



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:55 PM GMT

PDB ID : 4YLO
Title : E. coli Transcription Initiation Complex - 16-bp spacer and 4-nt RNA
Authors : Zuo, Y.; Steitz, T.A.
Deposited on : 2015-03-05
Resolution : 6.00 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 (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

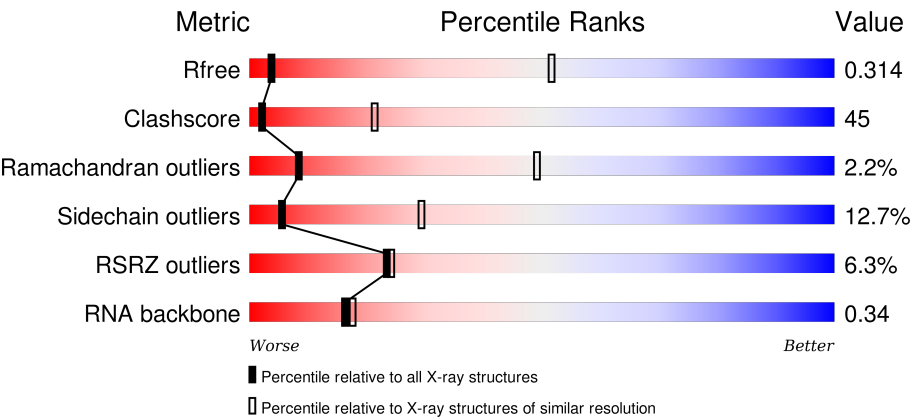
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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))
R_{free}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)
RNA backbone	2183	1103 (8.70-2.80)

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	242	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>47%40%8%5%</div></div>
1	B	242	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>41%47%6%6%</div></div>
1	G	242	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>41%48%7%5%</div></div>
1	H	242	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>45%44%5%6%</div></div>

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Mol	Chain	Length	Quality of chain
1	M	242	
1	N	242	
2	C	1342	
2	I	1342	
2	O	1342	
3	D	1407	
3	J	1407	
3	P	1407	
4	E	90	
4	K	90	
4	Q	90	
5	F	628	
5	L	628	
5	R	628	
6	1	49	
6	4	49	
6	7	49	
7	2	49	
7	5	49	
7	8	49	
8	3	4	
8	6	4	
8	9	4	

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
10	ZN	D	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94608 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	B	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	G	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	H	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	M	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	N	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP A7ZSI4
A	-5	HIS	-	expression tag	UNP A7ZSI4
A	-4	HIS	-	expression tag	UNP A7ZSI4
A	-3	HIS	-	expression tag	UNP A7ZSI4
A	-2	HIS	-	expression tag	UNP A7ZSI4
A	-1	HIS	-	expression tag	UNP A7ZSI4
A	0	HIS	-	expression tag	UNP A7ZSI4
B	-6	ALA	-	expression tag	UNP A7ZSI4
B	-5	HIS	-	expression tag	UNP A7ZSI4
B	-4	HIS	-	expression tag	UNP A7ZSI4
B	-3	HIS	-	expression tag	UNP A7ZSI4
B	-2	HIS	-	expression tag	UNP A7ZSI4
B	-1	HIS	-	expression tag	UNP A7ZSI4
B	0	HIS	-	expression tag	UNP A7ZSI4
G	-6	ALA	-	expression tag	UNP A7ZSI4
G	-5	HIS	-	expression tag	UNP A7ZSI4
G	-4	HIS	-	expression tag	UNP A7ZSI4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	HIS	-	expression tag	UNP A7ZSI4
G	-2	HIS	-	expression tag	UNP A7ZSI4
G	-1	HIS	-	expression tag	UNP A7ZSI4
G	0	HIS	-	expression tag	UNP A7ZSI4
H	-6	ALA	-	expression tag	UNP A7ZSI4
H	-5	HIS	-	expression tag	UNP A7ZSI4
H	-4	HIS	-	expression tag	UNP A7ZSI4
H	-3	HIS	-	expression tag	UNP A7ZSI4
H	-2	HIS	-	expression tag	UNP A7ZSI4
H	-1	HIS	-	expression tag	UNP A7ZSI4
H	0	HIS	-	expression tag	UNP A7ZSI4
M	-6	ALA	-	expression tag	UNP A7ZSI4
M	-5	HIS	-	expression tag	UNP A7ZSI4
M	-4	HIS	-	expression tag	UNP A7ZSI4
M	-3	HIS	-	expression tag	UNP A7ZSI4
M	-2	HIS	-	expression tag	UNP A7ZSI4
M	-1	HIS	-	expression tag	UNP A7ZSI4
M	0	HIS	-	expression tag	UNP A7ZSI4
N	-6	ALA	-	expression tag	UNP A7ZSI4
N	-5	HIS	-	expression tag	UNP A7ZSI4
N	-4	HIS	-	expression tag	UNP A7ZSI4
N	-3	HIS	-	expression tag	UNP A7ZSI4
N	-2	HIS	-	expression tag	UNP A7ZSI4
N	-1	HIS	-	expression tag	UNP A7ZSI4
N	0	HIS	-	expression tag	UNP A7ZSI4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			
2	I	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			
2	O	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			
3	P	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	K	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	Q	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			
5	L	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			
5	R	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	THR	-	expression tag	UNP P00579
L	-14	MET	-	expression tag	UNP P00579
L	-13	ARG	-	expression tag	UNP P00579
L	-12	GLY	-	expression tag	UNP P00579
L	-11	SER	-	expression tag	UNP P00579
L	-10	HIS	-	expression tag	UNP P00579
L	-9	HIS	-	expression tag	UNP P00579
L	-8	HIS	-	expression tag	UNP P00579
L	-7	HIS	-	expression tag	UNP P00579
L	-6	HIS	-	expression tag	UNP P00579
L	-5	HIS	-	expression tag	UNP P00579
L	-4	THR	-	expression tag	UNP P00579
L	-3	ASP	-	expression tag	UNP P00579
L	-2	GLN	-	expression tag	UNP P00579
L	-1	PHE	-	expression tag	UNP P00579
L	0	THR	-	expression tag	UNP P00579
R	-14	MET	-	expression tag	UNP P00579
R	-13	ARG	-	expression tag	UNP P00579
R	-12	GLY	-	expression tag	UNP P00579
R	-11	SER	-	expression tag	UNP P00579
R	-10	HIS	-	expression tag	UNP P00579
R	-9	HIS	-	expression tag	UNP P00579
R	-8	HIS	-	expression tag	UNP P00579
R	-7	HIS	-	expression tag	UNP P00579
R	-6	HIS	-	expression tag	UNP P00579
R	-5	HIS	-	expression tag	UNP P00579
R	-4	THR	-	expression tag	UNP P00579
R	-3	ASP	-	expression tag	UNP P00579
R	-2	GLN	-	expression tag	UNP P00579
R	-1	PHE	-	expression tag	UNP P00579
R	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a DNA chain called NT strand DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			
6	4	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			
6	7	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			

- Molecule 7 is a DNA chain called T strand DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	2	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			
7	5	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			
7	8	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			

- Molecule 8 is a RNA chain called RNA (5'-D*(GTP))-R(P*AP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	6	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	9	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	1	Total	Mg	0	0
			1	1		
9	J	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		

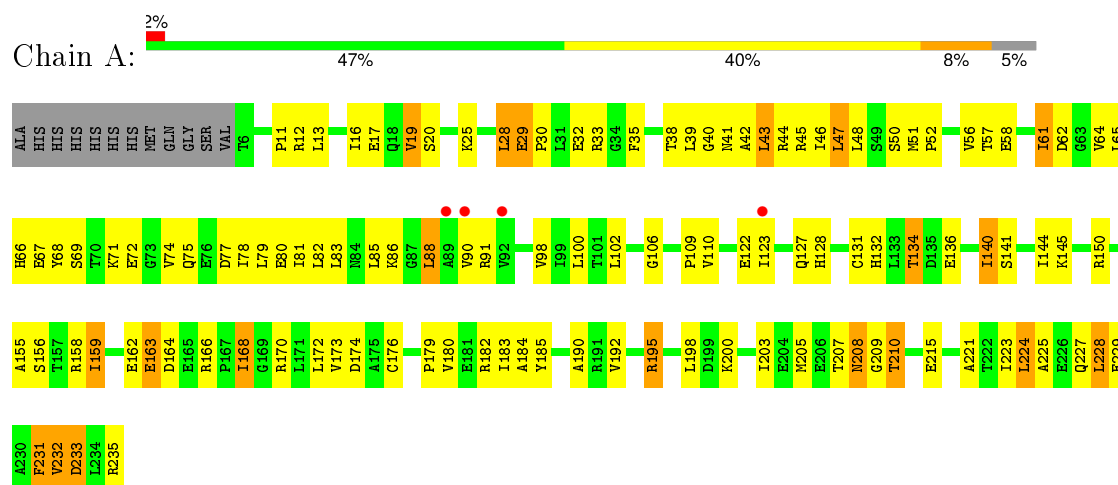
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	2	Total	Zn	0	0
			2	2		
10	J	2	Total	Zn	0	0
			2	2		
10	D	2	Total	Zn	0	0
			2	2		

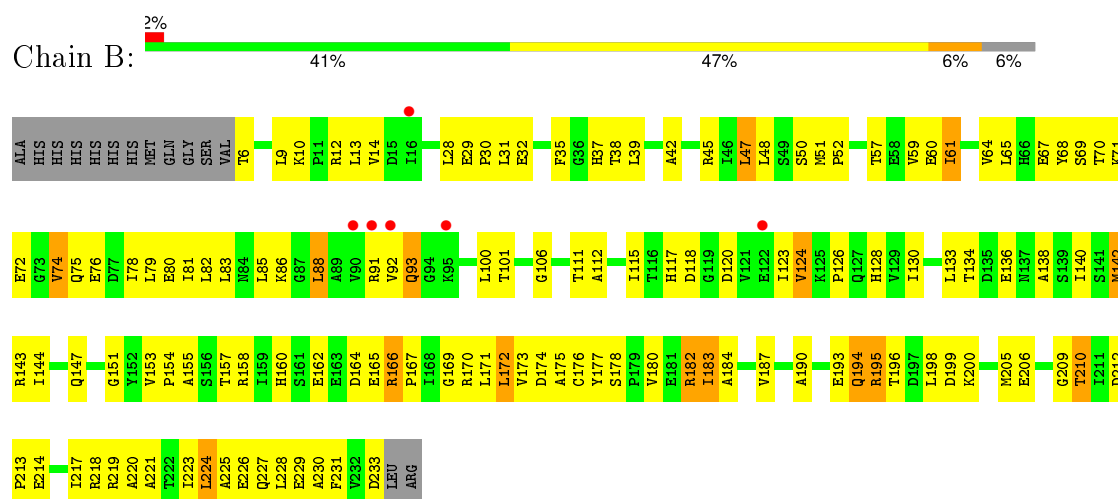
3 Residue-property plots

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.

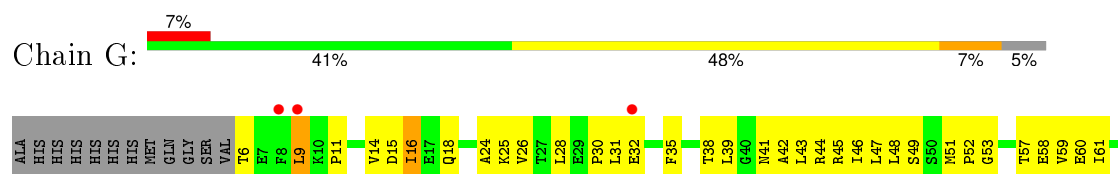
• Molecule 1: DNA-directed RNA polymerase subunit alpha

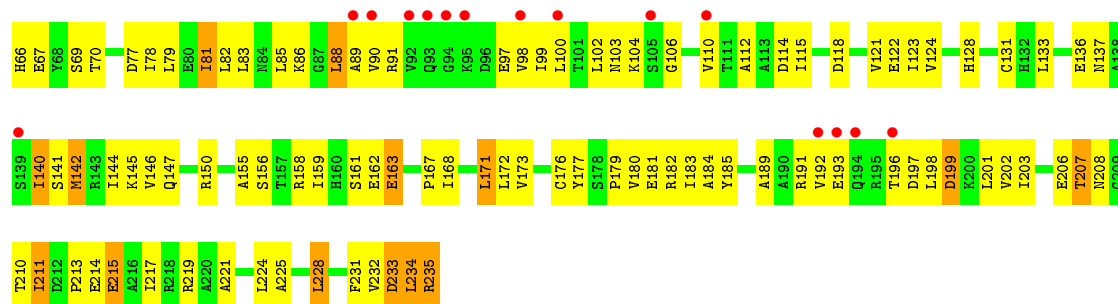


• Molecule 1: DNA-directed RNA polymerase subunit alpha

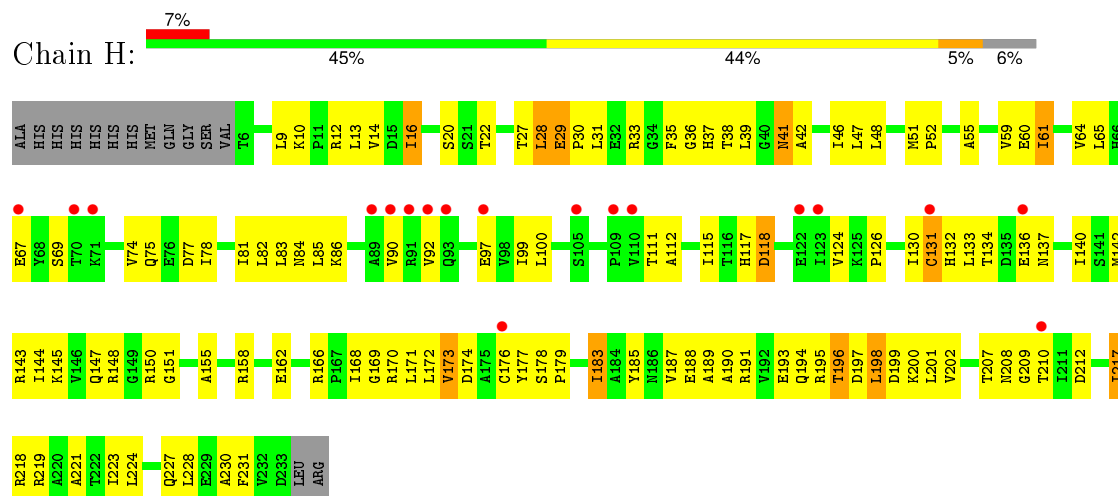


• Molecule 1: DNA-directed RNA polymerase subunit alpha

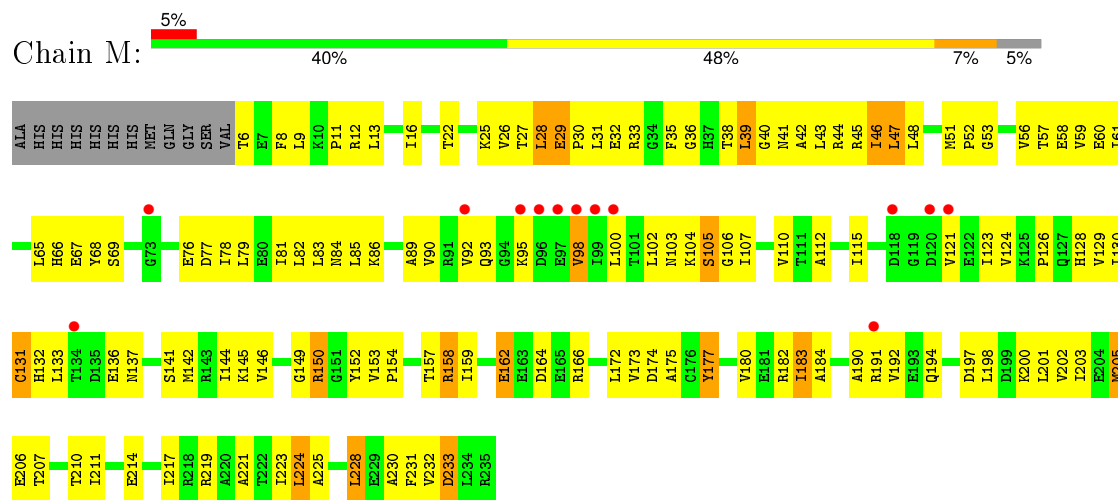




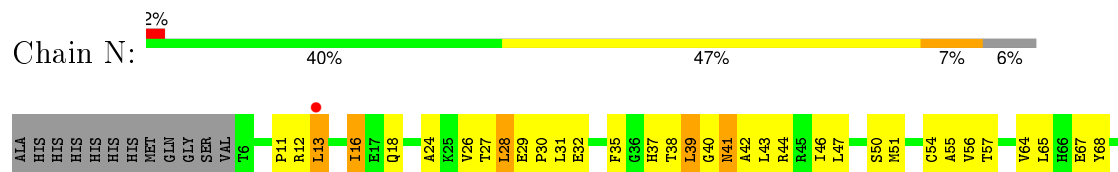
• Molecule 1: DNA-directed RNA polymerase subunit alpha

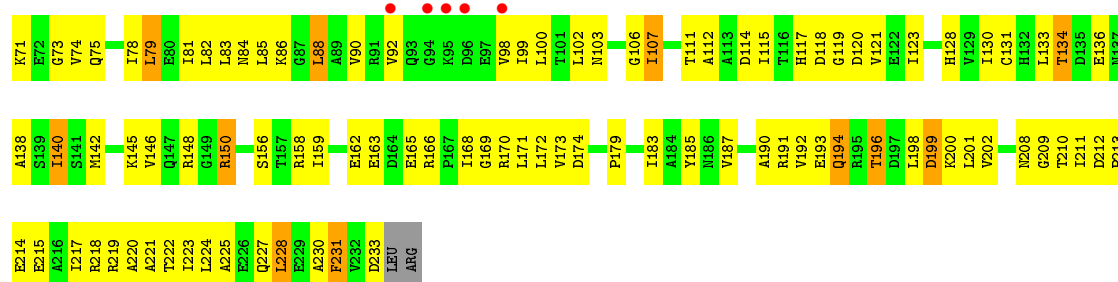


• Molecule 1: DNA-directed RNA polymerase subunit alpha

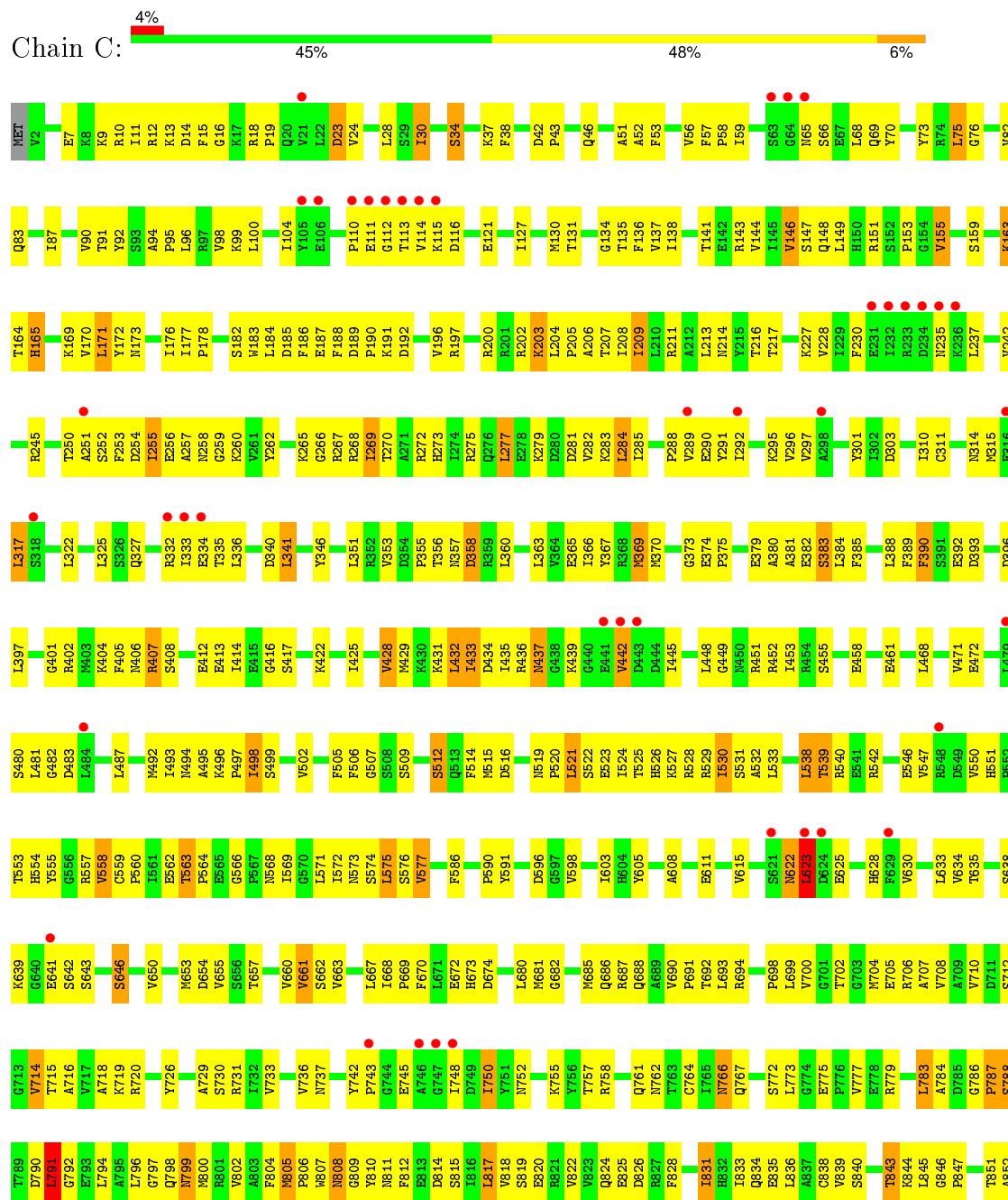


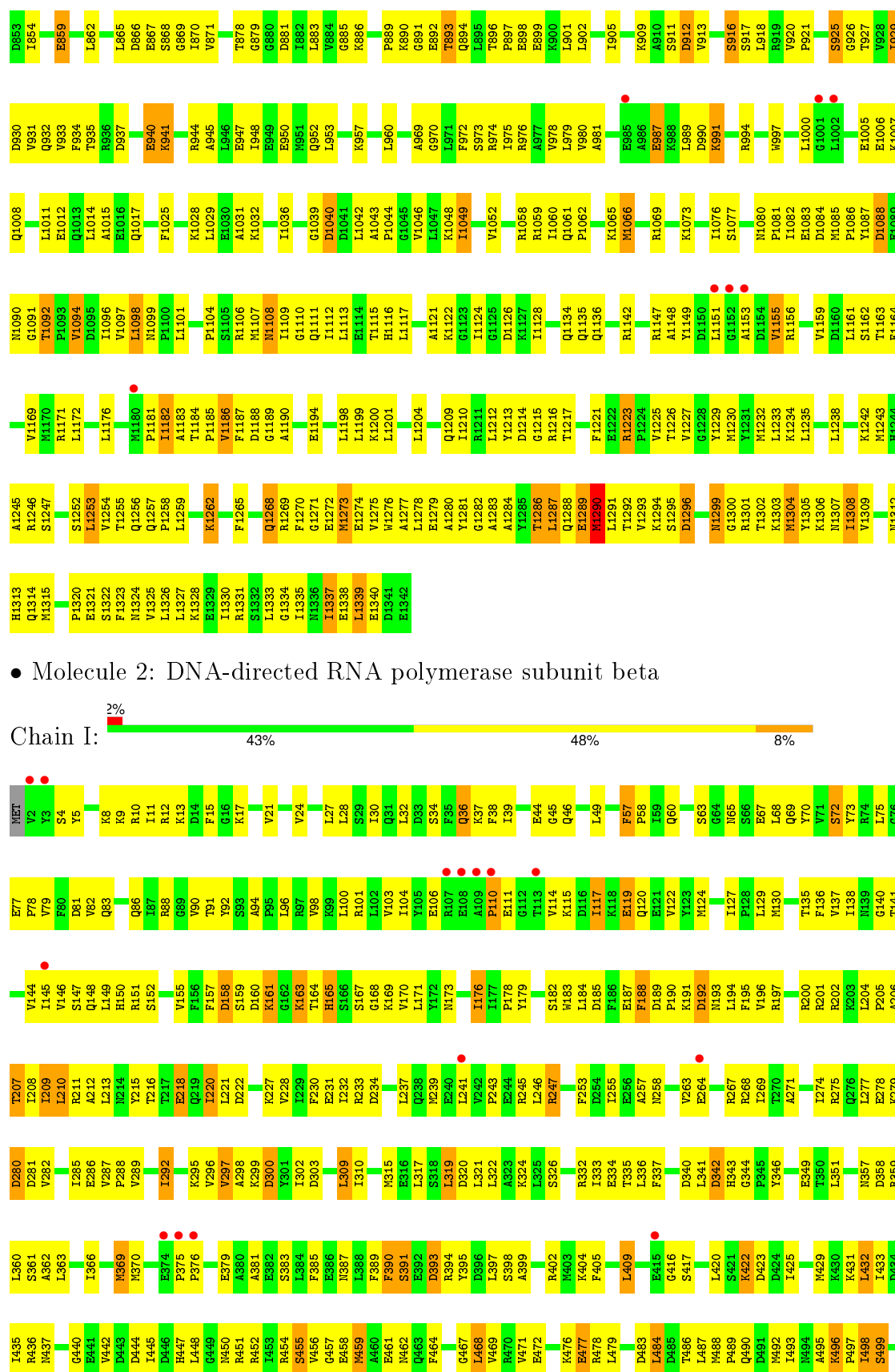
• Molecule 1: DNA-directed RNA polymerase subunit alpha

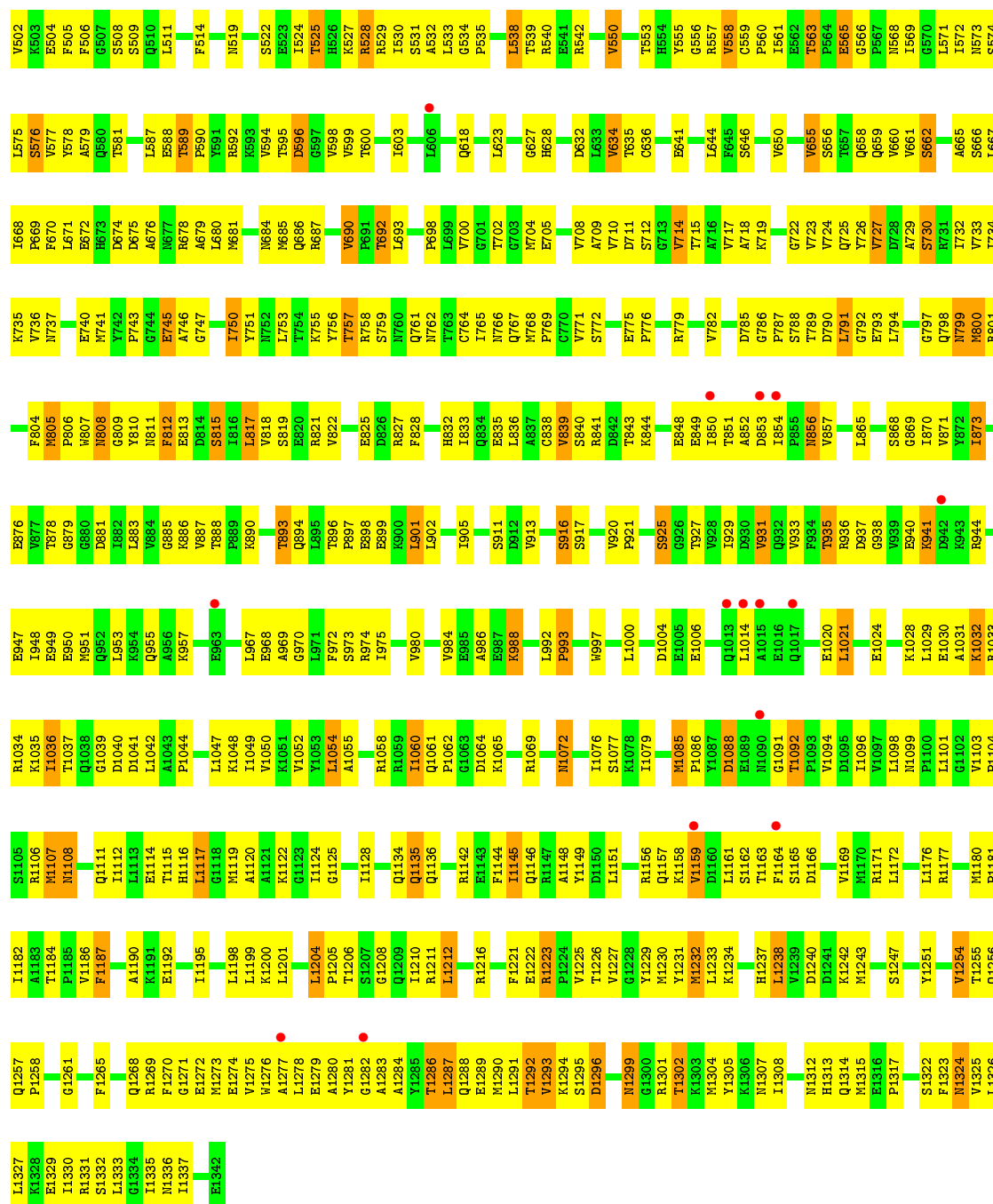




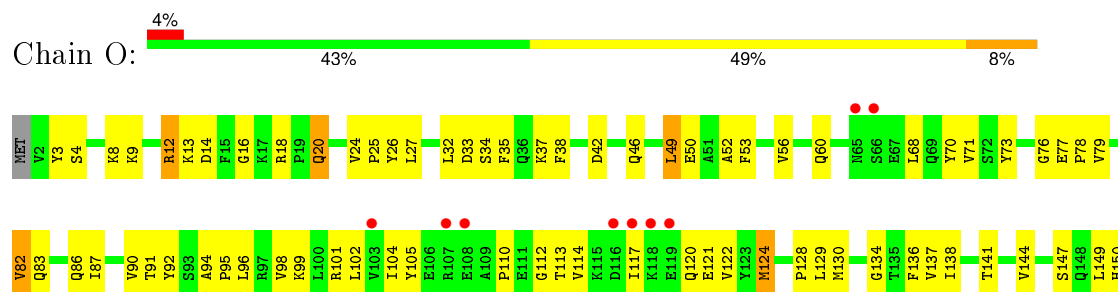
• Molecule 2: DNA-directed RNA polymerase subunit beta



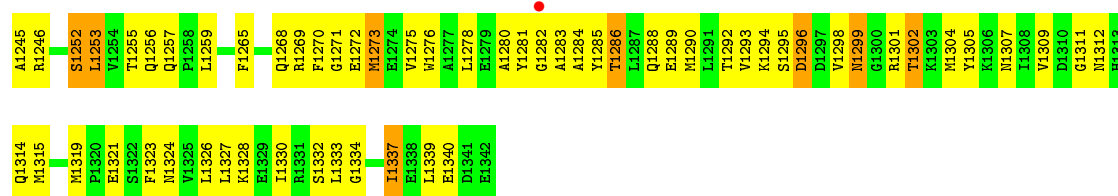




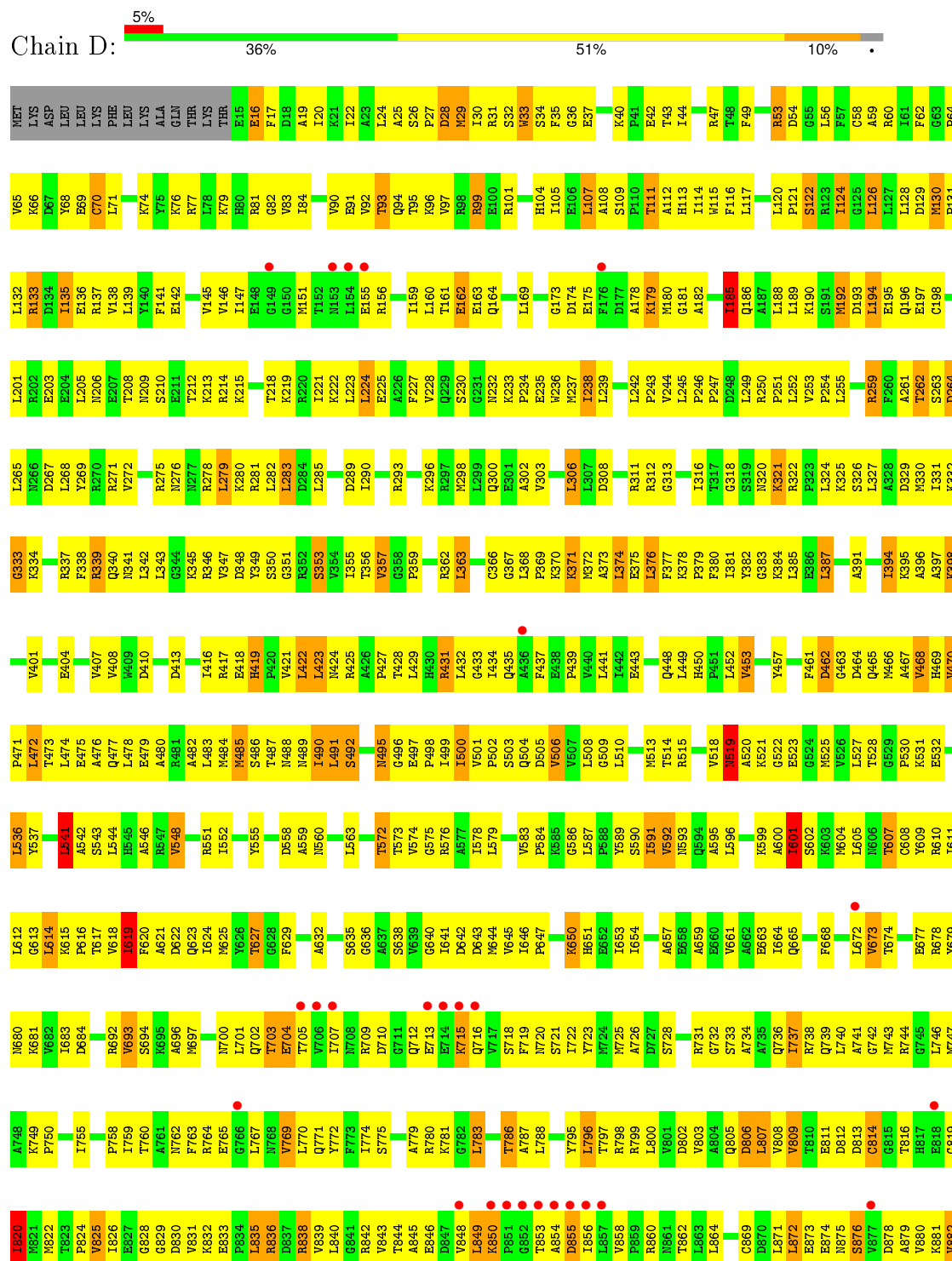
• Molecule 2: DNA-directed RNA polymerase subunit beta



E1174	H1099	L1014	T985	N856	G792	Q858	A579	F505	V428	V353	E286	N214	R151
H1175	P1100	L1017	R936	E859	E793	Q859	E583	S509	M429	D394	V287	Y215	S152
L1176	L1101	Q1017	D937	L862	L794	V660	V584	K431	K430	P356	P288	T216	P153
K1178	P1103	D1018	D942	L865	L796	V661	G585	L432	L433	P357	V289	T217	G154
H1179	H1019	H1020	K943	D866	G797	S662	F586	M514	L434	D358	L292	E218	V155
H1180	S1105	L1021	R944	D867	G798	G664	L587	M515	D434	P358	A293	F157	F156
P1181	R1106	L1022	A945	E867	N799	A685	P590	N519	I435	L363	G294	E225	F157
H1182	M1107	F1024	L946	S868	M800	S666	P590	F520	R436	L366	K296	E226	D156
A1183	N1108	F1025	E947	G869	R801	L687	V591	S521	N437	I366	K297	E227	K161
T1184	F1109	K1025	L948	R802	V802	I688	S592	L522	L437	V367	V296	I229	G162
P1185	E949	K1026	R803	I870	A803	P669	K593	E523	D443	R368	A298	E230	K163
H1186	E950	F804	F804	V871	F804	P670	T525	I524	D444	R369	K299	E231	T164
F1187	A951	M805	M805	E872	M805	L671	T525	T525	I445	H370	I232	I232	H165
D1188	Q952	P806	P806	E672	V599	H672	H526	H526	D446	R371	I302	R233	S166
G1189	L953	M807	M807	H673	T600	E673	E527	E527	H447	P372	D303	R234	S167
A1190	K954	N808	N808	D674	I603	D674	R528	R528	L448	G373	E304	R235	G168
H1195	Q955	G809	G809	D675	H604	D675	R529	R529	G449	G374	S305	R236	K169
L1197	A956	V810	V810	A676	H605	A676	I530	I530	N450	P375	T306	L237	V170
L1198	K957	N811	N811	M677	V605	M677	L533	L533	R451	P376	G307	Q238	L171
A1120	L960	F812	F812	R678	L606	R678	E537	E537	R452	T377	I310	R239	V172
G1123	L964	E813	E813	R679	A608	A679	G537	G537	I453	R378	C311	E240	N173
T1124	L965	D814	D814	L680	I609	L680	L538	L538	R454	E379	A312	V242	I177
H1125	Q965	S815	S815	A746	E610	A746	R540	R540	S455	P385	A313	R245	P178
D1126	L966	L817	L817	D749	A683	D749	E541	E541	M459	F389	N314	R246	Y179
K1127	L967	V818	V818	M753	N884	M753	E542	E542	F464	F390	K315	R247	R180
R1128	E968	N819	N819	L753	M885	L753	R541	R541	G467	S391	E316	R247	G181
M1129	A969	R820	R820	Y756	Q688	Y756	E546	E546	L468	G391	L317	A251	S182
A1130	G970	R821	R821	Y757	Q688	Y757	R547	R547	L468	S391	S318	S252	V183
M1131	L971	V822	V822	R758	A889	R758	R548	R548	L469	Y395	L319	F253	L184
L1132	F972	G823	G823	S759	R690	S759	R549	R549	R470	D396	D320	R253	D185
K1133	S973	R824	R824	M760	E625	M760	E551	E551	E471	L397	L322	I255	F186
G1134	R974	E825	E825	Q761	R891	Q761	R551	R551	V472	L397	A322	R260	S187
E1135	R975	D826	D826	Q762	R892	Q762	E551	E551	R402	M403	K324	K260	F188
R1136	R976	R827	R827	N762	L693	N762	E554	E554	M404	D189	L325	V261	D189
F1137	A977	F828	F828	T763	G627	T763	R554	R554	K476	K403	L326	Y262	P190
G1073	L978	T829	T829	G764	D896	G764	R557	R557	L481	K404	S326	Y262	K191
L1074	L978	R830	R830	I765	K697	I765	V558	V558	Q482	F405	K331	V263	D192
V1075	L979	I831	I831	N766	P898	N766	C559	C559	D483	M406	R332	E264	I193
S1077	A981	H832	H832	Q767	L693	Q767	P560	P560	L484	R407	I333	R265	L194
K1078	E985	I833	I833	Q767	V700	V700	I561	I561	D465	S408	E334	Q266	F195
P1081	L982	D834	D834	V771	G701	G701	S642	S642	I493	L409	T335	I269	V196
I1082	L982	E835	E835	S772	T702	T702	S643	S643	M494	L410	L336	T270	R197
E1083	P993	L836	L836	L773	G703	G703	L644	L644	P499	R411	F337	A271	I198
D1084	R994	C838	C838	V777	M704	M704	D711	D711	Q490	E412	R337	R272	D199
L1085	D995	V839	V839	E778	E705	E705	S638	S638	D491	E413	T338	H273	R200
P1086	R996	K914	K914	R779	R706	R706	R639	R639	M492	I414	R339	H273	R201
Y1087	K997	S840	S840	R779	A707	A707	S642	S642	I493	E415	I333	I274	R202
D1088	L1000	T843	T843	V782	V708	V708	S643	S643	M494	G416	E334	R275	K203
G1091	G1001	R844	R844	L783	A709	A709	S643	S643	M494	I419	D342	Q276	L204
D1092	L1002	D711	D711	L783	V710	V710	L644	L644	A495	R419	H343	L277	P205
P1093	T1003	E848	E848	D785	A784	A784	L644	L644	K496	L420	G344	E278	A206
V1094	D1004	T851	T851	G787	S712	S712	R647	R647	P497	S421	P345	R279	T207
D1095	E1005	A852	A852	S788	T715	T715	V652	V652	S499	K422	Y346	D280	I208
I1096	E1006	D853	D853	S788	A716	A716	M653	M653	A500	D424	I347	D281	I209
V1097	I929	R854	R854	T789	K719	K719	S656	S656	A501	I425	S348	V282	L210
L1098	L1011	P855	P855	R790	R719	R719	S656	S656	E504	V577	T350	K283	R211
				L791	R720	R720	T657	T657				I285	A212



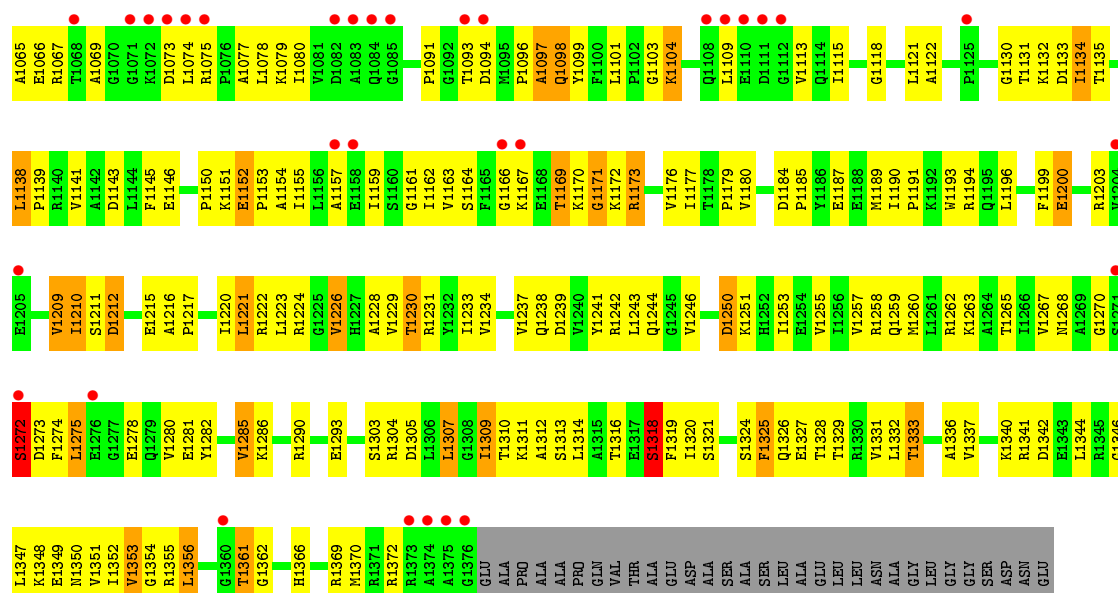
• Molecule 3: DNA-directed RNA polymerase subunit beta'





ALA	V1331	A1264	V1198	T1131	E1066	Y995	P926	T862	R798	M724	K650	V580	V506	V440
GLU	L1332	T1265	F1199	K1132	R1067	Y996	G927	L863	R799	M725	K650	M581	V507	L441
LEU	T1333	L1266	E1200	T1068	A1069	Y997	T928	L864	L801	G732	A657	I582	L508	I442
LEU	E1334	V1267	A1069	P998	P998	Y998	Q929	H865	R800	G732	A657	V583	G509	E443
ASN	V1337	A1268	R1203	L1138	G1071	Y999	L930	E866	V803	Q736	E658	P584	L510	G444
ALA	A1338	A1269	V1204	P1139	G1072	A1001	Y932	H868	Q805	I737	E659	K445	Y511	K445
GLY	A1339	G1270	E1205	P1140	D1073	V1002	Y935	H869	A804	I737	E660	G586	V512	I446
LEU	K1340	S1271	R1206	L1074	L1074	K1005	F935	D870	Q806	K738	A662	L587	M513	I447
GLY	D1273	D1208	D1208	L1144	P1075	G1006	A940	C869	L807	L740	Q665	P588	T514	Q448
SER	F1274	F1209	F1209	F1145	P1076	D1007	A941	D870	V808	A741	Q665	Y589	D516	H450
GLY	L1275	L1210	L1210	A1146	A1077	E1008	S942	D870	L807	G742	Q665	S590	C517	P451
ASP	E1278	R1148	D1212	A1147	K1078	E1009	S943	D870	V809	G743	S670	I581	V518	L452
ASN	G1279	P1153	P1217	P1153	A1083	E1010	S944	D870	T810	M743	S671	V592	M519	V453
GLU	G1280	A1154	H1218	A1154	Q1084	E1011	S945	D870	E811	K744	G671	I593	A520	Y457
GLY	E1281	I1155	H1219	I1155	G1085	E1012	S946	D870	D812	G745	G671	Q594	E523	Y458
GLY	E1282	L1156	I1220	L1156	N1086	E1013	S947	D870	L812	G746	V673	I594	E523	A459
GLY	E1283	E1157	L1221	E1157	D1087	E1014	S948	D870	C814	M747	V674	L596	E523	A460
GLY	E1284	E1158	L1222	E1158	V1088	E1015	S949	D870	G815	G748	A675	L596	E523	A461
GLY	E1285	E1159	L1223	E1159	L1089	E1016	S950	D870	T816	K749	G676	K599	V526	D460
GLY	E1286	E1160	G1224	E1160	P1091	E1017	S951	D870	H817	P750	Y679	A600	V526	F461
GLY	E1287	E1161	G1225	E1161	D1094	E1018	S952	D870	R821	S753	Y679	I601	P530	F462
GLY	E1288	E1162	H1226	E1162	Q1095	E1019	S953	D870	M822	M762	N690	S602	P530	A463
GLY	E1289	E1163	H1227	E1163	P1096	E1020	S954	D870	R823	M763	N690	K531	P530	A464
GLY	E1290	E1164	H1228	E1164	A1097	E1021	S955	D870	P824	M764	N690	K603	P530	A465
GLY	E1291	E1165	H1229	E1165	Q1098	E1022	S956	D870	R825	M765	N690	M604	P530	A466
GLY	E1292	E1166	H1230	E1166	Y1099	E1023	S957	D870	R826	M766	N690	L605	P530	A467
GLY	E1293	E1167	H1231	E1167	F1100	E1024	S958	D870	R827	M767	N690	K606	P530	A468
GLY	E1294	E1168	H1232	E1168	L1101	E1025	S959	D870	R828	M768	N690	L607	P530	A469
GLY	E1295	E1169	H1233	E1169	P1102	E1026	S960	D870	R829	M769	N690	L608	P530	A470
GLY	E1296	E1170	H1234	E1170	G1103	E1027	S961	D870	R830	M770	N690	V618	P530	A471
GLY	E1297	E1171	H1235	E1171	K1104	E1028	S962	D870	R831	M771	N690	I619	P530	A472
GLY	E1298	E1172	H1236	E1172	A1105	E1029	S963	D870	R832	M772	N690	F620	P530	A473
GLY	E1299	E1173	H1237	E1173	A1106	E1030	S964	D870	R833	M773	N690	A621	P530	A474
GLY	E1300	E1174	H1238	E1174	V1107	E1031	S965	D870	R834	M774	N690	D622	P530	A475
GLY	E1301	E1175	H1239	E1175	Q1108	E1032	S966	D870	R835	M775	N690	Y555	P530	A476
GLY	E1302	E1176	H1240	E1176	L1109	E1033	S967	D870	R836	M776	N690	I624	P530	A477
GLY	E1303	E1177	H1241	E1177	V1113	E1034	S968	D870	R837	M777	N690	I624	P530	A478
GLY	E1304	E1178	H1242	E1178	Q1114	E1035	S969	D870	R838	M778	N690	T627	P530	A479
GLY	E1305	E1179	H1243	E1179	I1115	E1036	S970	D870	R839	M779	N690	G628	P530	A480
GLY	E1306	E1180	H1244	E1180	S1116	E1037	S971	D870	R840	M780	N690	F629	P530	A481
GLY	E1307	E1181	H1245	E1181	S1117	E1038	S972	D870	R841	M781	N690	G561	P530	A482
GLY	E1308	E1182	H1246	E1182	S1118	E1039	S973	D870	R842	M782	N690	L562	P530	A483
GLY	E1309	E1183	H1247	E1183	S1119	E1040	S974	D870	R843	M783	N690	L563	P530	A484
GLY	E1310	E1184	H1248	E1184	S1120	E1041	S975	D870	R844	M784	N690	A632	P530	A485
GLY	E1311	E1185	H1249	E1185	S1121	E1042	S976	D870	R845	M785	N690	A633	P530	A486
GLY	E1312	E1186	H1250	E1186	S1122	E1043	S977	D870	R846	M786	N690	A634	P530	A487
GLY	E1313	E1187	H1251	E1187	S1123	E1044	S978	D870	R847	M787	N690	A635	P530	A488
GLY	E1314	E1188	H1252	E1188	S1124	E1045	S979	D870	R848	M788	N690	A636	P530	A489
GLY	E1315	E1189	H1253	E1189	S1125	E1046	S980	D870	R849	M789	N690	A637	P530	A490
GLY	E1316	E1190	H1254	E1190	S1126	E1047	S981	D870	R850	M790	N690	A638	P530	A491
GLY	E1317	E1191	H1255	E1191	S1127	E1048	S982	D870	R851	M791	N690	A639	P530	A492
GLY	E1318	E1192	H1256	E1192	S1128	E1049	S983	D870	R852	M792	N690	A640	P530	A493
GLY	E1319	E1193	H1257	E1193	S1129	E1050	S984	D870	R853	M793	N690	A641	P530	A494
GLY	E1320	E1194	H1258	E1194	S1130	E1051	S985	D870	R854	M794	N690	A642	P530	A495
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GLY	E1322	E1196	H1260	E1196	S1132	E1053	S987	D870	R856	M796	N690	A644	P530	A497
GLY	E1323	E1197	H1261	E1197	S1133	E1054	S988	D870	R857	M797	N690	A645	P530	A498
GLY	E1324	E1198	H1262	E1198	S1134	E1055	S989	D870	R858	M798	N690	A646	P530	A499
GLY	E1325	E1199	H1263	E1199	S1135	E1056	S990	D870	R859	M799	N690	A647	P530	A500
GLY	E1326	E1200	H1264	E1200	S1136	E1057	S991	D870	R860	M800	N690	A648	P530	A501
GLY	E1327	E1201	H1265	E1201	S1137	E1058	S992	D870	R861	M801	N690	A649	P530	A502
GLY	E1328	E1202	H1266	E1202	S1138	E1059	S993	D870	R862	M802	N690	A650	P530	A503
GLY	E1329	E1203	H1267	E1203	S1139	E1060	S994	D870	R863	M803	N690	A651	P530	A504
GLY	E1330	E1204	H1268	E1204	S1140	E1061	S995	D870	R864	M804	N690	A652	P530	A505
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GLY	E1334	E1208	H1272	E1208	S1144	E1065	S999	D870	R868	M808	N690	A656	P530	A509
GLY	E1335	E1209	H1273	E1209	S1145	E1066	S1000	D870	R869	M809	N690	A657	P530	A510
GLY	E1336	E1210	H1274	E1210	S1146	E1067	S1001	D870	R870	M810	N690	A658	P530	A511
GLY	E1337	E1211	H1275	E1211	S1147	E1068	S1002	D870	R871	M811	N690	A659	P530	A512
GLY	E1338	E1212	H1276	E1212	S1148	E1069	S1003	D870	R872	M812	N690	A660	P530	A513
GLY	E1339	E1213	H1277	E1213	S1149	E1070	S1004	D870	R873	M813	N690	A661	P530	A514
GLY	E1340	E1214	H1278	E1214	S1150	E1071	S1005	D870	R874	M814	N690	A662	P530	A515
GLY	E1341	E1215	H1279	E1215	S1151	E1072	S1006	D870	R875	M815	N690	A663	P530	A516
GLY	E1342	E1216	H1280	E1216	S1152	E1073	S1007	D870	R876	M816	N690	A664	P530	A517
GLY	E1343	E1217	H1281	E1217	S1153	E1074	S1008	D870	R877	M817	N690	A665	P530	A518
GLY	E1344	E1218	H1282	E1218	S1154	E1075	S1009	D870	R878	M818	N690	A666	P530	A519
GLY	E1345	E1219	H1283	E1219	S1155	E1076	S1010	D870	R879	M819	N690	A667	P530	A520
GLY	E1346	E1220	H1284	E1220	S1156	E1077	S1011	D870	R880	M820	N690	A668	P530	A521
GLY	E1347	E1221	H1285	E1221	S1157	E1078	S1012	D870	R881	M821	N690	A669	P530	A522
GLY	E1348	E1222	H1286	E1222	S1158	E1079	S1013	D870	R882	M822	N690	A670	P530	A523
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GLY	E1350	E1224	H1288	E1224	S1160	E1081	S1015	D870	R884	M824	N690	A672	P530	A525
GLY	E1351	E1225	H1289	E1225	S1161	E1082	S1016	D870	R885	M825	N690	A673	P530	A526
GLY	E1352	E1226	H1290	E1226	S1162	E1083	S1017	D870	R886	M826	N690	A674	P530	A527
GLY	E1353	E1227	H1291	E1227	S1163	E1084	S1018	D870	R887	M827	N690	A675	P530	A528
GLY	E1354	E1228	H1292	E1228	S1164	E1085	S1019	D870	R888	M828	N690	A676	P530	A529
GLY	E1355	E1229	H1293	E1229	S1165	E1086	S1020	D870	R889	M829	N690	A677	P530	A530
GLY	E1356	E1230	H1294	E1230	S1166	E1087	S1021	D870	R890	M830	N690	A678	P530	A531
GLY	E1357	E1231	H1295	E1231	S1167	E1088	S1022	D870	R891	M831	N690	A679	P530	A532
GLY	E1358	E1232	H1296	E1232	S1168	E1089	S1023	D870	R892	M832	N690	A680	P530	A533
GLY	E1359	E1233	H1297	E1233	S1169	E1090	S1024	D870	R893	M833	N690	A681	P530	A534
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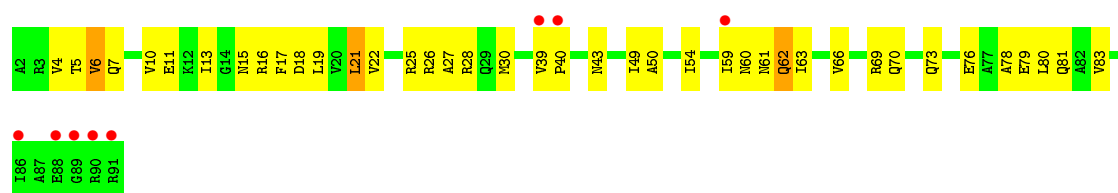




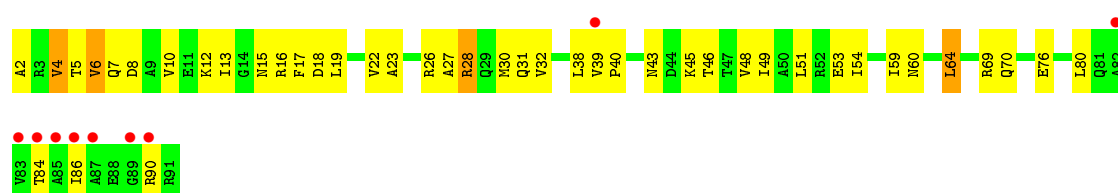
• Molecule 4: DNA-directed RNA polymerase subunit omega



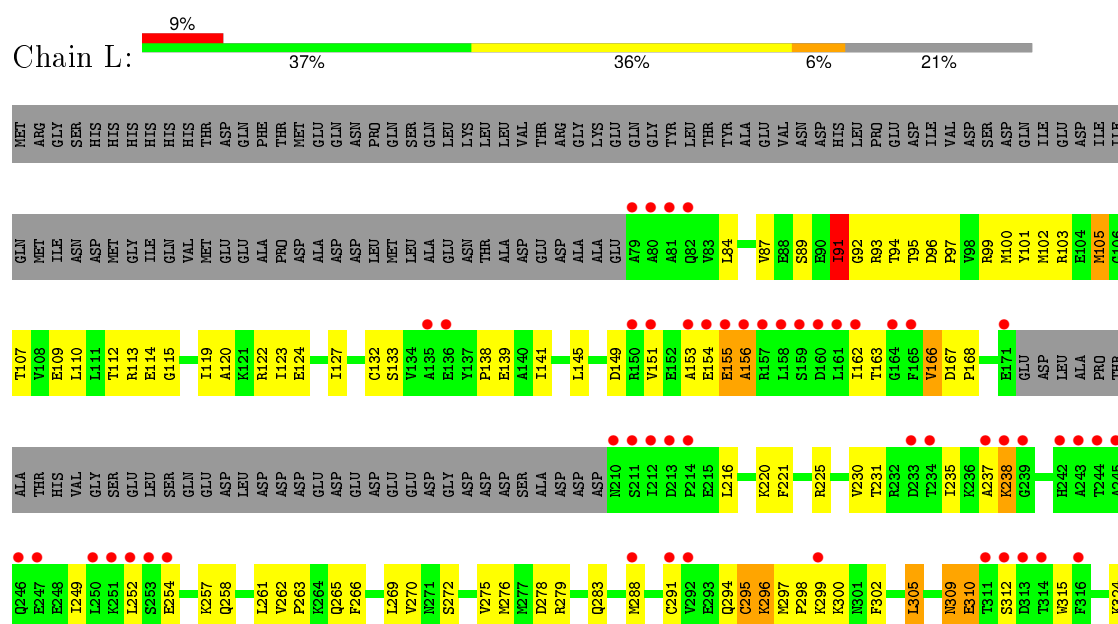
• Molecule 4: DNA-directed RNA polymerase subunit omega

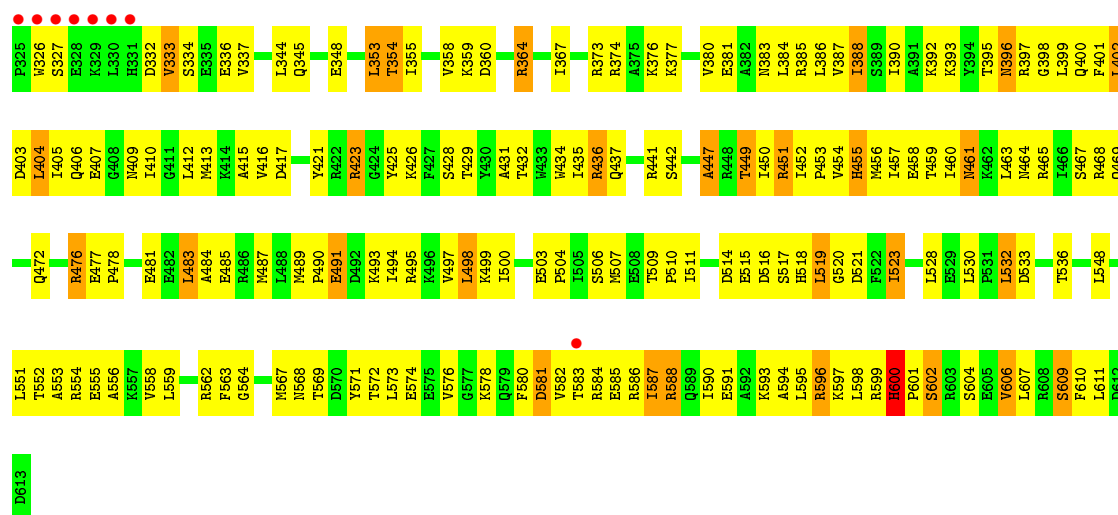


• Molecule 4: DNA-directed RNA polymerase subunit omega

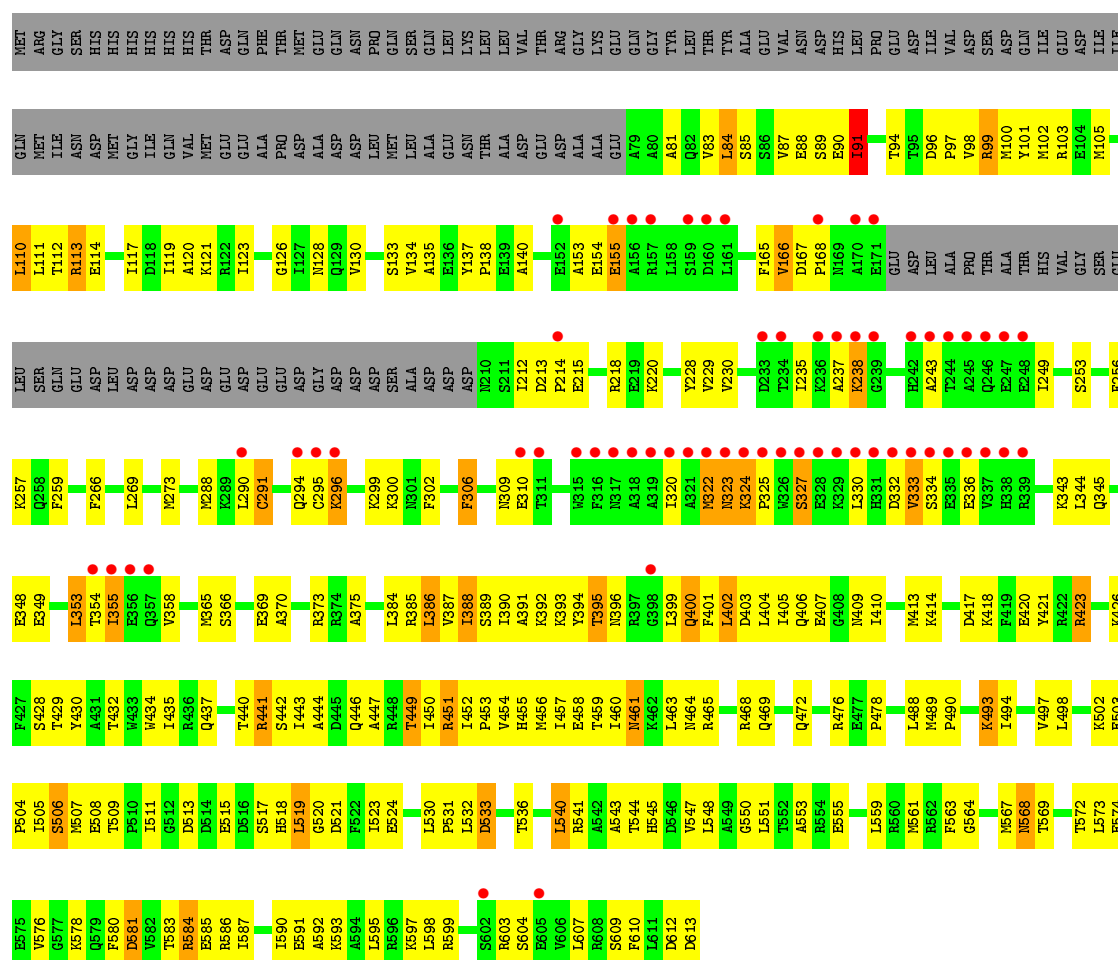


• Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 6: NT strand DNA (49-MER)

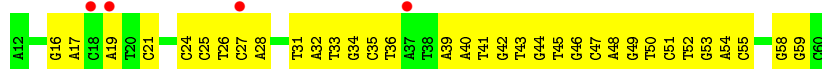




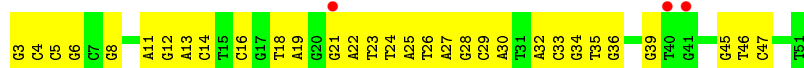
- Molecule 6: NT strand DNA (49-MER)



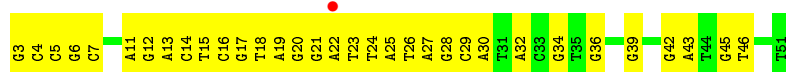
- Molecule 6: NT strand DNA (49-MER)



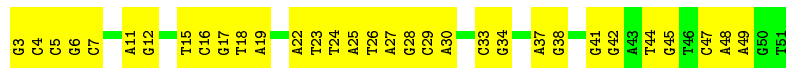
- Molecule 7: T strand DNA (49-MER)



- Molecule 7: T strand DNA (49-MER)



- Molecule 7: T strand DNA (49-MER)



- Molecule 8: RNA (5'-D*(GTP))-R(P*AP*GP*U)-3')



- Molecule 8: RNA (5'-D*(GTP))-R(P*AP*GP*U)-3')



G13
A14
G15
U16

- Molecule 8: RNA (5'-D(*(GTP))-R(P*AP*GP*U)-3')

Chain 9:

50%

50%

G13
A14
G15
U16

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	240.89Å 208.17Å 256.32Å 90.00° 119.31° 90.00°	Depositor
Resolution (Å)	39.95 – 6.00 39.95 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.95-6.00) 100.0 (39.95-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 6.13Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.227 , 0.314 0.227 , 0.314	Depositor DCC
R_{free} test set	2938 reflections (5.61%)	DCC
Wilson B-factor (Å ²)	343.5	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 254.0	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 55313 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	94608	wwPDB-VP
Average B, all atoms (Å ²)	238.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: GTP, 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	0.59	0/1809	0.85	2/2450 (0.1%)
1	B	0.57	0/1789	0.84	1/2425 (0.0%)
1	G	0.60	1/1809 (0.1%)	0.83	1/2450 (0.0%)
1	H	0.57	0/1789	0.79	1/2425 (0.0%)
1	M	0.63	0/1809	0.87	2/2450 (0.1%)
1	N	0.60	0/1789	0.87	0/2425
2	C	0.58	3/10745 (0.0%)	0.79	11/14499 (0.1%)
2	I	0.61	3/10745 (0.0%)	0.81	3/14499 (0.0%)
2	O	0.61	4/10745 (0.0%)	0.81	4/14499 (0.0%)
3	D	0.66	3/10729 (0.0%)	0.91	20/14487 (0.1%)
3	J	0.63	2/10729 (0.0%)	0.85	15/14487 (0.1%)
3	P	0.59	4/10729 (0.0%)	0.80	9/14487 (0.1%)
4	E	0.62	0/710	0.89	1/956 (0.1%)
4	K	0.56	0/710	0.72	0/956
4	Q	0.55	0/710	0.74	1/956 (0.1%)
5	F	0.56	2/4076 (0.0%)	0.77	1/5482 (0.0%)
5	L	0.59	0/4076	0.78	2/5482 (0.0%)
5	R	0.55	0/4076	0.77	2/5482 (0.0%)
6	1	0.39	0/1112	0.67	0/1706
6	4	0.51	1/1114 (0.1%)	0.73	0/1714
6	7	0.39	0/1115	0.70	0/1718
7	2	0.38	0/1136	0.66	0/1752
7	5	0.41	0/1137	0.69	0/1756
7	8	0.36	0/1137	0.68	0/1756
8	3	0.33	0/72	0.58	0/110
8	6	0.50	0/72	0.71	0/110
8	9	0.50	0/72	0.65	0/110
All	All	0.59	23/96541 (0.0%)	0.81	76/131629 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
3	P	0	1
All	All	0	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	316	GLU	CD-OE2	13.14	1.40	1.25
3	J	943	ARG	CZ-NH1	11.93	1.48	1.33
3	D	431	ARG	CZ-NH1	11.55	1.48	1.33
2	I	565	GLU	CB-CG	10.38	1.71	1.52
3	P	1152	GLU	CD-OE2	-9.69	1.15	1.25

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	359	LYS	CG-CD-CE	-8.94	85.08	111.90
3	D	431	ARG	NE-CZ-NH2	-8.33	116.13	120.30
3	J	943	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	M	29	GLU	C-N-CD	-7.94	103.14	120.60
3	D	376	LEU	CA-CB-CG	-7.68	97.62	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	943	ARG	Sidechain
3	P	210	SER	Peptide

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	1787	0	1813	190	0
1	B	1767	0	1789	200	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1787	0	1813	179	0
1	H	1767	0	1789	145	0
1	M	1787	0	1813	260	0
1	N	1767	0	1789	213	0
2	C	10576	0	10591	945	0
2	I	10576	0	10591	991	0
2	O	10576	0	10591	1002	1
3	D	10568	0	10781	1353	1
3	J	10568	0	10782	1175	0
3	P	10568	0	10780	1041	1
4	E	708	0	719	65	0
4	K	708	0	719	40	0
4	Q	708	0	719	46	0
5	F	4022	0	4083	368	1
5	L	4022	0	4083	367	0
5	R	4022	0	4083	348	0
6	1	996	0	557	71	0
6	4	996	0	555	103	1
6	7	996	0	554	69	0
7	2	1012	0	554	65	0
7	5	1012	0	553	62	0
7	8	1012	0	553	66	0
8	3	97	0	44	21	0
8	6	97	0	44	6	0
8	9	97	0	44	19	0
9	C	1	0	0	0	0
9	J	1	0	0	0	0
9	P	1	0	0	0	0
10	D	2	0	0	2	0
10	J	2	0	0	2	0
10	P	2	0	0	1	0
All	All	94608	0	92786	8368	3

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 45.

The worst 5 of 8368 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:359:LYS:NZ	5:F:359:LYS:CE	1.67	1.54
3:D:484:MET:CE	3:D:484:MET:SD	2.03	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:139:LEU:CD2	3:P:185:ILE:HD11	1.49	1.43
3:J:367:GLY:O	3:J:447:ILE:CG2	1.68	1.38
1:G:25:LYS:NZ	1:G:202:VAL:HG11	1.34	1.37

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:12:DA:O5'	6:4:60:DC:O5'[2_454]	1.86	0.34
5:F:482:GLU:OE2	2:O:275:ARG:NH2[2_455]	1.99	0.21
3:D:1282:TYR:OH	3:P:710:ASP:OD2[1_655]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/242 (94%)	210 (92%)	15 (7%)	3 (1%)	15	59
1	B	226/242 (93%)	207 (92%)	13 (6%)	6 (3%)	6	44
1	G	228/242 (94%)	211 (92%)	14 (6%)	3 (1%)	15	59
1	H	226/242 (93%)	207 (92%)	17 (8%)	2 (1%)	21	66
1	M	228/242 (94%)	209 (92%)	16 (7%)	3 (1%)	15	59
1	N	226/242 (93%)	207 (92%)	14 (6%)	5 (2%)	8	49
2	C	1339/1342 (100%)	1218 (91%)	98 (7%)	23 (2%)	11	55
2	I	1339/1342 (100%)	1210 (90%)	102 (8%)	27 (2%)	9	51
2	O	1339/1342 (100%)	1222 (91%)	87 (6%)	30 (2%)	8	49
3	D	1360/1407 (97%)	1210 (89%)	122 (9%)	28 (2%)	9	50
3	J	1360/1407 (97%)	1225 (90%)	110 (8%)	25 (2%)	11	53
3	P	1360/1407 (97%)	1208 (89%)	112 (8%)	40 (3%)	6	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	88/90 (98%)	82 (93%)	5 (6%)	1 (1%)	17	63
4	K	88/90 (98%)	83 (94%)	4 (4%)	1 (1%)	17	63
4	Q	88/90 (98%)	81 (92%)	6 (7%)	1 (1%)	17	63
5	F	493/628 (78%)	443 (90%)	34 (7%)	16 (3%)	5	40
5	L	493/628 (78%)	441 (90%)	36 (7%)	16 (3%)	5	40
5	R	493/628 (78%)	441 (90%)	36 (7%)	16 (3%)	5	40
All	All	11202/11853 (94%)	10115 (90%)	841 (8%)	246 (2%)	8	49

5 of 246 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	GLY
1	A	210	THR
2	C	113	THR
2	C	481	LEU
2	C	791	LEU

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	198/208 (95%)	171 (86%)	27 (14%)	5	27
1	B	196/208 (94%)	172 (88%)	24 (12%)	6	31
1	G	198/208 (95%)	169 (85%)	29 (15%)	4	24
1	H	196/208 (94%)	171 (87%)	25 (13%)	5	29
1	M	198/208 (95%)	171 (86%)	27 (14%)	5	27
1	N	196/208 (94%)	167 (85%)	29 (15%)	4	24
2	C	1156/1157 (100%)	1016 (88%)	140 (12%)	6	31
2	I	1156/1157 (100%)	1013 (88%)	143 (12%)	6	30
2	O	1156/1157 (100%)	1019 (88%)	137 (12%)	6	31
3	D	1135/1168 (97%)	968 (85%)	167 (15%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	1135/1168 (97%)	986 (87%)	149 (13%)	5	28
3	P	1135/1168 (97%)	989 (87%)	146 (13%)	5	29
4	E	74/74 (100%)	63 (85%)	11 (15%)	4	24
4	K	74/74 (100%)	70 (95%)	4 (5%)	27	64
4	Q	74/74 (100%)	68 (92%)	6 (8%)	15	50
5	F	439/554 (79%)	388 (88%)	51 (12%)	7	32
5	L	439/554 (79%)	382 (87%)	57 (13%)	5	28
5	R	439/554 (79%)	393 (90%)	46 (10%)	8	36
All	All	9594/10107 (95%)	8376 (87%)	1218 (13%)	5	29

5 of 1218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	727	VAL
3	J	568	SER
3	P	878	ASP
2	I	843	THR
3	J	29	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	725	GLN
3	J	690	ASN
3	P	1098	GLN
2	I	856	ASN
3	J	209	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	3/4 (75%)	1 (33%)	1 (33%)
8	6	3/4 (75%)	1 (33%)	1 (33%)
8	9	3/4 (75%)	1 (33%)	1 (33%)
All	All	9/12 (75%)	3 (33%)	3 (33%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	15	G
8	6	15	G
8	9	15	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	3	13	GTP
8	6	13	GTP
8	9	13	GTP

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	1	3
7	2	1
6	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	51:DC	O3'	52:DT	P	3.86
1	1	51:DC	O3'	52:DT	P	3.85
1	1	46:DG	O3'	47:DC	P	3.49
1	2	12:DG	O3'	13:DA	P	2.97
1	1	36:DT	O3'	37:DA	P	2.64

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/242 (95%)	0.03	4 (1%) 73 67	162, 207, 238, 299	0
1	B	228/242 (94%)	-0.11	6 (2%) 59 54	165, 211, 254, 284	0
1	G	230/242 (95%)	0.14	18 (7%) 16 19	175, 216, 259, 292	0
1	H	228/242 (94%)	0.45	18 (7%) 15 18	200, 264, 307, 325	0
1	M	230/242 (95%)	0.03	13 (5%) 27 27	155, 186, 230, 311	0
1	N	228/242 (94%)	-0.14	6 (2%) 59 54	162, 205, 248, 280	0
2	C	1341/1342 (99%)	0.06	49 (3%) 45 42	126, 243, 333, 427	0
2	I	1341/1342 (99%)	-0.03	29 (2%) 65 60	142, 196, 276, 345	0
2	O	1341/1342 (99%)	0.02	48 (3%) 46 43	126, 202, 287, 327	0
3	D	1362/1407 (96%)	0.11	69 (5%) 32 31	129, 204, 384, 437	0
3	J	1362/1407 (96%)	0.32	125 (9%) 11 15	145, 213, 344, 397	0
3	P	1362/1407 (96%)	0.24	105 (7%) 16 19	133, 223, 391, 441	0
4	E	90/90 (100%)	0.20	9 (10%) 9 14	138, 184, 398, 452	0
4	K	90/90 (100%)	0.30	8 (8%) 12 16	165, 213, 389, 436	0
4	Q	90/90 (100%)	0.36	9 (10%) 9 14	157, 202, 400, 463	0
5	F	497/628 (79%)	0.59	83 (16%) 2 8	176, 304, 513, 589	0
5	L	497/628 (79%)	0.29	59 (11%) 6 11	171, 277, 369, 399	0
5	R	497/628 (79%)	0.48	62 (12%) 5 10	170, 322, 414, 449	0
6	1	49/49 (100%)	0.02	2 (4%) 41 39	206, 263, 311, 333	0
6	4	49/49 (100%)	0.20	2 (4%) 41 39	50, 261, 289, 312	0
6	7	49/49 (100%)	0.41	4 (8%) 14 18	214, 295, 334, 336	0
7	2	49/49 (100%)	0.23	3 (6%) 25 25	186, 272, 334, 388	0
7	5	49/49 (100%)	0.15	1 (2%) 68 63	174, 257, 298, 371	0
7	8	49/49 (100%)	0.10	0 100 100	229, 300, 347, 427	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
8	3	3/4 (75%)	0.15	0	100 100	310, 310, 316, 331	0
8	6	3/4 (75%)	0.71	0	100 100	242, 242, 251, 272	0
8	9	3/4 (75%)	0.84	0	100 100	257, 257, 296, 373	0
All	All	11547/12159 (94%)	0.16	732 (6%)	23 24	50, 219, 383, 589	0

The worst 5 of 732 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	326	TRP	13.3
5	R	325	PRO	11.0
3	D	1054	THR	9.7
5	F	328	GLU	8.8
3	P	153	ASN	8.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
9	MG	C	1401	1/1	0.91	0.33	1.35	218,218,218,218	0
10	ZN	D	1502	1/1	0.97	0.21	1.32	172,172,172,172	0
10	ZN	J	1502	1/1	0.97	0.16	0.01	196,196,196,196	0
10	ZN	P	1502	1/1	0.90	0.15	-0.26	204,204,204,204	0
9	MG	P	1503	1/1	0.98	0.15	-1.08	187,187,187,187	0
10	ZN	P	1501	1/1	0.96	0.08	-1.40	252,252,252,252	0
10	ZN	J	1501	1/1	0.72	0.13	-1.70	218,218,218,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MG	J	1503	1/1	0.97	0.19	-1.76	204,204,204,204	0
10	ZN	D	1501	1/1	0.83	0.11	-1.77	215,215,215,215	0

6.5 Other polymers [i](#)

There are no such residues in this entry.