



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 02:06 PM BST

PDB ID : 2R92
Title : Elongation complex of RNA polymerase II with artificial RdRP scaffold
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on : 2007-09-12
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

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

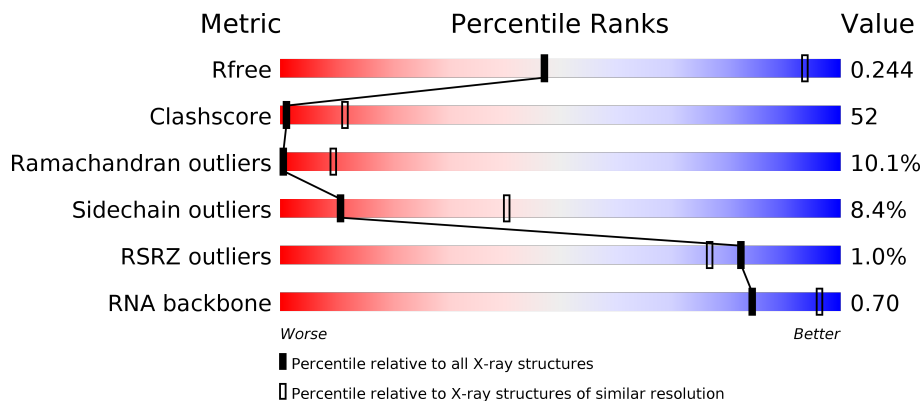
1 Overall quality at a glance

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.



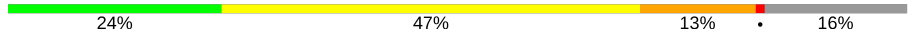
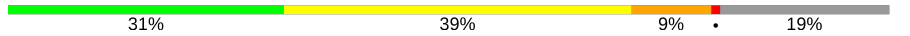
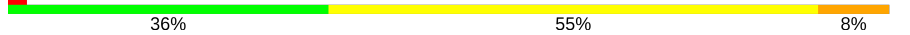

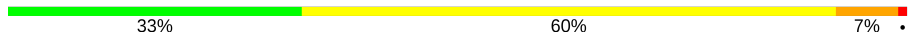
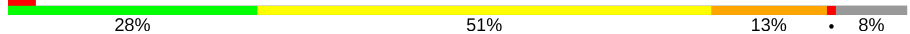
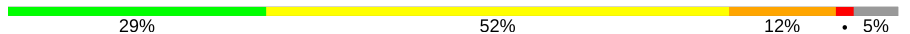
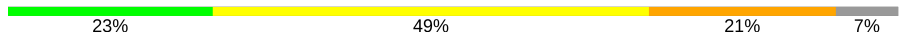
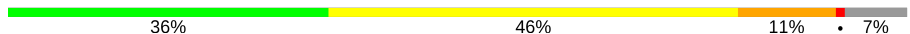

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 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	P	16	
2	T	17	
3	A	1733	
4	B	1224	

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Mol	Chain	Length	Quality of chain
5	C	318	
6	D	221	
7	E	215	
8	F	155	
9	G	171	
10	H	146	
11	I	122	
12	J	70	
13	K	120	
14	L	70	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 31611 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 (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	9	192	87	39	58	8	0	0	0

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*UP*UP*GP*AP*CP*GP*CP*CP*UP*GP*GP*UP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	10	208	94	36	69	9	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	1422	11194	7054	1959	2119	62	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	1112	8841	5596	1550	1640	55	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- 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	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	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	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	112	Total	C	N	O	S	0	0	0
			904	580	154	168	2			

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

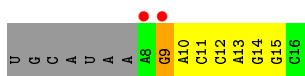
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

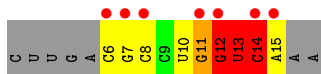
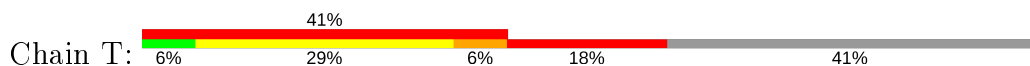
3 Residue-property plots [i](#)

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.

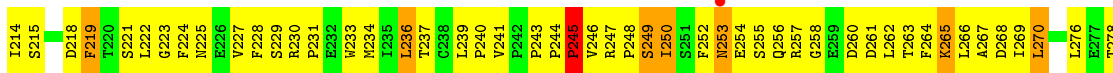
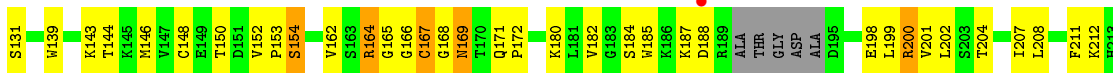
- Molecule 1: RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')



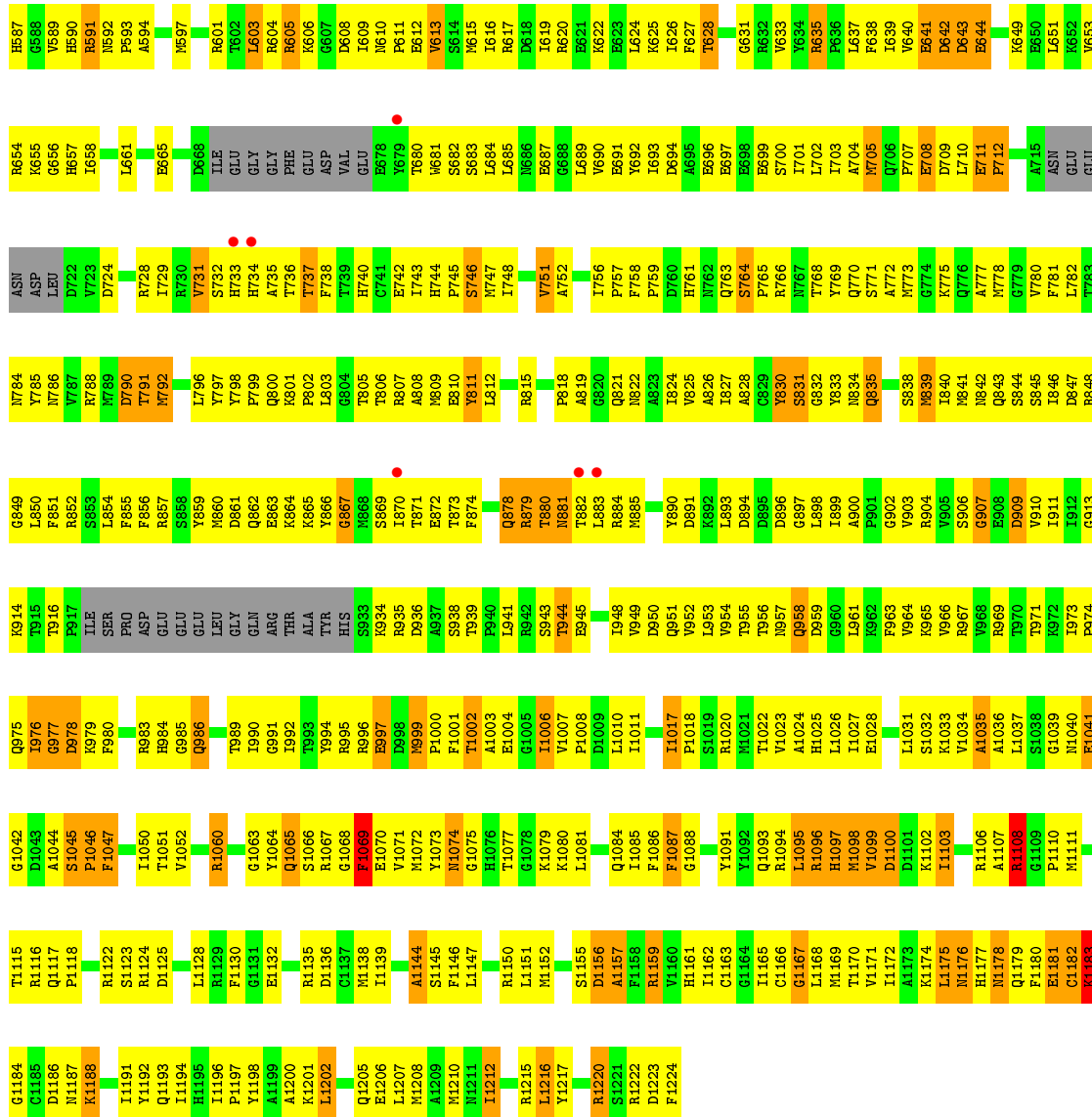
- Molecule 2: RNA (5'-R(*CP*UP*UP*GP*AP*CP*GP*CP*CP*UP*GP*GP*UP*CP*AP*AP*A)-3')



- Molecule 3: DNA-directed RNA polymerase II subunit RPB1

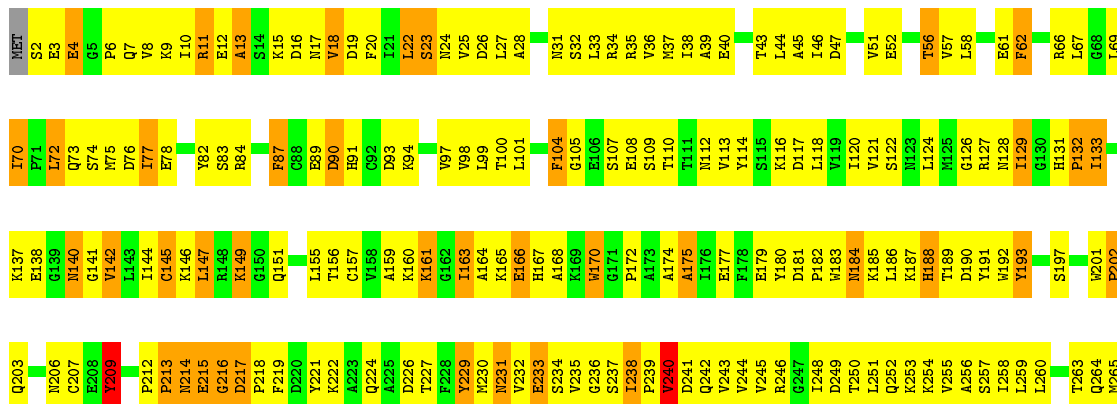


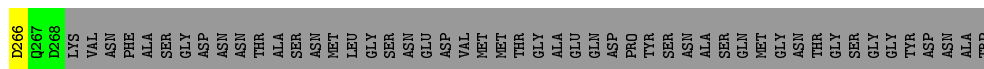
R1326	L1260	P1190	Y1119	Q1052	D885	L901	G835	G784	K687	I612	E542	S476	L413	K343
I1327	L1261	W1191	L1120	Q1053	I986	L902	R836	V785	V693	I613	L543	P477	D414	R344
Y1328	K1262	E1192	E1121	F1053	R987	N903	I837	G766	T694	F614	V546	Y478	L415	V345
N1329	L1193	L1192	R1122	L1054	L988	T904	Q838	Q767	K695	G615	N547	N479	R416	D346
N1330	L1263	R1194	H1123	R1055	D905	D905	R839	Q768	K696	V616	N548	D481	Y417	F347
S1331	E1264	H1124	H1125	R1056	R840	H906	R840	R774	E697	V617	M549	A481	S418	S348
F1332	M1265	L1197	A1125	W1058	L841	T907	L841	I775	A698	E618	L550	F482	K419	A349
L1333	M1266	D1198	A1126	H1059	R842	L908	R842	F779	K699	D483	D483	D483	R420	R350
M1267	D1127	D1127	D1127	P1060	R843	P1060	R843	F779	A699	M487	D423	M487	D423	M487
L1268	Q1128	Q1128	Q1128	E1061	R844	L913	R844	F779	A699	N488	D424	N488	I424	V352
T1271	E1129	E1129	E1129	E1062	L845	E914	L845	D781	L701	I425	Q425	I425	I353	I353
T1272	Q1130	Q1130	Q1130	M1063	E846	D846	E846	R781	L701	L426	Q427	L426	Q425	S354
L1273	I1134	I1134	I1134	V1064	R848	I919	R848	T783	H706	G623	G623	G623	G427	G355
M1274	R1135	R1135	R1135	G1065	R849	L920	R849	I784	H706	S625	I560	V491	Q427	D856
L1275	S1136	S1136	S1136	L1067	M849	G921	M849	L784	T709	R626	P561	P492	Y428	P357
L1276	A1137	A1137	A1137	L1068	Y852	Q926	Y852	H786	L710	G627	T562	Q493	G429	G429
T1277	I1138	I1138	I1138	I1007	R854	L929	R854	F787	R711	G628	P563	S494	W430	D362
E1280	A1139	A1139	A1139	Q1008	T855	Y933	T855	Q789	E712	L629	E495	R498	K431	Q363
E1281	Q1210	Q1210	Q1210	M1009	R856	Y934	R856	F787	R712	E496	E496	E496	V432	V364
E1282	G1211	G1211	G1211	Q1009	R857	Q935	R857	S788	S713	I630	I565	T497	V432	G365
E1283	I1212	I1212	I1212	Q1010	R858	Q936	R858	K789	F714	H631	I566	R498	R434	G366
E1284	R1214	R1214	R1214	A1010	R859	L936	R859	Y792	N717	V633	K567	A499	R434	P367
E1285	E1215	E1215	E1215	E1074	R860	L936	R860	P794	W719	V634	K568	A499	H435	P368
E1286	I1216	I1216	I1216	A1076	L861	L936	L861	E795	R720	V635	P570	E500	H435	P369
E1287	T1147	T1147	T1147	A1076	G861	D939	G861	S796	F721	O642	L571	Q503	D438	S369
E1288	I1148	I1148	I1148	A1076	R862	R940	R862	K797	W722	L504	M572	L504	I370	I370
E1289	A1149	A1149	A1149	M1079	R863	R941	R863	G798	L722	G505	S573	G505	D440	A371
K1290	S1150	S1150	S1150	T1080	R864	R941	R864	F799	M722	A506	A506	A506	P441	K372
V1291	I1151	I1151	I1151	L1081	R865	R942	R865	F799	L722	V507	V507	V507	P441	K373
P1292	I1152	I1152	I1152	ASN	R866	L943	R866	F799	E724	F646	K575	F646	L443	L374
S1293	Y1153	Y1153	Y1153	THR	R867	L943	R867	F799	A725	G647	Q576	P08	L443	L375
P1294	Y1154	Y1154	Y1154	PHE	R868	L943	R868	E801	W725	M648	I577	I577	M445	Y376
T1295	D1155	D1155	D1155	HLA	R867	L943	R867	S802	K728	I649	Q510	Q510	M446	P377
E1296	P1156	P1156	P1156	PRE	R868	L943	R868	S803	W736	I650	Q511	Q511	Q447	P377
E1297	T1161	T1161	T1161	ALA	R869	R942	R869	Y804	R731	Q650	S511	S511	L450	T381
E1298	V1162	V1162	V1162	ALA	R870	R942	R870	L805	L732	K651	S512	S512	L450	P382
E1299	I1163	I1163	I1163	ALA	R871	R942	R871	R806	L732	V652	P514	P514	H451	Y383
E1300	P1164	P1164	P1164	SER	R872	R942	R872	G807	W736	V653	G585	G585	K452	N384
E1301	E1165	E1165	E1165	K1092	R873	R942	R873	L808	M736	L657	I586	S516	K453	I385
E1302	D1166	D1166	D1166	K1093	D874	R942	D874	T809	K738	H658	I586	S516	S484	D386
E1303	L1236	L1236	L1236	R1094	A875	R942	A875	E812	F739	H659	R590	R518	M455	R387
M1304	I1237	I1237	I1237	Y1094	R878	R942	R878	F813	D739	S663	F591	P519	M456	L388
L1306	L1238	L1238	L1238	T1095	I878	R942	I878	F814	L740	T664	D592	G520	A457	V392
E1307	Q1170	Q1170	Q1170	S1096	L883	Q965	L883	F815	N741	G665	M521	M521	R458	H458
R1239	Q1171	Q1171	Q1171	G1097	L884	R966	L884	R816	N742	I668	I523	I523	V460	V392
G1310	F1174	F1174	F1174	R1097	L885	A967	L885	R816	V743	I668	I523	I523	V460	P396
V1311	S1175	S1175	S1175	R1100	L886	Q968	L886	M818	K744	D672	V524	V524	K461	R399
M1312	L1176	L1176	L1176	L1101	T885	Q969	T885	M818	Q745	D672	D526	D526	V462	P400
L1313	L1177	L1177	L1177	K1102	T886	R969	T886	M818	M746	I598	L598	L598	I463	P400
P1245	ASP	ASP	ASP	E1103	G887	T970	G887	R821	V747	S599	S599	S599	P464	G401
LYS	GLU	GLU	GLU	L1104	G888	H972	G888	E822	M748	T527	T527	T527	Y465	A402
SER	GLU	GLU	GLU	L1105	S889	H972	S889	E822	A749	L528	L528	L528	Y466	A402
LEU	ALA	ALA	ALA	M106	D890	I973	D890	I825	I499	I531	I531	I531	S466	K403
ASP	GLU	GLU	GLU	M107	A891	R977	A891	D826	G753	M603	M603	M603	Y467	Y404
ALA	GLN	GLN	GLN	Y1044	E894	P978	E894	T827	S754	F468	F468	F468	R469	I406
GLU	SER	SER	SER	Y1045	R895	S979	R895	V829	M757	L534	L534	L534	L470	R407
THR	PHE	PHE	PHE	P4114	R896	D980	R896	V829	I607	L534	L534	L534	M471	D408
ASP	ASP	ASP	ASP	S4115	R897	L961	R897	K830	I608	T535	T535	T535	L472	S409
GLU	ASP	ASP	ASP	L1116	R898	I982	R898	T831	M761	L536	L536	L536	L472	S409
A1254	Q1187	Q1187	Q1187	L1117	R899	I982	R899	T831	S762	I608	I608	I608	S473	G410
E1255	Q1188	Q1188	Q1188	S1047	R899	I982	R899	T831	A763	E684	E684	E684	V474	D411
E1256	S1189	S1189	S1189	I1049	D900	K984	D900	T834	A763	E684	E684	E684	T475	R412



• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

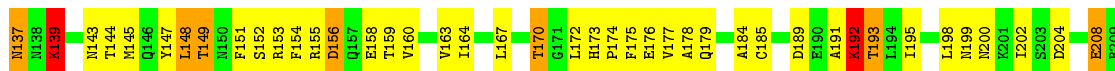
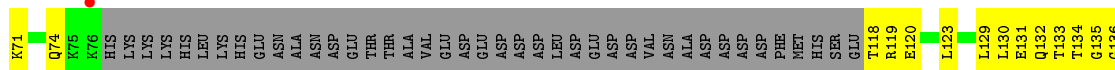
Chain C: 24% 47% 13% 16%





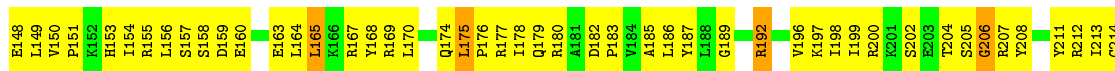
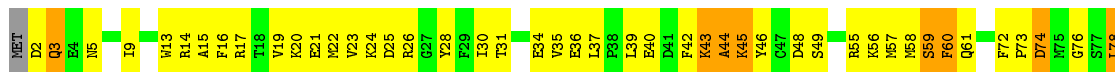
- Molecule 6: DNA-directed RNA polymerase II subunit RPB4

Chain D: 31% 39% 9% 19%



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

Chain E: 2% 36% 55% 8%

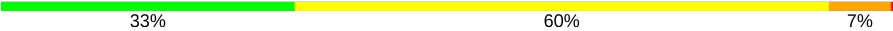


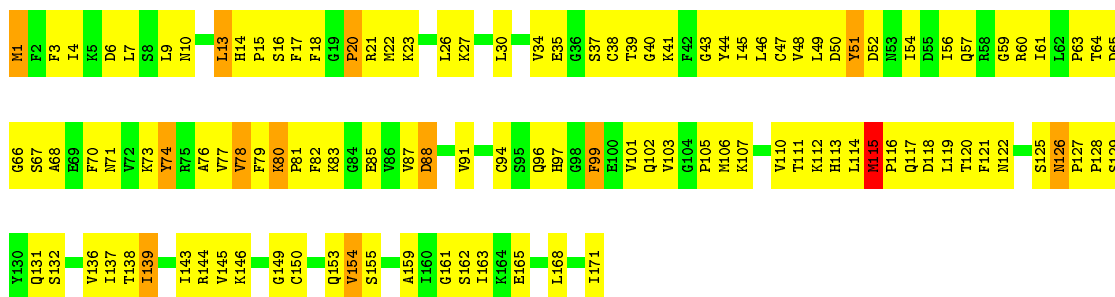
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 16% 35% 6% 43%



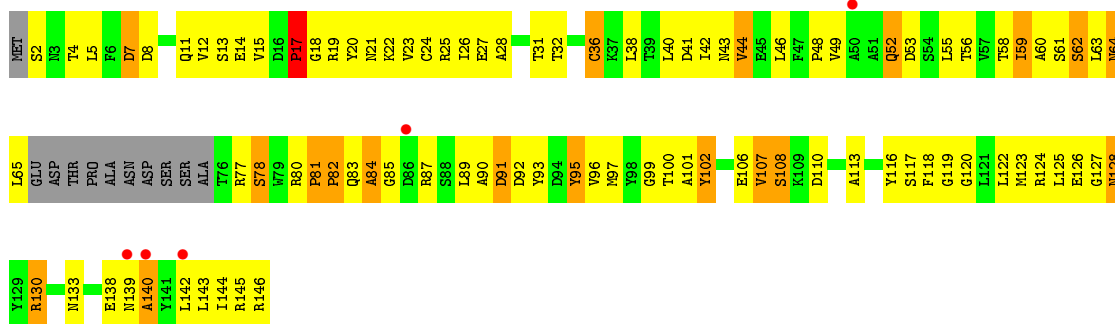
- Molecule 9: DNA-directed RNA polymerase II subunit RPB7

Chain G: 

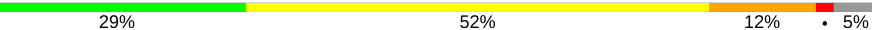


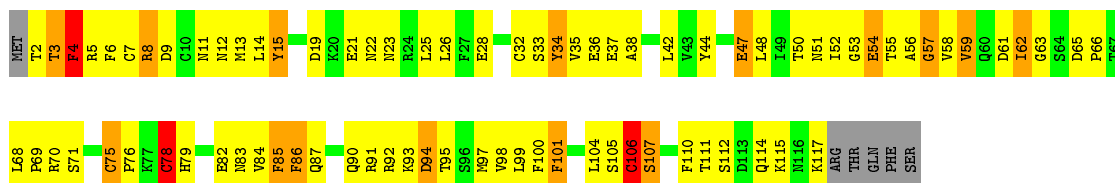
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

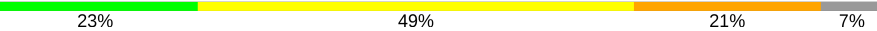


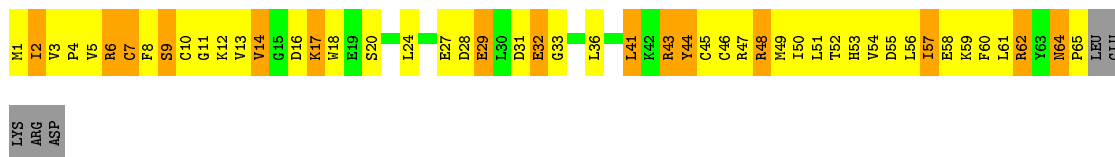
- Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



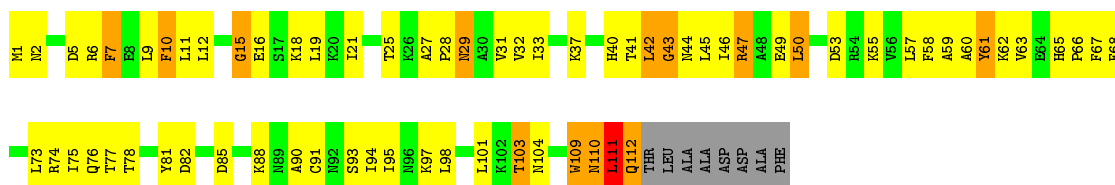
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 

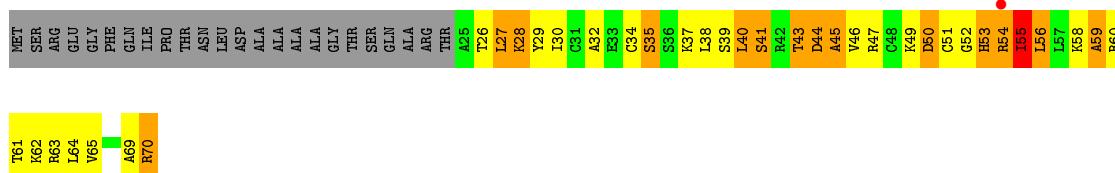


- Molecule 13: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.68Å 393.85Å 283.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 48.51 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.9 (48.51-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.246 0.205 , 0.244	Depositor DCC
R_{free} test set	2431 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.038 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31611	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: 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	P	0.63	0/215	0.81	0/334
2	T	0.71	0/231	1.32	5/358 (1.4%)
3	A	0.42	0/11394	0.73	7/15407 (0.0%)
4	B	0.41	0/9012	0.68	1/12149 (0.0%)
5	C	0.43	0/2138	0.71	0/2896
6	D	0.39	0/1444	0.66	0/1935
7	E	0.39	0/1788	0.63	0/2406
8	F	0.45	0/724	0.76	0/977
9	G	0.45	0/1368	0.72	0/1844
10	H	0.37	0/1102	0.62	0/1492
11	I	0.38	0/962	0.65	0/1295
12	J	0.47	0/541	0.75	0/727
13	K	0.45	0/922	0.68	0/1244
14	L	0.46	0/366	0.69	0/485
All	All	0.42	0/32207	0.71	13/43549 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1176	LEU	CA-CB-CG	13.45	146.23	115.30
2	T	12	G	N9-C1'-C2'	9.04	125.76	114.00
2	T	12	G	O4'-C1'-N9	8.14	114.72	108.20
2	T	13	U	O4'-C1'-N1	7.87	114.50	108.20
3	A	1176	LEU	CB-CA-C	-7.05	96.81	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	P	192	0	101	6	0
2	T	208	0	110	16	0
3	A	11194	0	11278	1259	0
4	B	8841	0	8874	1006	0
5	C	2101	0	2055	275	0
6	D	1434	0	1460	146	0
7	E	1752	0	1776	163	0
8	F	712	0	738	89	0
9	G	1340	0	1357	182	0
10	H	1084	0	1057	140	0
11	I	944	0	903	120	0
12	J	532	0	542	90	0
13	K	904	0	911	93	0
14	L	364	0	388	54	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	31611	0	31550	3310	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 52.

The worst 5 of 3310 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)
3:A:58:LEU:HD12	3:A:59:GLY:H	0.99	1.11
4:B:343:ILE:HG23	4:B:347:LYS:HB2	1.25	1.09
4:B:510:LYS:HG2	4:B:511:PRO:HD3	1.22	1.08
3:A:53:LEU:HD23	3:A:54:ASN:N	1.68	1.08
5:C:43:THR:HG22	5:C:44:LEU:H	0.98	1.07

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	
3	A	1412/1733 (82%)	1030 (73%)	249 (18%)	133 (9%)	0	11
4	B	1094/1224 (89%)	780 (71%)	214 (20%)	100 (9%)	1	12
5	C	264/318 (83%)	164 (62%)	64 (24%)	36 (14%)	0	4
6	D	174/221 (79%)	126 (72%)	30 (17%)	18 (10%)	0	9
7	E	212/215 (99%)	158 (74%)	36 (17%)	18 (8%)	1	12
8	F	86/155 (56%)	69 (80%)	9 (10%)	8 (9%)	0	11
9	G	169/171 (99%)	130 (77%)	33 (20%)	6 (4%)	3	30
10	H	131/146 (90%)	74 (56%)	36 (28%)	21 (16%)	0	3
11	I	114/122 (93%)	69 (60%)	30 (26%)	15 (13%)	0	5
12	J	63/70 (90%)	39 (62%)	10 (16%)	14 (22%)	0	1
13	K	110/120 (92%)	87 (79%)	15 (14%)	8 (7%)	1	16
14	L	44/70 (63%)	18 (41%)	10 (23%)	16 (36%)	0	0
All	All	3873/4565 (85%)	2744 (71%)	736 (19%)	393 (10%)	0	9

5 of 393 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	4	GLN
3	A	44	THR
3	A	48	ALA
3	A	54	ASN
3	A	57	ARG

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	
3	A	1245/1520 (82%)	1129 (91%)	116 (9%)	9	35
4	B	964/1061 (91%)	890 (92%)	74 (8%)	13	43
5	C	235/274 (86%)	212 (90%)	23 (10%)	8	33
6	D	160/200 (80%)	142 (89%)	18 (11%)	6	28
7	E	196/197 (100%)	188 (96%)	8 (4%)	30	59
8	F	78/137 (57%)	75 (96%)	3 (4%)	33	61
9	G	152/152 (100%)	140 (92%)	12 (8%)	12	42
10	H	119/128 (93%)	113 (95%)	6 (5%)	24	55
11	I	110/116 (95%)	99 (90%)	11 (10%)	7	32
12	J	60/65 (92%)	55 (92%)	5 (8%)	11	40
13	K	97/102 (95%)	87 (90%)	10 (10%)	7	31
14	L	40/57 (70%)	36 (90%)	4 (10%)	7	32
All	All	3456/4009 (86%)	3166 (92%)	290 (8%)	11	40

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	393	LYS
4	B	909	ASP
11	I	94	ASP
4	B	429	PHE
4	B	628	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	366	GLN
4	B	957	ASN
11	I	90	GLN
4	B	513	GLN

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Mol	Chain	Res	Type
4	B	538	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	8/16 (50%)	1 (12%)	0
2	T	9/17 (52%)	5 (55%)	2 (22%)
All	All	17/33 (51%)	6 (35%)	2 (11%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	P	9	G
2	T	11	G
2	T	12	G
2	T	13	U
2	T	14	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	12	G
2	T	13	U

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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	B	1
5	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2:SER	C	3:GLU	N	3.04
1	B	337:ARG	C	338:GLY	N	2.61

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	P	9/16 (56%)	2.00	2 (22%) 0 0	194, 200, 200, 200	0
2	T	10/17 (58%)	2.21	7 (70%) 0 0	180, 190, 200, 200	0
3	A	1422/1733 (82%)	-0.26	7 (0%) 91 87	56, 116, 175, 200	0
4	B	1112/1224 (90%)	-0.20	12 (1%) 80 74	57, 126, 188, 200	0
5	C	267/318 (83%)	-0.29	0 100 100	74, 110, 158, 180	0
6	D	178/221 (80%)	-0.26	1 (0%) 89 85	87, 133, 184, 198	0
7	E	214/215 (99%)	-0.24	4 (1%) 66 59	90, 159, 197, 200	0
8	F	88/155 (56%)	-0.52	0 100 100	65, 91, 129, 140	0
9	G	171/171 (100%)	-0.30	0 100 100	88, 112, 155, 163	0
10	H	135/146 (92%)	0.34	5 (3%) 41 34	139, 166, 190, 200	0
11	I	116/122 (95%)	0.06	0 100 100	114, 163, 191, 200	0
12	J	65/70 (92%)	-0.49	0 100 100	79, 108, 146, 153	0
13	K	112/120 (93%)	-0.31	0 100 100	81, 114, 139, 167	0
14	L	46/70 (65%)	0.02	1 (2%) 62 54	111, 166, 194, 196	0
All	All	3945/4598 (85%)	-0.21	39 (0%) 82 76	56, 123, 187, 200	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	471	LYS	5.2
1	P	9	G	4.6
3	A	1092	LYS	3.8
1	P	8	A	3.5
2	T	15	A	3.5

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 monosaccharides 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(\AA^2)	Q<0.9
15	ZN	A	1506	1/1	0.95	0.08	121,121,121,121	0
15	ZN	L	105	1/1	0.97	0.11	155,155,155,155	0
16	MG	A	1	1/1	0.97	0.18	79,79,79,79	0
15	ZN	I	203	1/1	0.99	0.16	120,120,120,120	0
15	ZN	I	204	1/1	0.99	0.04	181,181,181,181	0
15	ZN	C	302	1/1	1.00	0.13	82,82,82,82	0
15	ZN	A	1508	1/1	1.00	0.14	83,83,83,83	0
15	ZN	J	101	1/1	1.00	0.25	100,100,100,100	0
15	ZN	B	1307	1/1	1.00	0.22	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.