



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 09:39 pm GMT

PDB ID : 2A6H
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic sterptolydigin
Authors : Temiakov, D.; Zenkin, N.; Vassilyeva, M.N.; Perederina, A.; Tahirov, T.H.; Savkina, M.; Zorov, S.; Nikiforov, V.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Severinov, K.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

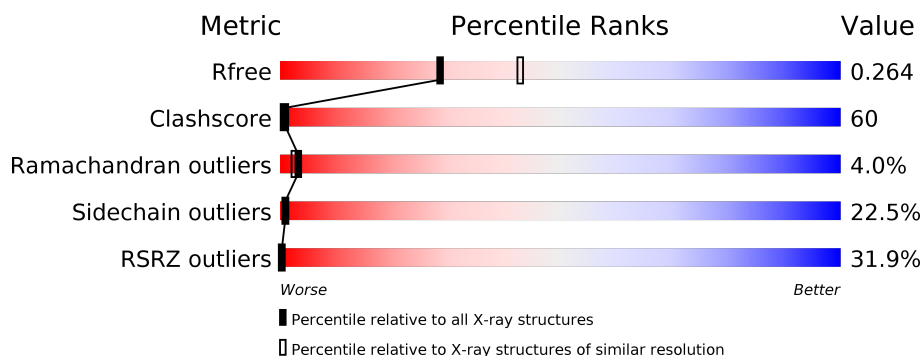
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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>21%</div> <div>16% 43% 13% 27%</div> </div>
1	B	315	<div> <div>23%</div> <div>16% 43% 13% 27%</div> </div>
1	K	315	<div> <div>19%</div> <div>23% 41% 8% 27%</div> </div>
1	L	315	<div> <div>26%</div> <div>20% 39% 12% 27%</div> </div>
2	C	1119	<div> <div>38%</div> <div>24% 57% 19%</div> </div>
2	M	1119	<div> <div>35%</div> <div>25% 55% 19%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div></div><div>23%</div><div>22%</div><div>52%</div><div>15%</div><div>•</div><div>9%</div></div>
3	N	1524	<div><div></div><div>24%</div><div>25%</div><div>49%</div><div>15%</div><div>•</div><div>9%</div></div>
4	E	99	<div><div></div><div>28%</div><div>27%</div><div>53%</div><div>15%</div><div>•</div><div>•</div></div>
4	O	99	<div><div></div><div>32%</div><div>24%</div><div>53%</div><div>18%</div><div>•</div><div>•</div></div>
5	F	423	<div><div></div><div>35%</div><div>20%</div><div>49%</div><div>11%</div><div>•</div><div>18%</div></div>
5	P	423	<div><div></div><div>30%</div><div>21%</div><div>49%</div><div>11%</div><div></div><div>18%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60908 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	1381	Total	C	N	O	S	0	0	0
			10728	6776	1912	2007	33			
3	N	1381	Total	C	N	O	S	0	0	0
			10728	6776	1912	2007	33			

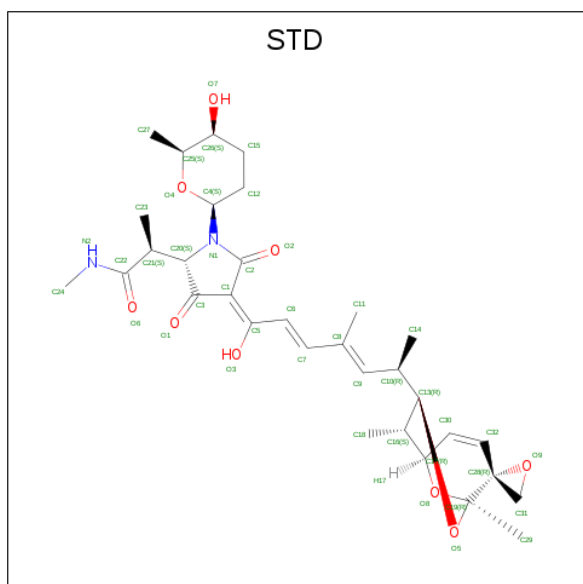
- Molecule 4 is a protein called RNA polymerase omega chain.

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
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	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	N	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 Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

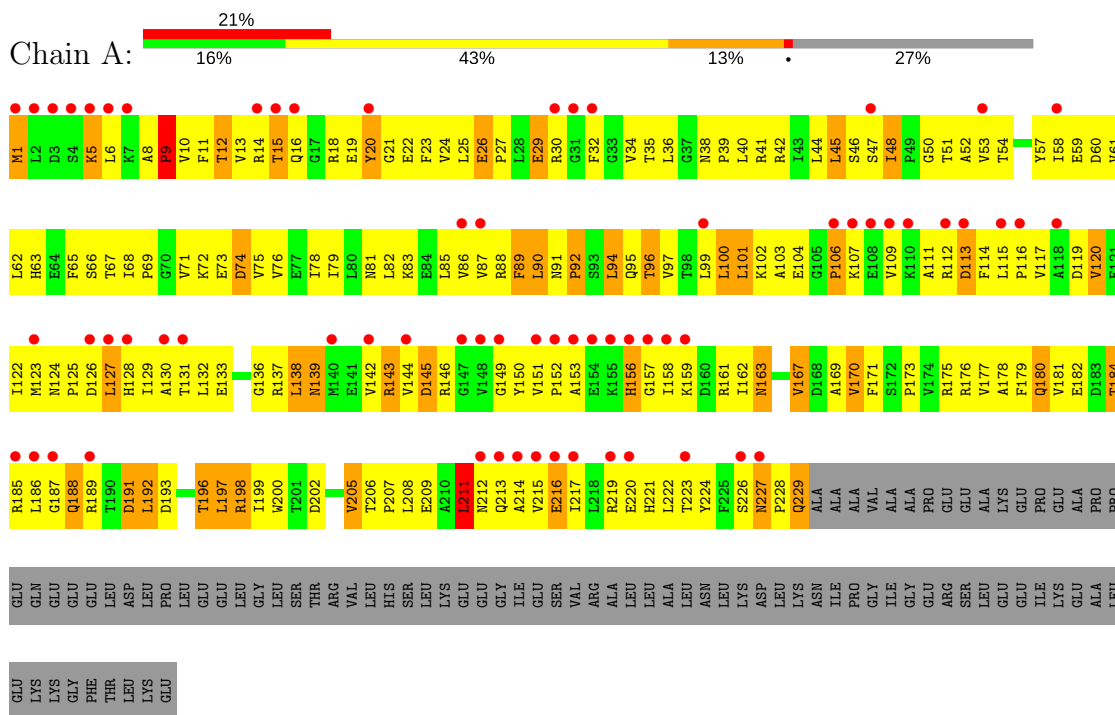
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	232	Total O 232 232	0	0
9	B	304	Total O 304 304	0	0
9	C	1144	Total O 1144 1144	0	0
9	D	1546	Total O 1546 1546	0	0
9	E	130	Total O 130 130	0	0
9	F	491	Total O 491 491	0	0
9	K	229	Total O 229 229	0	0
9	L	274	Total O 274 274	0	0
9	M	1072	Total O 1072 1072	0	0
9	N	1392	Total O 1392 1392	0	0
9	O	137	Total O 137 137	0	0
9	P	447	Total O 447 447	0	0

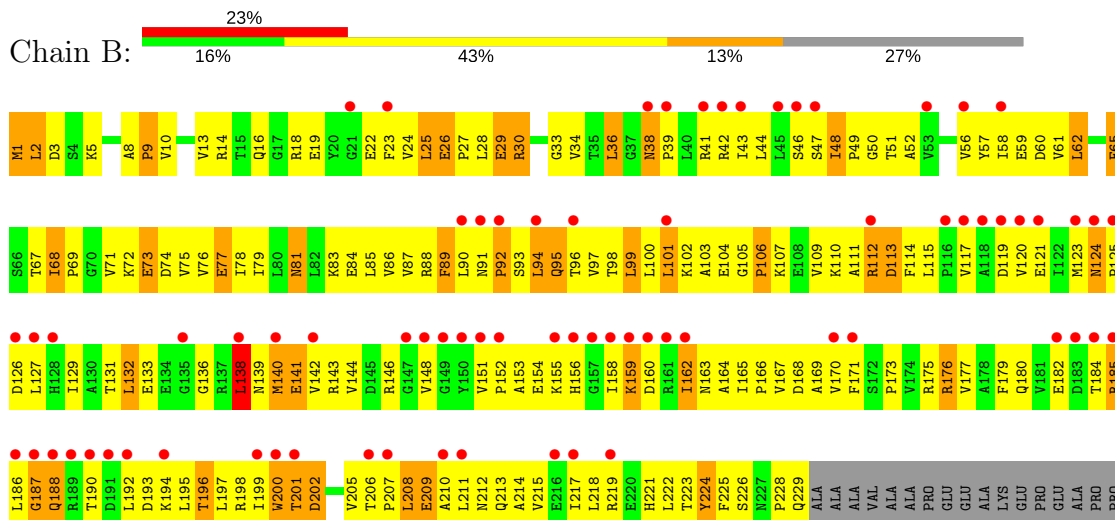
3 Residue-property plots

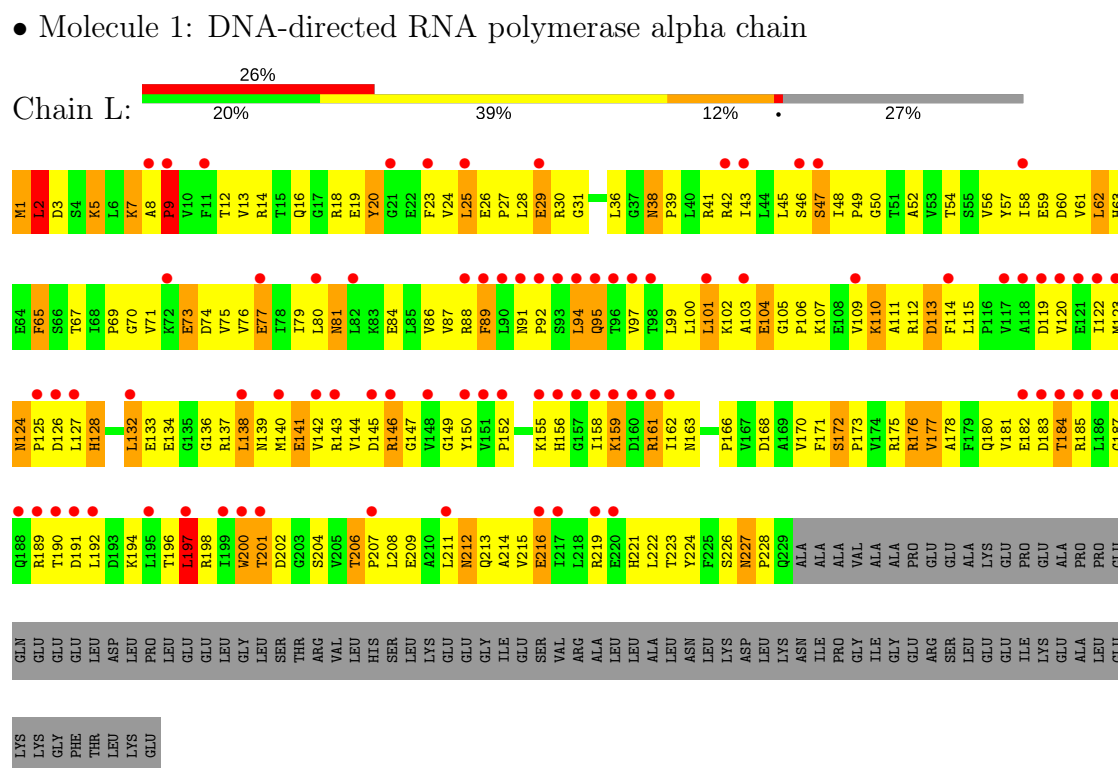
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

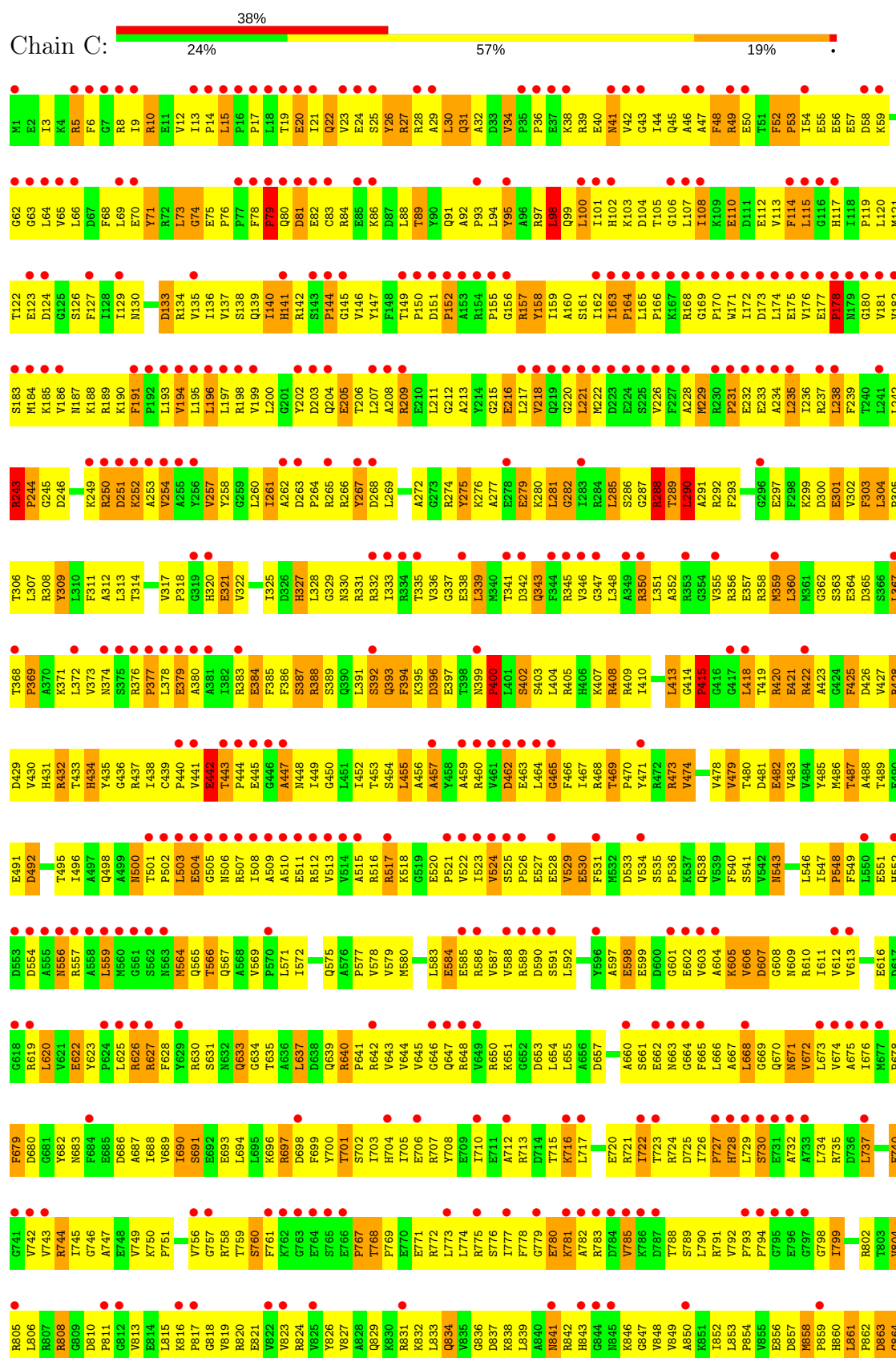


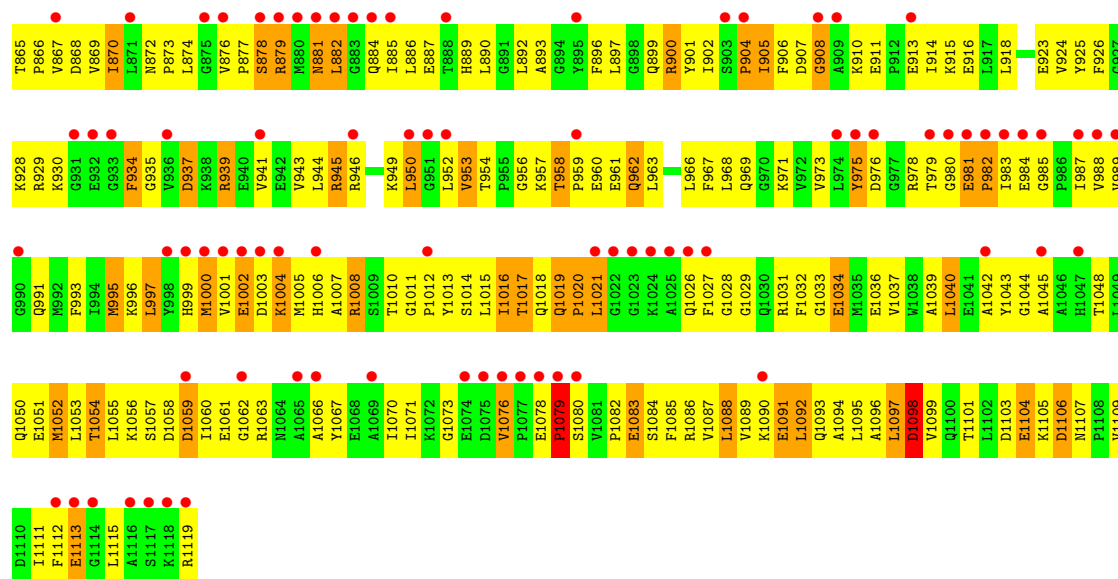
• Molecule 1: DNA-directed RNA polymerase alpha chain



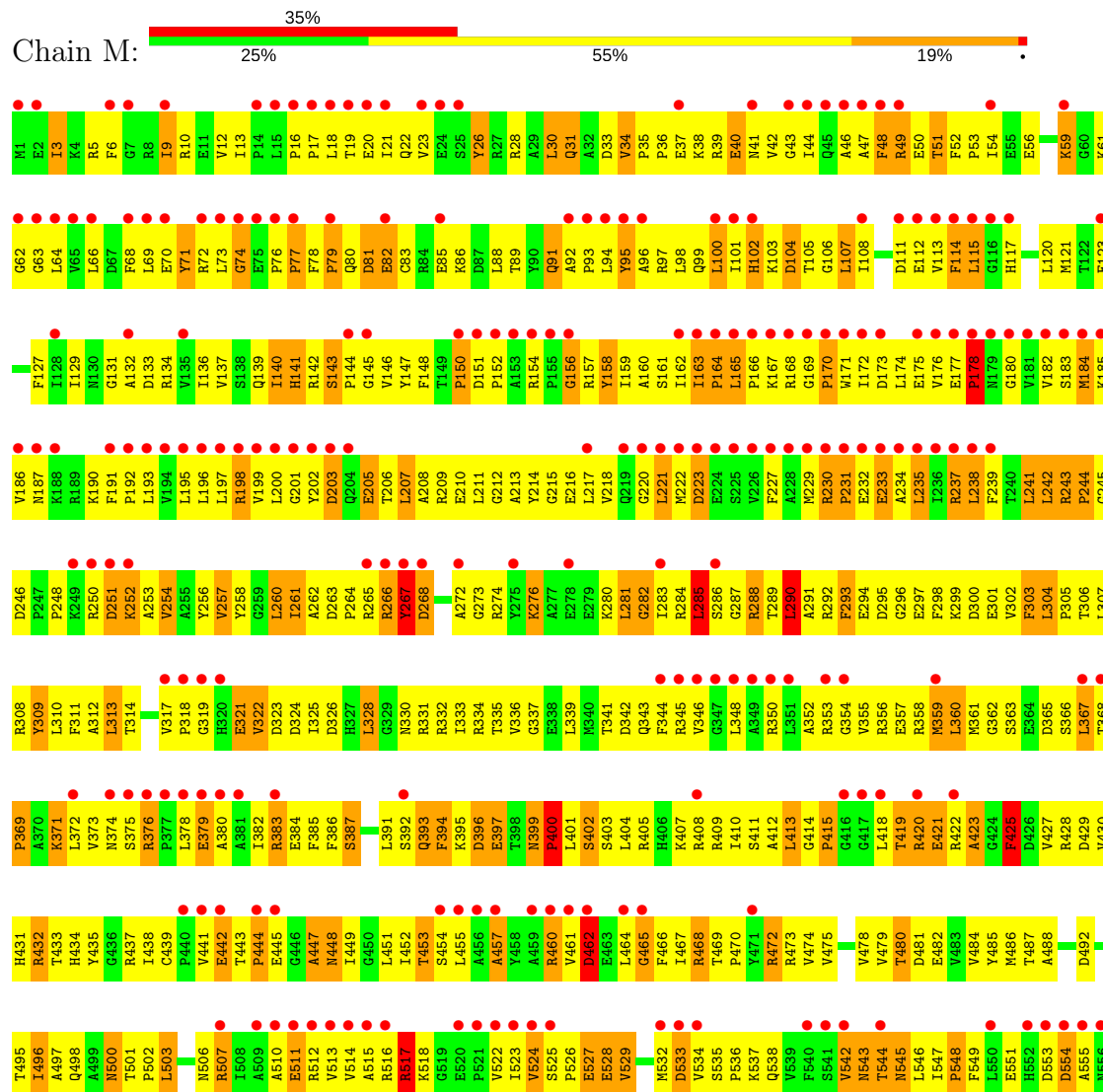


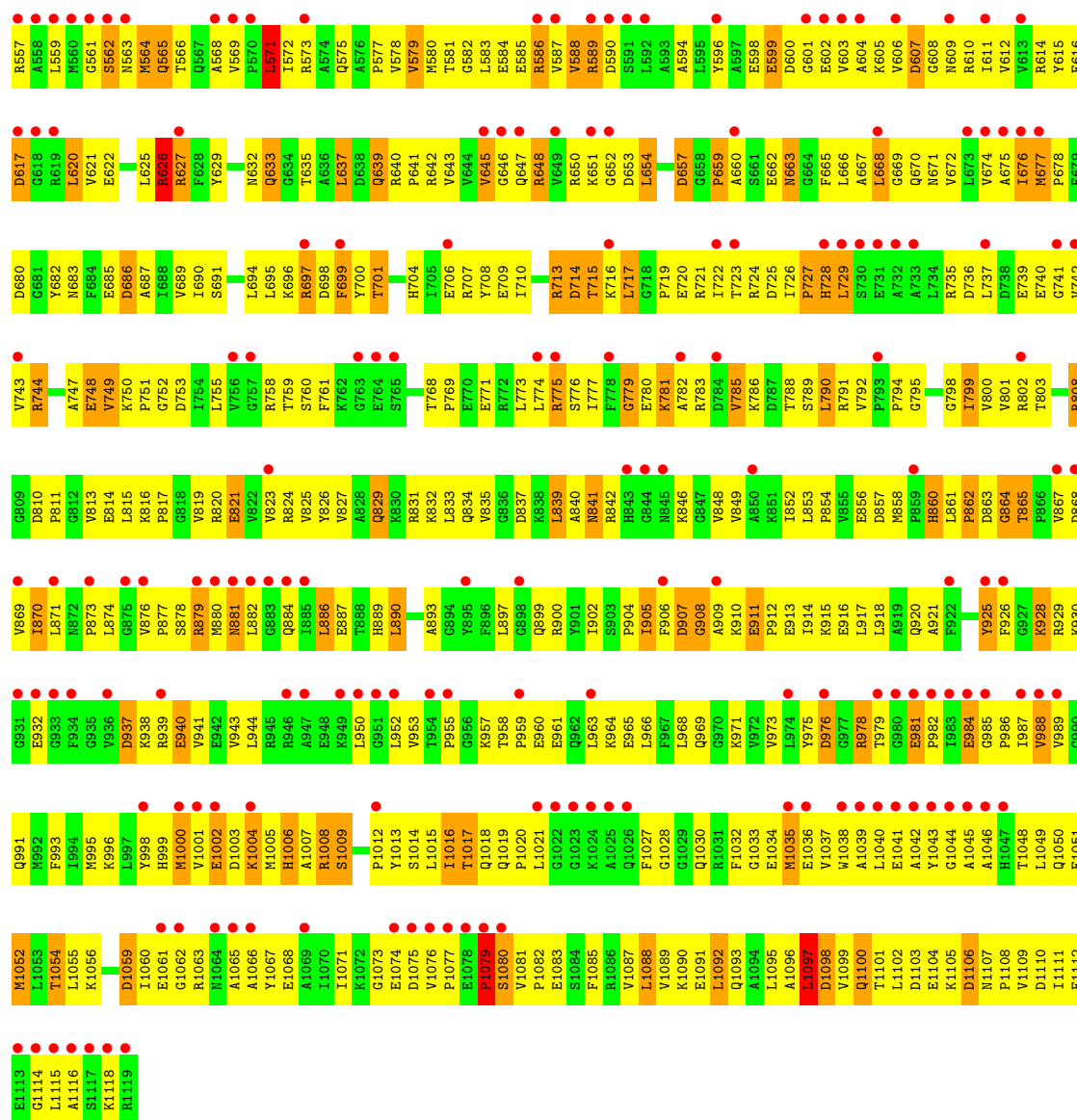
- Molecule 2: DNA-directed RNA polymerase beta chain



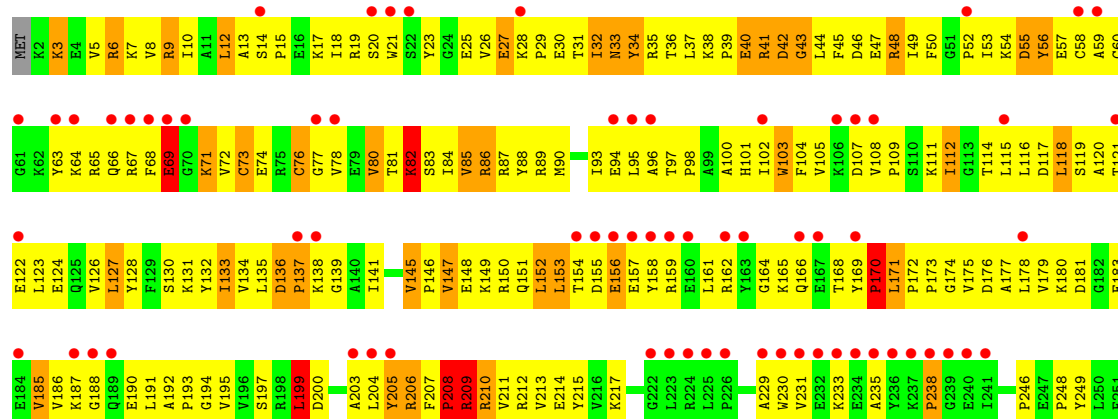


• Molecule 2: DNA-directed RNA polymerase beta chain





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

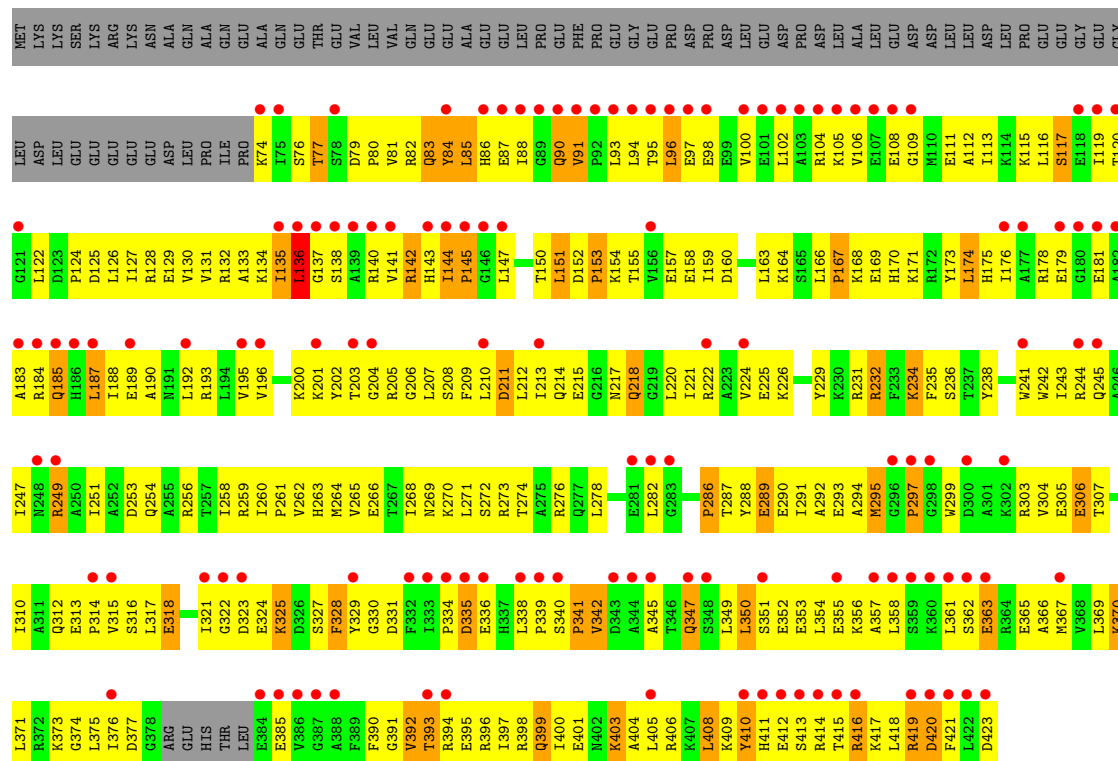


L1132	G1064	E874	A812	L751	D682	K621	G560	V499	D438	E374	ARG
R1133	L1065	T875	L813	L751	I683	R622	G561	R500	L439	E374	ALA
L1134	T1066	S876	A814	S752	K684	V623	A562	R501	V440	L378	GLU
R1135	V1067	R877	A815	S753	D685	P624	P563	F502	R441	A379	GLU
R1136	L1068	T944	H816	F754	E686	V625	E564	D503	N442	E381	GLY
R1137	E1069	R879	E817	A755	V687	S626	I565	D504	V443	A381	GLY
A1138	L1070	I880	R818	Q756	M688	G627	I566	S505	V444	E382	VAL
L1139	F1071	L881	C819	A757	D689	R628	I567	G506	V445	E385	VAL
L1140	L1072	R882	C820	F758	A690	S629	R568	N507	V446	E386	GLU
E1141	S1073	A883	R821	A759	R691	V630	N569	R508	V447	L387	LEU
A1142	S1074	R884	A822	R760	E692	I631	E570	P509	E448	L393	LYS
H1075	H1075	I885	L823	I761	E693	V632	K571	E510	S449	L394	GLY
G1076	F1012	I886	R824	Q762	E694	V633	K572	E511	Y450	E388	LEU
A1077	E1013	A887	A825	H763	I895	G634	K573	M512	D451	P390	GLU
R1078	L1074	R888	P826	L764	H696	P635	L574	I513	A391	A391	GLU
T1084	V955	A889	T827	S765	G697	Q636	E576	L513	S392	S392	GLU
A1085	V956	R890	K828	A766	K698	L637	E577	A454	L461	L461	ALA
L1148	P957	E891	R829	H767	V699	L639	V578	R455	G193	L394	PHE
L1086	E958	D892	A830	N768	L702	R640	D579	M456	V395	V395	LEU
R1087	E959	E893	G831	L769	N703	Q641	A590	E459	V396	V396	VAL
D1090	K960	R894	R832	L770	R704	G642	L581	A460	K397	K397	LEU
Y1093	Q961	V895	E833	S771	A705	G643	L582	A398	A398	A398	ARG
L1156	Y963	L964	T834	P772	A706	P644	D583	R399	R399	R399	ARG
L1094	L964	E898	S835	A773	P706	K646	N584	D523	Y401	Y401	GLU
T1095	E898	L899	V836	S774	L708	R647	E585	L524	P402	P402	ASP
R1096	E965	I900	C837	G775	H709	M648	R586	R525	F403	F403	GLU
L1159	E966	Q901	R839	E776	R710	M649	R587	P526	L465	L465	PRO
E1161	Q967	D903	L839	P777	A707	E650	E588	M527	E404	E404	VAL
L1098	R969	R903	V839	A777	P718	V651	A589	Q528	D405	D405	ALA
E1162	C1039	D904	L840	L787	V719	L652	S596	Q529	D406	D406	ALA
G1163	G1034	V904	R844	P781	Q714	P653	V591	D531	V407	V407	TYR
L1101	R1035	Q905	N845	S782	A715	R654	I591	G531	E408	E408	PHE
T1102	L971	Q906	N846	R783	Q715	P655	T592	G532	E471	E471	LEU
L1103	Q973	Q907	P846	D784	F716	R656	N593	G533	A410	A410	PRO
E1104	L974	K908	E848	L786	Q717	P657	P594	R534	T411	T411	VAL
L1105	E975	L910	A849	L787	V719	L657	G595	F535	G412	G412	GLY
L1106	G1040	S910	R850	G788	L720	L658	S596	A536	E474	E474	VAL
V1107	L1041	L911	L851	L789	L721	K659	D597	A537	D413	D413	MET
R1108	E1042	K912	A852	L790	Q724	R660	R598	T537	R414	R414	THR
E1109	G1043	D913	R853	Y791	S725	M661	P599	S538	V415	V415	PRO
L1172	L1044	L914	A854	L792	I726	E662	L600	D539	A416	A416	LEU
L1173	M1045	V915	H855	T793	I726	E663	R601	N541	ASN	ASN	MET
L1174	Q1046	Y916	C856	Q794	Q727	K664	S602	D542	P417	P417	VAL
L1175	K1047	Q917	I857	Q795	L728	G665	L603	L543	G418	G418	VAL
A1177	P1048	A918	V858	R796	H729	I666	T604	L544	V420	V420	HIS
L1178	S1049	F919	D859	K797	P730	A667	D605	Y544	K482	K482	GLY
E1179	E1051	R921	L860	E798	L731	P668	I606	R545	P484	P484	ILE
P1121	T1052	G923	Q861	K799	L731	N669	L607	R546	S485	S485	VAL
L1122	F1053	M924	V863	Q800	E734	V670	S608	L547	R486	R486	GLY
F1123	V1055	E925	V864	A802	F736	K671	N549	I548	A487	A487	LYS
L1124	P1056	K926	T865	A803	F737	A672	R550	N549	V427	V427	GLN
P1125	V1057	T927	V866	L804	N737	R674	N551	A490	K428	K428	PRO
D1126	R1058	R928	R867	E805	D739	R675	K491	D430	S429	S429	ALA
E1127	L1059	R929	R868	F806	F740	M676	R552	A492	D431	D431	ALA
V1128	S1059	R929	V869	A807	D741	L677	L554	R493	Y432	Y432	GLY
P1191	S1060	L930	G870	T808	G742	E678	K556	R495	R434	R434	LYS
L1192	E1063	L931	R871	P809	D743	R679	L557	L496	V435	V435	GLY
S1131	T999	L934	L873	E811	M745	R681	G620	V498	E497	E497	LEU
G1064	L1065	T875	L813	L751	D682	K621	G560	V499	D438	E374	ARG
L1066	T1066	S876	A814	S752	K684	V623	A562	R500	L439	E374	MET
V1067	R877	R877	A815	S753	D685	P624	P563	F502	R441	A379	PRO
L1068	T944	T944	H816	F754	E686	V625	E564	D503	N442	E381	ARG
E1069	R879	R879	E817	A755	V687	S626	I565	D504	V443	A381	GLN
L1070	I880	I880	R818	Q756	M688	G627	I566	S505	V444	E382	VAL
F1071	L881	L881	C819	A757	D689	R628	I567	G506	V445	E385	ARG
L1072	R882	R882	C820	F758	A690	S629	R568	N507	V446	E386	ALA
S1073	A883	A883	R821	A759	R691	V630	N569	R508	V447	H386	ALA
S1074	R884	R884	A822	R760	E692	I631	E570	P509	E448	L387	GLN
H1075	I885	I885	L823	I761	E693	V632	K571	E510	S449	L393	VAL
G1076	F1012	I886	R824	Q762	E694	V633	K572	E511	Y450	E388	VAL
A1077	E1013	A887	A825	H763	I895	G634	K573	M512	D451	P390	ALA
R1078	L1074	R888	P826	L764	H696	P635	L574	I513	A391	A391	GLU
T1084	V955	A889	T827	S765	G697	Q636	E576	L513	S392	S392	GLU
A1085	V956	R890	K828	A766	K698	L637	E577	A454	L461	L461	GLY
L1148	P957	E891	R829	H767	V699	L639	V578	R455	G193	L394	GLY
L1086	E958	D892	A830	N768	L702	R640	D579	M456	V395	V395	THR
R1087	E959	E893	G831	L769	N703	Q641	A590	E459	V396	V396	VAL
D1090	K960	R894	R832	L770	R704	G642	L581	A460	K397	K397	LEU
Y1093	Q961	V895	E833	S771	A705	P644	D583	A398	A398	A398	THR
L1156	Y963	L964	T834	P772	A706	P644	D583	R399	R399	R399	THR
L1094	L964	E898	S835	A773	P706	K646	N584	D523	Y401	Y401	PHE
T1095	E898	L899	V836	S774	L708	R647	E585	L524	P402	P402	LEU
R1096	E965	I900	C837	G775	H709	M648	R586	R525	F403	F403	GLU
L1159	E966	Q901	R839	E776	R710	M649	R587	P526	L465	L465	PRO
E1161	Q967	D903	L839	A777	A707	E650	E588	M527	E404	E404	VAL
L1098	R969	R903	V839	A777	P718	V651	A589	Q528	D405	D405	ALA
E1162	C1039	D904	L840	L787	V719	L652	S596	Q529	D406	D406	ALA
G1163	G1034	V904	R844	P781	Q714	P653	V591	D531	V407	V407	TYR
L1101	R1035	Q905	N845	S782	A715	R654	I591	G531	E408	E408	PHE
T1102	L971	Q906	N846	R783	Q715	P655	T592	G532	E471	E471	LEU
L1103	Q973	Q907	P846	D784	F716	R656	N593	G533	A410	A410	PRO
E1104	L974	K908	E848	L786	Q717	P657	P594	R534	T411	T411	VAL
L1105	E975	L910	A849	L787	V719	L657	G595	F535	G412	G412	GLY
L1106	G1040	S910	R850	G788	L720	L658	S596	A536	E474	E474	VAL
V1107	L1041	L911	L851	L789	L721	K659	D597	A537	D413	D413	MET
R1108	E1042	K912	A852	L790	Q724	R660	R598	T537	R414	R414	THR
E1109	G1043	D913	R853	Y791	S725	M661	P599	S538	V415	V415	PRO
L1172	L1044	L914	A854	L792	I726	E662	L600	D539	A416	A416	LEU
L1173	M1045	V915	H855	T793	I726	E663	R601	N541	ASN	ASN	MET
L1174	Q1046	Y916	C856	Q794	Q727	K664	S602	D542	P417	P417	VAL
L1175	K1047	Q917	I857	Q795	L728	G665	L603	L543	G418	G418	VAL
A1177	P1048	A918	V858	R796	H729	I666	T604	L544	V420	V420	HIS
L1178	S1049	F919	D859	K797	P730	A667	D605	Y544	K482	K482	GLY
E1179	E1051	R921	L860	E798	L731	P668	I606	R545	P484	P484	ILE
P1121	T1052	G923	Q861	K799	L731	N669	L607	R546	S485	S485	VAL
L1122	F1053	M924	V863	Q800	E734	V670	S608	L547	R486	R486	GLY
F1123	V1055	E925	V864	A802	F736	K671	N549	I548	A487	A487	LYS
L1124	P1056	K926	T865	A803	F737	A672	R550	N549	V427	V427	GLN
P1125	V1057	T927	V866	L804	N737	R674	N551	A490	K428	K428	PRO
D1126	R1058	R928	R867	E805	D739	R675	K491	D430	S429	S429	ALA
E1127	L1059	R929	R868	F806	F740	M676	R552	A492	D431	D431	ALA
V1128	S1059	R929	V869	A807	D741	L677	L554	R493	Y432	Y432	GLY
P1191	S1060	L930	G870	T808	G742	E678	K556	R495	R434	R434	LYS
L1192	E1063	L931	R871	P809	D743	R679	L557	L496	V435	V435	GLY
S1131	T999	L934	L873	E811	M745	R681	G620	V498	E497	E497	LEU









4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 34.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 91.0 (34.69-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.268 0.230 , 0.264	Depositor DCC
R_{free} test set	33251 reflections (5.76%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.079 for h,-h-k,-l 0.079 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	60908	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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	0.80	1/1838 (0.1%)	0.87	3/2498 (0.1%)
1	B	0.75	0/1838	0.84	6/2498 (0.2%)
1	K	0.75	0/1838	0.83	1/2498 (0.0%)
1	L	0.73	1/1838 (0.1%)	0.77	3/2498 (0.1%)
2	C	0.83	1/8997 (0.0%)	0.89	7/12164 (0.1%)
2	M	0.82	0/8997	0.90	10/12164 (0.1%)
3	D	0.82	0/10903	0.93	18/14736 (0.1%)
3	N	0.81	0/10903	0.93	19/14736 (0.1%)
4	E	0.82	0/783	0.96	0/1054
4	O	0.84	1/783 (0.1%)	0.95	1/1054 (0.1%)
5	F	0.72	0/2812	0.83	4/3781 (0.1%)
5	P	0.73	0/2812	0.82	3/3781 (0.1%)
All	All	0.80	4/54342 (0.0%)	0.90	75/73462 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	17	TYR	CD1-CE1	6.19	1.48	1.39
1	A	48	ILE	C-N	5.79	1.45	1.34
1	L	172	SER	N-CA	-5.30	1.35	1.46
2	C	191	PHE	C-N	5.26	1.44	1.34

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1389	LEU	CA-CB-CG	8.52	134.89	115.30
3	D	76	CYS	CA-CB-SG	8.24	128.84	114.00
3	D	199	LEU	CA-CB-CG	-8.01	96.89	115.30
2	M	165	LEU	C-N-CD	-7.94	103.13	120.60
3	N	199	LEU	CA-CB-CG	-7.89	97.16	115.30

There are no chirality outliers.

There are no planarity outliers.

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	239	0
1	B	1806	0	1861	210	0
1	K	1806	0	1861	178	0
1	L	1806	0	1861	205	0
2	C	8829	0	8933	1211	0
2	M	8829	0	8933	1154	0
3	D	10728	0	10809	1434	0
3	N	10728	0	10809	1309	0
4	E	769	0	775	89	0
4	O	769	0	775	118	0
5	F	2771	0	2844	364	0
5	P	2771	0	2844	336	0
6	D	43	0	31	4	0
6	N	43	0	31	6	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
9	A	232	0	0	42	0
9	B	304	0	0	53	0
9	C	1144	0	0	274	0
9	D	1546	0	0	310	0
9	E	130	0	0	20	0
9	F	491	0	0	108	0
9	K	229	0	0	33	0
9	L	274	0	0	51	0
9	M	1072	0	0	223	0
9	N	1392	0	0	261	0
9	O	137	0	0	26	0
9	P	447	0	0	72	0
All	All	60908	0	54228	6435	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 60.

The worst 5 of 6435 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:N:131:LYS:HG2	3:N:568:ARG:HG2	1.30	1.08
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.09	1.06
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.36	1.05
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.22	1.05
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.38	1.03

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%)	201 (88%)	21 (9%)	5 (2%)	7	8
1	B	227/315 (72%)	200 (88%)	21 (9%)	6 (3%)	6	6
1	K	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	13	18
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	9	11
2	C	1117/1119 (100%)	924 (83%)	143 (13%)	50 (4%)	3	2
2	M	1117/1119 (100%)	920 (82%)	149 (13%)	48 (4%)	3	2
3	D	1375/1524 (90%)	1129 (82%)	186 (14%)	60 (4%)	3	2
3	N	1375/1524 (90%)	1129 (82%)	181 (13%)	65 (5%)	2	1
4	E	93/99 (94%)	73 (78%)	16 (17%)	4 (4%)	3	2
4	O	93/99 (94%)	73 (78%)	16 (17%)	4 (4%)	3	2
5	F	341/423 (81%)	288 (84%)	42 (12%)	11 (3%)	4	3
5	P	341/423 (81%)	291 (85%)	37 (11%)	13 (4%)	3	3
All	All	6760/7590 (89%)	5632 (83%)	855 (13%)	273 (4%)	3	2

5 of 273 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	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%)	154 (76%)	48 (24%)	1	1
1	B	202/273 (74%)	162 (80%)	40 (20%)	1	1
1	K	202/273 (74%)	165 (82%)	37 (18%)	2	2
1	L	202/273 (74%)	156 (77%)	46 (23%)	1	1
2	C	941/941 (100%)	720 (76%)	221 (24%)	1	1
2	M	941/941 (100%)	722 (77%)	219 (23%)	1	1
3	D	1118/1279 (87%)	848 (76%)	270 (24%)	1	1
3	N	1118/1279 (87%)	860 (77%)	258 (23%)	1	1
4	E	83/87 (95%)	65 (78%)	18 (22%)	1	1
4	O	83/87 (95%)	67 (81%)	16 (19%)	1	1
5	F	295/370 (80%)	237 (80%)	58 (20%)	1	1
5	P	295/370 (80%)	245 (83%)	50 (17%)	2	2
All	All	5682/6446 (88%)	4401 (78%)	1281 (22%)	1	1

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

Mol	Chain	Res	Type
4	E	7	ASP
1	L	138	LEU
3	N	1372	VAL
4	E	89	MET

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Mol	Chain	Res	Type
5	F	399	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	337	HIS
1	L	227	ASN
4	O	28	GLN
1	K	38	ASN
1	K	227	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	8001	-	43,47,47	7.05	26 (60%)	46,73,73	2.59	10 (21%)
6	STD	N	8002	-	43,47,47	6.98	26 (60%)	46,73,73	2.74	9 (19%)

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	8001	-	-	0/31/101/101	0/4/5/5
6	STD	N	8002	-	-	2/31/101/101	0/4/5/5

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8001	STD	O5-C19	-27.86	1.18	1.43
6	N	8002	STD	O5-C19	-26.97	1.18	1.43
6	N	8002	STD	C23-C21	-14.10	1.21	1.53
6	D	8001	STD	C23-C21	-14.04	1.22	1.53
6	D	8001	STD	C18-C16	-12.94	1.25	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	8001	STD	O8-C17-C30	-6.62	105.06	111.66
6	N	8002	STD	O8-C17-C30	-6.43	105.26	111.66
6	D	8001	STD	O2-C2-C1	-3.38	122.49	130.53
6	N	8002	STD	O2-C2-C1	-3.16	123.01	130.53
6	D	8001	STD	O1-C3-C20	-2.17	122.71	124.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	8002	STD	C21-C22-N2-C24
6	N	8002	STD	O6-C22-N2-C24

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	8001	STD	4	0
6	N	8002	STD	6	0

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 [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%)	2.28	66 (28%) 0 0	31, 63, 90, 117	0
1	B	229/315 (72%)	2.69	74 (32%) 0 0	53, 90, 112, 118	0
1	K	229/315 (72%)	1.53	59 (25%) 0 0	33, 62, 87, 122	0
1	L	229/315 (72%)	3.11	82 (35%) 0 0	50, 87, 110, 125	0
2	C	1119/1119 (100%)	3.16	424 (37%) 0 0	25, 78, 104, 116	0
2	M	1119/1119 (100%)	2.82	396 (35%) 0 0	23, 72, 104, 115	0
3	D	1381/1524 (90%)	1.84	357 (25%) 0 0	27, 67, 107, 119	0
3	N	1381/1524 (90%)	1.85	373 (27%) 0 0	27, 68, 108, 120	0
4	E	95/99 (95%)	1.87	28 (29%) 0 0	44, 81, 108, 128	0
4	O	95/99 (95%)	1.95	32 (33%) 0 0	44, 75, 93, 105	0
5	F	345/423 (81%)	3.54	146 (42%) 0 0	55, 84, 107, 122	0
5	P	345/423 (81%)	3.06	129 (37%) 0 0	62, 84, 108, 116	0
All	All	6796/7590 (89%)	2.45	2166 (31%) 0 0	23, 73, 106, 128	0

The worst 5 of 2166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	405	ASP	71.3
3	N	406	ASP	57.5
1	A	1	MET	54.5
3	D	853	VAL	52.8
3	N	407	VAL	49.0

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

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

6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	STD	N	8002	43/43	0.76	0.15	27,35,41,48	0
6	STD	D	8001	43/43	0.86	0.13	25,35,40,43	0
8	MG	N	9002	1/1	0.88	0.51	53,53,53,53	0
8	MG	D	9001	1/1	0.94	0.19	29,29,29,29	0
7	ZN	N	7459	1/1	0.95	0.10	64,64,64,64	0
7	ZN	N	7413	1/1	0.99	0.11	65,65,65,65	0
7	ZN	D	7458	1/1	0.99	0.09	64,64,64,64	0
7	ZN	D	7412	1/1	0.99	0.06	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.