



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:43 PM GMT

PDB ID : 1Y1W
Title : Complete RNA Polymerase II elongation complex
Authors : Cramer, P.; Kettenberger, H.; Armache, K.-J.
Deposited on : 2004-11-19
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

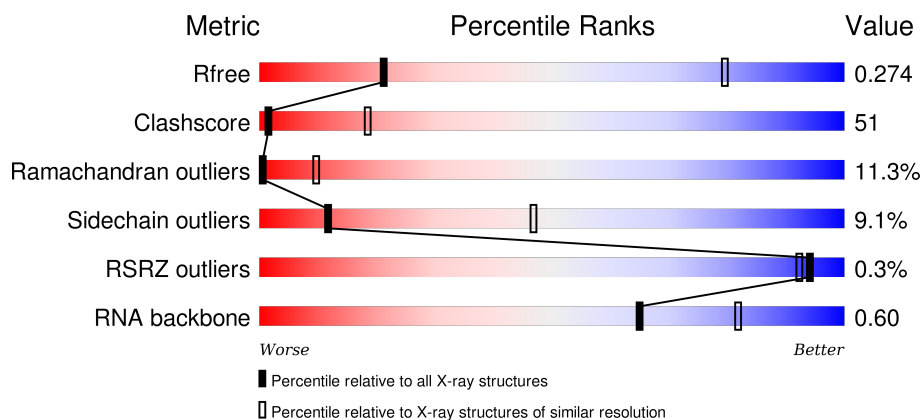
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	19	<div> <div>5%</div> <div>32%</div> <div>68%</div> </div>
2	N	7	<div> <div>14%</div> <div>14%</div> <div>71%</div> <div>14%</div> </div>
3	P	10	<div> <div>80%</div> <div>20%</div> </div>
4	A	1733	<div> <div>25%</div> <div>45%</div> <div>10%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31802 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 DNA chain called 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*C P*TP*GP*GP*TP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	19	Total	C	N	O	P	21	0	0
			387	185	67	116	19			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	7	Total	C	N	O	P	20	0	0
			141	69	27	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

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

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

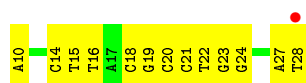
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

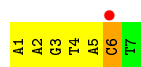
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

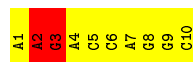
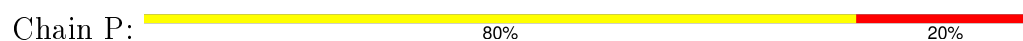
- Molecule 1: 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*AP*T)-3'



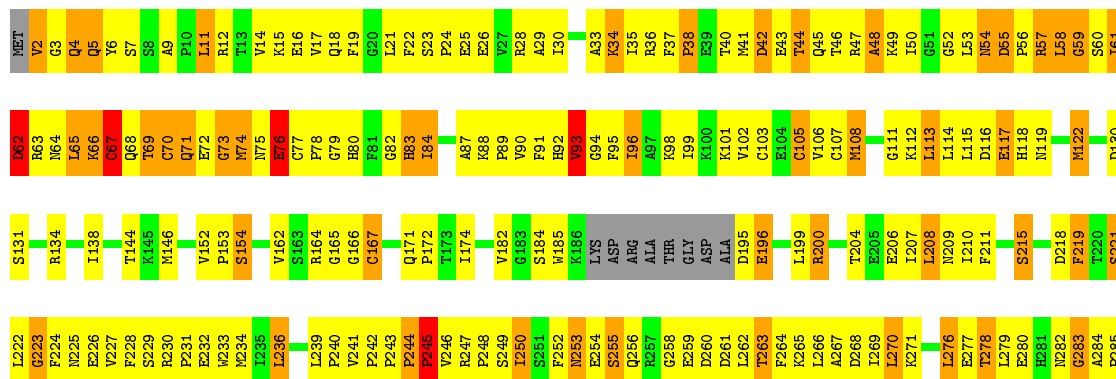
- Molecule 2: 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'



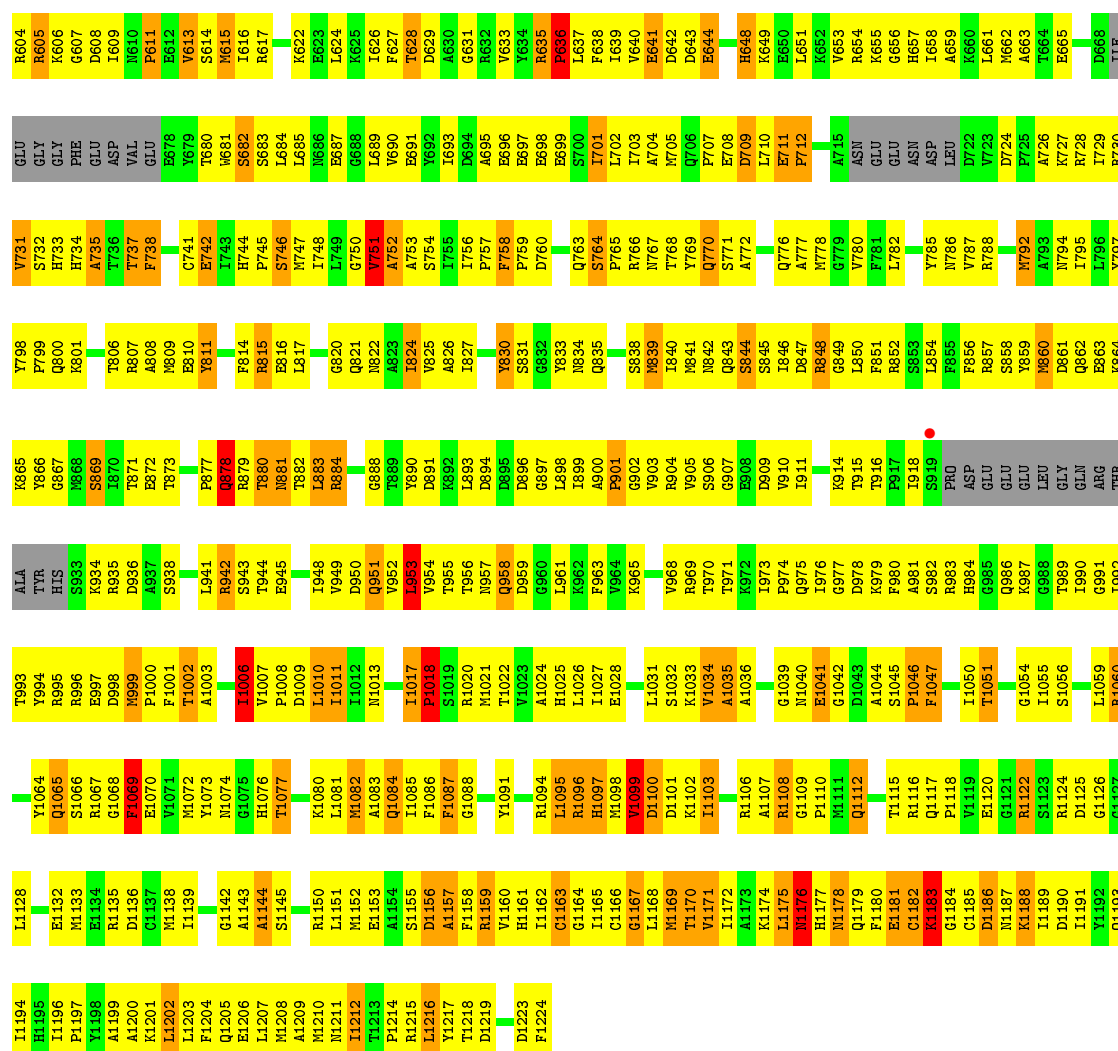
- Molecule 3: 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'



- Molecule 4: DNA-directed RNA polymerase II largest subunit

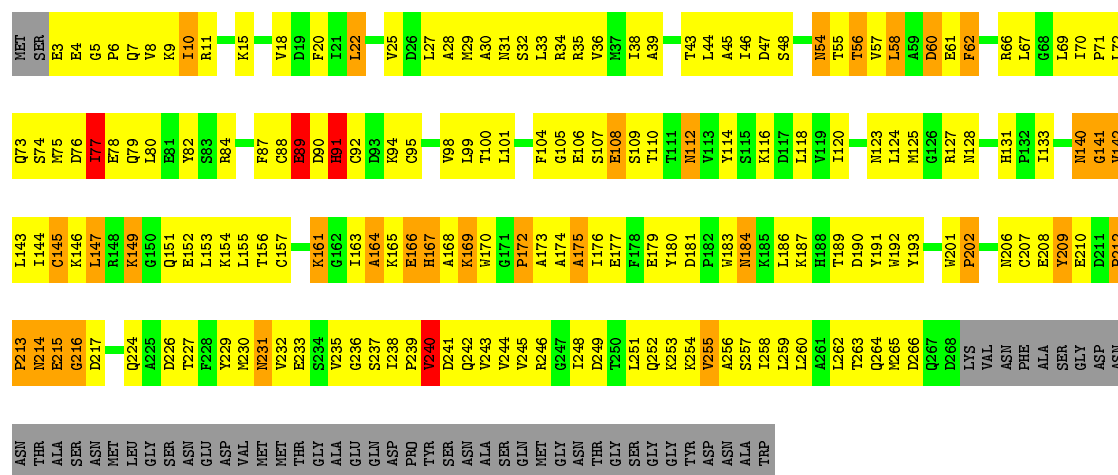


V1299	D1223	T1161	K1092	A1027	R961	G887	E822	I756	A684	G615	V551	G484	D423	F347	H286
K1300	L1224	V1162	K1093	T1028	R962	G888	G823	I757	E585	V616	H552	D485	I424	S348	H287
E1301		I1163	V1094	R1029	I963	S889	L324	I758	A687	E617	H553	E486	Q425	A349	A288
P1302	I1227	P1164	T1095	R1030	I964	D890	I825		K687	E618	H554	N487	Q427	R350	I289
K1303	M1228	E1165	S1096	V1031	Q965	A891	D826	M761	V690	K619	H555	N488	Y428	T351	E291
V1305		D1166	G1097	L1032	R966	R896	T827	T762	L691	K620	H556	N489	G428	V352	K291
L1306	D1231	E1167	V1098	Q1033	A967	R897	A828	A763	L692	T621	H557	H490	W430	I353	K292
E1307		I1168	R1099	E1034	Q968	R898	V829	C764	D693	G622	H558	E491	W430	S354	E293
T1308	L1236	I1169	R1100	Y1035	Q969	R898	R330	T765	V693	G623	H559	P492	W432	G355	S294
D1309	I1237	Q1170	T1070	L1037	R971	V899	A832	T766	K695	S624	H560	Q493	W432	D356	L295
V1310	K1102	K1171	K1102	T1038	R972	D900	A832	T767	K695	S625	H561		E433	P357	L296
G1311	L1172	H1173	L1105	L1039	R973	L901	E833	T768	E596	K626	H562	T487	R434	N358	D297
N1312	H1174	F1174	N1106	Q1040	I973	L902	E834	T769	A697	G627	H563	R498	H435		P298
L1313	S1175	S1175	V1107	A1041		R903	G835	V770	Q698	G628	H564	A499		V864	H299
S1314	V1242	L1176			S979	T904	I837		N700	L629	H565	E500	D438	V866	V300
V1316	ARG	LEU	M1110	W1044	L981	H906	Q838	R774	L701	I630	H566		N439		A301
V1317	PRO	ASP	M1111	V1045	L982	T907	R839	I775		H631	H567		D440		T302
M1317	LVS	GLU	K1112		R983	L908	R840	F779	T709	V632	H568		P441		V303
T1318	SER	GLU	T1113	N1048	K984	D909	L841	T780	L710	V632	H569		V442		K304
V1319	LEU	ALA	P1114	I1049	D985	P910	L842	I781	E711	V632	H570		L443		D305
P1320	ASP	GLU	S1115	E1050	I986	S911	K943	T782	E712		H571		F444		I306
	ALA	GLN	L1116	A1051	V987	L912	A844	T783	S713	C642	H572		N445		D307
		SER	T1117	Q1052	L988	L913	L845	L784	F714		H573		R446		I308
D1323	GLU	PHE	V1118	F1053		E914	E846	T785	E715	L645	H574	I511	Q447	T381	A309
P1324	THR	ASP	V1119	L1054	D982	I919	I848	I787		G647	H575	V512	P448	P382	G310
T1325	GLU		T1120	R1055	L993	L920	N849	T788	V719		H576	S533	S449	N383	Q311
R1326	A1284	Q1187	E1121	S1056	Q994	L920	N849	T789	E719	N648	H577	P514	L450	N384	P312
I1327	E1285	P1189	S1189	Y1057	E995	G921	N850	T790	R721	I649	H578	Q516	K452	N385	Q313
V1328	E1286	P1190	G1123	V1058	N996	D922	H852	T791	F722	Q650	H579	S517	K452	D386	A314
		H1124	H1124	H1059	L997		D853		L722	K651	H580	K518	N453	R387	L315
N1330	L1260	W1191		F1053	L998	Q926	N854		N723	G652	H584	P519	N455	L388	I316
S1331	K1261			P1060	L998		T855	F794	E724	V653	H585	C520	N456	V392	K317
F1332		L1193	D127	G1061	V999	L929	T856	T795	A725	N654	H586	M521	A457		S318
I1333	E1264	R1194	Q1130	E1062	R1001	D930	R857	T796	R726		H587		H458	P396	G319
D1334	L1195	L1195		M1063	L1001	R857	N858	T797		L658	H588	V524	R459		R320
I1335	T1266	A1196	L1133	G1065	K1003	Y933	S859	T798	K728	H659	H589	Q525	V460	H399	P321
M1336	M1267	L1197	I1134	N1004	R934	Q935	L860	T799	A729	D660	H590	D526	K463	P400	K323
E1337	L1268	D1198		E1005	L936	Q935	G861	V800	G730	G661	H591	T527	V462	G401	S324
V1339		R1199		L1066	L936	L936	N862	E801	R731	F662	H592	L528	I463	A402	I325
	I1271		E1139	A1068			V863	N802	L732	S663			P464	K403	K326
I1341	R1274	M1202	H1140	A1069	D939	D939	R864	S803	N736	T664	H595	I531	Y465	Y404	A327
E1342	Q1275		T1141	Q1070	Q1008	R940	Q865	T804	L737	G665	H596	R532	S466	W405	R328
A1343			T1142	S1071	N1009	R941	R866	L805	K738	L666	H597	K533	T467	A406	
G1344			L1143	I1072	A1010	F942	T867	R806	D739	G667	L598	L534	F468	K407	G331
R1345	L1207			G1073	Q1011	L943	Y868	G807	L740	D668	L599	T535	R469	D408	E332
A1346	T1208		T1147	P1075	D1013	V946	G869	L808	N741	T669	H600	L536	L470	S409	E333
V1347	V1282		I1148	A1014	E370	F947	E871	T809	N741	I670	H601	R537	N471	G410	G334
L1348	A1347		A1149	A1076	V1015	V943	D871	P810	N742	A671	D602		L472	D411	R335
V1349	M1284		S1150		T1016	G872	G872	Q811	V743	D672	H603	F540	S473	R412	I336
K1350			E1151	ASN	L1017	D949	N873	E812	K744	G673	H604	I541	V474	I413	R337
E1351	R1289		I1152	THR	F1018	D874	D874	F813	Q745	P674	H605	E542	T475	D143	G338
V1352	K1290		Y1153	PHE	C1019	N953	A875	F814	N746	T675	L606	L543	S476	L415	I339
	V1291		I1154	HIS	C1020	W954		F815	N746	T675	L607	D544	P477	R416	L340
V1355	P1292		D1155	PHE	L1021	P955	Q881	H816	V747	M676	H608	Q546	N478	Y417	N341
I1356	S1293		P1156	ALA	L1022	L956	S882	A817			H609	V545	N478	S418	K342
	P1294		D1157	GLY	A1023	P957	L883	N818	K752		H610	L547	A480	K419	K343
	T1295		P1158	VAL	S1024	R958	E884	G819	G753	E681		M548	D481	R420	R344
D1359			R1159	ALA	R1025	N959	T885	G820	S754			M549	F482	A421	V345
			K1221	SER	L1026	I960	I886	R821	F755	I683		L550	D483	G422	D346

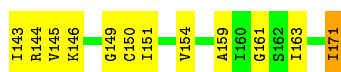


• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 27% 45% 10% 16%

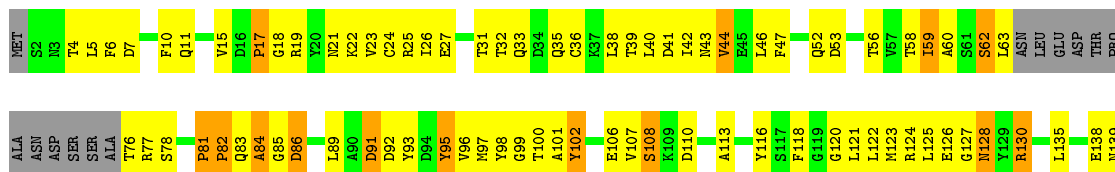


• Molecule 7: DNA-directed RNA polymerase II 32 kDa polypeptide



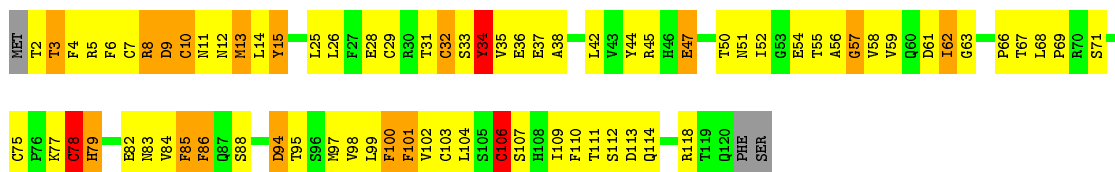
- Molecule 11: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H: 33% 47% 11% 9%



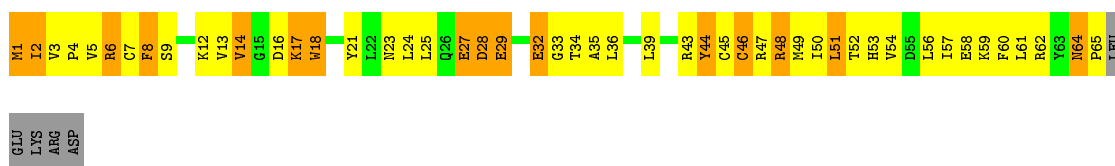
- Molecule 12: DNA-directed RNA polymerase II subunit 9

Chain I: 35% 47% 13% ..



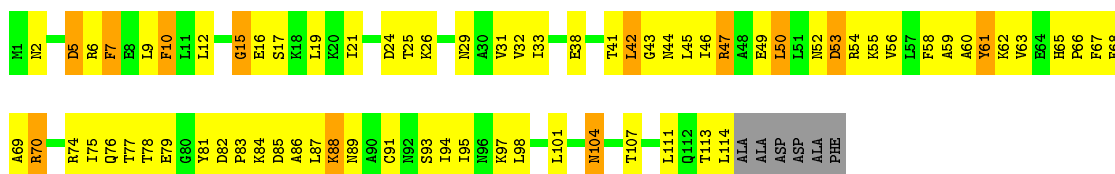
- Molecule 13: DNA-directed RNA polymerases I/II/III subunit 10

Chain J: 23% 47% 23% 7%



- Molecule 14: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 34% 51% 10% 5%



- Molecule 15: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L: 21% 30% 14% 34%





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.37Å 392.50Å 283.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 48.83 – 3.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 94.4 (48.83-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.10 (at 4.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.276 0.260 , 0.274	Depositor DCC
R_{free} test set	2054 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , -11.4	EDS
Estimated twinning fraction	0.210 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.209 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 101979 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	31802	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [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	T	1.15	1/432 (0.2%)	1.03	1/664 (0.2%)
2	N	1.74	1/158 (0.6%)	0.91	1/242 (0.4%)
3	P	1.17	2/240 (0.8%)	1.06	3/373 (0.8%)
4	A	0.50	0/11339	0.75	5/15334 (0.0%)
5	B	0.51	1/9008 (0.0%)	0.74	5/12146 (0.0%)
6	C	0.56	0/2133	0.76	0/2891
7	D	0.46	0/1365	0.71	0/1837
8	E	0.45	0/1788	0.64	0/2406
9	F	0.56	0/691	0.80	0/933
10	G	0.55	0/1368	0.76	0/1844
11	H	0.40	0/1086	0.65	0/1470
12	I	0.49	1/989 (0.1%)	0.72	0/1331
13	J	0.52	0/541	0.80	0/727
14	K	0.52	0/937	0.70	0/1265
15	L	0.47	0/365	0.74	0/485
All	All	0.54	6/32440 (0.0%)	0.75	15/43948 (0.0%)

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
5	B	0	1
6	C	0	1
All	All	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	10	DA	O3'-P	-9.11	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	6	DC	O3'-P	7.11	1.69	1.61
12	I	78	CYS	CB-SG	-6.30	1.71	1.82
3	P	3	G	P-OP1	-6.03	1.38	1.49
5	B	503	GLY	CA-C	6.02	1.61	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	10	DA	OP1-P-O3'	7.38	121.44	105.20
3	P	3	G	O5'-P-OP1	-7.04	99.36	105.70
3	P	2	A	C2'-C3'-O3'	6.95	124.82	113.70
2	N	6	DC	P-O3'-C3'	6.32	127.28	119.70
5	B	1185	CYS	N-CA-C	-6.23	94.17	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	503	GLY	Mainchain
6	C	82	TYR	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	T	387	0	216	24	0
2	N	141	0	81	8	0
3	P	214	0	111	13	0
4	A	11140	0	11217	1300	0
5	B	8836	0	8871	1003	0
6	C	2095	0	2051	255	0
7	D	1356	0	1319	117	0
8	E	1752	0	1776	148	0
9	F	679	0	701	86	0
10	G	1340	0	1357	157	0
11	H	1068	0	1040	110	0
12	I	971	0	930	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	532	0	542	94	0
14	K	919	0	929	93	0
15	L	363	0	387	45	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31802	0	31528	3238	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 51.

The worst 5 of 3238 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)
7:D:40:HIS:HB3	10:G:73:LYS:NZ	1.61	1.14
14:K:47:ARG:HH11	14:K:47:ARG:HB3	1.00	1.14
4:A:53:LEU:HD23	4:A:54:ASN:H	1.08	1.12
4:A:76:GLU:O	4:A:76:GLU:HG3	1.53	1.08
4:A:53:LEU:HD23	4:A:54:ASN:N	1.70	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
4	A	1406/1733 (81%)	936 (67%)	311 (22%)	159 (11%)	0 10
5	B	1096/1224 (90%)	740 (68%)	215 (20%)	141 (13%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	264/318 (83%)	166 (63%)	64 (24%)	34 (13%)	0	7
7	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	1	14
8	E	212/215 (99%)	154 (73%)	44 (21%)	14 (7%)	1	25
9	F	82/155 (53%)	63 (77%)	16 (20%)	3 (4%)	4	40
10	G	169/171 (99%)	133 (79%)	24 (14%)	12 (7%)	1	23
11	H	129/146 (88%)	85 (66%)	28 (22%)	16 (12%)	0	8
12	I	117/122 (96%)	79 (68%)	27 (23%)	11 (9%)	1	16
13	J	63/70 (90%)	34 (54%)	15 (24%)	14 (22%)	0	1
14	K	112/120 (93%)	87 (78%)	17 (15%)	8 (7%)	1	23
15	L	44/70 (63%)	17 (39%)	18 (41%)	9 (20%)	0	2
All	All	3867/4565 (85%)	2612 (68%)	817 (21%)	438 (11%)	0	10

5 of 438 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP
4	A	57	ARG

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	1239/1520 (82%)	1125 (91%)	114 (9%)	11	46
5	B	964/1061 (91%)	873 (91%)	91 (9%)	11	45
6	C	234/274 (85%)	213 (91%)	21 (9%)	12	47
7	D	140/200 (70%)	124 (89%)	16 (11%)	7	36
8	E	196/197 (100%)	188 (96%)	8 (4%)	37	73
9	F	74/137 (54%)	65 (88%)	9 (12%)	6	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	G	152/152 (100%)	139 (91%)	13 (9%)	13	50
11	H	117/128 (91%)	109 (93%)	8 (7%)	20	59
12	I	113/116 (97%)	98 (87%)	15 (13%)	5	30
13	J	60/65 (92%)	55 (92%)	5 (8%)	14	51
14	K	99/102 (97%)	90 (91%)	9 (9%)	12	47
15	L	40/57 (70%)	37 (92%)	3 (8%)	17	56
All	All	3428/4009 (86%)	3116 (91%)	312 (9%)	12	47

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	463	THR
5	B	901	PRO
12	I	78	CYS
5	B	485	ARG
5	B	636	PRO

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

Mol	Chain	Res	Type
5	B	484	ASN
5	B	975	GLN
11	H	131	ASN
5	B	516	ASN
5	B	734	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	1 (11%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	P	2	A

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 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

6.1 Protein, DNA and RNA chains

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	T	18/19 (94%)	0.43	1 (5%) 28 20	69, 103, 131, 137	0
2	N	6/7 (85%)	1.00	1 (16%) 2 3	97, 99, 108, 108	0
3	P	10/10 (100%)	0.34	0 100 100	80, 94, 125, 127	0
4	A	1416/1733 (81%)	-0.75	4 (0%) 94 92	21, 75, 151, 195	0
5	B	1112/1224 (90%)	-0.69	4 (0%) 93 90	20, 87, 156, 186	0
6	C	266/318 (83%)	-0.78	0 100 100	34, 71, 130, 150	0
7	D	177/221 (80%)	-0.55	0 100 100	43, 99, 137, 155	0
8	E	214/215 (99%)	-0.54	0 100 100	47, 132, 177, 181	0
9	F	84/155 (54%)	-0.92	0 100 100	21, 49, 93, 113	0
10	G	171/171 (100%)	-0.76	0 100 100	47, 76, 106, 122	0
11	H	133/146 (91%)	-0.32	0 100 100	91, 130, 165, 175	0
12	I	119/122 (97%)	-0.37	0 100 100	63, 122, 153, 191	0
13	J	65/70 (92%)	-0.87	0 100 100	37, 69, 113, 118	0
14	K	114/120 (95%)	-0.79	0 100 100	37, 75, 104, 118	0
15	L	46/70 (65%)	-0.33	0 100 100	73, 127, 160, 168	0
All	All	3951/4601 (85%)	-0.68	10 (0%) 94 92	20, 84, 156, 195	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	5.0
5	B	471	LYS	3.3
4	A	1175	SER	2.6
1	T	28	DT	2.5
5	B	470	LYS	2.3

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
16	ZN	C	319	1/1	0.99	0.09	-0.80	28,28,28,28	0
16	ZN	A	1734	1/1	0.98	0.09	-0.99	73,73,73,73	0
16	ZN	I	204	1/1	0.98	0.10	-1.19	141,141,141,141	0
16	ZN	L	105	1/1	0.99	0.10	-1.41	90,90,90,90	0
16	ZN	B	1307	1/1	1.00	0.08	-1.50	31,31,31,31	0
16	ZN	A	1735	1/1	0.99	0.05	-1.78	36,36,36,36	0
16	ZN	J	101	1/1	0.99	0.06	-2.14	45,45,45,45	0
16	ZN	I	203	1/1	0.99	0.08	-2.40	80,80,80,80	0
17	MG	A	1736	1/1	0.99	0.07	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.