



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 02:40 am BST

PDB ID : 3AOH
Title : RNA polymerase-Gfh1 complex (Crystal type 1)
Authors : Tagami, S.; Sekine, S.; Kumarevel, T.; Yamamoto, M.; Yokoyama, S.; RIKEN
Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2010-09-28
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

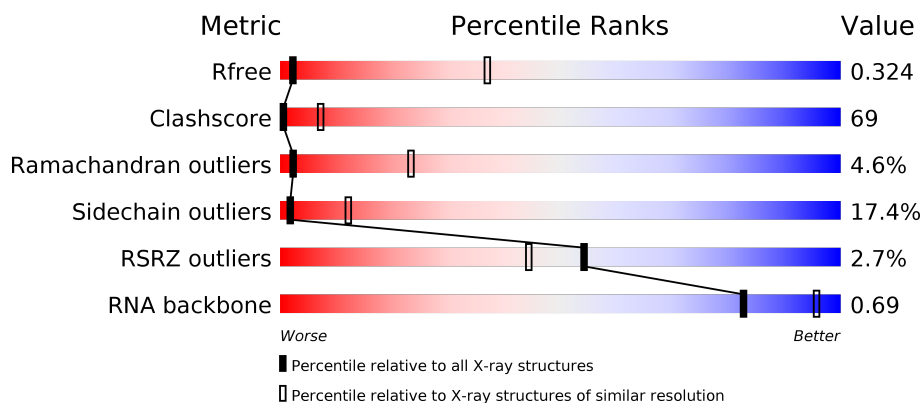
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)
RNA backbone	3102	1049 (5.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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>17%</div> <div>46%</div> <div>7%</div> <div>29%</div> </div>
1	B	315	<div> <div>21%</div> <div>41%</div> <div>9%</div> <div>29%</div> </div>
1	F	315	<div> <div>18%</div> <div>43%</div> <div>9%</div> <div>30%</div> </div>
1	G	315	<div> <div>22%</div> <div>40%</div> <div>8%</div> <div>29%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	315	
1	L	315	
2	C	1119	
2	H	1119	
2	M	1119	
3	D	1524	
3	I	1524	
3	N	1524	
4	E	99	
4	J	99	
4	O	99	
5	P	27	
6	Q	33	
7	X	156	
7	Y	156	
7	Z	156	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 74250 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	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	F	222	Total	C	N	O	S	0	0	0
			1750	1117	304	327	2			
1	G	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	K	222	Total	C	N	O	S	0	0	0
			1750	1117	304	327	2			
1	L	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1106	Total	C	N	O	S	0	0	0
			8733	5525	1558	1626	24			
2	H	1103	Total	C	N	O	S	0	0	0
			8710	5508	1555	1623	24			
2	M	1105	Total	C	N	O	S	0	0	0
			8729	5523	1557	1625	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1349	Total	C	N	O	S	0	0	0
			10651	6740	1888	1991	32			
3	I	1289	Total	C	N	O	S	0	0	0
			10182	6444	1804	1903	31			
3	N	1351	Total	C	N	O	S	0	0	0
			10667	6749	1891	1995	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			
4	J	92	Total	C	N	O	S	0	0	0
			749	478	130	137	4			
4	O	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a DNA chain called DNA (5'-D(*GP*GP*TP*CP*TP*GP*TP*AP*TP*CP*AP*CP*GP*AP*GP*CP*CP*AP*CP*CP*GP*CP*CP*GP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	6	Total	C	N	O	P	0	0	0
			120	56	22	36	6			

- Molecule 6 is a RNA chain called RNA (5'-R(*CP*CP*CP*CP*GP*GP*AP*AP*GP*AP*UP*CP*AP*UP*CP*UP*UP*CP*CP*GP*GP*GP*GP*GP*AP*U*GP*CP*GP*GP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Q	7	Total	C	N	O	P	0	0	0
			152	68	31	47	6			

- Molecule 7 is a protein called Anti-cleavage anti-GreA transcription factor Gfh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	X	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			
7	Y	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			
7	Z	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

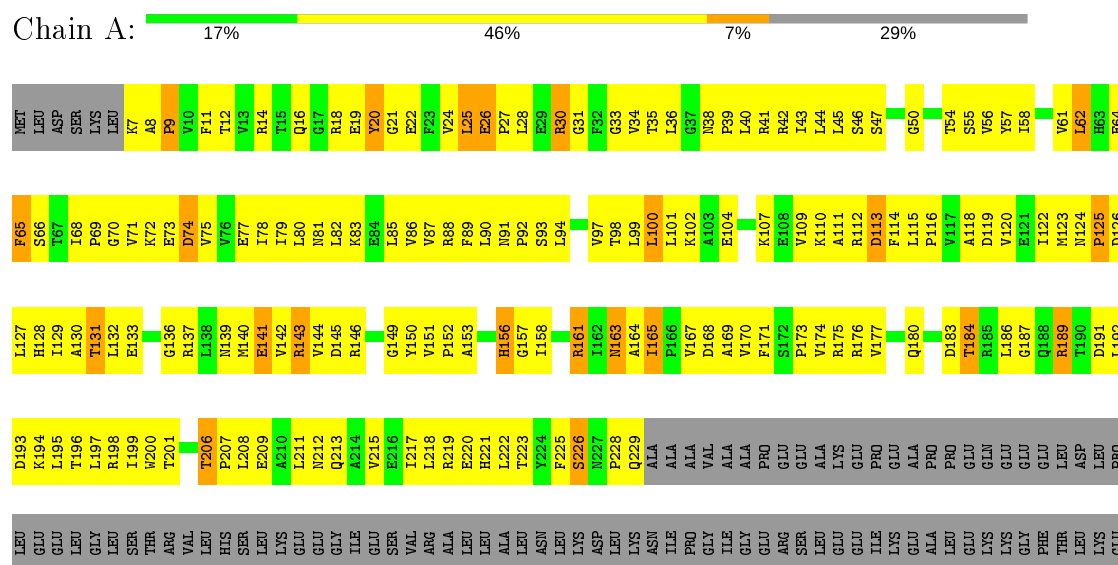
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

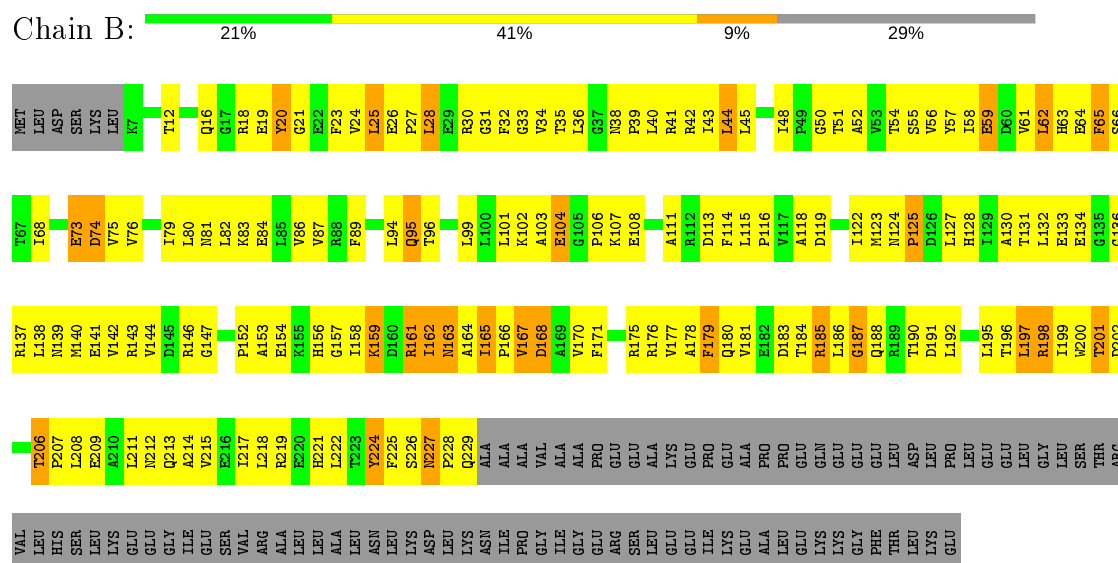
3 Residue-property plots

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

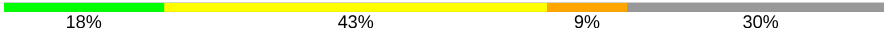
- Molecule 1: DNA-directed RNA polymerase subunit alpha

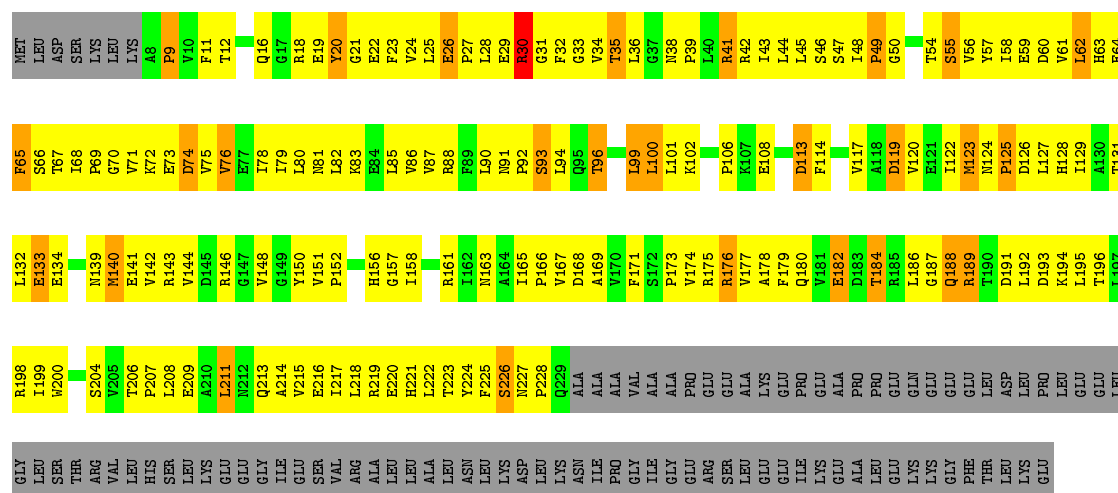


- Molecule 1: DNA-directed RNA polymerase subunit alpha




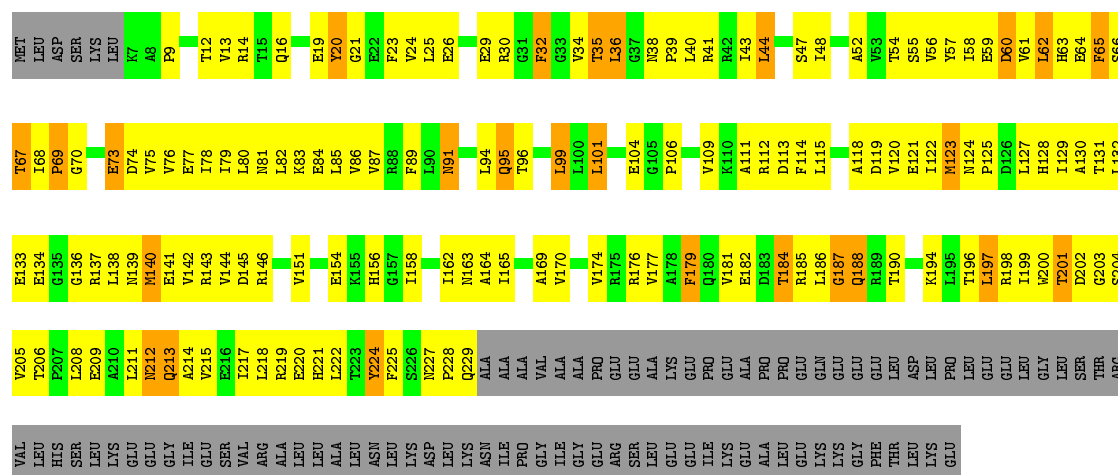
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain F: 




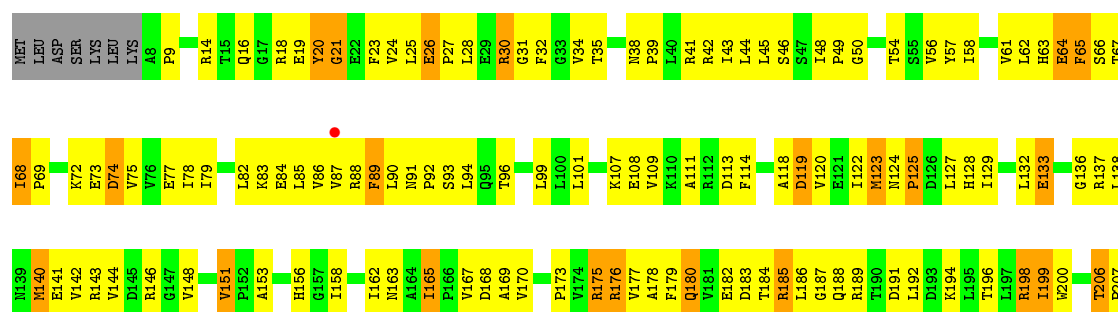
- Molecule 1: DNA-directed RNA polymerase subunit alpha

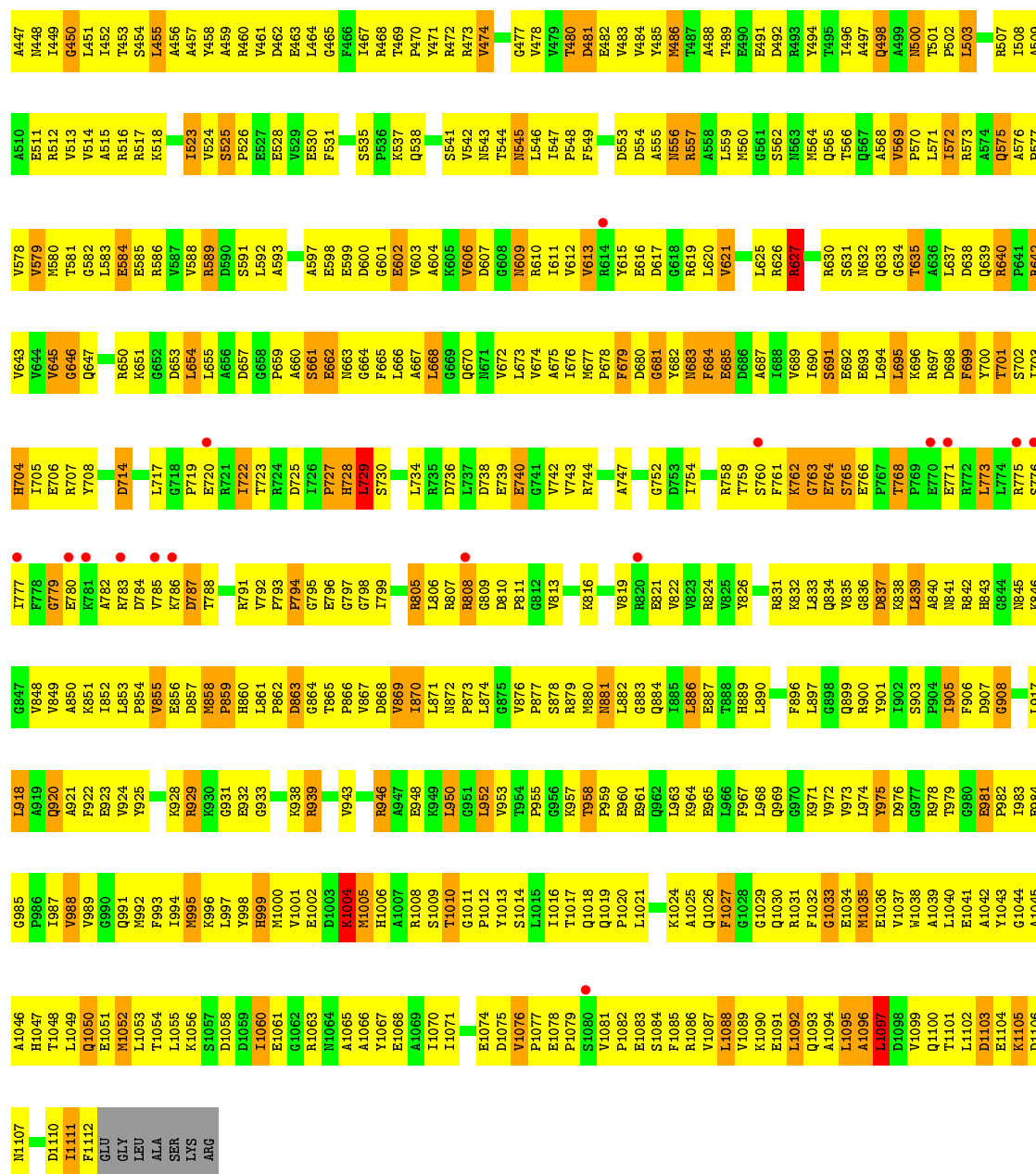
Chain G: 



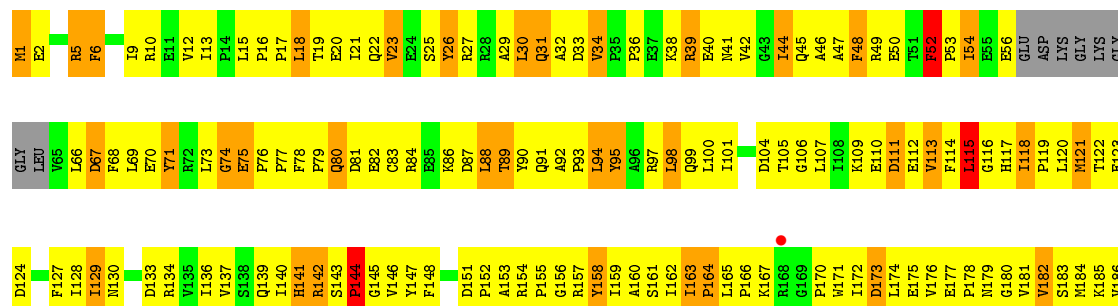
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain K: 



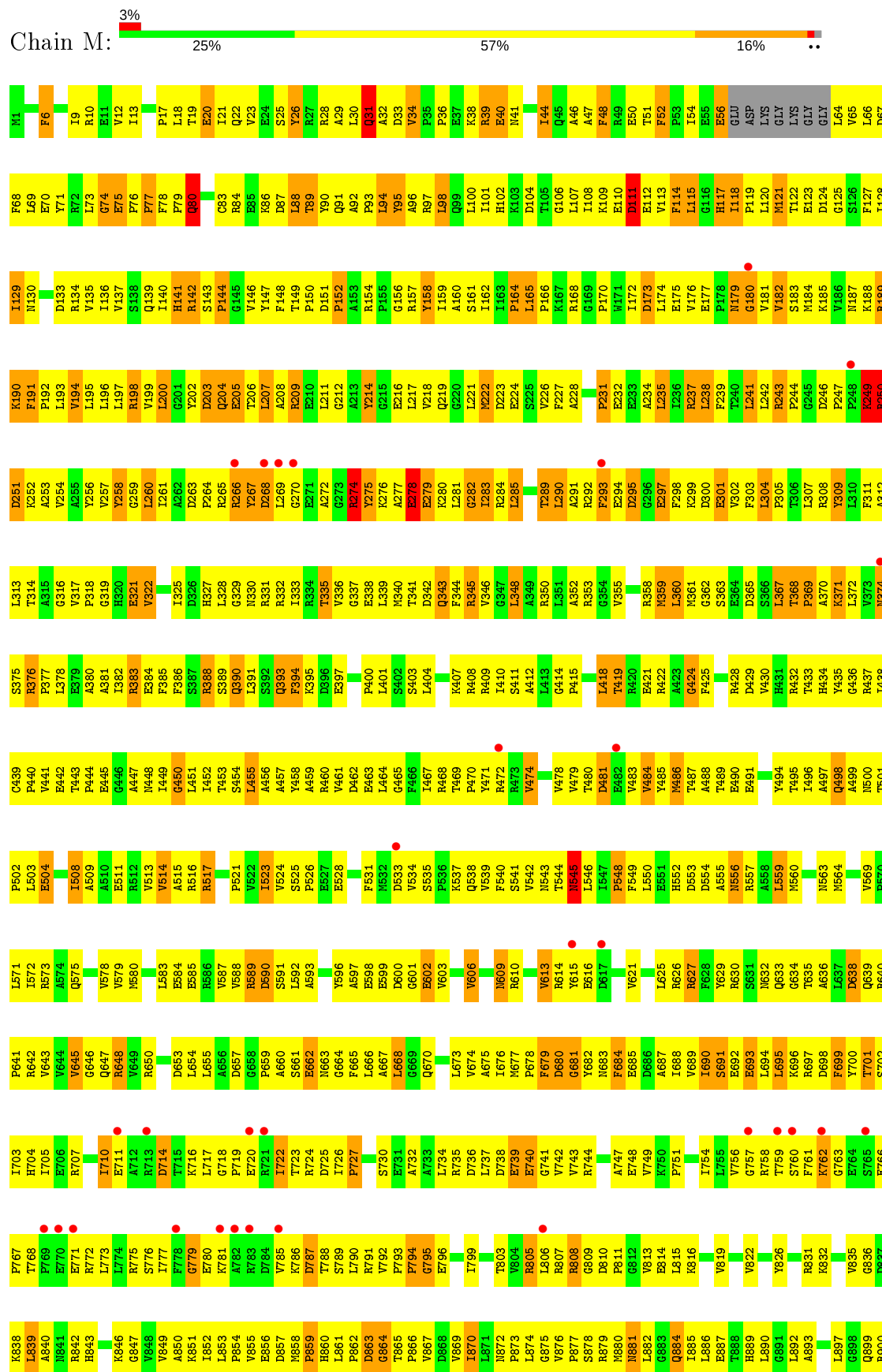


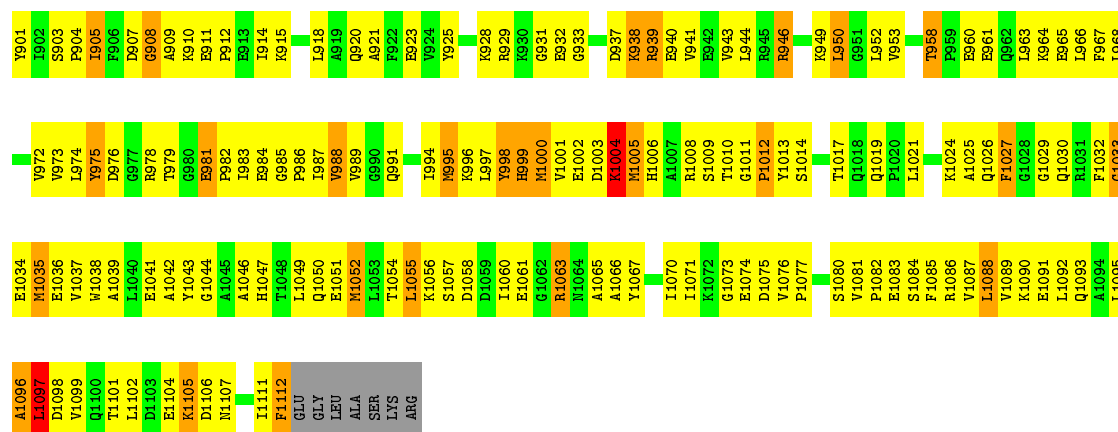
• Molecule 2: DNA-directed RNA polymerase subunit beta



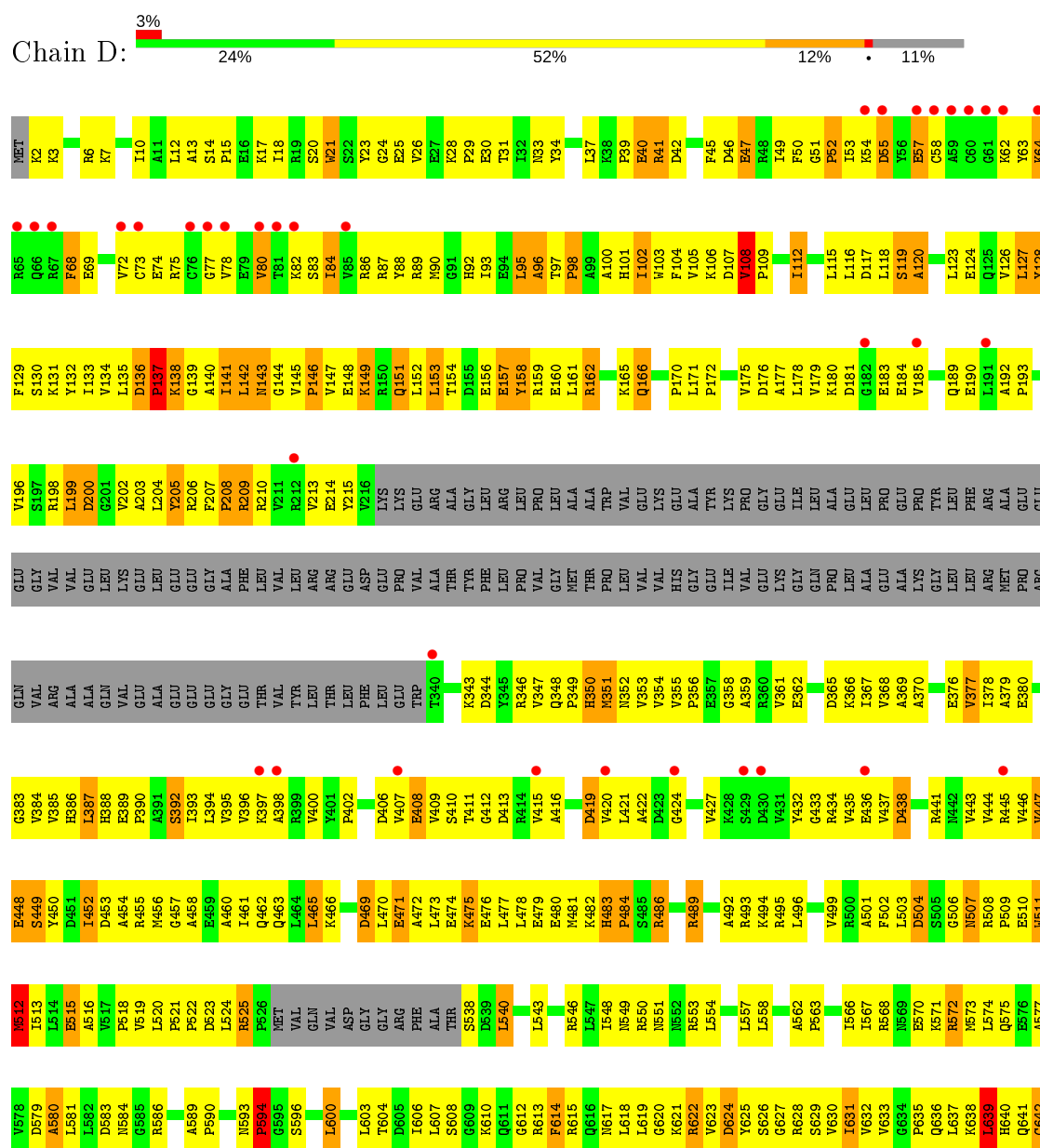


● Molecule 2: DNA-directed RNA polymerase subunit beta



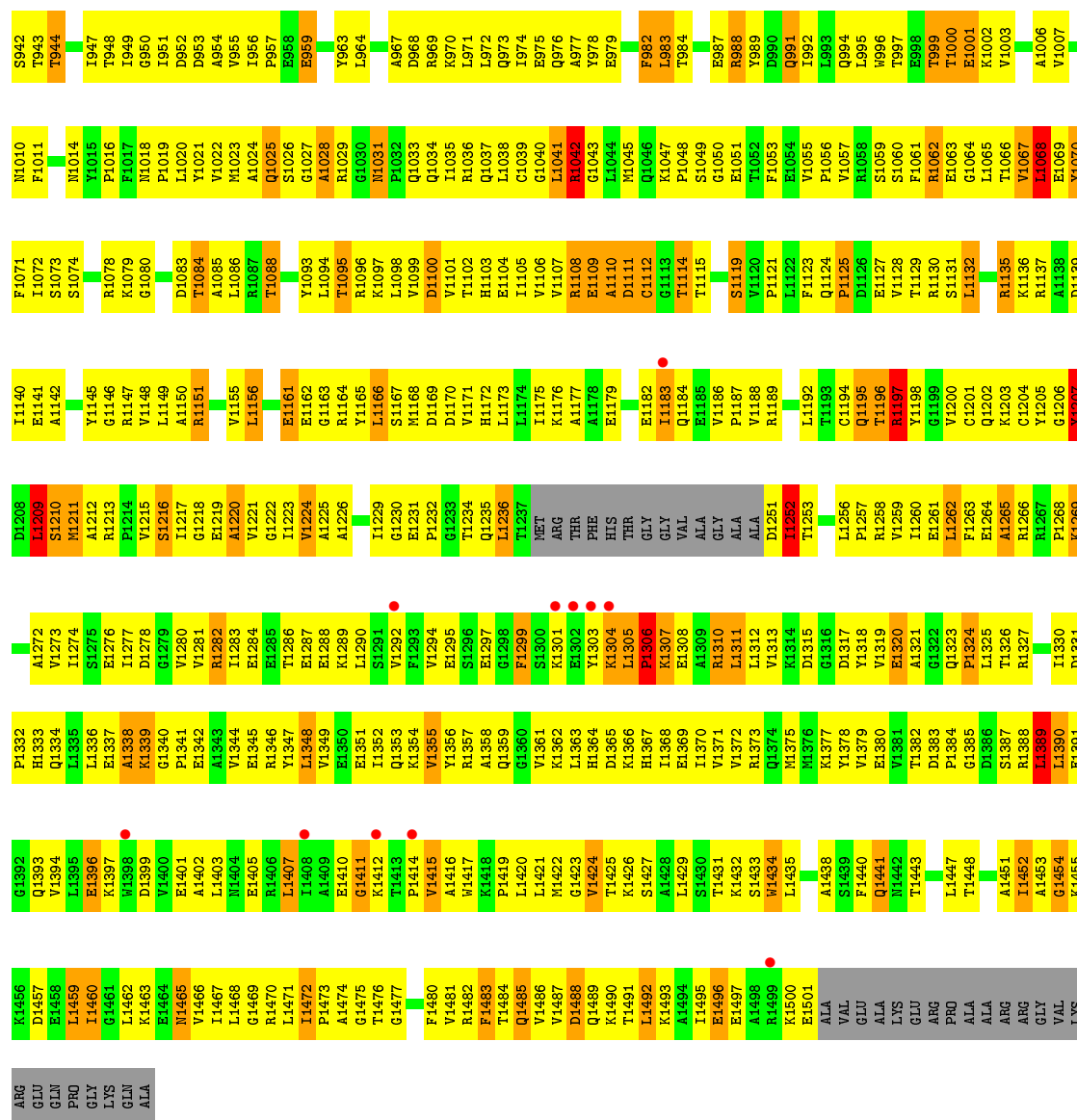


• Molecule 3: DNA-directed RNA polymerase subunit beta'

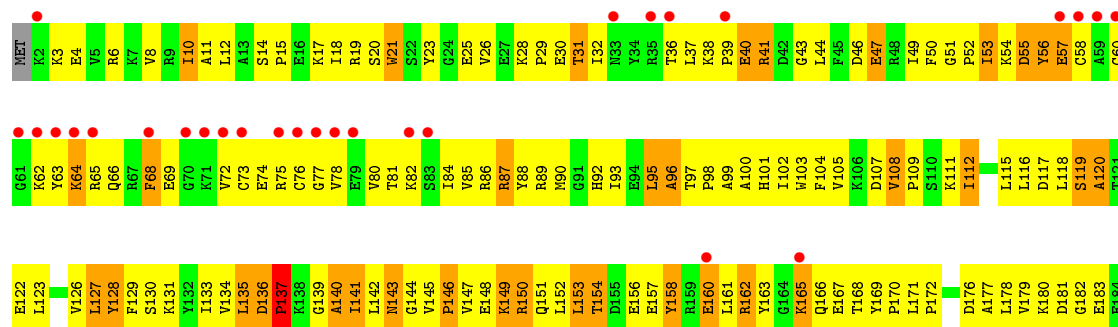




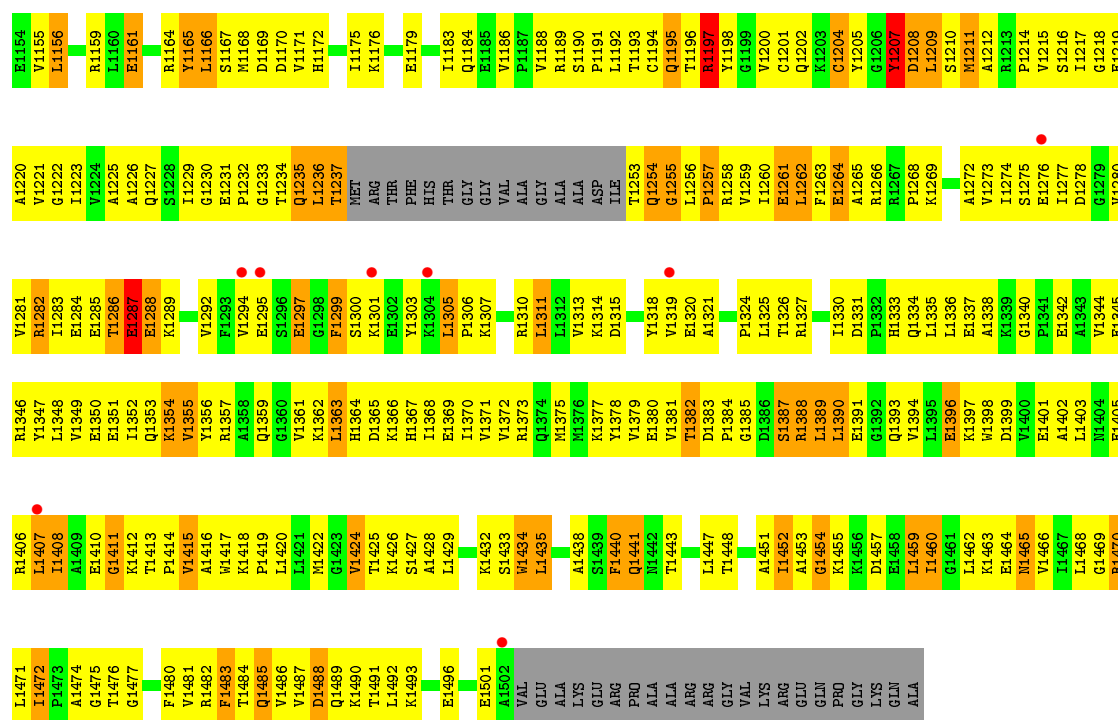




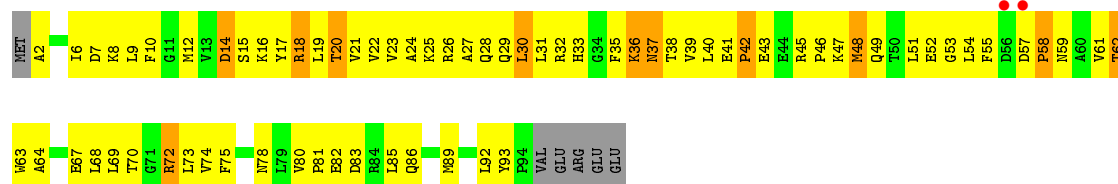
• Molecule 3: DNA-directed RNA polymerase subunit beta'



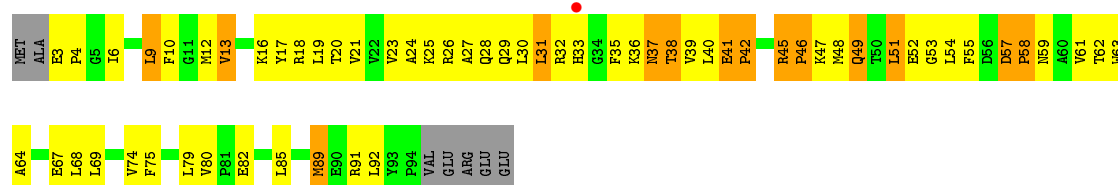
G1082	Y1093	L964	L899	V836	S771	R704	R640	R573	L503	V442	A370	V185
T1094	L1093	A967	L900	G637	P772	A705	Q641	L574	G506	V443	A376	Q188
T1095	P1032	A968	Q901	R838	A773	P706	G642	Q576	G507	V444	V377	E189
K1096	Q1034	R969	L902	L839	S774		G643	E576	R507	R445	I378	E190
L1098	I1035	K970	Q906	R340	G775	R709	L644	A577	P509	V446	A379	L191
V1099	R1036	L971	E907	R842	P777	L711	G646	D579	E510	E448	E380	A192
D1100	Q1037	L972	K908	R843	L778	G712	R647	A580	R511	A381	P193	
V1101	L1038	Q973	R909	R844	A779	I713	R648	L581	R512	E382		V196
T1102	G1039	E974	S910	R845	K780	Q714	L649	L582	I513	G383		S197
L1103	G1040	E975	L911	R846	P781	A715	L650	D583	I514	V384		R198
E1104	L1041	Q976	K912	D847	S782	F716	R651	D584	A516	G385		L199
L1105	R1042	A977	Q913	R848	R783	Q717	L652		V517	D453		D200
V1106	G1043	R978	L914	A849	D784	P718	F653	P590	P518	A454		G201
V1107	L1044	E979	V915	L850	I785	V719	G654	V591	V519	R388		V202
R1108	M1045	N980	Y916	L851	I786	L720	P655	T592	L520	GLU		A203
L1109	Q1046	G981	Q917	A852	L787	V721	F656	N593	P521	ALA		GLU
A1110	K1047	R982	R983	R853	G788	E722	L657	P594	P522	GLU		L204
L1111	P1048	L983	F919	V853	L789	G723	L658		D523	GLU		Y205
C1112	S1049	T984	L920	L857		Q724	G659	R598	L524	L393		R206
G1113	G1050	D985	R921	V858	I792	S725	R660	P599	R525	GLY		F207
T1114	E1051	R986	L922	D859	T793	I726	R661	L600	P526	GLU		P208
T1115	T1052	E987		L860	Q794	Q727			MET	THR		R209
R1116	Q1053	R988	E925	Q861	V795	L728	G664	L603	VAL	VAL		R210
E1117	E1054	Q989	K926	D862	R796	H729	G665	T604	GLN	TYR		V211
S1118	P1056	D990	T927	R863		F730	L666	D605	VAL	LEU		R212
L1119	I1057	Q991	A928	R864	K799	L731	A667	L606	ASP	THR		
V1120	R1058	I992	R929	T865	X800	V732	F668	L607	GLY	LEU		Y215
P1121	S1059		L930	R866	G801	C733	N669	S608	GLY	ASP		GLU
L1122	F1060	W996	L931	R867		E734	G609	X610	ARG	LEU		VAL
F1123	A1061	T997	L934	V863	L804	A735	A672	Q611	PHE	TRP		R210
Q1124	R1062	E998	K935	G870	E805	F736		Q612	ALA	TRP		R212
P1125	E1063	T999	T936	R871	F806	N737	R675	R613	TS37	ALA		
L1126	G1064	T1000	Y937	K872	R807	A738	L676	F614	SS38	V407		ALA
E1127	L1065	E1001	G938	L873	T808	D739	L677	R615	D539	E408		GLY
V1128	K1066	K1002	F939	R874	P809	F740	E678	R616	L540	E409		LEU
T1129	L1067	V1003	T940	T875	E810		R679	Q616		S410		ARG
R1130	L1068		F941	S876	E811	D743	D682	L618	L543	T411		LEU
S1131	E1069	V1007	S942	R877	A812	Q744		L619	T544	Q412		PRO
L1132	Y1070	F1011	T943	G878	L813	H748	L683	R620	R545	D413		VAL
R1135	F1071	E1012	T944	R879	A815	V749	K684	R621	R546	Q348		GLY
K1136	I1072	E1013	S945	L880	R816	P750	D685	R622	L547	P349		ALA
R1137	S1073	M1014	G946	L881	E817		E686	R623	E549	R483		ALA
D1138	S1074		T947	F882	R818	F754	R687	V623	R549	P484		TRP
L1140	K1079	P1019	D952	R883	R819			R624	R550	A485		VAL
E1141	G1080	L1020	D953	A889	A825	K760	V694	V630	R551	D419		GLU
L1144	D1083	Y1021	A954	R890	P826	I761	L695	T631	A562	V420		VAL
Y1145	T1084	V1022	R955	E891	R828	Q762	G696	V632	R488	L421		LYS
R1146	A1085	M1023	T956	D892	V829	H763	L697	V633	R489	R434		HIS
V1148	L1086	A1024	R957	E893	R830	L764	K698	R634	R495	A422		GLY
L1149	K1087	Q1025	E958	R894	G831	S765	V699	R635	E357	D423		GLY
A1150	L1088	S1026	E959	V895	R832	A766	V700	Q636	A490	G424		ILE
R1151	E1089	A1027	Q962	R897	R833	H767	L701	L637	X491			LYS
L1152	D1090	A1028	T834	R897	T834		L702	R638	A492	G433		VAL
V1153	S1091	R1029	Y963	E898	S835	L770	N703	L639	A563	R360		GLY
									P563	V361		GLY
									L554	E262		ILE
									G561	E436		GLN
									A562	V437		ALA
									R568	D438		LEU
									R569	L439		ALA
									E570	V440		PRO
									K571	V368		GLU
									R572	A369		ALA



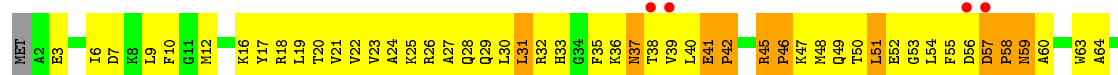
• Molecule 4: DNA-directed RNA polymerase subunit omega

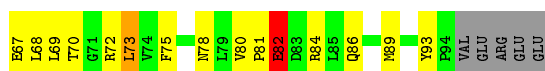


• Molecule 4: DNA-directed RNA polymerase subunit omega

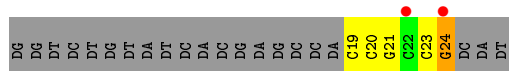


• Molecule 4: DNA-directed RNA polymerase subunit omega





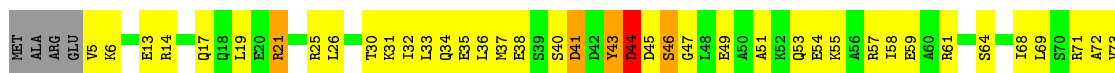
- Molecule 5: DNA (5'-D(*GP*GP*TP*CP*TP*GP*TP*AP*TP*CP*AP*CP*GP*AP*GP*CP*CP*AP*CP*CP*GP*CP*CP*GP*CP*AP*T)-3')



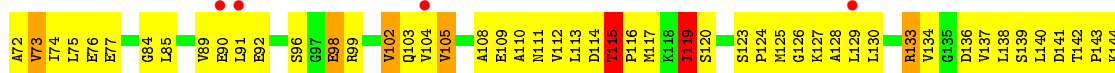
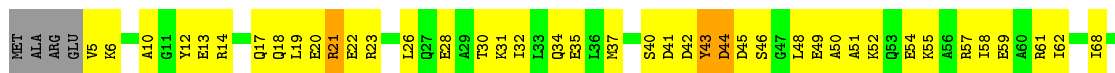
- Molecule 6: RNA (5'-R(*CP*CP*CP*CP*GP*GP*AP*AP*GP*AP*UP*CP*AP*UP*CP*UP*UP*CP*CP*GP*GP*GP*GP*GP*AP*U*GP*CP*GP*GP*CP*GP*G)-3')



- Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



- Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



- Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	192.76Å 260.70Å 198.56Å 90.00° 117.58° 90.00°	Depositor
Resolution (Å)	49.87 – 4.10 49.87 – 4.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.87-4.10) 97.0 (49.87-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 4.14Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.318 0.271 , 0.324	Depositor DCC
R_{free} test set	3932 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	136.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	74250	wwPDB-VP
Average B, all atoms (Å ²)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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: 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	0.44	0/1791	0.75	1/2436 (0.0%)
1	B	0.45	0/1791	0.71	0/2436
1	F	0.47	0/1782	0.76	0/2425
1	G	0.47	0/1791	0.73	0/2436
1	K	0.43	0/1782	0.72	0/2425
1	L	0.45	0/1791	0.71	0/2436
2	C	0.49	0/8900	0.84	12/12038 (0.1%)
2	H	0.52	1/8876 (0.0%)	0.85	13/12006 (0.1%)
2	M	0.48	0/8896	0.80	8/12033 (0.1%)
3	D	0.49	0/10832	0.81	8/14638 (0.1%)
3	I	0.50	0/10351	0.81	13/13979 (0.1%)
3	N	0.48	0/10848	0.81	10/14658 (0.1%)
4	E	0.53	1/768 (0.1%)	0.77	1/1035 (0.1%)
4	J	0.46	0/763	0.77	1/1028 (0.1%)
4	O	0.60	0/768	0.88	3/1035 (0.3%)
5	P	0.94	0/133	1.17	0/202
6	Q	1.22	0/170	1.09	1/265 (0.4%)
7	X	0.40	0/1178	0.74	1/1582 (0.1%)
7	Y	0.41	0/1178	0.74	1/1582 (0.1%)
7	Z	0.41	0/1178	0.76	0/1582
All	All	0.49	2/75567 (0.0%)	0.80	73/102257 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	H	0	1
2	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
3	N	0	1
5	P	0	1
6	Q	0	1
7	Z	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	258	TYR	CB-CG	-5.54	1.43	1.51
4	E	43	GLU	CB-CG	5.46	1.62	1.52

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1097	LEU	CA-CB-CG	10.26	138.90	115.30
3	D	142	LEU	CA-CB-CG	9.03	136.07	115.30
3	D	804	LEU	CA-CB-CG	-8.40	95.97	115.30
3	D	1209	LEU	N-CA-C	-8.10	89.14	111.00
3	N	1209	LEU	N-CA-C	-8.07	89.20	111.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	258	TYR	Sidechain
2	C	71	TYR	Sidechain
2	H	71	TYR	Sidechain
3	I	1070	TYR	Sidechain
2	M	258	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1805	210	0
1	B	1759	0	1805	226	0
1	F	1750	0	1792	251	0
1	G	1759	0	1805	230	0
1	K	1750	0	1792	199	0
1	L	1759	0	1805	196	0
2	C	8733	0	8834	1393	1
2	H	8710	0	8811	1418	2
2	M	8729	0	8831	1386	0
3	D	10651	0	10880	1742	2
3	I	10182	0	10418	1528	0
3	N	10667	0	10894	1632	1
4	E	754	0	769	96	0
4	J	749	0	764	106	0
4	O	754	0	769	107	0
5	P	120	0	67	10	0
6	Q	152	0	78	7	0
7	X	1169	0	1186	114	0
7	Y	1169	0	1186	129	0
7	Z	1169	0	1186	145	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
8	N	1	0	0	0	0
9	D	1	0	0	0	0
9	I	1	0	0	0	0
9	N	1	0	0	0	0
All	All	74250	0	75477	10329	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 69.

The worst 5 of 10329 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:H:282:GLY:O	2:H:283:ILE:HG13	1.34	1.25
3:D:1093:TYR:OH	3:D:1097:LYS:HE3	1.07	1.25
3:D:1093:TYR:OH	3:D:1097:LYS:CE	1.85	1.23
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.20	1.20
3:I:108:VAL:HB	3:I:109:PRO:HD3	1.20	1.19

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)
2:C:223:ASP:O	3:N:562:ALA:O[2_647]	1.66	0.54
3:D:562:ALA:O	2:H:223:ASP:O[2_646]	2.02	0.18
3:D:159:ARG:O	2:H:209:ARG:NH1[2_646]	2.15	0.05

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	221/315 (70%)	181 (82%)	33 (15%)	7 (3%)	4	30
1	B	221/315 (70%)	188 (85%)	28 (13%)	5 (2%)	6	36
1	F	220/315 (70%)	182 (83%)	32 (14%)	6 (3%)	5	33
1	G	221/315 (70%)	190 (86%)	27 (12%)	4 (2%)	8	40
1	K	220/315 (70%)	183 (83%)	29 (13%)	8 (4%)	3	28
1	L	221/315 (70%)	189 (86%)	26 (12%)	6 (3%)	5	33
2	C	1102/1119 (98%)	873 (79%)	169 (15%)	60 (5%)	2	21
2	H	1099/1119 (98%)	882 (80%)	157 (14%)	60 (6%)	2	21
2	M	1101/1119 (98%)	892 (81%)	150 (14%)	59 (5%)	2	21
3	D	1341/1524 (88%)	1055 (79%)	221 (16%)	65 (5%)	2	22
3	I	1281/1524 (84%)	1006 (78%)	216 (17%)	59 (5%)	2	23
3	N	1343/1524 (88%)	1068 (80%)	211 (16%)	64 (5%)	2	22
4	E	91/99 (92%)	71 (78%)	15 (16%)	5 (6%)	2	21
4	J	90/99 (91%)	71 (79%)	14 (16%)	5 (6%)	2	20
4	O	91/99 (92%)	70 (77%)	16 (18%)	5 (6%)	2	21
7	X	150/156 (96%)	119 (79%)	26 (17%)	5 (3%)	4	29
7	Y	150/156 (96%)	121 (81%)	26 (17%)	3 (2%)	7	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Z	150/156 (96%)	123 (82%)	21 (14%)	6 (4%)	3	25
All	All	9313/10584 (88%)	7464 (80%)	1417 (15%)	432 (5%)	2	23

5 of 432 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	226	SER
2	C	44	ILE
2	C	80	GLN
2	C	152	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	196/273 (72%)	170 (87%)	26 (13%)	4	21
1	B	196/273 (72%)	169 (86%)	27 (14%)	3	20
1	F	195/273 (71%)	160 (82%)	35 (18%)	2	11
1	G	196/273 (72%)	165 (84%)	31 (16%)	2	16
1	K	195/273 (71%)	168 (86%)	27 (14%)	3	20
1	L	196/273 (72%)	168 (86%)	28 (14%)	3	18
2	C	932/941 (99%)	740 (79%)	192 (21%)	1	7
2	H	930/941 (99%)	743 (80%)	187 (20%)	1	8
2	M	932/941 (99%)	761 (82%)	171 (18%)	1	10
3	D	1142/1279 (89%)	943 (83%)	199 (17%)	2	12
3	I	1092/1279 (85%)	902 (83%)	190 (17%)	2	12
3	N	1143/1279 (89%)	957 (84%)	186 (16%)	2	14
4	E	82/88 (93%)	70 (85%)	12 (15%)	3	18
4	J	82/88 (93%)	69 (84%)	13 (16%)	2	15
4	O	82/88 (93%)	69 (84%)	13 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	X	128/131 (98%)	114 (89%)	14 (11%)	6 26
7	Y	128/131 (98%)	109 (85%)	19 (15%)	3 17
7	Z	128/131 (98%)	109 (85%)	19 (15%)	3 17
All	All	7975/8955 (89%)	6586 (83%)	1389 (17%)	2 12

5 of 1389 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	504	GLU
3	I	678	GLU
3	N	1208	ASP
2	H	645	VAL
2	H	1097	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 249 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	406	HIS
3	I	593	ASN
3	N	1034	GLN
2	H	498	GLN
2	H	889	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Q	6/33 (18%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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 6 ligands modelled in this entry, 6 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](#)

There are no chain breaks in this entry.

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	223/315 (70%)	-0.30	0 100 100	81, 153, 225, 265	0
1	B	223/315 (70%)	-0.30	0 100 100	97, 154, 223, 265	0
1	F	222/315 (70%)	-0.36	0 100 100	84, 150, 216, 265	0
1	G	223/315 (70%)	-0.35	0 100 100	85, 150, 216, 248	0
1	K	222/315 (70%)	-0.06	1 (0%) 91 85	110, 167, 229, 262	0
1	L	223/315 (70%)	-0.23	0 100 100	103, 164, 222, 265	0
2	C	1106/1119 (98%)	-0.18	20 (1%) 68 59	70, 158, 243, 265	0
2	H	1103/1119 (98%)	-0.16	30 (2%) 54 44	73, 155, 251, 267	0
2	M	1105/1119 (98%)	-0.08	31 (2%) 53 42	79, 166, 255, 265	0
3	D	1349/1524 (88%)	-0.06	44 (3%) 46 37	74, 171, 259, 267	0
3	I	1289/1524 (84%)	-0.05	59 (4%) 32 27	70, 173, 259, 267	0
3	N	1351/1524 (88%)	-0.07	51 (3%) 40 32	76, 167, 254, 267	0
4	E	93/99 (93%)	-0.01	2 (2%) 62 52	114, 183, 262, 265	0
4	J	92/99 (92%)	-0.08	1 (1%) 80 72	92, 176, 254, 265	0
4	O	93/99 (93%)	-0.05	4 (4%) 35 29	99, 173, 246, 265	0
5	P	6/27 (22%)	1.66	2 (33%) 0 0	198, 198, 198, 198	0
6	Q	7/33 (21%)	2.30	4 (57%) 0 0	188, 198, 198, 198	0
7	X	152/156 (97%)	0.14	2 (1%) 77 68	105, 187, 241, 267	0
7	Y	152/156 (97%)	0.10	4 (2%) 56 45	99, 186, 246, 267	0
7	Z	152/156 (97%)	-0.07	1 (0%) 87 82	109, 171, 248, 267	0
All	All	9386/10644 (88%)	-0.11	256 (2%) 54 44	70, 166, 252, 267	0

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	763	GLY	6.7
2	H	765	SER	6.2
2	M	721	ARG	5.8
2	H	764	GLU	5.5
3	D	801	GLY	5.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MG	N	2006	1/1	0.90	0.48	94,94,94,94	0
9	MG	I	2005	1/1	0.92	0.36	94,94,94,94	0
9	MG	D	2004	1/1	0.97	0.08	94,94,94,94	0
8	ZN	D	2001	1/1	0.97	0.06	94,94,94,94	0
8	ZN	I	2002	1/1	0.99	0.07	94,94,94,94	0
8	ZN	N	2003	1/1	0.99	0.08	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.