



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 02:17 AM UTC

PDB ID : 3AOI / pdb_00003aoi
Title : RNA polymerase-Gfh1 complex (Crystal type 2)
Authors : Tagami, S.; Sekine, S.; Kumarevel, T.; Yamamoto, M.; Yokoyama, S.; RIKEN
Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2010-09-30
Resolution : 4.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

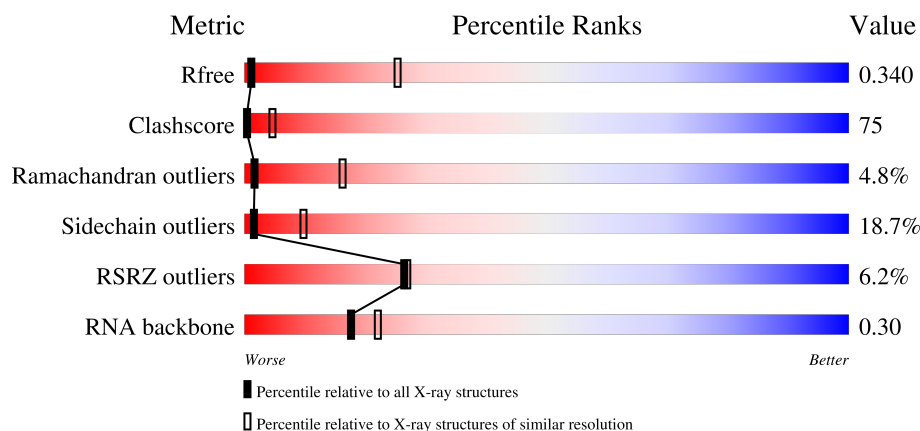
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)
RNA backbone	3983	1036 (5.50-3.10)

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 of 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	2% 17% 43% 10% 29%
1	B	315	3% 19% 40% 12% 29%
1	F	315	4% 19% 41% 10% 29%
1	G	315	3% 20% 38% 12% 29%

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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	
5	R	27	
5	T	27	
6	Q	32	
6	S	32	
6	U	32	
7	X	156	
7	Y	156	
7	Z	156	

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
9	MG	S	2005	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 73646 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	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	G	224	Total	C	N	O	S	0	0	0
			1764	1126	307	329	2			
1	K	225	Total	C	N	O	S	0	0	0
			1769	1129	308	330	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	1083	Total	C	N	O	S	0	0	0
			8550	5413	1525	1588	24			
2	H	1080	Total	C	N	O	S	0	0	0
			8524	5395	1521	1584	24			
2	M	1084	Total	C	N	O	S	0	0	0
			8555	5413	1528	1590	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1316	Total	C	N	O	S	0	0	0
			10384	6574	1840	1941	29			
3	I	1262	Total	C	N	O	S	0	0	0
			9965	6314	1765	1858	28			
3	N	1327	Total	C	N	O	S	0	0	0
			10475	6634	1852	1961	28			

- 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	93	Total	C	N	O	S	0	0	0
			754	481	131	138	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*A*CP*CP*GP*CP*CP*GP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	7	Total	C	N	O	P	0	0	0
			136	65	25	40	6			
5	R	6	Total	C	N	O	P	0	0	0
			119	57	24	33	5			
5	T	5	Total	C	N	O	P	0	0	0
			98	47	19	28	4			

- Molecule 6 is a RNA chain called RNA (5'-R(*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			
6	S	8	Total	C	N	O	P	0	0	0
			172	77	33	55	7			
6	U	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	154	Total	C	N	O	S	0	0	0
			1189	730	212	243	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 (CCD ID: ZN) (formula: Zn).

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

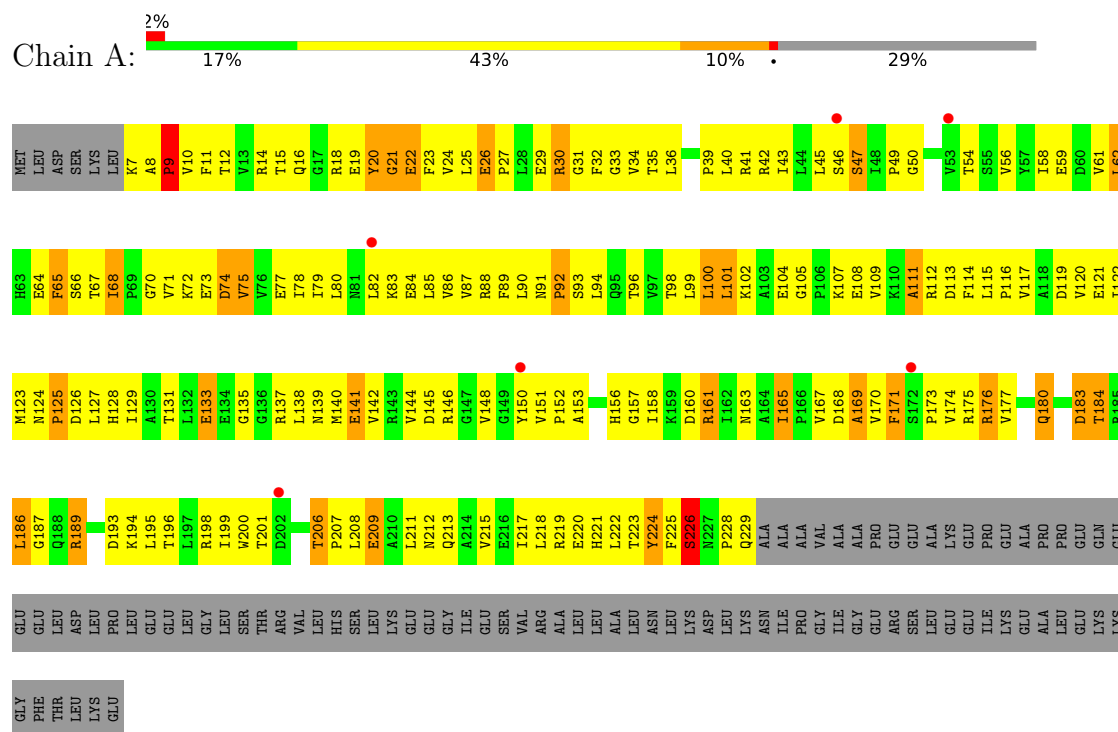
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

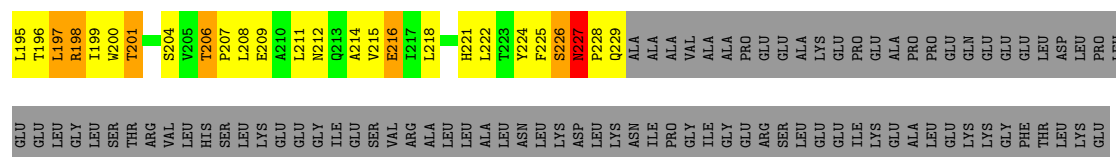
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total 1	Mg 1	0	0
9	N	1	Total 1	Mg 1	0	0
9	S	1	Total 1	Mg 1	0	0

3 Residue-property plots

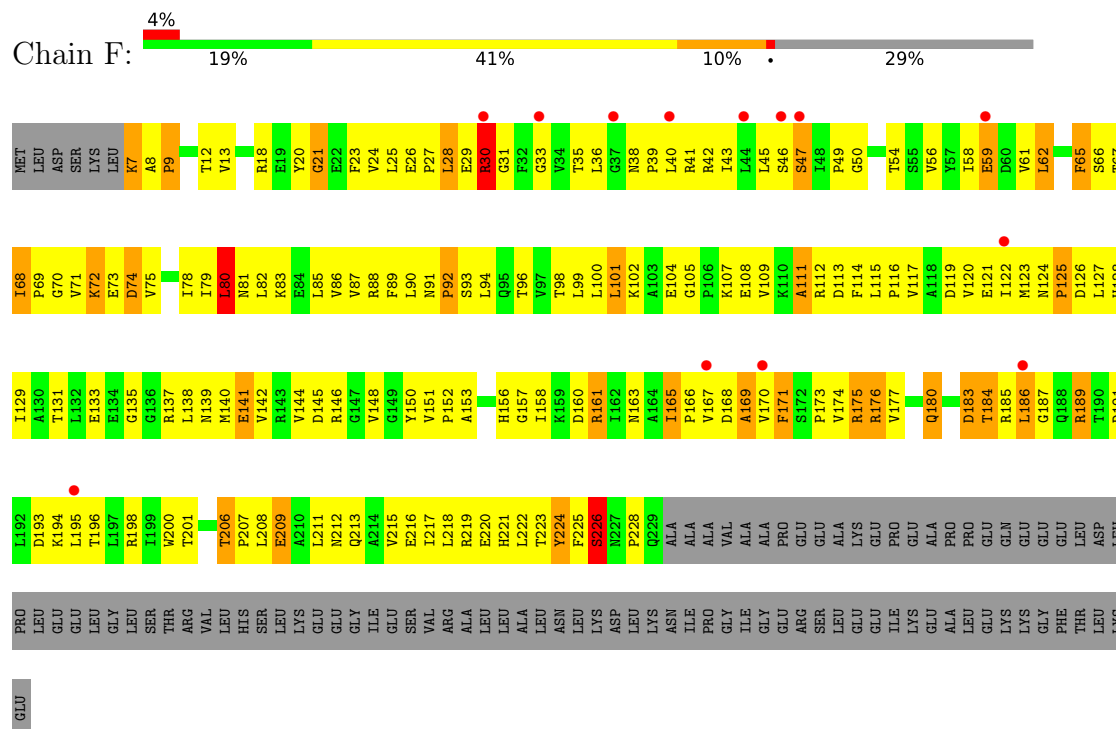
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

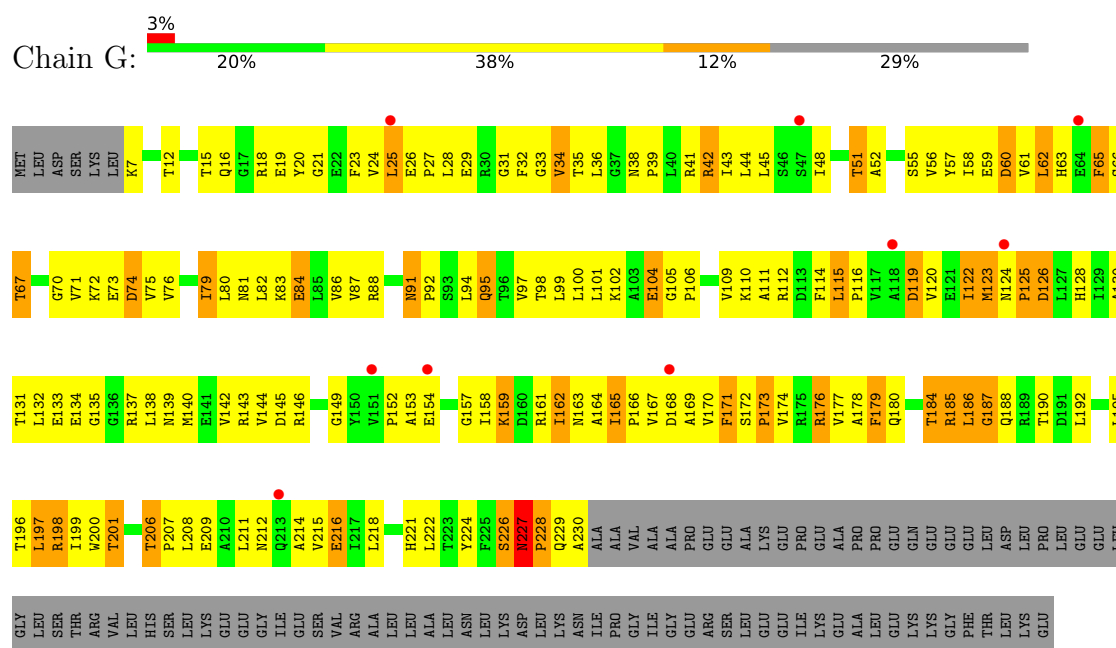




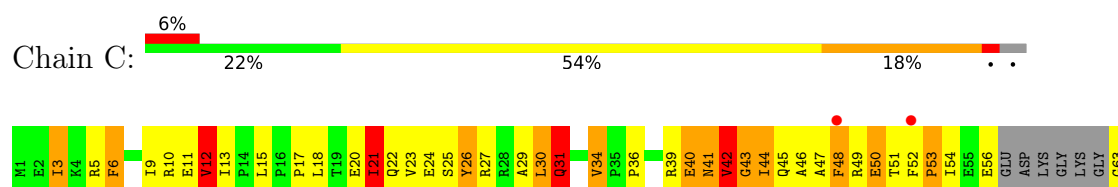
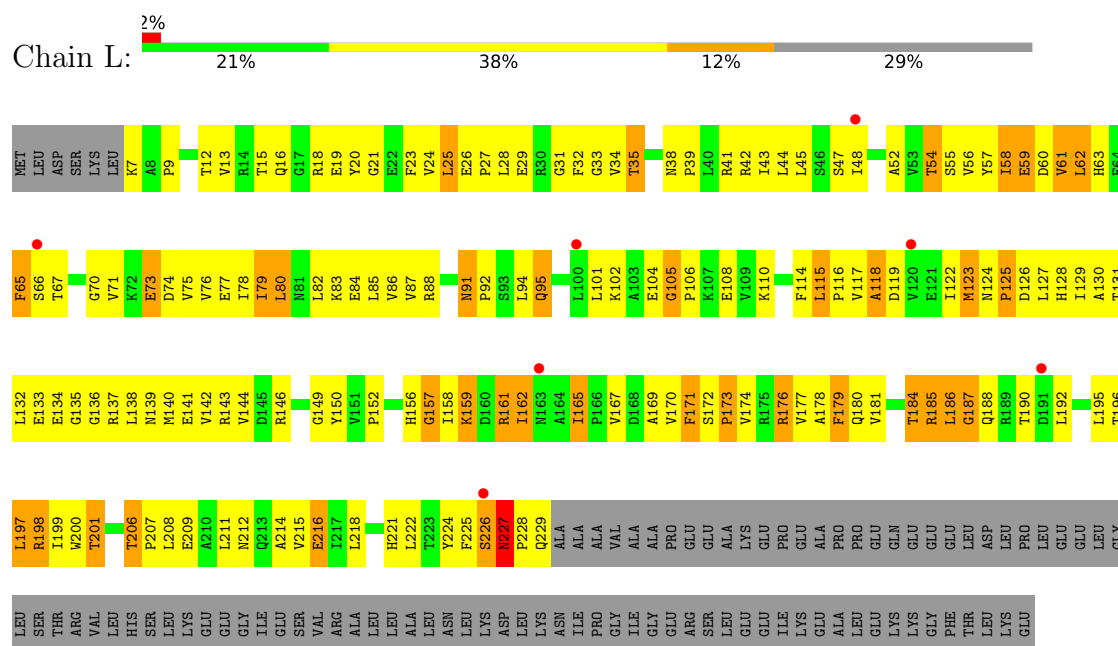
• Molecule 1: DNA-directed RNA polymerase subunit alpha



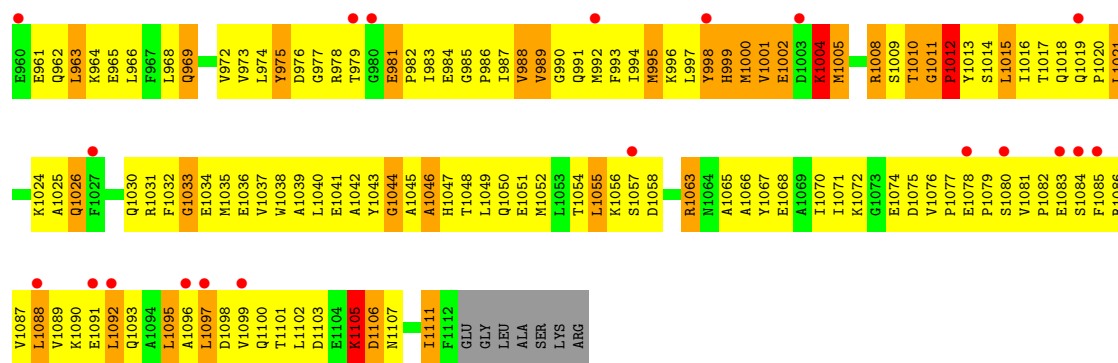
• Molecule 1: DNA-directed RNA polymerase subunit alpha



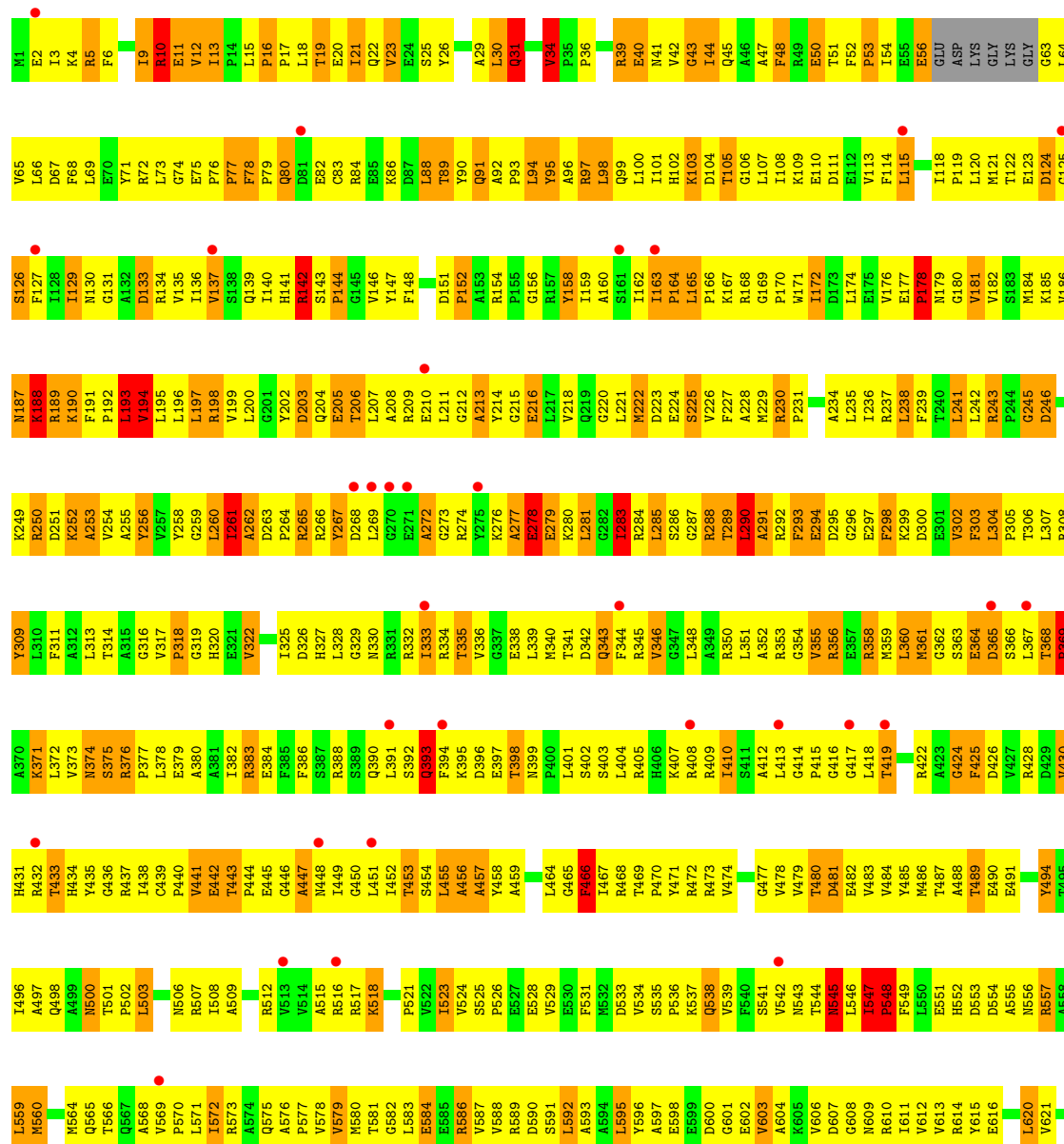
• Molecule 1: DNA-directed RNA polymerase subunit alpha

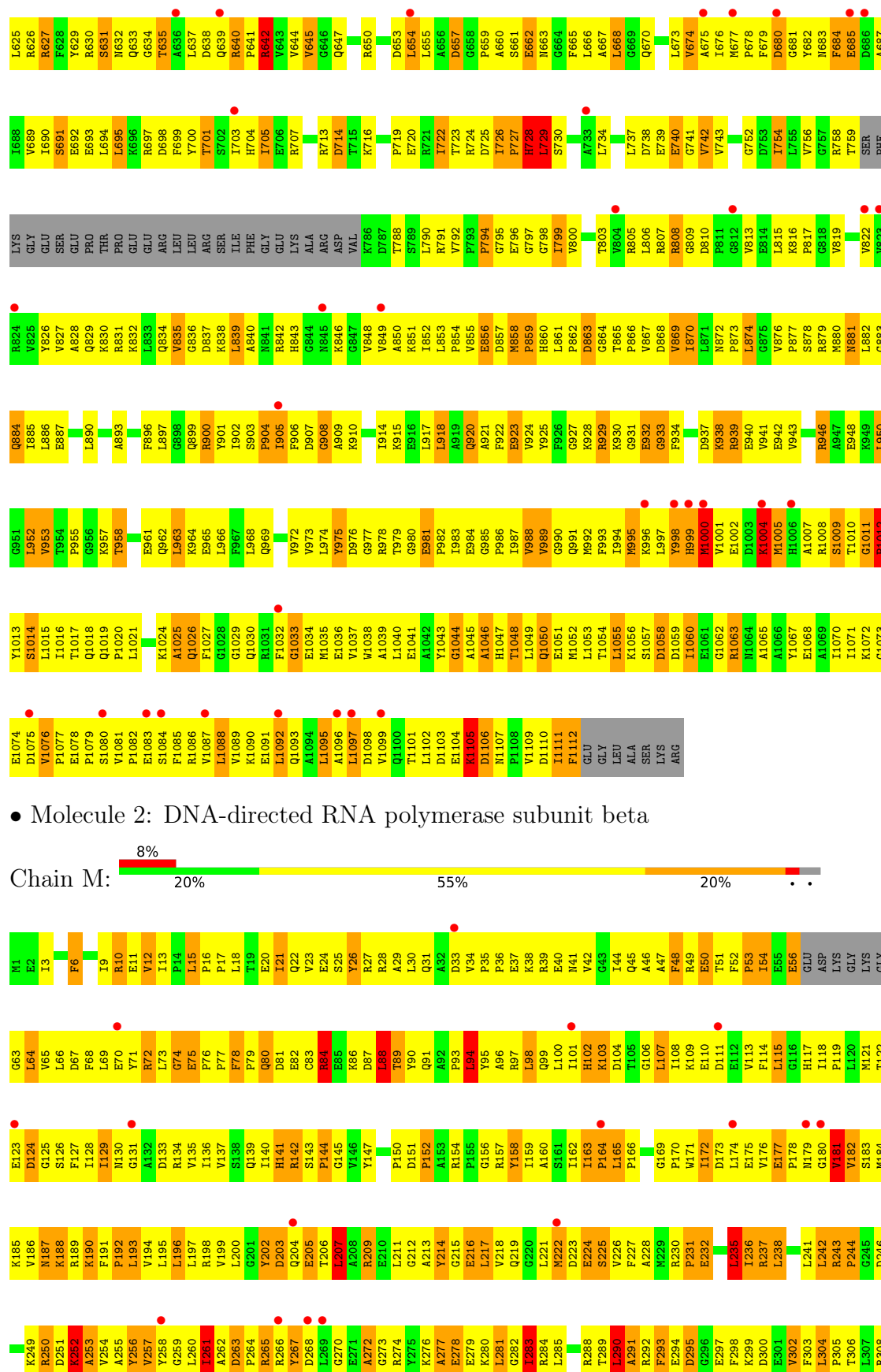


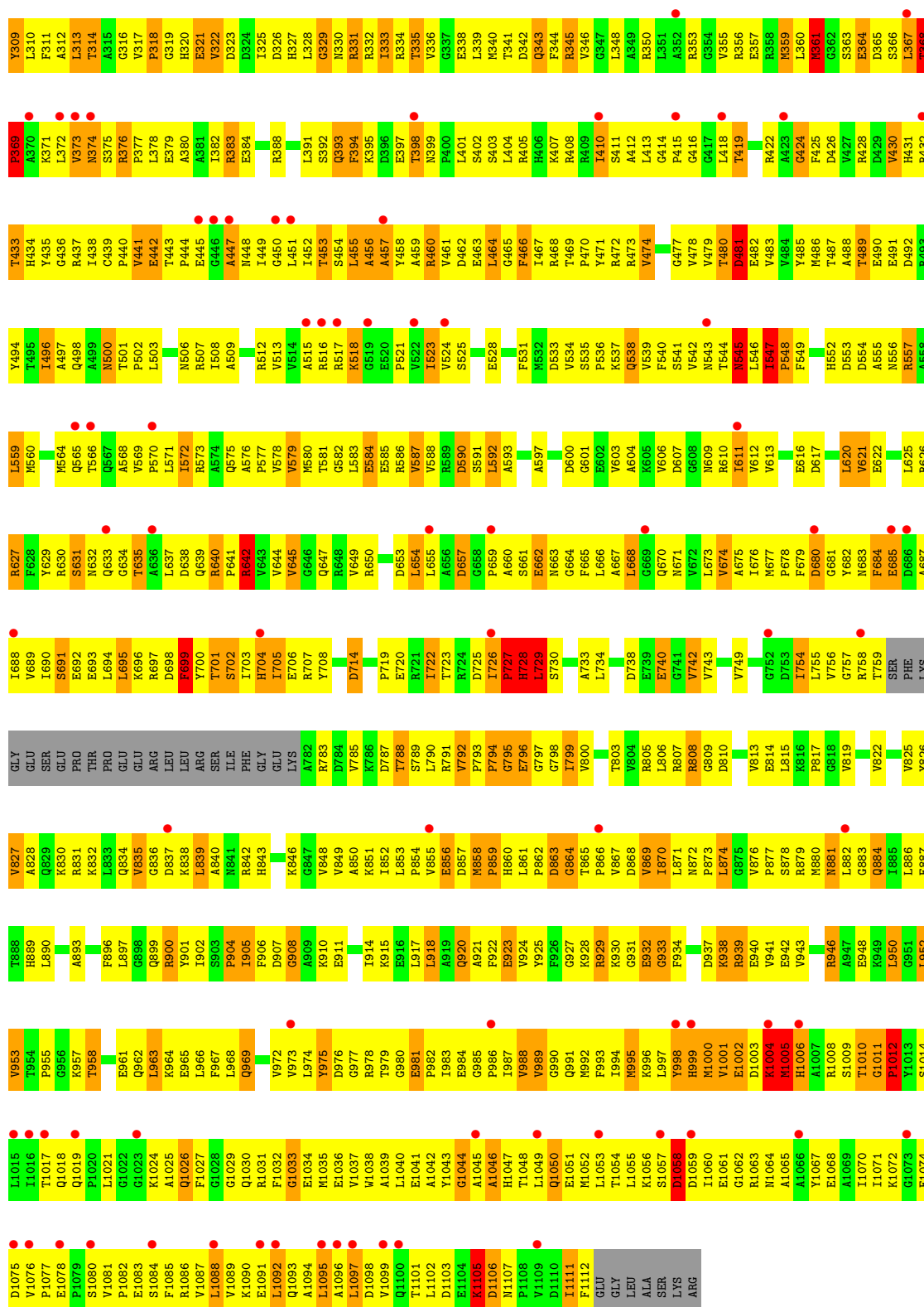
WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 2: DNA-directed RNA polymerase subunit beta



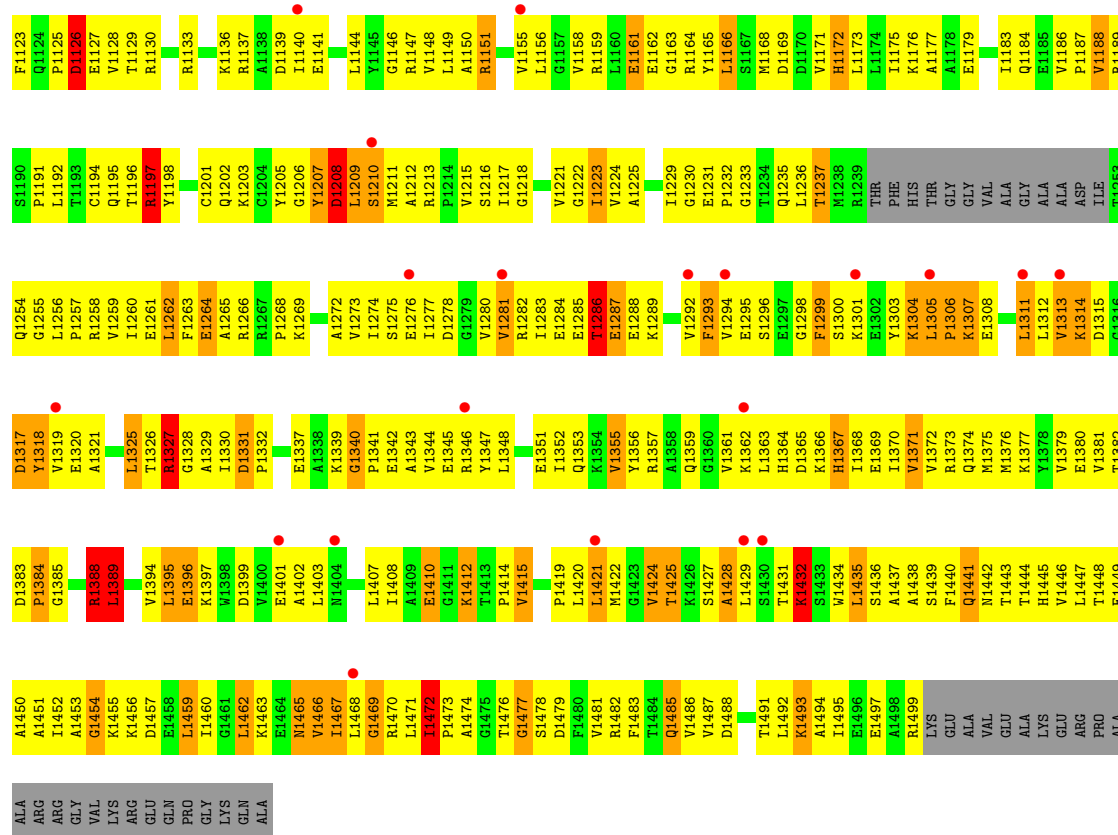




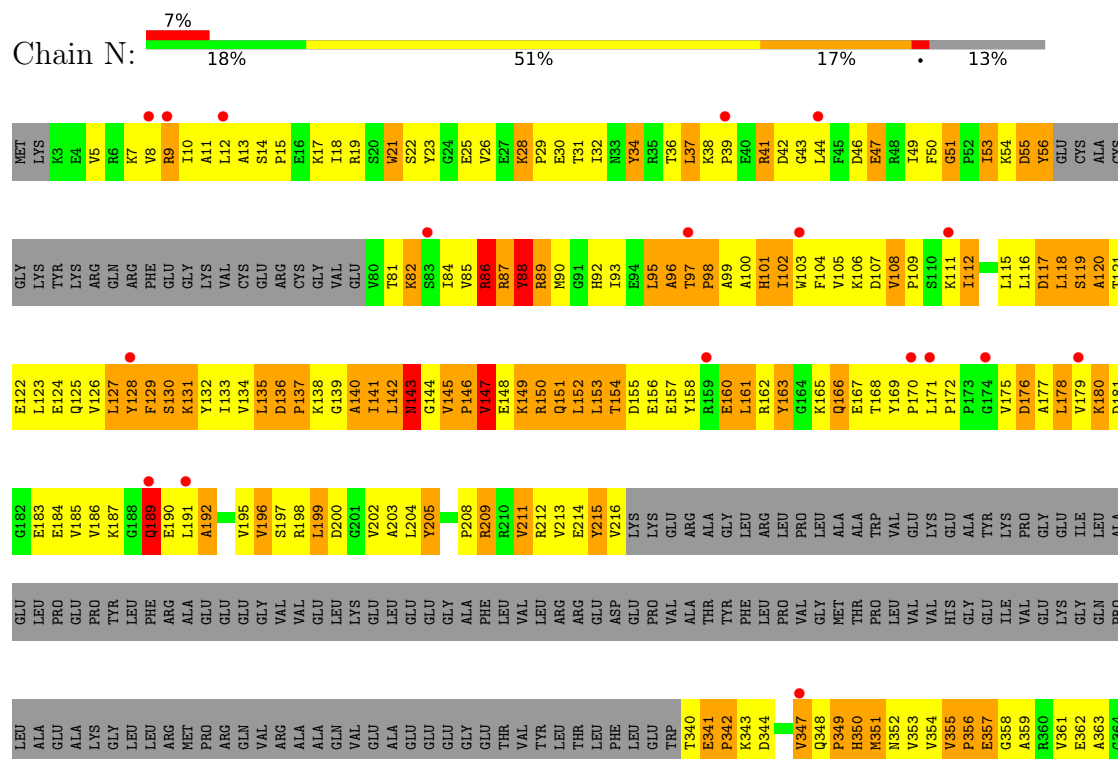




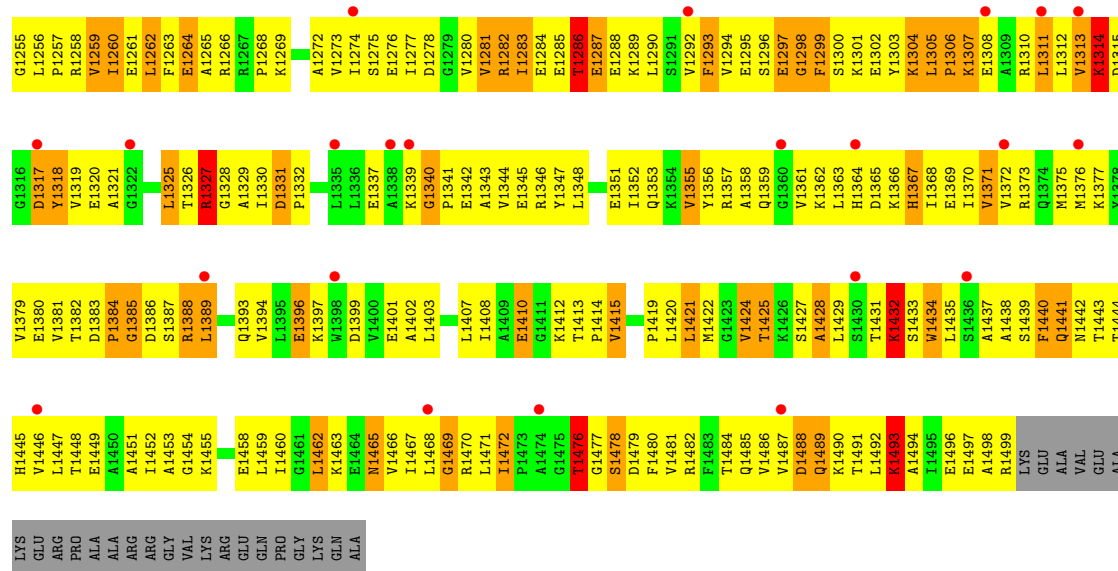
S1059	S1060	F1061	R1062	E1063	G1064	T1065	L1066	V1067	L1068	K1002	V1003				V1007	F1071	I1072	S1073	S1074	H1075							D1083	T1084	A1085	L1086	R1087	T1088	A1089	D1090	S1091	G1092	E1093	L1094	T1095	K1096	K1097	L1098	V1099	D1100	V1101	T1102	H1103	E1104	T1105	V1106	V1107	R1108	E1109	A1110	D1111	C1112	G1113	T1114	T1115	N1116	L1117	I1118	S1119	V1120	L1121	L1122																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
R929	L930	R931	D932	G970	K871	R872	L873	E874	S875	R876	P877	G878	R879	F941	S942	T943	T944	S945	G946	R947	V948						R884	R885	A886	E887	E888	A889	V890	E891	D892	E893	P957	E958	E959	K960	Y963	L964	D968	R969	K970	L971	L972	Q906	E907	K908	N909	S910	L911	K912	L913	L914	V915				R919	L920	T984	R985	R986	E987	Q923	W924	E925	K926	T927	A928																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
R867	Y868	M869	T808	K870	K871	R872	L873	E874	T875	S876	P877	G878	R879	F740	E805	F806	A807	T808	P809	A833	E810	E811	A812	L813	A814	A815	H816	E817	R818	G819	E820	V821	A822	L823	R824	A825	P826	I827	K828	V829	A830	R831	R832	T833	R834	S835	V836	G837	R838	Q901	L902	D903	Q906	E907	K908	N909	S910	L911	K912	L913	L914	V915	A918	F919	R920	R921	L922	G923	K924	V863	V864	T865	A928																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
R679	Q880	R881	D882	G883	K621	R622	V623	G624	Y625																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		



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



Q1195	R1130	V1067	K1002	Y937	T875	E811	T749	W688	Y625	L558	R495	R434	D365
T1196	S1131	L1068	V1003	G938	S876	A812	P750	D689	R628	G561	L496	V435	A386
R1197	L1132	E1069	V1007	F939	P877	L813	L751	A690	E497	A562	E497	V437	V368
Y1198	L1132	Y1070	V1007	T940	G878	A814	S752	L691	V499	P563	V499	D438	A369
G1199	R1136	F1071	F1011	F941	R879	A815	S753	E692	I631	E564	R500	L439	A370
C1201	R1137	I1072	F1011	S942	L881	A816	F754	E693	V632	I565	A501	V440	I371
A1138	R1137	T943	F1011	T943	F882	E817	A755	V694	V633	I566	F502	R441	D372
K1203	A1139	S1074	M1014	T944	F882	R818	Q756	I695	G634	I567	R502	R442	P373
K1203	A1139	S1074	M1014	T944	F882	R818	Q756	I695	G634	I567	R502	R442	P373
C1204	A1140	H1075	Y1015	S945	A883	G819	A757	H696	P335	I567	F502	R442	P373
Y1205	E1141	R1078	P1016	G946	R884	E820	E758	G697	R636	N569	D504	V443	E374
G1206	E1141	R1078	P1017	Y947	I885	E821	A759	G698	Q505	R569	S505	V444	E375
Y1207	A1142	T948	M1018	T948	V886	A822	A760	V699	L637	E570	G506	R445	E376
D1208	G1143	T949	P1019	T949	A887	L823	L761	V700	K638	K571	G507	V446	V377
L1209	L1144	A1082	L1020	G950	E888	N824	Q762	L701	L639	R572	R508	V447	I378
S1210	G1145	D1083	Y1021	I951	A889	A825	L763	L702	H640	M573	P509	E448	A379
M1211	G1146	T1084	Y1022	P952	V890	P826	L764	N703	Q641	L574	E510	S449	E380
A1212	R1147	A1085	M1023	D953	E891	R828	S765	R704	C642	Q575	W511	V450	A381
R1213	L1148	L1086	A1024	A954	D892	K827	A766	A705	G643	E576	N512	D451	E382
R1213	L1149	R1087	Q1025	V955	E893	V829	H767	P706	I644	A577	I513	L452	G383
P1214	A1150	T1088	S1026	I956	K894	A830	I768	T707	P645	V578	L514	D453	V384
V1215	R1151	T1089	G1027	P957	V895	G831	L769	L708	K646	D579	E515	A454	V385
S1216	E1152	D1090	A1028	E958	A896	R832	L770	R709	A580	A580	A516	R455	H386
I1217	E1152	S1091	R1029	E959	W897	E833	S771	R710	M648	L581	V517	M456	L387
G1218	V1155	G1092	G1030	E998	E898	T834	P772	L711	A649	D582	P513	C457	H388
E1219	L1156	Y1093	M1031	Y963	L899	S835	A773	G712	L650	D583	V519	A458	E389
A1220	L1156	L1094	P1032	L964	I900	V836	S774	I713	E851	N584	L520	A458	P390
V1221	L1160	T1095	Q1033	D968	Q901	G837	Q714	I714	L652	P521	P522	E459	A391
G1222	E1161	R1096	Q1034	R968	L902	R838	L778	A715	F652	R586	P522	I461	S392
I1223	E1162	K1097	I1035	R969	D903	L839	A779	F716	K654	D523	D523	Q462	I393
V1224	G1163	L1098	R1036	K970	K840	R890	A780	Q717	P655	L524	P524	Q463	L394
A1225	R1164	V1099	Q1037	L971	Y941	V841	S782	P718	F656	R525	R525	L464	V395
A1226	R1165	D1100	L1038	L972	Q907	V942	S782	V719	L657	T592	P526	L465	V396
Q1227	L1166	V1101	C1039	Q773	K908	F943	A783	L720	M593	VAL	VAL	E467	K397
S1228	M1167	T1102	G1040	E975	S910	A844	D784	E722	K660	GLN	GLN	E467	A398
I1229	E1168	H1103	L1041	E975	S910	N845	I785	E722	K660	VAL	VAL	D469	V400
G1230	D1169	E1104	R1042	Q976	L911	P846	L786	G723	R601	ASP	ASP	L470	Y401
E1231	D1170	I1105	G1043	A977	K912	D947	L787	Q724	R601	GLY	GLY	E471	P402
P1232	V1171	V1106	L1044	Y978	D913	E948	G788	S725	S602	GLY	GLY	A472	D406
G1233	R1172	V1107	M1045	E979	L914	A849	L789	I726	L603	ARG	ARG	L473	V407
T1234	L1173	R1108	Q1046	N980	V915	L850	Y790	Q727	T604	PHE	PHE	E474	E408
Q1235	E1174	E1109	K1047	Q981	L851	A852	Y791	L728	A667	I606	ALA	E475	V409
L1236	L1175	A1110	P1048	F982	A918	A852	I792	H729	P668	I607	THR	E476	V409
T1237	K1176	D1111	S1049	L983	F919	V853	T793	P730	N669	L607	THR	E476	V409
MET	A1177	C1112	G1050	T984	L920	V853	Q794	L731	V670	S538	D539	L477	T411
ARG	A1178	G1113	E1051	T984	R921	I857	V795	V732	K671	G609	D539	L478	T411
THR	E1179	T1114	T1052	E987	L922	V858	R796	C733	A672	K610	L540	E479	G412
PHE	Y1117	Y1117	F1053	R988	G923	D859	K797	E734	G611	Q611	L543	E480	D413
HIS	I1118	I1118	E1054	Y989	M924	L860	A798	A735	R675	R612	Y544	M481	R414
THR	S1119	S1119	V1055	D990	E925	Q861	K799	F736	M676	R613	R545	K482	V415
GLY	V1120	V1120	V1056	Q991	K926	D862	K800	N737	E678	F614	R545	H483	A416
GLY	E1185	E1185	V1057	I992	T927	V863	G801	A738	E678	R615	R545	P484	D419
VAL	P1186	P1121	R1058	L993	A928	V864	A802	D739	R679	Q616	R546	S495	V420
ALA	P1187	L1122	S1059	Q994	R929	T865	G803	F740	Q680	N617	Y548	R486	V420
ALA	V1188	F1123	S1060	L995	L930	V866	L804	F740	R681	L618	N549	A487	L421
GLY	R1189	R1189	P1061	A996	L931	R867	E805	D743	R681	L619	R550	R488	A422
ALA	S1190	P1125	R1062	T997	D932	Y868	F806	Q744	I683	G620	N551	R489	A422
D1251	P1191	D1126	E1063	E968	A933	M869	A807	M745	K684	K621	L554	A492	V427
I1252	L1192	E1127	G1064	T999	L934	R808	A746	M745	K684	R622	L554	A492	V427
T1253	T1193	L1128	L1065	T1000	K935	P809	V747	H748	E686	V623	L557	R493	Y432
Q1254	C1194	T1129	T1066	E1001	Y936	R872	E810	H748	P687	D624	L557	K494	G433



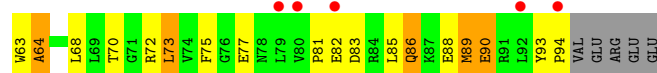
• Molecule 4: DNA-directed RNA polymerase subunit omega

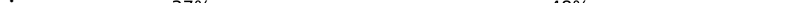


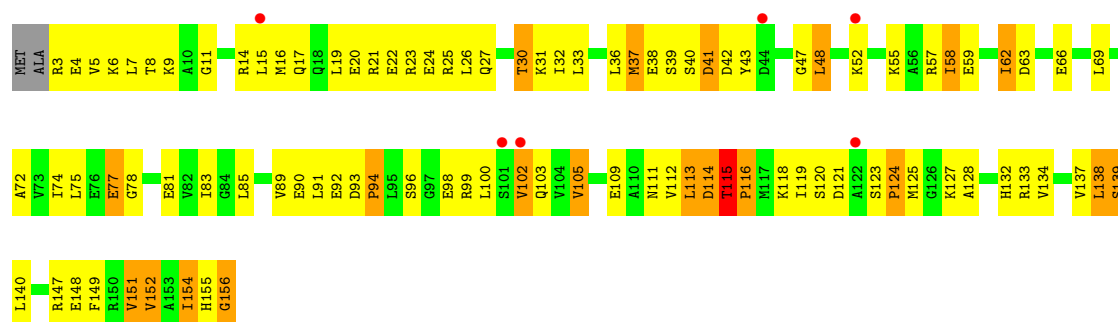
• Molecule 4: DNA-directed RNA polymerase subunit omega



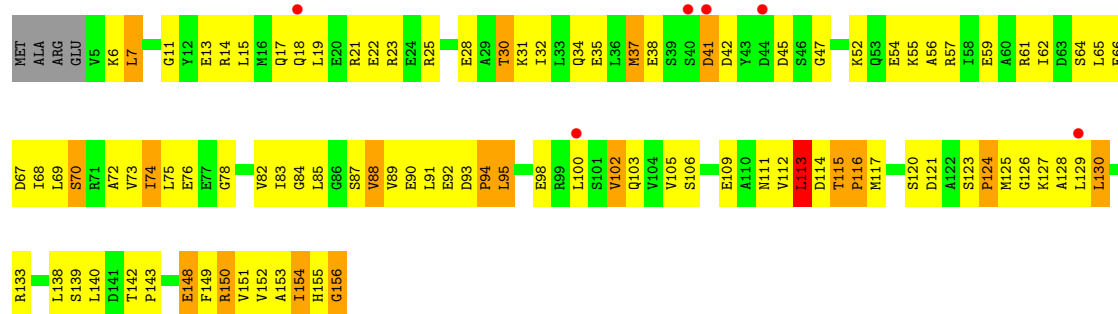
• Molecule 4: DNA-directed RNA polymerase subunit omega



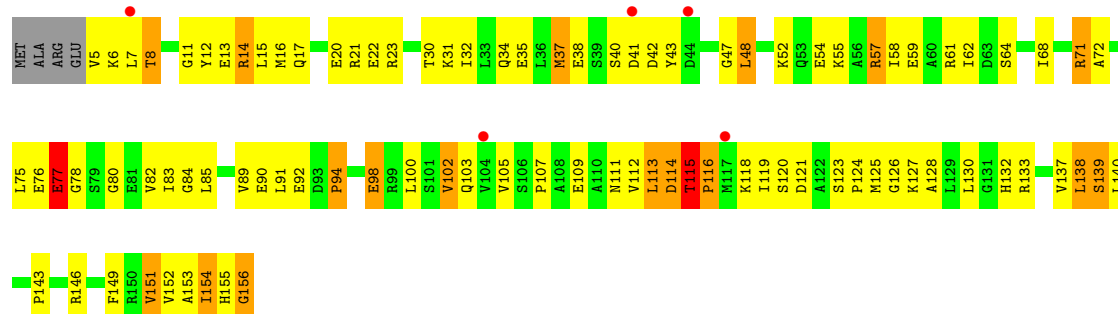
- Chain X: 



• 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	189.23Å 264.51Å 193.93Å 90.00° 116.68° 90.00°	Depositor
Resolution (Å)	47.57 – 4.30 47.57 – 4.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.57-4.30) 97.6 (47.57-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 4.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.317 , 0.338 0.320 , 0.340	Depositor DCC
R_{free} test set	3392 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	128.7	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 136.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.054 for l,-k,h	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	73646	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: MG, ZN

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	0/1791	1.16	18/2436 (0.7%)
1	B	0.58	0/1791	1.12	17/2436 (0.7%)
1	F	0.63	0/1791	1.14	17/2436 (0.7%)
1	G	0.60	0/1796	1.11	14/2443 (0.6%)
1	K	0.66	0/1801	1.16	19/2450 (0.8%)
1	L	0.59	0/1791	1.09	13/2436 (0.5%)
2	C	0.63	1/8713 (0.0%)	1.16	59/11785 (0.5%)
2	H	0.66	5/8686 (0.1%)	1.18	78/11750 (0.7%)
2	M	0.66	1/8717 (0.0%)	1.22	82/11792 (0.7%)
3	D	0.65	5/10559 (0.0%)	1.21	118/14272 (0.8%)
3	I	0.65	4/10131 (0.0%)	1.21	119/13685 (0.9%)
3	N	0.64	2/10653 (0.0%)	1.21	116/14403 (0.8%)
4	E	0.56	0/768	1.06	5/1035 (0.5%)
4	J	0.58	0/768	1.10	7/1035 (0.7%)
4	O	0.63	0/768	1.12	7/1035 (0.7%)
5	P	0.54	0/151	1.68	6/230 (2.6%)
5	R	0.52	0/133	1.32	5/203 (2.5%)
5	T	0.47	0/109	1.11	2/166 (1.2%)
6	Q	0.70	0/170	0.95	2/265 (0.8%)
6	S	0.85	0/192	0.86	0/299
6	U	0.72	0/170	0.94	2/265 (0.8%)
7	X	0.67	1/1198 (0.1%)	0.99	3/1608 (0.2%)
7	Y	0.70	1/1178 (0.1%)	0.98	2/1582 (0.1%)
7	Z	0.72	1/1178 (0.1%)	0.98	5/1582 (0.3%)
All	All	0.64	21/75003 (0.0%)	1.18	716/101629 (0.7%)

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	5
2	H	0	1
2	M	0	3
3	D	0	2
3	I	0	4
3	N	0	5
6	Q	0	1
6	S	0	1
All	All	0	22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	156	GLY	C-OXT	15.36	1.54	1.23
7	Y	156	GLY	C-OXT	15.28	1.54	1.23
7	X	156	GLY	C-OXT	10.41	1.44	1.23
3	I	604	THR	C-N	-8.26	1.23	1.34
3	N	447	VAL	CA-CB	-8.25	1.45	1.54

The worst 5 of 716 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	28	LYS	CA-C-N	16.16	140.03	119.84
3	D	28	LYS	C-N-CA	16.16	140.03	119.84
3	I	1209	LEU	N-CA-C	-14.35	89.28	109.95
3	N	1209	LEU	N-CA-C	-14.21	89.49	109.95
2	H	246	ASP	N-CA-C	13.35	120.14	108.13

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	267	TYR	Sidechain
2	C	589	ARG	Sidechain
2	C	642	ARG	Sidechain
2	C	71	TYR	Sidechain
2	C	735	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1759	0	1805	214	3
1	B	1759	0	1805	275	2
1	F	1759	0	1805	201	3
1	G	1764	0	1810	263	3
1	K	1769	0	1815	206	0
1	L	1759	0	1805	228	0
2	C	8550	0	8654	1463	1
2	H	8524	0	8626	1571	0
2	M	8555	0	8658	1578	1
3	D	10384	0	10615	1800	3
3	I	9965	0	10206	1752	1
3	N	10475	0	10699	1848	3
4	E	754	0	769	100	0
4	J	754	0	769	119	0
4	O	754	0	769	112	0
5	P	136	0	79	4	0
5	R	119	0	68	12	0
5	T	98	0	57	8	0
6	Q	152	0	78	10	0
6	S	172	0	88	12	0
6	U	152	0	79	12	0
7	X	1189	0	1205	150	0
7	Y	1169	0	1186	158	0
7	Z	1169	0	1186	148	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	N	1	0	0	0	0
9	S	1	0	0	0	0
All	All	73646	0	74636	11084	10

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 75.

The worst 5 of 11084 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:50:PHE:CD2	3:N:522:PRO:HD3	1.20	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:182:VAL:HG11	2:H:193:LEU:CD2	1.09	1.56
2:H:1090:LYS:HE3	3:I:90:MET:SD	1.45	1.55
2:H:182:VAL:CG1	2:H:193:LEU:HD21	1.13	1.55
3:I:783:ARG:NH1	7:Y:41:ASP:CB	1.67	1.53

The worst 5 of 10 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)
1:A:100:LEU:CD1	1:F:59:GLU:OE1[2_455]	1.51	0.69
3:D:1182:GLU:OE2	1:G:112:ARG:NE[1_655]	1.61	0.59
1:B:162:ILE:CG1	3:N:976:GLN:NE2[1_655]	1.90	0.30
1:A:100:LEU:CD1	1:F:59:GLU:CD[2_455]	1.97	0.23
2:C:223:ASP:O	3:N:562:ALA:O[2_444]	2.02	0.18

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%)	191 (86%)	22 (10%)	8 (4%)	2	20
1	B	221/315 (70%)	191 (86%)	27 (12%)	3 (1%)	9	39
1	F	221/315 (70%)	191 (86%)	20 (9%)	10 (4%)	2	17
1	G	222/315 (70%)	193 (87%)	26 (12%)	3 (1%)	9	39
1	K	223/315 (71%)	193 (86%)	21 (9%)	9 (4%)	2	18
1	L	221/315 (70%)	188 (85%)	28 (13%)	5 (2%)	5	28
2	C	1077/1119 (96%)	864 (80%)	150 (14%)	63 (6%)	1	14
2	H	1074/1119 (96%)	867 (81%)	145 (14%)	62 (6%)	1	14
2	M	1078/1119 (96%)	871 (81%)	149 (14%)	58 (5%)	1	15
3	D	1306/1524 (86%)	1062 (81%)	186 (14%)	58 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	1252/1524 (82%)	1012 (81%)	177 (14%)	63 (5%)	1	16
3	N	1317/1524 (86%)	1052 (80%)	196 (15%)	69 (5%)	1	15
4	E	91/99 (92%)	67 (74%)	17 (19%)	7 (8%)	1	10
4	J	91/99 (92%)	70 (77%)	14 (15%)	7 (8%)	1	10
4	O	91/99 (92%)	68 (75%)	16 (18%)	7 (8%)	1	10
7	X	152/156 (97%)	132 (87%)	16 (10%)	4 (3%)	4	25
7	Y	150/156 (96%)	135 (90%)	12 (8%)	3 (2%)	6	31
7	Z	150/156 (96%)	131 (87%)	16 (11%)	3 (2%)	6	31
All	All	9158/10584 (86%)	7478 (82%)	1238 (14%)	442 (5%)	2	16

5 of 442 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	GLY
2	C	23	VAL
2	C	40	GLU
2	C	44	ILE
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%)	166 (85%)	30 (15%)	3	13
1	B	196/273 (72%)	159 (81%)	37 (19%)	1	9
1	F	196/273 (72%)	171 (87%)	25 (13%)	4	17
1	G	196/273 (72%)	160 (82%)	36 (18%)	1	10
1	K	196/273 (72%)	164 (84%)	32 (16%)	2	12
1	L	196/273 (72%)	162 (83%)	34 (17%)	2	11
2	C	912/941 (97%)	718 (79%)	194 (21%)	1	6
2	H	909/941 (97%)	719 (79%)	190 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	912/941 (97%)	722 (79%)	190 (21%)	1	7
3	D	1113/1279 (87%)	917 (82%)	196 (18%)	2	11
3	I	1068/1279 (84%)	868 (81%)	200 (19%)	1	10
3	N	1124/1279 (88%)	921 (82%)	203 (18%)	2	10
4	E	82/88 (93%)	71 (87%)	11 (13%)	4	16
4	J	82/88 (93%)	73 (89%)	9 (11%)	6	22
4	O	82/88 (93%)	65 (79%)	17 (21%)	1	7
7	X	130/131 (99%)	110 (85%)	20 (15%)	2	13
7	Y	128/131 (98%)	103 (80%)	25 (20%)	1	8
7	Z	128/131 (98%)	109 (85%)	19 (15%)	3	14
All	All	7846/8955 (88%)	6378 (81%)	1468 (19%)	1	10

5 of 1468 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	62	THR
2	M	900	ARG
1	K	183	ASP
4	J	52	GLU
2	M	263	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 273 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	724	GLN
3	N	824	ASN
7	X	27	GLN
1	G	124	ASN
1	G	38	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Q	6/32 (18%)	1 (16%)	0
6	S	7/32 (21%)	2 (28%)	0
6	U	6/32 (18%)	3 (50%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	19/96 (19%)	6 (31%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Q	11	C
6	S	13	G
6	S	16	G
6	U	11	C
6	U	12	G

There are no RNA pucker outliers to report.

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 oligosaccharides 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 ⓘ

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%)	0.47	6 (2%) 56 43	82, 143, 203, 231	0
1	B	223/315 (70%)	0.43	8 (3%) 46 37	86, 150, 211, 231	0
1	F	223/315 (70%)	0.55	13 (5%) 29 28	88, 145, 202, 231	0
1	G	224/315 (71%)	0.52	9 (4%) 42 35	74, 150, 204, 231	0
1	K	225/315 (71%)	0.53	6 (2%) 56 43	77, 152, 205, 231	0
1	L	223/315 (70%)	0.49	7 (3%) 51 40	71, 146, 208, 231	0
2	C	1083/1119 (96%)	0.56	65 (6%) 27 27	46, 150, 225, 231	0
2	H	1080/1119 (96%)	0.60	65 (6%) 27 27	32, 148, 226, 231	0
2	M	1084/1119 (96%)	0.74	94 (8%) 16 19	51, 150, 227, 231	0
3	D	1316/1524 (86%)	0.59	66 (5%) 34 31	91, 161, 249, 285	0
3	I	1262/1524 (82%)	0.69	95 (7%) 20 23	91, 160, 246, 285	0
3	N	1327/1524 (87%)	0.73	110 (8%) 17 21	91, 162, 250, 284	0
4	E	93/99 (93%)	0.49	5 (5%) 31 29	91, 182, 231, 231	0
4	J	93/99 (93%)	0.42	3 (3%) 50 39	98, 176, 231, 231	0
4	O	93/99 (93%)	0.60	8 (8%) 16 19	90, 172, 231, 231	0
5	P	7/27 (25%)	0.62	0 100 100	199, 200, 200, 200	0
5	R	6/27 (22%)	0.68	0 100 100	200, 200, 200, 200	0
5	T	5/27 (18%)	0.89	0 100 100	199, 200, 200, 200	0
6	Q	7/32 (21%)	0.07	0 100 100	195, 200, 200, 200	0
6	S	8/32 (25%)	0.56	0 100 100	200, 200, 200, 200	0
6	U	7/32 (21%)	0.40	0 100 100	194, 200, 200, 200	0
7	X	154/156 (98%)	0.43	6 (3%) 43 36	97, 175, 229, 231	0
7	Y	152/156 (97%)	0.43	6 (3%) 43 36	88, 174, 228, 231	0
7	Z	152/156 (97%)	0.48	5 (3%) 49 39	95, 172, 228, 231	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	9270/10761 (86%)	0.62	577 (6%) 26 27	32, 156, 231, 285	0

The worst 5 of 577 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	355	VAL	8.4
3	I	1292	VAL	8.4
2	H	1097	LEU	8.4
3	D	1313	VAL	7.4
3	N	191	LEU	6.3

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 oligosaccharides 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. 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(Å ²)	Q<0.9
9	MG	S	2005	1/1	0.42	0.41	115,115,115,115	0
9	MG	N	2006	1/1	0.67	0.30	115,115,115,115	0
8	ZN	N	2001	1/1	0.97	0.04	115,115,115,115	0
9	MG	D	2004	1/1	0.99	0.06	115,115,115,115	0
8	ZN	I	2003	1/1	0.99	0.06	115,115,115,115	0
8	ZN	D	2002	1/1	0.99	0.03	115,115,115,115	0

6.5 Other polymers ⓘ

There are no such residues in this entry.