



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:10 PM GMT

PDB ID : 1IW7
Title : Crystal structure of the RNA polymerase holoenzyme from *Thermus thermophilus* at 2.6Å resolution
Authors : RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-04-22
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

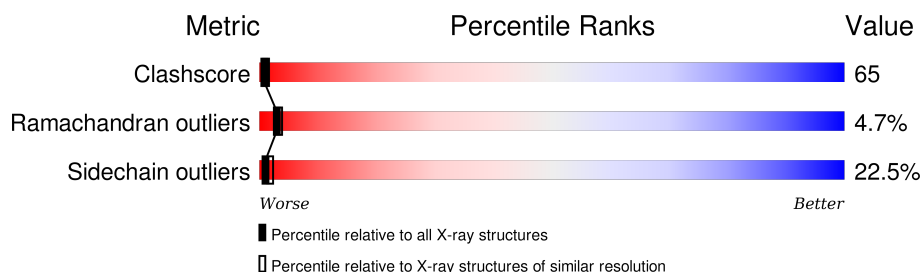
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
3	N	1524	<div><div></div><div>23%</div><div>51%</div><div>16%</div><div>•</div><div>9%</div></div>
4	E	99	<div><div></div><div>24%</div><div>56%</div><div>14%</div><div>•</div><div>•</div></div>
4	O	99	<div><div></div><div>24%</div><div>60%</div><div>11%</div><div>•</div><div>•</div></div>
5	F	423	<div><div></div><div>20%</div><div>47%</div><div>12%</div><div>•</div><div>18%</div></div>
5	P	423	<div><div></div><div>21%</div><div>44%</div><div>14%</div><div>•</div><div>18%</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 59529 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 RNA polymerase alpha subunit.

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 RNA polymerase beta subunit.

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 RNA polymerase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10801	6823	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10801	6823	1925	2020	33			

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

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-70 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	22	Total	Mg	0	0
			22	22		
6	D	118	Total	Mg	0	0
			118	118		
6	K	20	Total	Mg	0	0
			20	20		
6	E	6	Total	Mg	0	0
			6	6		
6	B	24	Total	Mg	0	0
			24	24		
6	C	63	Total	Mg	0	0
			63	63		
6	A	18	Total	Mg	0	0
			18	18		
6	N	92	Total	Mg	0	0
			92	92		
6	O	8	Total	Mg	0	0
			8	8		
6	L	19	Total	Mg	0	0
			19	19		
6	F	31	Total	Mg	0	0
			31	31		
6	M	64	Total	Mg	0	0
			64	64		

- Molecule 7 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Pb	0	0
			2	2		
7	N	2	Total	Pb	0	0
			2	2		

- Molecule 8 is water.

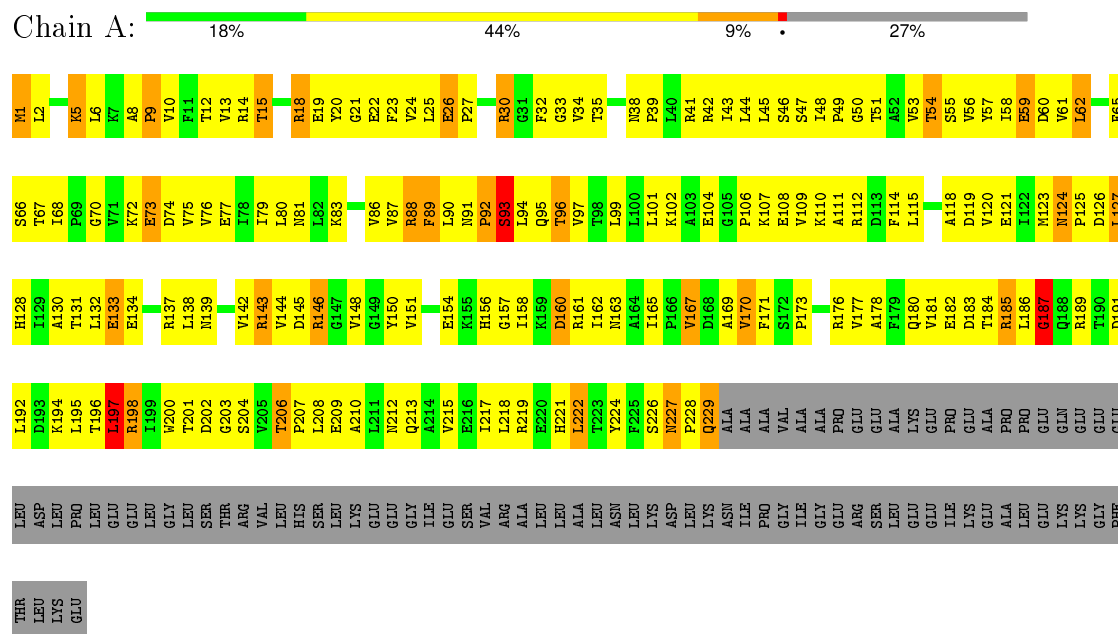
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	194	Total 194	O 194	0	0
8	B	193	Total 193	O 193	0	0
8	C	869	Total 869	O 869	0	0
8	D	1163	Total 1163	O 1163	0	0
8	E	114	Total 114	O 114	0	0
8	F	381	Total 381	O 381	0	0
8	K	161	Total 161	O 161	0	0
8	L	157	Total 157	O 157	0	0
8	M	822	Total 822	O 822	0	0
8	N	983	Total 983	O 983	0	0
8	O	114	Total 114	O 114	0	0
8	P	325	Total 325	O 325	0	0

3 Residue-property plots

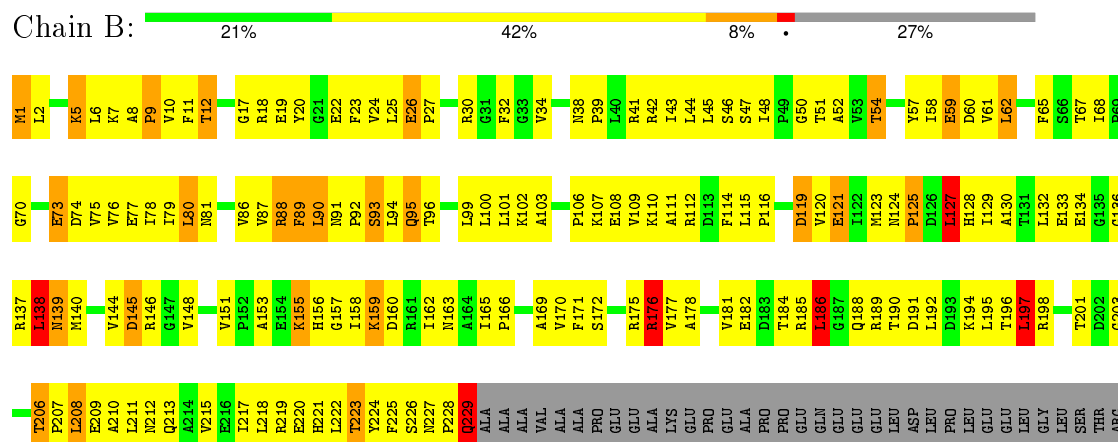
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: RNA polymerase alpha subunit



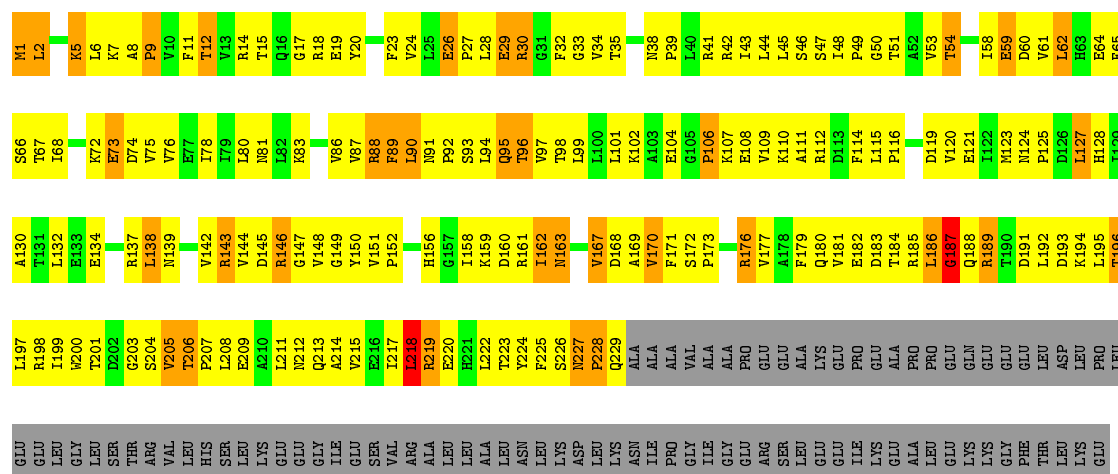
- Molecule 1: RNA polymerase alpha subunit



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THR
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LYS
GLU

• Molecule 1: RNA polymerase alpha subunit

Chain K: 17% 43% 11% 27%

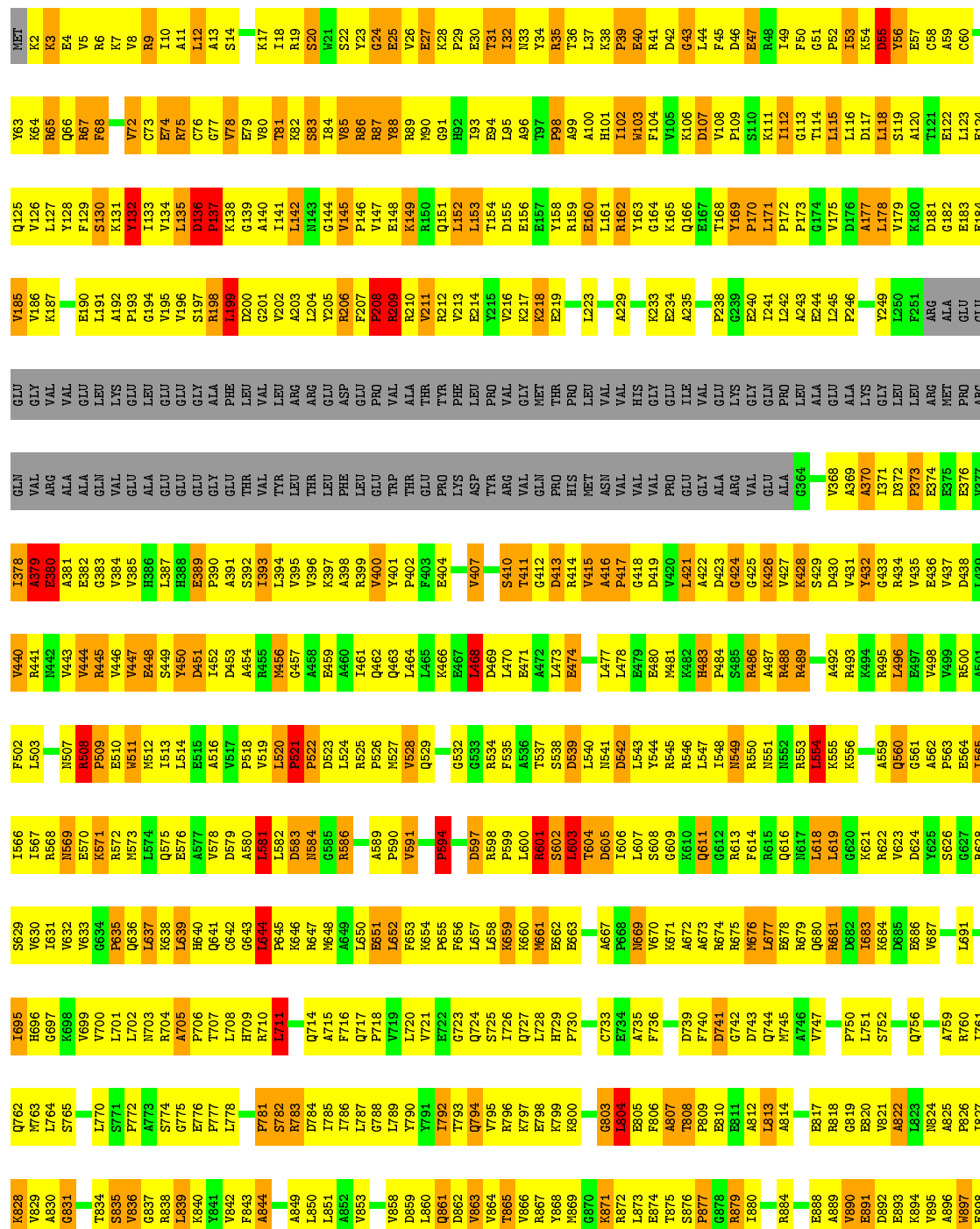


Q1093	R1031	L966	G898	Q834	G763	K696	A636	B573	I508	N448	E384	A315	A253	K188	F127
A1094	F1032	F967	Q899	D837	E766	R697	L637	A574	A409	I449	F385	G316	V254	R189	I128
L1095	G1033	L968	R900	D837	E766	D698	L637	A575	E510	L451	F386	G319	A255	R190	I129
A1096	E1034	Q969	Y901	K838	P767	F699	D638	A576	E511	L451	S387	G319	A256	F191	N130
L1097	M1035	Q970	I902	L839	P768	T700	Q639	P577	B512	I452	K388	R320	V257	G132	G131
D1098	E1036	K971	S903	A840	P769	T701	R640	V578	B513	T453	K389	R321	V258	L193	A132
V1099	V1037	P904	P904	R841	E770	S702	R641	V579	B514	S454	L391	V322	G259	V194	D133
W1038	W1038	I905	I905	R842	E771	I703	R642	M580	A515	L455	S392	D323	L260	R134	D134
A1039	P1100	R976	F906	R843	E772	H704	V643	G582	B516	A456	S392	D324	L261	L196	V135
L1040	L1040	G977	D907	R844	L773	E705	V644	L583	K318	A457	K395	I325	L197	L197	I136
E1041	E1041	R978	G908	R845	L774	E706	V645	L584	K319	A458	D363	I326	D263	K198	V137
A1042	A1042	T979	A909	K846	R775	R707	G646	E585	G519	A459	E397	H327	P264	V199	S138
E1043	E1043	K980	K910	G847	S776	V708	Q647	E586	E520	R460	T398	K328	K265	K200	Q139
K1005	K1005	E981	E911	R848	I777	E709	R648	R586	P521	V461	K399	L328	R266	L201	Q139
D1066	G1044	E981	E911	R848	I777	E709	R648	R586	P521	V461	K399	L328	R266	L201	Q139
N1107	A1045	R982	P912	R849	F778	I710	V649	V587	V522	D462	S402	R331	L269	Y202	H141
P1108	A1046	I983	E913	R850	G779	I710	R650	V588	V523	F582	R332	R332	L269	D203	R142
D1109	H1047	E984	E914	R851	E780	T715	R651	R589	S525	L464	S403	I333	Q270	Q204	S143
D1110	T1048	G985	K915	R852	K781	K716	G652	D590	S525	G465	L404	R344	E271	E205	P144
F1111	L1049	P986	E916	L853	A782	L717	D653	S591	P526	F466	R405	T335	G272	T206	G145
F1112	Q1050	I987	L917	R854	R783	G718	L654	L592	E527	L467	R406	V336	G273	L207	V146
L1115	M1052	F926	L918	R855	D784	P719	D657	A593	E528	R468	R407	G337	R274	A208	I147
A1116	L1053	Q920	A919	E856	K786	E720	G658	A594	E530	T469	R409	E338	Y275	R209	F148
S1117	T1054	Q991	Q920	D857	R787	R721	G659	L595	E530	P470	R409	L339	K276	E210	T149
K1118	L1055	M992	Q920	R858	T788	T722	R660	Y596	P531	Y471	S411	K340	A277	L211	P150
R1119	K1056	F993	F926	R860	S789	T723	R661	A597	N532	R472	A412	D342	E278	D151	D151
	S1057	K996	G927	R861	L790	D725	S662	E598	D533	R473	L413	Q343	E279	E216	P182
	I1060	L997	K928	R862	R791	T726	N663	D600	V534	V474	G414	F344	K280	L217	A153
	K1063	H999	E932	R863	V792	H728	G664	G601	P536	G476	P415	R345	G282	Q219	R154
	E1064	M1000	Q933	R864	G795	R729	L666	E602	K537	G477	G416	V346	G282	Q220	P155
	A1065	F934	F934	R865	G795	S730	L667	E603	Q538	V478	G417	G347	R284	L221	G156
	E1066	E1002	D937	R866	G795	S730	L668	E604	V539	T479	L418	L348	L285	M222	Y158
	Y1067	K1004	R937	R867	I799	L734	G669	R606	S541	D481	T419	R350	G287	S225	I159
	K1005	M1005	K938	R868	R305	R735	N671	D607	N543	E482	R422	L351	G288	S226	I162
	H1006	H1006	R939	R869	R306	D736	N672	G608	N544	V483	R422	A352	T289	F227	I163
	A1007	A1007	E940	R870	R307	D737	L673	R610	T544	V484	R423	V355	L290	A228	P164
	R1008	R1008	E941	R871	R307	D738	L674	R611	N545	Y485	R424	R356	L291	M229	L165
	S1009	S1009	E942	R872	R308	E739	A675	V612	L546	M486	R425	E357	R292	R230	P166
	T1010	T1010	E943	R873	R309	E740	A676	V613	T547	T487	V427	R292	F293	P231	K167
	D1075	D1075	R945	R874	R310	V742	L677	R614	P548	A488	R428	K359	G296	E232	R168
	P1076	P1076	R946	R875	R311	V743	P678	V615	L550	E490	V430	M359	G297	E233	G169
	P1077	S1014	R947	R876	R312	R744	P679	E616	E551	E491	H431	D365	E297	A234	P170
	E1078	L1015	E948	R877	R313	R744	D680	D617	E552	D492	R432	S366	K299	L235	H171
	P1079	I1016	K949	R878	R314	E747	G681	L620	D554	D493	R433	L367	K299	L236	I172
	S1080	T1017	L950	R879	R315	E748	Y682	V621	A555	Y494	R434	T368	D300	R237	D173
	V1081	Q1018	G951	R880	R316	E749	Y683	E622	N556	T495	R435	P369	E301	L238	L174
	P1082	Q1019	L952	R881	R317	K750	F684	E623	B557	I496	V436	P369	V302	F239	E175
	E1083	P1020	V953	R882	R318	P751	E685	E624	B558	A497	R437	A370	F303	T240	V176
	S1084	L1021	K957	R883	R319	G752	D686	L625	L559	Q498	I438	K371	P305	L241	E177
	F1085	G1022	T958	R884	R320	G752	D687	L626	E559	A499	C439	V372	T306	L242	F178
	V1087	K1024	R889	R885	R321	G752	A687	L627	E559	A499	C439	V373	T306	R243	R179
	L1088	F1027	E961	R886	R322	L755	V688	R626	M564	N500	P440	N374	R307	R244	G180
	V1089	G1028	Q962	R887	R323	L756	V689	R627	Q565	T501	P441	N374	R308	G245	V181
	K1090	L963	L963	R888	R324	G757	L690	R628	Q565	P502	R442	P377	V309	D246	V182
	E1091	L964	L964	R889	R325	G758	S691	R629	A568	L503	T443	E379	L310	P247	S183
	L1092	Q1030	E965	R890	R326	T759	E992	R630	A569	E504	T444	E379	L310	P247	S183
				R891	R327	S760	E993	S631	P570	G505	P445	E379	L310	P247	S183
				R892	R328	S761	E994	S632	L571	N506	G446	E379	L310	P247	S183
				R893	R329	S762	E995	S633	L572	R507	G447	E379	L310	P247	S183

• Molecule 2: RNA polymerase beta subunit

Chain M: 


M1	M2	M3	F6	G7	R8	I9	R10	E11	V12	I13	P14	L15	P16	P17	L18	R19	Y20	E21	Q22	E23	S25	Y26	R27	R28	A29	Q30	A32	D33	V34	P35	P36	E37	K38	R39	E40	V42	G43	I44	Q45	A46	A47	R49	E50	T51	F52	P53	I54	E55	E56	E57	D58	K59	G60	K61																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G62	G63	L64	V65	L67	F68	L69	E70	Y71	A72	L73	G74	E75	P76	P77	F78	P79	O80	D81	B82	C83	R84	E85	K86	D87	L88	T89	Y90	P92	A92	P93	L94	Y95	A96	R97	L98	Q99	L100	I101	H102	K103	D104	F105	G106	L107	I108	K109	E110	D111	E112	V113	F114	L115	G116	H117	I118	P119	L120	M121																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
T122	E123	D124	F127	I128	L129	M130	G131	A132	D133	R134	L135	I136	V137	S138	Q139	I140	S143	P144	G145	V146	F147	K148	T149	P150	D151	A153	R154	P155	G156	Y157	A158	I159	L162	P163	L165	P166	K167	R168	G169	P170	W171	I172	D173	L174	E175	V176	E177	P178	N179	G180	H181	V182	S183	G184																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
K185	V186	M187	K188	R189	A190	F191	P192	L193	V194	L196	L197	R198	V199	L200	G201	Y202	D203	Q204	E205	T206	L207	A208	R209	E210	L211	Y214	E215	E216	L217	G218	G219	G220	L221	W222	D223	V226	F227	A228	P229	R230	P231	E232	E233	L237	T238	F239	T240	L241	L242	R243	P244	G245	L246	P247	P248																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
K249	R250	D251	K252	A253	V254	A255	Y256	Y258	G259	L260	L261	A262	D263	P264	R265	R266	Y267	D268	L269	G270	E271	A272	R273	R274	Y275	K276	A277	E278	E279	K280	L281	G282	L283	R284	L285	S286	G287	R288	T289	L290	A291	R292	F293	G296	E297	F298	K299	D300	E301	F302	F303	L304	P305	T306	L307	R308	P309	Y309																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
L310	F311	A312	L313	T314	A315	G316	V317	P318	G319	E320	V321	D322	D323	G324	R325	H326	R327	L328	G329	R330	R331	R332	L333	R334	T335	V336	G337	E338	L339	R340	T341	D342	F343	V345	G347	L348	A349	R350	L351	A352	R353	V355	E357	R358	R359	L360	E364	D365	S366	L367	T368	P369	L370	K371																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
L372	V373	N374	S375	R376	P377	L378	A379	S380	R383	E384	F385	F386	S387	R388	S389	S392	Q393	F394	K395	R396	E397	R398	R399	P400	L401	S402	S403	L404	R405	R406	R407	R409	I410	R412	L413	G414	P415	L418	T419	R420	E421	R422	A423	G424	F425	D426	V427	D428	E429	A430	V431	H432	A433	L434	A435	L436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750																																																																																																																																																																																																													
P751	G752	D753	L754	L755	L756	G757	R758	L759	S760	R761	K762	G763	E766	P767	T768	F769	E770	E771	R772	L773	L774	R775	S776	L777	F778	G779	E780	E781	A782	R783	D784	L785	D786	L787	T788	S789	L790	R791	V792	G795	E796	G797	G798	L799	V800	T803	V804	R805	L806	R807	L808	N809	P810	G811	V812	V813	R814	G815	E816	D817	E822	Y823	P824																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
L625	R626	R627	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
E814	L815	K816	G818	V819	R820	E821	V822	R823	R824	R825	K826	G827	E828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	M1000	V1001	E1002	D1003	K1004	M1005	H1006	E1007	V1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A



GLU	A192	V126	R65	VAL	V1424	G1360	L1290	A1225	V1155	G1092	R1029	4967	L389
LEU	P193	L127	Q66	TI425	VI361	VI362	EL295	A1226	L1156	TI095	G1030	4968	1900
GLU	G194	Y128	R67	S1426	VI362	VI362	EL295	Q1227	VI158	TI096	G1031	4969	1901
GLY	V195	F129	F68	S1427	VI363	VI363	EL295	Q1228	VI159	TI097	G1032	4970	1902
ALA	V196	S130	E69	TI428	HI364	HI364	EL299	I1229	VI160	TI098	G1033	4971	1903
ALA	S197	K131	G70	TI429	HI365	HI365	EL300	I1230	VI161	TI099	G1034	4972	1904
PRO	R198	Y132	K71	VI430	VI366	VI366	VI301	EL301	VI162	TI100	G1035	4973	1905
LEU	L199	Y133	V72	TI431	HI367	HI367	VI304	EL302	VI163	TI101	G1036	4974	1906
VAL	D200	Y134	C73	VI432	HI368	HI368	VI305	EL303	VI164	TI102	G1037	4975	1907
LEU	G201	Y135	E74	VI433	HI369	HI369	VI306	EL304	VI165	TI103	G1038	4976	1908
ARG	V202	D136	R75	VI434	HI370	HI370	VI307	EL305	VI166	TI104	G1039	4977	1909
ARG	A203	P137	C76	VI435	VI372	VI372	VI308	EL306	VI167	TI105	G1040	4978	1910
GLY	K138	K137	G77	VI436	VI373	VI373	VI309	EL307	VI168	TI106	G1041	4979	1911
ASP	Y205	G139	V78	VI437	VI374	VI374	VI310	EL308	VI169	TI107	G1042	4980	1912
GLU	R206	A140	E79	VI438	VI375	VI375	VI311	EL309	VI170	TI108	G1043	4981	1913
PRO	F207	Y141	V80	VI439	VI376	VI376	VI312	EL310	VI171	TI109	G1044	4982	1914
VAL	P208	L142	T81	VI440	VI377	VI377	VI313	EL311	VI172	TI110	G1045	4983	1915
ALA	R209	K143	K82	VI441	VI378	VI378	VI314	EL312	VI173	TI111	G1046	4984	1916
ALA	R210	G144	S83	VI442	VI379	VI379	VI315	EL313	VI174	TI112	G1047	4985	1917
THR	V211	Y145	I84	VI443	VI380	VI380	VI316	EL314	VI175	TI113	G1048	4986	1918
THR	R212	P146	V85	VI444	VI381	VI381	VI317	EL315	VI176	TI114	G1049	4987	1919
PHE	V213	Y147	R86	VI445	VI382	VI382	VI318	EL316	VI177	TI115	G1050	4988	1920
LEU	E214	E148	R87	VI446	VI383	VI383	VI319	EL317	VI178	TI116	G1051	4989	1921
VAL	Y215	K149	Y88	VI447	VI384	VI384	VI320	EL318	VI179	TI117	G1052	4990	1922
GLY	V216	R150	R89	VI448	VI385	VI385	VI321	EL319	VI180	TI118	G1053	4991	1923
MET	K217	Q151	M90	VI449	VI386	VI386	VI322	EL320	VI181	TI119	G1054	4992	1924
THR	K218	L152	G91	VI450	VI387	VI387	VI323	EL321	VI182	TI120	G1055	4993	1925
PRO	E219	L153	R92	VI451	VI388	VI388	VI324	EL322	VI183	TI121	G1056	4994	1926
LEU	R220	T154	I93	VI452	VI389	VI389	VI325	EL323	VI184	TI122	G1057	4995	1927
VAL	A221	D155	E94	VI453	VI390	VI390	VI326	EL324	VI185	TI123	G1058	4996	1928
VAL	GLY	E156	L95	VI454	VI391	VI391	VI327	EL325	VI186	TI124	G1059	4997	1929
HIS	L227	E157	A96	VI455	VI392	VI392	VI328	EL326	VI187	TI125	G1060	4998	1930
GLY	A228	Y159	T97	VI456	VI393	VI393	VI329	EL327	VI188	TI126	G1061	4999	1931
ILE	K233	L161	P98	VI457	VI394	VI394	VI330	EL328	VI189	TI127	G1062	5000	1932
VAL	E234	R162	A99	VI458	VI395	VI395	VI331	EL329	VI190	TI128	G1063	5001	1933
GLY	Y238	Y163	H01	VI459	VI396	VI396	VI332	EL330	VI191	TI129	G1064	5002	1934
LYS	G239	Q166	I102	VI460	VI397	VI397	VI333	EL331	VI192	TI130	G1065	5003	1935
GLY	E240	E167	M03	VI461	VI398	VI398	VI334	EL332	VI193	TI131	G1066	5004	1936
PRO	I241	T168	F04	VI462	VI399	VI399	VI335	EL333	VI194	TI132	G1067	5005	1937
LEU	L242	Y169	P109	VI463	VI400	VI400	VI336	EL334	VI195	TI133	G1068	5006	1938
ALA	A243	P170	V108	VI464	VI401	VI401	VI337	EL335	VI196	TI134	G1069	5007	1939
ALA	P246	P172	S110	VI465	VI402	VI402	VI338	EL336	VI197	TI135	G1070	5008	1940
LYS	Y249	P173	K111	VI466	VI403	VI403	VI339	EL337	VI198	TI136	G1071	5009	1941
GLY	L250	A177	I112	VI467	VI404	VI404	VI340	EL338	VI199	TI137	G1072	5010	1942
LEU	P251	L178	G113	VI468	VI405	VI405	VI341	EL339	VI200	TI138	G1073	5011	1943
ARG	ALA	V179	L115	VI469	VI406	VI406	VI342	EL340	VI201	TI139	G1074	5012	1944
MET	GLU	K180	L116	VI470	VI407	VI407	VI343	EL341	VI202	TI140	G1075	5013	1945
PRO	GLU	D181	L117	VI471	VI408	VI408	VI344	EL342	VI203	TI141	G1076	5014	1946
ARG	GLU	G182	L118	VI472	VI409	VI409	VI345	EL343	VI204	TI142	G1077	5015	1947
ARG	GLU	L183	S119	VI473	VI410	VI410	VI346	EL344	VI205	TI143	G1078	5016	1948
VAL	GLY	V185	A120	VI474	VI411	VI411	VI347	EL345	VI206	TI144	G1079	5017	1949
ARG	VAL	V186	T121	VI475	VI412	VI412	VI348	EL346	VI207	TI145	G1080	5018	1950
ALA	VAL	K187	E122	VI476	VI413	VI413	VI349	EL347	VI208	TI146	G1081	5019	1951
ALA	GLU	E190	L123	VI477	VI414	VI414	VI350	EL348	VI209	TI147	G1082	5020	1952
GLN	LEU	E191	E124	VI478	VI415	VI415	VI351	EL349	VI210	TI148	G1083	5021	1953
VAL	LYS	L191	Q125	VI479	VI416	VI416	VI352	EL350	VI211	TI149	G1084	5022	1954
				VI480	VI417	VI417	VI353	EL351	VI212	TI150	G1085	5023	1955
				VI481	VI418	VI418	VI354	EL352	VI213	TI151	G1086	5024	1956
				VI482	VI419	VI419	VI355	EL353	VI214	TI152	G1087	5025	1957
				VI483	VI420	VI420	VI356	EL354	VI215	TI153	G1088	5026	1958
				VI484	VI421	VI421	VI357	EL355	VI216	TI154	G1089	5027	1959
				VI485	VI422	VI422	VI358	EL356	VI217	TI155	G1090	5028	1960
				VI486	VI423	VI423	VI359	EL357	VI218	TI156	G1091	5029	1961
				VI487	VI424	VI424	VI360	EL358	VI219	TI157	G1092	5030	1962
				VI488	VI425	VI425	VI361	EL359	VI220	TI158	G1093	5031	1963
				VI489	VI426	VI426	VI362	EL360	VI221	TI159	G1094	5032	1964
				VI490	VI427	VI427	VI363	EL361	VI222	TI160	G1095	5033	1965
				VI491	VI428	VI428	VI364	EL362	VI223	TI161	G1096	5034	1966
				VI492	VI429	VI429	VI365	EL363	VI224	TI162	G1097	5035	1967
				VI493	VI430	VI430	VI366	EL364	VI225	TI163	G1098	5036	1968
				VI494	VI431	VI431	VI367	EL365	VI226	TI164	G1099	5037	1969
				VI495	VI432	VI432	VI368	EL366	VI227	TI165	G1100	5038	1970
				VI496	VI433	VI433	VI369	EL367	VI228	TI166	G1101	5039	1971
				VI497	VI434	VI434	VI370	EL368	VI229	TI167	G1102	5040	1972
				VI498	VI435	VI435	VI371	EL369	VI230	TI168	G1103	5041	1973
				VI499	VI436	VI436	VI372	EL370	VI231	TI169	G1104	5042	1974
				VI500	VI437	VI437	VI373	EL371	VI232	TI170	G1105	5043	1975
				VI501	VI438	VI438	VI374	EL372	VI233	TI171	G1106	5044	1976
				VI502	VI439	VI439	VI375	EL373	VI234	TI172	G1107	5045	1977
				VI503	VI440	VI440	VI376	EL374	VI235	TI173	G1108	5046	1978
				VI504	VI441	VI441	VI377	EL375	VI236	TI174	G1109	5047	1979
				VI505	VI442	VI442	VI378	EL376	VI237	TI175	G1110	5048	1980
				VI506	VI443	VI443	VI379	EL377	VI238	TI176	G1111	5049	1981
				VI507	VI444	VI444	VI380	EL378	VI239	TI177	G1112	5050	1982
				VI508	VI445	VI445	VI381	EL379	VI240	TI178	G1113	5051	1983
				VI509	VI446	VI446	VI382	EL380	VI241	TI179	G1114	5052	1984
				VI510	VI447	VI447	VI383	EL381	VI242	TI180	G1115	5053	1985
				VI511	VI448	VI448	VI384	EL382	VI243	TI181	G1116	5054	1986
				VI512	VI449	VI449	VI385	EL383	VI244	TI182	G1117	5055	1987
				VI513	VI450	VI450	VI386	EL384	VI245	TI183	G1118	5056	1988
				VI514	VI451	VI451	VI387	EL385	VI246	TI184	G1119	5057	1989
				VI515	VI452	VI452	VI388	EL386	VI247	TI185	G1120	5058	1990
				VI516	VI453	VI453	VI389	EL387	VI248	TI186	G1121	5059	1991
				VI517	VI454	VI454	VI390	EL388	VI249	TI187	G1122	5060	1992
				VI518	VI455	VI455	VI391	EL389	VI250	TI188	G1123	5061	1993
				VI519	VI456	VI456	VI392	EL390	VI251	TI189	G1124	5062	1994
				VI520	VI457	VI457	VI393	EL391	VI252	TI190	G1125	5063	1995
				VI521	VI458	VI458	VI394	EL392	VI253	TI191	G1126	5064	1996
				VI522	VI459	VI459	VI395	EL393	VI254	TI192	G1127	5065	1997
				VI523	VI460	VI460	VI396	EL394	VI255	TI193	G1128	5066	1998
				VI524	VI461	VI461	VI397	EL395	VI256	TI194	G1129	5067	1999
				VI525	VI462	VI462	VI398	EL396	VI257	TI195	G1130	5068	2000
				VI526	VI463	VI463	VI399	EL					



● Molecule 5: RNA polymerase sigma-70 subunit

Chain P:  21% 44% 14% 18%

WET	LEU	L126	E189	P261	I326	F390
LYS	ASP	I127	A190	P262	S327	G391
LYS	LEU	E128	M191	H263	F328	V392
SER	GLU	L129	L192	M264	Y329	T393
LYS	GLU	V130	V265	G330	G330	R394
ARG	GLU	V131	L194	E266	D331	E395
LYS	GLU	R132	V195	T267	F332	R396
ASN	GLU	A133	V196	L268	I333	I397
ALA	ASP	K134	S197	M269	P334	R398
GLN	LEU	I135	I198	T270	D335	Q399
ALA	PRO	L136	A199	E336	E336	I400
GLN	ILE	G137	K200	L271	H337	E401
GLU	PRO	S138	T274	L274	L338	N402
ALA	K74	A139	G204	A275	P339	K403
GLN	I75	R140	R205	R276	S340	A404
GLU	S76	V141	G206	Q277	P341	L405
THR	T77	R142	L207	L278	V342	R406
GLU	S78	H143	S208	Q279	D343	K407
VAL	D79	I144	F209	Q280	A344	L408
LEU	P80	P145	L210	E281	Q347	K409
VAL	V81	G146	L211	L282	R410	Y410
GLN	R82	L147	L212	G283	S348	H411
GLU	Q83	K148	I213	R284	L349	E412
GLU	Y84	E149	Q214	E285	L350	S413
ALA	L85	T150	E215	P286	S351	R414
GLU	H86	L151	G216	T287	S351	T415
GLU	E87	D152	N217	Y288	L354	R416
LEU	I88	P153	Q218	E289	E355	K417
PRO	G89	K154	G219	E290	K356	L418
GLU	Q90	T155	L220	I291	A357	R419
PHE	Y91	V156	I221	A292	L358	D420
PRO	P92	I159	R222	G293	S359	F421
GLU	L93	L94	A223	M295	K360	L422
GLY	L94	Q161	V224	G296	L361	
GLY	T95	E225	E225	P297		
PRO	L96	K162	K226	G298	R364	
ASP	E97	L163	R232	H299	E365	
PRO	E98	K164	R232	D300	A366	
ASP	E99	S165	F233	A301	M367	
LEU	V100	L166	R234	K302	V368	
GLU	E101	P167	F235	R303	L369	
ASP	L102	K168	S236	V304	K370	
PRO	K105	E169	A239	E305	L371	
LEU	V106	H170	T240	E306	R372	
ALA	M110	K171	W241	T307	K373	
GLU	I113	Y173	W242	L308	G374	
ASP	K114	L174	I243	K309	I375	
LEU	S117	H175	R249	I310	D377	
ASP	E118	I176	A250	P314	G378	
LEU	I119	R178	I251	V315	ARG	
PRO	T120	E181	D253	L317	GLU	
GLU	G121	A182	R256	E318	HIS	
GLY	L122	R184	T257	T319	THR	
GLY	D123	L187	R258	P320	LEU	
GLY	P124	I188	I260	I321	E384	
				E324	E385	
				K325	F389	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59529	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PB, 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	0.68	0/1838	0.87	4/2498 (0.2%)
1	B	0.68	0/1838	0.85	7/2498 (0.3%)
1	K	0.66	1/1838 (0.1%)	0.85	5/2498 (0.2%)
1	L	0.67	0/1838	0.90	4/2498 (0.2%)
2	C	0.72	3/8997 (0.0%)	0.97	30/12164 (0.2%)
2	M	0.73	2/8997 (0.0%)	0.97	26/12164 (0.2%)
3	D	0.71	8/10979 (0.1%)	1.01	52/14844 (0.4%)
3	N	0.73	6/10979 (0.1%)	1.02	38/14844 (0.3%)
4	E	0.72	0/783	1.01	2/1054 (0.2%)
4	O	0.71	0/783	1.02	2/1054 (0.2%)
5	F	0.90	8/2812 (0.3%)	1.08	20/3781 (0.5%)
5	P	0.85	4/2812 (0.1%)	1.12	20/3781 (0.5%)
All	All	0.73	32/54494 (0.1%)	0.99	210/73678 (0.3%)

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	3
3	N	0	3
5	F	0	1
All	All	0	7

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	GLU	CG-CD	13.42	1.72	1.51
5	F	401	GLU	CB-CG	13.27	1.77	1.52
5	P	401	GLU	CG-CD	13.01	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	401	GLU	CB-CG	12.94	1.76	1.52
5	F	423	ASP	C-OXT	11.47	1.45	1.23

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	229	GLN	CA-C-O	17.63	157.12	120.10
5	P	416	ARG	NE-CZ-NH1	13.69	127.14	120.30
2	C	243	ARG	C-N-CD	-12.01	94.19	120.60
2	M	163	ILE	C-N-CD	-11.12	96.14	120.60
3	D	380	GLU	CA-C-O	-11.07	96.85	120.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	132	TYR	Sidechain
3	D	379	ALA	Peptide
3	D	380	GLU	Mainchain
5	F	421	PHE	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	247	0
1	B	1806	0	1861	213	0
1	K	1806	0	1861	216	0
1	L	1806	0	1861	213	0
2	C	8829	0	8933	1312	0
2	M	8829	0	8933	1273	0
3	D	10801	0	10887	1543	0
3	N	10801	0	10885	1539	0
4	E	769	0	775	94	0
4	O	769	0	775	106	0
5	F	2771	0	2843	392	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	2771	0	2844	429	0
6	A	18	0	0	0	0
6	B	24	0	0	0	0
6	C	63	0	0	0	0
6	D	118	0	0	1	0
6	E	6	0	0	0	0
6	F	31	0	0	0	0
6	K	20	0	0	0	0
6	L	19	0	0	0	0
6	M	64	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	22	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	A	194	0	0	44	0
8	B	193	0	0	50	0
8	C	869	0	0	254	0
8	D	1163	0	0	325	0
8	E	114	0	0	30	0
8	F	381	0	0	67	0
8	K	161	0	0	49	0
8	L	157	0	0	52	0
8	M	822	0	0	266	0
8	N	983	0	0	291	0
8	O	114	0	0	30	0
8	P	325	0	0	75	0
All	All	59529	0	54319	7072	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 65.

The worst 5 of 7072 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)
5:F:419:ARG:CG	5:F:419:ARG:CB	1.76	1.60
5:P:401:GLU:CB	5:P:401:GLU:CG	1.76	1.56
5:F:401:GLU:CB	5:F:401:GLU:CG	1.77	1.55
3:N:218:LYS:CB	8:N:9902:HOH:O	1.85	1.18
1:A:94:LEU:HD21	1:A:119:ASP:HB2	1.26	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	201 (88%)	21 (9%)	5 (2%)	8	15
1	B	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	15	30
1	K	227/315 (72%)	199 (88%)	24 (11%)	4 (2%)	11	21
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	15	30
2	C	1117/1119 (100%)	923 (83%)	139 (12%)	55 (5%)	3	3
2	M	1117/1119 (100%)	928 (83%)	135 (12%)	54 (5%)	3	3
3	D	1388/1524 (91%)	1119 (81%)	196 (14%)	73 (5%)	2	2
3	N	1388/1524 (91%)	1113 (80%)	200 (14%)	75 (5%)	2	2
4	E	93/99 (94%)	72 (77%)	13 (14%)	8 (9%)	1	1
4	O	93/99 (94%)	71 (76%)	15 (16%)	7 (8%)	1	1
5	F	341/423 (81%)	295 (86%)	31 (9%)	15 (4%)	3	4
5	P	341/423 (81%)	288 (84%)	34 (10%)	19 (6%)	2	2
All	All	6786/7590 (89%)	5608 (83%)	857 (13%)	321 (5%)	3	3

5 of 321 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLY
2	C	111	ASP
2	C	152	PRO
2	C	231	PRO
2	C	244	PRO

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%)	165 (82%)	37 (18%)	2	3
1	B	202/273 (74%)	164 (81%)	38 (19%)	2	3
1	K	202/273 (74%)	160 (79%)	42 (21%)	1	2
1	L	202/273 (74%)	161 (80%)	41 (20%)	1	2
2	C	941/941 (100%)	730 (78%)	211 (22%)	1	2
2	M	941/941 (100%)	718 (76%)	223 (24%)	1	1
3	D	1123/1279 (88%)	865 (77%)	258 (23%)	1	2
3	N	1123/1279 (88%)	841 (75%)	282 (25%)	1	1
4	E	83/87 (95%)	68 (82%)	15 (18%)	2	3
4	O	83/87 (95%)	68 (82%)	15 (18%)	2	3
5	F	295/370 (80%)	232 (79%)	63 (21%)	1	2
5	P	295/370 (80%)	239 (81%)	56 (19%)	2	3
All	All	5692/6446 (88%)	4411 (78%)	1281 (22%)	1	2

5 of 1281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	234	LYS
2	M	57	GLU
3	N	1332	PRO
5	F	324	GLU
1	K	170	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1489	GLN
1	L	95	GLN
3	N	1374	GLN
4	E	33	HIS

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Mol	Chain	Res	Type
1	K	38	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 489 ligands modelled in this entry, 489 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.