



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:56 AM UTC

PDB ID : 1Y1W / pdb_00001y1w
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

<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
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

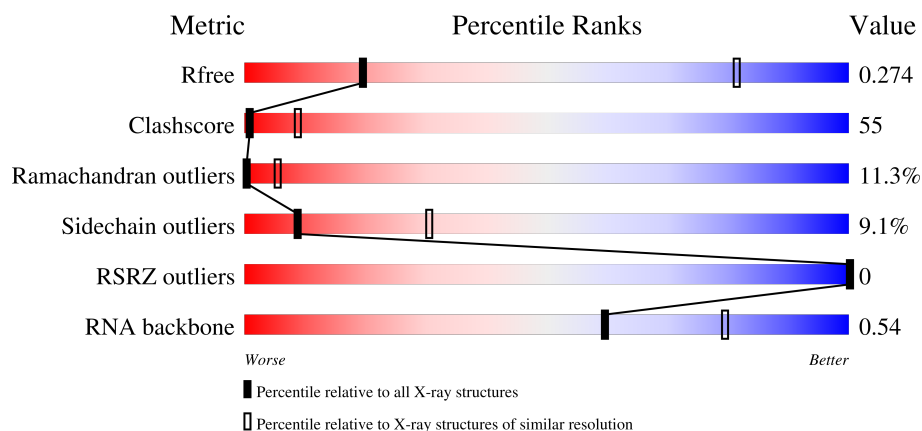
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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 ≥ 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	T	19	32% 63% 5%
2	N	7	14% 71% 14%
3	P	10	80% 20%
4	A	1733	22% 45% 13% • 18%

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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*CP*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 (CCD ID: ZN) (formula: Zn).

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

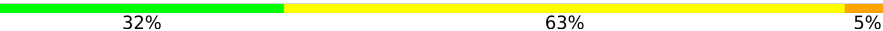
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

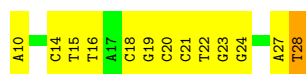
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

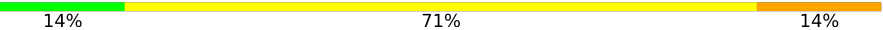
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

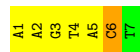
- Molecule 1: 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*AP*T)-3'

Chain T: 

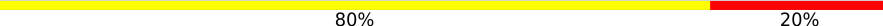


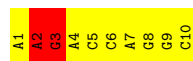
- Molecule 2: 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'

Chain N: 



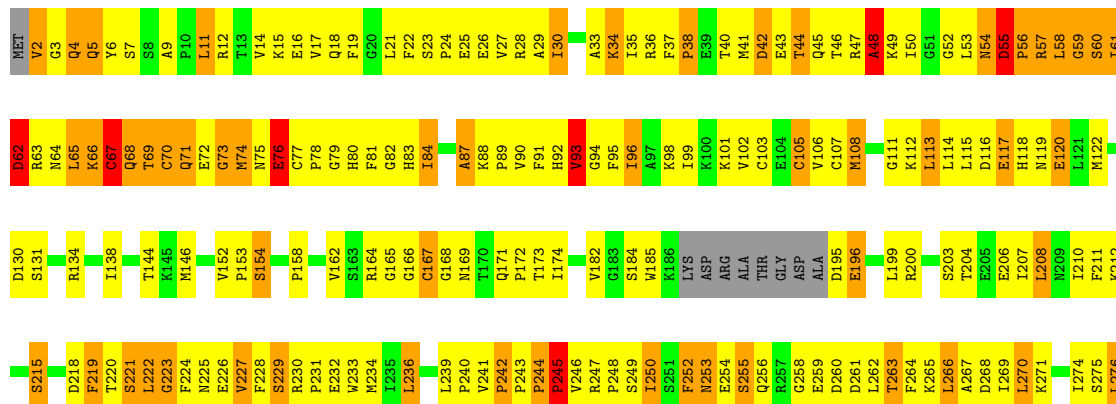
- Molecule 3: 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'

Chain P: 

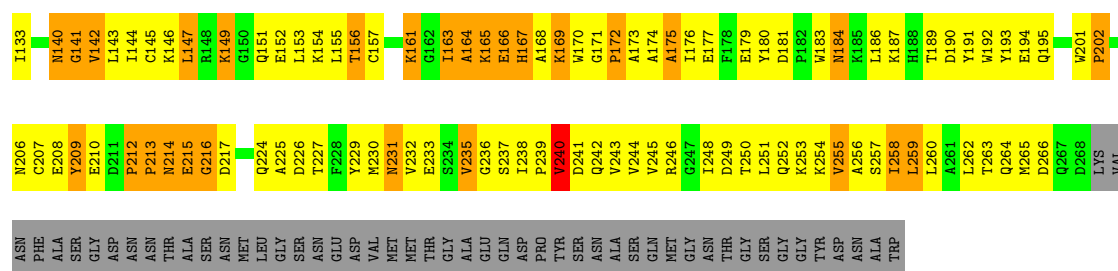


- Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A: 

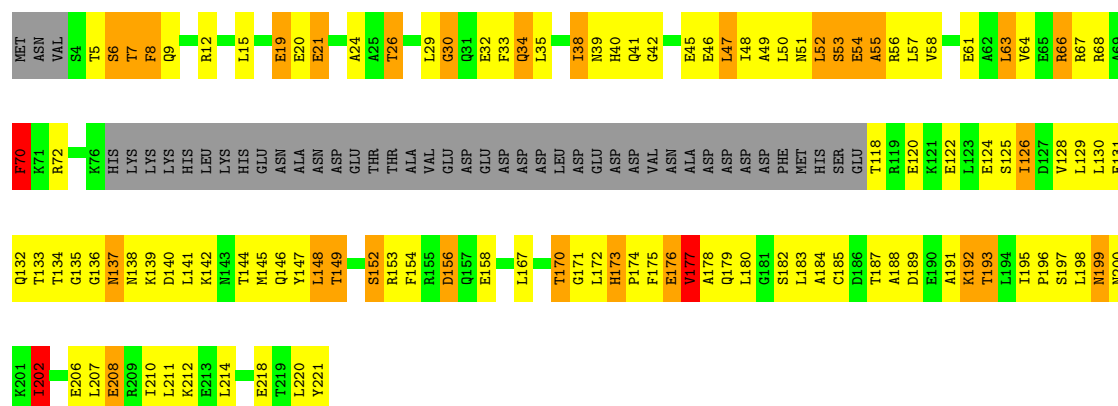


D1188	S1189	A1125	M1063	L1000	V863	V863	E801	L737	D668	P600	T539	V474	I413	G338	E277
S1189	S1189	A1125	V1064	R1001	I864	I864	M802	K738	T689	K601	F540	T475	D414	N339	T278
P1190	P1190	D1127	G1065	G1002	Q865	Q865	S803	D739	I670	D602	I542	S476	L415	L340	L279
W1191	W1191	G1128	V1066	K1003	F866	F866	Y804	A671	A671	N603	E542	P477	R416	M341	E280
L1192	L1192	L1067	L1067	N1004	I867	I867	L805	N741	D672	G604	L543	Y478	G342	G342	H281
L1193	L1193	Q1130	A1068	E1005	Y868	Y868	R806	N742	G673	M605	D544	N479	S418	K343	H282
R1194	R1194	A1069	A1069	I1006	C869	C869	C807	V743	P674	L606	Q545	A480	R344	R344	G283
L1195	L1195	Q1070	Q1070	I1007	E870	E870	L808	K744	T675	I607	V546	D481	V345	V345	A284
L1196	L1196	S1071	F942	Q1008	D872	D872	T809	K745	T676	L608	L547	P482	D346	D346	P285
L1197	L1197	L1072	F941	M1009	K873	K873	P810	M746	M676	D609	N548	D483	F347	F347	H286
L1198	L1198	G1073	L943	A1010	Q811	Q811	Q811	V747	I679	G610	M549	G422	S348	S348	H287
R1199	R1199	E1074	Y946	Q1011	E812	E812	F813	T680	T680	G611	L550	D485	A349	A349	A288
A1200	A1200	R1012	F947	R1012	F813	F813	F814	G750	F681	I612	Y551	E486	Q425	Q425	I289
A1076	A1076	A1014	F947	D1013	F814	F814	F814	S751	T682	I613	W552	M487	L436	L436	E290
M1079	M1079	A1014	Y948	A1014	F815	F815	F815	K752	T683	F614	V553	N488	Q427	Q427	E291
L1141	L1141	D949	Y948	V1015	H877	H877	H816	G753	A684	G615	P554	L489	Y428	Y428	A292
L1143	L1143	Q950	G950	I878	I878	I878	A817	S754	G685	V616	D555	H490	G429	G429	E293
K1144	K1144	G950	G950	I878	I878	I878	A817	S754	G685	V616	D555	H490	G429	G429	S294
T1147	T1147	Q950	G950	I878	I878	I878	A817	S754	G685	V616	D555	H490	G429	G429	S294
I1148	I1148	Q950	G950	I878	I878	I878	A817	S754	G685	V616	D555	H490	G429	G429	L295
A1149	A1149	HIS	PHE	L1021	T885	T885	E822	A759	T621	T621	I560	T497	W430	W430	L296
S1150	S1150	PHE	PHE	L1022	T885	T885	E822	A759	T621	T621	I560	T497	W430	W430	Q297
E1151	E1151	ALA	PHE	L1023	G887	G887	L824	M761	D692	G623	T562	R499	R434	R434	F298
I1152	I1152	GLY	GLY	S1024	G888	G888	R825	S762	V693	S624	P563	A499	H435	H435	H299
Y1153	Y1153	VAL	VAL	R1025	S889	S889	R826	A763	T694	S625	A564	E500	V364	V364	V300
Y1154	Y1154	ALA	ALA	A1026	D890	D890	T827	G764	K695	M626	I565	Q503	D438	D438	A301
L1155	L1155	SER	SER	A1027	A891	A891	R828	V765	G696	G627	I566	L504	M439	M439	T302
P1156	P1156	K1092	K1092	T1028	V829	V829	V829	G766	A697	G628	K667	C505	D440	D440	T303
L1093	L1093	R1029	R1029	R1029	R830	R830	K830	Q767	A697	G628	K667	C505	V442	V442	M304
Y1094	Y1094	R1030	R1030	R1030	R831	R831	T831	Q768	A699	G629	P568	A506	W443	W443	D305
T1095	T1095	L1037	L1037	L1037	R832	R832	A832	S769	N700	H631	P570	V507	F444	F444	N306
S1096	S1096	L1032	L1032	L1032	E833	E833	A833	S769	N700	H631	P570	V507	F444	F444	D367
G1097	G1097	Q1033	Q1033	Q1033	D900	D900	T834	R774	T709	V632	L571	P508	M445	M445	I308
V1098	V1098	E1034	E1034	E1034	L901	L901	G835	I775	L710	V633	W572	I511	R446	R446	A309
R1100	R1100	R1036	R1036	R1036	L902	L902	Y836	A776	R711	K637	S573	V512	Q447	Q447	G310
L1101	L1101	L1037	L1037	L1037	N903	N903	T837	A776	R711	K637	S573	V512	Q447	Q447	Q311
K1102	K1102	L1037	L1037	L1037	T904	T904	Q838	F777	E712	C642	K575	P514	L450	L450	Q313
E1103	E1103	T1038	T1038	T1038	D905	D905	R839	G778	S713	C642	K575	P514	L450	L450	Q313
L1104	L1104	Q1040	Q1040	Q1040	T907	T907	R840	G778	S713	C642	K575	P514	L450	L450	A314
L1105	L1105	L1049	L1049	L1049	L908	L908	L841	V780	E715	L645	L578	N517	M453	M453	L315
N1106	N1106	V1107	V1107	V1107	D909	D909	K843	D716	G647	F646	S579	K518	S454	S454	Q316
V1107	V1107	V1107	V1107	V1107	P910	P910	A844	R783	N717	G647	V580	P519	M455	M455	K317
M1110	M1110	M1110	M1110	M1110	S911	S911	L845	L784	V718	L649	I582	C520	M456	M456	S318
L1111	L1111	L1111	L1111	L1111	L912	L912	L846	L784	V718	L649	I582	C520	M456	M456	G319
L1112	L1112	L1112	L1112	L1112	L913	L913	E846	P785	R720	K651	N584	V524	H458	H458	P321
T1113	T1113	L1113	L1113	L1113	E914	E914	D847	H786	F721	V652	G585	Q525	V460	V460	V322
P1114	P1114	L1114	L1114	L1114	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	K323
S1115	S1115	L1115	L1115	L1115	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	S324
L1116	L1116	L1116	L1116	L1116	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	I325
L1117	L1117	L1117	L1117	L1117	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	G401
L1118	L1118	L1118	L1118	L1118	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	I326
L1119	L1119	L1119	L1119	L1119	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	R326
L1120	L1120	L1120	L1120	L1120	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	A327
L1121	L1121	L1121	L1121	L1121	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	R328
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L1123	L1123	L1123	L1123	L1123	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	R332
L1124	L1124	L1124	L1124	L1124	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	E333
L1125	L1125	L1125	L1125	L1125	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	G334
L1126	L1126	L1126	L1126	L1126	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	R335
L1127	L1127	L1127	L1127	L1127	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	I336
L1128	L1128	L1128	L1128	L1128	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	R337
L1129	L1129	L1129	L1129	L1129	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1130	L1130	L1130	L1130	L1130	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1131	L1131	L1131	L1131	L1131	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1132	L1132	L1132	L1132	L1132	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
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L1136	L1136	L1136	L1136	L1136	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1137	L1137	L1137	L1137	L1137	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
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L1145	L1145	L1145	L1145	L1145	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1146	L1146	L1146	L1146	L1146	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1147	L1147	L1147	L1147	L1147	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1148	L1148	L1148	L1148	L1148	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1149	L1149	L1149	L1149	L1149	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1150	L1150	L1150	L1150	L1150	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1151	L1151	L1151	L1151	L1151	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1152	L1152	L1152	L1152	L1152	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1153	L1153	L1153	L1153	L1153	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1154	L1154	L1154	L1154	L1154	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1155	L1155	L1155	L1155	L1155	E914	E914	T848	F787	L722	V653	I586	D526	P400	P400	
L1156	L1156	L1156	L1156	L1156	E914	E914	T848	F787	L722	V653	I586	D526	P400	P4	



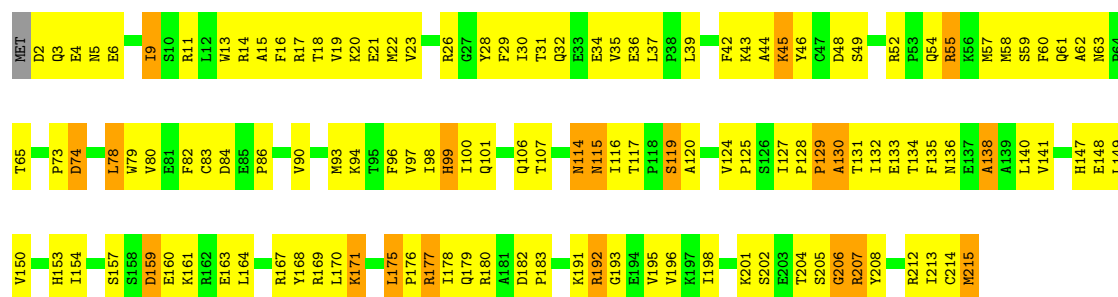
• Molecule 7: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D: 28% 38% 13% 20%



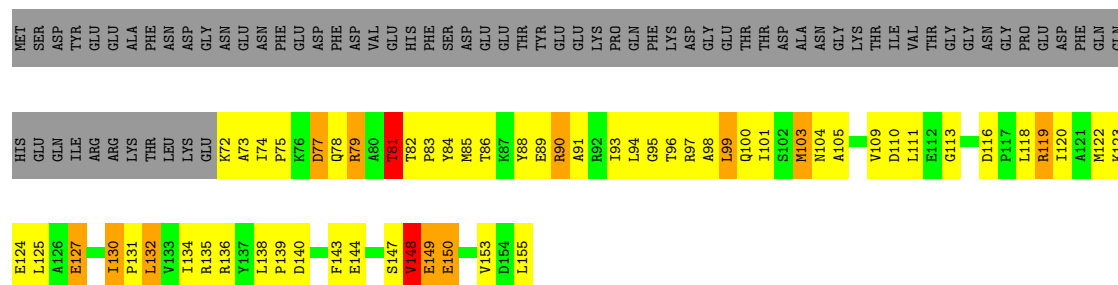
• Molecule 8: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 39% 51% 9%

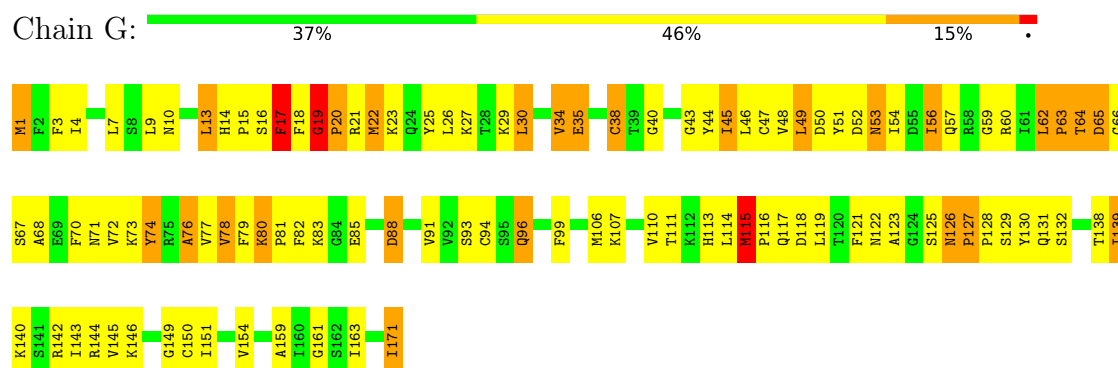


• Molecule 9: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

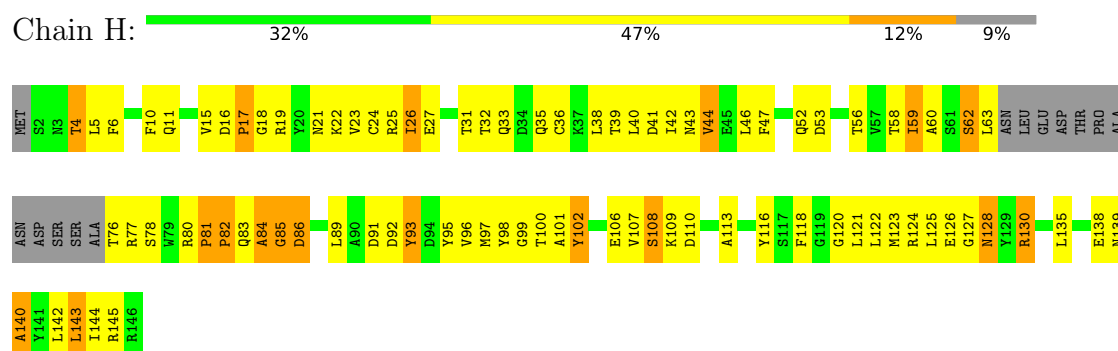
Chain F: 16% 30% 7% 46%



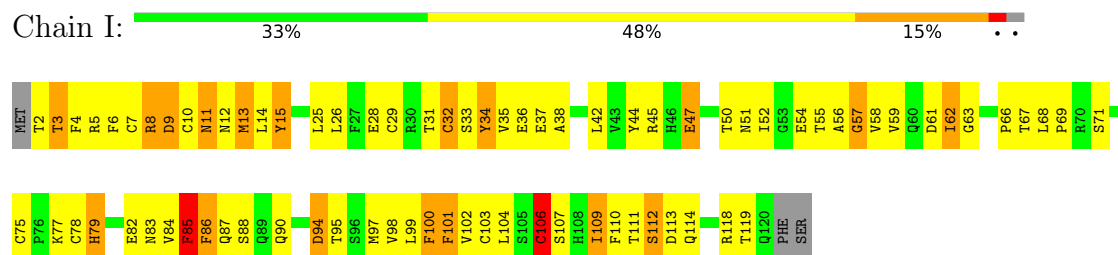
- Molecule 10: DNA-directed RNA polymerase II 19 kDa polypeptide



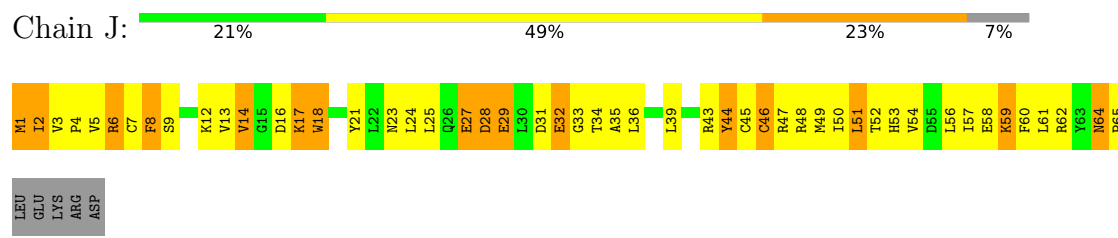
- Molecule 11: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



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



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



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





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 50.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 94.4 (50.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.276 0.260 , 0.274	Depositor DCC
R_{free} test set	2439 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 114.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.207 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.206 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.87	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.67	1/432 (0.2%)	1.05	1/664 (0.2%)
2	N	1.08	1/158 (0.6%)	0.97	0/242
3	P	0.79	1/240 (0.4%)	1.07	3/373 (0.8%)
4	A	0.63	2/11339 (0.0%)	1.13	88/15334 (0.6%)
5	B	0.63	6/9008 (0.1%)	1.09	68/12146 (0.6%)
6	C	0.69	2/2133 (0.1%)	1.14	18/2891 (0.6%)
7	D	0.55	0/1365	1.18	16/1837 (0.9%)
8	E	0.52	0/1788	1.03	15/2406 (0.6%)
9	F	0.71	0/691	1.20	6/933 (0.6%)
10	G	0.63	0/1368	1.16	16/1844 (0.9%)
11	H	0.45	0/1086	1.01	6/1470 (0.4%)
12	I	0.52	0/989	1.07	5/1331 (0.4%)
13	J	0.60	0/541	1.05	1/727 (0.1%)
14	K	0.57	0/937	1.08	7/1265 (0.6%)
15	L	0.54	0/365	0.97	0/485
All	All	0.62	13/32440 (0.0%)	1.10	250/43948 (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
5	B	0	1
6	C	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	469	GLN	CA-C	7.52	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	10	DA	O3'-P	-7.29	1.50	1.61
5	B	504	ARG	N-CA	7.09	1.55	1.46
5	B	503	GLY	CA-C	6.81	1.61	1.51
6	C	89	GLU	N-CA	-6.39	1.38	1.46

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1185	CYS	N-CA-C	-15.47	94.17	113.97
4	A	452	LYS	N-CA-C	-14.08	95.94	111.14
7	D	54	GLU	N-CA-C	-11.61	99.64	114.04
4	A	466	SER	N-CA-C	10.56	124.75	112.72
7	D	26	THR	N-CA-C	-10.21	98.54	112.94

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	1407	0
5	B	8836	0	8871	1076	0
6	C	2095	0	2051	273	0
7	D	1356	0	1319	128	0
8	E	1752	0	1776	156	0
9	F	679	0	701	91	0
10	G	1340	0	1357	166	0
11	H	1068	0	1040	113	0
12	I	971	0	930	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	532	0	542	95	0
14	K	919	0	929	103	0
15	L	363	0	387	46	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	3486	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 55.

The worst 5 of 3486 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:HB3	14:K:47:ARG:HH11	1.00	1.14
4:A:53:LEU:HD23	4:A:54:ASN:H	1.08	1.12
4:A:76:GLU:HG3	4:A:76:GLU:O	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 5
5	B	1096/1224 (90%)	740 (68%)	215 (20%)	141 (13%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	264/318 (83%)	166 (63%)	64 (24%)	34 (13%)	0	4
7	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	0	9
8	E	212/215 (99%)	154 (73%)	44 (21%)	14 (7%)	1	15
9	F	82/155 (53%)	63 (77%)	16 (20%)	3 (4%)	2	22
10	G	169/171 (99%)	133 (79%)	24 (14%)	12 (7%)	1	14
11	H	129/146 (88%)	85 (66%)	28 (22%)	16 (12%)	0	4
12	I	117/122 (96%)	79 (68%)	27 (23%)	11 (9%)	0	10
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	14
15	L	44/70 (63%)	17 (39%)	18 (41%)	9 (20%)	0	1
All	All	3867/4565 (85%)	2612 (68%)	817 (21%)	438 (11%)	0	5

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%)	1121 (90%)	118 (10%)	8	28
5	B	964/1061 (91%)	874 (91%)	90 (9%)	8	29
6	C	234/274 (85%)	216 (92%)	18 (8%)	12	35
7	D	140/200 (70%)	118 (84%)	22 (16%)	2	15
8	E	196/197 (100%)	188 (96%)	8 (4%)	27	49
9	F	74/137 (54%)	65 (88%)	9 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	G	152/152 (100%)	137 (90%)	15 (10%)	7	27
11	H	117/128 (91%)	110 (94%)	7 (6%)	17	42
12	I	113/116 (97%)	101 (89%)	12 (11%)	6	24
13	J	60/65 (92%)	56 (93%)	4 (7%)	15	39
14	K	99/102 (97%)	91 (92%)	8 (8%)	11	34
15	L	40/57 (70%)	38 (95%)	2 (5%)	22	45
All	All	3428/4009 (86%)	3115 (91%)	313 (9%)	9	30

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	D	120	GLU
11	H	143	LEU
7	D	152	SER
9	F	103	MET
13	J	9	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	538	ASN
5	B	1179	GLN
12	I	12	ASN
5	B	744	HIS
5	B	1015	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 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 ⓘ

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	0 100 100	69, 103, 131, 137	0
2	N	6/7 (85%)	-0.48	0 100 100	97, 99, 108, 108	0
3	P	10/10 (100%)	-0.90	0 100 100	80, 94, 125, 127	0
4	A	1416/1733 (81%)	-1.00	0 100 100	21, 75, 151, 195	0
5	B	1112/1224 (90%)	-0.97	0 100 100	20, 87, 156, 186	0
6	C	266/318 (83%)	-1.06	0 100 100	34, 71, 130, 150	0
7	D	177/221 (80%)	-1.00	0 100 100	43, 99, 137, 155	0
8	E	214/215 (99%)	-0.96	0 100 100	47, 132, 177, 181	0
9	F	84/155 (54%)	-1.11	0 100 100	21, 49, 93, 113	0
10	G	171/171 (100%)	-1.05	0 100 100	47, 76, 106, 122	0
11	H	133/146 (91%)	-0.84	0 100 100	91, 130, 165, 175	0
12	I	119/122 (97%)	-0.87	0 100 100	63, 122, 153, 191	0
13	J	65/70 (92%)	-1.10	0 100 100	37, 69, 113, 118	0
14	K	114/120 (95%)	-1.11	0 100 100	37, 75, 104, 118	0
15	L	46/70 (65%)	-0.88	0 100 100	73, 127, 160, 168	0
All	All	3951/4601 (85%)	-0.99	0 100 100	20, 84, 156, 195	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

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($\text{\AA}^2$)	Q<0.9
16	ZN	A	1734	1/1	1.00	0.02	73,73,73,73	0
16	ZN	A	1735	1/1	1.00	0.01	36,36,36,36	0
16	ZN	B	1307	1/1	1.00	0.01	31,31,31,31	0
16	ZN	C	319	1/1	1.00	0.01	28,28,28,28	0
16	ZN	I	203	1/1	1.00	0.01	80,80,80,80	0
16	ZN	I	204	1/1	1.00	0.02	141,141,141,141	0
16	ZN	J	101	1/1	1.00	0.02	45,45,45,45	0
16	ZN	L	105	1/1	1.00	0.01	90,90,90,90	0
17	MG	A	1736	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.