



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:47 AM UTC

PDB ID : 4WQT / pdb_00004wqt
Title : Thermus thermophilus RNA polymerase complexed with an RNA cleavage stimulating factor (a GreA/Gfh1 chimeric protein)
Authors : Murayama, Y.; Sekine, S.; Yokoyama, S.
Deposited on : 2014-10-22
Resolution : 4.40 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

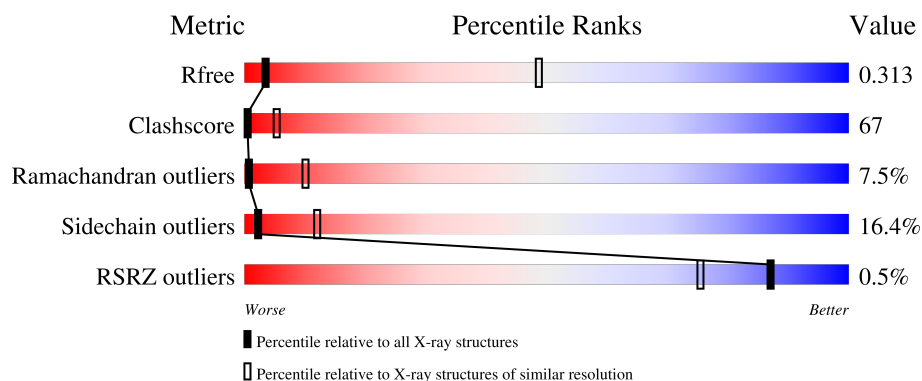
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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.



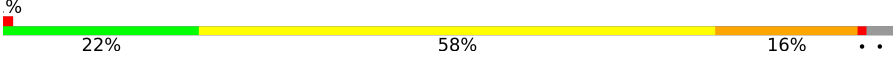
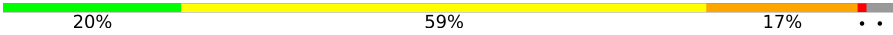
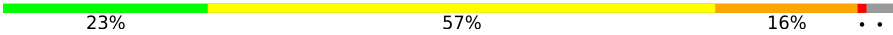
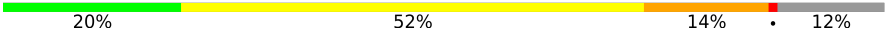
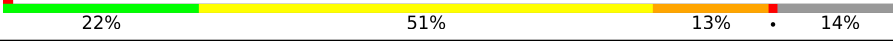
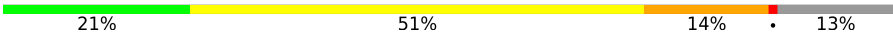
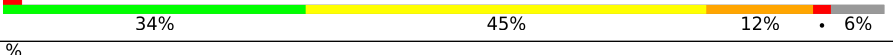
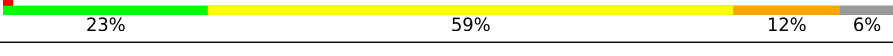
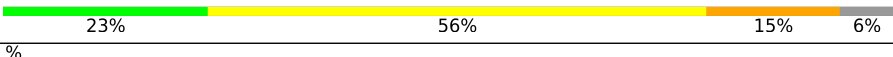
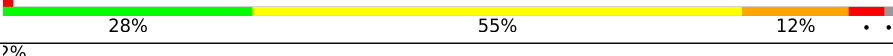
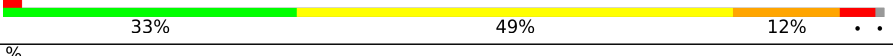
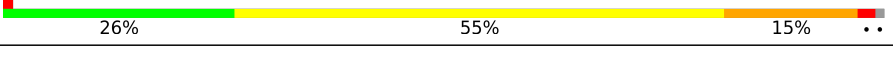
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	
1	B	315	
1	F	315	
1	G	315	
1	K	315	

Continued on next page...

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Mol	Chain	Length	Quality of chain
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	X	156	
5	Y	156	
5	Z	156	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 73369 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	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			
1	F	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	G	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	K	225	Total	C	N	O	S	0	0	0
			1769	1129	308	330	2			
1	L	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1080	Total	C	N	O	S	0	0	0
			8521	5392	1520	1585	24			
2	H	1081	Total	C	N	O	S	0	0	0
			8530	5398	1522	1586	24			
2	M	1080	Total	C	N	O	S	0	0	0
			8521	5392	1520	1585	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0	0
			10513	6654	1864	1965	30			
3	I	1318	Total	C	N	O	S	0	0	0
			10396	6583	1842	1942	29			
3	N	1323	Total	C	N	O	S	0	0	0
			10440	6613	1849	1949	29			

- 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 protein called RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	154	Total	C	N	O	S	0	0	0
			1200	736	218	242	4			
5	Y	154	Total	C	N	O	S	0	0	0
			1200	736	218	242	4			
5	Z	154	Total	C	N	O	S	0	0	0
			1200	736	218	242	4			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

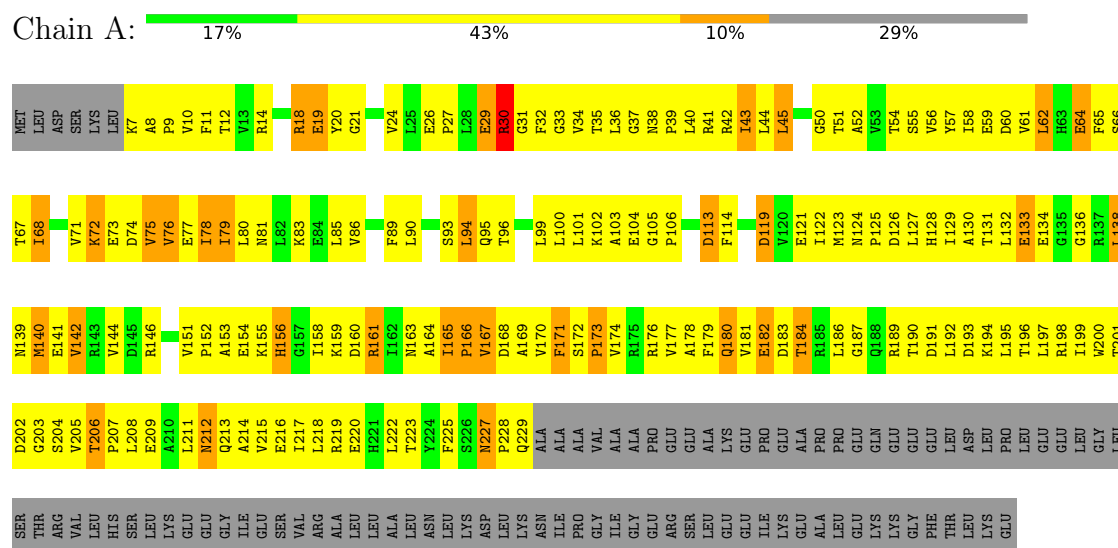
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

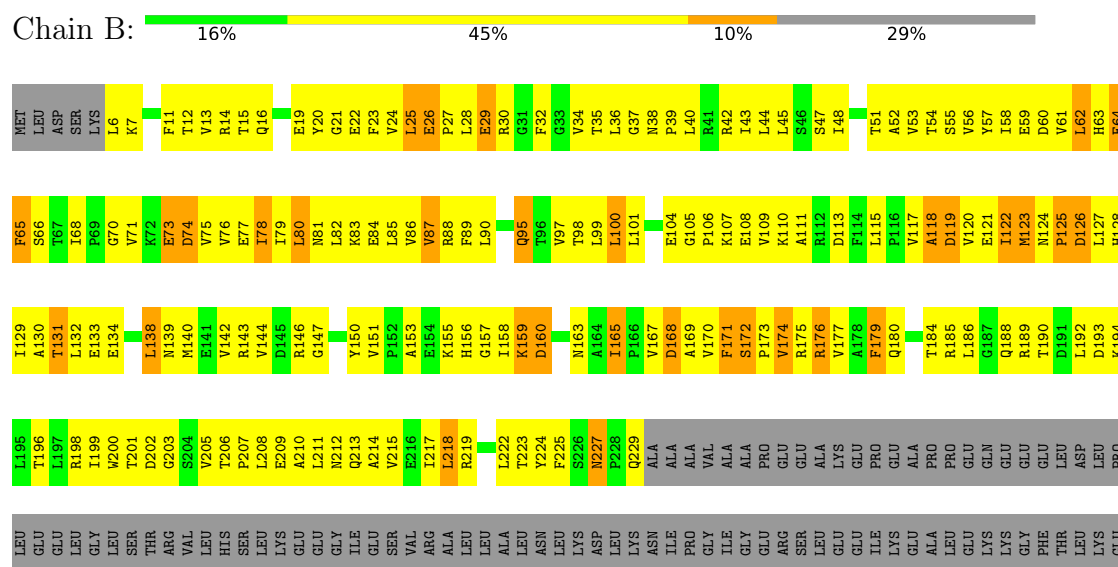
3 Residue-property plots

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.

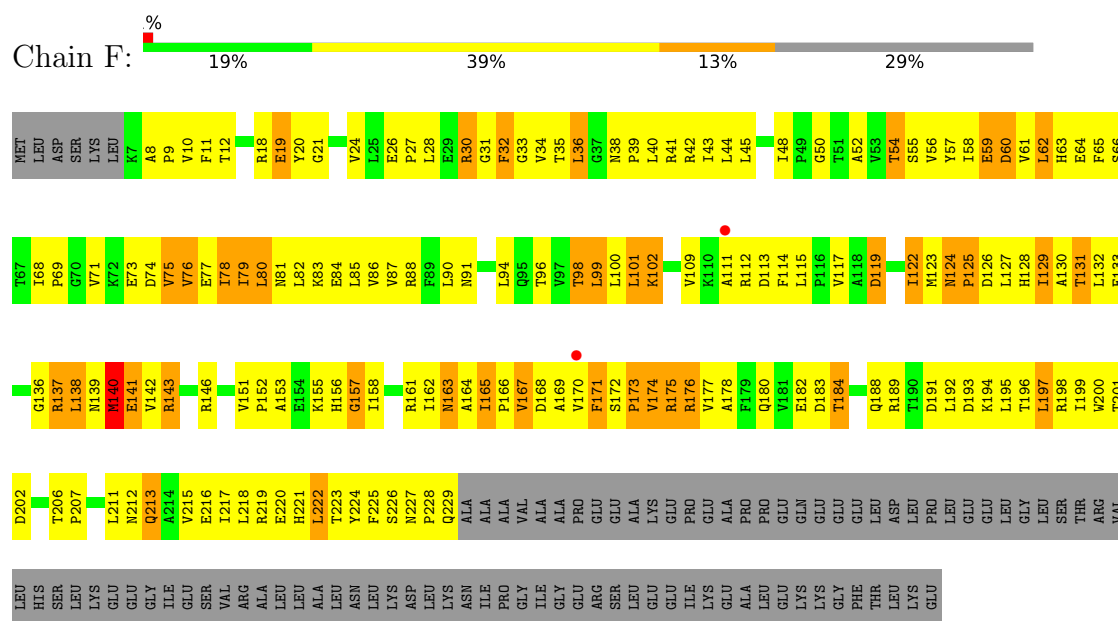
• Molecule 1: DNA-directed RNA polymerase subunit alpha



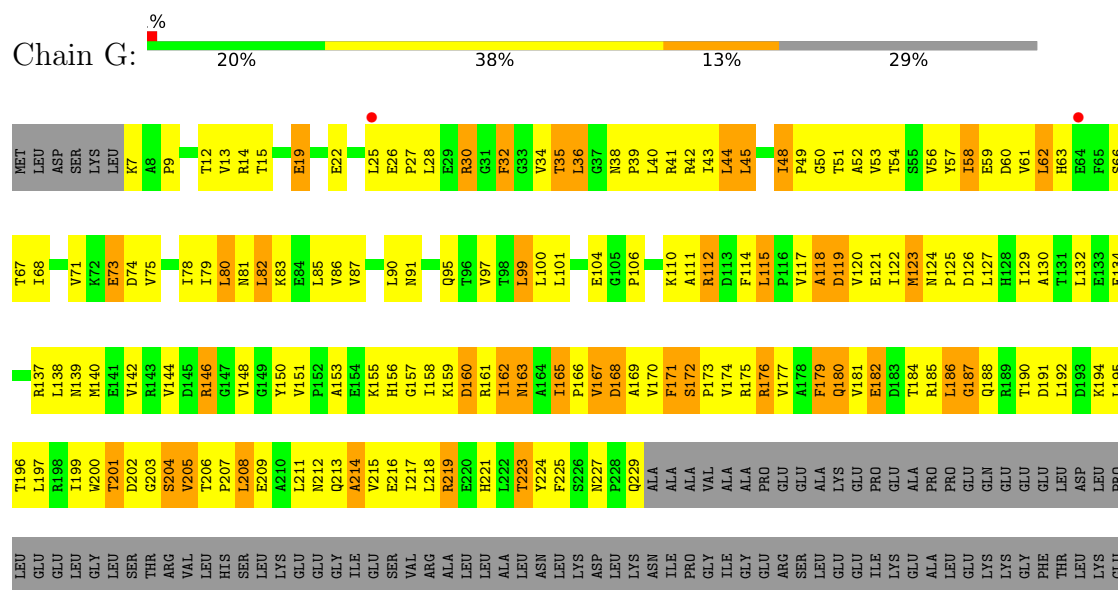
• Molecule 1: DNA-directed RNA polymerase subunit alpha



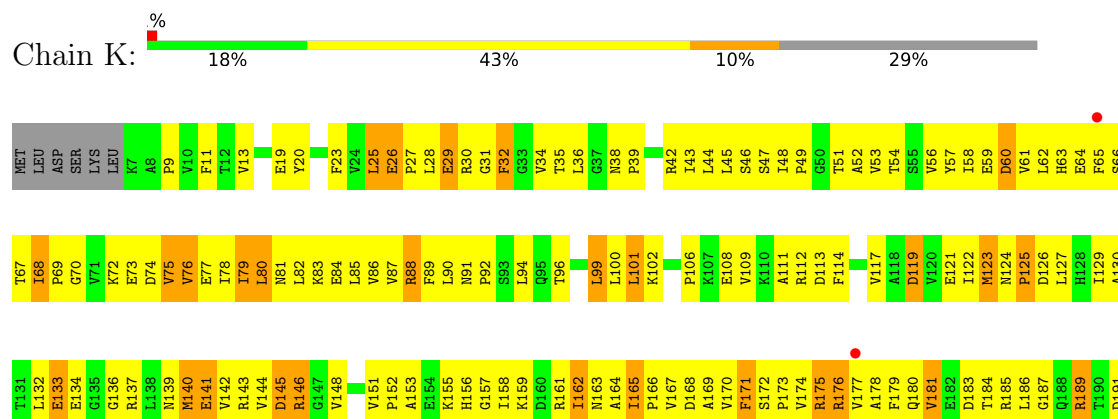
• Molecule 1: DNA-directed RNA polymerase subunit alpha

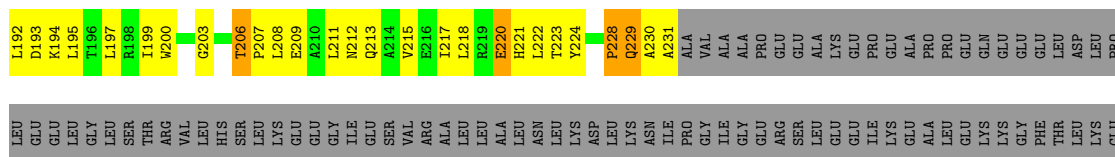


• Molecule 1: DNA-directed RNA polymerase subunit alpha

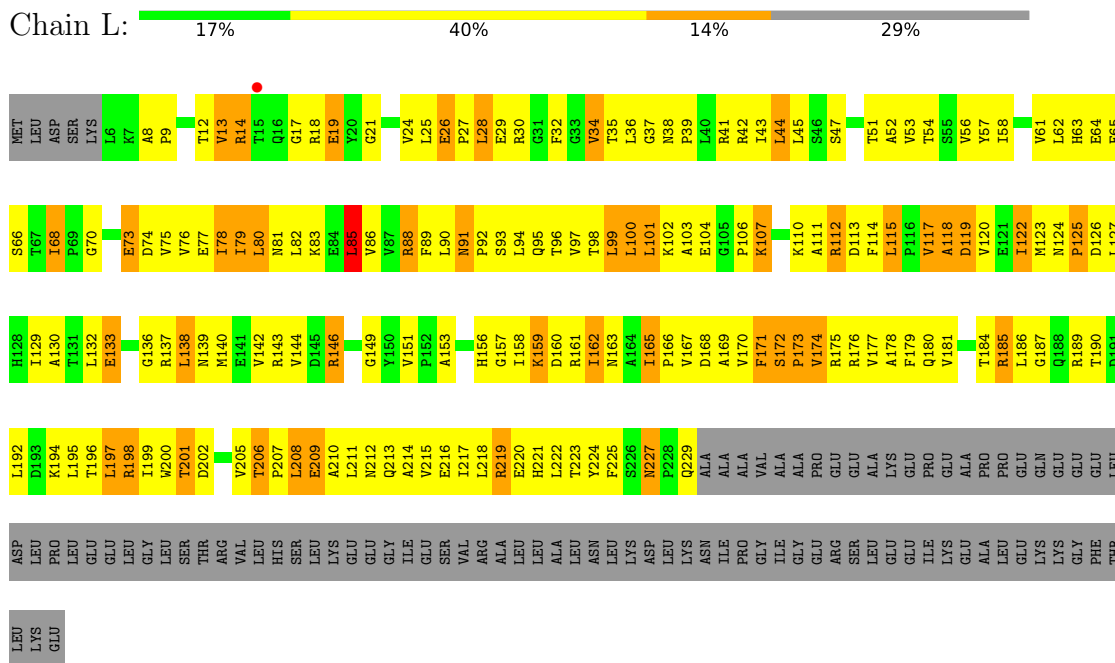


• Molecule 1: DNA-directed RNA polymerase subunit alpha

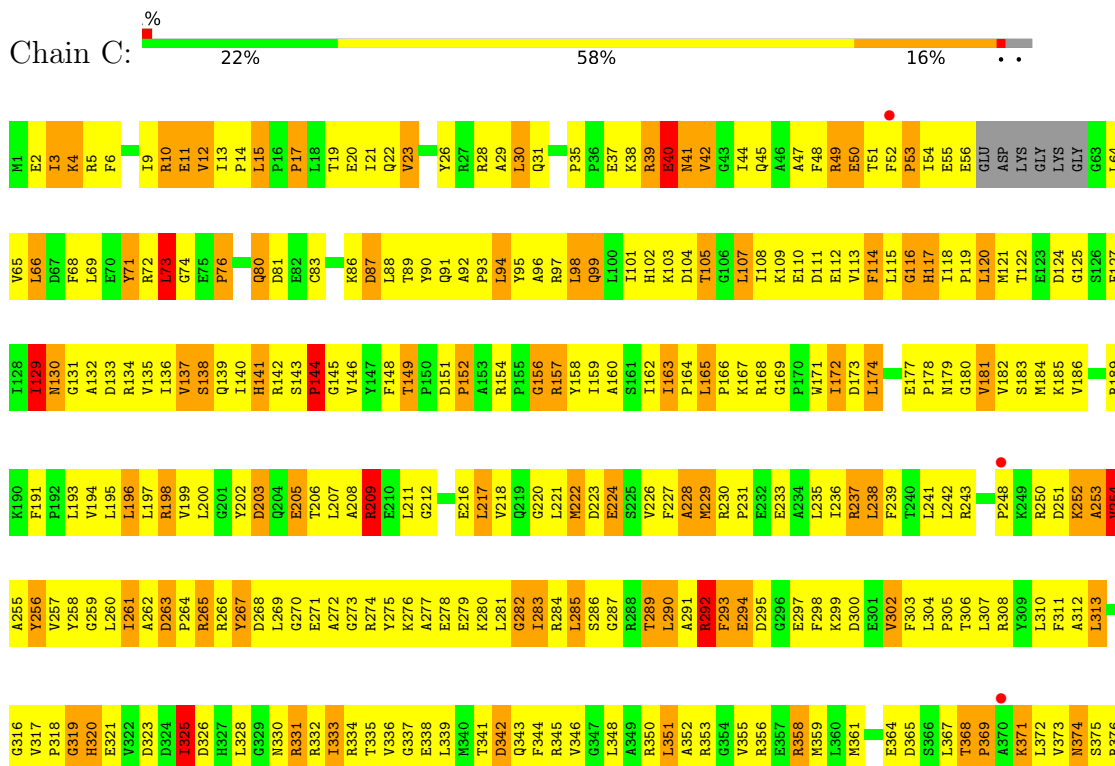


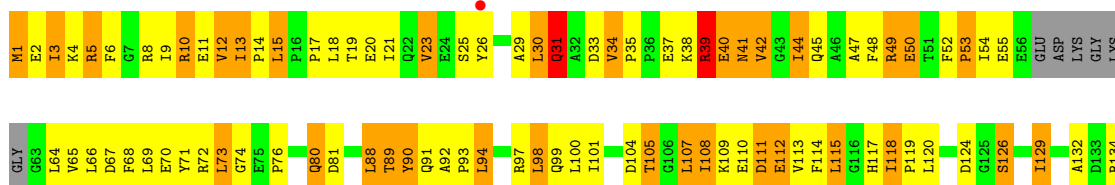


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta



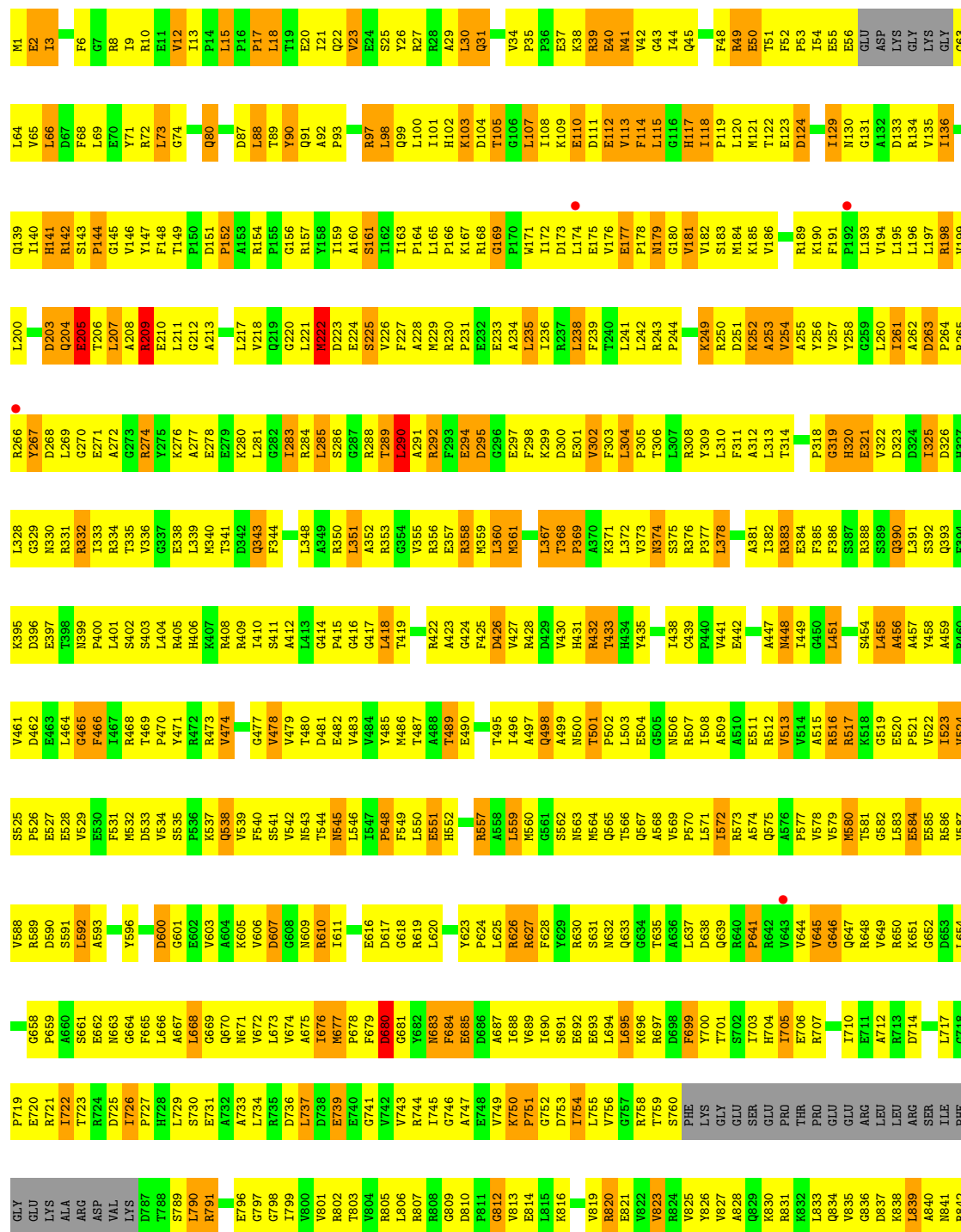


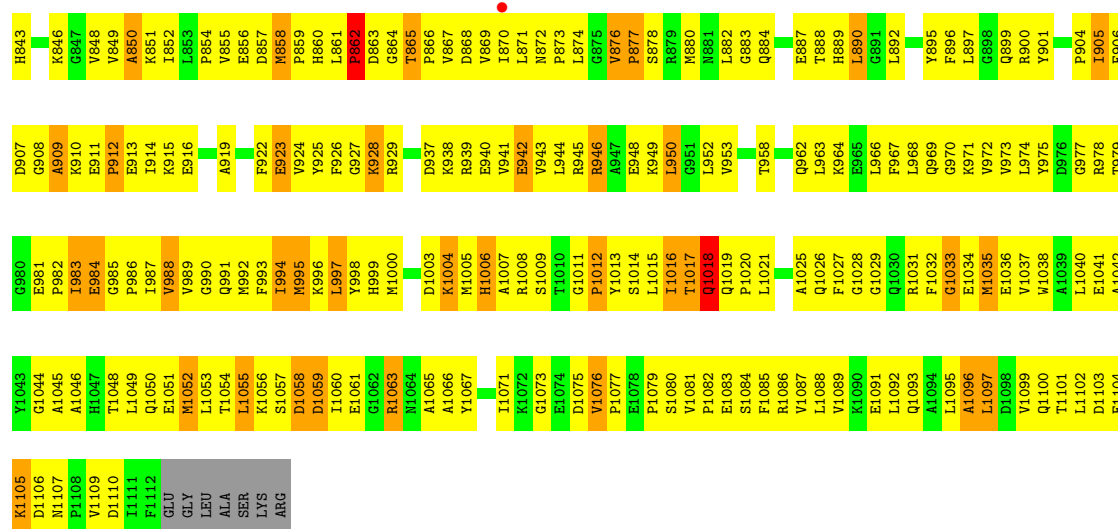
WORLDWIDE
PDB
PROTEIN DATA BANK



● Molecule 2: DNA-directed RNA polymerase subunit beta

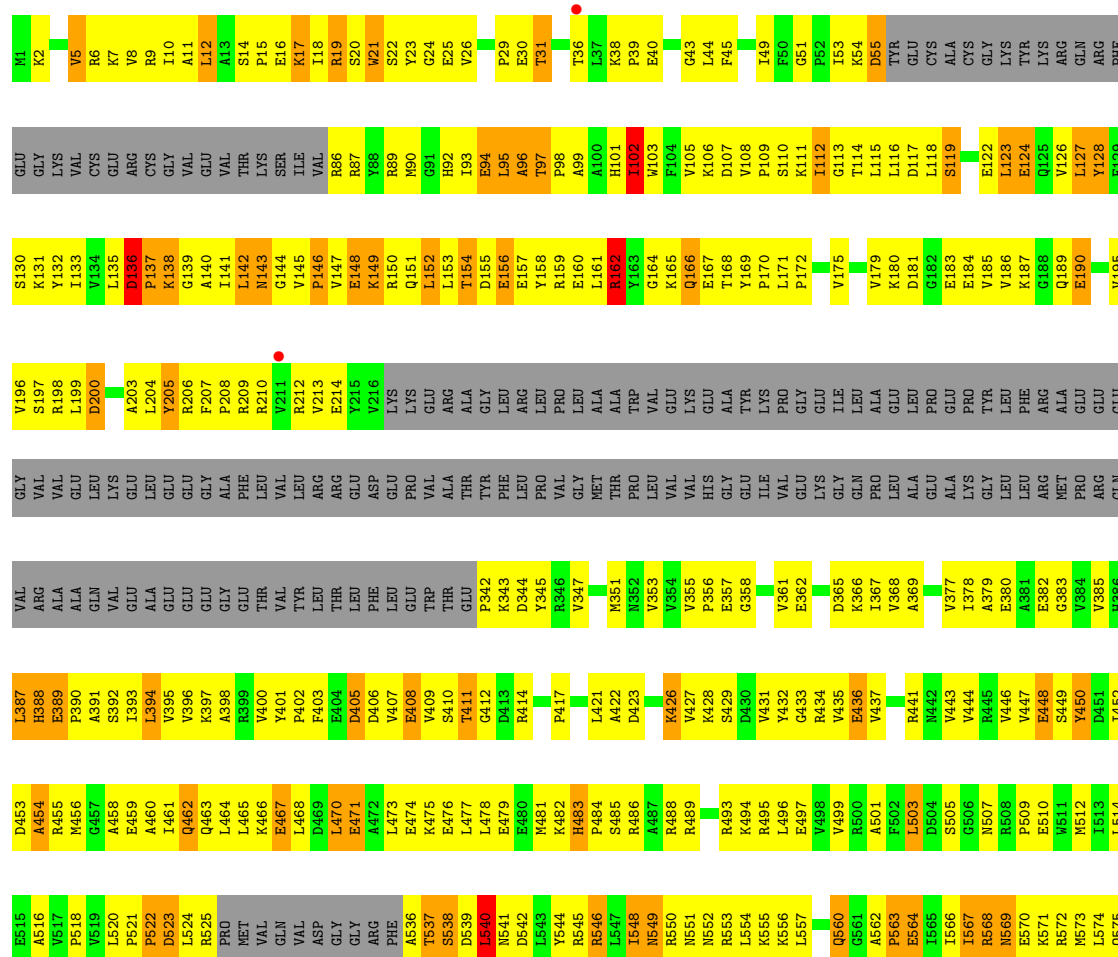
Chain M: 23% 57% 16% . .



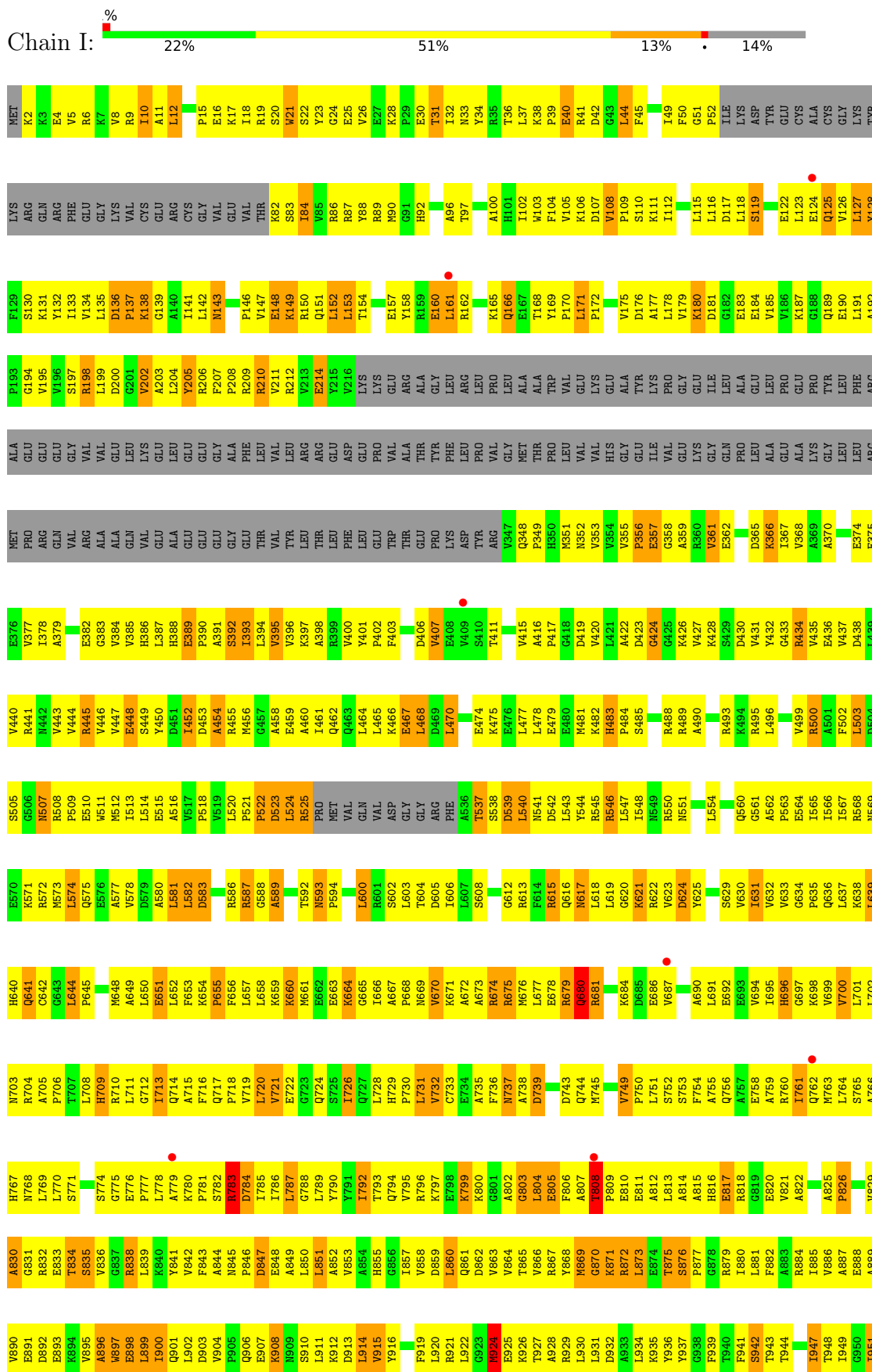


• Molecule 3: DNA-directed RNA polymerase subunit beta'

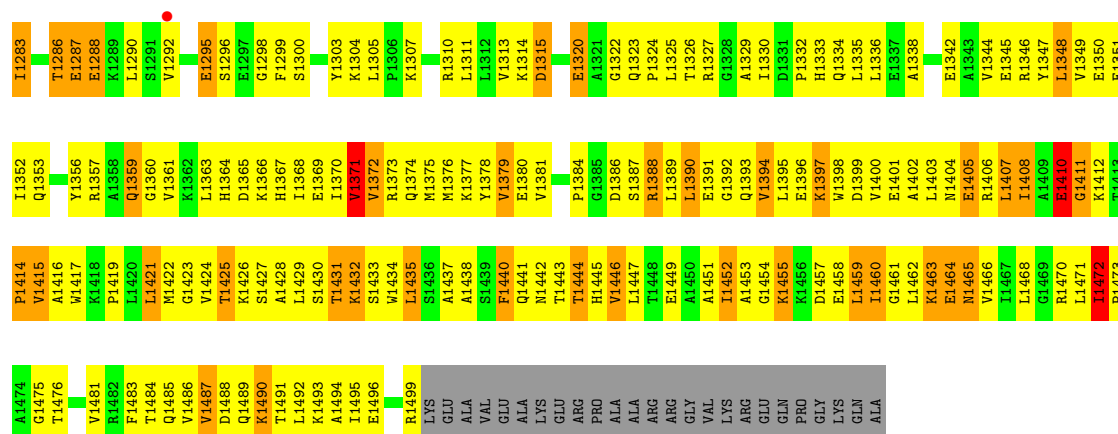
Chain D: 20% 52% 14% 12%



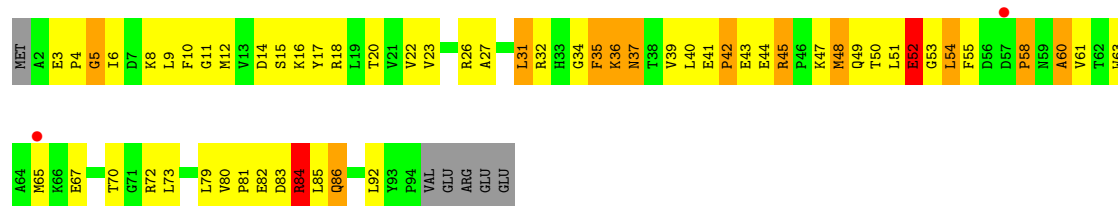
- Molecule 3: DNA-directed RNA polymerase subunit beta'



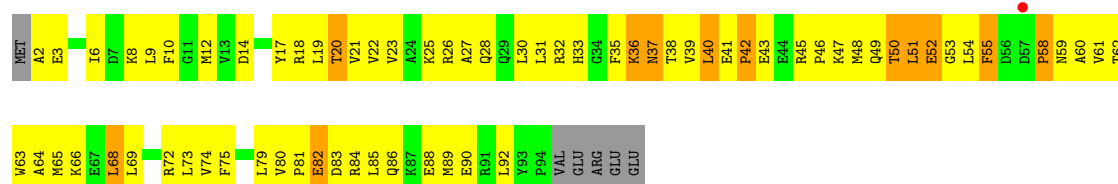
G1218	L1156	T1095	S1026	E958	H987	G837	P777	L711	K646	L574	M511	V443	E380
E1219	G1157	R1096	G1027	E959	E995	R838	L778	G712	R647	Q575	M512	V446	A381
A1220	L1158	K1097	A1028	R989	L779	L839	A780	Q714	R648	E576	L513	V447	E382
V1221	R1159	L1098	R1029	I900	K780	K840	K781	Q715	A649	A577	L514	G383	ARG
G1222	L1160	V1099	G1030	L901	Y841	R841	W781	A715	E651	V578	E515	V384	GLN
I1223	E1161	D1100	M1031	L964	W842	W842	S782	F716	E651	D579	E516	V385	VAL
V1224	E1162	V1101	G1031	E965	D903	F843	R783	Q717	L652	A580	V517	Y450	ARG
A1225	G1163	T1102	Q1034	E966	V904	A844	D784	F718	F653	L581	F518	D451	ALA
A1226	H1103	H1103	I1035	A967	P905	N845	L785	W719	K654	L582	V519	L452	ALA
Q1227	Y1165	E1104	R1036	D968	Q906	R846	L786	L720	D583	E389	L520	E389	GLN
S1228	L1166	T1105	Q1037	R969	E907	D847	L787	W721	F656	N584	P521	A454	VAL
I1229	S1167	V1106	L1038	K908	K908	E848	G788	E722	L657	G585	P522	G585	GLU
G1230	M1168	V1107	C1039	L971	N909	A849	L789	Q727	L658	R586	D523	M456	ALA
E1231	D1169	R1103	G1040	L972	S910	L850	W790	Q727	K659	E589	L524	G457	GLU
P1232	D1170	E1109	R1041	Q973	K912	L851	Y791	L728	R660	P590	R525	A458	GLU
	L1171	A1110	L1042	I974	N912	A852	L792	W729	M661	P591	P526	E458	GLY
Q1235	H1172	D1111	G1043	E975	D913	R853	Q794	F730		V591	M527	A460	GLY
L1236	L1173	C1112	L1044	Q976	L914	A854	Q794	L731		V592	V528	V396	GLU
T1237	L1174	G1113	M1045	A977	V915	R855	W795	W732		N593	Q462	A398	THR
RET	I1175	T1114	Q1046	E978	Y916	G856	R796	C733		P594	Q463	R399	VAL
ARG	K1176	T1115	K1047	E979	Q917	L857	K797	E734		P599	ASP	L464	TYR
THR	A1177	M1116	P1048	M980	A918	W858	K798	A735		L600	GLY	L465	GLY
PHE	A1178	Y1117	S1049	G981	F919	D859	K799	F736		A672	LEU	K466	THR
HIS	E1179	I1118	G1050	F982	L920	L860	K800	A737		A673	ARG	P402	THR
THR		S1119	E1051	L983	R921	Q861	G801	W745		S602	PHE	E467	LEU
GLY	E1182	V1120	T1052	T984	L922	D862	A802	A746		L603	ALA	L468	PHE
GLY	I1183	P1121	F1053	D985	G923	R863	G803	W747			T537	D469	LEU
VAL	V1186	L1122	E1054	R986	N924	L864	L804	F740		T606	S538	L470	GLU
ALA	P1187	Q1123	V1055	E987	E925	T865	E805	D743		L607	GLY	E471	TRP
GLY	L1188	Q1124	P1056	R988	K926	W866	F806	Q744		L540	D539	A472	E408
ALA	V1189	P1125	V1057	Y989	T927	R867	A807	Q744		R613	L540	L473	THR
ALA	R1189	D1126	R1058	D990	A928	Y868	T808	W745		N541	E474	E474	GLU
ASP	S1190	E1127	S1059	Q991	R929	R869	P809	A746		D542	D542	K475	P342
ILE	P1191	V1128	S1060	L992	L930	G870	E811	W747		L543	G412		G412
	T1192	R1130	Q984	L993	L931	K871	E811	W748		R346	D413	Y345	Y345
	T1193	R1131	L995	L996	L934	E874	A814	S752		V347	R414	V347	V347
	C1194	L1132	L1065		K935	T875	A815			M351	V415		M351
P1257	Q1195	R1133	T1066	T999	Y936	S876	H816			V354	D419		V354
R1258	R1196	L1134	V1067	T1000	Y937	P877	E817	Q756		V355	V420		V355
V1259	R1197	R1135	L1068	E1001	Q938	G878	R818	Q756		P356	L421		P356
E1261	G1198	K1136	E1069	K1002	F939	R879	Q819	E758		E357	A422		E357
L1262	V1200	R1137		V1003	T940	T880	E820	W759		G358	D423		G358
F1263	Q1201	I1072	S1073	T1004	F941	L881	W821	A759		R489	G424		R489
E1264	K1202	S1073	H1075		S942	F882	A822	W760		A492	G425		R360
A1265	C1204	A1142	S1074	V1007	T943	A883	L823	Q762		R493	K426		V361
R1267	Y1205	G1143	H1075		T944	R884	R824	W763		K494	K427		D365
K1269	Y1207	L1144	A1082	N1010		T885	A825	L764		L496	S429		K366
A1270	D1208	G1146	D1083	Y1015	T947	W886	P826	W765		V499	D430		I367
R1271	L1209	R1147	T1084	P1016	T948	A887	I827	A766		L503	V431		V368
A1272	S1210	V1148	A1085	P1017	Y949	E889	R828	W767		L503	Y432		A369
V1273	M1211	L1149	L1086	N1018	G950	A889	W829	N703		D504	G433		A370
I1274	A1212	A1150	R1087	L1019	P952	E891	A830	L769		E564	R434		R434
S1275	R1213	R1151	L1087	L1020	D953	D892	R832	W771		S505	V435		E374
E1276	P1214	E1152	S1091	Y1021	A954	E893	E833	S771		L566	L439		E375
I1277	V1215	V1153	G1092	Y1022	Y955	R894	T834	S774		N507	V440		E376
D1278	S1216	E1154	Y1093	M1023	P956	W895	S835	L644		R508	R441		I378
	I1217	V1155	L1094		P957	A896	W836	E776		E510	N442		A379



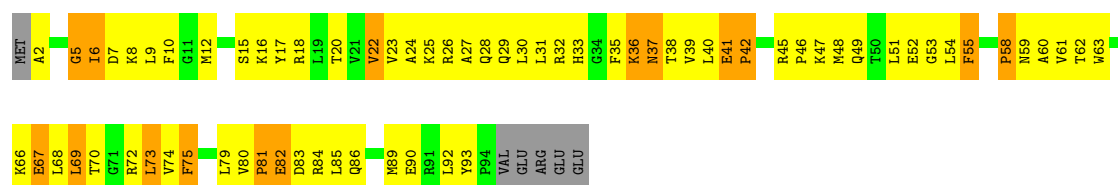
- Molecule 4: DNA-directed RNA polymerase subunit omega



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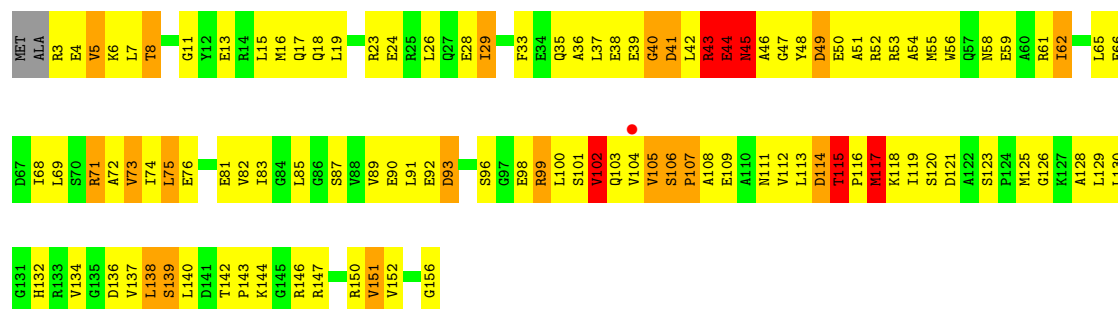


- Molecule 4: DNA-directed RNA polymerase subunit omega

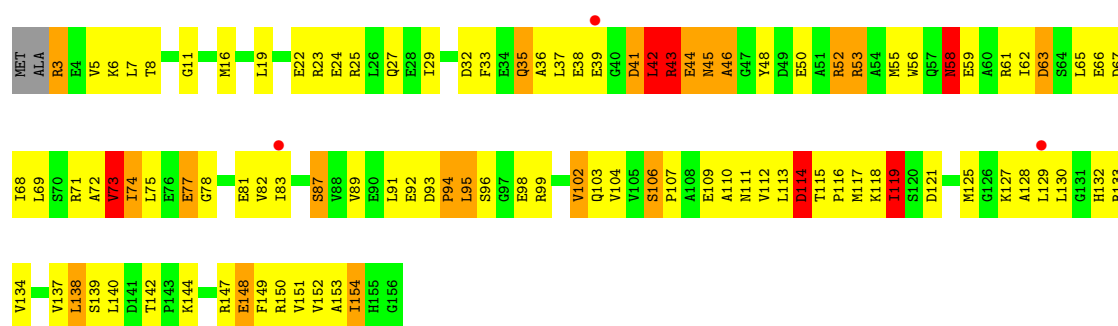


- Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)

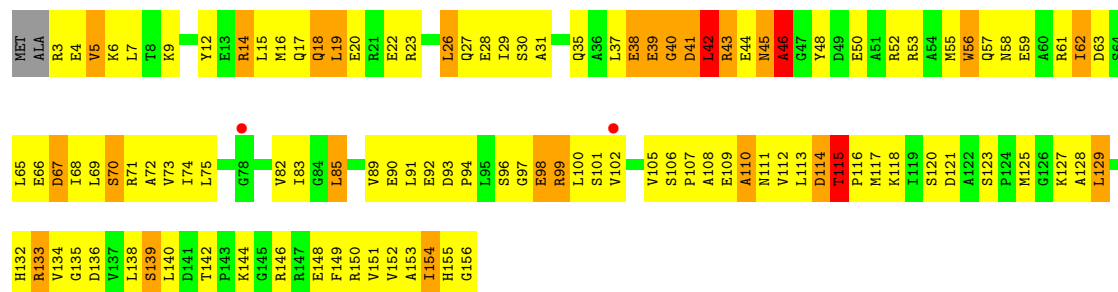




- Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)



- Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	189.57Å 263.77Å 195.85Å 90.00° 116.83° 90.00°	Depositor
Resolution (Å)	45.79 – 4.40 45.79 – 4.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (45.79-4.40) 96.3 (45.79-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.260 , 0.313 0.260 , 0.313	Depositor DCC
R_{free} test set	3149 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	151.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 216.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.129 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	73369	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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	0.61	0/1791	0.91	4/2436 (0.2%)
1	B	0.65	0/1799	0.92	0/2447
1	F	0.65	0/1791	0.89	1/2436 (0.0%)
1	G	0.65	0/1791	0.89	0/2436
1	K	0.56	0/1801	0.84	0/2450
1	L	0.62	1/1799 (0.1%)	0.88	0/2447
2	C	0.64	2/8683 (0.0%)	0.91	4/11747 (0.0%)
2	H	0.66	0/8692	0.90	5/11758 (0.0%)
2	M	0.63	1/8683 (0.0%)	0.91	7/11747 (0.1%)
3	D	0.66	0/10692	0.92	10/14452 (0.1%)
3	I	0.63	0/10571	0.89	6/14288 (0.0%)
3	N	0.64	3/10617 (0.0%)	0.89	11/14350 (0.1%)
4	E	0.62	0/768	0.87	2/1035 (0.2%)
4	J	0.65	0/768	0.88	0/1035
4	O	0.66	0/768	0.89	0/1035
5	X	0.87	1/1212 (0.1%)	1.10	10/1629 (0.6%)
5	Y	0.82	2/1212 (0.2%)	1.11	5/1629 (0.3%)
5	Z	0.84	2/1212 (0.2%)	1.17	7/1629 (0.4%)
All	All	0.65	12/74650 (0.0%)	0.91	72/100986 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	41	ASP	CA-C	-7.13	1.43	1.52
5	Z	46	ALA	N-CA	7.05	1.55	1.46
2	C	1037	VAL	CA-CB	-6.59	1.46	1.54
5	X	44	GLU	CA-C	-6.54	1.45	1.52
5	Y	41	ASP	N-CA	-6.05	1.39	1.46

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	144	GLY	N-CA-C	-9.10	103.65	114.48
3	D	712	GLY	N-CA-C	-7.67	105.89	114.40
5	X	115	THR	CA-C-N	-7.05	110.09	120.46
5	X	115	THR	C-N-CA	-7.05	110.09	120.46
5	X	40	GLY	N-CA-C	-7.01	100.03	112.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1805	264	0
1	B	1767	0	1816	270	0
1	F	1759	0	1805	266	0
1	G	1759	0	1805	251	0
1	K	1769	0	1815	242	0
1	L	1767	0	1816	234	0
2	C	8521	0	8619	1253	0
2	H	8530	0	8632	1363	0
2	M	8521	0	8619	1190	0
3	D	10513	0	10743	1601	0
3	I	10396	0	10627	1471	0
3	N	10440	0	10682	1460	0
4	E	754	0	769	97	0
4	J	754	0	769	106	0
4	O	754	0	769	128	0
5	X	1200	0	1194	143	0
5	Y	1200	0	1194	148	0
5	Z	1200	0	1194	128	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	N	1	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
7	N	1	0	0	0	0
All	All	73369	0	74673	9980	0

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 67.

The worst 5 of 9980 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:41:ASP:OD1	5:Y:48:TYR:HB2	1.38	1.19
1:F:54:THR:HG22	1:F:158:ILE:HG13	1.26	1.17
2:H:983:ILE:HD12	3:I:944:THR:HA	1.23	1.16
2:M:565:GLN:HA	2:M:995:MET:HE1	1.22	1.14
1:G:99:LEU:HD13	1:G:142:VAL:HG23	1.29	1.13

There are no symmetry-related clashes.

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%)	167 (76%)	41 (19%)	13 (6%)	1	13
1	B	222/315 (70%)	171 (77%)	43 (19%)	8 (4%)	2	20
1	F	221/315 (70%)	166 (75%)	41 (19%)	14 (6%)	1	13
1	G	221/315 (70%)	168 (76%)	43 (20%)	10 (4%)	2	17
1	K	223/315 (71%)	173 (78%)	39 (18%)	11 (5%)	1	16
1	L	222/315 (70%)	165 (74%)	47 (21%)	10 (4%)	2	17
2	C	1074/1119 (96%)	774 (72%)	213 (20%)	87 (8%)	1	9
2	H	1075/1119 (96%)	766 (71%)	223 (21%)	86 (8%)	1	9
2	M	1074/1119 (96%)	765 (71%)	222 (21%)	87 (8%)	1	9
3	D	1326/1524 (87%)	943 (71%)	271 (20%)	112 (8%)	0	9
3	I	1308/1524 (86%)	958 (73%)	247 (19%)	103 (8%)	1	9
3	N	1313/1524 (86%)	953 (73%)	258 (20%)	102 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	91/99 (92%)	66 (72%)	18 (20%)	7 (8%)	1	10
4	J	91/99 (92%)	62 (68%)	22 (24%)	7 (8%)	1	10
4	O	91/99 (92%)	58 (64%)	27 (30%)	6 (7%)	1	12
5	X	152/156 (97%)	125 (82%)	21 (14%)	6 (4%)	2	18
5	Y	152/156 (97%)	118 (78%)	23 (15%)	11 (7%)	1	11
5	Z	152/156 (97%)	119 (78%)	24 (16%)	9 (6%)	1	13
All	All	9229/10584 (87%)	6717 (73%)	1823 (20%)	689 (8%)	1	10

5 of 689 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	171	PHE
1	A	228	PRO
1	B	118	ALA
1	B	126	ASP

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%)	168 (86%)	28 (14%)	3	15
1	B	197/273 (72%)	162 (82%)	35 (18%)	2	10
1	F	196/273 (72%)	159 (81%)	37 (19%)	1	9
1	G	196/273 (72%)	159 (81%)	37 (19%)	1	9
1	K	196/273 (72%)	165 (84%)	31 (16%)	2	13
1	L	197/273 (72%)	154 (78%)	43 (22%)	1	6
2	C	909/941 (97%)	754 (83%)	155 (17%)	2	11
2	H	910/941 (97%)	752 (83%)	158 (17%)	2	11
2	M	909/941 (97%)	764 (84%)	145 (16%)	2	12
3	D	1124/1279 (88%)	945 (84%)	179 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	1114/1279 (87%)	949 (85%)	165 (15%)	3	14
3	N	1120/1279 (88%)	939 (84%)	181 (16%)	2	12
4	E	82/88 (93%)	69 (84%)	13 (16%)	2	13
4	J	82/88 (93%)	71 (87%)	11 (13%)	4	16
4	O	82/88 (93%)	69 (84%)	13 (16%)	2	13
5	X	128/129 (99%)	108 (84%)	20 (16%)	2	13
5	Y	128/129 (99%)	108 (84%)	20 (16%)	2	13
5	Z	128/129 (99%)	106 (83%)	22 (17%)	2	11
All	All	7894/8949 (88%)	6601 (84%)	1293 (16%)	2	12

5 of 1293 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	217	LEU
3	N	959	GLU
2	M	383	ARG
2	M	209	ARG
3	N	12	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 269 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	552	ASN
3	N	748	HIS
5	X	57	GLN
1	G	63	HIS
1	F	229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 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 [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%)	-0.19	0 100 100	89, 173, 228, 279	0
1	B	224/315 (71%)	-0.17	0 100 100	108, 172, 229, 282	0
1	F	223/315 (70%)	-0.26	2 (0%) 81 67	83, 162, 225, 270	0
1	G	223/315 (70%)	-0.20	2 (0%) 81 67	91, 153, 211, 230	0
1	K	225/315 (71%)	-0.20	2 (0%) 81 67	116, 192, 249, 279	0
1	L	224/315 (71%)	-0.20	1 (0%) 88 77	89, 167, 217, 242	0
2	C	1080/1119 (96%)	-0.21	7 (0%) 85 73	80, 168, 245, 311	0
2	H	1081/1119 (96%)	-0.23	5 (0%) 87 75	67, 161, 239, 339	0
2	M	1080/1119 (96%)	-0.19	5 (0%) 87 75	80, 174, 247, 315	0
3	D	1334/1524 (87%)	-0.24	3 (0%) 91 83	83, 172, 251, 342	0
3	I	1318/1524 (86%)	-0.21	10 (0%) 82 69	65, 181, 280, 356	0
3	N	1323/1524 (86%)	-0.24	4 (0%) 90 80	77, 176, 260, 310	0
4	E	93/99 (93%)	0.00	2 (2%) 62 49	115, 192, 279, 362	0
4	J	93/99 (93%)	-0.12	1 (1%) 78 63	115, 177, 268, 293	0
4	O	93/99 (93%)	-0.30	0 100 100	88, 176, 245, 261	0
5	X	154/156 (98%)	-0.15	1 (0%) 85 73	146, 228, 282, 303	0
5	Y	154/156 (98%)	0.16	3 (1%) 66 52	157, 237, 315, 379	0
5	Z	154/156 (98%)	-0.06	2 (1%) 75 60	133, 219, 288, 356	0
All	All	9299/10584 (87%)	-0.21	50 (0%) 87 75	65, 175, 259, 379	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Y	129	LEU	3.9
4	E	57	ASP	3.8
4	E	65	MET	3.6

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Mol	Chain	Res	Type	RSRZ
3	I	161	LEU	3.3
2	C	1080	SER	3.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
7	MG	I	1602	1/1	0.57	0.30	114,114,114,114	0
7	MG	N	1602	1/1	0.57	0.18	182,182,182,182	0
6	ZN	I	1601	1/1	0.91	0.07	666,666,666,666	0
7	MG	D	2002	1/1	0.94	0.06	130,130,130,130	0
6	ZN	N	1601	1/1	0.95	0.05	333,333,333,333	0
6	ZN	D	2001	1/1	0.97	0.04	221,221,221,221	0

6.5 Other polymers [i](#)

There are no such residues in this entry.