



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2016 – 05:31 PM EDT

PDB ID : 4YLP
Title : E. coli Transcription Initiation Complex - 16-bp spacer and 5-nt RNA
Authors : Zuo, Y.; Steitz, T.A.
Deposited on : 2015-03-05
Resolution : 5.50 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

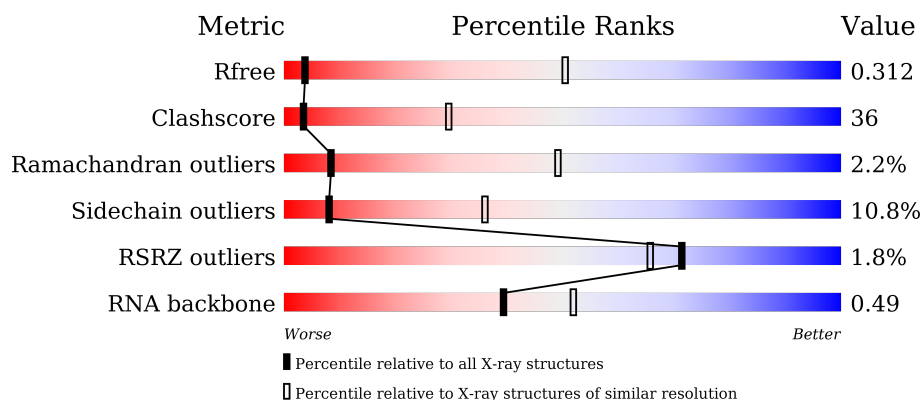
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)
RNA backbone	2183	1101 (7.80-2.80)

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	
1	B	242	
1	G	242	
1	H	242	

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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	5	
8	6	5	
8	9	5	

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	MG	P	1503	-	-	-	X
9	ZN	D	1502	-	-	X	-
9	ZN	P	1501	-	-	X	-
9	ZN	P	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94668 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'-R*(GTP))-R(P*AP*GP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3	5	Total	C	N	O	P	0	0	0
			117	48	20	42	7			
8	6	5	Total	C	N	O	P	0	0	0
			117	48	20	42	7			
8	9	5	Total	C	N	O	P	0	0	0
			117	48	20	42	7			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

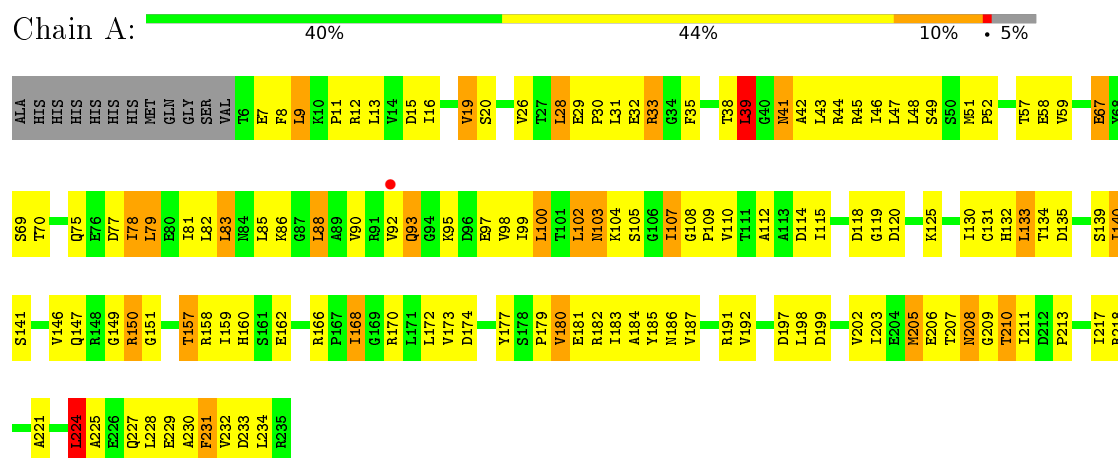
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	1	Total	Mg	0	0
			1	1		
10	J	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		

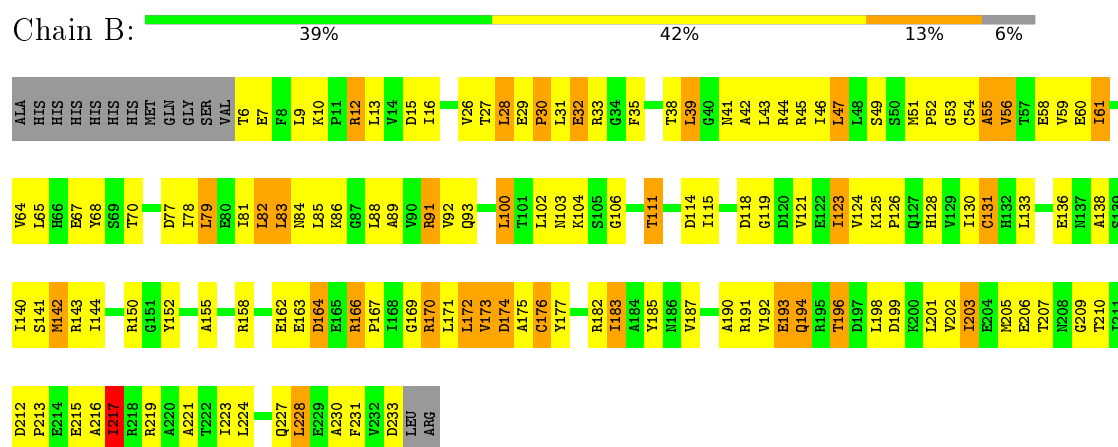
3 Residue-property plots

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.

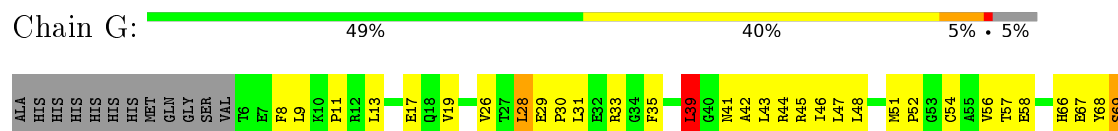
• Molecule 1: DNA-directed RNA polymerase subunit alpha

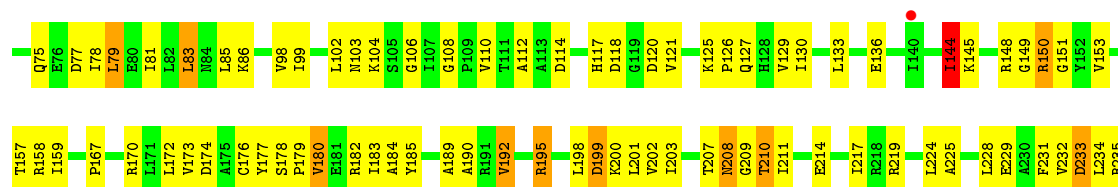


• Molecule 1: DNA-directed RNA polymerase subunit alpha

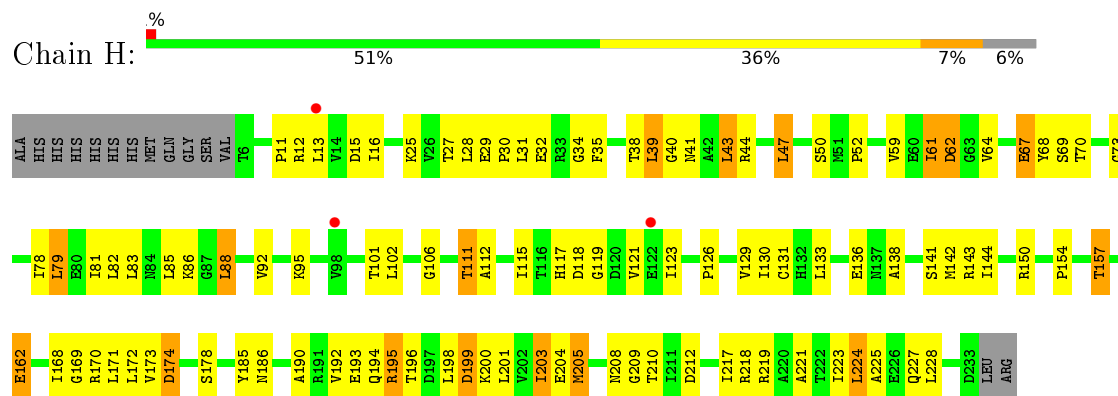


• Molecule 1: DNA-directed RNA polymerase subunit alpha

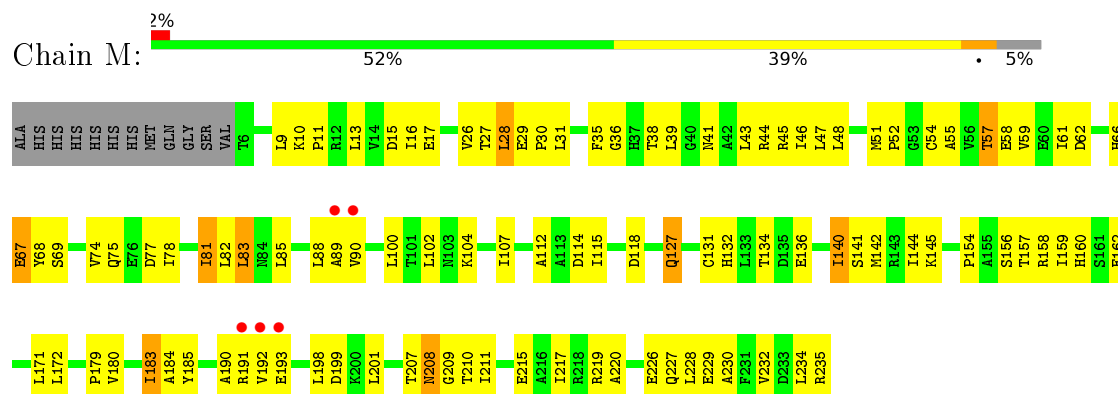




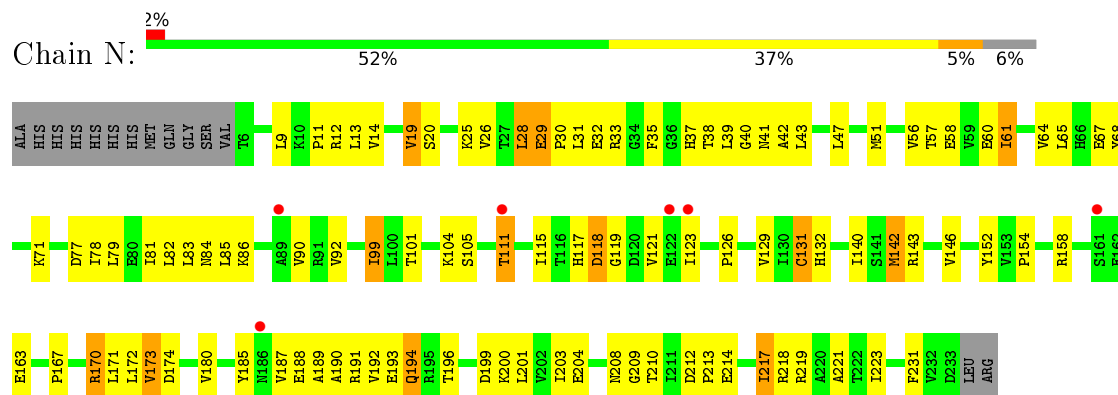
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



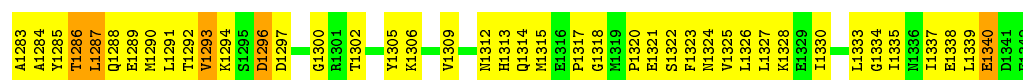
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

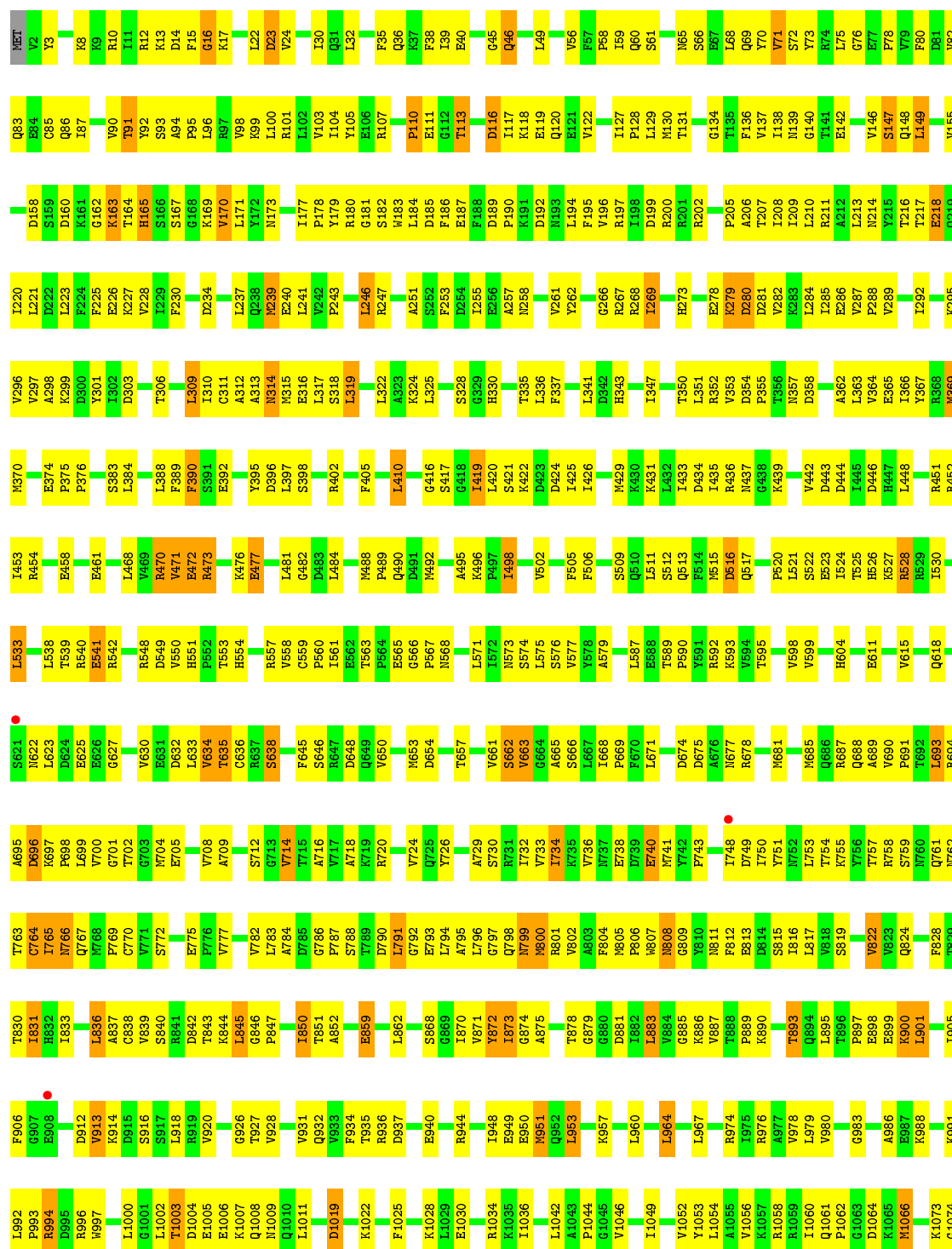


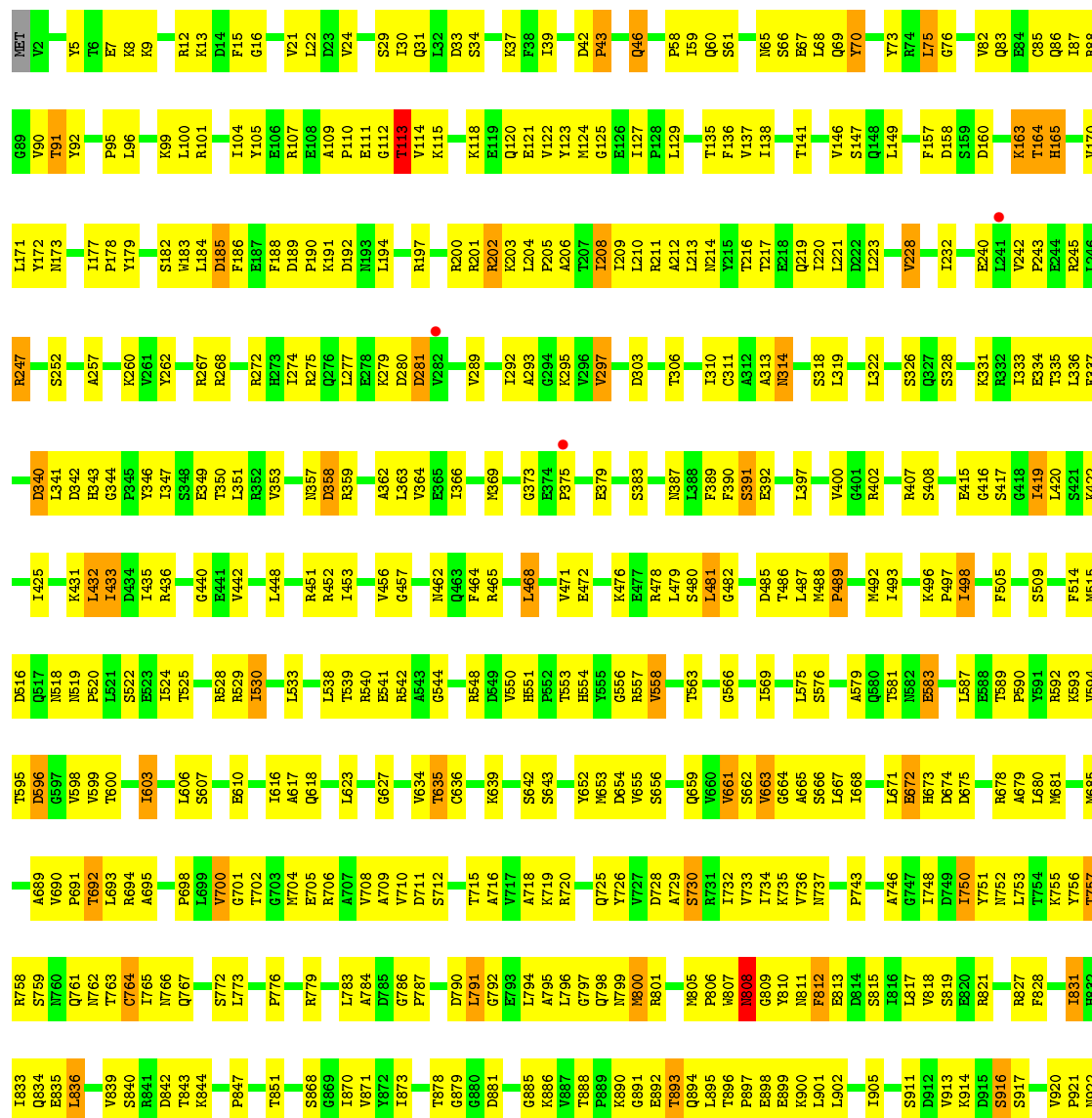
I1210	Q1136	I1060	F972	T888	M805	V736	G684	I569	Q490	L409	L325	E249	A174	T91	Y2	Y3	Y6	E7	V8	K9	R10	I11	K13	F15	G16	K17	R18	V21	P25	Y26	L27	L28	S29	I30	Q31	D32	D33	S34	F35	Q36	L49	F57	P58	S61	Y70	Y73	R74	L75	G76	V82	Q83	E84	C85	Q86	S87	R88	G89	V90							
R1211	A1139	Q1061	I975	P889	P806	D739	A665	I573	D491	L410	I333	T250	A175	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
L1212	K1140	P1062	I975	T896	M807	D739	S666	S574	M492	L410	I333	A251	I176	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
G1215	R1216	D1064	L979	P897	G809	M741	I668	S575	M494	E413	I333	A252	I177	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
R1217	R1142	K1065	V980	E898	Y810	M741	I669	S576	M495	E414	I335	A253	I178	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
G1218	I1145	M1066	V984	E899	M811	A746	I670	S577	M496	E415	I336	A254	I179	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
E1219	Q1146	R1069	V984	E900	F812	G747	I671	S578	M497	E416	I337	A255	I180	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
Q1220	Y1149	S1077	K988	L901	S815	I748	E672	S579	M498	E417	I338	A256	I181	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
F1221	D1150	K1078	L992	A904	L817	I750	D673	S580	M499	E418	I339	A257	I182	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
E1222	L1151	I1079	P993	I905	S818	I751	D674	S581	M500	E419	I340	A258	I183	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
P1224	R1156	I1082	D995	F906	S819	I752	D675	S582	M501	E420	I341	A259	I184	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
V1225	K1157	E1083	R996	K909	E820	I753	D676	S583	M502	E421	I342	A260	I185	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
V1226	K1158	P1086	M997	A910	S821	I754	D677	S584	M503	E422	I343	A261	I186	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
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Y1229	S1162	D1088	L1000	D812	S823	I756	D679	S586	M505	E424	I345	A263	I188	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
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K1234	S1165	T1092	E1005	S917	S826	I759	D682	S589	M508	E427	I348	A266	I191	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
L1238	D1166	P1093	E1006	L918	S827	I760	D683	S590	M509	E428	I349	A267	I192	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
V1239	V1169	V1094	K1007	R919	S828	I761	D684	S591	M510	E429	I350	A268	I193	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
D1240	R1170	D1095	Q1010	V920	S829	I762	D685	S592	M511	E430	I351	A269	I194	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
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R1246	A1172	M1099	E1012	G926	S831	I764	D687	S594	M513	E432	I353	A271	I196	Y92	Y93	Y94	Y95	P96	R97	V98	E106	I183	P110	F186	G112	V113	K115	V122	P123	M124	I127	P128	L129	M130	T131	T132	D133	F136	V137	I138	M139	G140	T141	Q146	L149	V146	S147	L149	S152	P153	G154	V155	F156	F157	D158	S159	D160	K163	T164	C165	H166	S167	G168	R169	M173
S1247	A1173	P1100	Q1013	T927																																																													



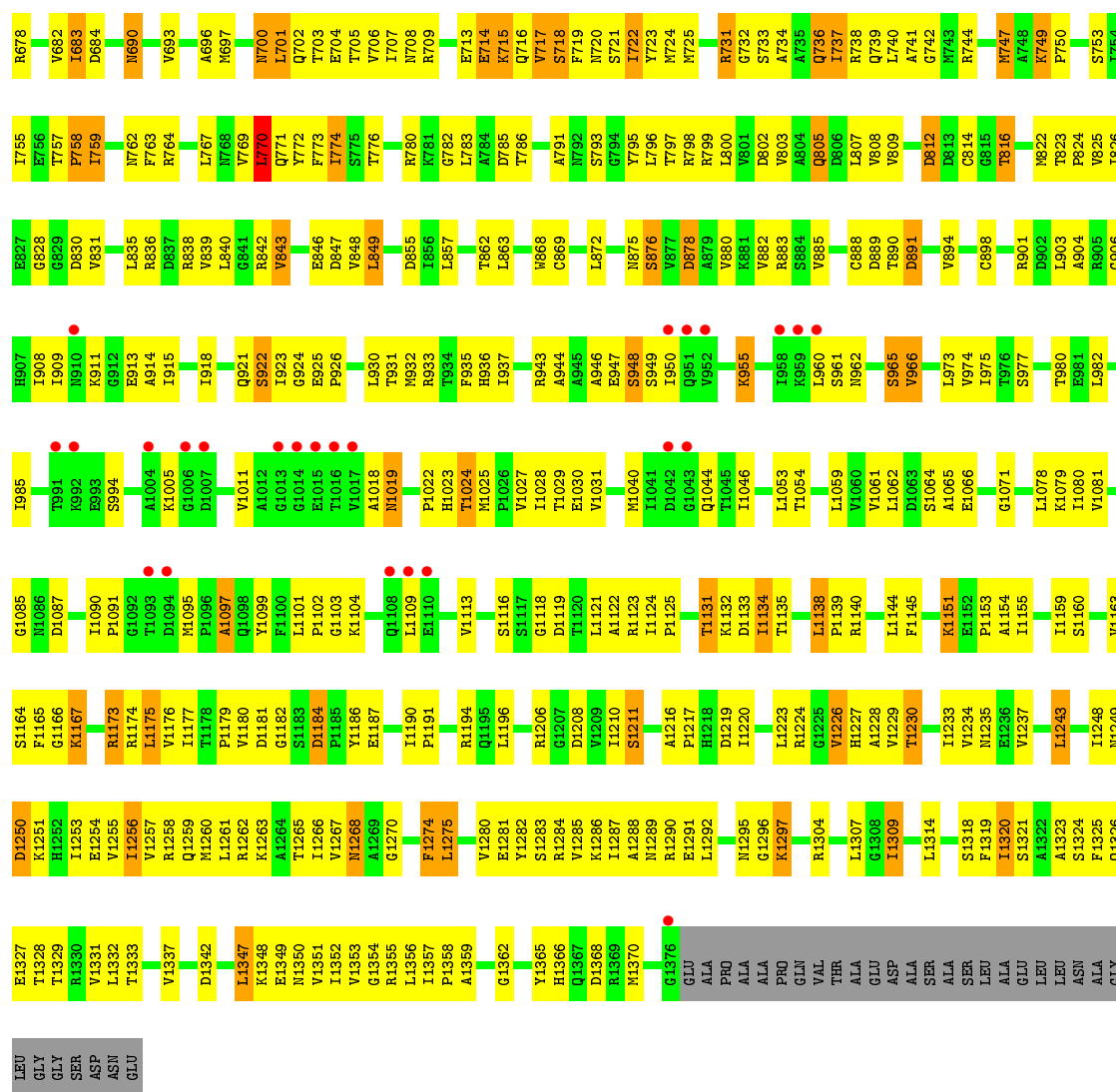
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 44% 49% 7%

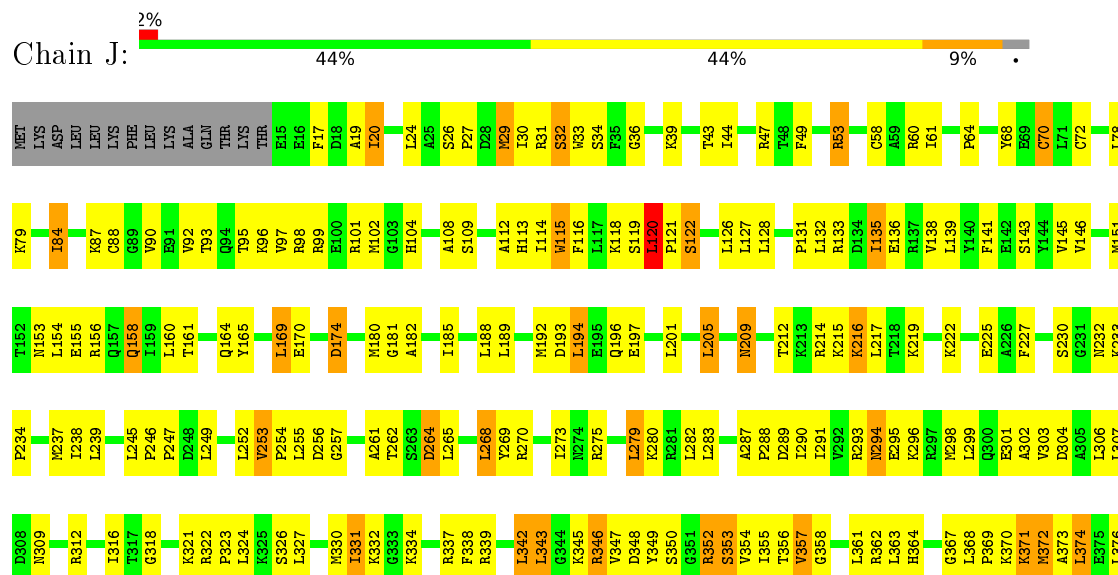






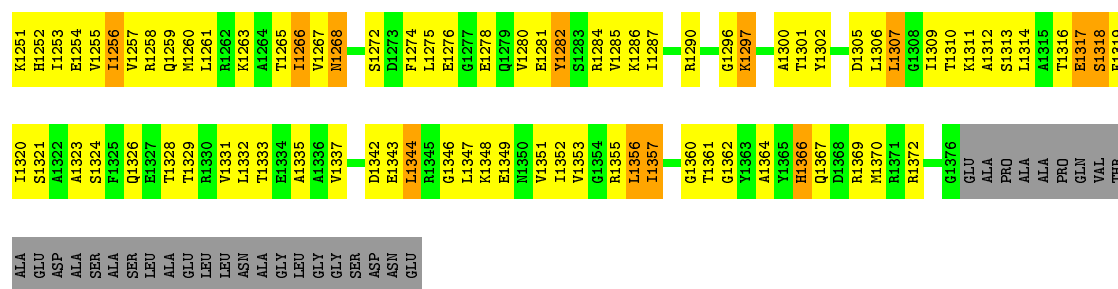


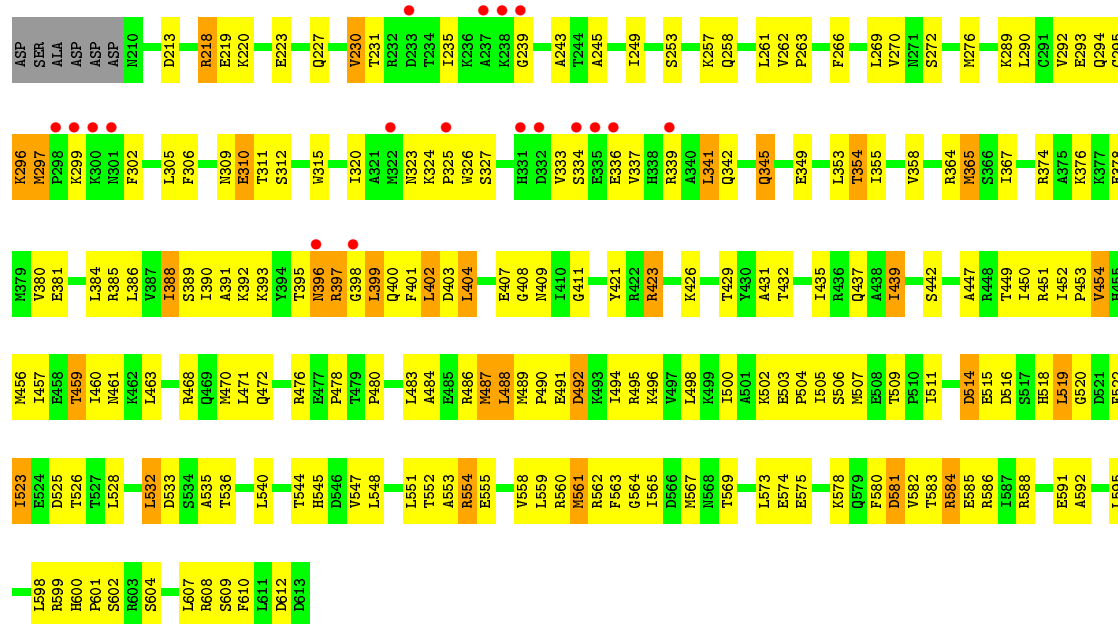
• Molecule 3: DNA-directed RNA polymerase subunit beta'



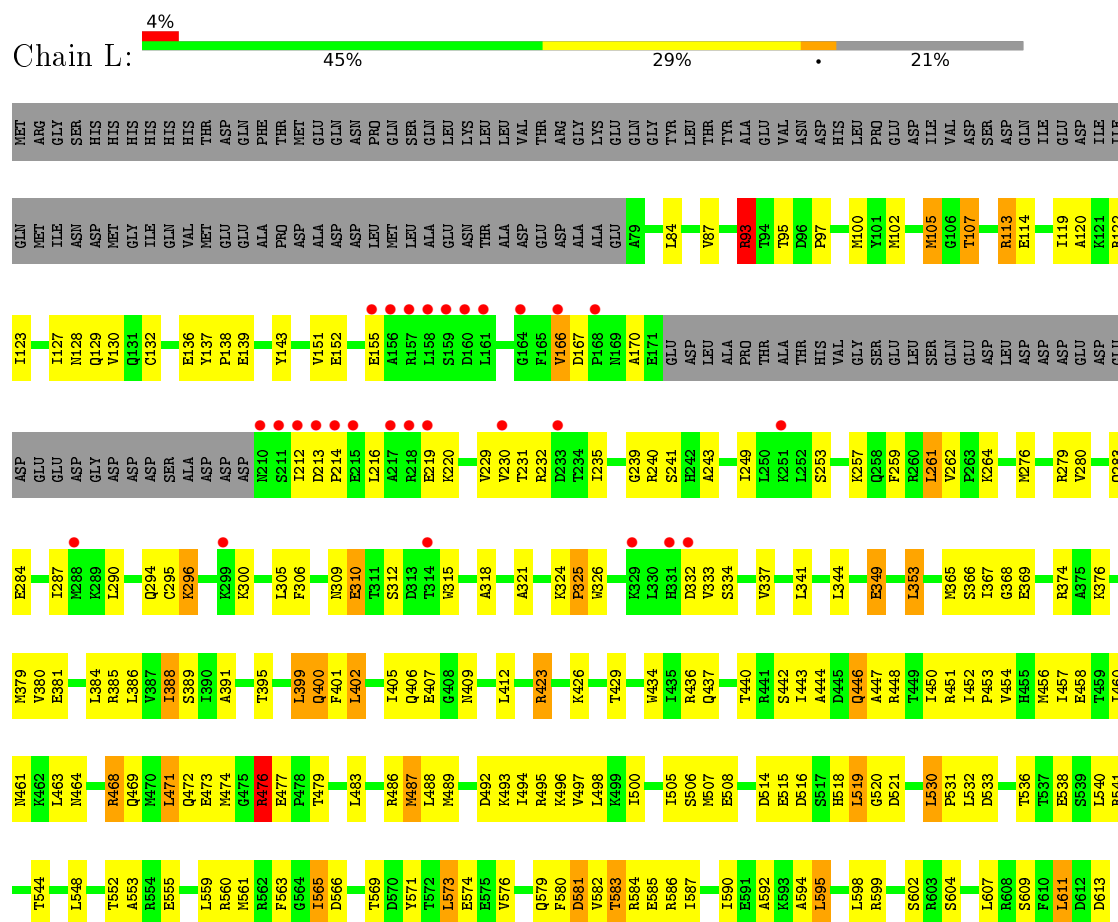


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K1170	K1079	T980	H897	T823	K749	L672	L597	W518	K370	R297	L217	L139	C70	LYS
G1171	I1080	R984	C898	R824	P750	V673	G597	M519	K371	M298	I221	Y140	L71	ASP
L1172	V1081	L985	R899	V825	V673	T674	K598	A520	M372	L299	C72	L141	C72	LEU
R1173	G901	R901	G901	I826	G752	G752	K599	M525	A373	Q300	L224	E142	K74	LEU
R1174	Q1084	R990	D902	E827	S753	R678	A600	I601	L374	E351	A256	Y145	K75	LEU
L1175	G1085	D902	D902	G828	S753	R678	I601	L596	E375	A302	C256	Y146	Y75	PHE
V1176	R1086	L903	L903	V831	I754	R681	S802	L527	L376	V303	P227	Y147	K76	LEU
I1177	D1087	E993	L903	V831	I755	V682	K603	T528	F377	L306	N232	E148	R77	ALA
V1180	P1091	S994	I909	L835	I759	V682	M604	G529	K378	L306	N232	E148	L78	GLN
D1181	M098	P998	R910	R836	I759	V682	L605	P530	K379	L306	N232	E148	L78	THR
D1184	M1096	P998	R911	R836	I759	V682	L605	P530	K379	L306	N232	E148	L78	LYS
E1187	A1097	V1002	E915	R836	F763	V686	M606	E532	L381	R311	L289	L154	C85	THR
M1188	L1101	K1005	R918	V843	L767	V693	L541	L541	F382	G313	L240	E155	E86	E15
M1189	G1103	Q1010	T844	T844	V769	V693	L541	L541	G383	R314	T240	E155	K87	A19
I1190	K1104	A1018	E945	E945	L770	V693	L541	L541	K384	G318	L242	Q157	C88	I20
P1191	A1105	M1019	E945	E945	L770	V693	L541	L541	L385	S319	P243	Q158	G89	I21
K1192	V1106	W1020	G924	G924	V772	M699	L541	L541	L385	N320	V244	I159	V90	I22
L1196	V1107	L849	E925	E925	F773	N700	L541	L541	K398	K321	L245	E162	E91	I23
Q1108	Q1108	P1021	P926	K850	I774	Q702	L541	L541	K399	P247	P247	Y165	T93	A23
L1109	L1109	P1022	P926	K850	S775	Q702	L541	L541	E402	S326	P247	Y165	Q94	A25
G1201	L1114	H1023	L930	T853	T776	T703	L541	L541	E403	L327	P247	Y165	T95	S26
V1209	Q1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
S1211	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
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I1218	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
I1219	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
I1220	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
I1221	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
I1222	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
I1223	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
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I1225	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
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I1249	S1117	M1025	E954	E954	T776	T703	L541	L541	E404	L327	P247	Y165	T95	A25
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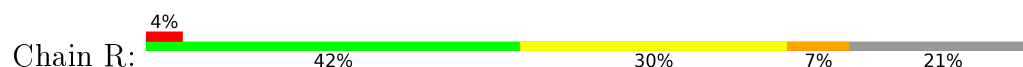




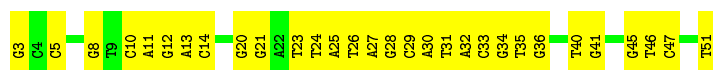
- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD

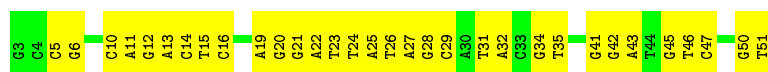


Chain 2:  39% 61%



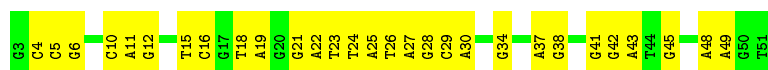
- Molecule 7: T strand DNA (49-MER)

Chain 5:  35% 65%




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

Chain 8:  41% 59%



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

Chain 3:  80% 20%



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

Chain 6:  40% 40% 20%



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

Chain 9:  40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	237.67Å 204.99Å 248.84Å 90.00° 116.86° 90.00°	Depositor
Resolution (Å)	39.98 – 5.50 39.98 – 5.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.98-5.50) 98.1 (39.98-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 5.37Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.231 , 0.313 0.231 , 0.312	Depositor DCC
R_{free} test set	3384 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	324.1	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 168.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	94668	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: 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	0.63	0/1809	0.91	5/2450 (0.2%)
1	B	0.58	0/1789	0.87	3/2425 (0.1%)
1	G	0.60	0/1809	0.87	2/2450 (0.1%)
1	H	0.59	0/1789	0.87	2/2425 (0.1%)
1	M	0.53	0/1809	0.76	1/2450 (0.0%)
1	N	0.55	0/1789	0.81	1/2425 (0.0%)
2	C	0.56	0/10745	0.78	5/14499 (0.0%)
2	I	0.58	1/10745 (0.0%)	0.78	5/14499 (0.0%)
2	O	0.53	0/10745	0.75	4/14499 (0.0%)
3	D	0.57	1/10729 (0.0%)	0.80	9/14487 (0.1%)
3	J	0.59	1/10729 (0.0%)	0.85	16/14487 (0.1%)
3	P	0.57	1/10729 (0.0%)	0.80	5/14487 (0.0%)
4	E	0.53	0/710	0.71	0/956
4	K	0.62	1/710 (0.1%)	0.82	0/956
4	Q	0.54	0/710	0.77	0/956
5	F	0.51	0/4076	0.73	1/5482 (0.0%)
5	L	0.53	0/4076	0.75	3/5482 (0.1%)
5	R	0.54	1/4076 (0.0%)	0.75	3/5482 (0.1%)
6	1	0.34	0/1114	0.68	0/1714
6	4	1.27	1/1114 (0.1%)	0.91	4/1714 (0.2%)
6	7	0.40	0/1115	0.66	0/1718
7	2	0.35	0/1136	0.67	0/1752
7	5	0.33	0/1136	0.68	0/1752
7	8	0.41	0/1137	0.66	0/1756
8	3	0.38	0/94	0.67	0/144
8	6	0.42	0/94	0.64	0/144
8	9	0.28	0/94	0.68	0/144
All	All	0.57	7/96608 (0.0%)	0.79	69/131735 (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	P	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	51	DC	O3'-P	40.58	2.09	1.61
2	I	638	SER	CB-OG	16.07	1.63	1.42
3	D	955	LYS	CE-NZ	10.97	1.76	1.49
4	K	91	ARG	C-O	7.42	1.37	1.23
3	P	681	LYS	CG-CD	5.15	1.70	1.52

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	4	51	DC	OP1-P-O3'	15.55	139.42	105.20
6	4	51	DC	P-O3'-C3'	15.39	138.17	119.70
6	4	51	DC	O3'-P-O5'	-10.32	84.38	104.00
3	J	120	LEU	C-N-CD	-9.82	99.00	120.60
1	N	29	GLU	C-N-CD	-9.03	100.74	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	1276	GLU	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	209	0
1	B	1767	0	1789	217	0
1	G	1787	0	1813	166	0
1	H	1767	0	1789	160	0
1	M	1787	0	1813	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1767	0	1789	116	0
2	C	10576	0	10591	815	0
2	I	10576	0	10591	916	0
2	O	10576	0	10591	739	0
3	D	10568	0	10781	927	1
3	J	10568	0	10780	1017	0
3	P	10568	0	10783	901	0
4	E	708	0	719	39	0
4	K	708	0	719	38	0
4	Q	708	0	719	47	0
5	F	4022	0	4083	280	0
5	L	4022	0	4083	220	0
5	R	4022	0	4083	298	0
6	1	996	0	555	65	1
6	4	996	0	556	71	0
6	7	996	0	554	60	1
7	2	1012	0	554	55	1
7	5	1012	0	554	53	0
7	8	1012	0	553	48	0
8	3	117	0	55	10	0
8	6	117	0	55	6	0
8	9	117	0	55	6	0
9	D	2	0	0	2	0
9	J	2	0	0	1	0
9	P	2	0	0	5	0
10	D	1	0	0	0	0
10	J	1	0	0	0	0
10	P	1	0	0	0	0
All	All	94668	0	92820	6810	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 36.

The worst 5 of 6810 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:255:ILE:CG1	2:I:255:ILE:CD1	1.74	1.59
3:D:955:LYS:NZ	3:D:955:LYS:CE	1.76	1.48
3:P:514:THR:HG21	3:P:596:LEU:CD1	1.48	1.42
3:J:421:VAL:CG1	3:J:469:HIS:O	1.70	1.40
3:P:1095:MET:SD	3:P:1173:ARG:NH2	1.97	1.38

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)
7:2:3:DG:O5'	7:2:51:DT:O3'[2_657]	1.64	0.56
3:D:1174:ARG:NH2	6:1:17:DA:OP1[2_657]	2.10	0.10
6:7:12:DA:O5'	6:7:60:DC:O3'[2_546]	2.13	0.07

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%)	213 (93%)	11 (5%)	4 (2%)	11	53
1	B	226/242 (93%)	204 (90%)	14 (6%)	8 (4%)	4	39
1	G	228/242 (94%)	211 (92%)	14 (6%)	3 (1%)	15	59
1	H	226/242 (93%)	205 (91%)	17 (8%)	4 (2%)	11	53
1	M	228/242 (94%)	215 (94%)	12 (5%)	1 (0%)	39	80
1	N	226/242 (93%)	208 (92%)	12 (5%)	6 (3%)	6	44
2	C	1339/1342 (100%)	1220 (91%)	97 (7%)	22 (2%)	12	56
2	I	1339/1342 (100%)	1226 (92%)	88 (7%)	25 (2%)	10	52
2	O	1339/1342 (100%)	1235 (92%)	82 (6%)	22 (2%)	12	56
3	D	1360/1407 (97%)	1212 (89%)	120 (9%)	28 (2%)	9	50
3	J	1360/1407 (97%)	1212 (89%)	113 (8%)	35 (3%)	7	45
3	P	1360/1407 (97%)	1214 (89%)	111 (8%)	35 (3%)	7	45
4	E	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
4	K	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
4	Q	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
5	F	493/628 (78%)	449 (91%)	30 (6%)	14 (3%)	6	44
5	L	493/628 (78%)	444 (90%)	30 (6%)	19 (4%)	4	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	493/628 (78%)	447 (91%)	30 (6%)	16 (3%)	5	41
All	All	11202/11853 (94%)	10167 (91%)	793 (7%)	242 (2%)	8	49

5 of 242 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	THR
1	B	209	GLY
2	C	165	HIS
2	C	808	ASN
2	C	812	PHE

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%)	166 (84%)	32 (16%)	3	20
1	B	196/208 (94%)	163 (83%)	33 (17%)	2	19
1	G	198/208 (95%)	180 (91%)	18 (9%)	12	44
1	H	196/208 (94%)	171 (87%)	25 (13%)	5	29
1	M	198/208 (95%)	183 (92%)	15 (8%)	16	53
1	N	196/208 (94%)	179 (91%)	17 (9%)	13	46
2	C	1156/1157 (100%)	1027 (89%)	129 (11%)	7	34
2	I	1156/1157 (100%)	1038 (90%)	118 (10%)	9	38
2	O	1156/1157 (100%)	1044 (90%)	112 (10%)	10	40
3	D	1135/1168 (97%)	1009 (89%)	126 (11%)	8	34
3	J	1135/1168 (97%)	1003 (88%)	132 (12%)	7	32
3	P	1135/1168 (97%)	1014 (89%)	121 (11%)	8	36
4	E	74/74 (100%)	71 (96%)	3 (4%)	37	71
4	K	74/74 (100%)	65 (88%)	9 (12%)	6	31
4	Q	74/74 (100%)	68 (92%)	6 (8%)	15	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	439/554 (79%)	395 (90%)	44 (10%)	9	38
5	L	439/554 (79%)	401 (91%)	38 (9%)	13	46
5	R	439/554 (79%)	384 (88%)	55 (12%)	6	30
All	All	9594/10107 (95%)	8561 (89%)	1033 (11%)	8	36

5 of 1033 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	734	ILE
3	J	567	THR
3	P	1177	ILE
2	I	836	LEU
2	I	1337	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	1116	HIS
3	J	690	ASN
3	P	1114	GLN
2	I	1307	ASN
3	J	341	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	4/5 (80%)	0	1 (25%)
8	6	4/5 (80%)	0	1 (25%)
8	9	3/5 (60%)	0	0
All	All	11/15 (73%)	0	2 (18%)

There are no RNA backbone outliers to report.

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	3	13	GTP
8	6	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	4	2
7	2	1
6	1	1
7	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	46:DG	O3'	47:DC	P	5.33
1	1	46:DG	O3'	47:DC	P	4.95
1	2	12:DG	O3'	13:DA	P	2.74
1	5	11:DA	O3'	12:DG	P	2.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	51:DC	O3'	52:DT	P	2.09

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%)	-0.42	1 (0%) 93 90	134, 152, 183, 205	0
1	B	228/242 (94%)	-0.56	0 100 100	136, 167, 199, 236	0
1	G	230/242 (95%)	-0.31	1 (0%) 93 90	139, 162, 198, 240	0
1	H	228/242 (94%)	-0.41	3 (1%) 79 73	141, 176, 208, 242	0
1	M	230/242 (95%)	-0.21	5 (2%) 65 60	159, 179, 209, 245	0
1	N	228/242 (94%)	-0.16	6 (2%) 59 54	169, 201, 249, 272	0
2	C	1341/1342 (99%)	-0.34	3 (0%) 95 94	107, 166, 250, 351	0
2	I	1341/1342 (99%)	-0.37	4 (0%) 94 92	98, 172, 227, 283	0
2	O	1341/1342 (99%)	-0.35	4 (0%) 94 92	113, 174, 222, 263	0
3	D	1362/1407 (96%)	-0.22	26 (1%) 70 64	112, 184, 269, 324	0
3	J	1362/1407 (96%)	-0.22	23 (1%) 73 67	100, 172, 323, 386	0
3	P	1362/1407 (96%)	-0.17	33 (2%) 62 57	117, 182, 291, 333	0
4	E	90/90 (100%)	0.06	5 (5%) 28 27	136, 169, 350, 413	0
4	K	90/90 (100%)	-0.10	8 (8%) 12 14	112, 152, 324, 363	0
4	Q	90/90 (100%)	-0.31	4 (4%) 38 35	128, 171, 328, 364	0
5	F	497/628 (79%)	-0.11	24 (4%) 34 31	154, 271, 387, 434	0
5	L	497/628 (79%)	0.07	28 (5%) 28 27	138, 281, 365, 402	0
5	R	497/628 (79%)	-0.13	23 (4%) 36 34	146, 261, 390, 426	0
6	1	49/49 (100%)	-0.35	0 100 100	205, 265, 288, 289	0
6	4	49/49 (100%)	-0.34	2 (4%) 41 37	181, 228, 278, 302	0
6	7	49/49 (100%)	-0.40	1 (2%) 68 62	184, 228, 266, 277	0
7	2	49/49 (100%)	-0.53	0 100 100	192, 268, 291, 312	0
7	5	49/49 (100%)	-0.29	0 100 100	163, 232, 279, 326	0
7	8	49/49 (100%)	-0.52	0 100 100	166, 227, 262, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
8	3	4/5 (80%)	0.14	0	100	100	230, 234, 236, 245	0
8	6	4/5 (80%)	0.02	0	100	100	220, 221, 224, 239	0
8	9	4/5 (80%)	0.31	0	100	100	215, 221, 224, 236	0
All	All	11550/12162 (94%)	-0.26	204 (1%)	71	66	98, 182, 331, 434	0

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	211	SER	11.0
3	D	959	LYS	7.6
5	L	212	ILE	6.8
5	R	211	SER	6.7
3	P	1004	ALA	6.4

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
10	MG	P	1503	1/1	0.98	0.31	2.10	170,170,170,170	0
9	ZN	J	1502	1/1	0.96	0.17	0.85	144,144,144,144	0
9	ZN	D	1502	1/1	0.98	0.15	0.54	181,181,181,181	0
10	MG	J	1503	1/1	0.99	0.20	-0.30	145,145,145,145	0
9	ZN	P	1502	1/1	0.96	0.14	-0.44	158,158,158,158	0
10	MG	D	1503	1/1	0.99	0.16	-0.63	141,141,141,141	0
9	ZN	J	1501	1/1	0.94	0.07	-0.97	211,211,211,211	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	ZN	D	1501	1/1	0.93	0.06	-1.46	220,220,220,220	0
9	ZN	P	1501	1/1	0.93	0.08	-1.57	206,206,206,206	0

6.5 Other polymers [i](#)

There are no such residues in this entry.