wwPDB X-ray Structure Validation Summary Report (i)

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

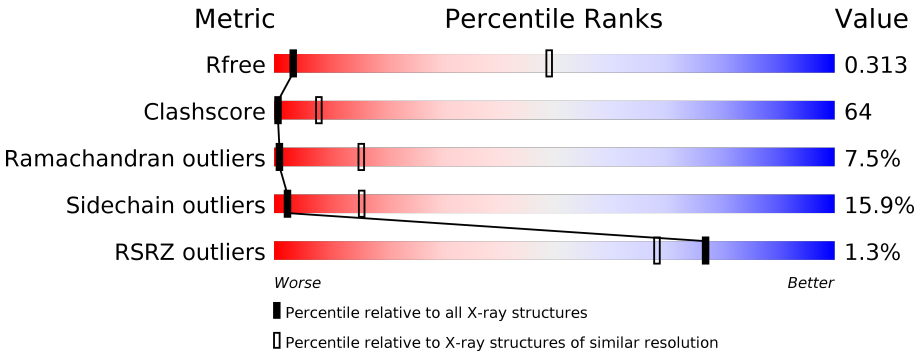
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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 <=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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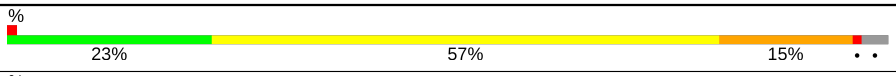
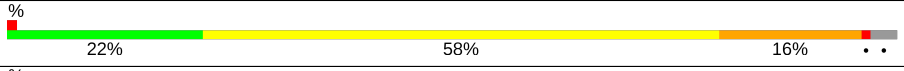
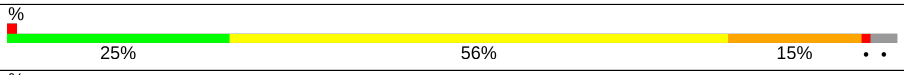
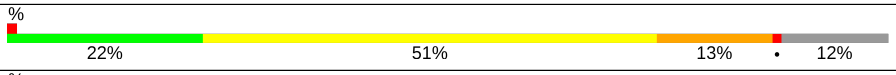
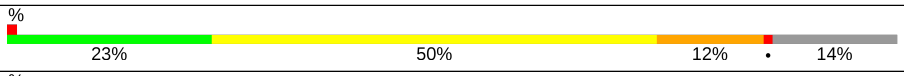
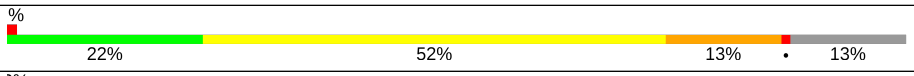
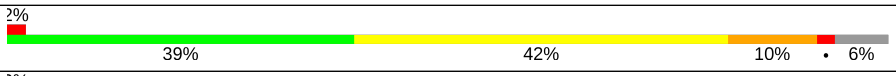
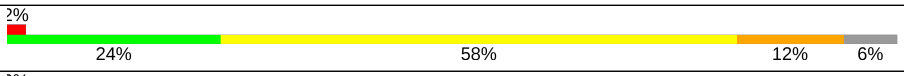
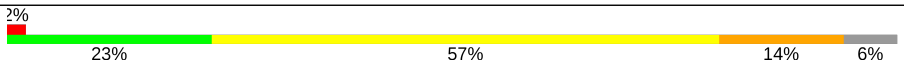
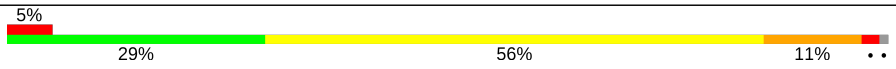
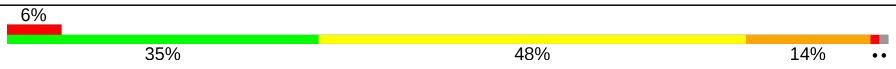
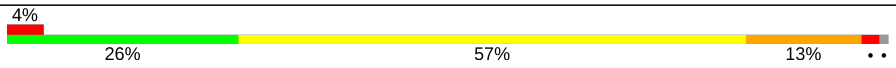
Mol	Chain	Length	Quality of chain
2	C	1119	
2	H	1119	
2	M	1119	
3	D	1524	
3	I	1524	
3	N	1524	
4	E	99	
4	J	99	
4	O	99	
5	X	156	
5	Y	156	
5	Z	156	

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 (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).

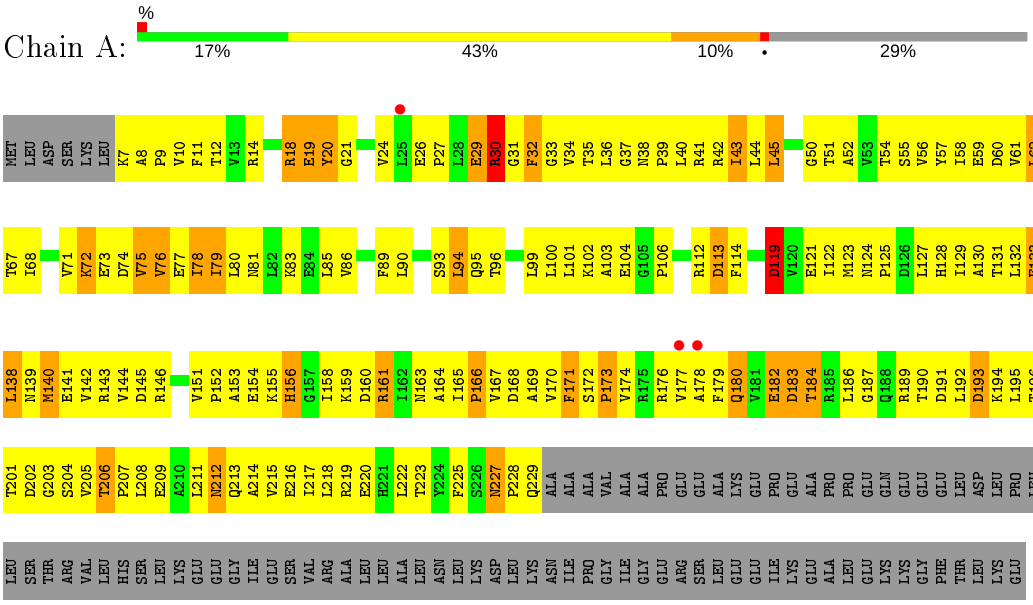
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

3 Residue-property plots (i)

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.

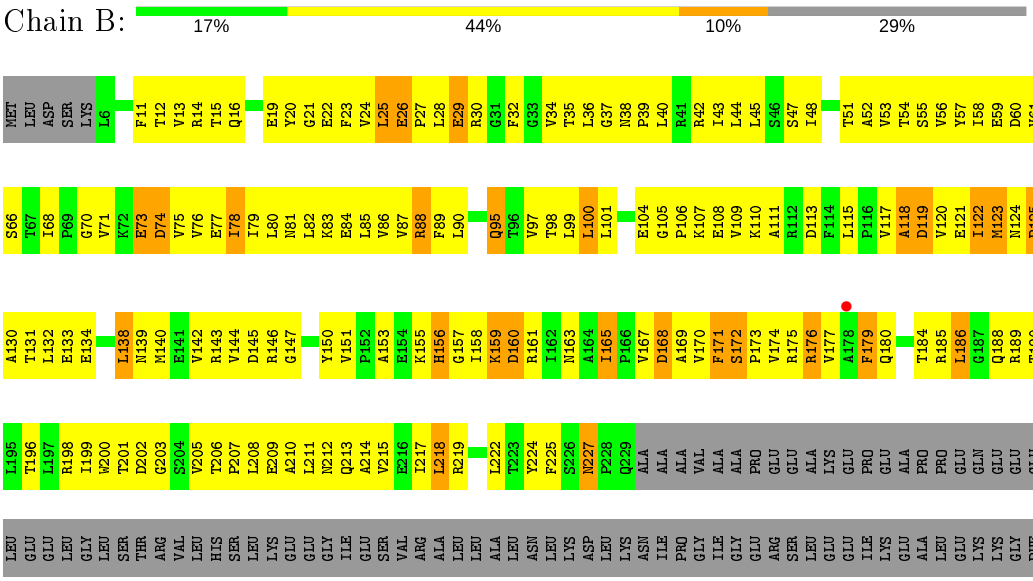
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



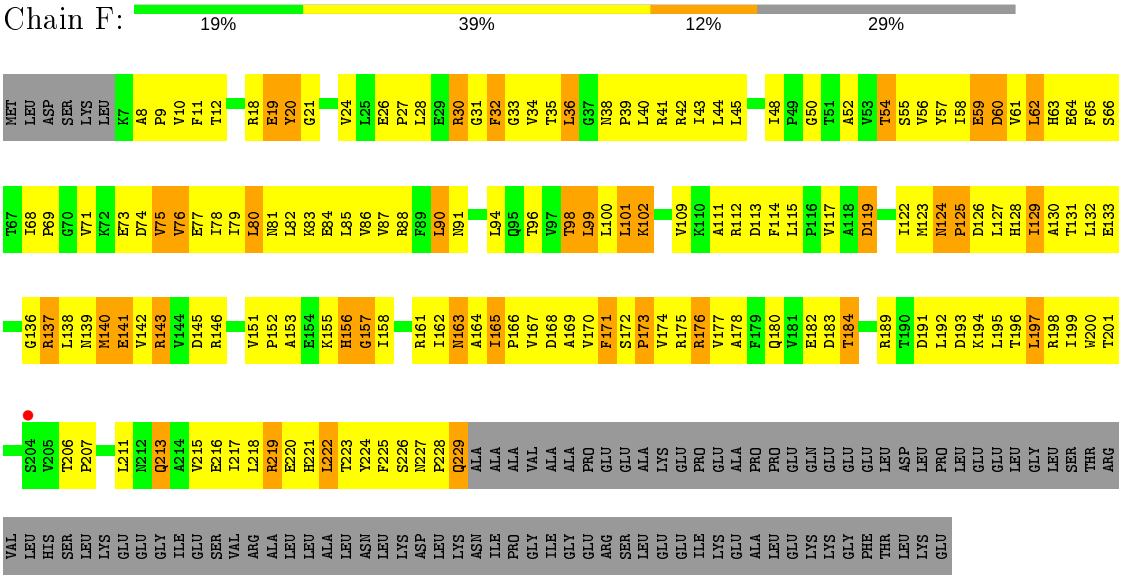
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



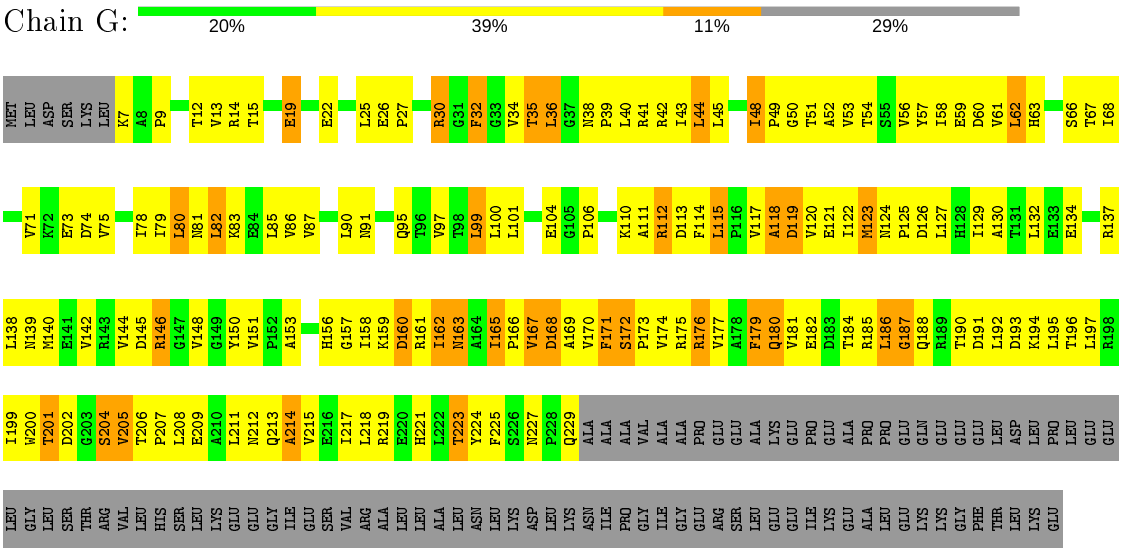
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain F:



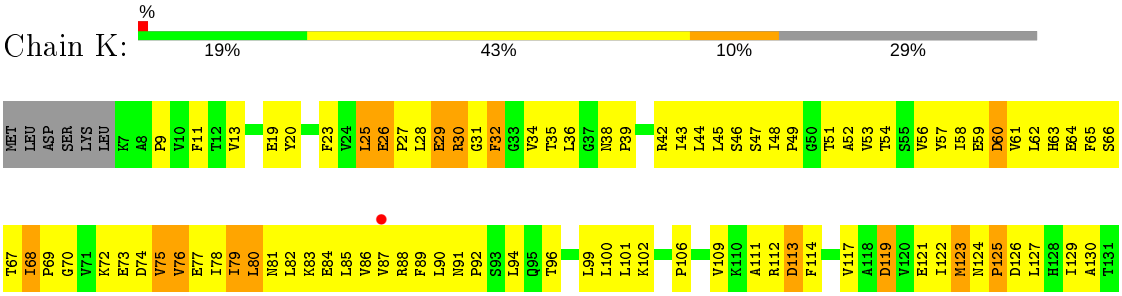
• Molecule 1: DNA-directed RNA polymerase subunit alpha

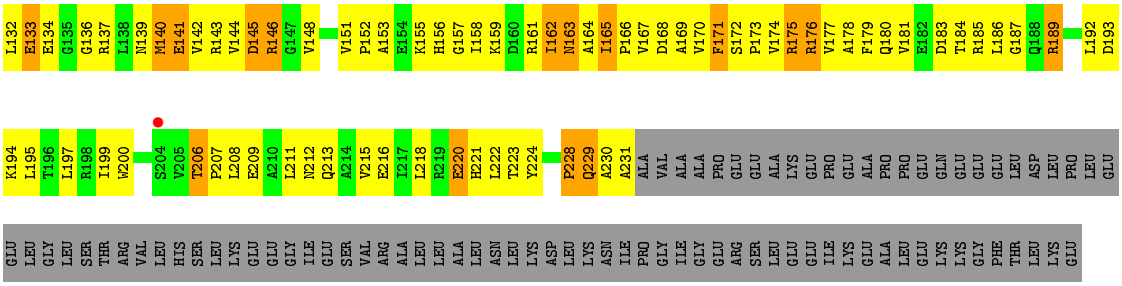
Chain G:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

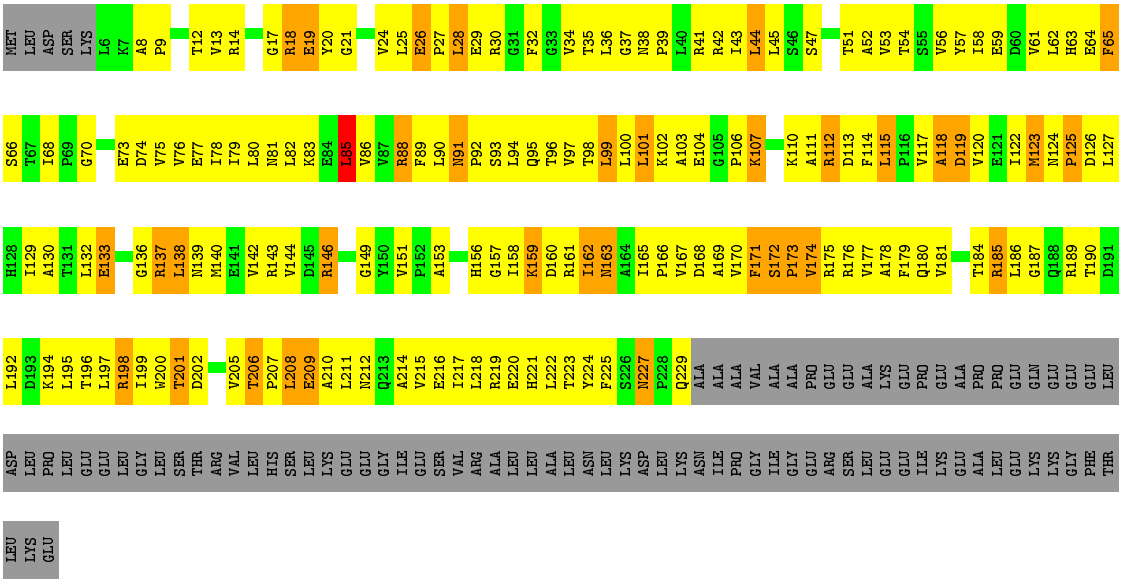
Chain K:





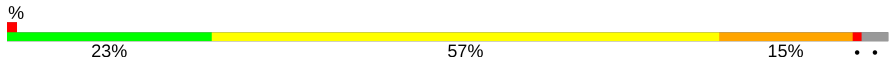
• Molecule 1: DNA-directed RNA polymerase subunit alpha

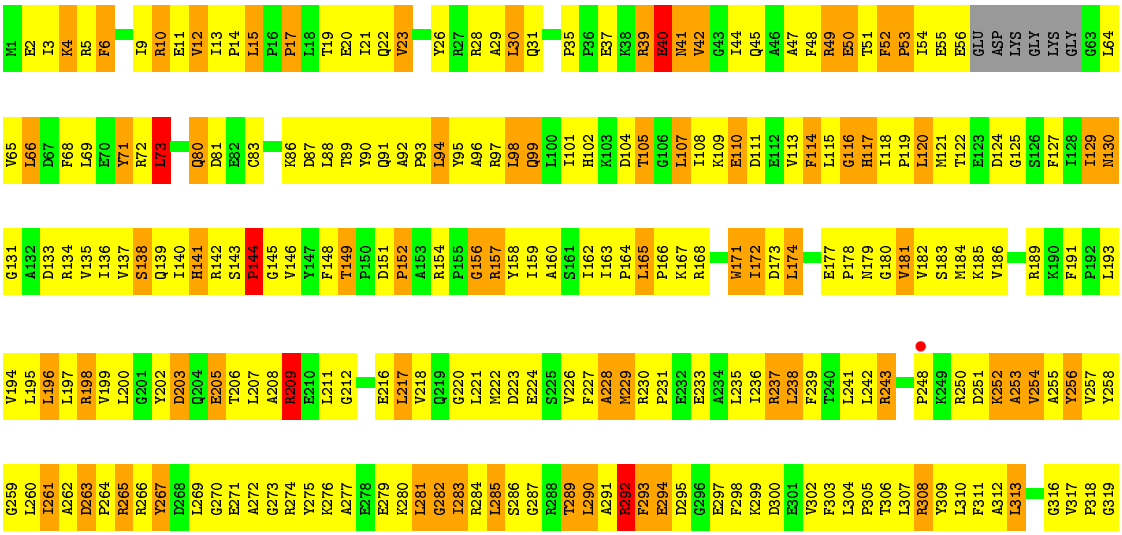
Chain L:

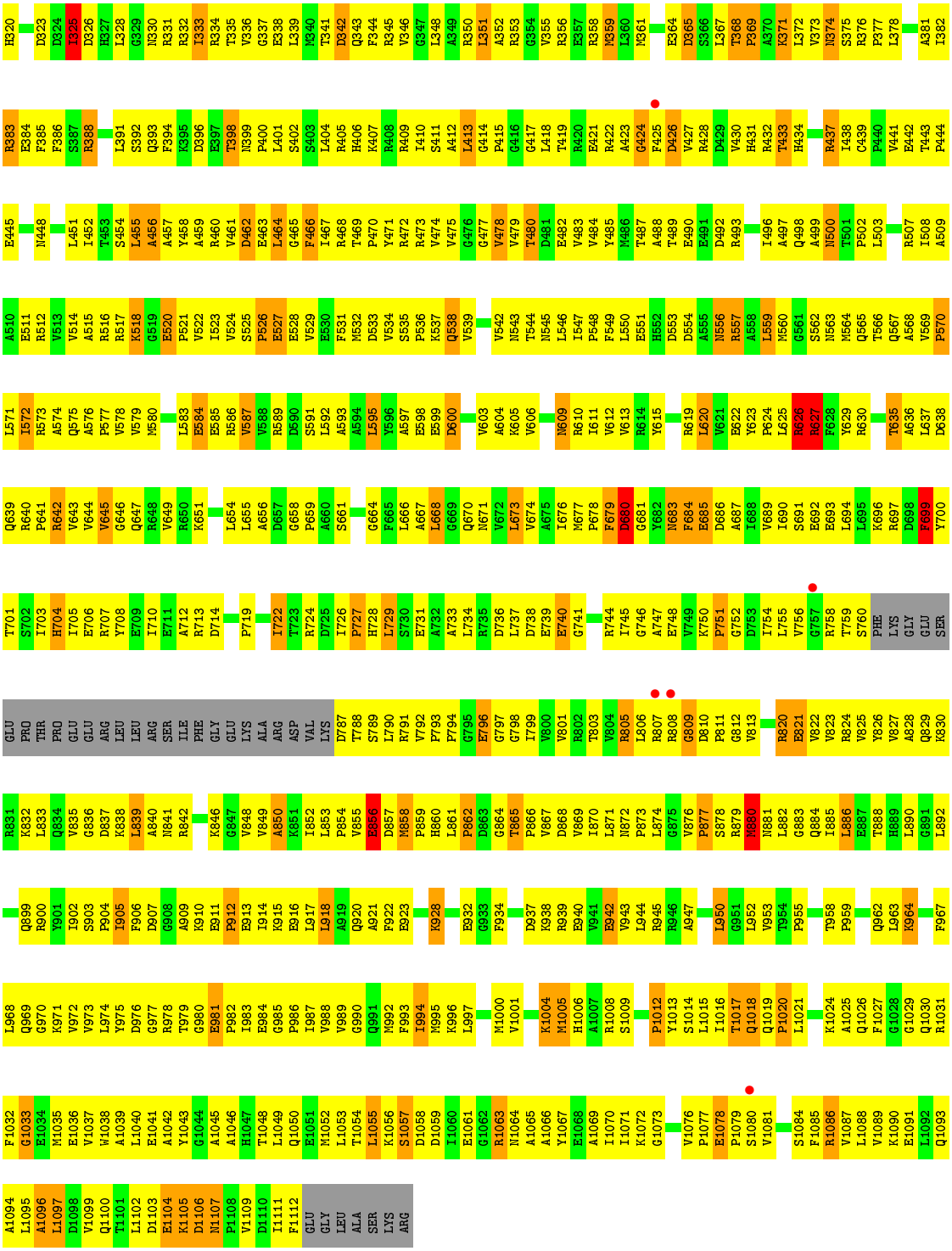


• Molecule 2: DNA-directed RNA polymerase subunit beta

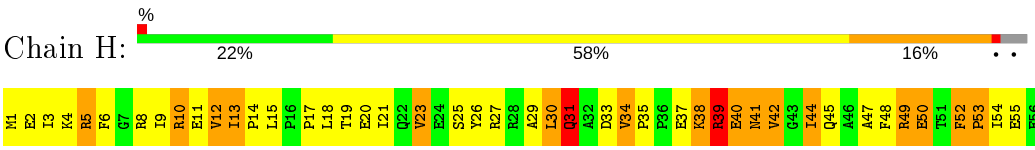
Chain C:

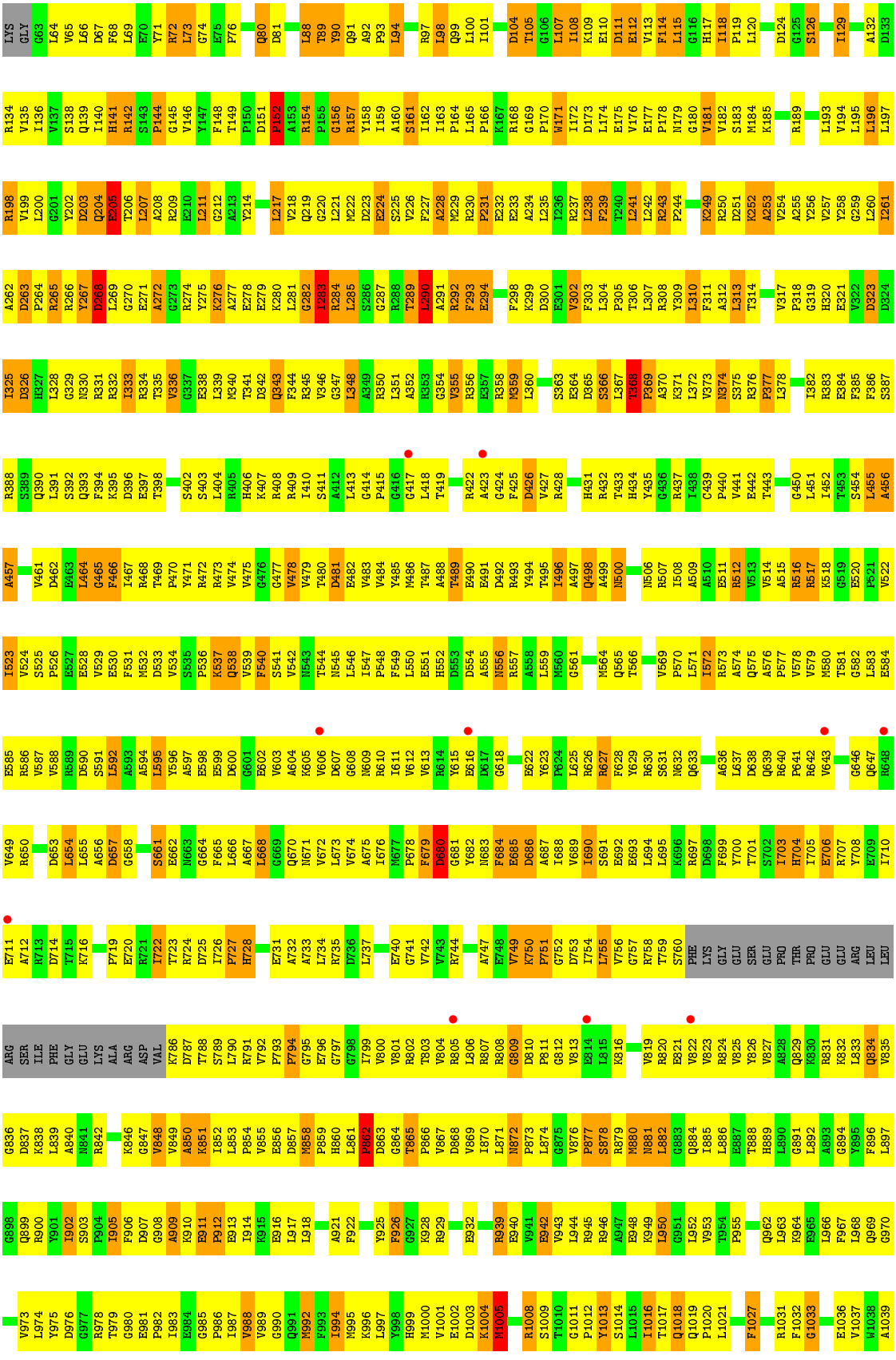


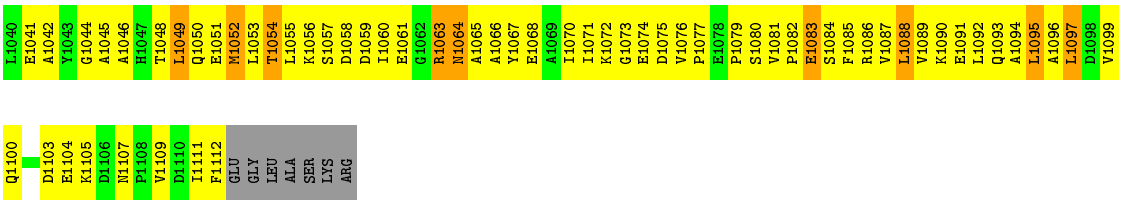




- Molecule 2: DNA-directed RNA polymerase subunit beta

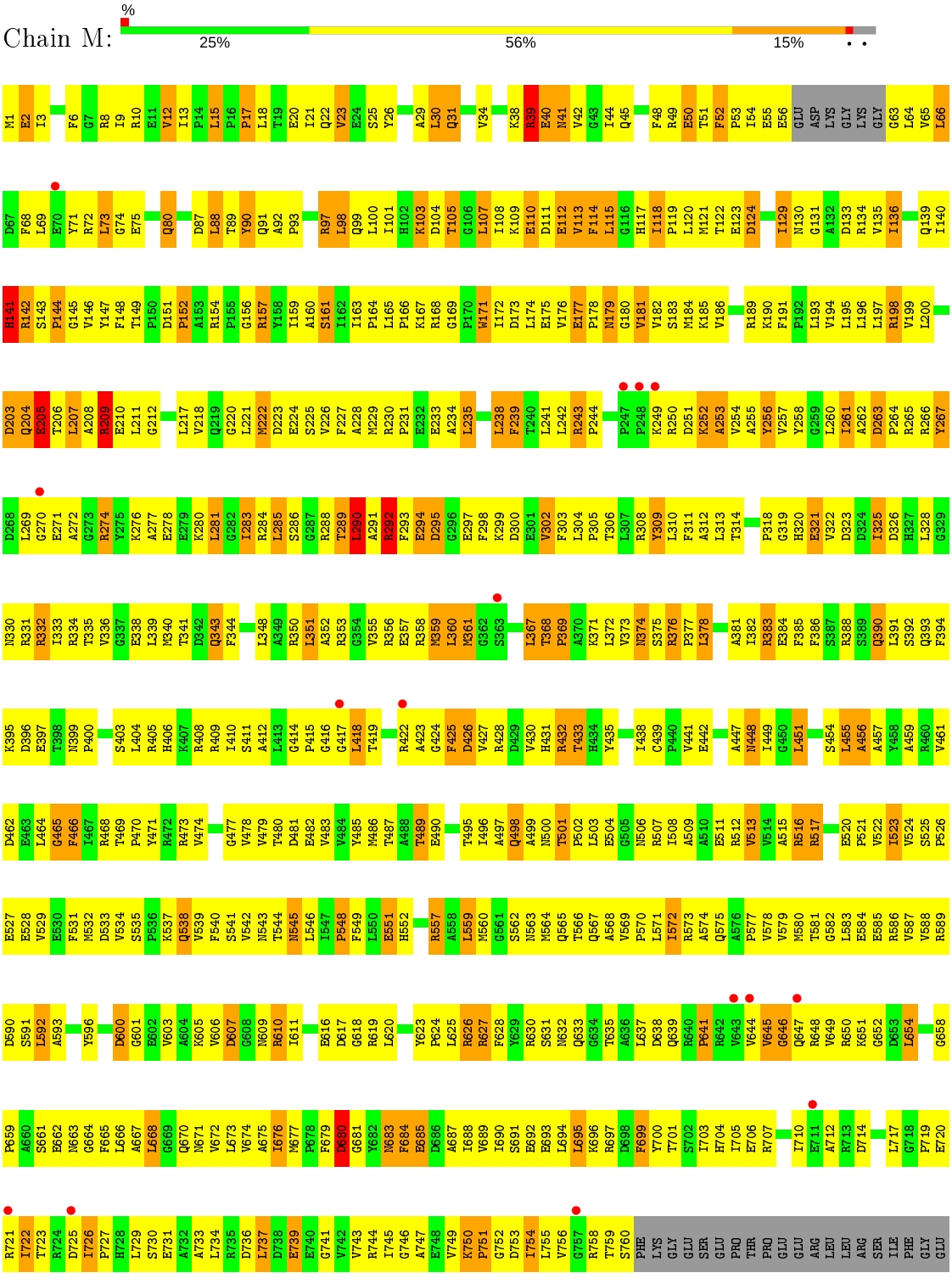


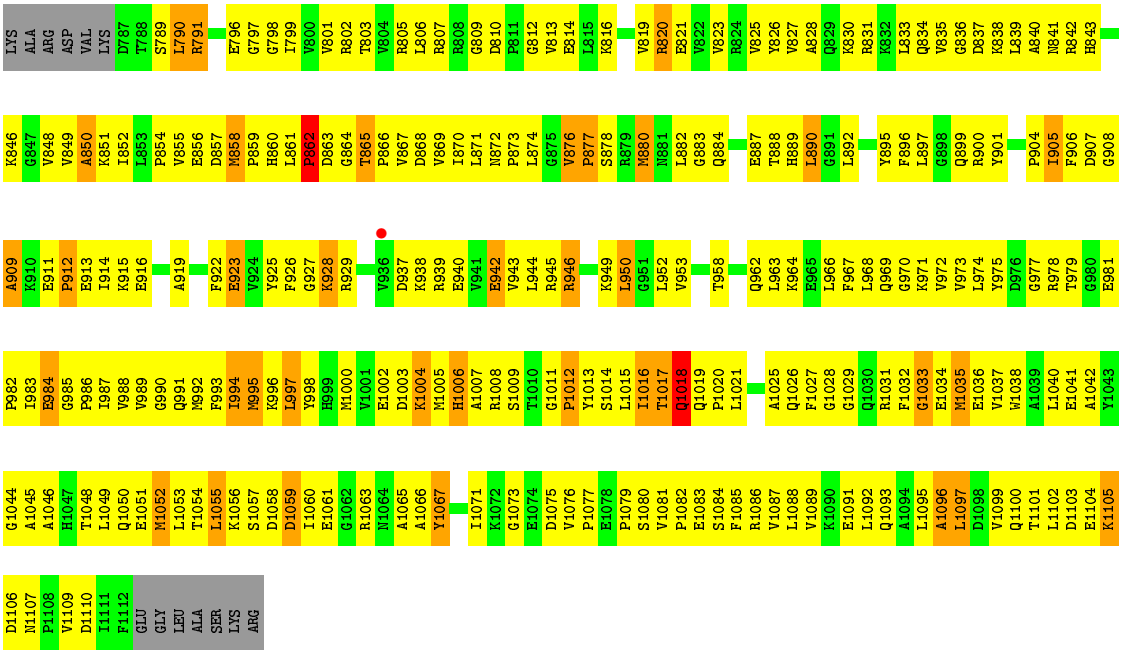




- Molecule 2: DNA-directed RNA polymerase subunit beta

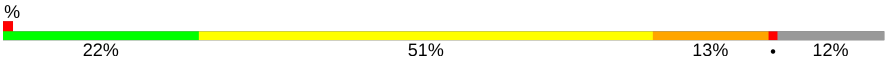
Chain M:

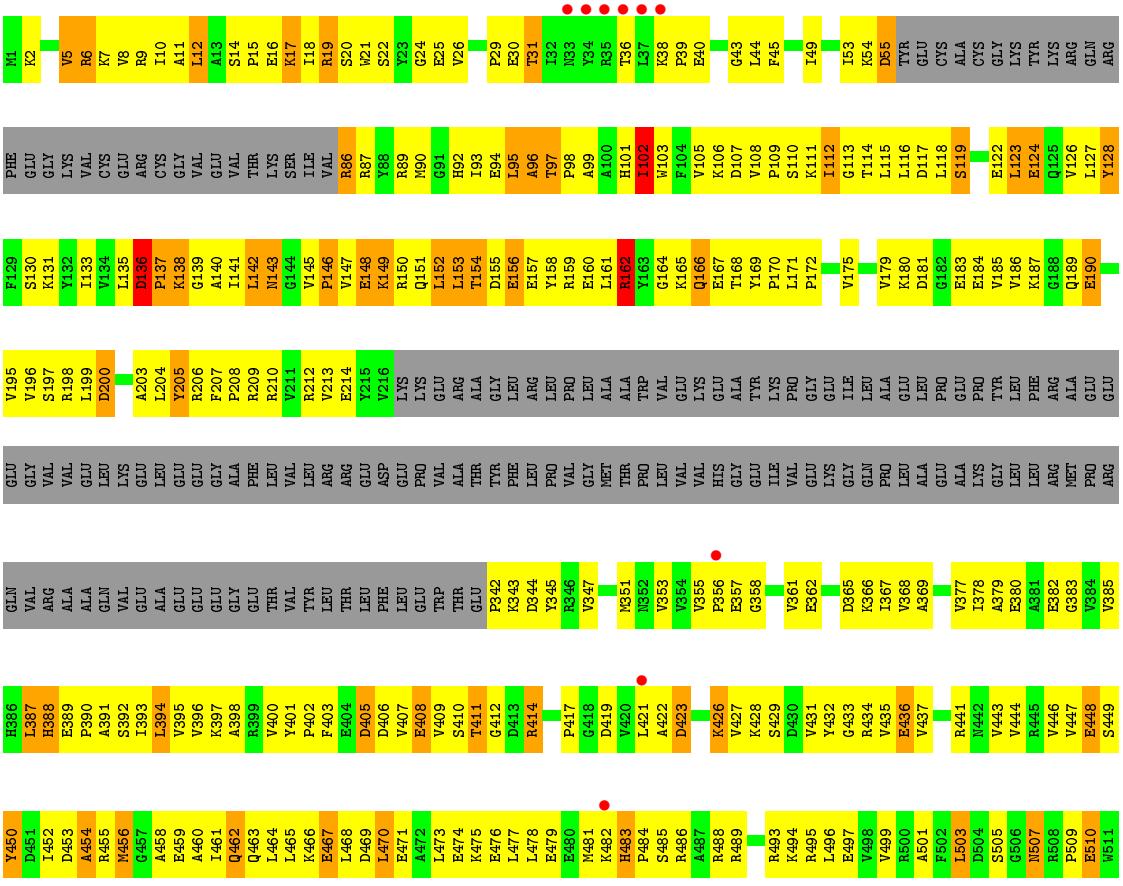


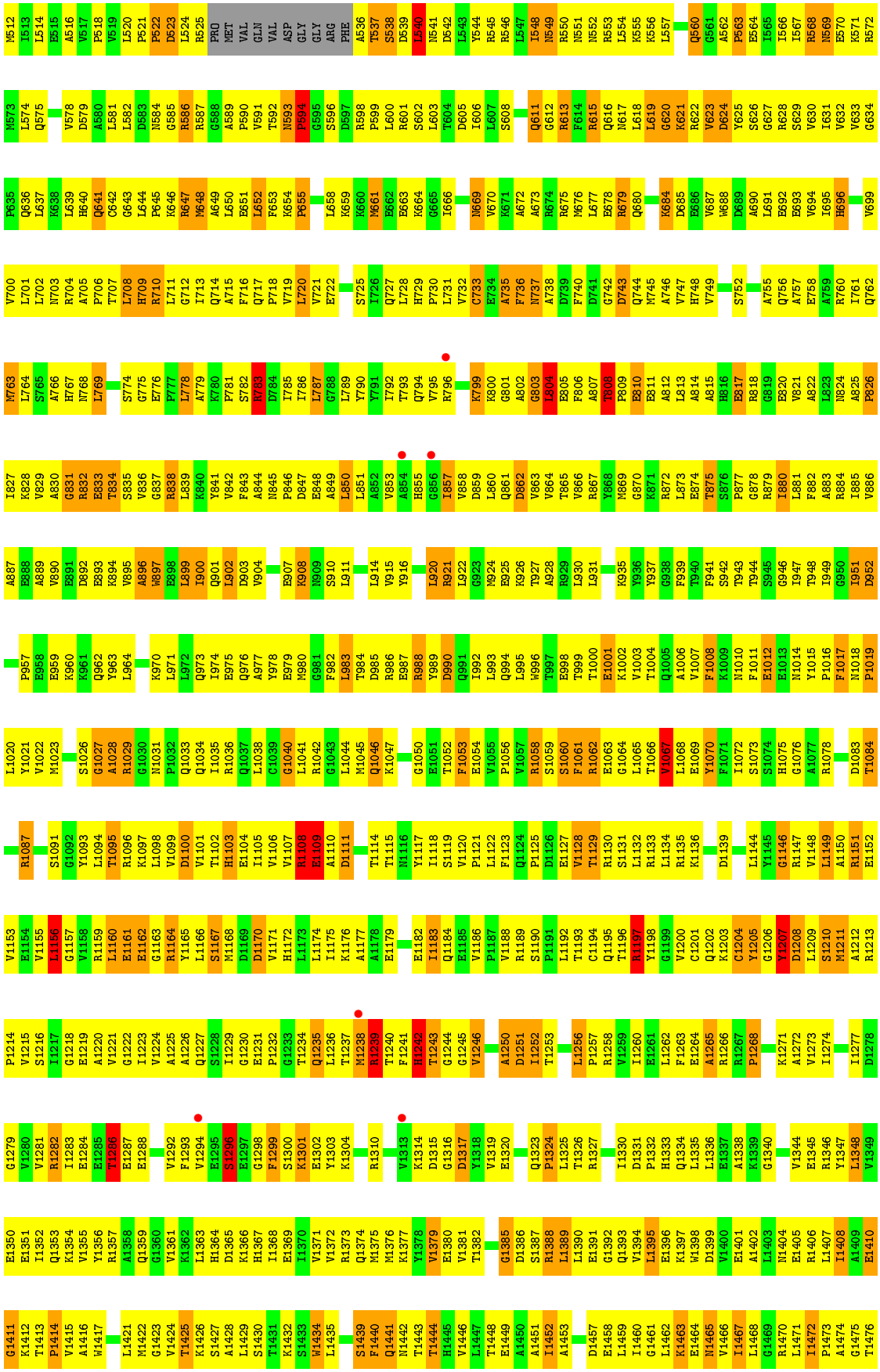


- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

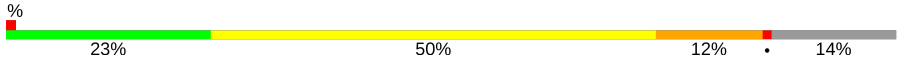


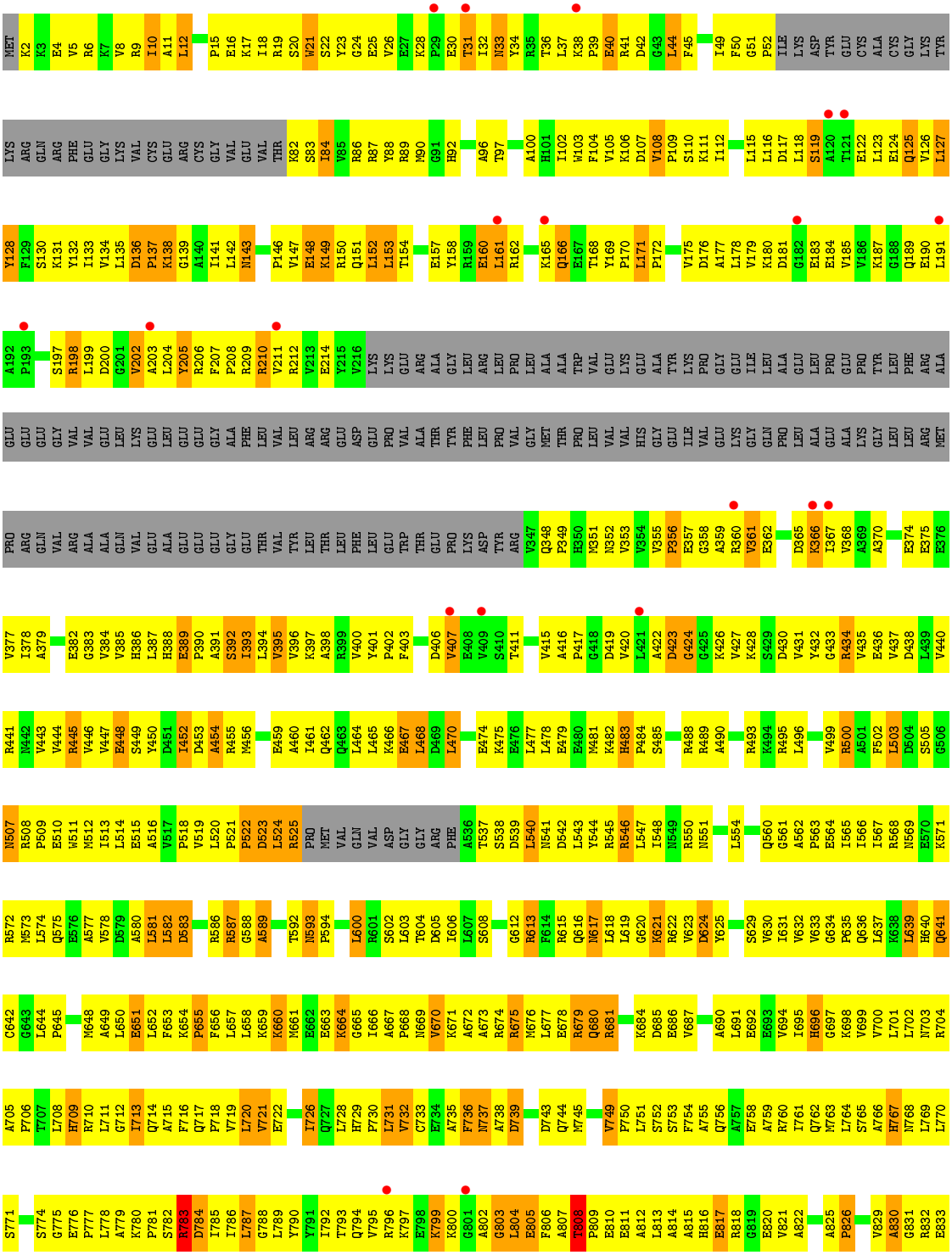


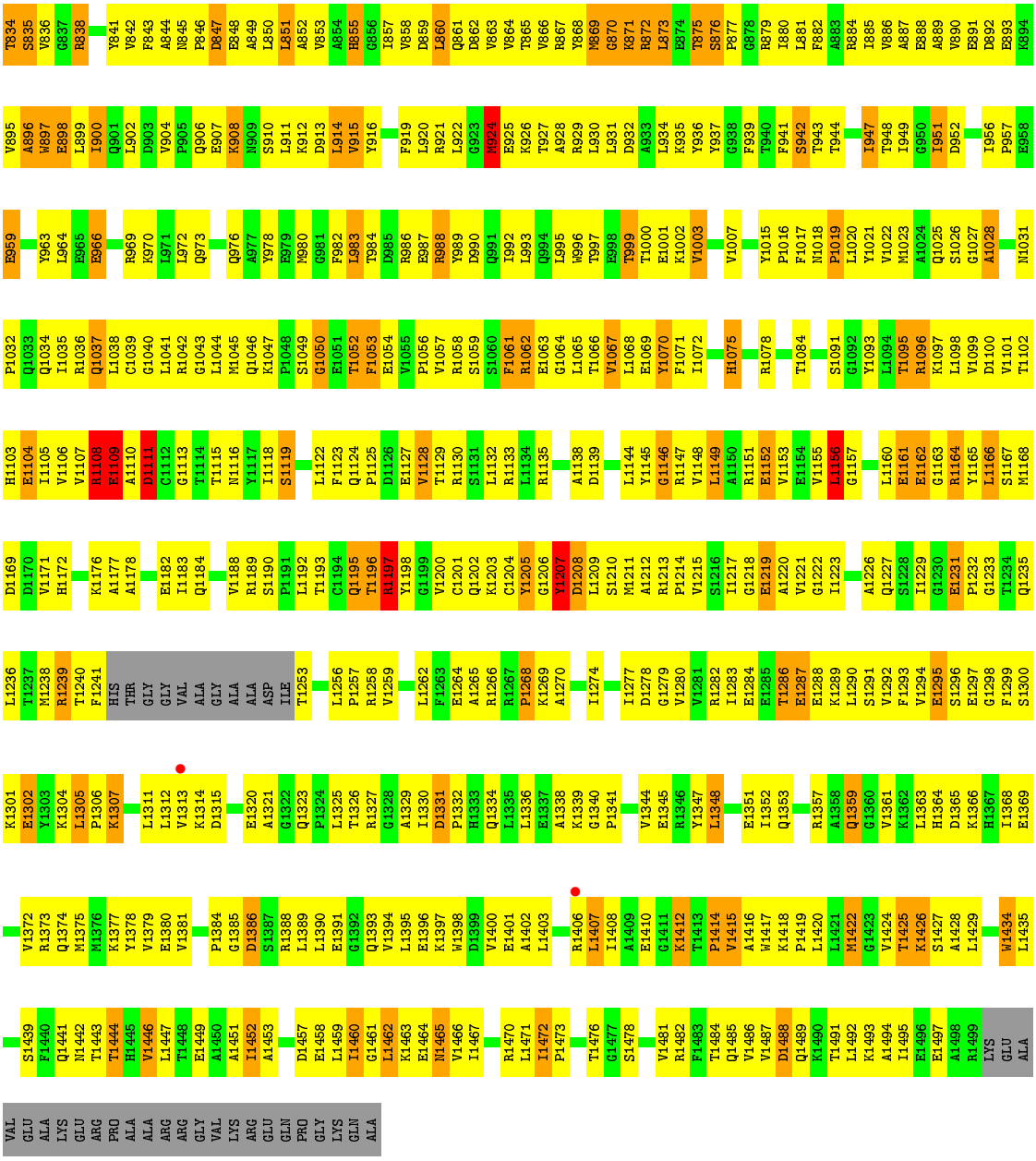


- Molecule 3: DNA-directed RNA polymerase subunit beta'

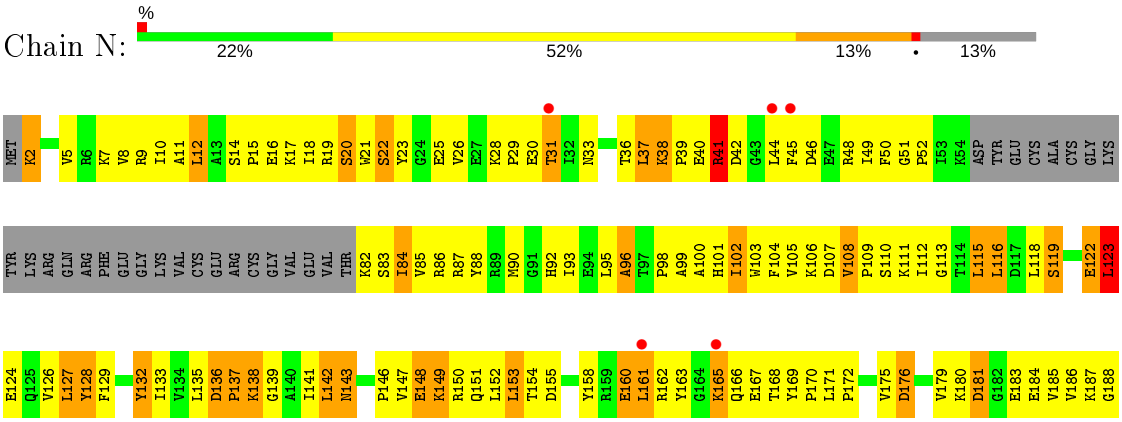
Chain I:

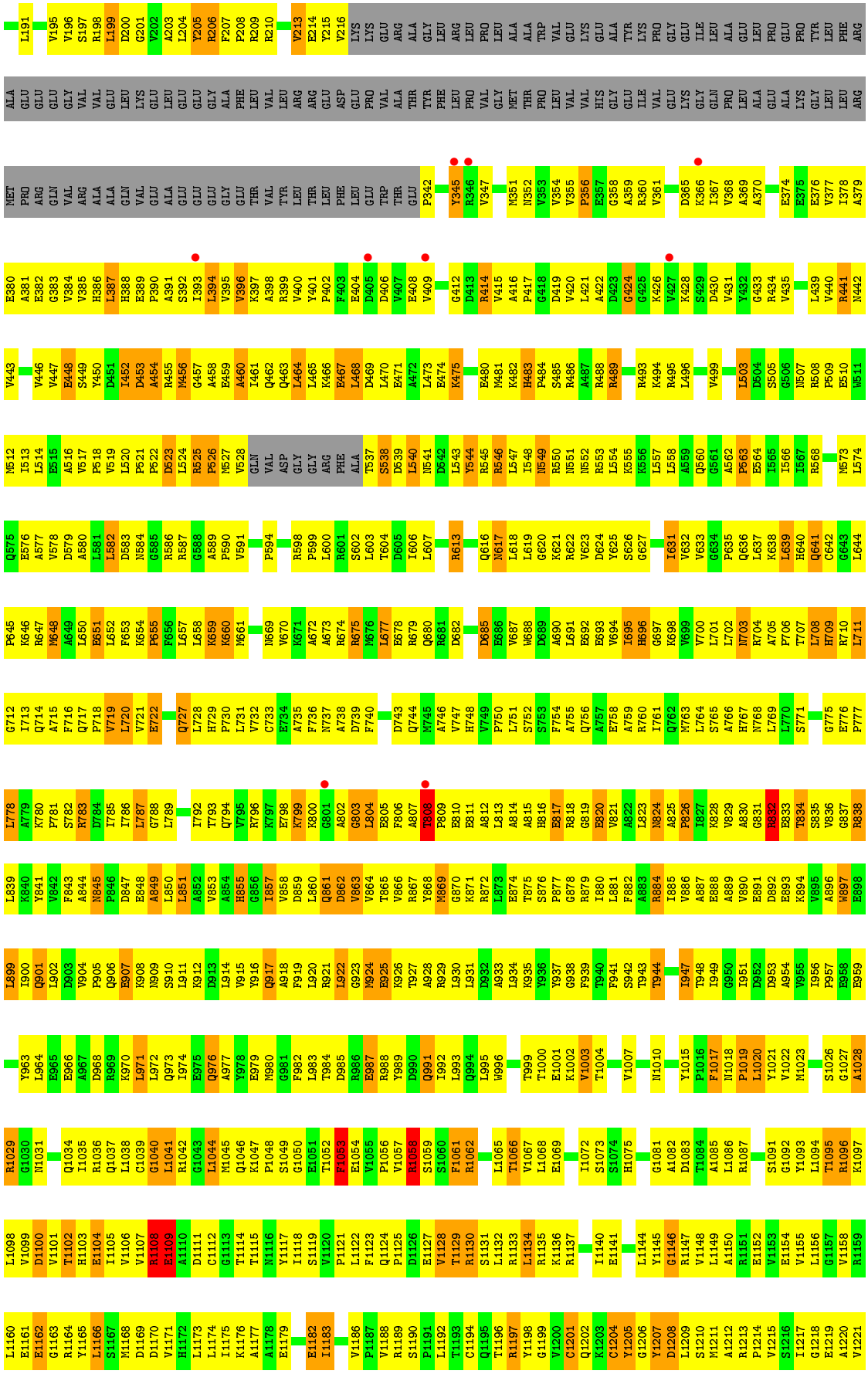


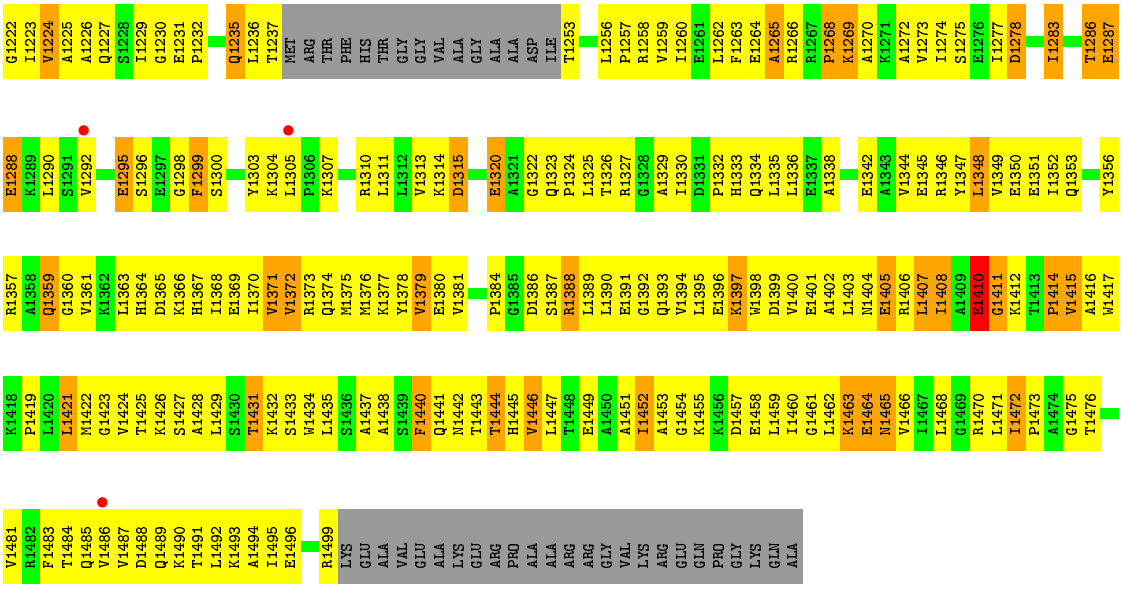




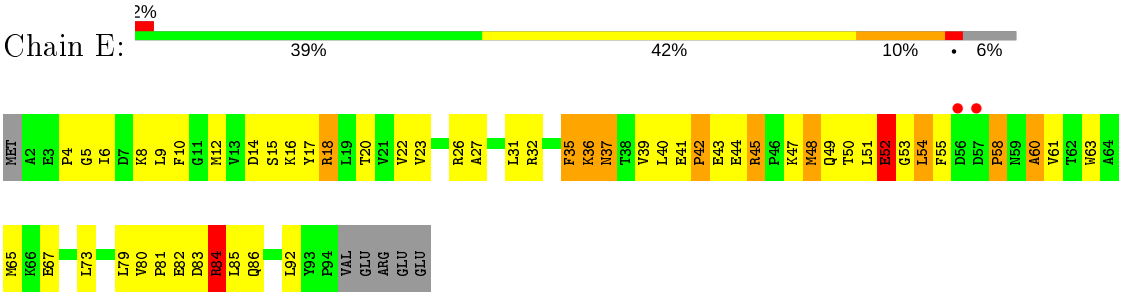
• Molecule 3: DNA-directed RNA polymerase subunit beta'



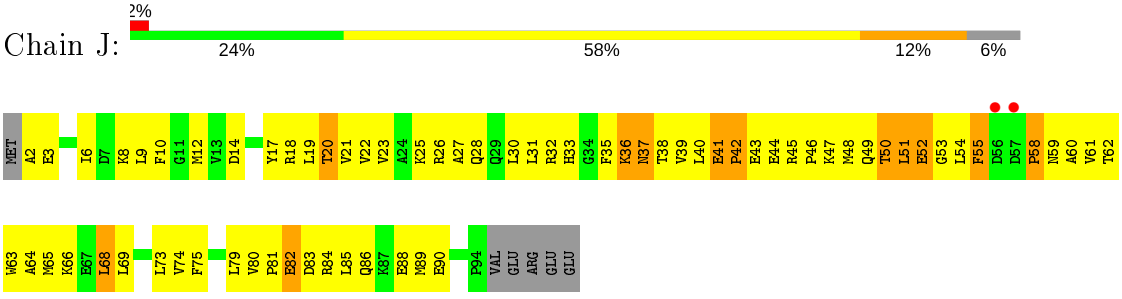




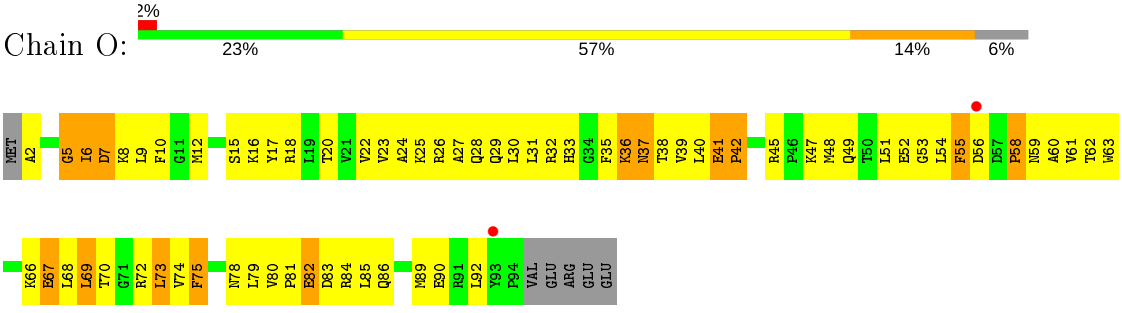
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega

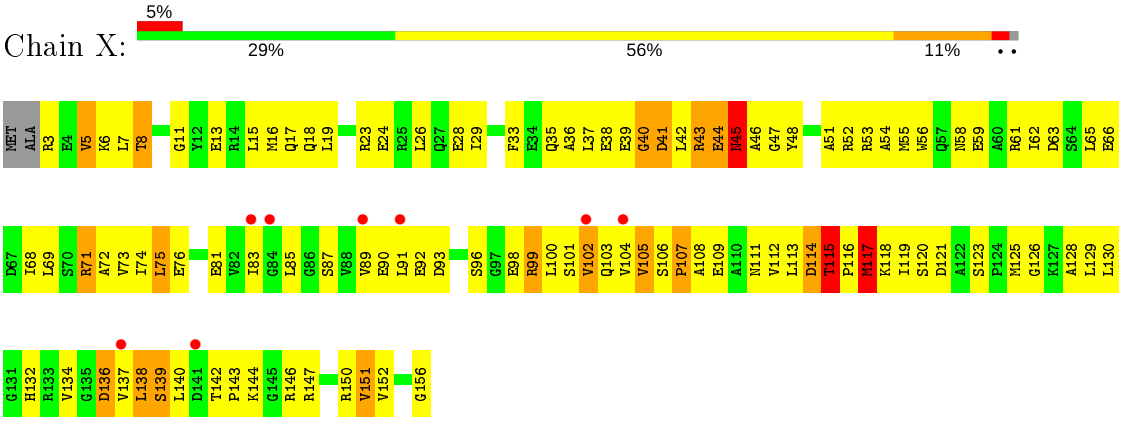


• Molecule 4: DNA-directed RNA polymerase subunit omega



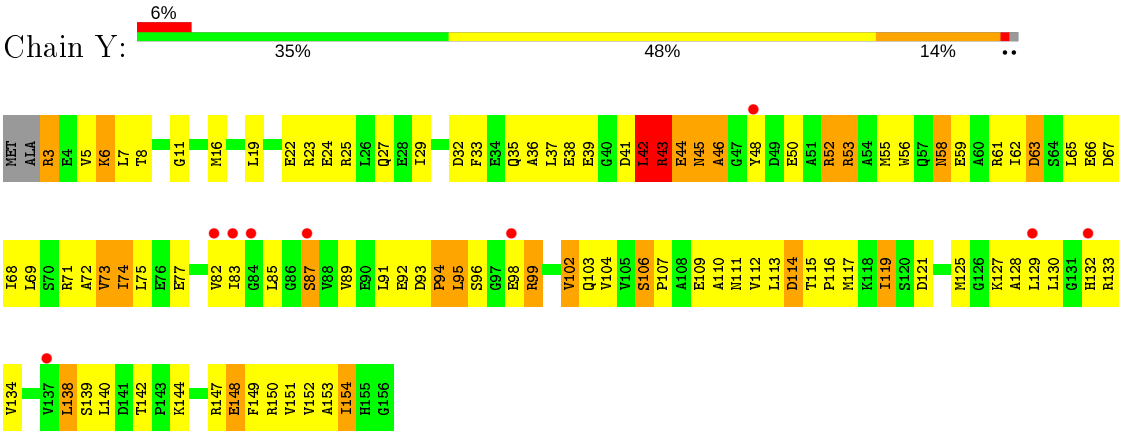
• Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)

Chain X:



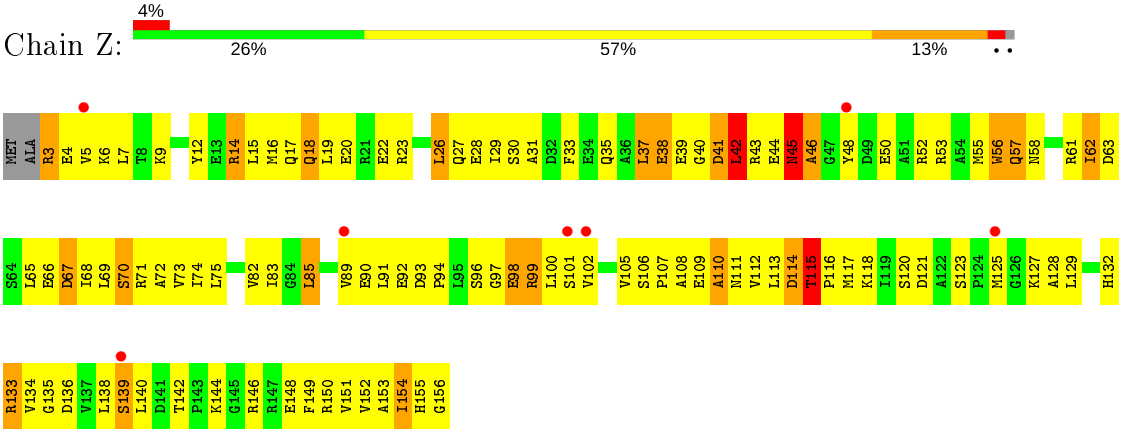
• Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)

Chain Y:



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

Chain Z:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (3.01%)	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)	0.22 , 136.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.129 for l,-k,h	Xtriage
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

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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	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(^{o})	Ideal(^{o})
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 (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	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

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, 95^{th} 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, 95^{th} 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
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.