



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:07 PM UTC

PDB ID : 1Y1Y / pdb_00001y1y
Title : RNA Polymerase II-TFIIS-DNA/RNA 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

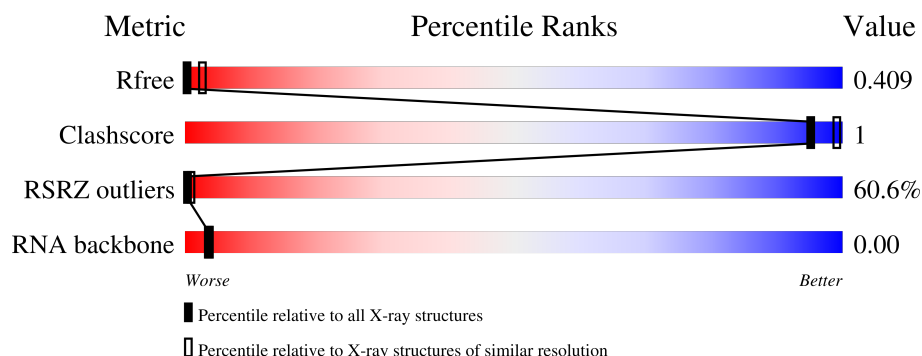
1 Overall quality at a glance

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)
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	7	100% 100%
2	P	4	75% 100%
3	A	1733	54% 82% 18%
4	B	1224	55% 91% 9%
5	C	318	55% 84% 16%
6	D	221	44% 80% 20%

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Mol	Chain	Length	Quality of chain
7	E	215	60% 99% .
8	F	155	30% 54% 46%
9	G	171	62% 99% .
10	H	146	38% 91% 9%
11	I	122	47% 98% .
12	J	70	61% 93% 7%
13	K	120	60% 95% 5%
14	L	70	39% 66% 34%
15	S	179	34% 95% . .

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 4112 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*TP*AP*CP*GP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	T	7	Total P 7 7	0	0	7

- Molecule 2 is a RNA chain called 5'-R(P*AP*GP*GP*C)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	P	4	Total P 4 4	0	0	4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	A	1426	Total C 1426 1426	0	0	1426

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	B	1112	Total C 1112 1112	8	0	1112

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	266	Total C 266 266	0	0	266

- Molecule 6 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	D	177	Total C 177 177	0	0	177

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	E	214	Total	C	0	0	214
			214	214			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	F	84	Total	C	0	0	84
			84	84			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	G	171	Total	C	0	0	171
			171	171			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	H	133	Total	C	0	0	133
			133	133			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	I	119	Total	C	0	0	119
			119	119			

- Molecule 12 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	J	65	Total	C	0	0	65
			65	65			

- Molecule 13 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	K	114	Total	C	0	0	114
			114	114			

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	L	46	Total	C	0	0	46
			46	46			

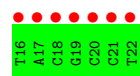
- Molecule 15 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	S	174	Total	C	0	0	174
			174	174			

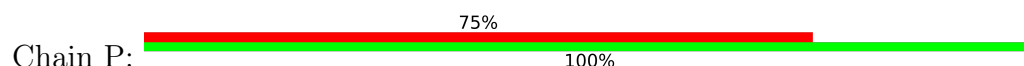
3 Residue-property plots

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.

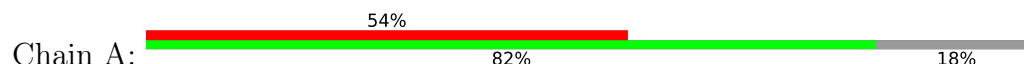
- Molecule 1: 5'-D(P*TP*AP*CP*GP*CP*CP*T)-3'



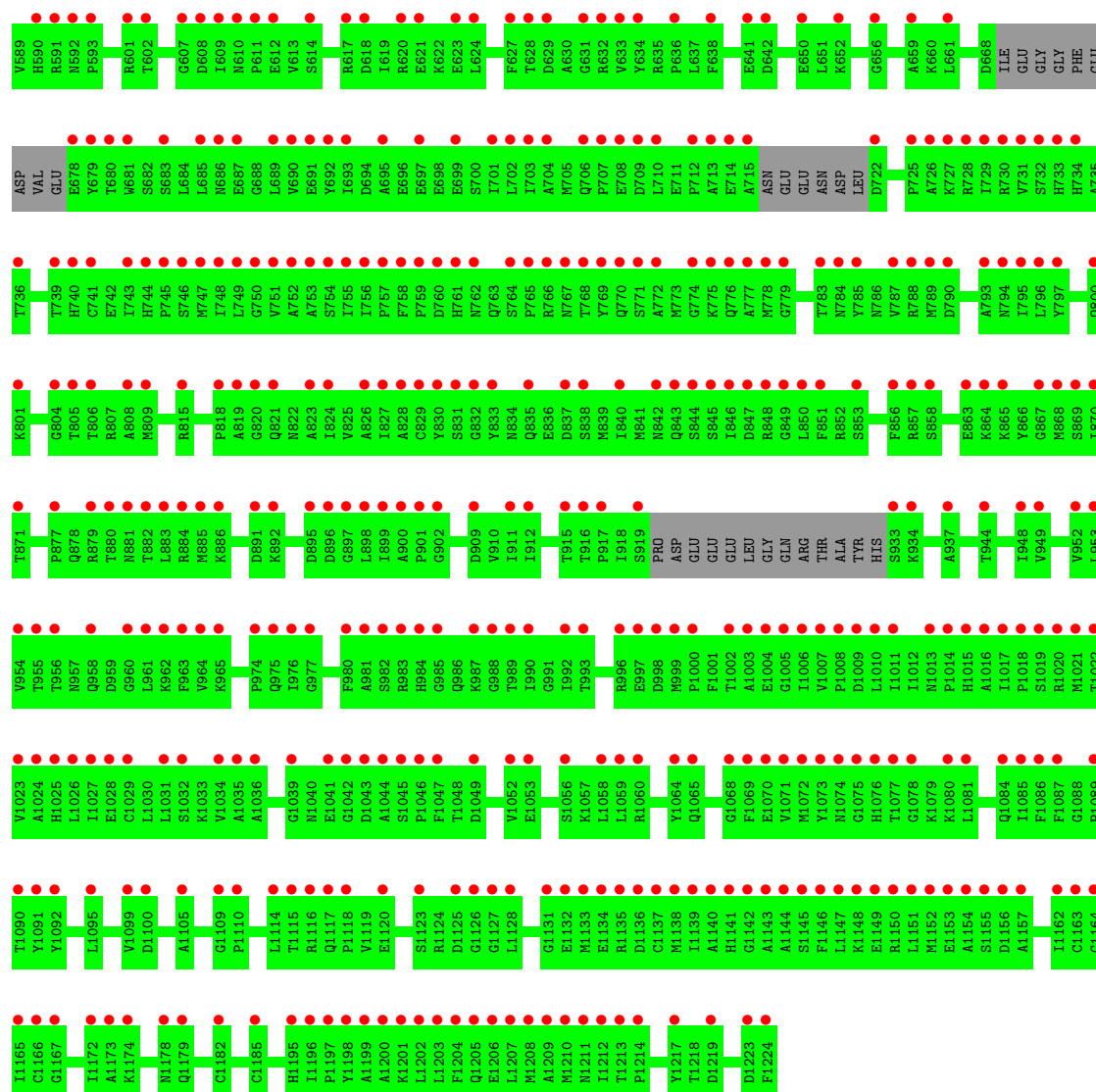
- Molecule 2: 5'-R(P*AP*GP*GP*C)-3'



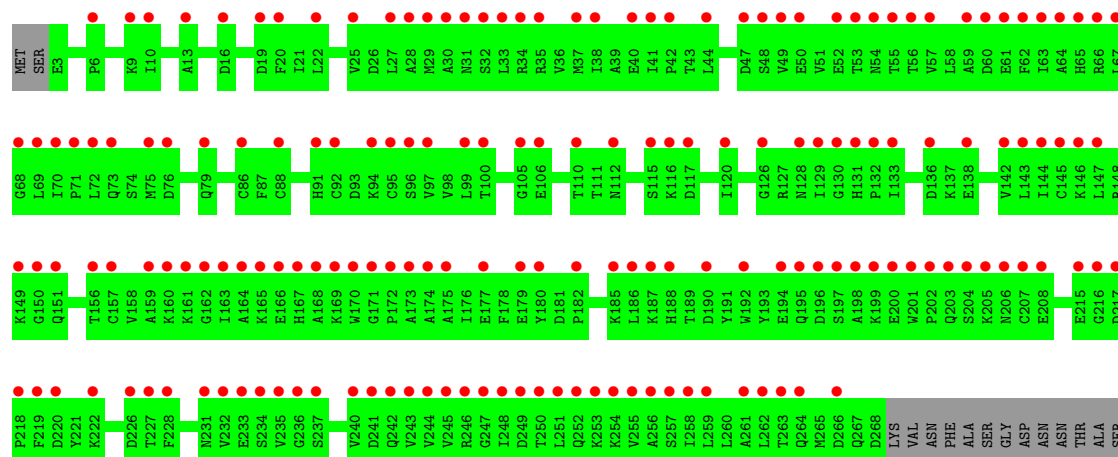
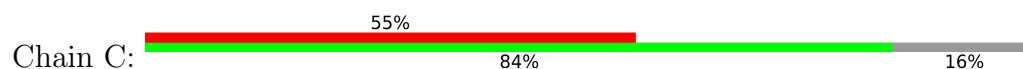
- Molecule 3: DNA-directed RNA polymerase II largest subunit



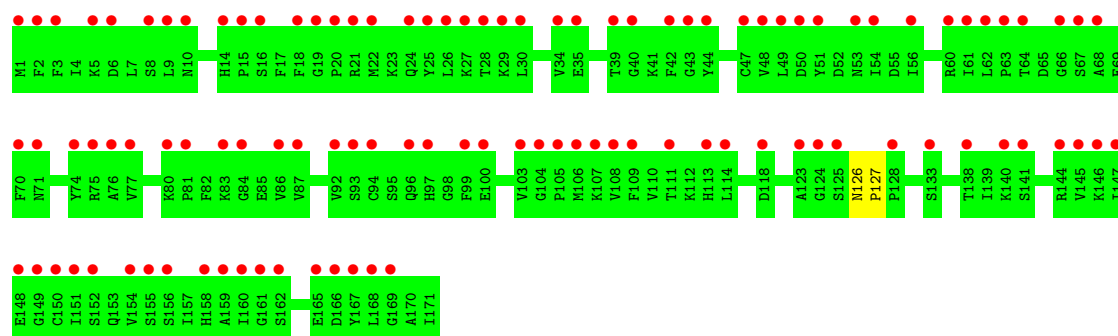
M466	K518	L582	Q650	V719	D781	A844	E914	Q994	M1063	E1129	A1200	L1268	L1348	M466
A457	P519	P583	V652	R720	T783	E846	G916	K994	G1065	Q1130	A1201	E1269	Y1349	A457
H458	C520	N584	V653	F721	R782	E846	G916	E995	V1066	A1131	D1206	M1270	K1350	H458
R459	N521	G585	N654	L722	P785	M849	L920	N996	L1067	K1132	L1206	T1271	V1352	R459
V460	G522	I586	F655	R723	H785	V850	G921	L998	A1068	L1133	M1209	L1273	V1353	V460
K461			W656	E724	H786	H851	G921	V999	A1069	L1134	W1209	L1273	V1353	K461
V462	D526	Q589	W656	R725	F787	H851	D922	L1000	Q1070	R1135	G1210	R1274	N1354	V462
I463	T527	R590	L657	R726	S788	H852	D923	L1000	S1070	S1136	Q1211	G1275	V1355	I463
P464	L528	L598	L658		R789	D853	K924	R1001	T1071	V1212	V1136	V1276	V1355	P464
V465	C529	S599	H659		D790	H854	L925	G1002	I1072	A1137	G1213		A1357	V465
S466	G530	G594	N660	A729	T793	T855	Q926		G1073	T1141	E1214	Y1287	S1358	S466
	Y531	T595	G661	R731	S793	T856	V927		E1074	L1142	R1215		D1359	
L470	H532	T596	F662	L732	P794		L928		P1075	L1143	R1216			L470
M471		L597	S663	A733	E795	S859	L929	Q1008	A1076	K1144	Q1217	P1292	V1363	M471
L472	T535	L598	T664	E734	S796	L860		M1009	T1077	Q1145	K1218	S1293	V1363	L472
S473	L536	S599	G665	W735	K797	L860	K934	A1010	Q1078	V1146	T1219	P1294	R1366	S473
V474	B537	P600	I666	W736	G798	N862	Q935	Q1011	M1079	L1146	F1220	G1296	H1366	V474
T475	D538		G667	L737		H863	L936	R1012	T1080	A1149	K1221	E1297	M1368	T475
S476	T539	N603	D668	K738	E801	L864	V937	D1013	L1081	S1150	N1222	E1301	L1369	S476
P477	F540	L598	T669	D739	N802	Q865	K938	A1014	N1082	E1151	D1223	E1301	L1370	P477
L478	I541	L606	R677	W746	S803	F866	D939	T1015	F1083	L1152	L1371	L1274	A1370	L478
Y479	E542	L607	E678	N741	H904	L867	R940	T1016	F1084	Y1153	F1225	V1372	V1372	Y479
M480	L543	I606	I679	W742	L805	H868	K941	L1017		L1154	V1226	L1373	D1373	M480
D481	D544	G610	P674	V743	R806	G869	F942	F1018	A1087	D1155	T1227	L1306		D481
F482	Q545	Q611	T675	K744	G807	E870	V946	C1019	G1088	P1156	W1228	L1306	T1376	F482
D483	L612	I612	M676	Q745	L808	D871	F947	C1020	S1091	S1160	S1229	Q1377	T1376	D483
G484	L547	T613	R677	M746	T809	G872		L1021	K1092	T1161	E1230	Q1378	Q1378	G484
D485	N548	F614	E678	W747	P810	D873	A952	R1023	K1093	E1165	E1234	G1379	G1379	D485
E486	M549	G615	I679	M748	Q811	D874	L952	S1024	V1094	D1166		K1380	G1380	E486
M487	L550	V616	T682	A749	E512	A875	A952	R1025	K1094	E1165	E1234	L1381	G1380	M487
M488	Y551	E618	L683	G750	F913	A876	N953	L1026	S1096	D1166		L1382	G1380	M488
L489	W552	E618	A684	S751	R814	H877	W954	T1026	T1096	L1237	L1238	L1382	G1380	L489
H490	V553	L598	E685	K752	F815	L878	P955	A1027	G1097	L1169	R1239	L1382	G1380	H490
V491	P564	T621	G685	G753	H816	E879	L956	T1028	V1098	L1170	C1240	M1318	V1384	V491
P492	D555	V622	A686	S754	A817	K880	L960	R1029	P1099	H1173	R1241	T1318	F1389	P492
Q493	W566	G623			M618	Q881	L960	R1030	R1100		V1242		R1389	Q493
S494	D577	S624	K689	M757	G819	S882	L960	Q1033	L1101	L1176	V1243		M1390	S494
E495	G558	N625	V690	A758	G820	L883	L963	Q1033	K1102	L1176	V1243		R1391	E495
A496	V559	L626	L691	L759	G820	D884	L963	Q1033	E1103	LEU	ARG	D1323	M1391	A496
T497	T560	T607	D692	A761	R821	T885	Q965	ASP	L1104	ASP	LYS	P1324	M1392	T497
R498	P561	G628	V693	Q761	G823	L886	N966	GLU	L1105	GLU	SER	T1325	M1393	R498
A499	T562	L629	T694	S762	G823	G887	A967	W1044	N1106	GLU	LEU	R1326	G1395	A499
E500	P563	L630	Q698	A763	L825	G888	Q968	V1045	V1107	ALA	ASP	T1329	A1396	E500
L501	A564	H631	T698	C764	D826	G888	Q969	L1046	A1108	GLU	ALA	M1330	L1397	L501
Q503	I565	V632		V765	T827		Q969	S1047	A1108	GLN	THR	S1331	M1398	Q503
L504	I566	V633	T703	G766	A828	A892	I973	M1048	M1111	GLU		F1332	C1400	L504
C505		T634		Q767		R836	D974	I1049		PHE	GLU	I1333	S1401	C505
A506	K569		H706	Q768	T831	R836	D974	I1049	P1114	ASP	A1254	D1334	F1402	A506
V507	L571	G638	G707	S769	A832	R897	H975	E1050	S1115	Q1187	E1254	I1334	F1402	V507
P508	W572	P639	M708	V770	E833	R898	T976	A1051	L1116	Q1188	A1254	E1340	F1402	P508
L509	S573	Q640	T709	E771	T834	V899	K977	F1052	L1116	Q1188	A1254	E1340	F1402	L509
Q510	Q574	L710	L710	G772	T834	D900	P978	F1053	T1117	S1189	D1257	L1341	F1402	Q510
I511	G574	V641	R711	K773	G835	N903	L983	R1055	E1121	P1190	H1258	G1340	F1402	I511
V512	K575	C542	E712	R774	L837	N903	L983	R1055	P1122	W1191	M1259	I1341	F1402	V512
S513	A643		S713	L775	T837	N903	L983	R1055	P1122	W1191	M1259	I1341	F1402	S513
P514	L577	F714	L714	I775	Q838	T907	K984	V1057	G1123	Q1187	E1254	I1341	F1402	P514
Q515	L578	E715	E715	R777	R839	L908	D985	L1058	H1124	Q1187	E1254	I1341	F1402	Q515
S516	S579	G647	T716	G778	R840	S911	L912	P1060	A1125	E1196	L1261	L1341	F1402	S516
N517	W580	N648	N717	F779	L841	S911	L912	P1060	A1125	E1196	L1261	L1341	F1402	N517
F517	A581		N719	V750	V642	S911	L912	P1060	A1125	E1196	L1261	L1341	F1402	F517



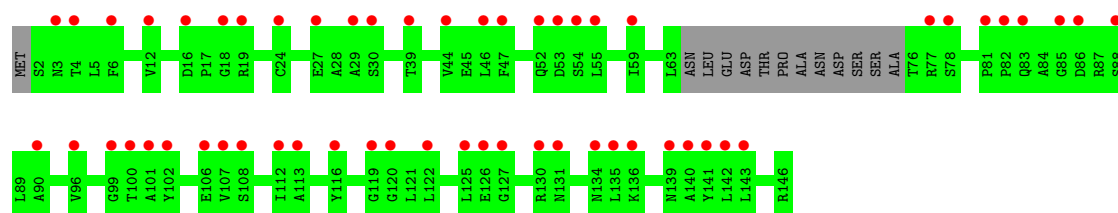
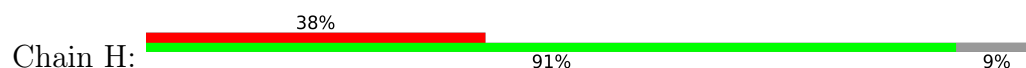
• Molecule 5: DNA-directed RNA polymerase II 45 kDa polypeptide



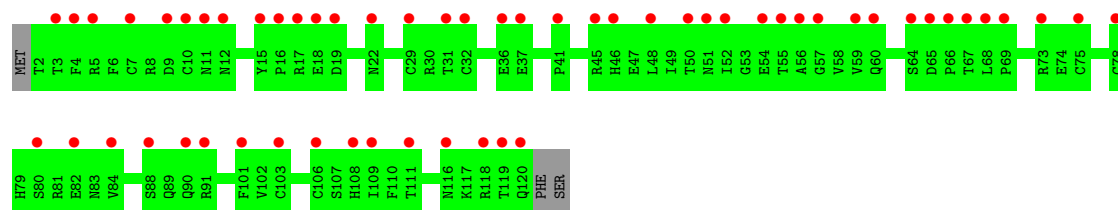




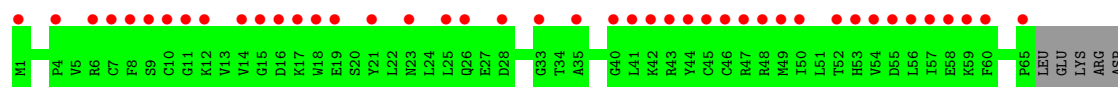
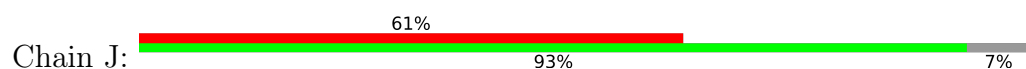
- Molecule 10: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



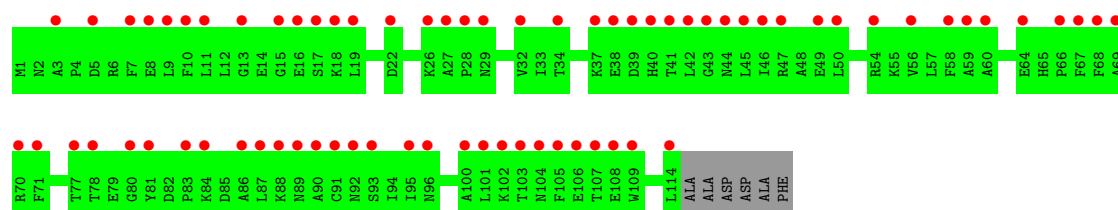
- Molecule 11: DNA-directed RNA polymerase II subunit 9



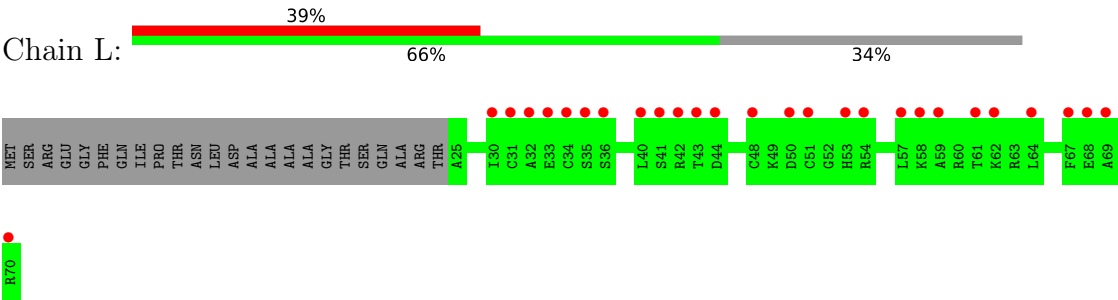
- Molecule 12: DNA-directed RNA polymerases I/II/III subunit 10



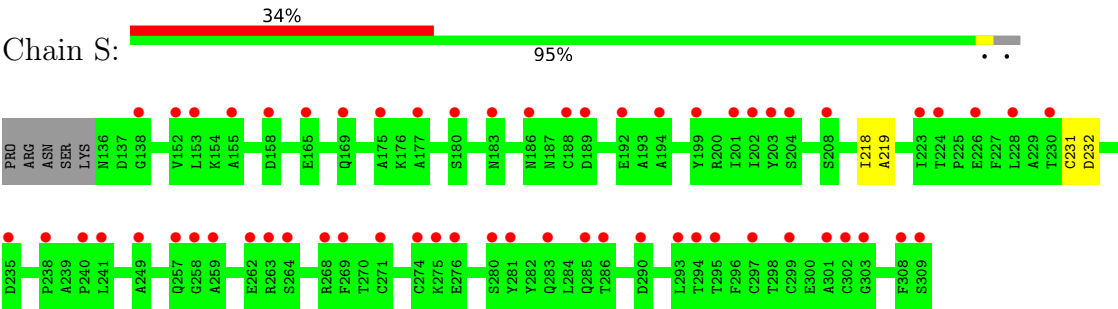
- Molecule 13: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 14: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



- Molecule 15: Transcription elongation factor S-II



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.20Å 395.70Å 282.10Å 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) 98.6 (50.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 4.00Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.281 , (Not available) 0.413 , 0.409	Depositor DCC
R_{free} test set	2038 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	106.8	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	9.76 , 298.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	4112	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

5.1 Standard geometry [i](#)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	T	7	0	0	0	0
2	P	4	0	0	0	0
3	A	1426	0	0	1	0
4	B	1112	0	0	0	0
5	C	266	0	0	0	0
6	D	177	0	0	0	0
7	E	214	0	0	1	0
8	F	84	0	0	0	0
9	G	171	0	0	1	0
10	H	133	0	0	0	0
11	I	119	0	0	0	0
12	J	65	0	0	0	0
13	K	114	0	0	0	0
14	L	46	0	0	0	0
15	S	174	0	0	2	0
All	All	4112	0	0	5	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 1.

All (5) 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)
15:S:218:ILE:CA	15:S:219:ALA:CA	2.73	0.66
9:G:126:ASN:CA	9:G:127:PRO:CA	2.78	0.62
3:A:447:GLN:CA	3:A:448:PRO:CA	2.83	0.56
15:S:231:CYS:CA	15:S:232:ASP:CA	2.86	0.53
7:E:128:PRO:CA	7:E:129:PRO:CA	2.90	0.49

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	0/4	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

There are no ligands in this entry.

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	7/7 (100%)	5.60	7 (100%) 0 0	68, 74, 104, 109	0
2	P	4/4 (100%)	3.74	3 (75%) 0 0	82, 86, 92, 95	0
3	A	1426/1733 (82%)	3.54	941 (65%) 0 1	19, 69, 145, 200	0
4	B	1104/1224 (90%)	3.28	670 (60%) 0 1	22, 82, 164, 198	0
5	C	266/318 (83%)	3.55	174 (65%) 0 1	38, 77, 136, 162	0
6	D	177/221 (80%)	2.56	97 (54%) 0 1	41, 93, 159, 174	0
7	E	214/215 (99%)	3.34	129 (60%) 0 1	39, 110, 172, 189	0
8	F	84/155 (54%)	2.77	46 (54%) 0 1	19, 53, 95, 117	0
9	G	171/171 (100%)	2.98	106 (61%) 0 1	43, 72, 110, 129	0
10	H	133/146 (91%)	2.49	56 (42%) 0 1	81, 132, 175, 192	0
11	I	119/122 (97%)	2.32	57 (47%) 0 1	64, 125, 171, 216	0
12	J	65/70 (92%)	3.78	43 (66%) 0 1	48, 72, 126, 138	0
13	K	114/120 (95%)	3.02	72 (63%) 0 1	40, 84, 137, 146	0
14	L	46/70 (65%)	2.97	27 (58%) 0 1	68, 134, 166, 187	0
15	S	174/179 (97%)	2.03	60 (34%) 1 2	50, 50, 124, 138	0
All	All	4104/4755 (86%)	3.23	2488 (60%) 0 1	19, 80, 159, 216	0

The worst 5 of 2488 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	110	PHE	42.0
3	A	1061	GLY	30.8
3	A	69	THR	29.8
3	A	1437	GLY	28.6
9	G	104	GLY	26.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.