



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:26 AM GMT

PDB ID : 2CW0
Title : Crystal structure of Thermus thermophilus RNA polymerase holoenzyme at 3.3 angstroms resolution
Authors : Tuske, S.; Sarafianos, S.G.; Wang, X.; Hudson, B.; Sineva, E.; Mukhopadhyay, J.; Birktoft, J.J.; Leroy, O.; Ismail, S.; Clark Jr., A.D.; Dharia, C.; Napoli, A.; Laptenko, O.; Lee, J.; Borukhov, S.; Ebright, R.H.; Arnold, E.
Deposited on : 2005-06-15
Resolution : 3.30 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

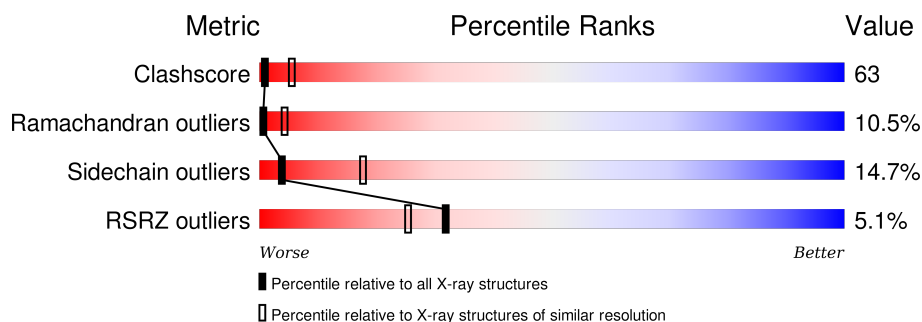
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	A	315	<div> <div>18%</div> <div>44%</div> <div>10%</div> <div>27%</div> </div>
1	B	315	<div> <div>10%</div> <div>19%</div> <div>43%</div> <div>11%</div> <div>27%</div> </div>
1	K	315	<div> <div>23%</div> <div>38%</div> <div>10%</div> <div>27%</div> </div>
1	L	315	<div> <div>3%</div> <div>17%</div> <div>48%</div> <div>8%</div> <div>27%</div> </div>
2	C	1119	<div> <div>5%</div> <div>25%</div> <div>59%</div> <div>14%</div> </div>
2	M	1119	<div> <div>4%</div> <div>24%</div> <div>59%</div> <div>15%</div> </div>
3	D	1524	<div> <div>5%</div> <div>20%</div> <div>52%</div> <div>18%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53962 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 protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			
5	P	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	N	2	Total	Zn	0	0
			2	2		

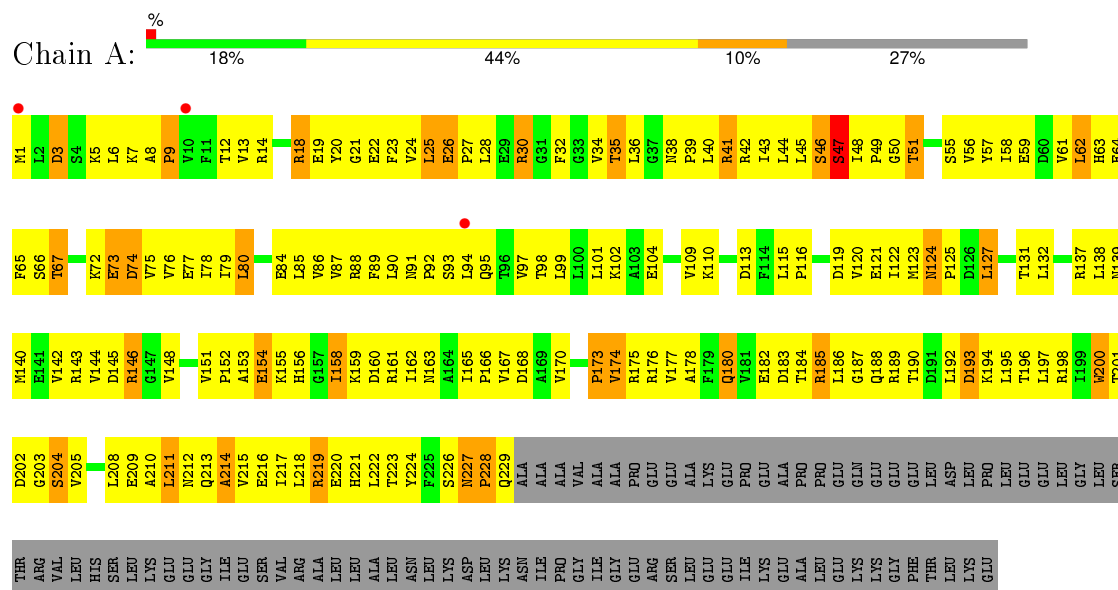
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

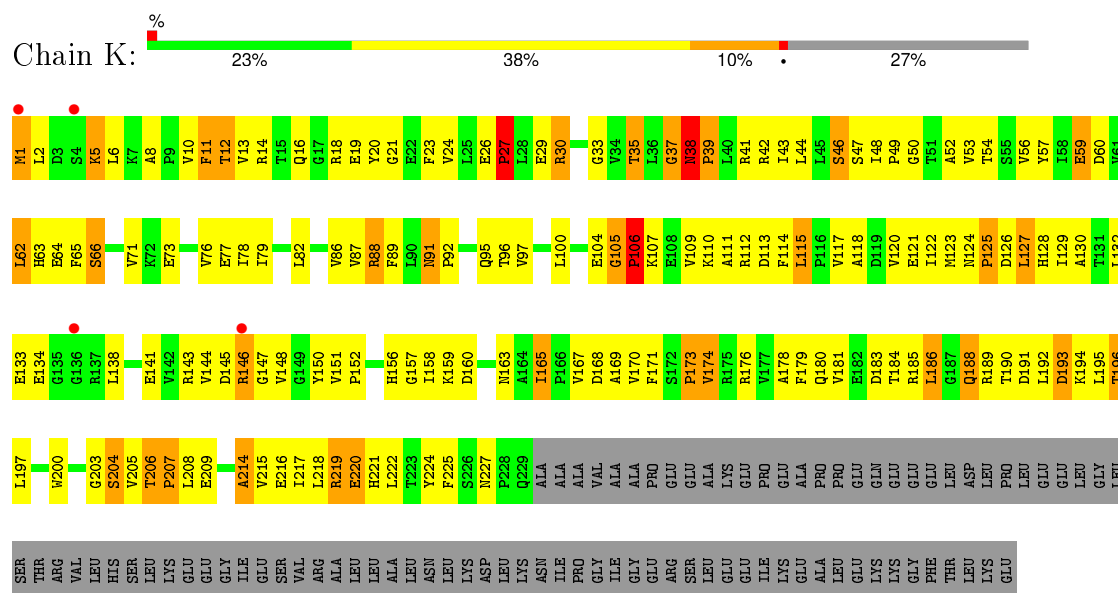
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: DNA-directed RNA polymerase alpha chain



LYS
LYS
GLY
PHE
THR
LEU
LYS
GLU

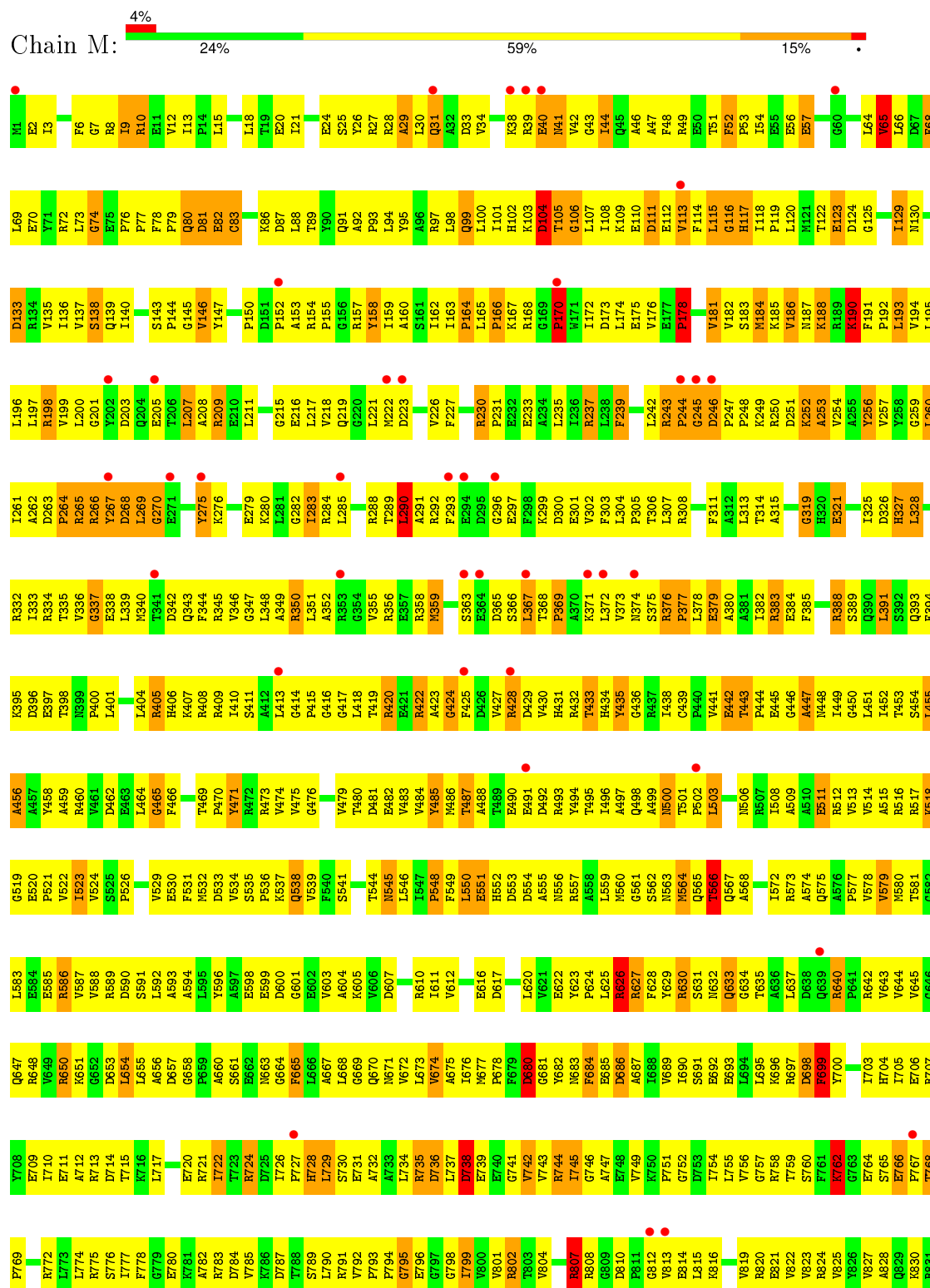
• Molecule 1: DNA-directed RNA polymerase alpha chain

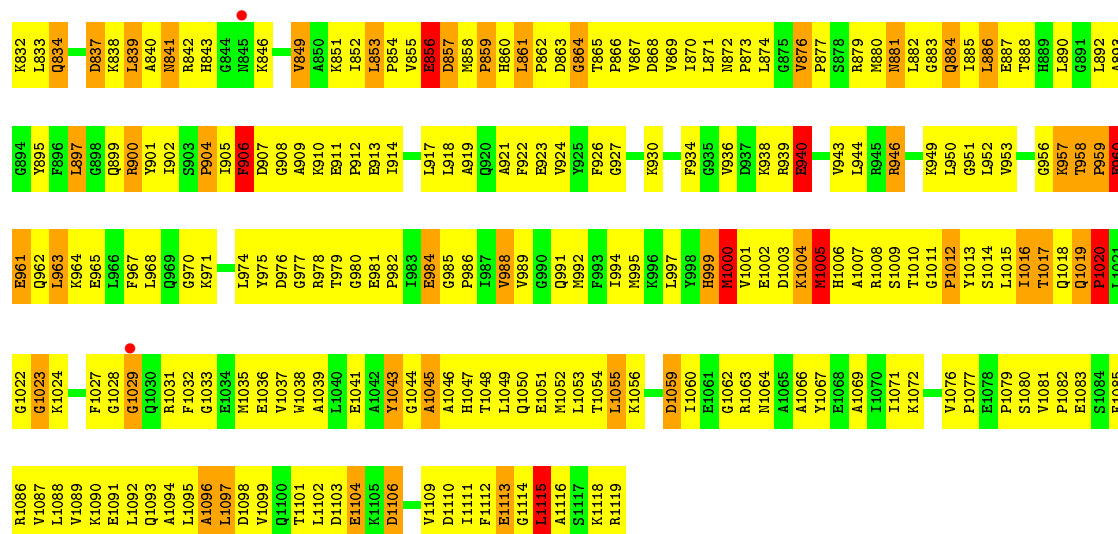


G1022	L952	L886	V825	G763	L695	N632	L571	M506	P444	S375	L313	R250	K188	S126	G63
G1023	K957	E887	Y826	E764	K696	Q633	L572	R507	E445	R376	T314	D251	R189	F127	L64
K1024		T888		S765	R697	G634	R573	I508	G446	P377	A315	K252	K190	I128	V65
F1027	E960	H889	Q829	E766	D698	T635	A574	A509	A447	L378	G316	A253	F191	I129	L66
G1028	G991	G891	K830	T767	F699	A636	Q575	V513	N448	E379	V317		P192	M130	D67
G1029	L963	L892	K832	T768	T701	D638	A576	V514	I449		R318	Y256	L193	G131	F68
Q1030	K964	A893	L833	E770	S702	Q639	P577	M514	G450		G319	V257	V194	A182	L69
R1031	E965		K834	E771	T703	R640	V578	A515	L451		R320	Y258	L195	D133	L69
G1032	L966	F896	V835	R772	H704	P641	M580	R517	A452		F321	Y259	L196	R134	E70
G1033	F967	G836	G836	R773		G642	K518	K518	T453		R386	L261	L197	V135	R72
G1034	L968	G898	D837	L774	R707	V643	G582	G519	S454		S387	L260	R198	I136	L73
M1035	Q935	Q838	K838	R775	Y708	V644	L583	M520	S454		R388	A262	R199	V137	G74
E1036	G970	R900	L839	S776	E709	V645	E584	P521	L455		S389	D263	L200	S138	E75
V1037	K971	A840	A840	I777	E710	G646	E585		Y458		Q990	P264	G201	Q139	F76
W1038	V972	I902	R842		E711	Q647	R586	V522	A459		L391	R265	Y202	Q139	F77
	V973	S903	R843	E780	A712	R648	V587	V524			S392	R266	D203	I140	F78
E1041	L974	P904	H843	K781	R713	V649	V588	S525	D462		Q393	Y267	Q204	P144	Q80
A1042	K975	R905	G844	A782	A712	R650	R589		L464		K395	D268	T206	G145	D81
Y1043	D976	F906	N845	T883	L717	K651	D590		G465		R396	G270	L207	V146	E82
G1044	G977	D907	K846	D784	G718	D653	S591	V529	F466		E397	E271	A208	Y147	
A1045	R978		V848	V785		L654	A593	F531	R468		T398	A272	R209	T149	K86
A1046	T979		V849	D787	R721	L655	A594	M532	T469		V336	G273	E210	P150	D87
H1047	G980	E911	A850	T788	T722		A594	D533	P470		G337	R274	L211	D151	L88
T1048	E981	P912	K851	S789	R724		L595	M533	Y471		E338	Y275	G212		T89
L1049	P982	E913										K276			
Q1050	L914	K915	L852	L790	D725	P659	A597	S535	R472		R340	A277	G215	A153	Y90
E1051	E984	E916	L853	R791	I726	A660	E598	P536	R473		R406	E278	E216	R154	K86
M1052	G985	R916	P854	V792	T727	S661	E599	K537	V474		K407	E279	L217	P155	Q91
L1053	P986	L917	V855	H728	H728	E662	D600	Q538	V475		R408	K280	V218	G156	L94
T1054	L987	L918	B856	P793	L729	N663	G601	V539	G476		R409	L281			Y95
L1055	V988	G795	D857	G794	S730	G664	B602	F540	G477		I410	G282	L221	Y158	A96
K1056	G989	R920	M858	E796	E731	F665	B603	S541	V478		G346	G282	M222	I159	R97
S1057	E990	A921	R860	G797		L666	A604	V542	V479		L348	R284	E223	A180	L98
D1058	Q991	F922	H861	G798	L734	A667	G605	N543	T480		A349	L285	D224	S161	Q99
D1059	N992	E923	L861	I799	R735	L668	V606	T544	D481		R350	S286	S225	I162	L100
F993	F993	V924	D862	V800	D736	G669	D607	N545	G416		L361	G287	V226	I163	I101
		Y925	D863	V801	L737	Q670	G608	L546	G417		A352	R388	F227	I163	H102
K996	K996	F926	G864	R802	D738	M671	M609	I547	L418		R353	T289	A228	L165	K103
L997	L997	G927	T865	T803	E739	V672	R610	F548	T419		G354	L290	F229	P166	D104
Y1067	Y998	K928	P866	V804	G740	L673	V611	L550	M486		V355	A291	R230	K167	G106
	H999	R929	V867	R805	G741	V674	V612	F549	T487		R356	R292	P231	R168	T105
A1066			D868	L806	V742	A675	V613	E551	A488		G357	F293	E232	G169	L107
I1070	I1003	F934	V869	R807	V743	L676	R614	H552	T489		R358		E233	P170	L108
I1071	K1004	G935	L870	R808	R744	M677	Y615		E490		G359	G296	E234	M171	K109
	M1005	V936	L871	G809	I745	P678	E516		D492		L360		L235	I172	E110
E1074		D937	N872	D810	E748	F679	D617		D429		R361	K299	I236	D173	D111
D1075	K938	R937	P873	P811	V749	D680	G681		V430		G362	D300	R237	L174	E112
V1076	R939	R939	L874	G812	V750	G681	V621		H431		S363	E301	L238	E175	V113
	G1011	E940	G875	V813	K750	V682	E622		R432		R364	V302	F239		F114
P1079	P1012		V876	E814	P751	M683	G561		T433		D365	F303	T240	P178	L115
S1080	Y1013	V943	R877	L815	G752	F684	P624		H434		S366	L304	L241	M179	G116
V1081	S1014	L944	S878	V823	K750	P684	Y623		R494		G367	L304	L241	M179	G116
P1082	L1015	R945	R879	P824	V751	M683	P624		V435		T368	P305	L242	G180	H117
G1083	P1016	R946	V875	L425	G685	M685	L425		G436		T306	T306	R243	V181	I118
E1084	L1017	R947	N880	R626	L755	V689	R626		R437		R369	L307	P244	V182	P119
S1084	T1017	A947	N881	R627		M689	R627		R438		A370	R308	G245	S183	
F1085	Q1018	E948	L882	E821	R758	P691	F628		P502		K371	Y309	D246	M184	
R1086	Q1019	R949	L882	E822	T759	S691	Y629		L503		L372	L310	P247	K185	
T1087	P1020	G884	Q884	V823	S760	E692	R630		E504		V373	F311	P248	V186	
L1088	L1021	G951	R885	R824	K762	L694	S631		G505		N374	A312	K249	G125	

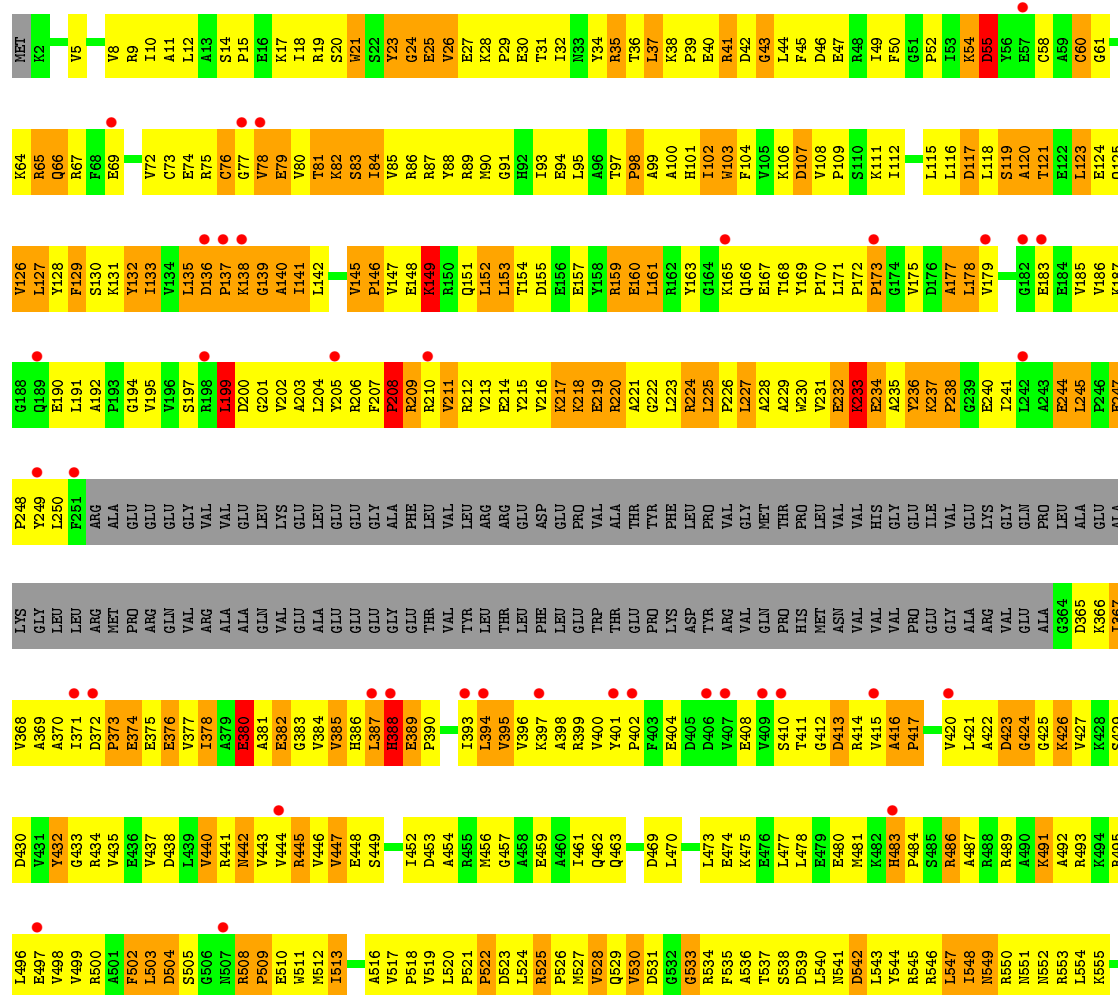
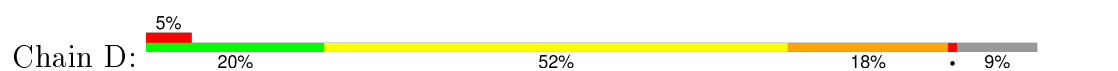


• Molecule 2: DNA-directed RNA polymerase beta chain





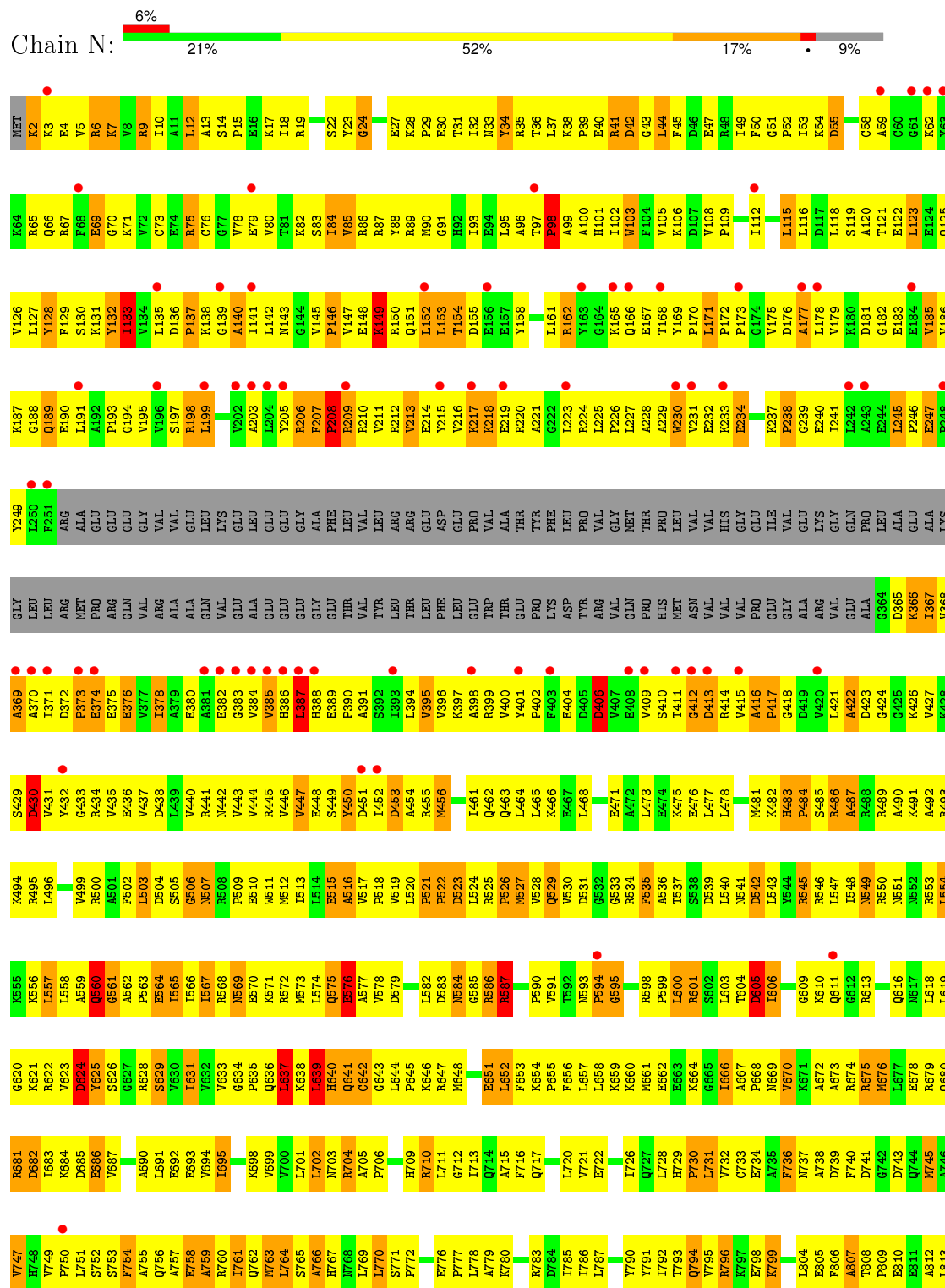
• Molecule 3: DNA-directed RNA polymerase beta' chain



S1486	R1310	G1248	P1187	Q1124	E1083	V1003	A933	L973	E806	D743	R681	L618	L558
A1437	L1311	A1249	V1188	P1125	G1064	T1004	L934	E974	F806	Q744	D682	L619	A559
A1438	L1312	A1250	R1189	D1126	T1066	Q1005	R935	T975	A807	R745	G620	G620	Q560
S1375	V1313	D1251	S1190	E1127	T1066	A1006	Y936	S976	T808	G684	K621	K621	G561
K1314	K1314	I1252	P1191	T1128	V1067	V1007	Y937	P877	P809	D685	K622	K622	A563
T1253	D1315	T1253	L1192	T1129	L1068	F1008	G938	G878	E810	E686	V623	V623	P563
Q1254	G1316	Q1254	R1193	R1130	E1069	K1009	F939	R879	E811	L751	D624	D624	E564
L1255	D1317	L1255	Q1195	S1131	T1070	R1010	F940	L881	A812	S752	Y625	Y625	E688
L1256	V1318	L1256	T1196	L1132	F1071	F1011	T941	L880	L813	S753	S626	S626	I566
P1257	R1319	P1257	R1197	R1133	S1072	E1012	A814	P882	A814	F754	K627	K627	I567
R1258	V1320	R1258	Y1198	L1134	S1073	E1013	S945	R883	A815	A755	R628	R628	R658
V1259	G1321	V1259	G1199	R1135	S1074	N1014	S946	R884	R816	Q756	S629	S629	N569
I1260	G1322	I1260	V1200	K1136	S1075	K1015	G946	T885	E817	A757	V630	V630	E570
E1261	Q1323	E1261	C1201	R1137	G1076	P1016	I947	V886	R818	E758	I631	I631	K571
L1262	P1324	L1262	Q1202	A1138	A1077	F1017	T948	A887	G819	A759	V632	V632	R572
F1263	L1325	F1263	R1203	D1139	R1078	E1018	T949	E888	E820	R760	V633	V633	M573
E1264	T1326	E1264	K1204	I1140	K1079	P1019	G950	A889	G897	G697	G634	G634	A579
A1265	R1327	A1265	Y1205	E1141	G1080	L1020	I951	V890	V821	I761	L574	L574	L574
R1266	G1328	R1266	G1206	A1142	G1081	Y1021	D952	E891	G824	Y763	P635	P635	Q575
L1267	T1329	L1267	Y1207	G1143	A1082	V1022	D953	D892	A825	L764	L637	L637	E576
P1268	D1330	P1268	D1208	L1144	D1083	M1023	A954	E893	P826	L702	K638	K638	A577
G1329	I1331	G1329	L1209	Y1145	T1084	A1024	V955	K894	R827	S765	L639	L639	V578
L1330	H1332	L1330	S1210	G1146	A1085	Q1025	V956	V895	K828	A766	L639	L639	D579
E1331	K1333	E1331	R1211	R1147	L1086	S1026	P957	A896	V829	R767	H640	H640	A580
A1332	D1334	A1332	A1212	V1148	R1087	G1027	E958	K897	A896	A768	Q641	Q641	L581
L1335	L1335	L1335	R1213	L1149	T1088	A1028	E959	E898	A830	P706	G642	G642	L582
L1336	E1337	L1336	P1214	A1150	A1089	R1029	K960	E899	G831	L770	D583	D583	D583
G1337	T1338	G1337	V1215	R1151	G1092	G1030	L964	I900	R832	S771	L644	L644	N584
I1338	P1340	I1338	S1216	L1153	Y1093	M1032	N969	L902	R833	P772	P645	P645	G585
Q1389	E1342	Q1389	I1217	V1154	L1094	Q1033	K970	K903	T834	A773	K646	K646	R586
G1392	A1403	G1392	G1218	V1155	T1095	Q1034	K970	V904	V835	S774	R647	R647	R587
L1393	N1404	L1393	E1219	L1156	R1096	I1035	I971	P905	R838	G775	M648	M648	G588
V1394	E1405	V1394	A1220	L1156	K1097	G1040	Q976	S910	P846	P777	A649	A649	A589
L1395	L1406	L1395	V1221	R1159	L1098	Q1036	L972	K906	Y841	L778	L650	L650	P590
E1396	P1407	E1396	I1222	E1161	Y1099	L1038	Q973	K908	R842	A779	L652	L652	T592
K1397	A1409	K1397	I1223	E1162	D1100	G1039	E975	N909	F843	R780	K654	K654	N593
L1400	L1348	L1400	V1224	E1163	V1101	G1040	Q976	S910	P846	P781	P655	P655	G595
E1401	E1350	E1401	A1225	G1163	T1102	L1041	A977	L911	Y842	S782	P656	P656	S596
G1411	L1349	G1411	I1226	R1164	H1103	R1042	Y978	K912	P846	D784	L657	L657	D597
K1412	N1404	K1412	A1227	L1165	E1104	G1043	T984	L914	A849	L785	L658	L658	R598
P1414	E1405	P1414	S1228	Y1166	T1105	L1044	D985	V915	L850	L786	K659	K659	P599
L1415	L1406	L1415	I1229	L1167	V1106	M1045	D986	K916	L850	L787	K660	K660	L600
V1416	E1407	V1416	G1230	S1167	V1107	Q1046	R986	Y916	V853	L788	M661	M661	R601
A1417	K1354	A1417	E1231	M1168	R1108	Q1046	E987	Q917	V853	G788	B662	B662	S602
E1418	V1355	E1418	P1232	D1169	E1109	P1048	R988	A918	V858	L789	B663	B663	L603
F1482	T1356	F1482	G1233	D1170	R1109	F1048	R989	L918	V858	Y790	L604	L604	T604
T1484	R1357	T1484	T1234	V1171	A1110	G1049	D990	F919	D859	R791	P668	P668	D605
Q1485	A1358	Q1485	Q1235	H1172	D1111	G1050	D990	L920	L860	T792	P669	P669	I606
V1486	Q1359	V1486	L1236	L1173	C1112	E1051	Q991	R921	Q861	T793	L607	L607	L607
L1487	G1360	L1487	T1237	L1174	G1113	T1052	L992	L922	D862	Q794	V670	V670	V670
D1488	V1361	D1488	M1238	L1175	T1114	F1053	L993	G923	V863	V795	K671	K671	S603
Q1489	K1362	Q1489	R1239	K1176	T1115	E1054	Q994	E924	V864	R796	A672	A672	G609
A1422	L1363	A1422	E1239	R1177	N1116	Y1055	L995	E925	T865	A735	A673	A673	K610
S1427	H1364	S1427	T1240	A1177	Y1117	P1056	V996	K926	V866	R797	K674	K674	Q611
A1428	D1365	A1428	F1241	E1178	Y1117	A1178	K926	T927	R867	K799	R675	R675	G612
L1429	K1366	L1429	R1242	E1179	S1118	Y1057	T997	T927	R867	A737	R676	R676	K613
S1430	E1367	S1430	T1243	L1305	S1119	R1058	E998	A928	X668	K800	R677	R677	F614
T1431	H1367	T1431	G1244	E1182	V1120	S1059	T999	R929	X668	G801	L677	L677	R615
K1432	L1368	K1432	G1245	I1183	P1121	S1060	F1000	L930	R869	A802	B678	B678	R615
E1436	E1369	E1436	V1246	L1122	F1061	K871	L804	D932	G870	F740	Q616	Q616	Q616
A1437	L1370	A1437	G1247	L1122	F1061	K871	L804	D932	G870	F740	Q616	Q616	Q616
V1439	E1437	V1439	A1247	V1186	F1123	R1062	K1002	D932	R872	G742	Q680	Q680	N617

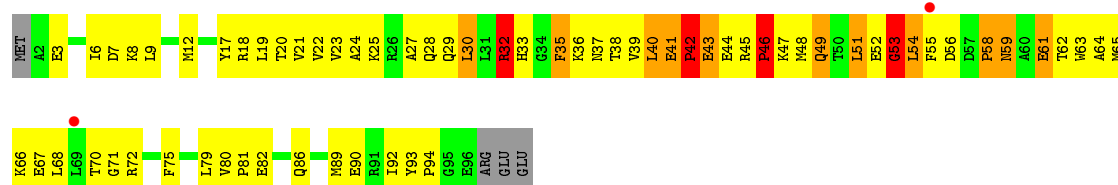
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LYS	
GLU	
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PRO	
ALA	
ALA	
ARG	
ARG	
GLY	
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ARG	
GLU	
GLN	
PRO	
GLY	
LYS	
GLN	
ALA	

• Molecule 3: DNA-directed RNA polymerase beta' chain

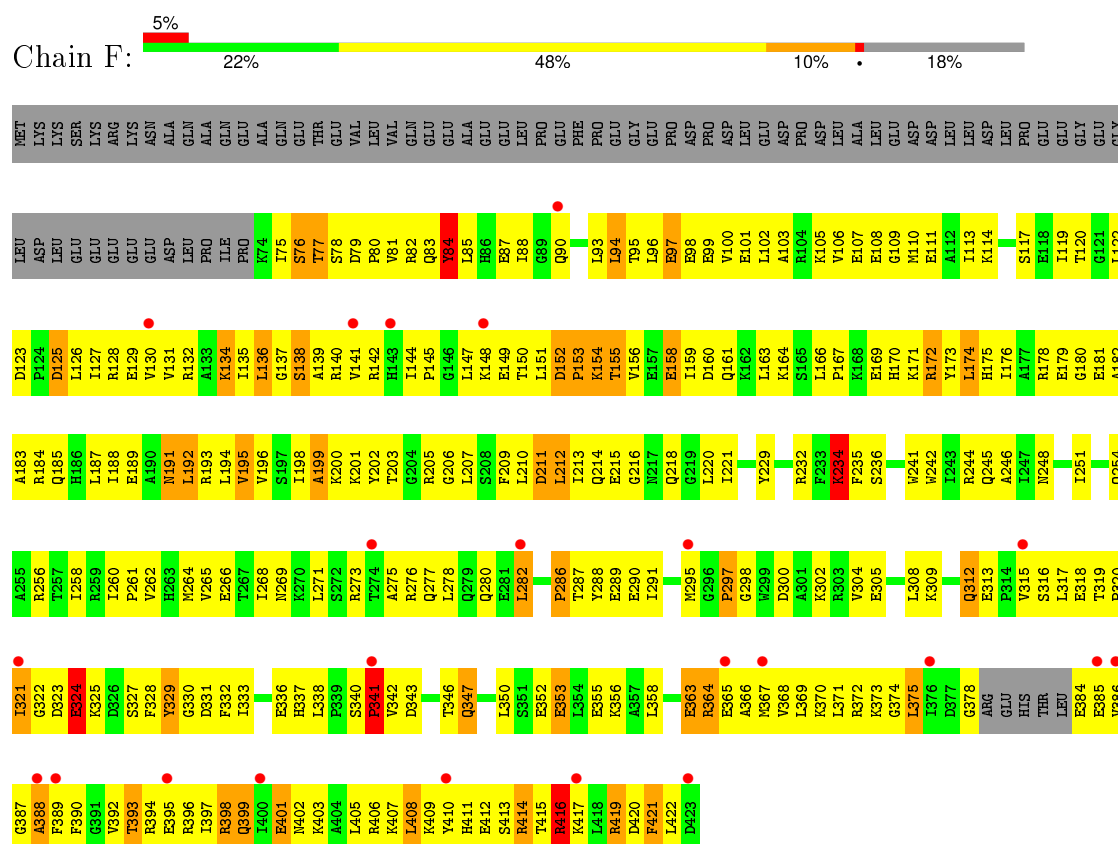
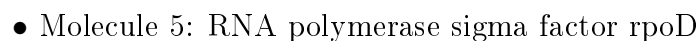




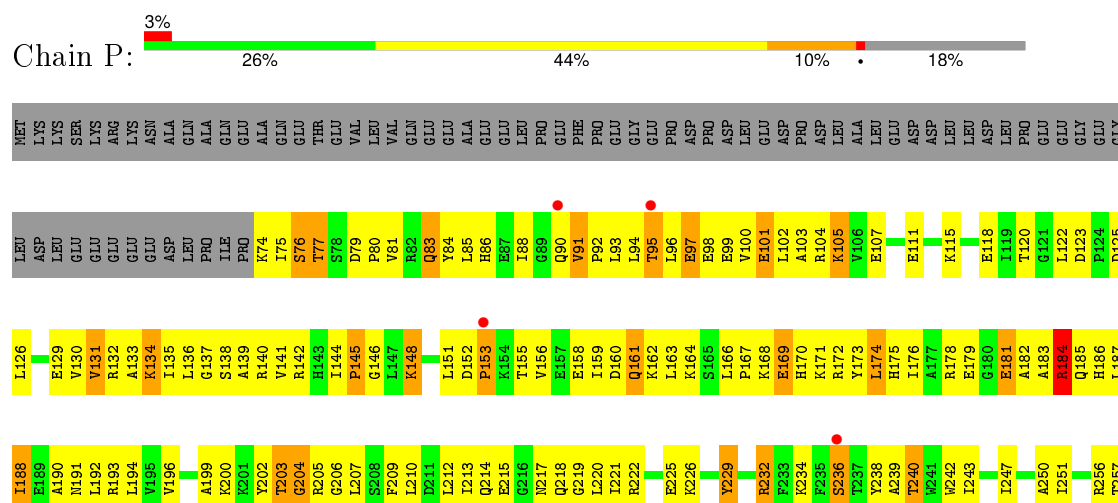
- Chain E: 

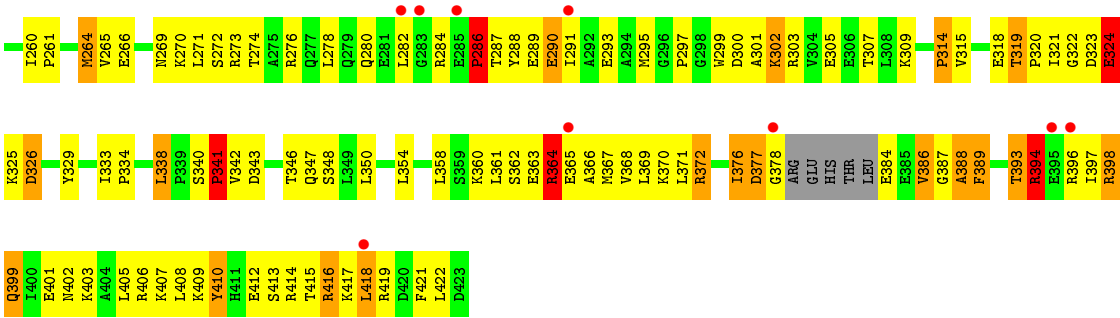


- WORLDWIDE
PDB
PROTEIN DATA BANK



- Molecule 5: RNA polymerase sigma factor rpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.15Å 236.15Å 249.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.87 – 3.30	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 47.2 (29.87-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.282 , 0.320 0.286 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 8.9	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 115957 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	53962	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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

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	A	0.46	0/1838	0.75	0/2498
1	B	0.36	0/1838	0.64	0/2498
1	K	0.46	0/1838	0.75	0/2498
1	L	0.39	0/1838	0.68	0/2498
2	C	0.45	0/8997	0.79	8/12164 (0.1%)
2	M	0.46	0/8997	0.79	8/12164 (0.1%)
3	D	0.48	0/11165	0.83	16/15088 (0.1%)
3	N	0.46	0/11165	0.81	15/15088 (0.1%)
4	E	0.42	0/783	0.80	3/1054 (0.3%)
4	O	0.42	0/783	0.80	1/1054 (0.1%)
5	F	0.40	0/2836	0.73	0/3812
5	P	0.41	0/2836	0.72	0/3812
All	All	0.45	0/54914	0.78	51/74228 (0.1%)

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
3	D	0	1
3	N	0	3
5	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1209	LEU	N-CA-C	-10.12	83.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	728	HIS	N-CA-C	7.66	131.69	111.00
2	C	728	HIS	N-CA-C	7.62	131.58	111.00
3	N	1209	LEU	N-CA-C	-7.26	91.39	111.00
2	M	319	GLY	N-CA-C	-7.22	95.05	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	132	TYR	Sidechain
5	F	84	TYR	Sidechain
3	N	1015	TYR	Sidechain
3	N	1318	TYR	Sidechain
3	N	132	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	A	1806	0	1861	249	0
1	B	1806	0	1861	193	0
1	K	1806	0	1861	190	0
1	L	1806	0	1861	208	0
2	C	8829	0	8933	1143	0
2	M	8829	0	8933	1183	0
3	D	10975	0	11211	1723	0
3	N	10975	0	11210	1681	0
4	E	769	0	775	94	0
4	O	769	0	775	83	0
5	F	2793	0	2873	301	0
5	P	2793	0	2873	364	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
All	All	53962	0	55027	6830	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 63.

The worst 5 of 6830 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:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.21	1.20
2:C:1016:ILE:HD13	2:C:1016:ILE:H	1.06	1.16
3:D:907:GLU:HG2	3:D:1027:GLY:H	1.02	1.16
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.22	1.15
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.27	1.15

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	
1	A	227/315 (72%)	167 (74%)	39 (17%)	21 (9%)	1	6
1	B	227/315 (72%)	177 (78%)	37 (16%)	13 (6%)	2	16
1	K	227/315 (72%)	161 (71%)	39 (17%)	27 (12%)	0	3
1	L	227/315 (72%)	166 (73%)	44 (19%)	17 (8%)	1	10
2	C	1117/1119 (100%)	781 (70%)	226 (20%)	110 (10%)	1	5
2	M	1117/1119 (100%)	769 (69%)	215 (19%)	133 (12%)	0	3
3	D	1388/1524 (91%)	941 (68%)	293 (21%)	154 (11%)	0	3
3	N	1388/1524 (91%)	907 (65%)	332 (24%)	149 (11%)	0	4
4	E	93/99 (94%)	67 (72%)	17 (18%)	9 (10%)	1	5
4	O	93/99 (94%)	59 (63%)	20 (22%)	14 (15%)	0	1
5	F	341/423 (81%)	241 (71%)	67 (20%)	33 (10%)	1	5
5	P	341/423 (81%)	249 (73%)	57 (17%)	35 (10%)	1	4
All	All	6786/7590 (89%)	4685 (69%)	1386 (20%)	715 (10%)	1	4

5 of 715 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	B	3	ASP
1	B	118	ALA
1	B	160	ASP
2	C	7	GLY

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	
1	A	202/273 (74%)	177 (88%)	25 (12%)	6	25
1	B	202/273 (74%)	172 (85%)	30 (15%)	4	17
1	K	202/273 (74%)	173 (86%)	29 (14%)	4	19
1	L	202/273 (74%)	182 (90%)	20 (10%)	10	37
2	C	941/941 (100%)	808 (86%)	133 (14%)	4	20
2	M	941/941 (100%)	805 (86%)	136 (14%)	4	18
3	D	1170/1279 (92%)	970 (83%)	200 (17%)	2	12
3	N	1170/1279 (92%)	980 (84%)	190 (16%)	3	14
4	E	83/87 (95%)	72 (87%)	11 (13%)	5	21
4	O	83/87 (95%)	70 (84%)	13 (16%)	3	15
5	F	300/370 (81%)	264 (88%)	36 (12%)	6	27
5	P	300/370 (81%)	269 (90%)	31 (10%)	9	34
All	All	5796/6446 (90%)	4942 (85%)	854 (15%)	4	18

5 of 854 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1462	LEU
1	L	156	HIS
3	N	1326	THR
4	E	66	LYS

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Mol	Chain	Res	Type
5	F	416	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1442	ASN
1	L	38	ASN
3	N	1441	GLN
3	D	1489	GLN
1	K	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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	A	229/315 (72%)	-0.02	3 (1%) 79 74	41, 64, 87, 113	0
1	B	229/315 (72%)	0.70	30 (13%) 5 3	47, 121, 143, 143	0
1	K	229/315 (72%)	-0.12	4 (1%) 73 67	28, 63, 88, 111	0
1	L	229/315 (72%)	0.18	8 (3%) 48 40	41, 79, 99, 117	0
2	C	1119/1119 (100%)	0.12	55 (4%) 33 27	12, 67, 133, 143	0
2	M	1119/1119 (100%)	0.09	43 (3%) 44 37	6, 71, 122, 133	0
3	D	1392/1524 (91%)	0.12	71 (5%) 32 25	7, 60, 125, 143	0
3	N	1392/1524 (91%)	0.22	93 (6%) 21 17	5, 65, 134, 143	0
4	E	95/99 (95%)	0.10	2 (2%) 67 60	54, 84, 100, 106	0
4	O	95/99 (95%)	0.10	1 (1%) 82 78	46, 86, 117, 121	0
5	F	345/423 (81%)	0.19	23 (6%) 21 17	48, 81, 113, 121	0
5	P	345/423 (81%)	0.03	13 (3%) 44 37	47, 73, 110, 123	0
All	All	6818/7590 (89%)	0.14	346 (5%) 32 25	5, 70, 129, 143	0

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	181	VAL	9.0
2	C	271	GLU	9.0
3	D	1240	THR	8.9
3	N	1245	GLY	8.0
3	N	371	ILE	7.8

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 [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
6	ZN	D	1526	1/1	0.97	0.19	-0.84	78,78,78,78	0
6	ZN	N	1525	1/1	0.91	0.13	-1.05	108,108,108,108	0
6	ZN	N	1526	1/1	0.93	0.05	-1.42	72,72,72,72	0
6	ZN	D	1525	1/1	0.74	0.07	-1.91	107,107,107,107	0
7	MG	N	1527	1/1	0.96	0.10	-	29,29,29,29	0
7	MG	D	1527	1/1	0.84	0.15	-	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.