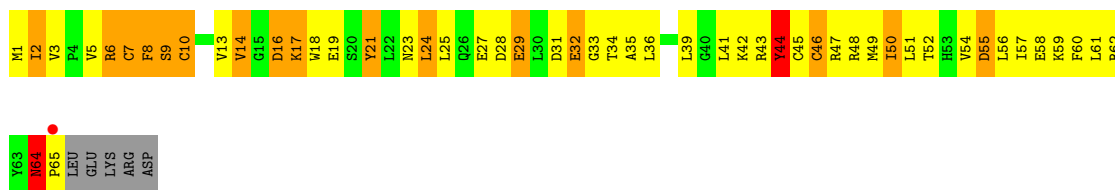
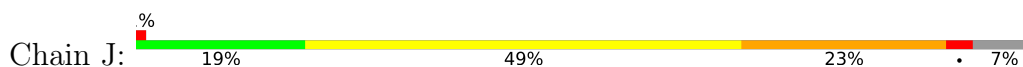
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



- Molecule 10: DNA-directed RNA polymerase II subunit 9

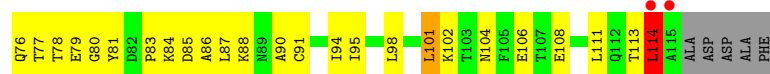
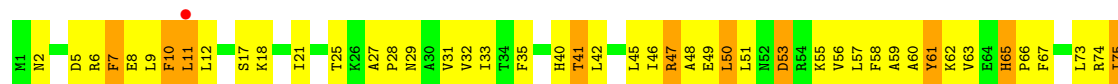


- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

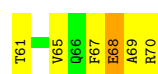
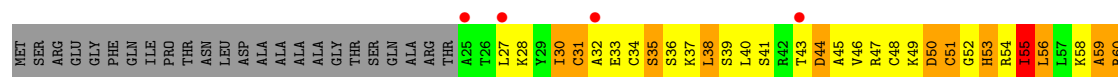


- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide





- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.59Å 399.81Å 286.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.80) 99.8 (50.00-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.252 , 0.273 0.213 , 0.240	Depositor DCC
$R_{free}$ test set	8121 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.4	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 84.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, 5BU, 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	R	0.80	3/652 (0.5%)	1.08	3/1017 (0.3%)
2	A	0.59	2/11339 (0.0%)	1.11	86/15334 (0.6%)
3	B	0.57	0/9008	1.16	76/12146 (0.6%)
4	C	0.56	0/2133	1.16	18/2891 (0.6%)
5	D	0.54	0/1365	1.09	13/1837 (0.7%)
6	E	0.51	0/1788	1.09	15/2406 (0.6%)
7	F	0.71	0/691	1.17	6/933 (0.6%)
8	G	0.58	0/1368	1.20	13/1844 (0.7%)
9	H	0.45	0/1086	0.97	4/1470 (0.3%)
10	I	0.43	0/989	1.16	11/1331 (0.8%)
11	J	0.59	0/541	1.14	3/727 (0.4%)
12	K	0.52	0/942	0.98	4/1272 (0.3%)
13	L	0.62	0/365	1.03	3/485 (0.6%)
All	All	0.58	5/32267 (0.0%)	1.12	255/43693 (0.6%)

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	R	0	2
11	J	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	28	5BU	O3'-P	7.88	1.64	1.56
1	R	12	5BU	O3'-P	7.34	1.63	1.56
2	A	1273	LEU	CA-C	5.47	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	17	5BU	O3'-P	5.07	1.61	1.56
2	A	250	ILE	CA-CB	5.02	1.61	1.54

The worst 5 of 255 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	508	LEU	N-CA-C	-22.89	86.78	108.75
3	B	275	TYR	N-CA-C	-14.72	95.27	113.23
2	A	56	PRO	N-CA-C	-13.55	100.59	114.68
3	B	1185	CYS	N-CA-C	-13.49	95.36	114.12
3	B	464	GLY	N-CA-C	-11.63	100.04	115.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	44	TYR	Sidechain
1	R	2	C	Sidechain
1	R	5	C	Sidechain

## 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	666	0	331	42	0
2	A	11140	0	11217	1183	0
3	B	8836	0	8871	984	0
4	C	2095	0	2051	253	0
5	D	1356	0	1319	127	0
6	E	1752	0	1776	142	0
7	F	679	0	701	60	0
8	G	1340	0	1357	144	0
9	H	1068	0	1040	126	0
10	I	971	0	928	92	0
11	J	532	0	542	93	0
12	K	924	0	934	86	0
13	L	363	0	386	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	31731	0	31453	3118	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 49.

The worst 5 of 3118 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)
5:D:40:HIS:HB3	8:G:73:LYS:NZ	1.60	1.16
2:A:1329:THR:HG22	2:A:1331:SER:H	1.01	1.12
3:B:827:ILE:HG12	3:B:1012:ILE:HD11	1.18	1.11
3:B:463:THR:HB	3:B:465:ASN:HB2	1.32	1.10
1:R:3:A:OP2	3:B:531:GLN:HB3	1.50	1.10

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
2	A	1406/1733 (81%)	973 (69%)	278 (20%)	155 (11%)	<b>0</b> <b>5</b>
3	B	1096/1224 (90%)	754 (69%)	214 (20%)	128 (12%)	<b>0</b> <b>4</b>
4	C	264/318 (83%)	172 (65%)	62 (24%)	30 (11%)	<b>0</b> <b>5</b>
5	D	173/221 (78%)	116 (67%)	36 (21%)	21 (12%)	<b>0</b> <b>4</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	212/215 (99%)	155 (73%)	42 (20%)	15 (7%)	1	12
7	F	82/155 (53%)	72 (88%)	9 (11%)	1 (1%)	10	40
8	G	169/171 (99%)	133 (79%)	19 (11%)	17 (10%)	0	7
9	H	129/146 (88%)	89 (69%)	23 (18%)	17 (13%)	0	3
10	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	0	8
11	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
12	K	113/120 (94%)	83 (74%)	25 (22%)	5 (4%)	2	19
13	L	44/70 (63%)	19 (43%)	16 (36%)	9 (20%)	0	1
All	All	3868/4565 (85%)	2684 (69%)	761 (20%)	423 (11%)	0	5

5 of 423 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	31	SER
2	A	48	ALA
2	A	55	ASP
2	A	57	ARG
2	A	58	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	1239/1520 (82%)	1133 (91%)	106 (9%)	10	33
3	B	964/1061 (91%)	840 (87%)	124 (13%)	4	20
4	C	234/274 (85%)	211 (90%)	23 (10%)	7	29
5	D	140/200 (70%)	123 (88%)	17 (12%)	5	21
6	E	196/197 (100%)	185 (94%)	11 (6%)	19	45
7	F	74/137 (54%)	63 (85%)	11 (15%)	3	16
8	G	152/152 (100%)	134 (88%)	18 (12%)	5	22
9	H	117/128 (91%)	112 (96%)	5 (4%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	113/116 (97%)	97 (86%)	16 (14%)	3	17
11	J	60/65 (92%)	51 (85%)	9 (15%)	3	16
12	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
13	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	3428/4009 (86%)	3076 (90%)	352 (10%)	7	27

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	22	LEU
7	F	110	ASP
4	C	89	GLU
5	D	180	LEU
8	G	56	ILE

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

Mol	Chain	Res	Type
3	B	538	ASN
3	B	1179	GLN
10	I	11	ASN
3	B	587	HIS
3	B	975	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	31/31 (100%)	16 (51%)	3 (9%)

5 of 16 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	3	A
1	R	6	A
1	R	7	C
1	R	8	U
1	R	9	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	2	C
1	R	5	C
1	R	6	A

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

4 non-standard protein/DNA/RNA residues are 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
1	5BU	R	27	1	19,22,23	0.50	0	27,32,35	1.43	4 (14%)
1	5BU	R	17	1	19,22,23	0.40	0	27,32,35	1.16	1 (3%)
1	5BU	R	12	1	19,22,23	1.31	1 (5%)	27,32,35	1.59	6 (22%)
1	5BU	R	28	1	19,22,23	1.93	1 (5%)	27,32,35	1.57	4 (14%)

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
1	5BU	R	27	1	-	2/7/25/26	0/2/2/2
1	5BU	R	17	1	-	0/7/25/26	0/2/2/2
1	5BU	R	12	1	-	0/7/25/26	0/2/2/2
1	5BU	R	28	1	-	4/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	28	5BU	BR-C5	7.53	2.06	1.88
1	R	12	5BU	BR-C5	4.89	1.99	1.88

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	R	27	5BU	BR-C5-C4	4.75	123.49	118.02
1	R	28	5BU	C6-C5-C4	-4.15	116.46	120.67
1	R	28	5BU	O3'-C3'-C2'	4.09	124.92	111.82
1	R	17	5BU	BR-C5-C4	3.70	122.28	118.02
1	R	12	5BU	C1'-N1-C6	3.50	126.92	121.15

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	R	27	5BU	O4'-C4'-C5'-O5'
1	R	28	5BU	O4'-C4'-C5'-O5'
1	R	28	5BU	C3'-C4'-C5'-O5'
1	R	27	5BU	C3'-C4'-C5'-O5'
1	R	28	5BU	C4'-C5'-O5'-P

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	27	5BU	1	0
1	R	17	5BU	3	0
1	R	12	5BU	4	0
1	R	28	5BU	4	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	R	23/31 (74%)	0.51	2 (8%) 16 16	86, 105, 133, 157	0
2	A	1416/1733 (81%)	0.01	42 (2%) 52 36	22, 86, 159, 180	0
3	B	1112/1224 (90%)	0.22	45 (4%) 42 30	26, 95, 168, 180	0
4	C	266/318 (83%)	-0.10	4 (1%) 72 50	47, 82, 139, 156	0
5	D	177/221 (80%)	0.40	9 (5%) 33 25	56, 108, 156, 177	0
6	E	214/215 (99%)	0.52	12 (5%) 30 23	56, 141, 179, 180	0
7	F	84/155 (54%)	-0.34	2 (2%) 59 41	28, 59, 98, 122	0
8	G	171/171 (100%)	-0.05	2 (1%) 76 54	54, 82, 124, 133	0
9	H	133/146 (91%)	0.79	12 (9%) 15 16	105, 144, 178, 180	0
10	I	119/122 (97%)	0.36	5 (4%) 40 29	82, 135, 166, 180	0
11	J	65/70 (92%)	-0.13	1 (1%) 72 50	48, 78, 125, 133	0
12	K	115/120 (95%)	-0.27	3 (2%) 57 39	45, 83, 113, 143	0
13	L	46/70 (65%)	0.76	4 (8%) 16 16	73, 139, 174, 179	0
All	All	3941/4596 (85%)	0.13	143 (3%) 46 32	22, 92, 168, 180	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	56	PRO	7.1
3	B	882	THR	7.1
2	A	1081	LEU	6.2
9	H	63	LEU	5.7
2	A	1205	LYS	5.5

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	5BU	R	27	21/22	0.76	0.12	140,148,161,171	0
1	5BU	R	28	21/22	0.77	0.11	130,138,155,167	0
1	5BU	R	12	21/22	0.86	0.10	96,112,134,153	0
1	5BU	R	17	21/22	0.90	0.10	88,105,129,149	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
14	ZN	I	1122	1/1	0.97	0.05	176,176,176,176	0
14	ZN	A	2456	1/1	0.98	0.06	73,73,73,73	0
14	ZN	L	1071	1/1	0.98	0.04	114,114,114,114	0
14	ZN	B	2225	1/1	0.99	0.02	66,66,66,66	0
14	ZN	I	1121	1/1	0.99	0.05	85,85,85,85	0
15	MG	A	2458	1/1	0.99	0.07	20,20,20,20	0
14	ZN	J	1066	1/1	1.00	0.05	65,65,65,65	0
14	ZN	A	2457	1/1	1.00	0.01	46,46,46,46	0
14	ZN	C	1269	1/1	1.00	0.02	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.