



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:25 AM 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

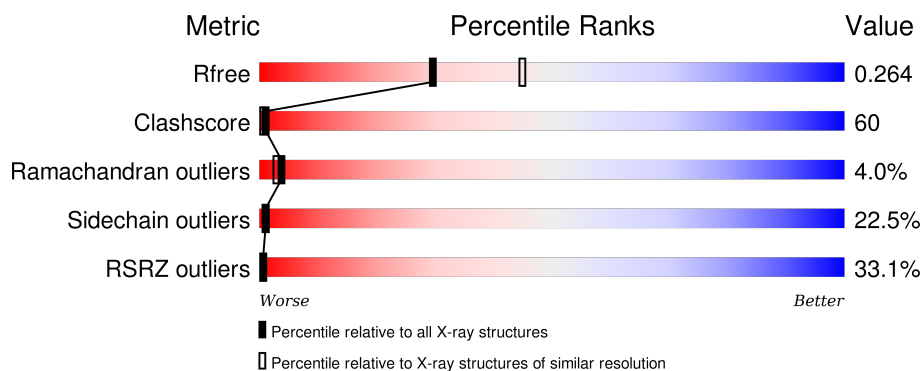
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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>22%</div> <div> <div>16%</div> <div>43%</div> <div>13%</div> <div>27%</div> </div> </div>
1	B	315	<div> <div>24%</div> <div> <div>16%</div> <div>43%</div> <div>13%</div> <div>27%</div> </div> </div>
1	K	315	<div> <div>20%</div> <div> <div>23%</div> <div>41%</div> <div>8%</div> <div>27%</div> </div> </div>
1	L	315	<div> <div>28%</div> <div> <div>20%</div> <div>39%</div> <div>12%</div> <div>27%</div> </div> </div>
2	C	1119	<div> <div>40%</div> <div> <div>24%</div> <div>57%</div> <div>19%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	M	1119	<div><div></div><div>36%</div><div>25%</div><div>55%</div><div>19%</div><div></div></div>
3	D	1524	<div><div></div><div>25%</div><div>22%</div><div>52%</div><div>15%</div><div>9%</div><div></div></div>
3	N	1524	<div><div></div><div>25%</div><div>25%</div><div>49%</div><div>15%</div><div>9%</div><div></div></div>
4	E	99	<div><div></div><div>29%</div><div>27%</div><div>53%</div><div>15%</div><div></div><div></div></div>
4	O	99	<div><div></div><div>33%</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>18%</div><div></div></div>
5	P	423	<div><div></div><div>31%</div><div>21%</div><div>49%</div><div>11%</div><div>18%</div><div></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			

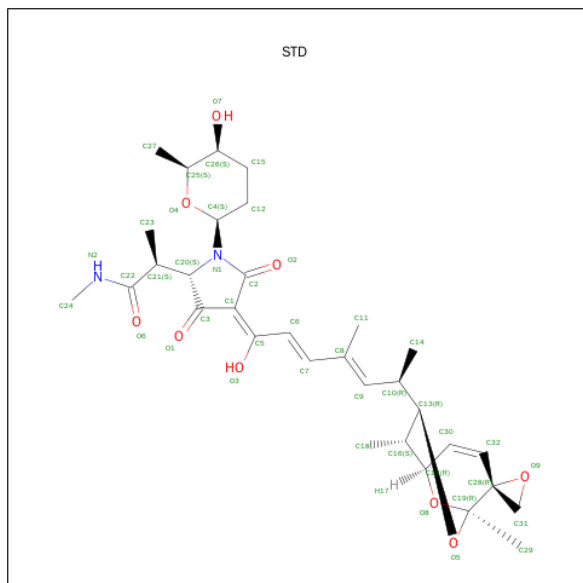
- Molecule 4 is a protein called RNA polymerase omega chain.

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

- Molecule 6 is STREPTOLYDIGIN (three-letter code: STD) (formula: C₃₂H₄₄N₂O₉).



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

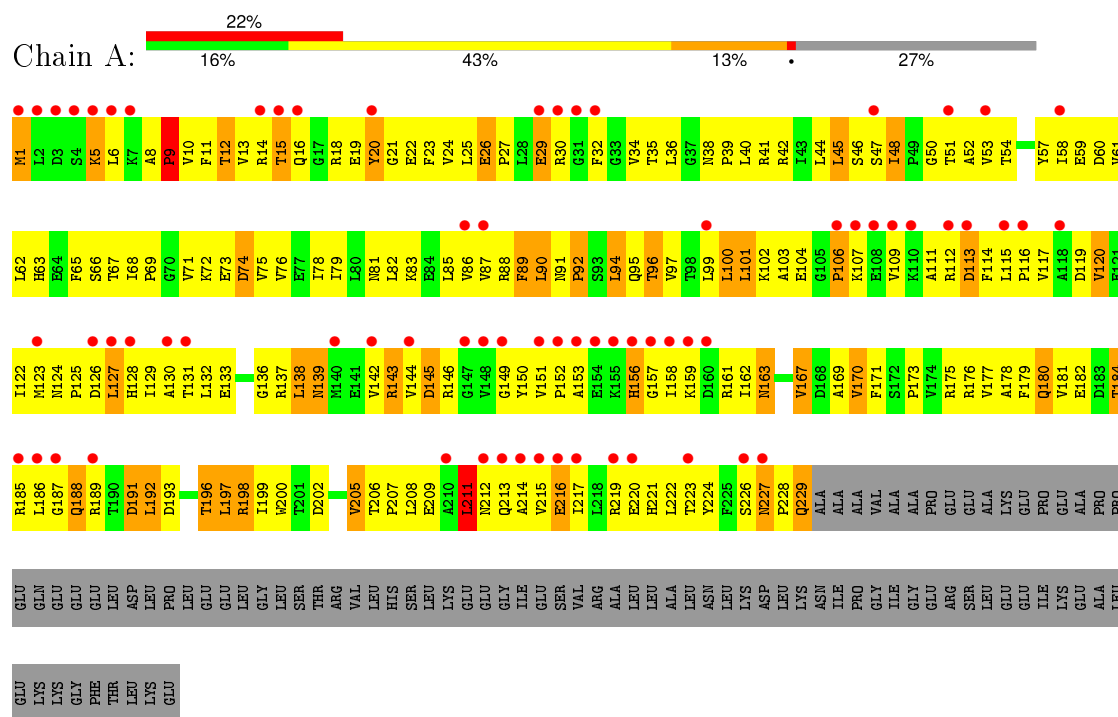
- Molecule 9 is water.

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

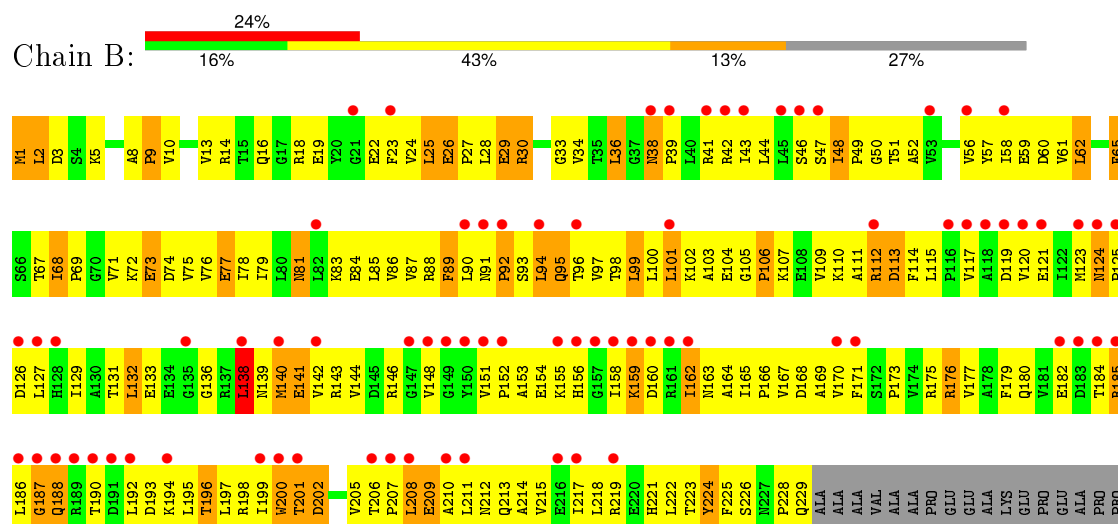
3 Residue-property plots

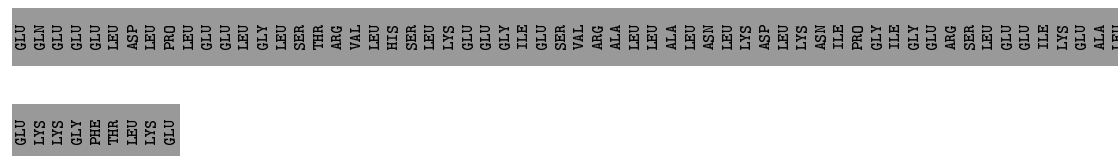
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase alpha chain

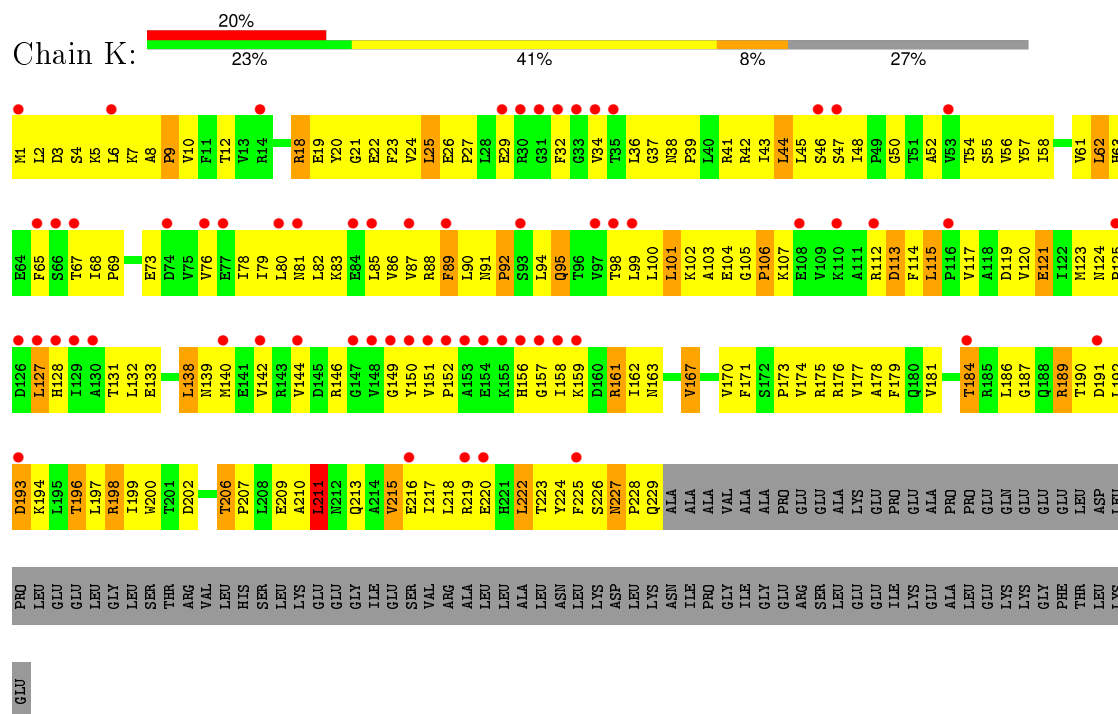


• Molecule 1: DNA-directed RNA polymerase alpha chain

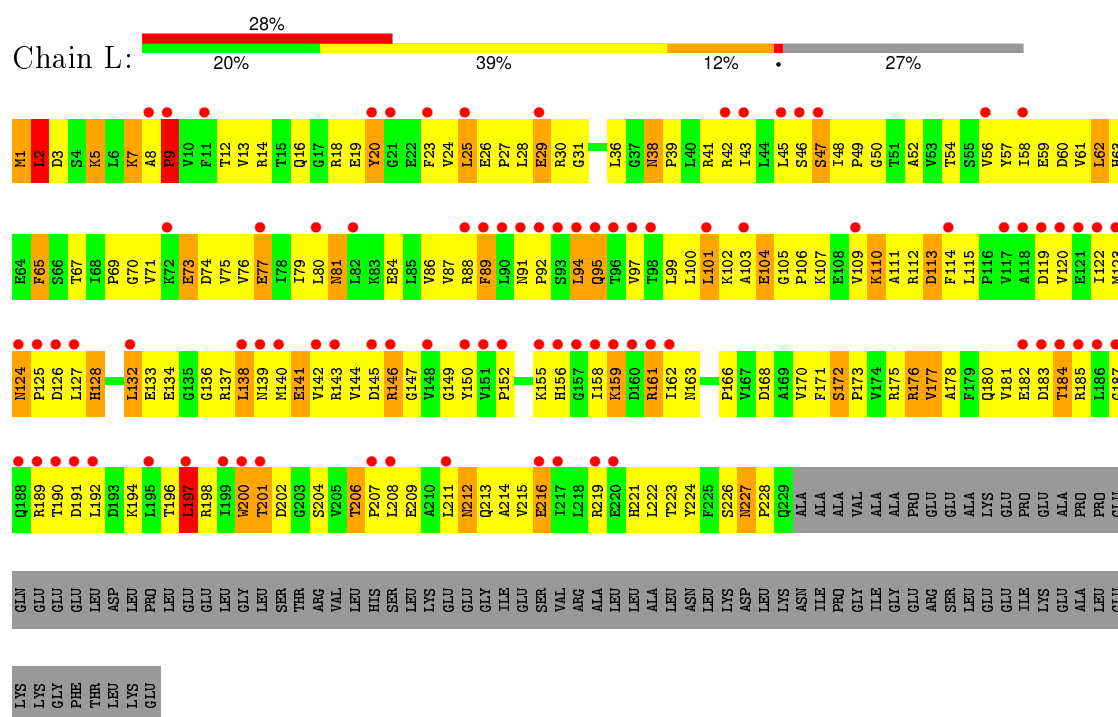




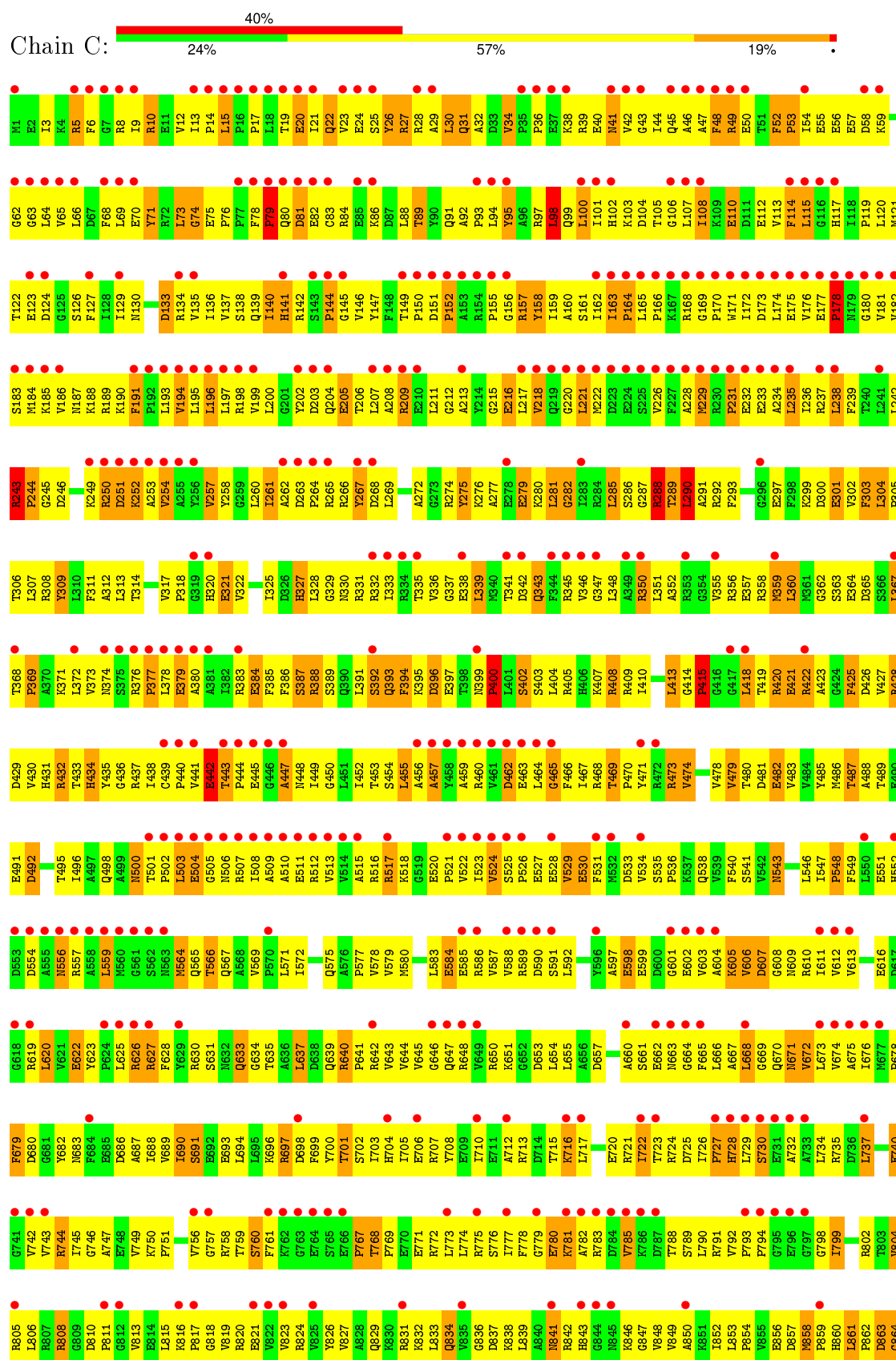
• Molecule 1: DNA-directed RNA polymerase alpha chain

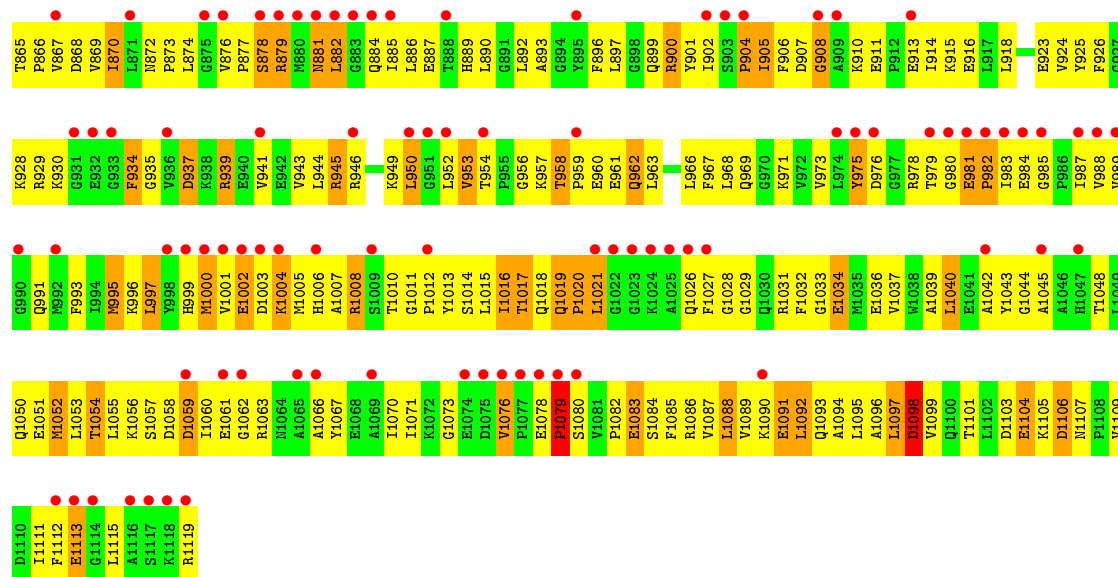


• Molecule 1: DNA-directed RNA polymerase alpha chain



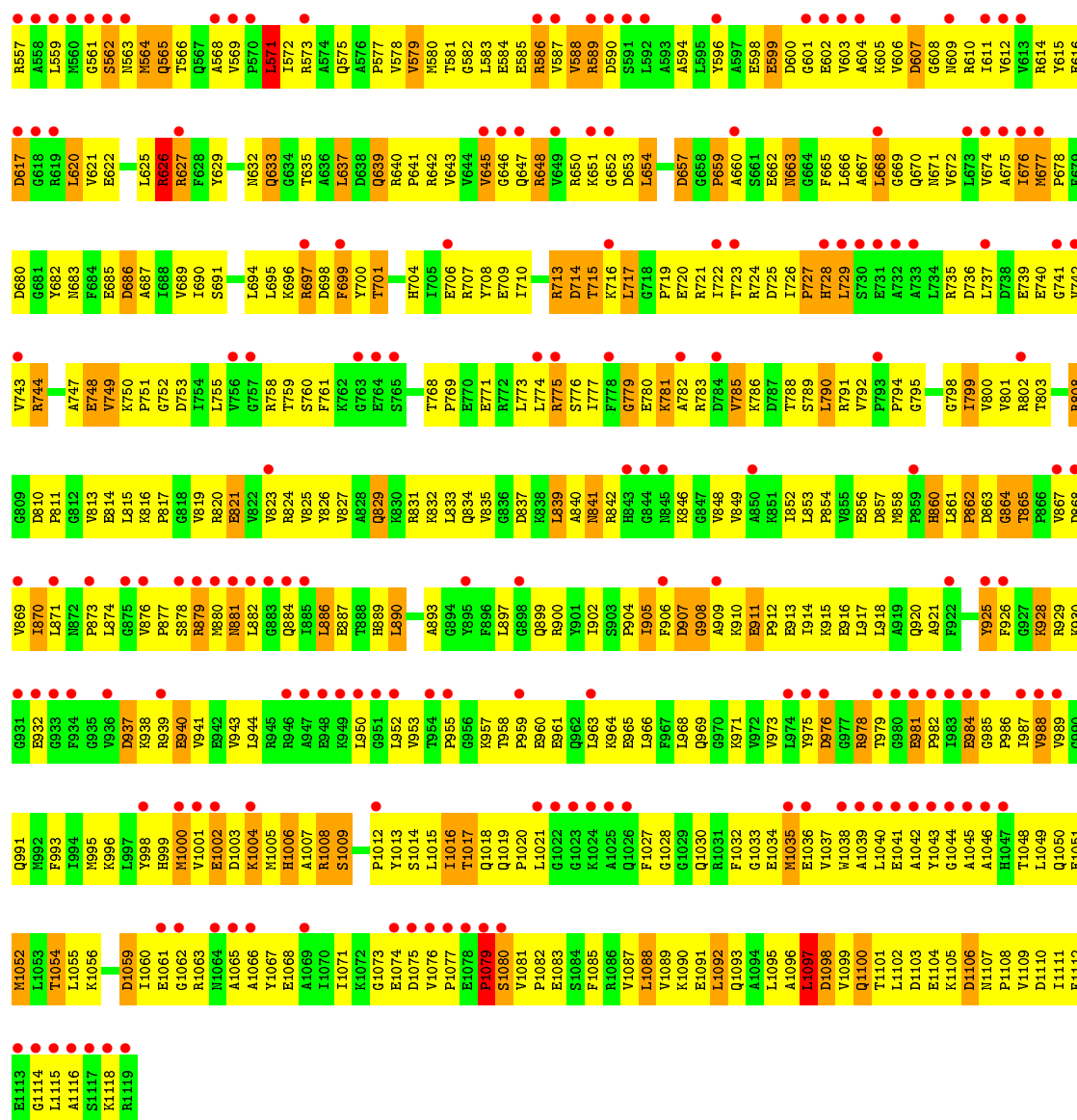
• Molecule 2: DNA-directed RNA polymerase beta chain



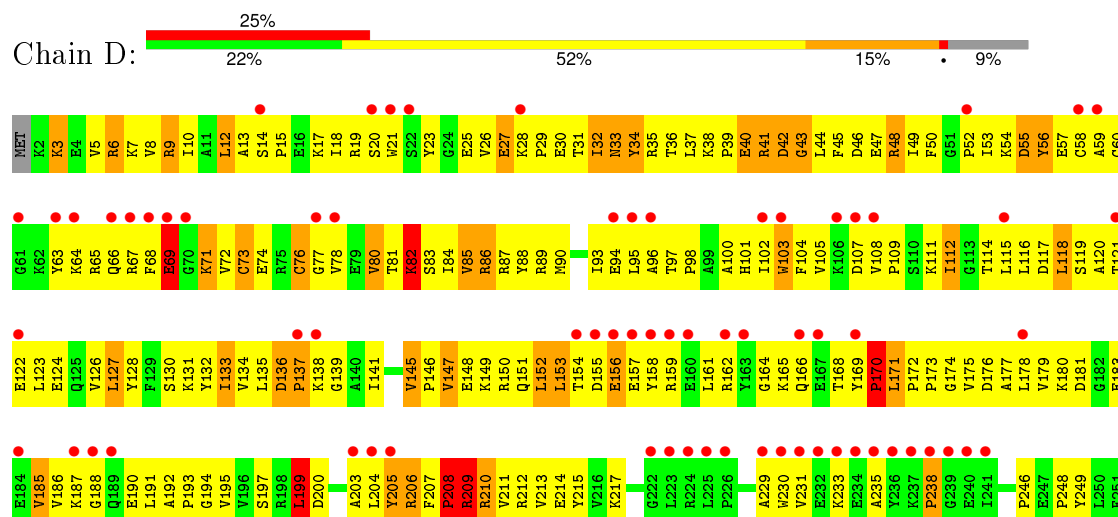


• Molecule 2: DNA-directed RNA polymerase beta chain

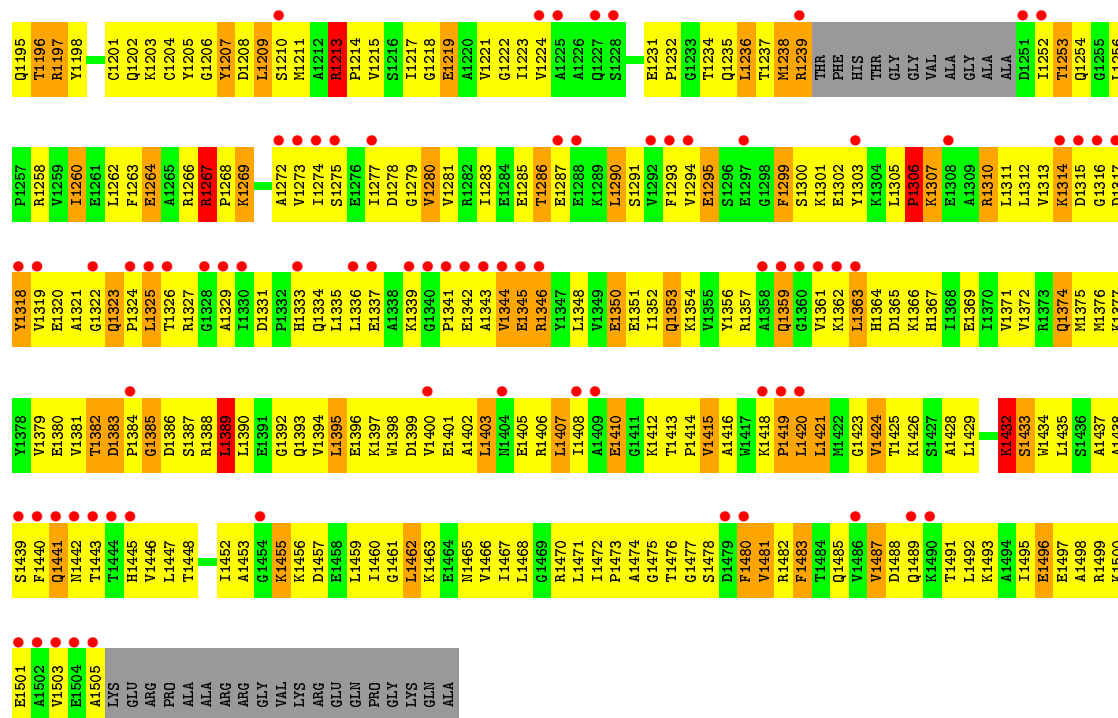




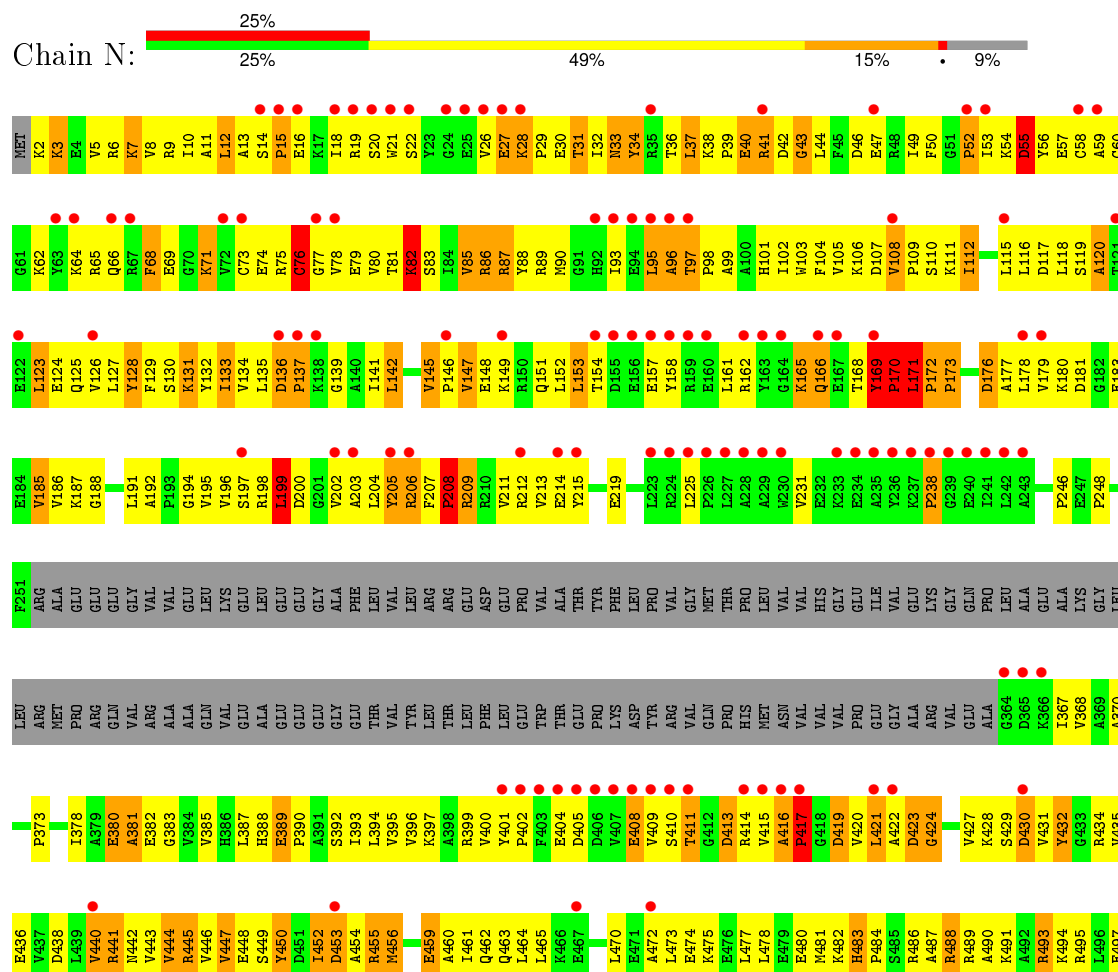
● Molecule 3: DNA-directed RNA polymerase beta' chain



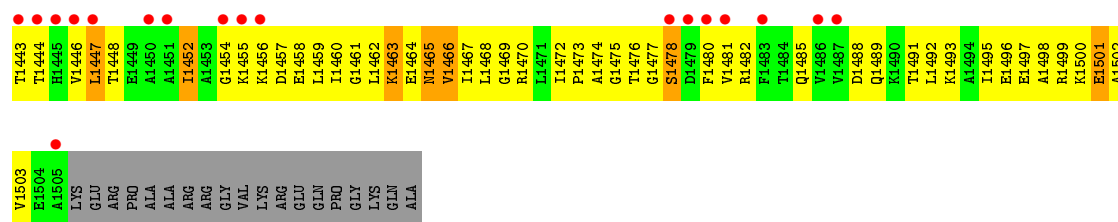
L1132	L1065	G1064	T1000	E874	A812	L751	D682	K621	Q560	V499	D438	E374	ARG
R1133	L1066	L1067	E1001	T875	E813	L751	E883	R622	G561	R500	L439	E374	ALA
L1134	V1067	V1068	K1002	S876	A814	S752	K684	R623	A562	R501	V440	L378	GLU
K1136	L1068	L1069	V1003	R877	A815	S753	D685	D624	P563	F502	R441	A379	GLU
R1137	E1069	E1070	T1004	G878	B816	F754	E886	S626	E564	L503	N442	E380	GLY
A1138	L1070	L1071	Q1005	R879	R817	A755	V687	S627	S565	D504	V443	A381	GLY
L1139	A1006	G946	Q1006	I880	R818	F756	M888	G627	S505	S506	R444	E382	VAL
F1071	V1007	I947	A1008	L881	G819	Q757	D889	R628	G506	G507	R445	E382	VAL
F1008	F1008	T948	F1008	R882	E820	E758	A690	S629	R568	N507	V446	V385	GLU
S1073	K1009	I949	A883	R884	R821	A759	L691	V630	N569	R508	V447	H386	LEU
S1074	M1010	G950	A884	R884	A822	R760	E892	V631	E570	P509	E448	L387	LYS
H1075	F1011	I951	L885	I885	L833	I761	E893	V632	K571	E510	S449	H388	GLU
G1076	E1012	D952	V886	R886	L834	Q762	E894	V633	R572	H511	Y450	E389	LEU
A1077	E1013	D953	A887	A887	A825	M763	I895	G634	R573	M512	D451	P390	GLU
R1078	M1014	A954	E888	E888	R826	L764	H696	P635	L574	I513	I452	A391	GLU
T1084	Y1015	V955	R889	R889	P826	L764	H696	P635	L574	I513	I452	A391	GLU
A1085	I956	I956	E890	E890	R827	Q636	E697	L637	E576	A516	D453	S392	GLY
L1086	P957	P957	R891	R891	K828	A766	K698	L637	E576	A516	D453	S392	GLY
L1087	E958	E958	D892	D892	V829	H767	V699	L639	V578	V517	R455	L394	PHE
D1090	K960	K960	E893	E893	A830	M768	V699	L639	V578	V517	R455	L394	LEU
Y1093	K994	K994	R894	R894	E831	L769	L702	R640	D579	V519	V396	V396	VAL
L1094	R895	R895	R895	R895	R832	L770	M703	R641	A580	L520	E459	K397	LEU
T1095	Q961	Q961	A896	A896	E833	S771	R704	G642	L581	P522	A460	A398	ARG
R1096	Y963	Y963	E898	E898	T834	S772	A705	G643	L582	I461	I461	A399	ARG
L1097	L964	L964	R898	R898	S835	A773	T706	R646	D583	Q463	Q463	V401	LEU
E1098	E966	E966	R899	R899	V836	S774	T707	R647	D584	L524	L464	P402	ASP
Q1033	E965	E965	I899	I899	G837	G775	L708	R647	D585	R525	L464	P402	GLU
R1034	K970	K970	Q900	Q900	R838	P776	R709	M648	R586	P526	L465	F403	PRO
I1035	L971	L971	R901	R901	E839	P777	R710	M649	R587	M527	K466	E404	VAL
L1036	L972	L972	R902	R902	L839	P777	R710	M649	R587	M527	K466	E404	VAL
Q1037	Q973	Q973	R903	R903	F843	P781	I713	L650	E588	Q528	L467	D405	ALA
E1103	I974	I974	R904	R904	E844	S782	Q714	E651	A589	Q529	L468	D406	THR
C1039	E975	E975	V905	V905	D845	R783	A715	E652	V591	D531	L470	V530	TYR
G1040	Q976	Q976	S910	S910	D846	S784	Q715	E653	S596	D532	L471	V531	PHE
L1041	A977	A977	L911	L911	E846	D784	A716	E654	S597	G532	E472	V409	LEU
R1042	Y978	Y978	K912	K912	D847	D785	Q717	E655	S598	G533	A473	T411	PRO
G1043	G979	G979	D913	D913	E847	D786	Q718	E656	S599	R534	L474	G412	GLY
L1044	M980	M980	L914	L914	D848	D787	A719	E657	S599	R534	L474	G412	GLY
M1045	G981	G981	V915	V915	E849	D788	Q720	E658	S599	R534	L474	G412	GLY
Q1046	F982	F982	Y916	Y916	L850	L787	L720	E659	S599	R534	L474	G412	GLY
K1047	L983	L983	Q917	Q917	L851	L788	L721	E660	S599	R534	L474	G412	GLY
P1048	T984	T984	A918	A918	L852	L789	V721	E661	S599	R534	L474	G412	GLY
S1049	D985	D985	F919	F919	E853	L791	Q724	E662	S599	R534	L474	G412	GLY
E1051	R986	R986	L920	L920	A854	L792	S725	E663	S599	R534	L474	G412	GLY
T1052	E987	E987	R921	R921	E855	L793	I726	E664	S599	R534	L474	G412	GLY
F1053	Y989	Y989	L922	L922	E856	Q794	Q727	E665	S599	R534	L474	G412	GLY
E1054	D990	D990	G923	G923	E857	L795	L728	E666	S599	R534	L474	G412	GLY
V1055	Q991	Q991	E925	E925	E858	L796	H729	E667	S599	R534	L474	G412	GLY
P1056	L992	L992	R926	R926	E859	L797	P730	E668	S599	R534	L474	G412	GLY
P1057	L993	L993	T927	T927	E860	L798	L731	E669	S599	R534	L474	G412	GLY
L1058	Q994	Q994	A928	A928	E861	L799	E734	E670	S599	R534	L474	G412	GLY
E1059	L995	L995	R929	R929	E862	L800	E735	E671	S599	R534	L474	G412	GLY
S1060	W996	W996	L930	L930	E863	L801	F736	E672	S599	R534	L474	G412	GLY
R1061	E997	E997	I931	I931	E864	L802	F737	E673	S599	R534	L474	G412	GLY
F1062	T999	T999	L934	L934	E865	L803	F738	E674	S599	R534	L474	G412	GLY
L1063	E1063	E1063	L934	L934	E866	L804	F739	E675	S599	R534	L474	G412	GLY
L1064	E1064	E1064	L934	L934	E867	L805	D739	E676	S599	R534	L474	G412	GLY
L1065	E1065	E1065	L934	L934	E868	L806	D740	E677	S599	R534	L474	G412	GLY
L1066	E1066	E1066	L934	L934	E869	L807	D741	E678	S599	R534	L474	G412	GLY
L1067	E1067	E1067	L934	L934	E870	L808	G742	E679	S599	R534	L474	G412	GLY
L1068	E1068	E1068	L934	L934	E871	L809	G743	E680	S599	R534	L474	G412	GLY
L1069	E1069	E1069	L934	L934	E872	L810	Q744	E681	S599	R534	L474	G412	GLY
L1070	E1070	E1070	L934	L934	E873	L811	Q745	E682	S599	R534	L474	G412	GLY
L1071	E1071	E1071	L934	L934	E874	L812	Q746	E683	S599	R534	L474	G412	GLY
L1072	E1072	E1072	L934	L934	E875	L813	Q747	E684	S599	R534	L474	G412	GLY
L1073	E1073	E1073	L934	L934	E876	L814	Q748	E685	S599	R534	L474	G412	GLY
L1074	E1074	E1074	L934	L934	E877	L815	Q749	E686	S599	R534	L474	G412	GLY
L1075	E1075	E1075	L934	L934	E878	L816	Q750	E687	S599	R534	L474	G412	GLY
L1076	E1076	E1076	L934	L934	E879	L817	Q751	E688	S599	R534	L474	G412	GLY
L1077	E1077	E1077	L934	L934	E880	L818	Q752	E689	S599	R534	L474	G412	GLY
L1078	E1078	E1078	L934	L934	E881	L819	Q753	E690	S599	R534	L474	G412	GLY
L1079	E1079	E1079	L934	L934	E882	L820	Q754	E691	S599	R534	L474	G412	GLY
L1080	E1080	E1080	L934	L934	E883	L821	Q755	E692	S599	R534	L474	G412	GLY
L1081	E1081	E1081	L934	L934	E884	L822	Q756	E693	S599	R534	L474	G412	GLY
L1082	E1082	E1082	L934	L934	E885	L823	Q757	E694	S599	R534	L474	G412	GLY
L1083	E1083	E1083	L934	L934	E886	L824	Q758	E695	S599	R534	L474	G412	GLY
L1084	E1084	E1084	L934	L934	E887	L825	Q759	E696	S599	R534	L474	G412	GLY
L1085	E1085	E1085	L934	L934	E888	L826	Q760	E697	S599	R534	L474	G412	GLY
L1086	E1086	E1086	L934	L934	E889	L827	Q761	E698	S599	R534	L474	G412	GLY
L1087	E1087	E1087	L934	L934	E890	L828	Q762	E699	S599	R534	L474	G412	GLY
L1088	E1088	E1088	L934	L934	E891	L829	Q763	E700	S599	R534	L474	G412	GLY
L1089	E1089	E1089	L934	L934	E892	L830	Q764	E701	S599	R534	L474	G412	GLY
L1090	E1090	E1090	L934	L934	E893	L831	Q765	E702	S599	R534	L474	G412	GLY
L1091	E1091	E1091	L934	L934	E894	L832	Q766	E703	S599	R534	L474	G412	GLY
L1092	E1092	E1092	L934	L934	E895	L833	Q767	E704	S599	R534	L474	G412	GLY
L1093	E1093	E1093	L934	L934	E896	L834	Q768	E705	S599	R534	L474	G412	GLY
L1094	E1094	E1094	L934	L934	E897	L835	Q769	E706	S599	R534	L474	G412	GLY
L1095	E1095	E1095	L934	L934	E898	L836	Q770	E707	S599	R534	L474	G412	GLY
L1096	E1096	E1096	L934	L934	E899	L837	Q771	E708	S599	R534	L474	G412	GLY
L1097	E1097	E1097	L934	L934	E900	L838	Q772	E709	S599	R534	L474	G412	GLY
L1098	E1098	E1098	L934	L934	E901	L839	Q773	E710	S599	R534	L474	G412	GLY
L1099	E1099	E1099	L934	L934	E902	L840	Q774	E711	S599	R534	L474	G412	GLY
L1100	E1100	E1100	L934	L934	E903	L841	Q775	E712	S599	R534	L474	G412	GLY
L1101	E1101	E1101	L934	L934	E904	L842	Q776	E713	S599	R534	L474	G412	GLY
L1102	E1102	E1102	L934	L934	E905	L843	Q777	E714	S599	R534	L474	G412	GLY
L1103	E1103	E1103	L934	L934	E906	L844	Q778	E715	S599	R534	L474	G412	GLY
L1104	E1104	E1104	L934	L934	E907	L845	Q779	E716	S599	R534	L474	G412	GLY
L1105	E1105	E1105	L934	L934	E908	L846	Q780	E717	S599	R534	L474	G412	GLY
L1106	E1106	E1106	L934	L934	E909	L847	Q781	E718	S599	R534	L474	G412	GLY
L1107	E1107	E1107	L934	L934	E910	L848	Q782	E719	S599	R534	L474	G412	GLY
L1108	E1108	E1108	L934	L934	E911	L849	Q783	E720	S599	R534	L474	G412	GLY
L1109	E1109	E1109	L934	L934	E912	L850	Q784	E721	S599	R534	L474	G412	GLY
L1110	E1110	E1110	L934	L934	E913	L851	Q785	E722	S599	R534	L474	G412	GLY
L1111	E1111	E1111	L934	L934	E914	L852	Q786	E723	S599	R534	L474	G41	



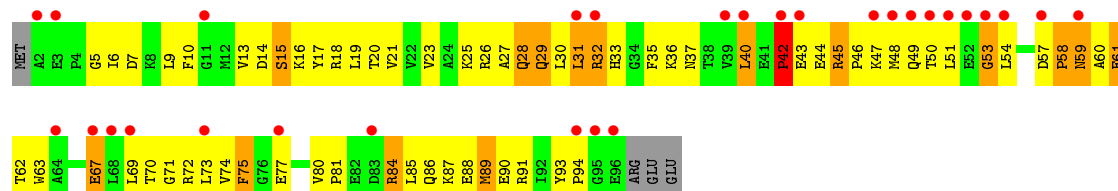
• Molecule 3: DNA-directed RNA polymerase beta' chain



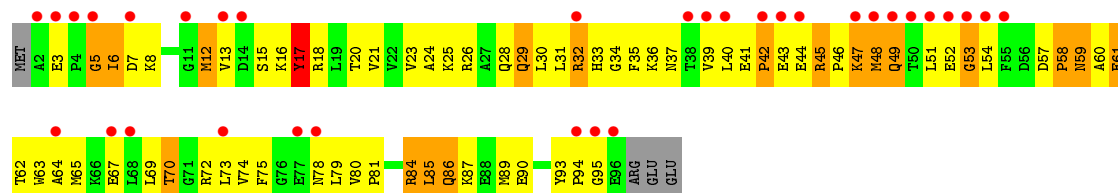




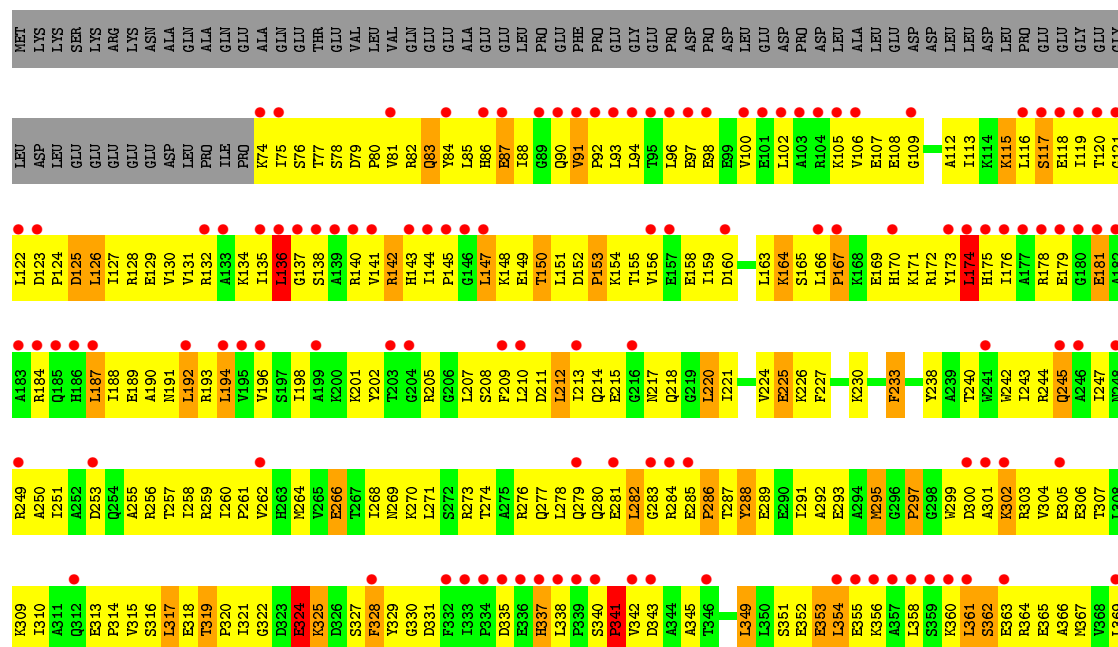
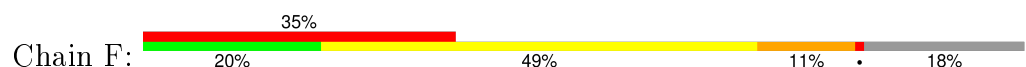
• Molecule 4: RNA polymerase omega chain

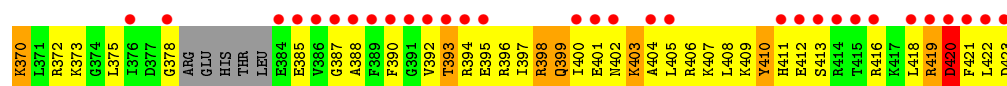


• Molecule 4: RNA polymerase omega chain

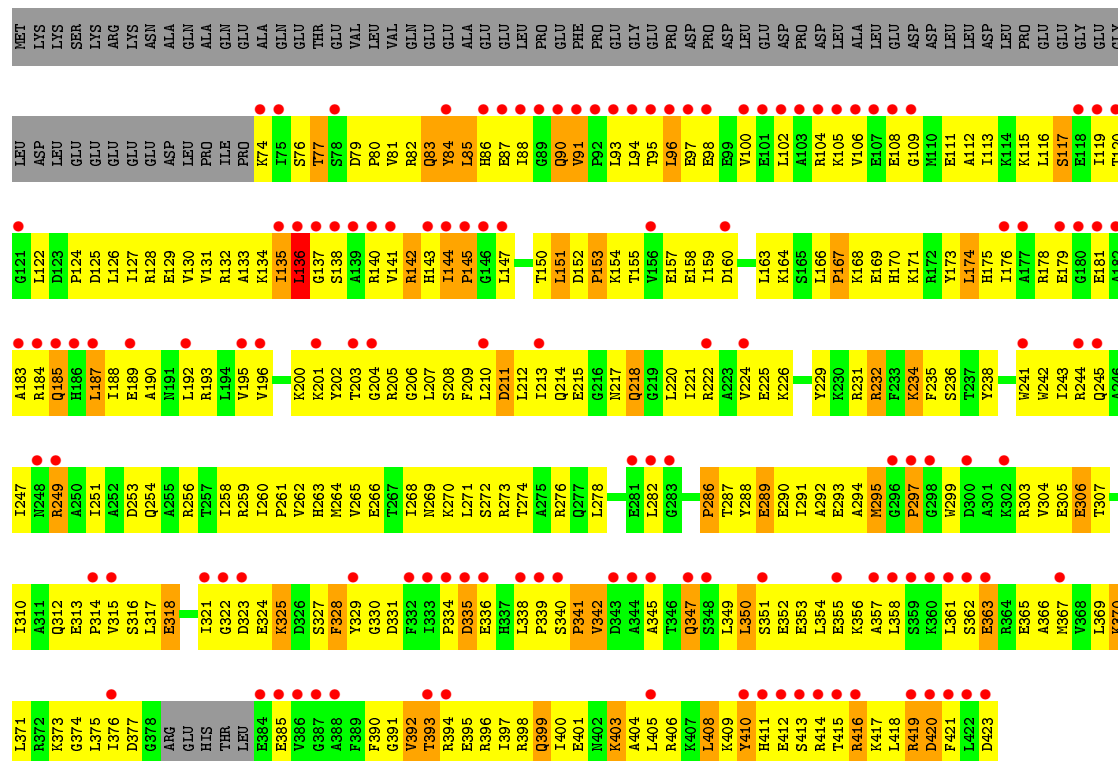
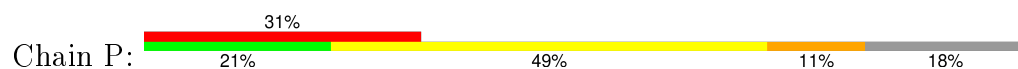


• Molecule 5: RNA polymerase sigma factor rpoD





● Molecule 5: RNA polymerase sigma factor rpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	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 (6.12%)	DCC
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
Estimated twinning fraction	0.499 for -h,-k,l 0.079 for h,-h-k,-l 0.079 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 577129 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)	8	9
1	B	227/315 (72%)	200 (88%)	21 (9%)	6 (3%)	7	6
1	K	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	15	21
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	11	13
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%)	3	2
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%)	5	4
5	P	341/423 (81%)	291 (85%)	37 (11%)	13 (4%)	4	3
All	All	6760/7590 (89%)	5632 (83%)	855 (13%)	273 (4%)	4	3

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	2
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%)	2	2
5	F	295/370 (80%)	237 (80%)	58 (20%)	1	2
5	P	295/370 (80%)	245 (83%)	50 (17%)	2	3
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	7.92	25 (58%)	41,73,73	2.56	10 (24%)
6	STD	N	8002	-	43,47,47	8.00	25 (58%)	41,73,73	2.61	11 (26%)

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8001	STD	O5-C19	-29.36	1.18	1.42
6	N	8002	STD	O5-C19	-28.41	1.18	1.42
6	N	8002	STD	C16-C17	-24.86	1.29	1.53
6	D	8001	STD	C16-C17	-23.37	1.31	1.53
6	N	8002	STD	C23-C21	-13.50	1.21	1.53

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	8001	STD	C20-N1-C2	-7.17	103.15	112.31
6	N	8002	STD	C20-N1-C2	-7.04	103.32	112.31
6	D	8001	STD	O8-C17-C30	-6.56	105.06	111.69
6	N	8002	STD	O8-C17-C30	-6.38	105.26	111.69
6	D	8001	STD	O2-C2-N1	-4.54	118.39	125.99

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%)	2.40	70 (30%) 1 1	31, 63, 90, 117	0
1	B	229/315 (72%)	2.83	76 (33%) 0 1	53, 90, 112, 118	0
1	K	229/315 (72%)	1.63	62 (27%) 1 1	33, 62, 87, 122	0
1	L	229/315 (72%)	3.27	88 (38%) 0 0	50, 87, 110, 125	0
2	C	1119/1119 (100%)	3.32	446 (39%) 0 0	25, 78, 104, 116	0
2	M	1119/1119 (100%)	2.97	407 (36%) 0 0	23, 72, 104, 115	0
3	D	1381/1524 (90%)	1.95	376 (27%) 1 1	27, 67, 107, 119	0
3	N	1381/1524 (90%)	1.97	386 (27%) 1 1	27, 68, 108, 120	0
4	E	95/99 (95%)	1.99	29 (30%) 1 1	44, 81, 108, 128	0
4	O	95/99 (95%)	2.07	33 (34%) 0 0	44, 75, 93, 105	0
5	F	345/423 (81%)	3.70	149 (43%) 0 0	55, 84, 107, 122	0
5	P	345/423 (81%)	3.21	130 (37%) 0 0	62, 84, 108, 116	0
All	All	6796/7590 (89%)	2.58	2252 (33%) 0 1	23, 73, 106, 128	0

The worst 5 of 2252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	405	ASP	73.9
3	N	406	ASP	59.6
1	A	1	MET	56.9
3	D	853	VAL	54.9
3	N	407	VAL	50.9

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
6	STD	N	8002	43/43	0.76	0.15	0.05	27,35,41,48	0
6	STD	D	8001	43/43	0.86	0.13	-0.38	25,35,40,43	0
7	ZN	N	7413	1/1	0.99	0.11	-0.94	65,65,65,65	0
7	ZN	D	7412	1/1	0.99	0.06	-1.46	58,58,58,58	0
7	ZN	N	7459	1/1	0.95	0.10	-1.63	64,64,64,64	0
7	ZN	D	7458	1/1	0.99	0.09	-2.30	64,64,64,64	0
8	MG	D	9001	1/1	0.94	0.19	-	29,29,29,29	0
8	MG	N	9002	1/1	0.88	0.51	-	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.