



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:29 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

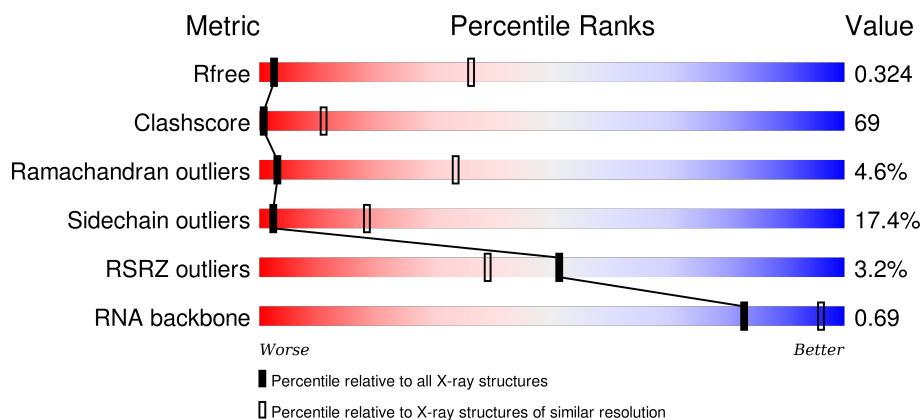
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)
RNA backbone	2183	1079 (5.04-2.80)

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	315	
1	B	315	
1	F	315	
1	G	315	

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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		

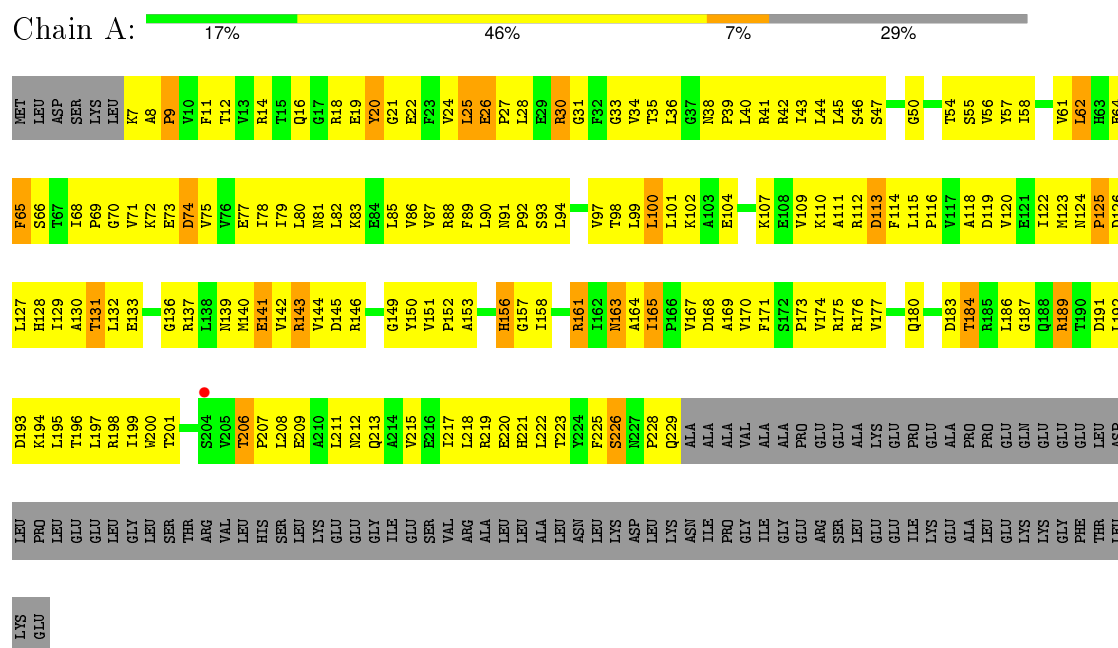
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

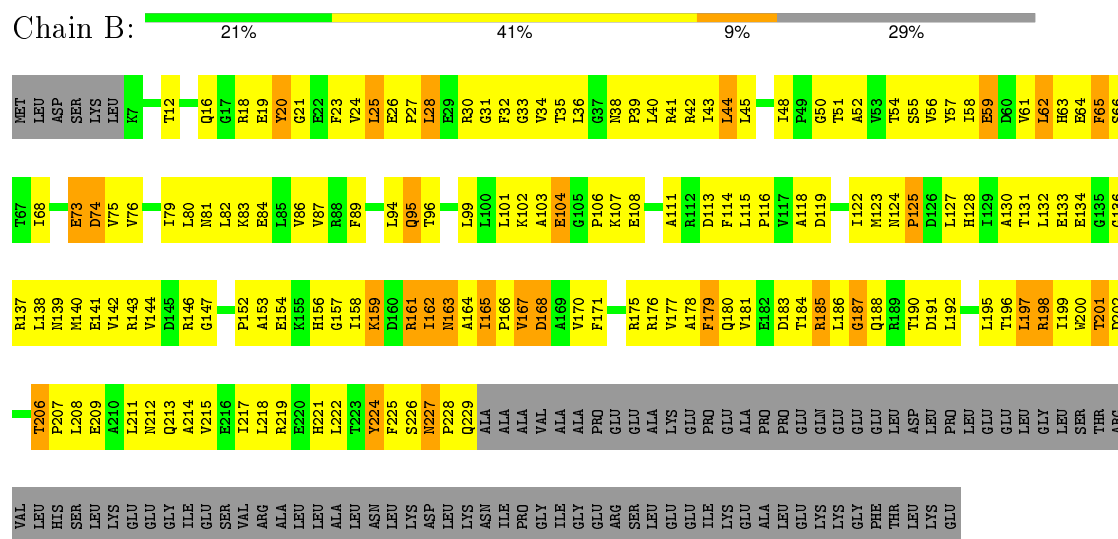
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

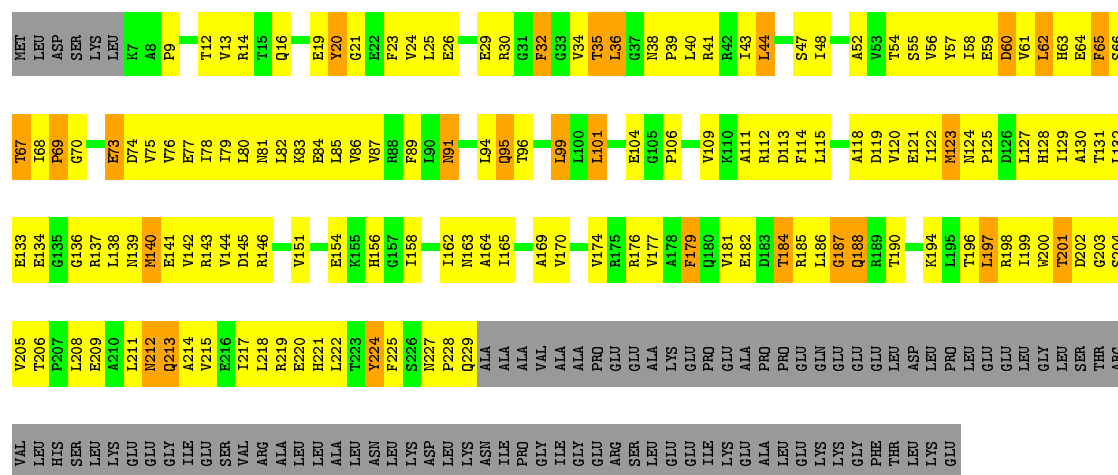
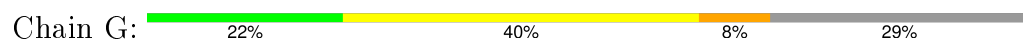
• Molecule 1: DNA-directed RNA polymerase subunit alpha



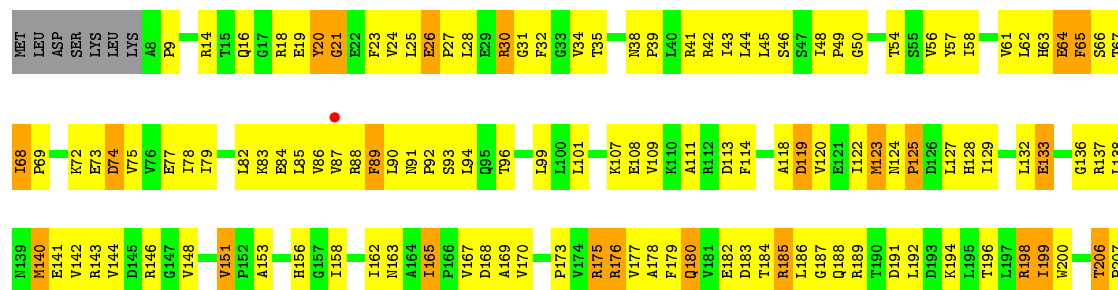
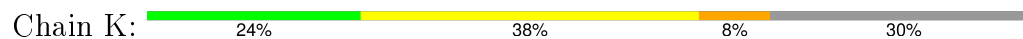
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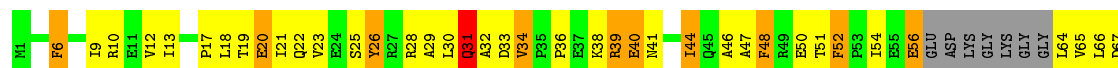


Chain F: 18% 43% 9% 30%



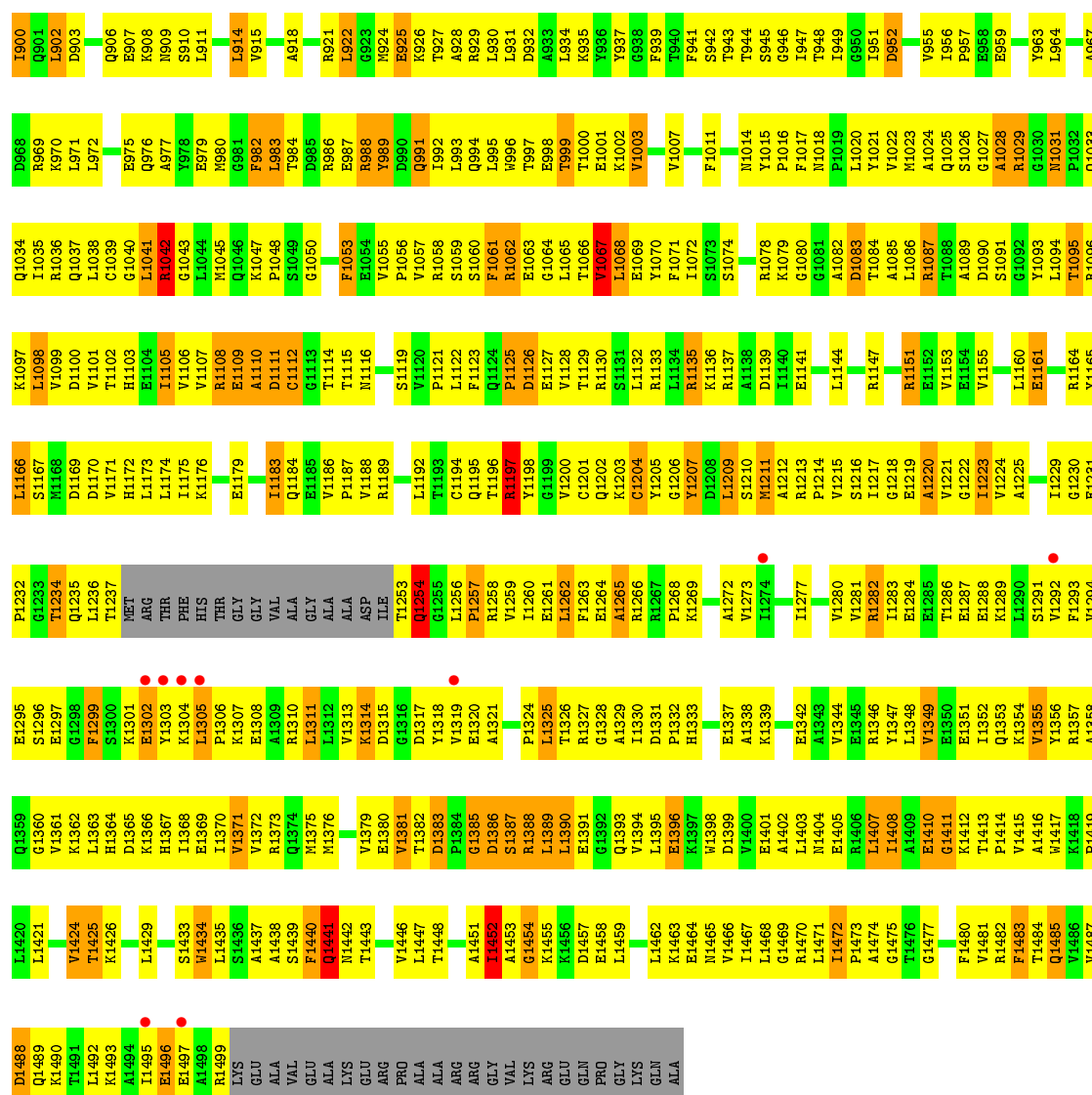
- Molecule 1: DNA-directed RNA polymerase subunit alpha



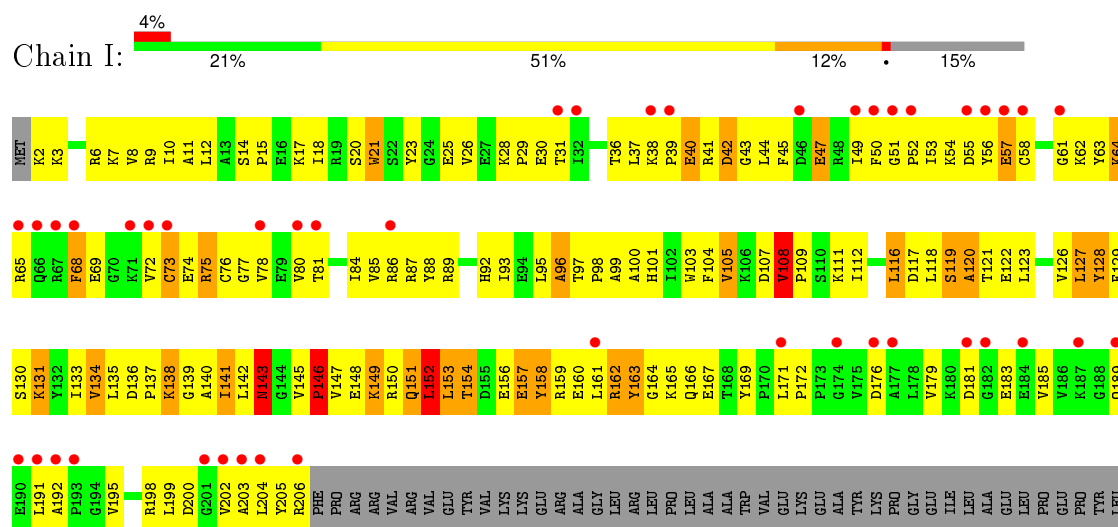


E1034	M1035	V972	Y901	K838	P767	I703	P641	L571	P502	C439	S375	L313	D251	K190	I129	F68
M1036	V973	V973	I902	L839	I768	H704	R642	L572	L503	P440	R376	T314	K252	F191	M130	L69
V1037	L974	V974	S903	R840	P769	I705	V643	A574	B504	V441	R377	A315	A253	L193		E70
M1038	R842	R842	I905	V645	E706	E706	V644	Q575		E442	L378	G316	V254	L194	D133	Y71
A1039	B843	B843	R906	G646	R707	R707	G646		A509	T443	A379	V317	A255	V195	R134	L73
L1040	G977	G977	D907	Q647	I710	I710	Q647	V678	A510	P445	A380	G318	A256	L196	V135	G74
E1041	R978	R978	G908	R648	E711	E711	R648	V579	B511	E447	A381	G319	V257	L197	V136	E75
A1042	T979	T979	A909	V649	A712	A712	V649	P580	B512	I448	R383	E321	G259	R198	P137	P76
Y1043	G980	G980	K910	R650	R713	R713	R650		V513	I449	F385	V322	I261	L200	I140	F78
G1044	E981	E981	E911		D714	D714		L583	V514	L449	F385		G262	G201	H141	P79
A1045	P982	P982	P912	D653	T715	T715	D653	E584	A515	G450	F386	I325	A262	Y202	R142	G80
A1046	K850	K850	E913	L654	R716	R716	L654	E585	R516	L451	F387	R326	D263	G202	R142	
H1047	L852	L852	K915	L655	L717	L717	L655	R586	R517	L452	R388	R327	P264	D203	S143	C83
T1048	L853	L853	K915	A656	G718	G718	A656	V587		T453	R389	L328	R266	Q204	P144	R84
L1049	P854	P854		D657	P719	P719	D657	V588	P521	S454	Q390	G329	R266	E205	G145	E85
Q1050	R855	R855	E919	G658	E720	E720	G658	R589	V522	L455	S392	N330	Y267	T206	V146	E86
E1051	E856	E856	A819	P659	R721	R721	P659	I523	I523	A456	S392	R331	D268	L207	Y147	X86
M1052	D857	D857	Q920	A660	I722	I722	A660	V524	V524	A457	Q393	R332	L269	A208	F148	D87
L1053	R858	R858	A821	S661	T723	T723	S661	L592	S525	Y458	F394	R333	G270	R209	T149	L88
T1054	F922	F922	F922	E662	R724	R724	E662	A593	P526	A459	K395	R334	E271	E210	P150	T89
Q991	G991	G991		N663	I726	I726	N663	Y596	B527	V461	D396	T335	A272	L211	D151	Q91
I1055	I994	I994	Y925	F665	I726	I726	F665	A597	E528	R460	D396	V335	G273	G212	P152	Q91
S1056	N995	N995		L666	P727	P727	L666	E598		D462	R374	G337	R273	A213	A153	A92
S1057	K996	K996		A667			A667	E599		E463	L401	L339	K276	Y214	R154	P93
D1058	L997	L997		L668			L668			L464	S402	R340	A277	G215	P155	L94
D1059	T865	T865	K928	G669	E731	E731	G669	D600	D533	G465	S402	R340	A277	E216	G156	Y95
I1060	R866	R866	K930	E669	A732	A732	E669	G601	V534	F466	S403	T341	E278	L217	R157	A96
E1061	E867	E867	G931	D670	E733	E733	D670	E541	S541	L467	L404	D342	E279	V218	Y158	R97
G1062	M1000	M1000	G795	E670	A734	A734	E670	P536	P536	R468	A412	Q343	K280	Q219	I159	L98
R1063	V1001	V1001	E932	L734	R735	R735	L734	K537	K537	T469	K407	R344	L281	G220	A160	Q99
M1064	G933	G933		L673	R736	R736	L673	Q538	Q538	P470	R408	R345	G282	L221	S161	L100
A1065	L870	L870		V674	L737	L737	V674	V539	V539	Y471	R409	V346	L283	M222	I162	I101
A1066	L871	L871	D937	A675	R738	R738	A675	P540	P540	R472	S411	L348	K284	E223	P163	H102
Y1067	N872	N872	K938	L676	E739	E739	L676	R610	R610	R473	S411	L348	E279	E224	P164	K103
I1070	P873	P873	R939	N677	R740	R740	N677	R610	R610	V474	A412	A349	K285	S225	L165	D104
A1071	L874	L874	E940	P678	R805	R805	P678	V542	V542		I413	R350	T289	V226	P166	T105
R1072	G875	G875	V941	P679	L806	L806	P679	N543	N543	V478	G414	L351	L290	F227	K187	G106
G1073	V876	V876	E942	D680	G741	G741	D680	T544	T544	V479	G415	A352	A291	A228	R168	L107
I1074	P877	P877	V943	G681	V742	V742	G681	B545	B545	T480		R353	R292	E228	G169	I108
E1075	S878	S878	L944	V682	R743	R743	V682	L546	L546	T481		G354	F293	E232	W171	K109
V1076	R879	R879	R945	N683	R744	R744	N683	D817	D817	D481	T419	V355	E294	E232	E110	E110
P1077	N880	N880	R946	P684	A747	A747	P684	P548	P548	V483	R420	R358	D295	E233	I172	D111
	N881	N881		E685	E748	E748	E685	F549	F549	V484	E421	K359	G296	A234	D173	E112
	L882	L882	K949	V686	V749	V749	V686	L550	L550	Y485	R422	R359	E297	L235	L174	V113
	G883	G883	L850	A687	R750	R750	A687	B551	B551	V486	A423	L360	F298	L235	E175	F114
	Q884	Q884	G951	L688	P751	P751	L688	D552	D552	T487	G424	N361	K299	L238	V176	L115
	T885	T885	V953	V689			V689	D554	D554	A488	F425	G362	D300	L238	E177	G116
	L886	L886		I690	I754	I754	I690	A555	A555	T489		S363	E301	F239	P178	H117
	E887	E887		S691	L755	L755	S691	N556	N556	E490		E364	V302	T240	M179	I118
	T888	T888		E692	V756	V756	E692	R630	R630	E491	R428	D365	F303	L241	G180	F119
	H889	H889		E693	G757	G757	E693	S631	S631		D429	D365	L304	L242	V181	L120
	L890	L890		L694	R758	R758	L694	N632	N632	Y494	V430	S366	L304	R243	P182	M121
	G891	G891		L695	T759	T759	L695	Q633	Q633	T495	H431	L367	T306	P244	S183	T122
	L892	L892		G696	S760	S760	G696	G634	G634	T496	R432	T368	L307	G245	E123	M184
	A893	A893		R697	R761	R761	R697	T635	T635	A497	T433	P369	R308	D246	K185	D124
				D698	K762	K762	D698	N563	N563		H434	A370	Y309	P247	V186	G125
	L897	L897		F699	G763	G763	F699	L837	L837	Q498	Y435	K371	Y309	P247	V187	G126
	G898	G898		T700	E764	E764	T700	D638	D638	A499	G436	L372	L310	P248	K187	S126
	Q899	Q899		T701	S765	S765	T701	Q639	Q639	N500	F437	L372	F311	R249	K188	F127
	R900	R900		S702	E766	E766	S702	R640	R640	T501	I438	N374	A312	R250	R189	I128

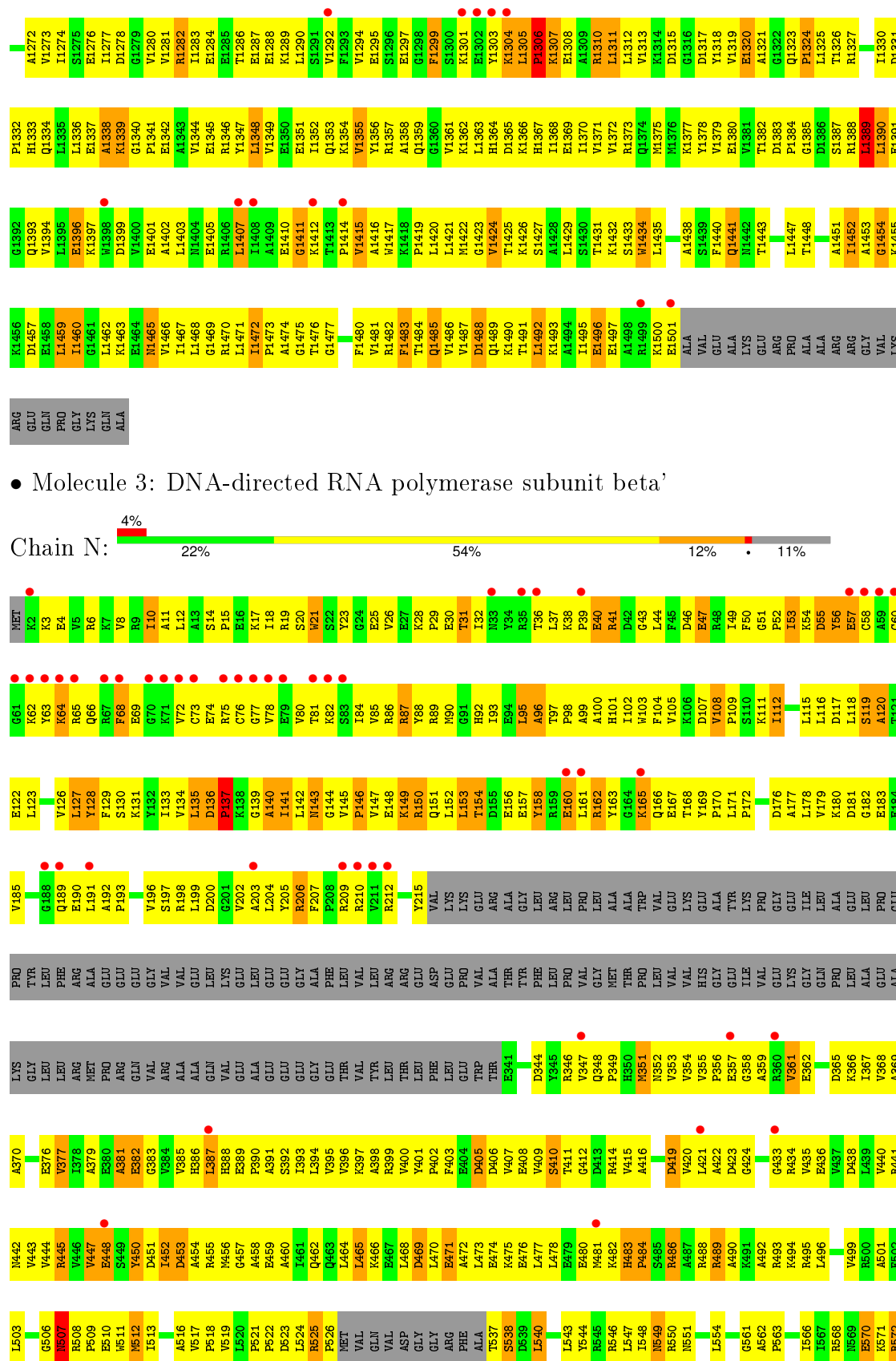




• Molecule 3: DNA-directed RNA polymerase subunit beta'





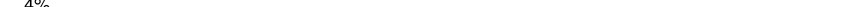


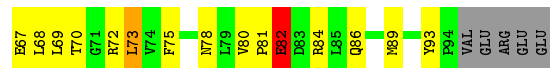
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E1405	R1406	L1407	L1408	A1409	E1410	G1411	K1412	T1413	P1414	V1415	A1416	H1417	K1418	P1419	L1420	L1421	M1422	G1423	L1424	V1425	T1426	K1427	A1428	L1429	K1432	S1433	W1434	L1435	A1436	S1437	F1440	N1442	T1443	L1447	T1448	A1451	I1452	A1453	G1454	K1455	K1456	T1457	E1458	I1459	L1460	G1461	L1462	K1463	E1464	N1465	V1466	E1401	I1467	L1468	G1469																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
E1345	R1346	Y1347	L1348	E1349	E1350	E1351	I1352	Q1353	V1354	V1355	V1356	R1357	A1358	Q1359	G1360	V1361	K1362	L1363	H1364	D1365	K1366	H1367	I1368	E1369	I1370	V1371	V1372	R1373	Q1374	M1375	K1377	F1440	N1442	T1443	L1447	P1384	G1385	D1386	S1387	R1388	L1389	E1391	Q1392	Q1393	V1394	L1395	E1396	K1397	W1398	D1399	G1400	E1401	I1402	L1403	N1404																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
V1280	V1281	L1282	I1283	E1284	E1285	T1286	E1287	E1288	K1289	V1292	F1293	V1294	E1295	G1296	E1297	G1298	F1299	S1300	K1301	E1302	Y1303	H1304	L1305	P1306	K1307	R1310	L1311	L1312	V1313	K1314	D1315	Y1318	V1319	E1320	A1321	P1324	L1325	T1326	R1327	I1330	D1331	P1332	H1333	Q1334	L1335	L1336	E1337	A1338	K1339	G1340	P1341	E1401	I1402	L1403	N1404																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
E1219	A1220	V1221	G1222	I1223	V1224	A1225	L1226	Q1227	S1228	I1229	G1230	E1231	P1232	G1233	T1234	Q1235	L1236	T1237	MET	ARG	THR	PRE	HIS	THR	GLY	GLY	VAL	ALA	ALA	ALA	ASP	I1253	Q1254	G1255	L1256	P1257	V1259	I1260	E1261	L1262	F1263	E1264	A1265	R1266	G1267	P1268	K1269	A1272	V1273	I1274	S1275	E1276	I1277	D1278	G1279																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
V1153	E1154	L1155	L1156	R1159	L1160	E1161	R1164	L1165	L1166	S1167	M1168	D1169	L1170	V1171	H1172	I1175	K1176	E1179	I1183	Q1184	E1185	V1186	P1187	L1188	R1189	S1190	L1191	F1192	L1193	C1194	Q1195	T1196	R1197	Y1198	G1199	V1200	C1201	Q1202	Q1203	C1204	Y1205	G1206	Y1207	D1208	L1209	S1210	M1211	A1212	R1213	P1214	V1215	S1216	G1218																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
S1091	G1092	Y1093	L1094	T1095	R1096	K1097	L1098	V1099	V1100	T1102	H1103	E1104	I1105	V1106	V1107	R1108	E1109	A1110	D1111	C1112	G1113	T1114	T1115	N1116	Y1117	I1118	S1119	V1120	P1121	L1122	F1123	Q1124	P1125	D1126	E1127	V1128	T1129	R1130	L1131	L1132	R1135	K1136	L1137	A1138	D1139	E1140	E1141	L1144	Y1145	G1146	R1147	V1148	L1149	A1150	R1151	E1152																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
R1029	G1030	M1031	Q1032	Q1033	Q1034	L1035	R1036	Q1037	C1038	L1039	G1040	E1041	R1042	G1043	V1044	M1045	G1046	K1047	P1048	D1111	C1112	E1051	T1052	L1053	E1054	P1055	V1056	S1119	V1057	R1058	L1059	S1060	F1061	R1062	G1064	T1065	L1066	Y1067	L1068	E1069	Y1070	F1071	I1072	S1073	S1074	H1075	R1078	K1079	G1080	D1083	Y1084	G1085	L1086	R1087	T1088	D1090																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
E988	L899	Q900	R838	Q901	L839	K840	Y841	V842	L897	R898	K899	L902	Q906	E907	K908	N909	S910	R846	L911	K912	E913	L914	V915	L850	L787	L851	Q917	A918	F919	L893	T994	D985	R986	E987	R988	Y989	D990	Q991	R992	L995	Y996	F1001	T997	E998	T999	T1000	E1001	K1002	V1003	V1007	F1011	E1012	E1013	Y1015	P1016	F1017	M1018	P1019	D953	A989	V890	E991	V955	M1022	R956	D892	E933	K994	E986	E959	A996	W897																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
S835	V836	G837	R838	Q901	L839	K840	Y841	V842	L897	R898	K899	L902	Q906	E907	K908	N909	S910	R846	L911	K912	E913	L914	V915	L850	L787	L851	Q917	A918	F919	L893	T994	D985	R986	E987	R988	Y989	D990	Q991	R992	L995	Y996	F1001	T997	E998	T999	T1000	E1001	K1002	V1003	V1007	F1011	E1012	E1013	Y1015	P1016	F1017	M1018	P1019	D953	A989	V890	E991	V955	M1022	R956	D892	E933	K994	E986	E959	A996	W897																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
S771	P772	S773	S774	S775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
R704	A705	P706	R707	R708	R709	R710	L711	G712	Q713	Q714	Q715	Q716	Q717	Q718	Q719	Q720	Q721	Q722	Q723	Q724	Q725	Q726	Q727	Q728	Q729	Q730	Q731	Q732	Q733	Q734	Q735	Q736	Q737	Q738	Q739	Q740	Q741	Q742	Q743	Q744	Q745	Q746	Q747	Q748	Q749	Q750	Q751	Q752	Q753	Q754	Q755	Q756	Q757	Q758	Q759	Q760	Q761	Q762	Q763	Q764	Q765	Q766	Q767	Q768	Q769	Q770	Q771	Q772	Q773	Q774	Q775	Q776	Q777	Q778	Q779	Q780	Q781	Q782	Q783	Q784	Q785	Q786	Q787	Q788	Q789	Q790	Q791	Q792	Q793	Q794	Q795	Q796	Q797	Q798	Q799	Q800	Q801	Q802	Q803	Q804	Q805	Q806	Q807	Q808	Q809	Q810	Q811	Q812	Q813	Q814	Q815	Q816	Q817	Q818	Q819	Q820	Q821	Q822	Q823	Q824	Q825	Q826	Q827	Q828	Q829	Q830	Q831	Q832	Q833	Q834	Q835	Q836	Q837	Q838	Q839	Q840	Q841	Q842	Q843	Q844	Q845	Q846	Q847	Q848	Q849	Q850	Q851	Q852	Q853	Q854	Q855	Q856	Q857	Q858	Q859	Q860	Q861	Q862	Q863	Q864	Q865	Q866	Q867	Q868	Q869	Q870	Q871	Q872	Q873	Q874	Q875	Q876	Q877	Q878	Q879	Q880	Q881	Q882	Q883	Q884	Q885	Q886	Q887	Q888	Q889	Q890	Q891	Q892	Q893	Q894	Q895	Q896	Q897	Q898	Q899	Q900	Q901	Q902	Q903	Q904	Q905	Q906	Q907	Q908	Q909	Q910	Q911	Q912	Q913	Q914	Q915	Q916	Q917	Q918	Q919	Q920	Q921	Q922	Q923	Q924	Q925	Q926	Q927	Q928	Q929	Q930	Q931	Q932	Q933	Q934	Q935	Q936	Q937	Q938	Q939	Q940	Q941	Q942	Q943	Q944	Q945	Q946	Q947	Q948	Q949	Q950	Q951	Q952	Q953	Q954	Q955	Q956	Q957	Q958	Q959	Q960	Q961	Q962	Q963	Q964	Q965	Q966	Q967	Q968	Q969	Q970	Q971	Q972	Q973	Q974	Q975	Q976	Q977	Q978	Q979	Q980	Q981	Q982	Q983	Q984	Q985	Q986	Q987	Q988	Q989	Q990	Q991	Q992	Q993	Q994	Q995	Q996	Q997	Q998	Q999	Q1000	Q1001	Q1002	Q1003	Q1004	Q1005	Q1006	Q1007	Q1008	Q1009	Q1010	Q1011	Q1012	Q1013	Q1014	Q1015	Q1016	Q1017	Q1018	Q1019	Q1020	Q1021	Q1022	Q1023	Q1024	Q1025	Q1026	Q1027	Q1028	Q1029	Q1030	Q1031	Q1032	Q1033	Q1034	Q1035	Q1036	Q1037	Q1038	Q1039	Q1040	Q1041	Q1042	Q1043	Q1044	Q1045	Q1046	Q1047	Q1048	Q1049	Q1050	Q1051	Q1052	Q1053	Q1054	Q1055	Q1056	Q1057	Q1058	Q1059	Q1060	Q1061	Q1062	Q1063	Q1064	Q1065	Q1066	Q1067	Q1068	Q1069	Q1070	Q1071	Q1072	Q1073	Q1074	Q1075	Q1076	Q1077	Q1078	Q1079	Q1080	Q1081	Q1082	Q1083	Q1084	Q1085	Q1086	Q1087	Q1088	Q1089	Q1090	Q1091	Q1092	Q1093	Q1094	Q1095	Q1096	Q1097	Q1098	Q1099	Q1100	Q1101	Q1102	Q1103	Q1104	Q1105	Q1106	Q1107	Q1108	Q1109	Q1110	Q1111	Q1112	Q1113	Q1114	Q1115	Q1116	Q1117	Q1118	Q1119	Q1120	Q1121	Q1122	Q1123	Q1124	Q1125	Q1126	Q1127	Q1128	Q1129	Q1130	Q1131	Q1132	Q1133	Q1134	Q1135	Q1136	Q1137	Q1138	Q1139	Q1140	Q1141	Q1142	Q1143	Q1144	Q1145	Q1146	Q1147	Q1148	Q1149	Q1150	Q1151	Q1152	Q1153	Q1154	Q1155	Q1156	Q1157	Q1158	Q1159	Q1160	Q1161	Q1162	Q1163	Q1164	Q1165	Q1166	Q1167	Q1168	Q1169	Q1170	Q1171	Q1172	Q1173	Q1174	Q1175	Q1176	Q1177	Q1178	Q1179	Q1180	Q1181	Q1182	Q1183	Q1184	Q1185	Q1186	Q1187	Q1188	Q1189	Q1190	Q1191	Q1192	Q1193	Q1194	Q1195	Q1196	Q1197	Q1198	Q1199	Q1200	Q1201	Q1202	Q1203	Q1204	Q1205	Q1206	Q1207	Q1208	Q1209	Q1210	Q1211	Q1212	Q1213	Q1214	Q1215	Q1216	Q1217	Q1218	Q1219	Q1220	Q1221	Q1222	Q1223	Q1224	Q1225	Q1226	Q1227	Q1228	Q1229	Q1230	Q1231	Q1232	Q1233	Q1234	Q1235	Q1236	Q1237	Q1238	Q1239	Q1240	Q1241	Q1242	Q1243	Q1244	Q1245	Q1246	Q1247	Q1248	Q1249	Q1250	Q1251	Q1252	Q1253	Q1254	Q1255	Q1256	Q1257	Q1258	Q1259	Q1260	Q1261	Q1262	Q1263	Q1264	Q1265	Q1266	Q1267	Q1268	Q1269	Q1270	Q1271	Q1272	Q1273	Q1274	Q1275	Q1276	Q1277	Q1278	Q1279	Q1280	Q1281	Q1282	Q1283	Q1284	Q1285	Q1286	Q1287	Q1288	Q1289	Q1290	Q1291	Q1292	Q1293	Q1294	Q1295	Q1296	Q1297	Q1298	Q1299	Q1300	Q1301	Q1302	Q1303	Q1304	Q1305	Q1306	Q1307	Q1308	Q1309	Q1310	Q1311	Q1312	Q1313	Q1314	Q1315	Q1316	Q1317	Q1318	Q1319	Q1320	Q1321	Q1322	Q1323	Q1324	Q1325	Q1326	Q1327	Q1328	Q1329	Q1330	Q1331	Q1332	Q1333	Q1334	Q1335	Q1336	Q1337	Q1338	Q1339	Q1340	Q1341	Q1342	Q1343	Q1344	Q1345	Q1346	Q1347	Q1348	Q1349	Q1350	Q1351	Q1352	Q1353	Q1354	Q1355	Q1356	Q1357	Q1358	Q1359	Q1360	Q1361	Q1362	Q1363	Q1364	Q1365	Q1366	Q1367	Q1368	Q1369	Q1370	Q1371	Q1372	Q1373	Q1374	Q1375	Q1376	Q1377	Q1378	Q1379	Q1380	Q1381	Q1382	Q1383	Q1384	Q1385	Q1386	Q1387	Q1388





- [illegible]



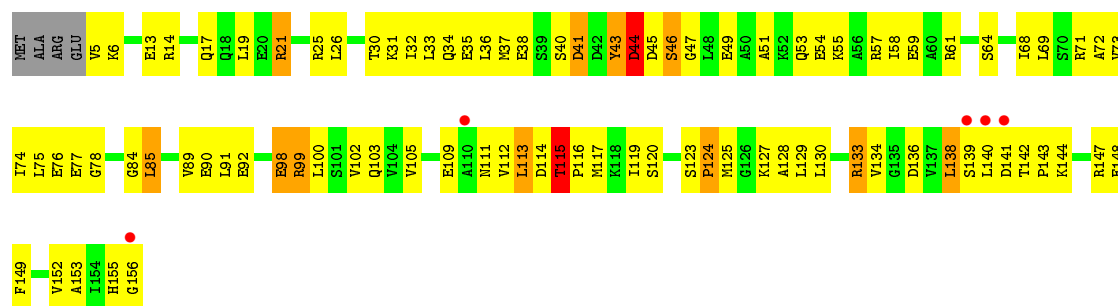
- Chain O: 



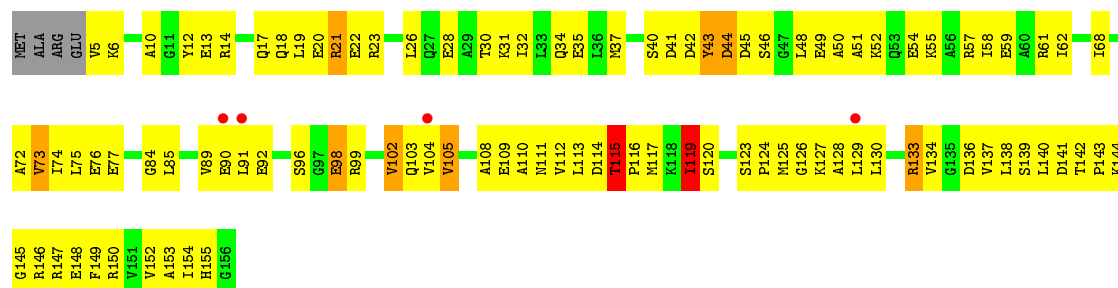
- Chain P: 
- 

- Chain Q:
-
- | Category | Percentage |
|----------|------------|
| Red | 12% |
| Green | 12% |
| Yellow | 6% |
| Red | 1% |
| Grey | 79% |

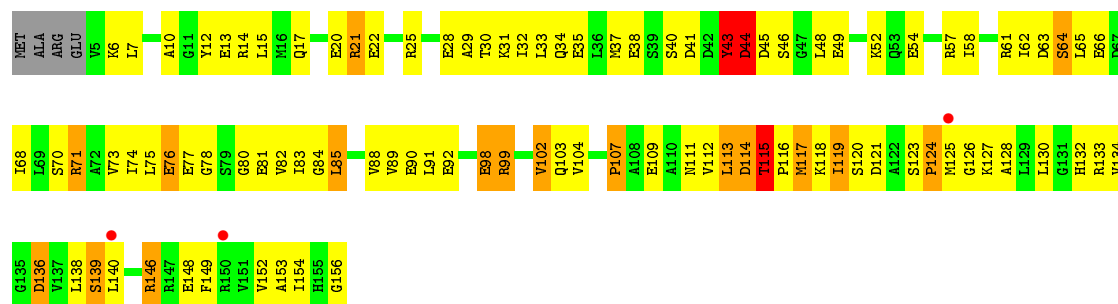
- Chain X: 



• 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%)	DCC
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 , 83.3	EDS
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 131785 reflections	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, 0.375 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: 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%)	5	43
1	B	221/315 (70%)	188 (85%)	28 (13%)	5 (2%)	8	50
1	F	220/315 (70%)	182 (83%)	32 (14%)	6 (3%)	6	47
1	G	221/315 (70%)	190 (86%)	27 (12%)	4 (2%)	11	55
1	K	220/315 (70%)	183 (83%)	29 (13%)	8 (4%)	4	41
1	L	221/315 (70%)	189 (86%)	26 (12%)	6 (3%)	6	47
2	C	1102/1119 (98%)	873 (79%)	169 (15%)	60 (5%)	2	30
2	H	1099/1119 (98%)	882 (80%)	157 (14%)	60 (6%)	2	30
2	M	1101/1119 (98%)	892 (81%)	150 (14%)	59 (5%)	2	30
3	D	1341/1524 (88%)	1055 (79%)	221 (16%)	65 (5%)	3	32
3	I	1281/1524 (84%)	1006 (78%)	216 (17%)	59 (5%)	3	33
3	N	1343/1524 (88%)	1068 (80%)	211 (16%)	64 (5%)	3	32
4	E	91/99 (92%)	71 (78%)	15 (16%)	5 (6%)	2	30
4	J	90/99 (91%)	71 (79%)	14 (16%)	5 (6%)	2	29
4	O	91/99 (92%)	70 (77%)	16 (18%)	5 (6%)	2	30
7	X	150/156 (96%)	119 (79%)	26 (17%)	5 (3%)	5	43
7	Y	150/156 (96%)	121 (81%)	26 (17%)	3 (2%)	9	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Z	150/156 (96%)	123 (82%)	21 (14%)	6 (4%)	4	37
All	All	9313/10584 (88%)	7464 (80%)	1417 (15%)	432 (5%)	3	33

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%)	5	30
1	B	196/273 (72%)	169 (86%)	27 (14%)	4	29
1	F	195/273 (71%)	160 (82%)	35 (18%)	2	17
1	G	196/273 (72%)	165 (84%)	31 (16%)	3	23
1	K	195/273 (71%)	168 (86%)	27 (14%)	4	29
1	L	196/273 (72%)	168 (86%)	28 (14%)	4	28
2	C	932/941 (99%)	740 (79%)	192 (21%)	1	12
2	H	930/941 (99%)	743 (80%)	187 (20%)	1	13
2	M	932/941 (99%)	761 (82%)	171 (18%)	2	16
3	D	1142/1279 (89%)	943 (83%)	199 (17%)	2	18
3	I	1092/1279 (85%)	902 (83%)	190 (17%)	2	18
3	N	1143/1279 (89%)	957 (84%)	186 (16%)	3	22
4	E	82/88 (93%)	70 (85%)	12 (15%)	4	26
4	J	82/88 (93%)	69 (84%)	13 (16%)	3	23
4	O	82/88 (93%)	69 (84%)	13 (16%)	3	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	X	128/131 (98%)	114 (89%)	14 (11%)	8	39
7	Y	128/131 (98%)	109 (85%)	19 (15%)	4	26
7	Z	128/131 (98%)	109 (85%)	19 (15%)	4	26
All	All	7975/8955 (89%)	6586 (83%)	1389 (17%)	2	18

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%)	-0.26	1 (0%) 93 90	81, 153, 225, 265	0
1	B	223/315 (70%)	-0.27	0 100 100	97, 154, 223, 265	0
1	F	222/315 (70%)	-0.33	0 100 100	84, 150, 216, 265	0
1	G	223/315 (70%)	-0.31	0 100 100	85, 150, 216, 248	0
1	K	222/315 (70%)	-0.02	1 (0%) 91 88	110, 167, 229, 262	0
1	L	223/315 (70%)	-0.19	0 100 100	103, 164, 222, 265	0
2	C	1106/1119 (98%)	-0.14	24 (2%) 65 55	70, 158, 243, 265	0
2	H	1103/1119 (98%)	-0.13	31 (2%) 56 45	73, 155, 251, 267	0
2	M	1105/1119 (98%)	-0.04	36 (3%) 50 38	79, 166, 255, 265	0
3	D	1349/1524 (88%)	-0.02	53 (3%) 43 33	74, 171, 259, 267	0
3	I	1289/1524 (84%)	-0.01	67 (5%) 31 23	70, 173, 259, 267	0
3	N	1351/1524 (88%)	-0.03	57 (4%) 40 31	76, 167, 254, 267	0
4	E	93/99 (93%)	0.04	2 (2%) 65 55	114, 183, 262, 265	0
4	J	92/99 (92%)	-0.04	2 (2%) 65 55	92, 176, 254, 265	0
4	O	93/99 (93%)	-0.01	4 (4%) 39 29	99, 173, 246, 265	0
5	P	6/27 (22%)	1.87	3 (50%) 0 1	198, 198, 198, 198	0
6	Q	7/33 (21%)	2.65	4 (57%) 0 1	188, 198, 198, 198	0
7	X	152/156 (97%)	0.20	5 (3%) 50 38	105, 187, 241, 267	0
7	Y	152/156 (97%)	0.15	4 (2%) 59 48	99, 186, 246, 267	0
7	Z	152/156 (97%)	-0.03	3 (1%) 68 58	109, 171, 248, 267	0
All	All	9386/10644 (88%)	-0.07	297 (3%) 51 39	70, 166, 252, 267	0

The worst 5 of 297 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	763	GLY	6.9
2	H	765	SER	6.4
2	M	721	ARG	6.0
3	D	801	GLY	5.8
2	H	764	GLU	5.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	ZN	N	2003	1/1	0.98	0.08	-1.07	94,94,94,94	0
8	ZN	D	2001	1/1	0.97	0.06	-1.17	94,94,94,94	0
8	ZN	I	2002	1/1	0.99	0.07	-1.19	94,94,94,94	0
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

6.5 Other polymers [i](#)

There are no such residues in this entry.