



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 06:46 am BST

PDB ID : 4WQT
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

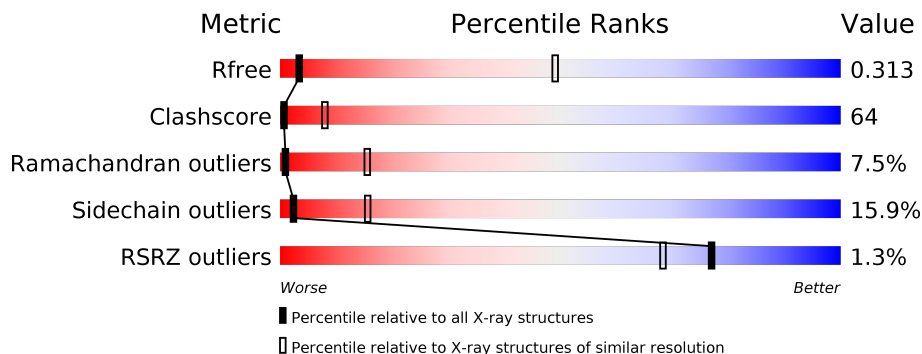
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	 % 17% 43% 10% 29%
1	B	315	 17% 44% 10% 29%
1	F	315	 19% 39% 12% 29%
1	G	315	 20% 39% 11% 29%
1	K	315	 % 19% 43% 10% 29%
1	L	315	 16% 43% 11% 29%

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Mol	Chain	Length	Quality of chain
2	C	1119	<p>%</p> <p>23% 57% 15% . .</p>
2	H	1119	<p>%</p> <p>22% 58% 16% . .</p>
2	M	1119	<p>%</p> <p>25% 56% 15% . .</p>
3	D	1524	<p>%</p> <p>22% 51% 13% . 12%</p>
3	I	1524	<p>%</p> <p>23% 50% 12% . 14%</p>
3	N	1524	<p>%</p> <p>22% 52% 13% . 13%</p>
4	E	99	<p>2%</p> <p>39% 42% 10% . 6%</p>
4	J	99	<p>2%</p> <p>24% 58% 12% 6%</p>
4	O	99	<p>2%</p> <p>23% 57% 14% 6%</p>
5	X	156	<p>5%</p> <p>29% 56% 11% . .</p>
5	Y	156	<p>6%</p> <p>35% 48% 14% . .</p>
5	Z	156	<p>4%</p> <p>26% 57% 13% . .</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	223	Total 1759	C 1123	N 306	O 328	S 2	0	0	0
1	B	224	Total 1767	C 1129	N 307	O 329	S 2	0	0	0
1	F	223	Total 1759	C 1123	N 306	O 328	S 2	0	0	0
1	G	223	Total 1759	C 1123	N 306	O 328	S 2	0	0	0
1	K	225	Total 1769	C 1129	N 308	O 330	S 2	0	0	0
1	L	224	Total 1767	C 1129	N 307	O 329	S 2	0	0	0

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

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

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

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

- 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 (three-letter code: ZN) (formula: Zn).

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

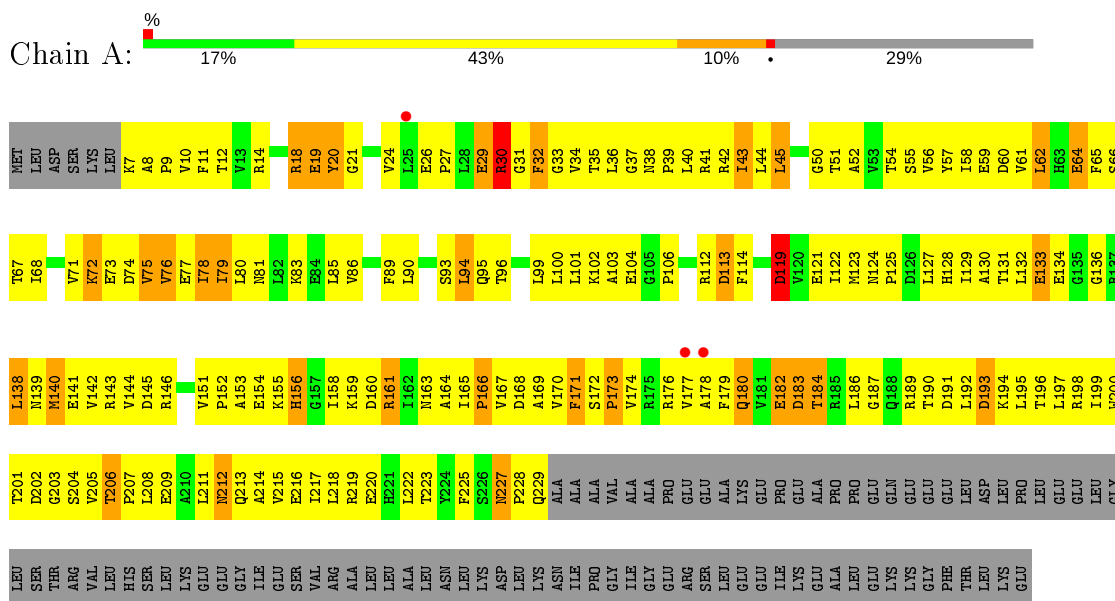
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

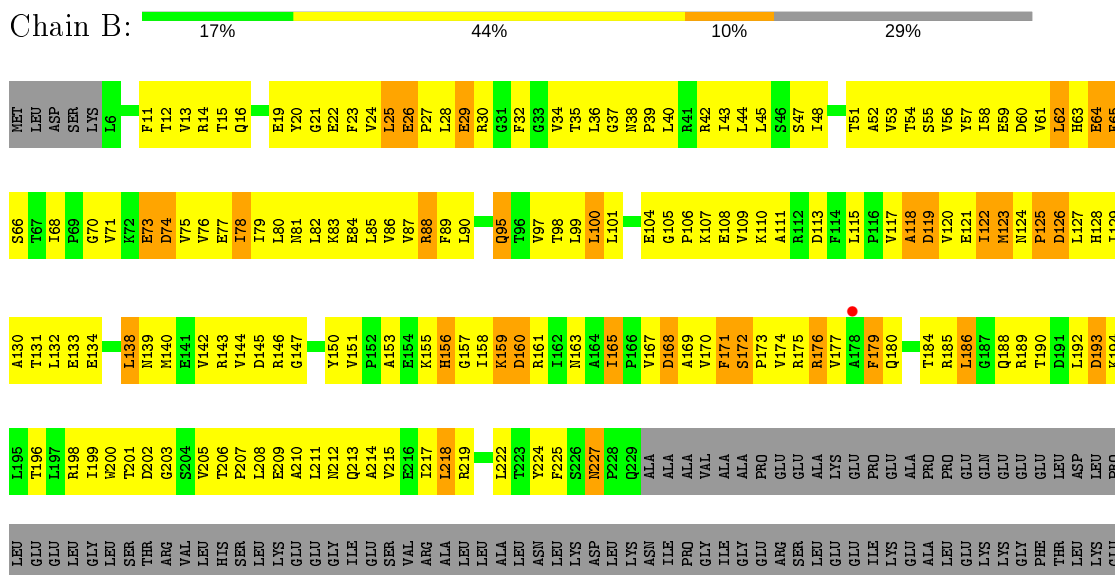
3 Residue-property plots

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

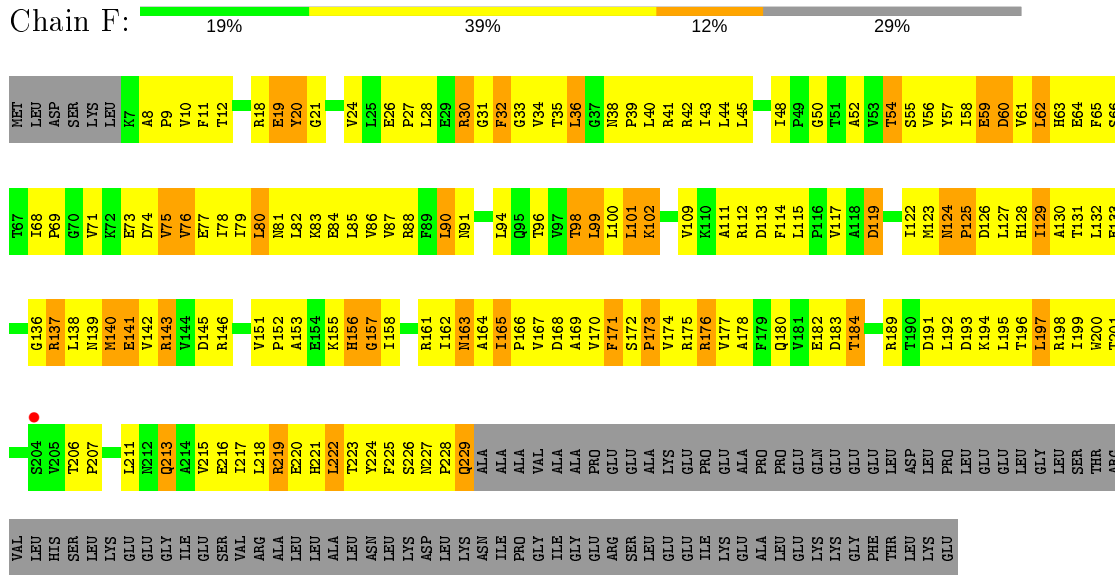
- Molecule 1: DNA-directed RNA polymerase subunit alpha



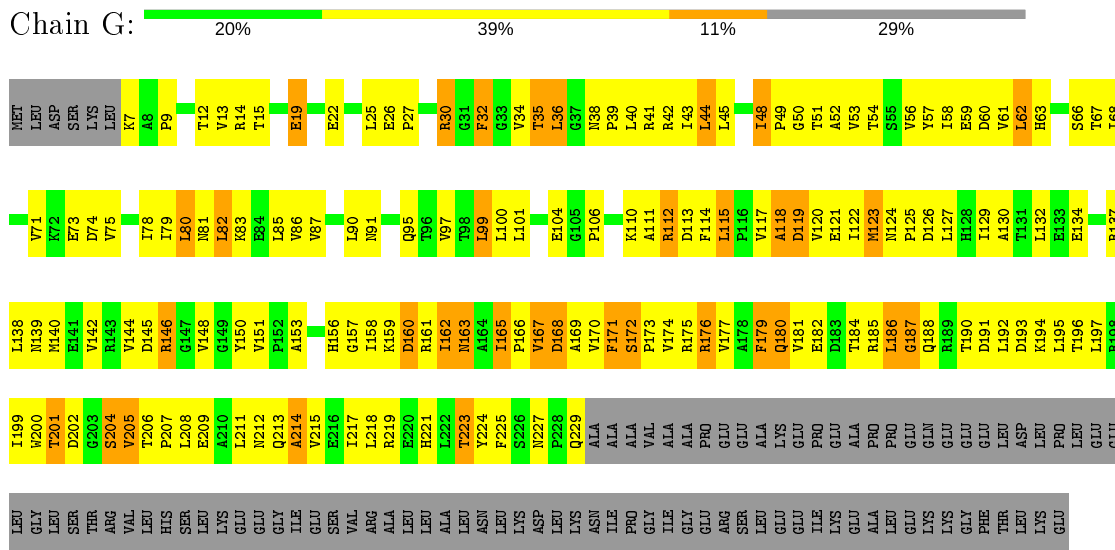
- Molecule 1: DNA-directed RNA polymerase subunit alpha



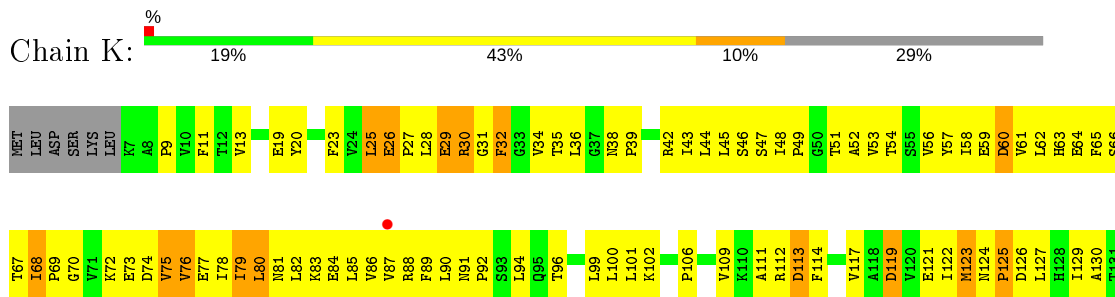
• Molecule 1: DNA-directed RNA polymerase subunit alpha

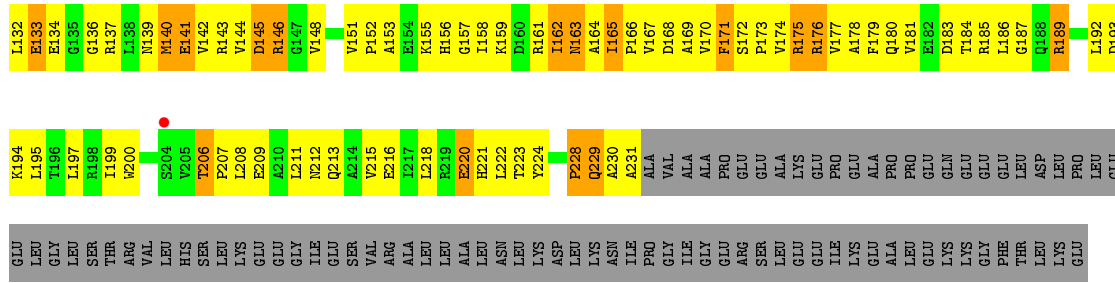


• Molecule 1: DNA-directed RNA polymerase subunit alpha

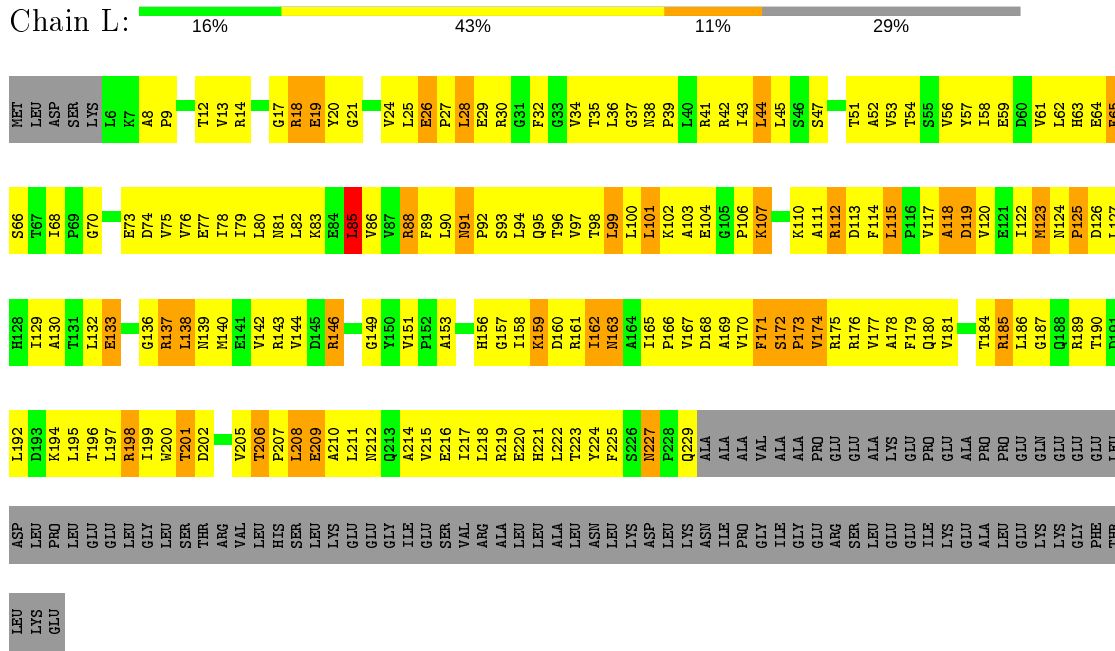


• Molecule 1: DNA-directed RNA polymerase subunit alpha

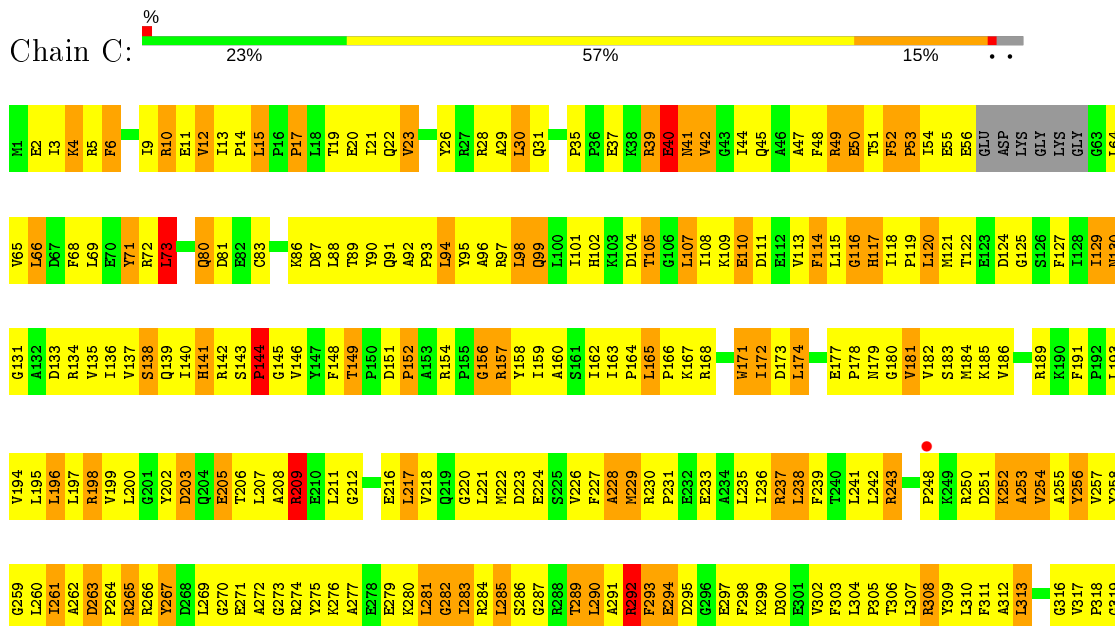


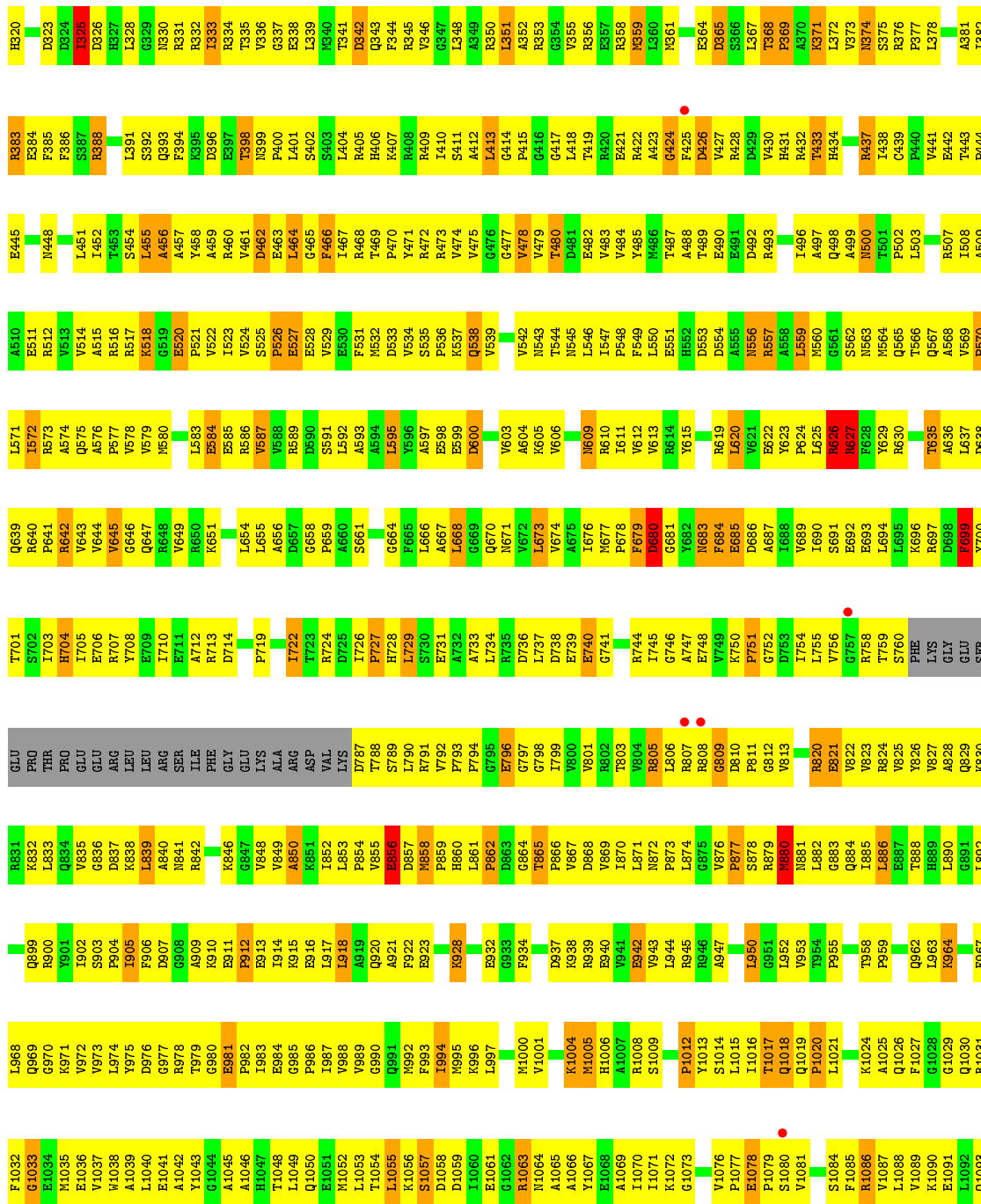


• Molecule 1: DNA-directed RNA polymerase subunit alpha

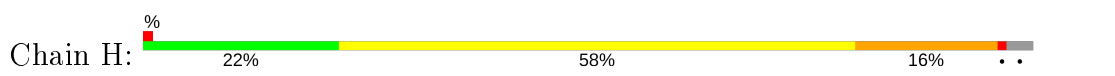


• Molecule 2: DNA-directed RNA polymerase subunit beta

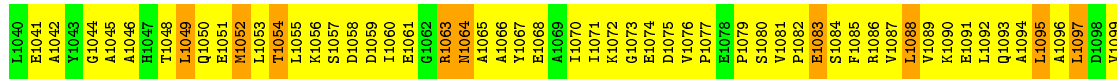




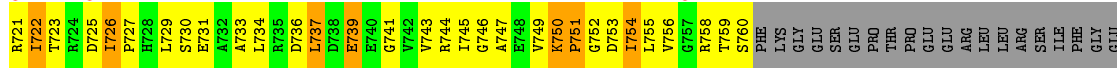
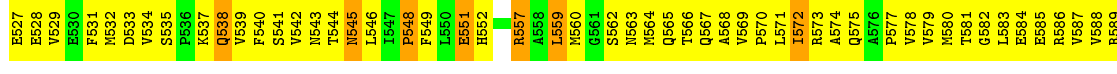
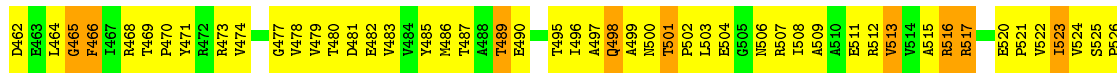
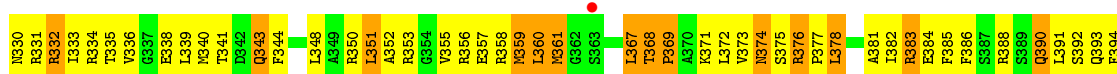
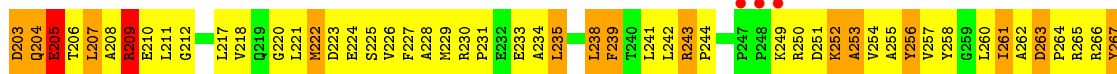
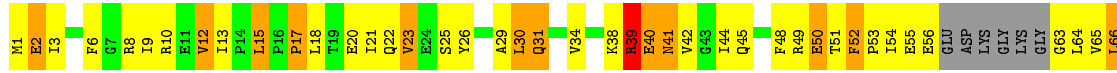
● Molecule 2: DNA-directed RNA polymerase subunit beta

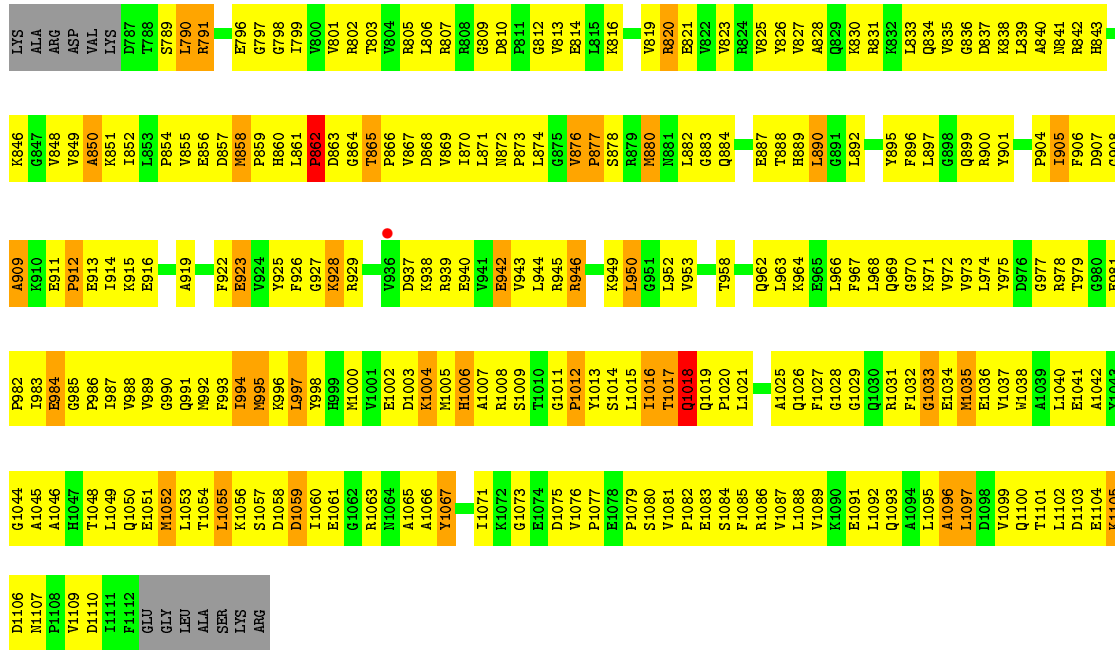


V973	G898	G886	ARG	E711	V649	E585	I593	R388	I325	A262	R198	LYS
L974	Q899	D837	SER	A712	R650	R986	V624	S389	D826	D263	V199	GLY
Y975	R900	K838	ILE	R713	V653	V587	S525	S390	P264	P264	L200	GLY
D976	Y901	L839	PHE	D714	D653	V688	P526	L391	E327	R265	G201	L64
G977	I902	A840	GLY	K715	R654	R689	E527	S392	G329	R265	Y202	V65
R978	S903	N641	GLU	T716	L655	D590	E528	Q393	R267	Y267	D203	L66
R979	P904	R842	LYS	K716	A656	S591	V529	F384	R331	D688	O204	D67
G980	I905	R842	ALA	P719	D657	L592	E530	K395	R332	L269	H141	F66
G981	F906	K846	ARG	E720	G658	A593	F531	D396	I333	G270	R142	L69
G982	D907	G847	ASP	I721	S661	A594	M532	E397	R334	A271	S143	E70
G983	G908	V848	VAL	I722	L595	L595	D533	E397	T335	A272	P144	E71
G984	A909	R849	K766	R723	E662	V596	V534	T398	V356	G273	G145	R72
G985	K910	A850	D787	R724	N663	A597	S585	S402	G337	R274	V146	R73
G986	E911	K851	T788	D725	G664	E598	F536	S403	E338	Y275	Y147	G74
G987	R912	L852	S789	I726	F665	E599	R537	L404	R340	K276	F148	E75
G988	E913	L853	L790	P727	L666	D600	O538	L404	M349	A277	T149	E76
G989	I914	P854	R791	H728	A667	G601	V539	H406	T341	E278	P150	E77
G990	R915	R855	R792	D736	V674	D607	L546	K407	G347	R284	D151	R78
G991	E916	E856	P793	L737	A675	N609	L547	G414	L348	L285	R157	R79
G992	L917	R862	I798	R744	V676	R610	F548	P415	R350	G287	Y158	A92
G993	L918	D863	V800	E740	I677	R611	F549	G416	R351	R288	A160	P83
G994	E921	R864	R801	G741	R678	V612	L550	G417	L352	T289	S161	L94
G995	R922	P865	T803	V742	F679	R613	E551	T487	R353	L290	I162	R97
G996	F922	L866	R804	V743	D680	R614	H552	A488	G354	A291	I163	L98
G997	Y925	D868	R805	R744	G681	V615	S563	T489	V355	R392	P164	Q99
G998	F926	R869	L806	Y682	Y682	E616	D554	E490	R356	F293	L165	L100
G999	G927	R870	R807	M683	M683	E617	M556	A423	E357	E294	L166	L101
G1000	R927	L871	R808	F684	F684	O618	R556	G424	R358	F298	K167	D104
G1001	E930	N872	D810	E749	E685	O619	M564	F425	M359	K299	R168	T105
G1002	R941	P873	T804	K750	D686	R623	O565	G426	R360	A294	G169	G106
G1003	E942	L874	R811	P751	A687	V623	O566	Y494	L360	D300	P170	G107
G1004	R943	G875	G812	G752	I688	R624	T566	Y495	S863	E301	M771	E112
G1005	L944	V876	V813	D753	V689	L625	M500	F436	E364	V302	L172	E113
G1006	R945	P877	E814	I754	V690	R626	N500	A437	E365	R303	M179	F114
G1007	R946	S878	L815	L755	S691	R627	A510	I438	D366	F311	G180	G116
G1008	A947	R879	K316	V756	E692	F628	A511	C439	R432	R311	V181	H117
G1009	E948	M880	V819	G757	E693	V629	O565	P440	L304	P305	E175	I118
G1010	K949	N881	R820	R758	L694	R630	A574	V441	L367	T306	V176	P119
G1011	L944	L882	R821	I759	L695	S631	Q575	E442	D369	L307	E177	L120
G1012	R945	P877	E814	G759	L695	M632	M506	T443	S863	R307	P178	E114
G1013	R946	S878	L815	L755	S691	R627	A509	I438	E364	Y309	M179	L115
G1014	A947	R879	K316	V756	E692	F628	A510	C439	D366	R311	G180	G116
G1015	E948	M880	V819	G757	E693	V629	A511	P440	R432	F311	V181	H117
G1016	K949	N881	R820	R758	L694	R630	A574	V441	L367	P305	E175	I118
G1017	L944	L882	R821	I759	L695	S631	Q575	E442	D369	T306	V176	P119
G1018	G951	G853	E821	PHE	R697	M632	M506	T443	S863	R307	P178	E114
G1019	L952	Q854	V822	LYS	D698	O633	A509	I438	E364	Y309	M179	L115
G1020	P953	L855	V823	GLY	D699	O633	A510	C439	D366	R311	G180	G116
G1021	T954	L856	R824	GLU	F699	R640	A511	P440	R432	F311	V181	H117
G1022	P955	F857	V825	GLU	Y700	L637	R512	V441	L367	P305	E175	I118
G1023	P955	F857	V826	SER	T701	D638	R513	E442	D369	T344	K252	P119
G1024	Q962	T868	V827	GLU	S702	O639	V514	T443	S863	R377	K252	L120
G1025	L963	L859	A828	GLU	I703	R640	V515	L378	E364	L378	A253	K185
G1026	K964	G891	Q829	TRP	H704	R641	A515	G450	D366	V317	V254	D124
G1027	E965	L892	K330	PRO	I705	R642	R517	L451	R382	F311	A255	G125
G1028	L966	R893	R831	GLU	E706	V643	K518	L452	R383	H320	Y256	S126
G1029	F967	G894	K832	GLU	R707	V643	M580	T453	L493	H320	V257	I129
G1030	L968	F895	L833	ARG	R708	O646	S454	S454	E384	H320	Y256	I129
G1031	F969	F896	Q834	LEU	E709	O647	G582	L455	F385	V322	G259	L194
G1032	G970	L897	V835	LEU	I710	R648	E584	A456	S387	D324	I261	L196
G1033	G970	L897	V835	LEU	I710	R648	E584	A456	S387	D324	I261	D133

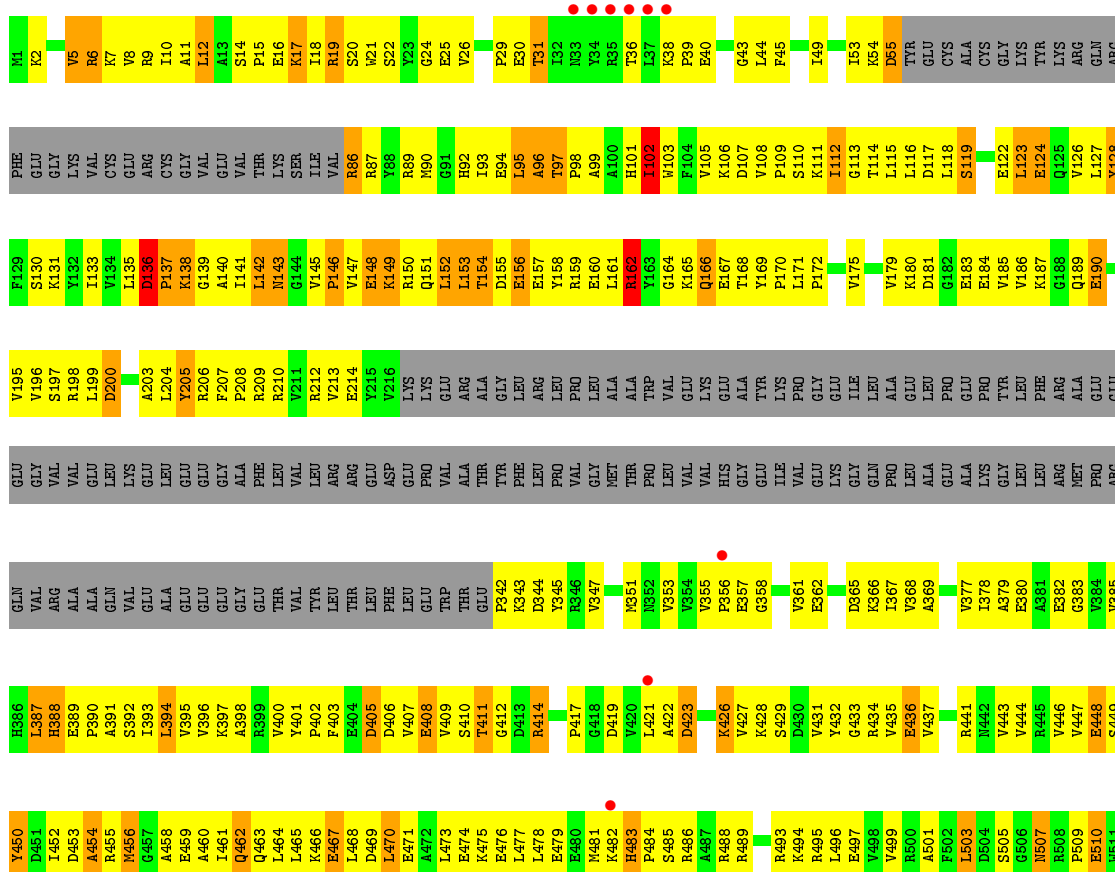


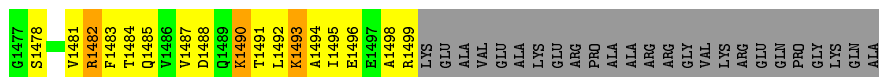
• Molecule 2: DNA-directed RNA polymerase subunit beta



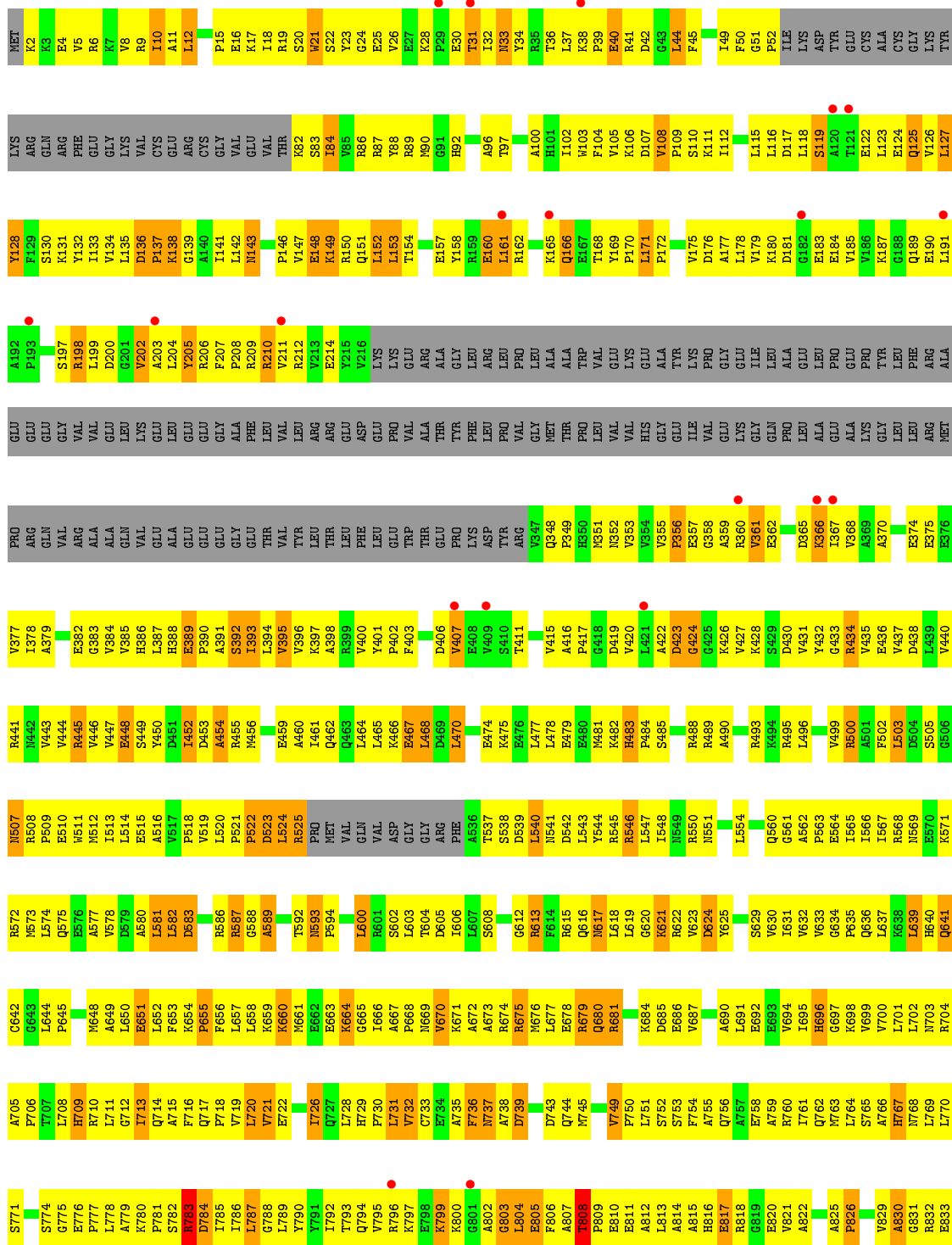
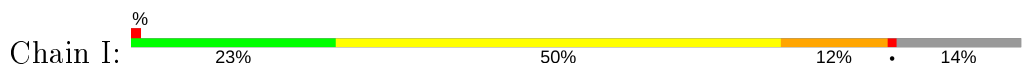


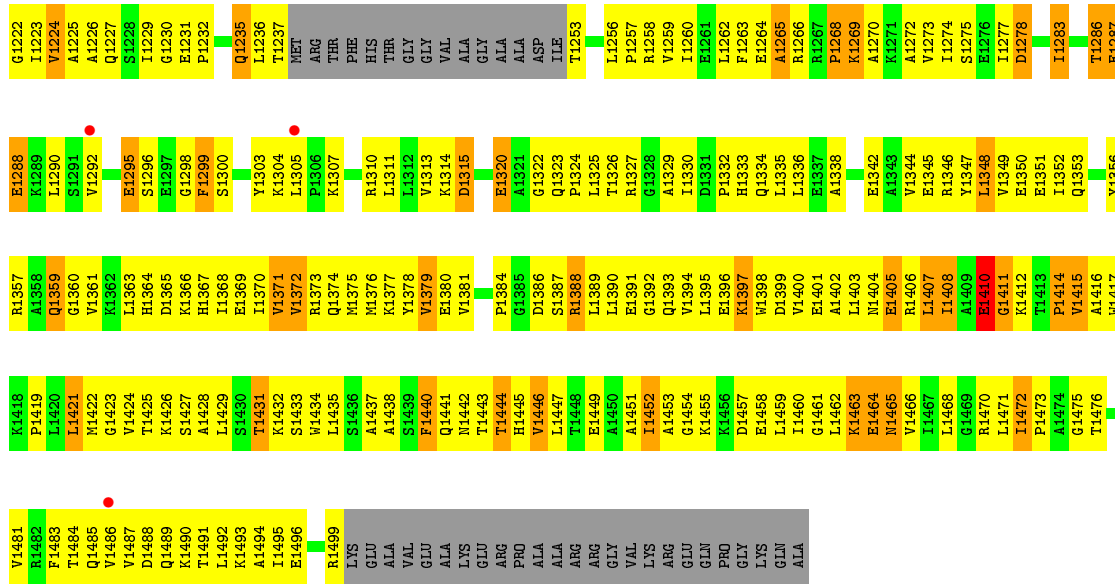
● Molecule 3: DNA-directed RNA polymerase subunit beta'



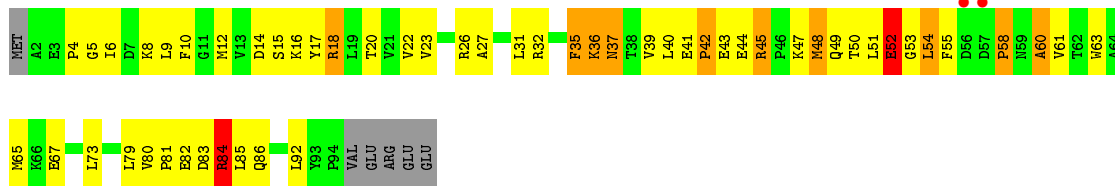


• Molecule 3: DNA-directed RNA polymerase subunit beta'

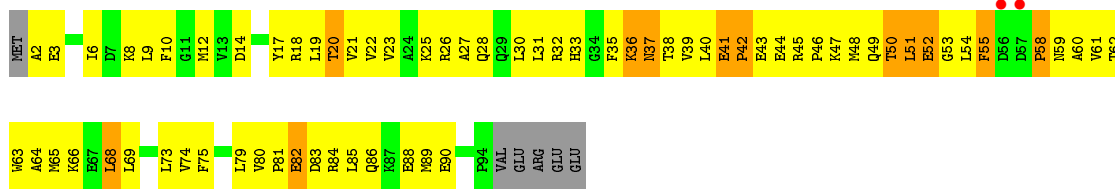




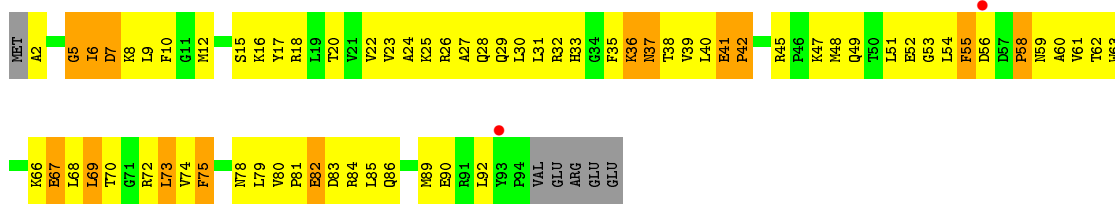
• Molecule 4: DNA-directed RNA polymerase subunit omega



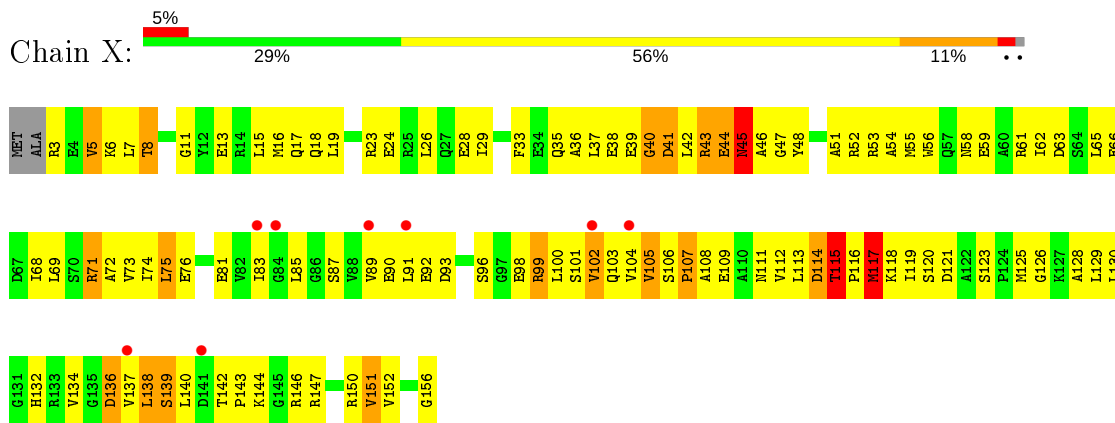
• Molecule 4: DNA-directed RNA polymerase subunit omega



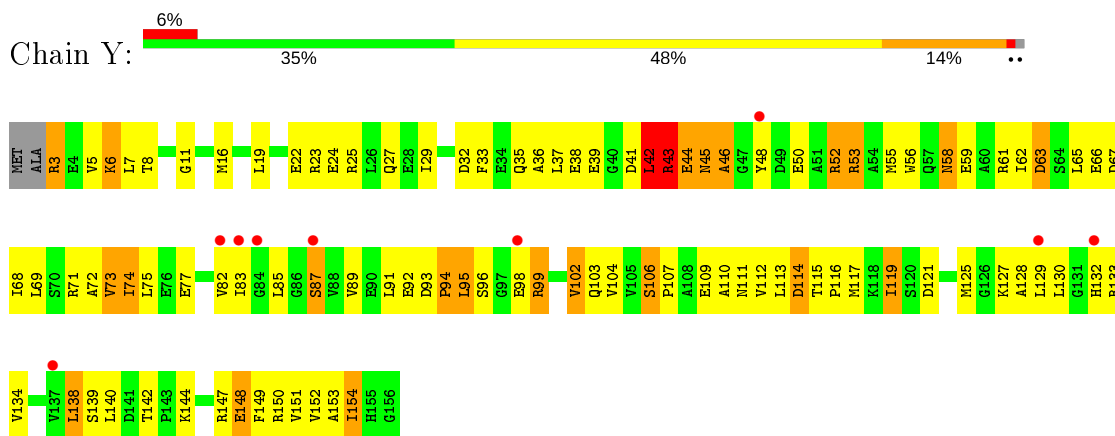
• Molecule 4: DNA-directed RNA polymerase subunit omega



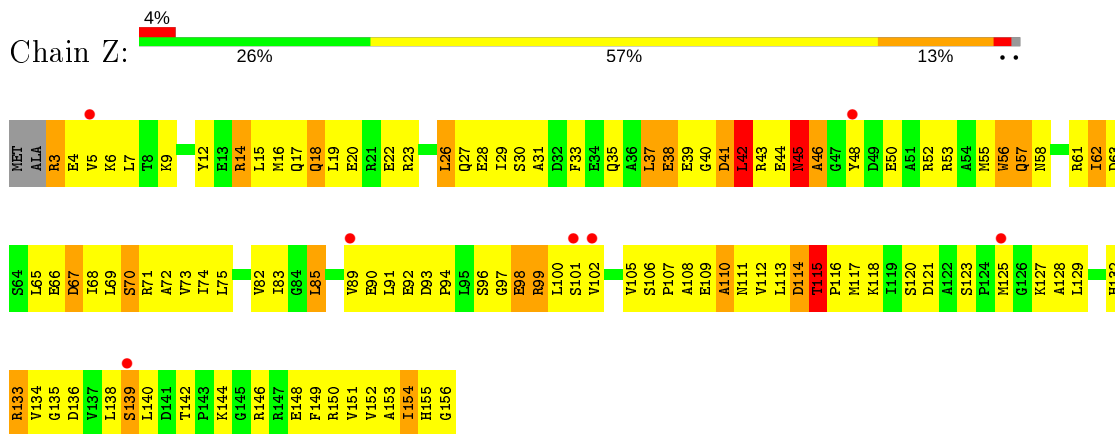
• Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)



• 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) 96.5 (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)	Xtrriage
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 (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	151.2	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 136.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtrriage
Estimated twinning fraction	0.129 for l,-k,h	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	73369	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/1791	0.64	0/2436
1	B	0.51	0/1799	0.65	0/2447
1	F	0.51	0/1791	0.66	0/2436
1	G	0.51	0/1791	0.68	0/2436
1	K	0.45	0/1801	0.60	0/2450
1	L	0.51	0/1799	0.65	0/2447
2	C	0.51	0/8683	0.63	0/11747
2	H	0.53	0/8692	0.64	0/11758
2	M	0.49	0/8683	0.63	0/11747
3	D	0.52	0/10692	0.65	1/14452 (0.0%)
3	I	0.50	0/10571	0.62	0/14288
3	N	0.50	0/10617	0.63	0/14350
4	E	0.49	0/768	0.62	0/1035
4	J	0.51	0/768	0.63	0/1035
4	O	0.53	0/768	0.62	0/1035
5	X	0.68	0/1212	0.81	1/1629 (0.1%)
5	Y	0.64	0/1212	0.82	1/1629 (0.1%)
5	Z	0.62	0/1212	0.87	2/1629 (0.1%)
All	All	0.51	0/74650	0.65	5/100986 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	37	LEU	CB-CG-CD1	-6.64	99.71	111.00
5	Z	42	LEU	CA-CB-CG	5.91	128.89	115.30
5	X	40	GLY	N-CA-C	-5.23	100.03	113.10
5	Y	85	LEU	CA-CB-CG	-5.07	103.64	115.30
3	D	1242	HIS	N-CA-C	-5.02	97.45	111.00

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	257	0
1	B	1767	0	1816	262	0
1	F	1759	0	1805	253	0
1	G	1759	0	1805	236	0
1	K	1769	0	1815	236	0
1	L	1767	0	1816	230	0
2	C	8521	0	8619	1196	0
2	H	8530	0	8632	1294	0
2	M	8521	0	8619	1131	0
3	D	10513	0	10743	1508	0
3	I	10396	0	10627	1408	0
3	N	10440	0	10682	1391	0
4	E	754	0	769	86	0
4	J	754	0	769	99	0
4	O	754	0	769	124	0
5	X	1200	0	1194	142	0
5	Y	1200	0	1194	139	0
5	Z	1200	0	1194	125	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	9501	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 64.

The worst 5 of 9501 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
1:G:99:LEU:HD13	1:G:142:VAL:HG23	1.29	1.13
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.28	1.12

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	20
1	B	222/315 (70%)	171 (77%)	43 (19%)	8 (4%)	3	28
1	F	221/315 (70%)	166 (75%)	41 (19%)	14 (6%)	1	19
1	G	221/315 (70%)	168 (76%)	43 (20%)	10 (4%)	2	24
1	K	223/315 (71%)	173 (78%)	39 (18%)	11 (5%)	2	23
1	L	222/315 (70%)	165 (74%)	47 (21%)	10 (4%)	2	24
2	C	1074/1119 (96%)	774 (72%)	213 (20%)	87 (8%)	1	14
2	H	1075/1119 (96%)	766 (71%)	223 (21%)	86 (8%)	1	14
2	M	1074/1119 (96%)	765 (71%)	222 (21%)	87 (8%)	1	14
3	D	1326/1524 (87%)	943 (71%)	271 (20%)	112 (8%)	1	13
3	I	1308/1524 (86%)	958 (73%)	247 (19%)	103 (8%)	1	14
3	N	1313/1524 (86%)	953 (73%)	258 (20%)	102 (8%)	1	15
4	E	91/99 (92%)	66 (72%)	18 (20%)	7 (8%)	1	15
4	J	91/99 (92%)	62 (68%)	22 (24%)	7 (8%)	1	15
4	O	91/99 (92%)	58 (64%)	27 (30%)	6 (7%)	1	18
5	X	152/156 (97%)	125 (82%)	21 (14%)	6 (4%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Y	152/156 (97%)	118 (78%)	23 (15%)	11 (7%)	1	16
5	Z	152/156 (97%)	119 (78%)	24 (16%)	9 (6%)	1	20
All	All	9229/10584 (87%)	6717 (73%)	1823 (20%)	689 (8%)	1	15

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 [i](#)

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%)	163 (83%)	33 (17%)	2	14
1	B	197/273 (72%)	161 (82%)	36 (18%)	1	11
1	F	196/273 (72%)	160 (82%)	36 (18%)	1	11
1	G	196/273 (72%)	163 (83%)	33 (17%)	2	14
1	K	196/273 (72%)	168 (86%)	28 (14%)	3	18
1	L	197/273 (72%)	160 (81%)	37 (19%)	1	10
2	C	909/941 (97%)	763 (84%)	146 (16%)	2	15
2	H	910/941 (97%)	762 (84%)	148 (16%)	2	14
2	M	909/941 (97%)	763 (84%)	146 (16%)	2	15
3	D	1124/1279 (88%)	948 (84%)	176 (16%)	2	16
3	I	1114/1279 (87%)	951 (85%)	163 (15%)	3	17
3	N	1120/1279 (88%)	946 (84%)	174 (16%)	2	16
4	E	82/88 (93%)	69 (84%)	13 (16%)	2	15
4	J	82/88 (93%)	70 (85%)	12 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	82/88 (93%)	68 (83%)	14 (17%)	2	13
5	X	128/129 (99%)	111 (87%)	17 (13%)	4	20
5	Y	128/129 (99%)	108 (84%)	20 (16%)	2	16
5	Z	128/129 (99%)	104 (81%)	24 (19%)	1	10
All	All	7894/8949 (88%)	6638 (84%)	1256 (16%)	2	15

5 of 1256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	679	PHE
3	I	842	VAL
3	N	1295	GLU
2	H	799	ILE
3	I	171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 239 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	872	ASN
3	I	845	ASN
3	N	1334	GLN
2	H	899	GLN
3	I	549	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q<0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/315 (70%)	-0.30	3 (1%) 77 68	89, 173, 228, 279	0
1	B	224/315 (71%)	-0.33	1 (0%) 92 87	108, 172, 229, 282	0
1	F	223/315 (70%)	-0.39	1 (0%) 92 87	83, 162, 225, 270	0
1	G	223/315 (70%)	-0.45	0 100 100	91, 153, 211, 230	0
1	K	225/315 (71%)	-0.17	2 (0%) 84 77	116, 192, 249, 279	0
1	L	224/315 (71%)	-0.43	0 100 100	89, 167, 217, 242	0
2	C	1080/1119 (96%)	-0.33	6 (0%) 89 84	80, 168, 245, 311	0
2	H	1081/1119 (96%)	-0.35	10 (0%) 84 77	67, 161, 239, 339	0
2	M	1080/1119 (96%)	-0.30	16 (1%) 73 64	80, 174, 247, 315	0
3	D	1334/1524 (87%)	-0.28	15 (1%) 80 72	83, 172, 251, 342	0
3	I	1318/1524 (86%)	-0.22	22 (1%) 70 61	65, 181, 280, 356	0
3	N	1323/1524 (86%)	-0.26	17 (1%) 77 68	77, 176, 260, 310	0
4	E	93/99 (93%)	-0.07	2 (2%) 62 52	115, 192, 279, 362	0
4	J	93/99 (93%)	-0.26	2 (2%) 62 52	115, 177, 268, 293	0
4	O	93/99 (93%)	-0.17	2 (2%) 62 52	88, 176, 245, 261	0
5	X	154/156 (98%)	0.12	8 (5%) 27 24	146, 228, 282, 303	0
5	Y	154/156 (98%)	0.21	9 (5%) 23 19	157, 237, 315, 379	0
5	Z	154/156 (98%)	0.07	7 (4%) 33 28	133, 219, 288, 356	0
All	All	9299/10584 (87%)	-0.27	123 (1%) 77 68	65, 175, 259, 379	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	56	ASP	7.0
4	E	57	ASP	6.3
3	I	211	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
2	C	807	ARG	5.2
5	Y	129	LEU	4.7

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	N	1602	1/1	0.91	0.38	182,182,182,182	0
6	ZN	I	1601	1/1	0.94	0.07	666,666,666,666	0
6	ZN	N	1601	1/1	0.95	0.06	333,333,333,333	0
7	MG	I	1602	1/1	0.95	1.08	114,114,114,114	0
6	ZN	D	2001	1/1	0.97	0.06	221,221,221,221	0
7	MG	D	2002	1/1	0.97	0.17	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.