



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:26 am GMT

PDB ID : 1ZYR
Title : Structure of Thermus thermophilus RNA polymerase holoenzyme in complex with the antibiotic streptolydigin
Authors : Tuske, S.; Sarafianos, S.G.; Wang, X.; Hudson, B.; Sineva, E.; Mukhopadhyay, J.; Birktoft, J.J.; Leroy, O.; Ismail, S.; Clark, A.D.; Dharia, C.; Napoli, A.; Laptenko, O.; Lee, J.; Borukhov, S.; Ebright, R.H.; Arnold, E.
Deposited on : 2005-06-10
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

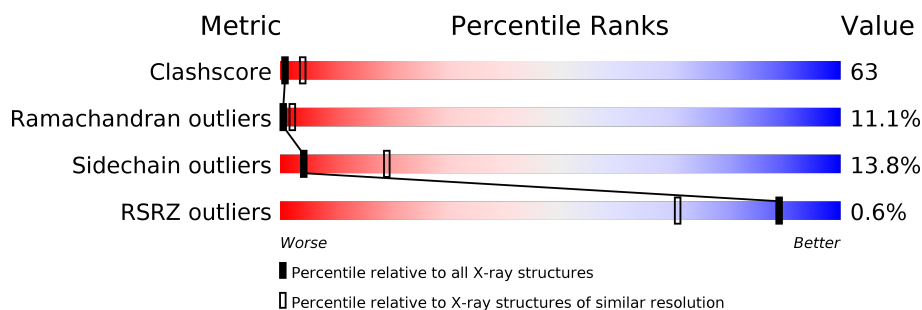
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	
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	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ZN	N	9003	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54048 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 subunit 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			

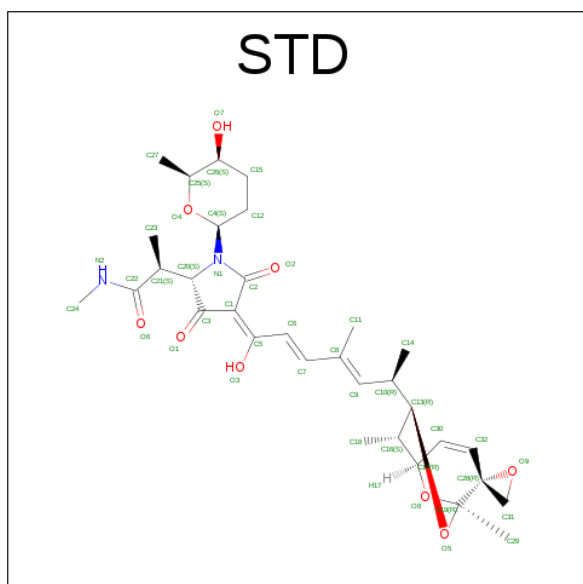
- Molecule 4 is a protein called DNA-directed RNA polymerase omega chain.

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 DNA-directed RNA polymerase sigma chain.

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 STREPTOLYDIGIN (three-letter code: STD) (formula: $C_{32}H_{44}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			43	32	2	9		
6	M	1	Total	C	N	O	0	0
			43	32	2	9		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

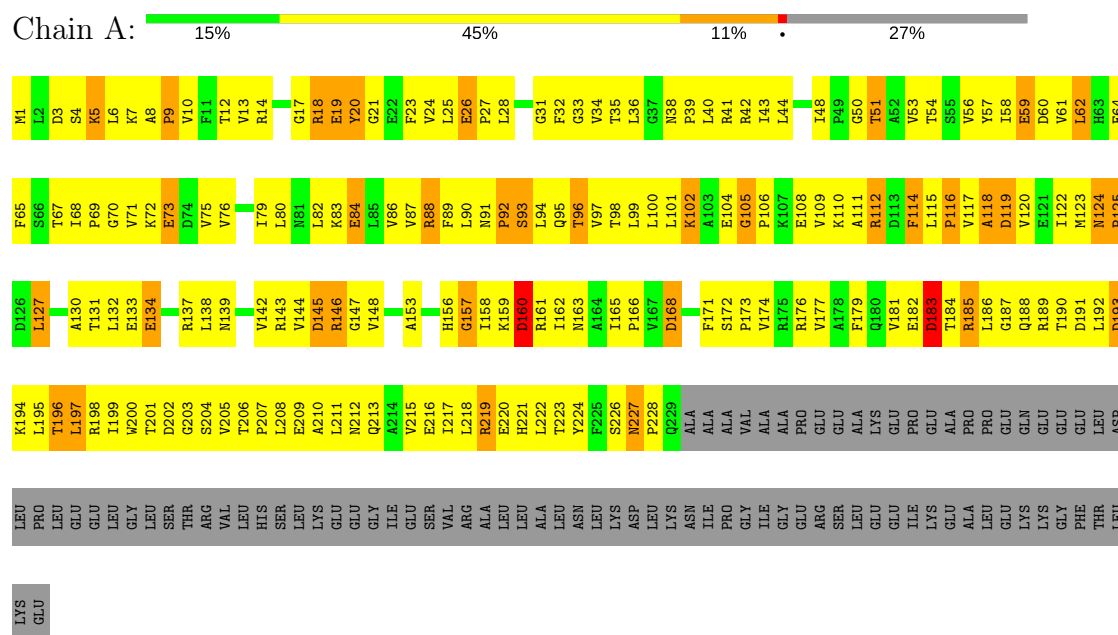
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

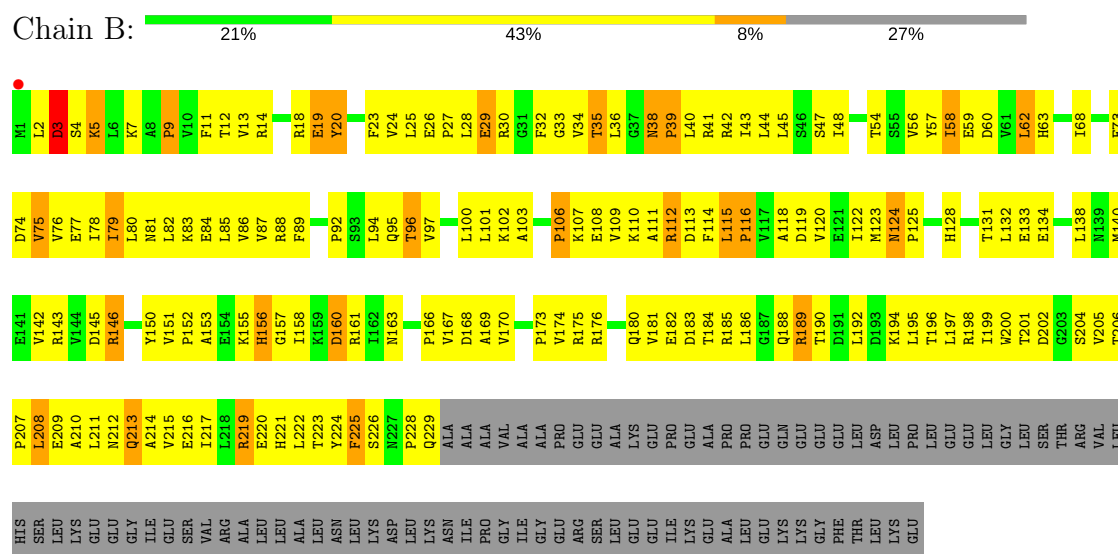
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA-directed RNA polymerase alpha chain



• Molecule 1: DNA-directed RNA polymerase alpha chain



[illegible]

Chain L: 21% 41% 11% 27%

Category	Percentage	Count
Red	21%	21
Orange	41%	41
Yellow	11%	11
Grey	27%	27

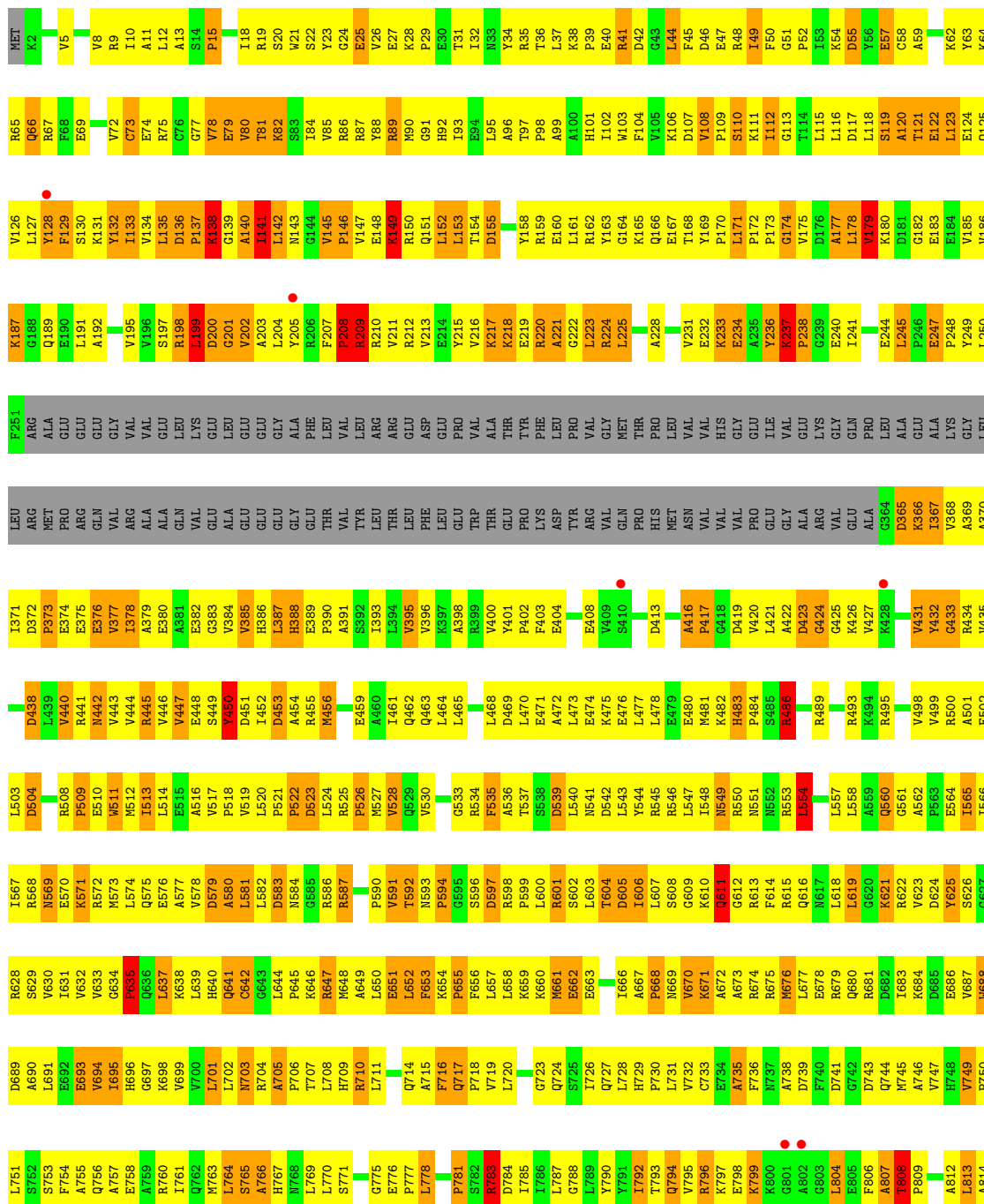
Chain C:

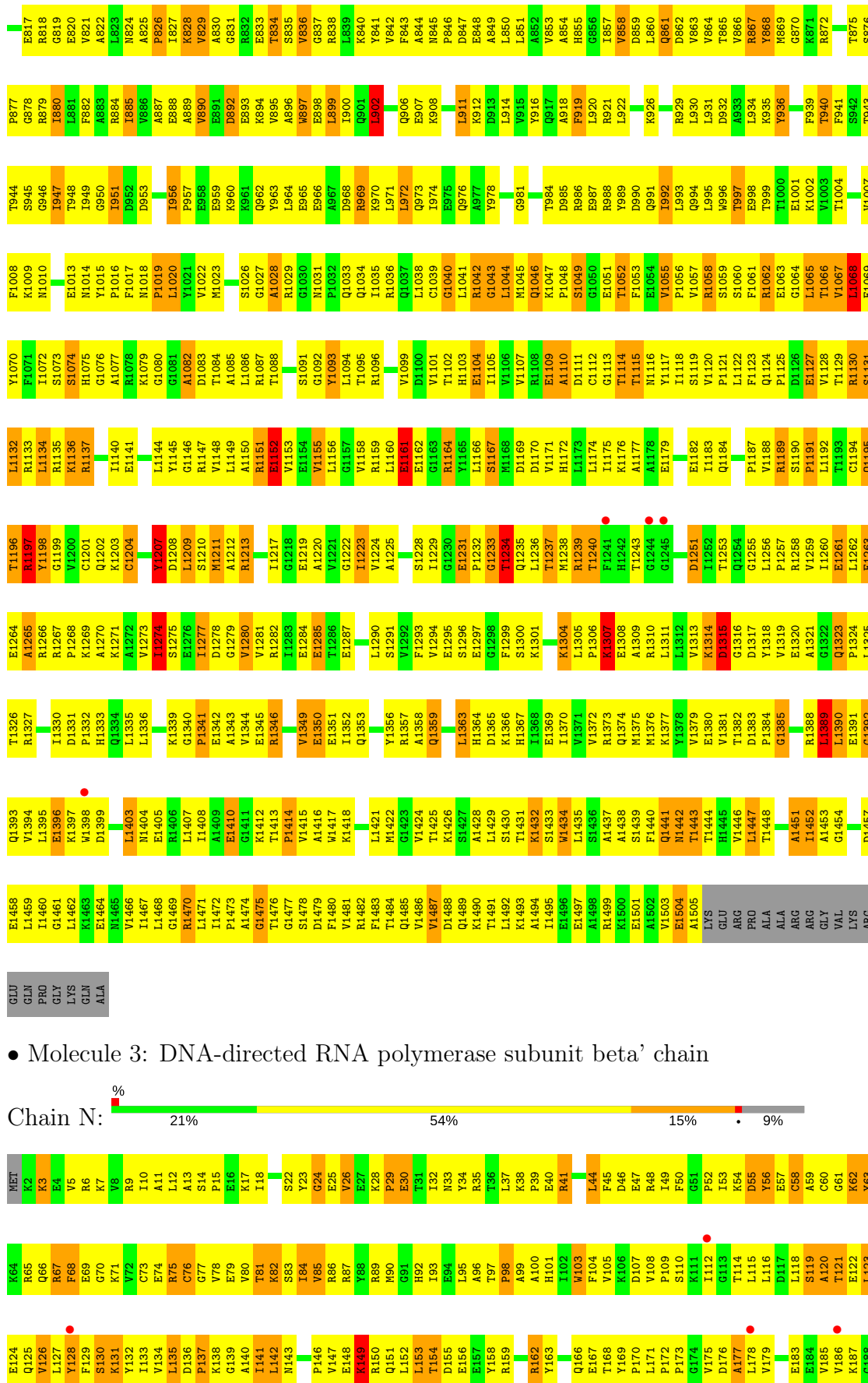
Node Label	Category
E1	Green
E2	Green
E3	Green
R4	Green
R5	Green
R6	Green
G7	Green
H8	Green
T9	Green
R10	Green
E11	Green
V12	Green
H13	Green
P14	Green
L15	Green
P16	Green
P17	Green
L18	Green
T19	Green
E20	Green
E21	Green
Q22	Green
Q23	Green
E24	Green
S25	Green
V26	Green
R27	Green
R28	Green
A29	Green
L30	Green
Q31	Green
V34	Green
P35	Green
P36	Green
E37	Green
K38	Green
R39	Green
E40	Green
V41	Green
V42	Green
Q43	Green
L44	Green
Q45	Green
F46	Green
R49	Green
E50	Green
T51	Green
F52	Green
P53	Green
I54	Green
E57	Green
L64	Green
V65	Green
L66	Green
P67	Green
F69	Green
E70	Green
T71	Green
R72	Green
L73	Green
G74	Green
E75	Green
T76	Green
P77	Green
F78	Green
P79	Green
Q80	Green
D81	Green
E82	Green
C83	Green
L88	Green
T89	Green
Q90	Green
Q91	Green
A92	Green
P93	Green
L94	Green
Y95	Green
A96	Green
R97	Green
L100	Green
I101	Green
H102	Green
H103	Green
D104	Green
T105	Green
G106	Green
L107	Green
T108	Green
K109	Green
E110	Green
D111	Green
E112	Green
V113	Green
F114	Green
L115	Green
G116	Green
H117	Green
I118	Green
M121	Green
T122	Green
E123	Green
D124	Green
F127	Green
I128	Green
I129	Green
M130	Green
G131	Green
A132	Green
D133	Green
F134	Green
E13	Yellow
E14	Yellow
E15	Yellow
R16	Yellow
R17	Yellow
R18	Yellow
G19	Yellow
H20	Yellow
T21	Yellow
R22	Yellow
E23	Yellow
E24	Yellow
S25	Yellow
V26	Yellow
R27	Yellow
R28	Yellow
A29	Yellow
L30	Yellow
Q31	Yellow
V34	Yellow
P35	Yellow
P36	Yellow
E37	Yellow
K38	Yellow
R39	Yellow
E40	Yellow
V41	Yellow
V42	Yellow
Q43	Yellow
L44	Yellow
Q45	Yellow
F46	Yellow
R49	Yellow
E50	Yellow
T51	Yellow
F52	Yellow
P53	Yellow
I54	Yellow
E57	Yellow
L64	Yellow
V65	Yellow
L66	Yellow
P67	Yellow
F69	Yellow
E70	Yellow
T71	Yellow
R72	Yellow
L73	Yellow
G74	Yellow
E75	Yellow
T76	Yellow
P77	Yellow
F78	Yellow
P79	Yellow
Q80	Yellow
D81	Yellow
E82	Yellow
C83	Yellow
L88	Yellow
T89	Yellow
Q90	Yellow
Q91	Yellow
A92	Yellow
P93	Yellow
L94	Yellow
Y95	Yellow
A96	Yellow
R97	Yellow
L100	Yellow
I101	Yellow
H102	Yellow
H103	Yellow
D104	Yellow
T105	Yellow
G106	Yellow
L107	Yellow
T108	Yellow
K109	Yellow
E110	Yellow
D111	Yellow
E112	Yellow
V113	Yellow
F114	Yellow
L115	Yellow
G116	Yellow
H117	Yellow
I118	Yellow

V1109	H1047	G980	L1917	V855	T788	E720	G658	L595	V529	D462	T398	V330	D263	L196	V135
D1110	T1048	E981	L918	E856	S789	R721	P659	Y596	E530	E463	T398	R331	P264	L197	I136
I1111	L1049	P982	A919	M857	L790	I722	A660	A597	F531	L460	S403	R332	R265	R198	S138
F1112	Q1050	R983	Q920	M858	R791	T723	S661	E598		G465	L404	I333	R266	V199	I137
E1113	E1051	E984	E1051	E859	F792	R724	M663	E599	V534	F466	R334	R335	R267	L200	Q139
G1114	M1052	G985	F922	H860	F793	R725	N662	D600	S535	I467	H406	T335	G201	G201	I140
L1115	L1053	P986	E923	L861	F794	I726	G664	G601	P536	R468	K407	V336	D268	Y202	H141
K1118	T1054	L987	F924	P862	G795	F727	F665	E602	K537	T469	R408	G337	E271	D203	R142
R1119	L1055	V988	F925	D863	E796	H728	L666	V603	Q538	R472	A409	E338	A272	Q204	S143
	K1056	V989	F926	G864	E797	I729	A667	A604	V539	Y471			G273	E205	P144
	S1057	G990	G927	T865	I799	S730	L668	K605	F540	R472				T206	G145
	D1058			P866	V800	L734	G669	V606	S541	R473	A412	T341	K276	L207	V146
	D1059	F993	K929	V867	V801	R735	M671	D607	V542	V474	G414	D342	A277	X208	I147
			K930	D868	R802	R736	M672	G808	N543	V475	P415	Q343	E278	R209	F148
		R996	G931	V969	R805	D737	L673	N609	T544		G416		E279	E210	T149
		L997		I870	R806	D738	A675	I611	N545	V478			K280	E211	P150
				L871	R807	G741	M676	V613					D151	G220	D151
		M1000	G935	N872	D810	V742	A677	V612	L547	T480	L418	L348	G282	G220	P152
		Y1001	V936	P873	P811	V743	M677	V613	P548	D481	R420	R350	I283	L221	A153
		E1002	K938	L874	P812	R744	M678	Y615	F549	E482	E421	L351	R284	K222	R154
		D1003	R939	G875	G812		F679	E616	L560	V483	R422	R352	L285	D223	P155
		K1004	E940	P876	V813		D680	E617	S551	V484	A423	R353	G224	E224	G156
		M1005	V941	S877	V814		G681	G618	D553	M486	F425	V355	R288	G225	R157
		H1006	E942	S878	L815	A747	G682	R619	D554	T487	D426	R356	T269	V226	Y158
		A1007	V943	M880	K816	E748	N683	L620	A555	A488	V427	E357	L260	F227	I159
		R1008	L944	N881		V749	P684	V621	N556	T489			A291	A228	A160
		S1009		L882	V819	R750	E685	E622		E490			R292	R229	
		V1010	R945	G883	D823	I754	D686	L625	L559	E491	V430	S363	G296	R230	I163
		G1011	A947	K884	R824	L755	P688	G626	M560	D492	H431	E364	E297	P231	P164
		P1012	E948	I885	V825	R756	V689	R627	S562	Y494	R432		F298	E232	L165
		Y1013	K949	L886	R826	G757	L690	F628	N563	L496	P433		K299	R237	P170
		S1014	L960	E987	A827		S691	G629	M564	A497	G436		D300	L238	W171
		L1015	G951	T888	Q829	T759	E692	S631		Q498	R437		V302	F239	I172
		T1017	L953	L890	K830	F761	L694	N632	Q567		I438	L372	F363	T240	D173
		F1085	G891	L892	R831	K762	L695	Q633	A568	T501	C439	V373	L304	L241	L174
		L1021	L892	A893	R832	E766	K696	A636	P570	P502	P440	N374	P305	L242	E175
		K1024	G894	G994	L833	T767	D698	D638	L571	L503	V441	S375		R243	V176
		F1027	Y895	P896	V835	T768	P699	D639	I572		T443	P377	Y309	P244	E177
			L897		D836	F769	Y700	Q639	Q575	I508	P444	L378		G245	P178
		Q1030	L963	L897	D837	E770	T701	R640	A576		E445	E379	A312	D246	N179
		A1031	K964	R900	R838	E771		P641	P577	V513	G446	A381	L313	P247	G180
		F1032	E965	Y901	L839	R772	H704	R642	V578	V514	N448	A382	T314	P248	V181
		G1033	L966	I902	A840	L773	T705	V643	V579	A515	N447	I382	A315	R249	V182
		A1034	F967	S903	N841	L774	E706	V644	M580	R516	I449	R383	G316	R250	S183
		L1035	L968	P904	R842	R775	R707	V645		R517	G450	E384	V317	D251	M184
		D1036	Q969	I905	H843	S776	Y708	G646	L583	K518	L451	F385	P318	K252	K185
		V1037	G970	F906	S844	I777	E709	Q647	E584	G519	I452	F386	G319	A253	V186
		Q1038	K971	D907	R845		I710		E585	E520	T453		H320	V254	N187
		A1039	V972	K910	R846	E780	R713	R650	R586	P521	S454		G321	A255	K188
		L1040	V973	E911	V849	K781	T714	K651	V587	V522	L455	Q390	V322	Y256	R189
		E1041	L974	E912	T715	A783	T715	D652	R589	I523	A456	L391		V257	K190
		F1104	K975	P912	K851	D784	K716	L854	D590	V524	A457	S392	I325	Y258	F191
		K1105	D976	E913	R851	D784	K716	L854	S891	S825	Y458		D326	G259	P192
		D1106	G977	I914	L852	K786	L717	L655	A459	P526	A459	K396	H327	L260	L193
		N1107	K978	L853	P854	K786	L717	A656	L592	E527			L328	T261	V194
		P1108	T979	E916		F719		D657		E528	V461		G329	A262	L195

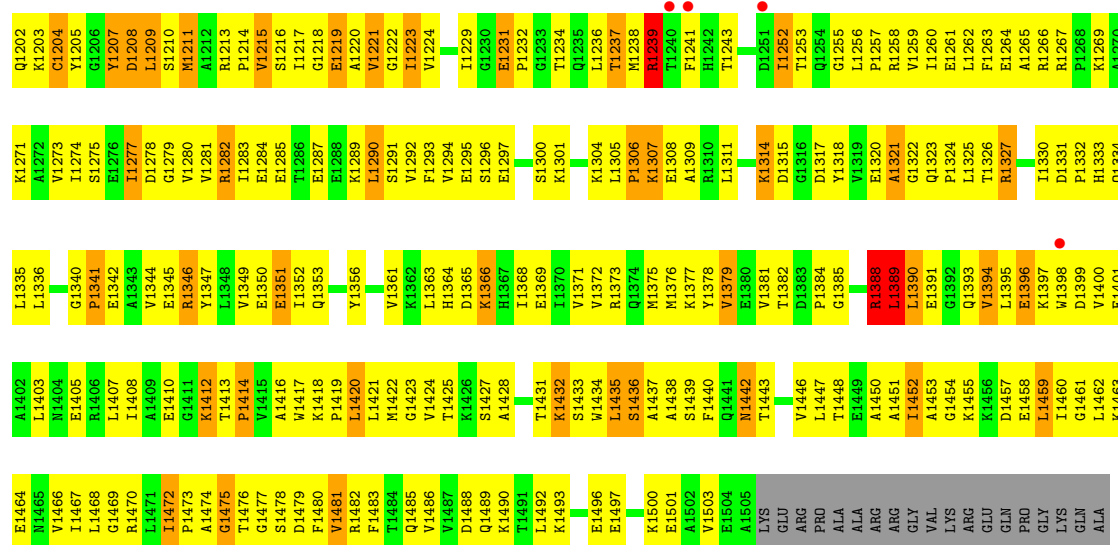
• Molecule 2: DNA-directed RNA polymerase beta chain





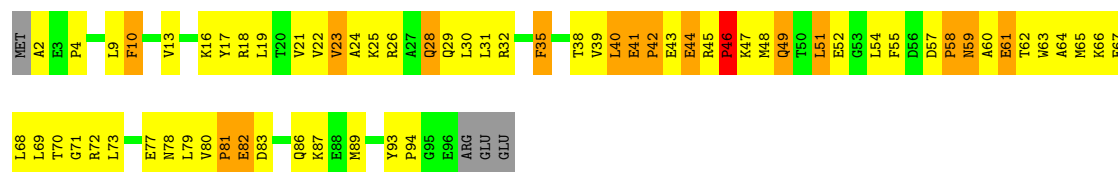


R1135	E1069	L1144	E1007	L873	A812	P750	D885	Y625	A559	L496	E436	D372	Q189
K1136	Y1070	T1145	V1007	E874	L813	L751	E886	S626	Q560	E497	V437	P373	E190
R1137	F1071	G1146	F1008	S875	A814	S752	W688	G627	G561	V498	D438	E374	L191
A1138	L1072	R1147	K1009	S876	A815	S753	W689	R628	A562	V499	L439	E375	A192
R1139	S1073	R1148	P1010	P877	H816	F754	D889	S629	S663	R500	V440	E376	P193
S1074	S1074	L1149	F1011	G878	E817	A755	A690	V630	E564	A501	R441	V377	G194
H1075	H1075	T1150	E1012	R879	R818	Q756	L691	I631	I565	F502	M442	I378	V195
		R1078	Y1015	I880	G819	A757	E692	V632	I566	L503	V443	A381	V196
		K1079	F1016	L881	E820	E758	E693	V633	I567	D504	V444	E382	S197
		R1147	F1017	A882	V821	A759	R658	G634	S505	G506	V445	G383	L198
		T1084	N1018	A883	A822	R760	I695	P635	N669	G506	V446	G383	L199
		A1085	S945	R884	L823	I761	V699	V636	E570	N507	V447	V384	
		L1086	E946	T885	N824	Q762	V699	L637	K571	E448	V448	V385	V202
		R1087	I947	V886	A825	H763	V700	K638	R572	S449	V449	H386	A203
			Y1021	A887	P826	L764	L701	L639	M573	E510	V450	L387	L204
			M1023	E888	I827	S765	L702	H640	L574	M511	D451	L387	L205
				A889	K828	A766	N703	Q641	Q675	L513	D452	E389	Y206
				V890	V829	H767	R704	G642	E576	L514	D453	P390	F207
				E891	A830	W768	A705	G643	A577	E515	D454	A391	P208
				D892	G831	L769	P706	L644	V578	A516	R455	S392	R209
				E893	R832	L770	L770	P645	D579	V517	M456	I393	R210
				K894	E833	S771	L708	R647	L582	P518	G457	L394	V211
				V895	T834	F772	H709	K647	A458	V519	A458	V395	ARG
				A896	S835	A773	R710	M648	D583	L520	V459	V396	R212
				W897	V836	S774	L711	M649	N584	P521	A460	K397	V213
				E898	G837	G775	G712	L650	G585	P522	I461	A398	ASP
				L899	R838	E776	I713	E561	R587	D523	Q462	R399	GLU
				I900	L839	P777	L714	L652	L524	R526	Q463	V400	V216
				Q901	K840	L778	A715	F653	R587	P526	L464	Y401	K218
				E965	Y941	A779	F716	G654	P590	R527	L465	P402	E219
				E966	R942	K780	Q717	P655	V591	M527	K466	F403	R220
				A967	V943	S781	P718	P656	T592	V528	E467	E404	ASP
				D968	F905	S782	V719	P657	N593	Q529	L468	D405	G222
				R969	N845	R783	L720	L658	P594	V530	D469	D406	G221
				L971	P846	F784	V721	K659	S596	G533	L470	V409	R224
				K908	D847	I786	E722	K660	D597	R534	E471	S410	L225
					E848	L786	G723	M661	R598	F535	L473	T411	P226
				L911	A849	L787	Q724	E562	P599	A536	E474	G412	L227
				K912	L850	G788		E563	L600	T537	K475	D413	W230
				D913	L851	L789	Q727	K664	R601	S538	R414	R415	V231
				L914	A852	Y790	L728	G665	S602	D539	L477	V415	E232
				V915	V853	Y791	H729	I666	L603	L540	L478	A416	K233
				Y916	A854	L792	P730	A667	L604		E479	P417	E234
				Y917	H855	T793	L731	P668	T604		E480		
				Q917	G856	Q794	V732	M669	D605	L543	E481	L421	K237
				A918	I857	Y795		V670	L606	Y544	K482	A422	P238
				F919	V858	R796	F736	K671	L607	R545	K483	D423	GLU
				L920	D859	K797	N737	A672	S608	R546	H483	G424	GLY
				R921	L860	E798	A738	A673	G609	I548	S485	G425	E240
				L922	Q861	K799	D739	R674		N549	R486	K426	I241
				G923	D862	K800	F740	R675	R613	R550	A487	V427	L242
				M924	V863		D741	M676	N617	N551	K488	K428	PRO
				E925	V864		Q742	L677	G742	N552	R489	S429	A243
				K926	E805		D743	E678	L618	R554	K366	D430	L244
				T927	F806		Q744	R679	L619	R553	A490	V431	P246
				A928	A807		M745	Q680	G620	L554	K491	Y432	E247
				R929	Y868		A746	R681	K621	K555	A492	G433	P248
				L930	M869		P809	D682	R622	A566	R493	G434	GLY
				L931	K871		H748	I683	G623	R494	A370	R434	LEU
				D932	K871		H748	I683	G623	R494	A370	R434	F251
				A933	R872		V749	K684	D624	L558	R495	V435	
L1155	D1090	L1156	S1091	L1157	G1092	L1158	Y1093	G1027	Y955	S1026	G1027		
L1156	S1091	L1157	G1092	L1158	Y1093	G1027	Y955	S1026	G1027	Y955	S1026		
L1157	G1092	L1158	Y1093	G1027	Y955	S1026	G1027	Y955	S1026	G1027	Y955		
L1158	Y1093	G1027	Y955	S1026	G1027	Y955	S1026	G1027	Y955	S1026	G1027		
L1159	G1027	Y955	S1026	G1027	Y955	S1026	G1027	Y955	S1026	G1027	Y955		
L1160	Y1094	L1161	T1095	R1029	G1030	G1030	G1030	G1030	G1030	G1030	G1030		
L1161	T1095	R1029	G1030	G1030	G1030	G1030	G1030	G1030	G1030	G1030	G1030		
L1162	R1096	E1161	K1097	P1032	L1098	E1162	K1097	P1032	L1098	E1162	K1097		
L1163	K1097	P1032	L1098	E1162	K1097	P1032	L1098	E1162	K1097	P1032	L1098		
L1164	P1032	L1098	E1162	K1097	P1032	L1098	E1162	K1097	P1032	L1098	E1162		
L1165	L1099	G1033	Q1033	Q1033	Q1033	Q1033	Q1033	Q1033	Q1033	Q1033	Q1033		
L1166	D1100	L1167	T1101	L1168	H1102	S1167	T1102	L1169	E1104	L1170	V1106		
L1167	T1101	L1168	H1102	S1167	T1102	L1169	E1104	L1170	V1106	L1171	H1107		
L1168	H1102	S1167	T1102	L1169	E1104	L1170	V1106	L1171	H1107	L1172	R1108		
L1169	E1104	L1170	V1106	L1171	H1107	L1172	R1108	E1109	G1043	L1044	L1044		
L1170	V1106	L1171	H1107	L1172	R1108	E1109	G1043	L1044	L1044	L1044	L1044		
L1171	H1107	L1172	R1108	E1109	G1043	L1044	L1044	L1044	L1044	L1044	L1044		
L1172	R1108	E1109	G1043	L1044	L1044	L1044	L1044	L1044	L1044	L1044	L1044		
L1173	E1109	G1043	L1044	L1044	L1044	L1044	L1044	L1044	L1044	L1044	L1044		
L1174	L1044	L1044	L1044	L1044	L1044	L1044	L1044	L1044	L1044	L1044	L1044		
L1175	A1110	L1176	K1176	A1177	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1176	K1176	A1177	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1177	A1177	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1178	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1179	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1180	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1181	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1182	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1183	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1184	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1185	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1186	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1187	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1188	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1189	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1190	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1191	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1192	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1193	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1194	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1195	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1196	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1197	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1198	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1199	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		
L1200	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112	G1112		



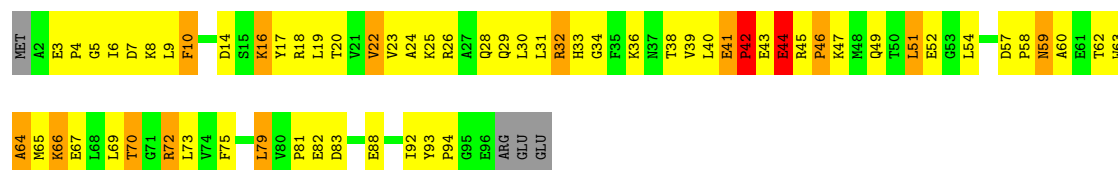
• Molecule 4: DNA-directed RNA polymerase omega chain

Chain E: 29% 51% 15%



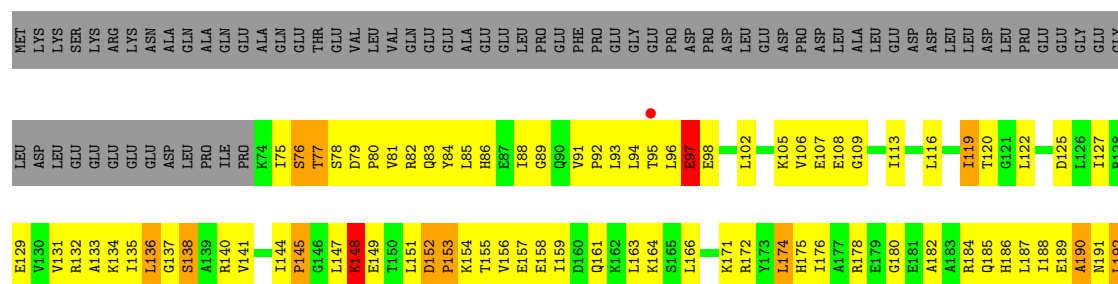
• Molecule 4: DNA-directed RNA polymerase omega chain

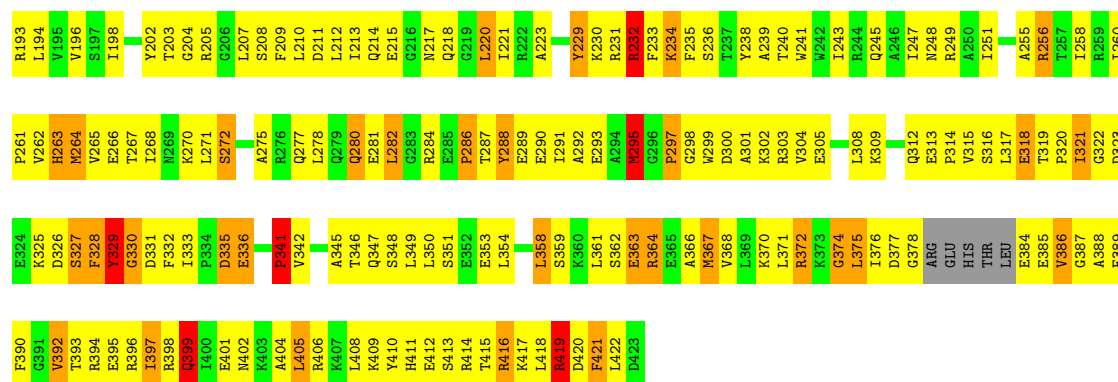
Chain O: 31% 49% 13%



• Molecule 5: DNA-directed RNA polymerase sigma chain

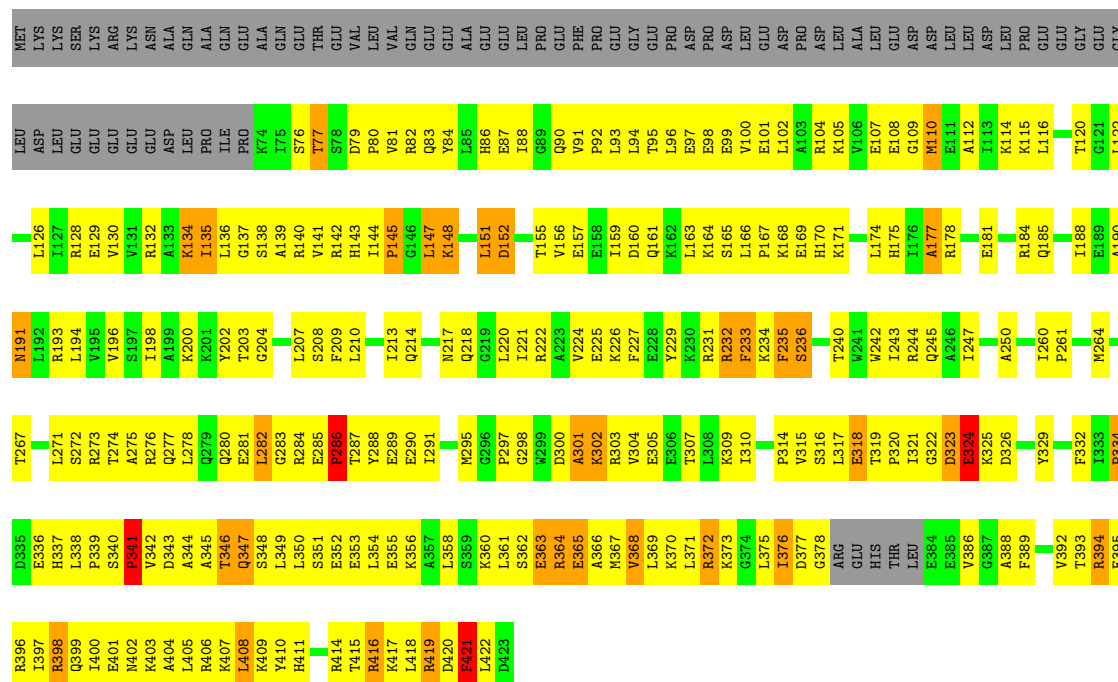
Chain F: 23% 47% 10% 18%





• Molecule 5: DNA-directed RNA polymerase sigma chain

Chain P: 24% 48% 8% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	237.00Å 237.00Å 250.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.89 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.9 (30.00-3.00) 42.8 (29.89-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.261 , 0.281 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , -24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	54048	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STD, 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	0.43	0/1838	0.76	0/2498
1	B	0.38	0/1838	0.64	0/2498
1	K	0.46	0/1838	0.75	0/2498
1	L	0.39	0/1838	0.66	0/2498
2	C	0.45	0/8997	0.76	5/12164 (0.0%)
2	M	0.44	0/8997	0.76	5/12164 (0.0%)
3	D	0.46	0/11165	0.78	13/15088 (0.1%)
3	N	0.45	0/11165	0.78	14/15088 (0.1%)
4	E	0.40	0/783	0.77	2/1054 (0.2%)
4	O	0.44	0/783	0.82	1/1054 (0.1%)
5	F	0.41	0/2836	0.70	1/3812 (0.0%)
5	P	0.41	0/2836	0.69	0/3812
All	All	0.44	0/54914	0.76	41/74228 (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
2	C	0	1
3	D	0	1
3	N	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	81	THR	N-CA-C	-7.96	89.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	728	HIS	N-CA-C	7.59	131.49	111.00
4	O	49	GLN	N-CA-C	7.23	130.53	111.00
3	N	1209	LEU	N-CA-C	-7.22	91.50	111.00
3	D	1209	LEU	N-CA-C	-7.04	92.00	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	258	TYR	Sidechain
3	D	132	TYR	Sidechain
3	N	625	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	279	0
1	B	1806	0	1861	211	0
1	K	1806	0	1861	232	0
1	L	1806	0	1861	210	0
2	C	8829	0	8933	1148	0
2	M	8829	0	8933	1178	0
3	D	10975	0	11213	1653	0
3	N	10975	0	11212	1616	0
4	E	769	0	775	99	0
4	O	769	0	775	87	0
5	F	2793	0	2873	320	0
5	P	2793	0	2873	362	0
6	D	43	0	44	10	0
6	M	43	0	44	8	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
All	All	54048	0	55119	6892	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 6892 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)
2:C:673:LEU:HD23	2:C:867:VAL:HA	1.22	1.20
3:N:172:PRO:HB3	3:N:178:LEU:HD22	1.22	1.16
3:D:141:ILE:H	3:D:141:ILE:HD12	1.11	1.16
2:C:857:ASP:HB2	2:C:978:ARG:HG2	1.29	1.15
3:D:1304:LYS:H	3:D:1304:LYS:HD3	1.03	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%)	163 (72%)	48 (21%)	16 (7%)	1	7
1	B	227/315 (72%)	167 (74%)	46 (20%)	14 (6%)	2	10
1	K	227/315 (72%)	154 (68%)	45 (20%)	28 (12%)	0	1
1	L	227/315 (72%)	169 (74%)	41 (18%)	17 (8%)	1	6
2	C	1117/1119 (100%)	768 (69%)	229 (20%)	120 (11%)	0	2
2	M	1117/1119 (100%)	758 (68%)	222 (20%)	137 (12%)	0	1
3	D	1388/1524 (91%)	940 (68%)	286 (21%)	162 (12%)	0	2
3	N	1388/1524 (91%)	916 (66%)	317 (23%)	155 (11%)	0	2
4	E	93/99 (94%)	66 (71%)	17 (18%)	10 (11%)	0	2
4	O	93/99 (94%)	56 (60%)	25 (27%)	12 (13%)	0	1
5	F	341/423 (81%)	239 (70%)	57 (17%)	45 (13%)	0	1
5	P	341/423 (81%)	250 (73%)	54 (16%)	37 (11%)	0	2
All	All	6786/7590 (89%)	4646 (68%)	1387 (20%)	753 (11%)	0	2

5 of 753 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	160	ASP
1	A	188	GLN
1	B	3	ASP
1	B	96	THR

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%)	171 (85%)	31 (15%)	3	15
1	B	202/273 (74%)	178 (88%)	24 (12%)	6	25
1	K	202/273 (74%)	172 (85%)	30 (15%)	3	16
1	L	202/273 (74%)	175 (87%)	27 (13%)	4	20
2	C	941/941 (100%)	829 (88%)	112 (12%)	6	25
2	M	941/941 (100%)	816 (87%)	125 (13%)	4	20
3	D	1170/1279 (92%)	972 (83%)	198 (17%)	2	12
3	N	1170/1279 (92%)	1000 (86%)	170 (14%)	4	17
4	E	83/87 (95%)	71 (86%)	12 (14%)	4	17
4	O	83/87 (95%)	72 (87%)	11 (13%)	4	20
5	F	300/370 (81%)	261 (87%)	39 (13%)	5	21
5	P	300/370 (81%)	281 (94%)	19 (6%)	21	57
All	All	5796/6446 (90%)	4998 (86%)	798 (14%)	4	19

5 of 798 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1442	ASN
1	L	1	MET
3	N	1190	SER
4	E	46	PRO

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Mol	Chain	Res	Type
5	F	341	PRO

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	1489	GLN
1	L	212	ASN
3	N	1334	GLN
5	F	90	GLN
1	K	124	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	STD	D	1525	-	43,47,47	2.17	14 (32%)	46,73,73	1.86	8 (17%)
6	STD	M	1120	-	43,47,47	2.00	12 (27%)	46,73,73	2.31	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	STD	D	1525	-	-	0/31/101/101	0/2/5/5
6	STD	M	1120	-	-	0/31/101/101	0/2/5/5

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1120	STD	O9-C28	-4.55	1.37	1.43
6	M	1120	STD	C20-C3	-3.69	1.49	1.53
6	D	1525	STD	O9-C28	-3.52	1.38	1.43
6	D	1525	STD	C4-N1	-2.47	1.42	1.45
6	D	1525	STD	C28-C32	2.09	1.53	1.50

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1525	STD	C29-C19-C28	-5.48	108.73	113.34
6	M	1120	STD	C29-C19-C28	-5.03	109.10	113.34
6	M	1120	STD	O8-C17-C30	-2.63	109.04	111.66
6	D	1525	STD	C21-C22-N2	-2.56	112.40	116.52
6	M	1120	STD	C6-C7-C8	-2.35	122.68	126.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1525	STD	10	0
6	M	1120	STD	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.58	0 100 100	32, 58, 89, 110	0
1	B	229/315 (72%)	-0.52	1 (0%) 92 77	45, 96, 120, 124	0
1	K	229/315 (72%)	-0.56	0 100 100	24, 57, 82, 111	0
1	L	229/315 (72%)	-0.62	0 100 100	43, 78, 96, 117	0
2	C	1119/1119 (100%)	-0.55	5 (0%) 92 77	21, 67, 123, 137	0
2	M	1119/1119 (100%)	-0.54	3 (0%) 93 82	21, 69, 120, 130	0
3	D	1392/1524 (91%)	-0.53	10 (0%) 87 67	20, 64, 107, 125	0
3	N	1392/1524 (91%)	-0.48	19 (1%) 75 49	20, 64, 125, 140	0
4	E	95/99 (95%)	-0.56	0 100 100	52, 82, 99, 102	0
4	O	95/99 (95%)	-0.52	0 100 100	46, 86, 114, 119	0
5	F	345/423 (81%)	-0.57	1 (0%) 93 82	53, 77, 97, 104	0
5	P	345/423 (81%)	-0.57	0 100 100	47, 81, 97, 108	0
All	All	6818/7590 (89%)	-0.53	39 (0%) 89 71	20, 69, 118, 140	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	406	ASP	5.8
3	D	802	ALA	5.5
3	D	205	TYR	5.4
3	D	801	GLY	4.9
3	N	224	ARG	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	ZN	N	9003	1/1	0.99	0.24	4.31	55,55,55,55	0
7	ZN	N	9004	1/1	0.99	0.23	1.07	56,56,56,56	0
7	ZN	D	9001	1/1	0.99	0.20	0.52	56,56,56,56	0
7	ZN	D	9002	1/1	0.98	0.22	0.46	47,47,47,47	0
6	STD	M	1120	43/43	0.92	0.20	0.05	39,51,53,56	0
6	STD	D	1525	43/43	0.95	0.17	-0.32	39,59,62,63	0
8	MG	D	9901	1/1	0.97	0.13	-	20,20,20,20	0
8	MG	N	9902	1/1	0.96	0.22	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.