wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2023 – 10:49 PM EDT

PDB ID	:	3EQL
Title	:	Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic myxopyronin
Authors	:	Vassylyev, D.G.; Vassylyeva, M.N.; Artsimovitch, I.
Deposited on	:	2008-09-30
Resolution	:	2.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

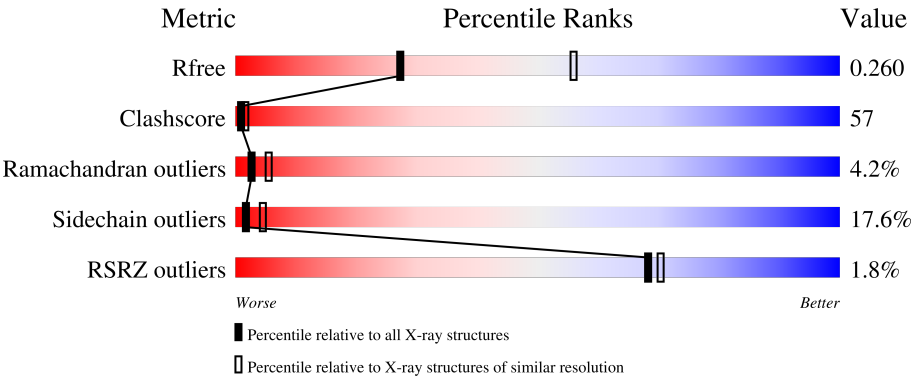
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 <=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	18% 44% 10% • 27%
1	B	315	3% 19% 44% 9% 27%
1	K	315	20% 42% 10% • 27%
1	L	315	17% 46% 9% • 27%
2	C	1119	25% 58% 16% •

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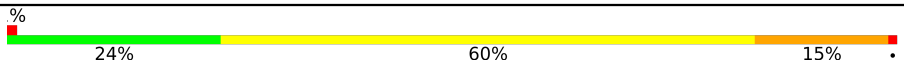
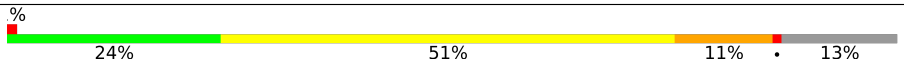
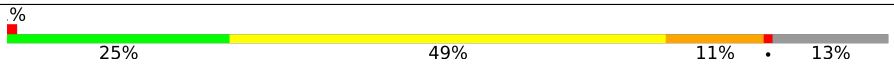
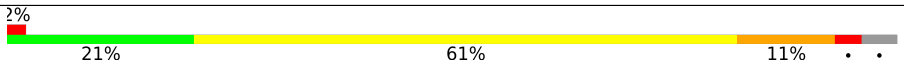
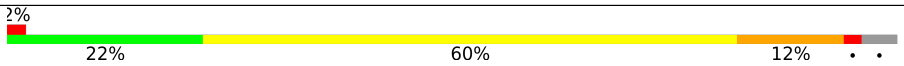
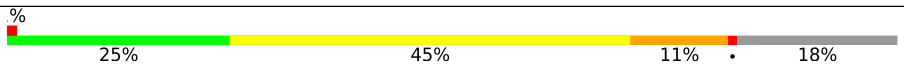
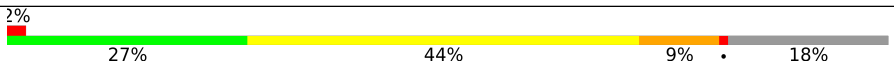
Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 57340 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	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			
3	N	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
4	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

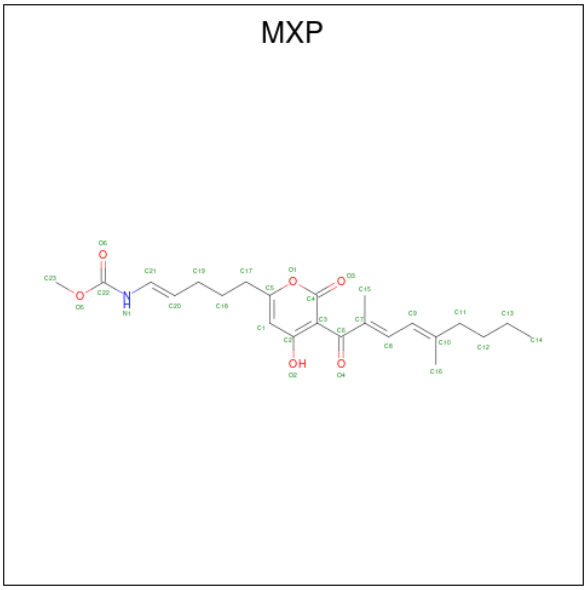
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	N	2	Total	Zn	0	0
			2	2		

- Molecule 7 is Myxopyronin B (three-letter code: MXP) (formula: $C_{23}H_{31}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			30	23	1	6		
7	N	1	Total	C	N	O	0	0
			30	23	1	6		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is water.

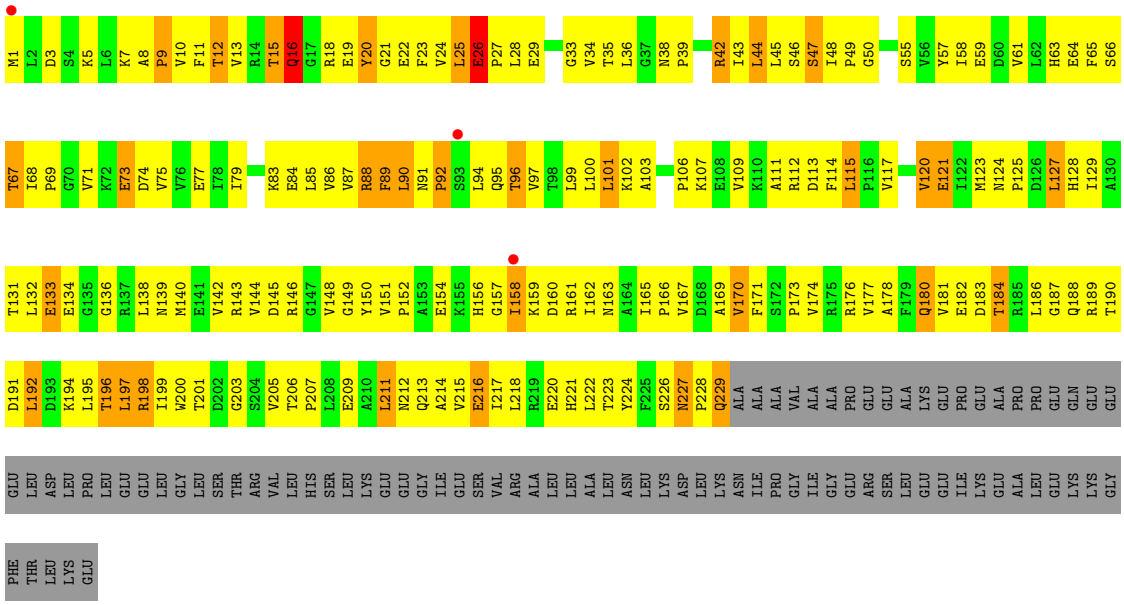
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	141	Total O 141 141	0	0
9	B	149	Total O 149 149	0	0
9	C	704	Total O 704 704	0	0
9	D	927	Total O 927 927	0	0
9	E	82	Total O 82 82	0	0
9	F	305	Total O 305 305	0	0
9	K	152	Total O 152 152	0	0
9	L	148	Total O 148 148	0	0
9	M	680	Total O 680 680	0	0
9	N	864	Total O 864 864	0	0
9	O	84	Total O 84 84	0	0
9	P	260	Total O 260 260	0	0

3 Residue-property plots (i)

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.

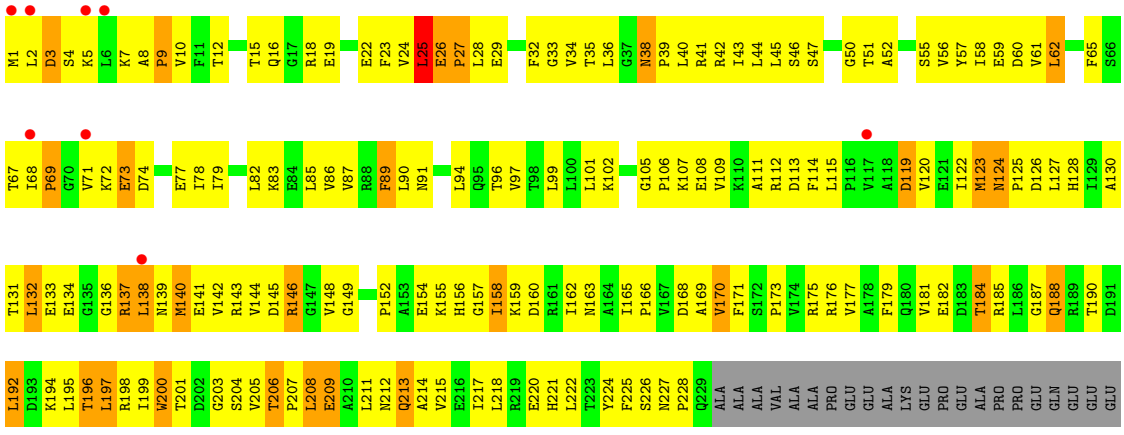
• Molecule 1: DNA-directed RNA polymerase subunit alpha

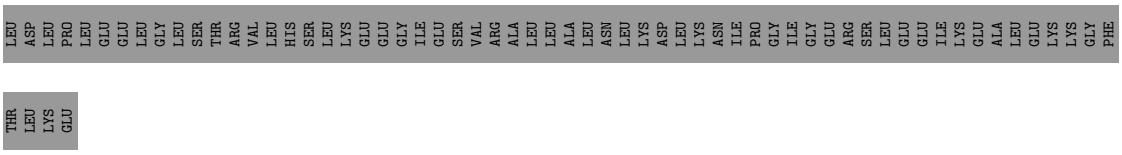
Chain A:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

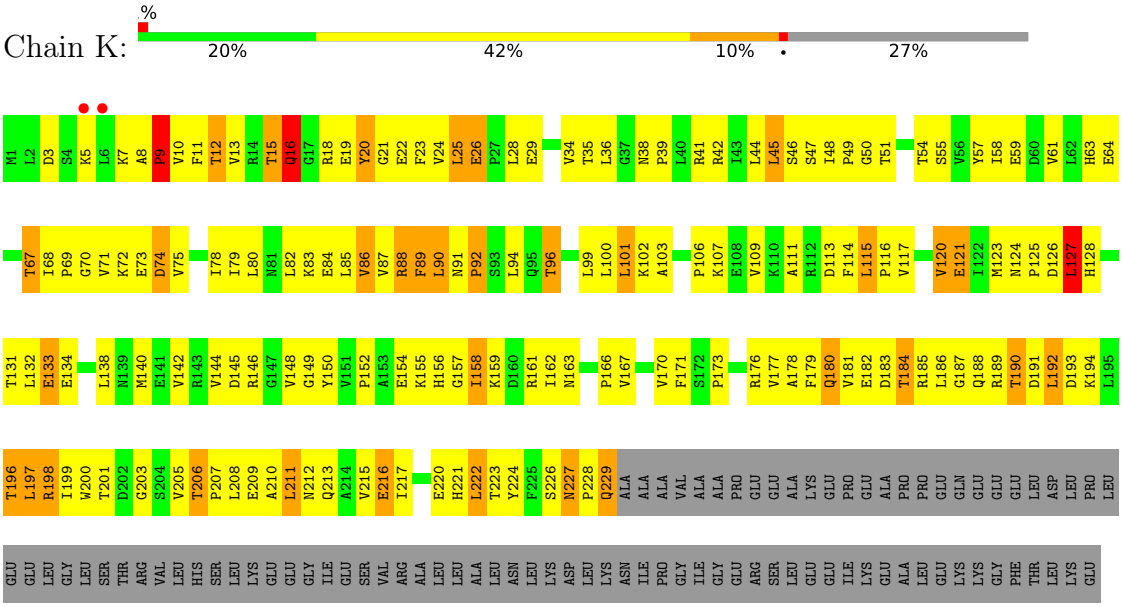
Chain B:





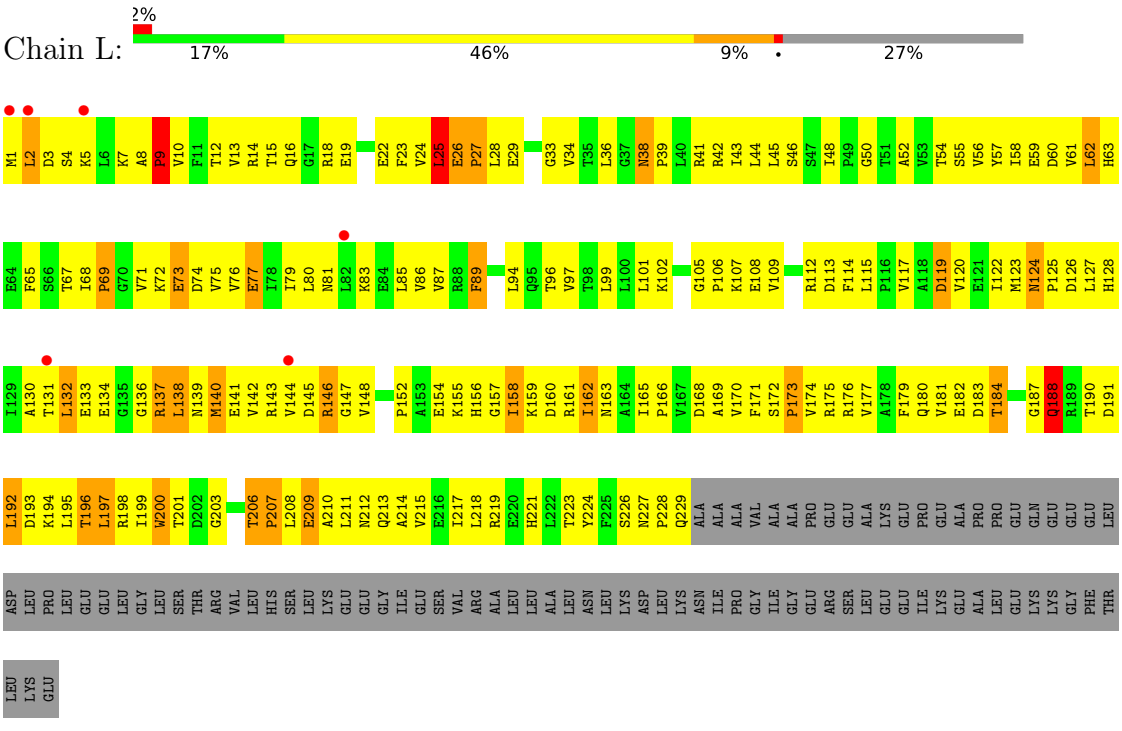
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain K:



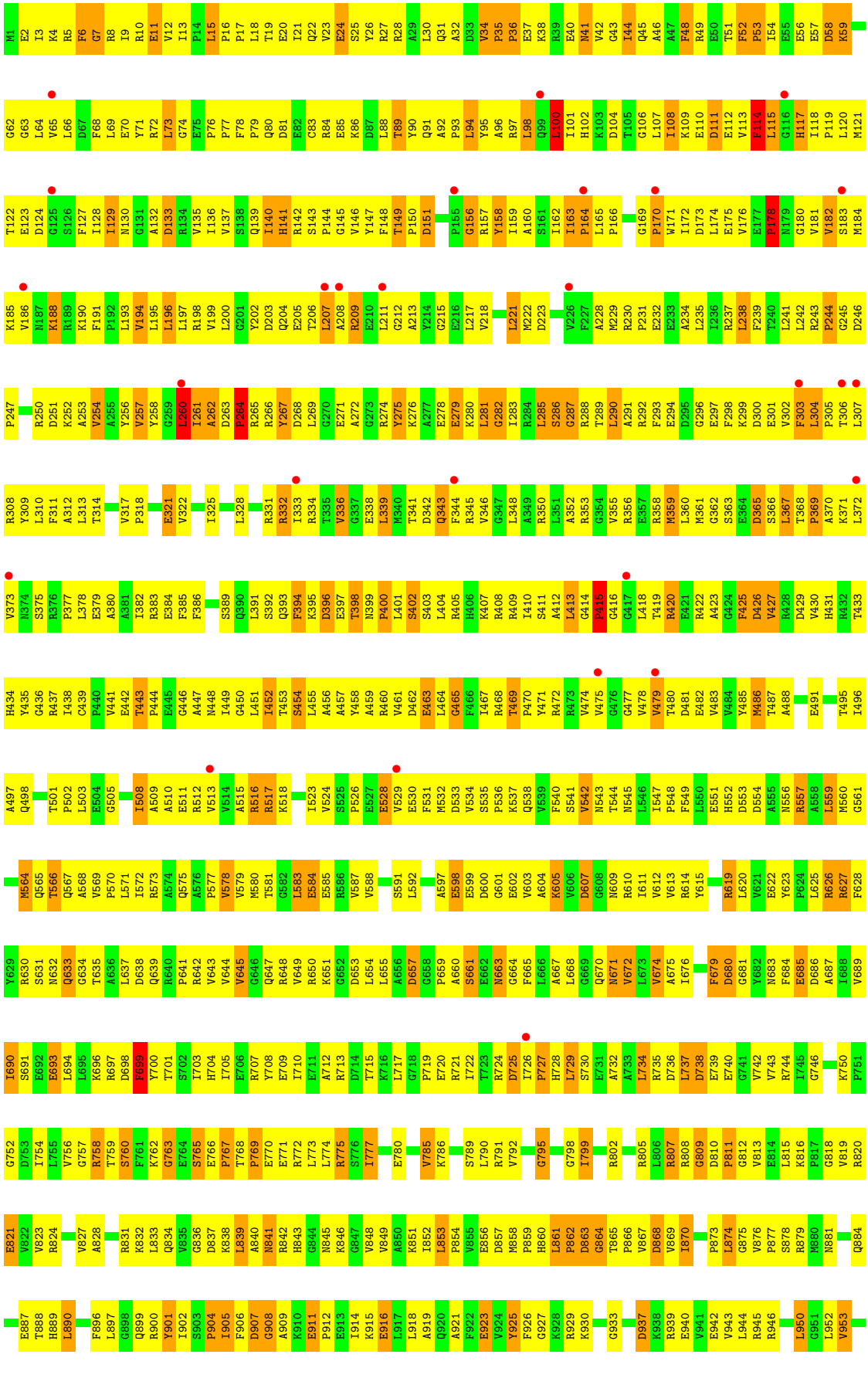
• Molecule 1: DNA-directed RNA polymerase subunit alpha

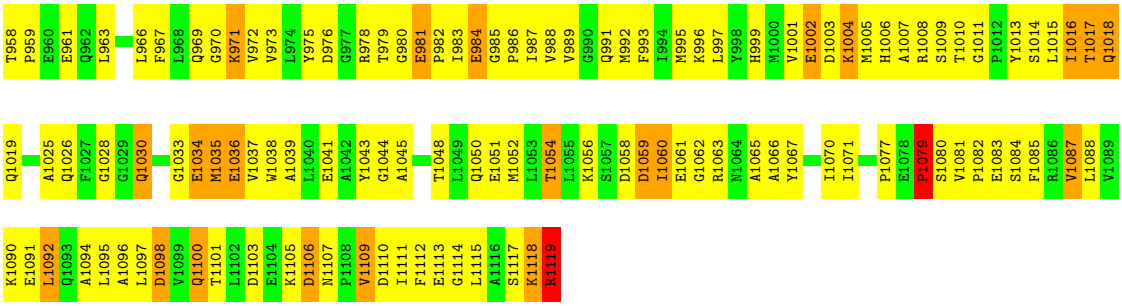
Chain L:



• Molecule 2: DNA-directed RNA polymerase subunit beta

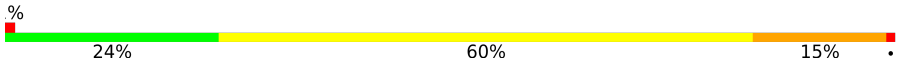
Chain C:

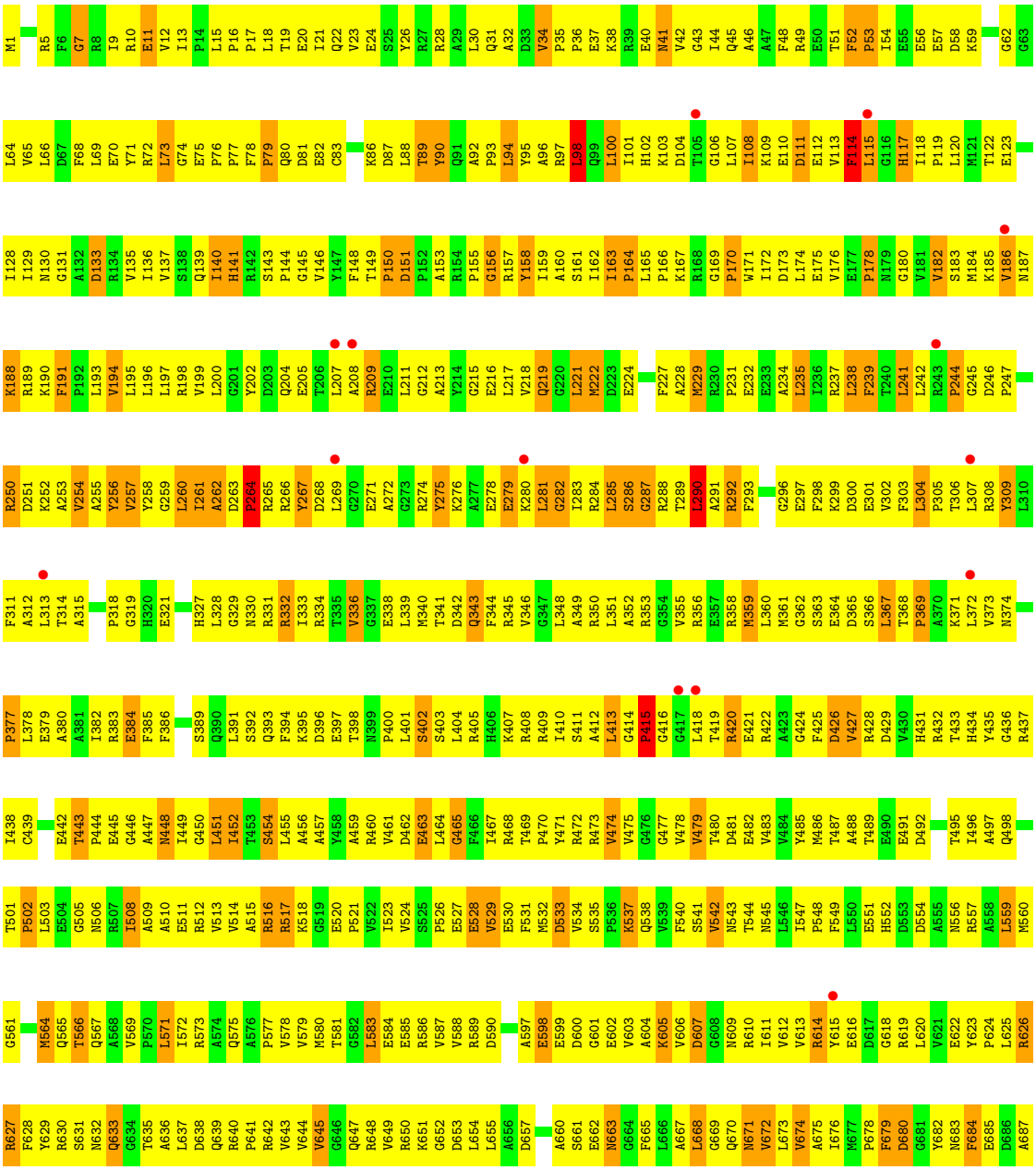


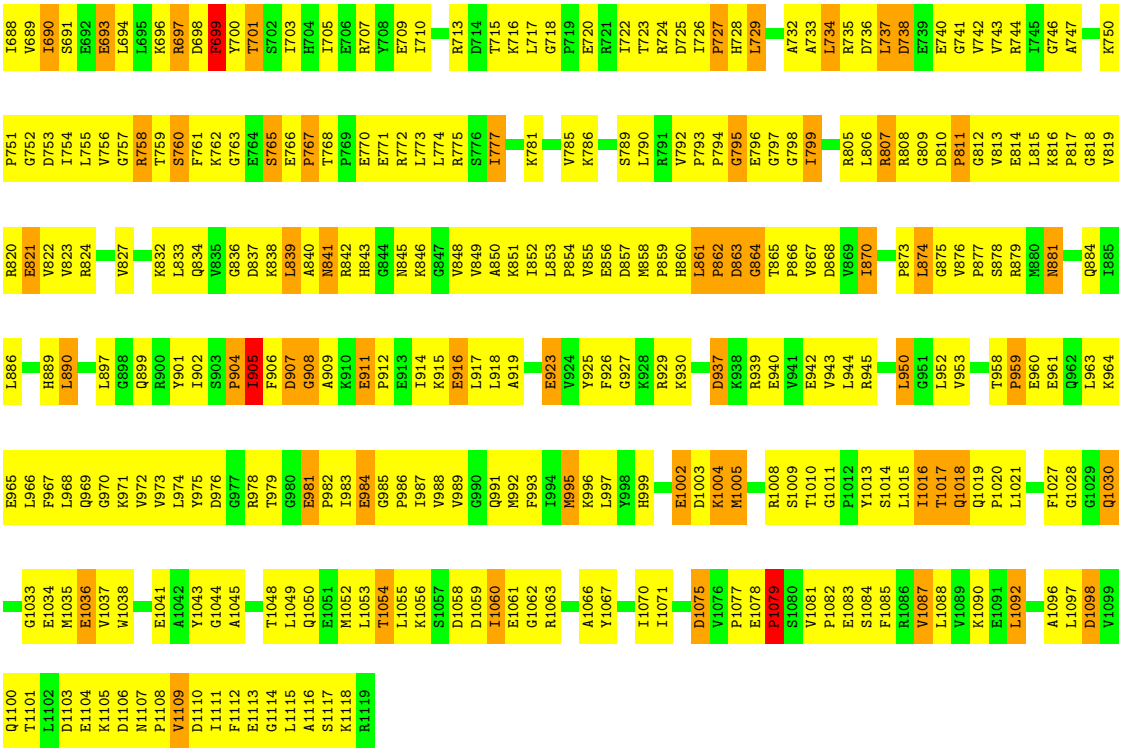


• Molecule 2: DNA-directed RNA polymerase subunit beta

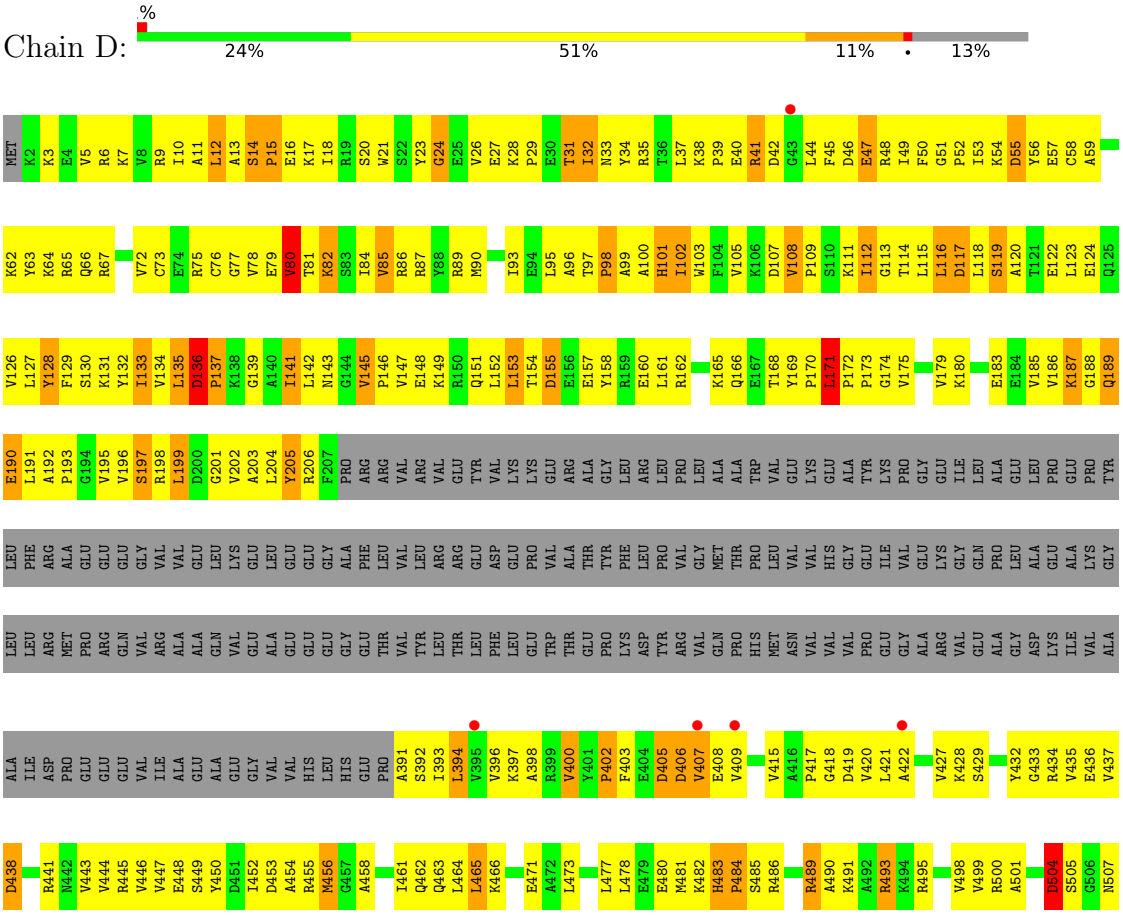
Chain M:

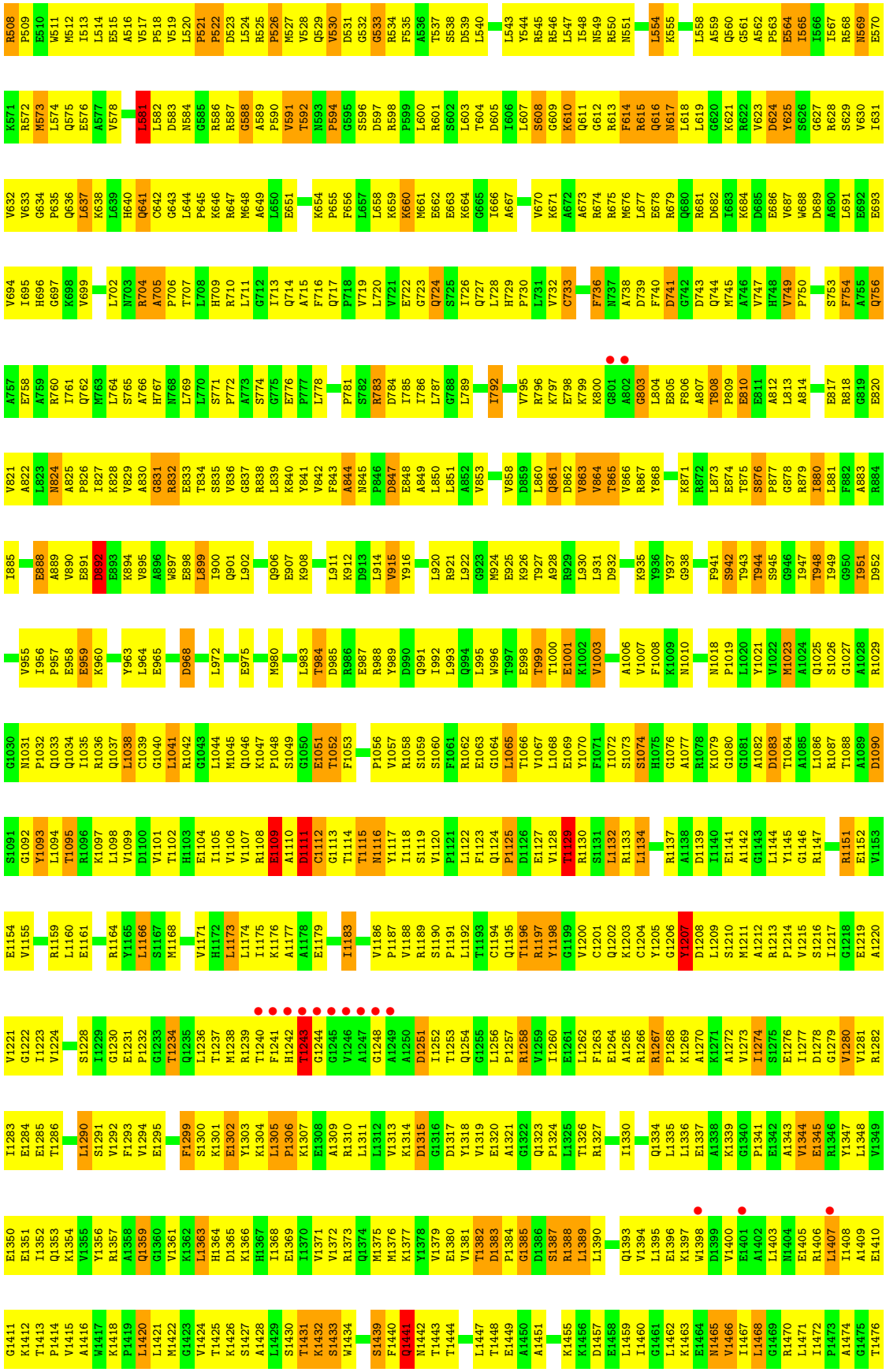




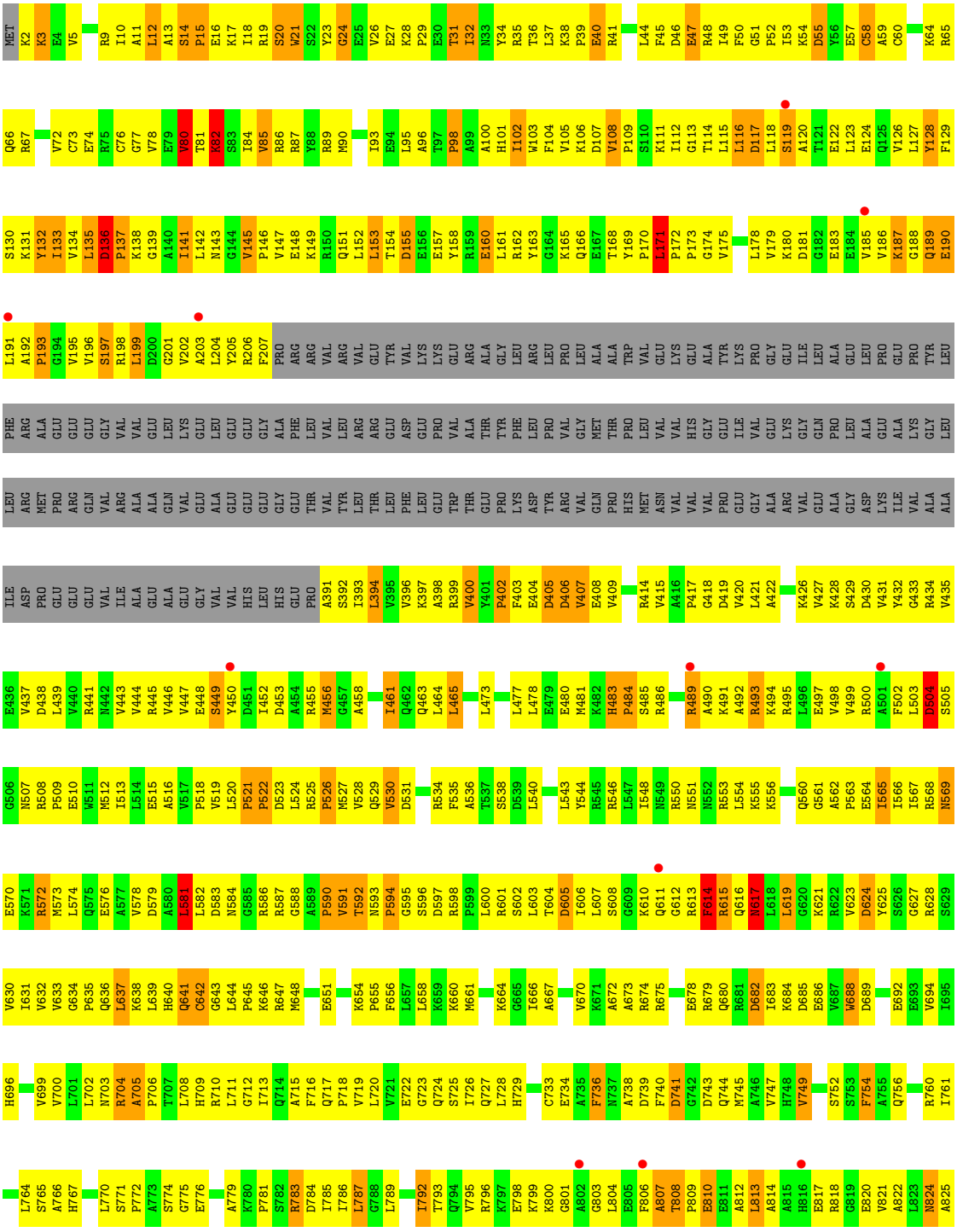


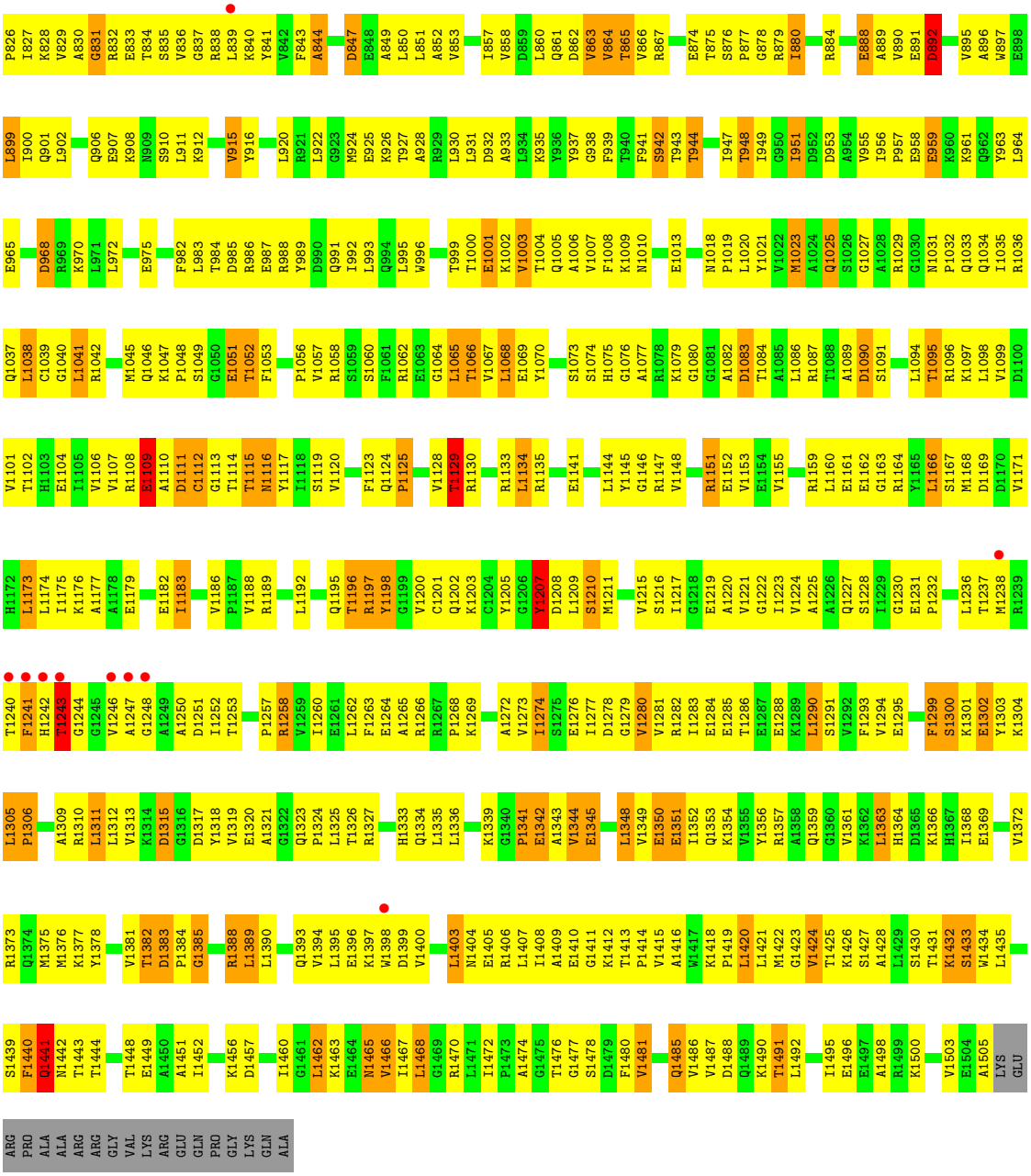
• Molecule 3: DNA-directed RNA polymerase subunit beta'



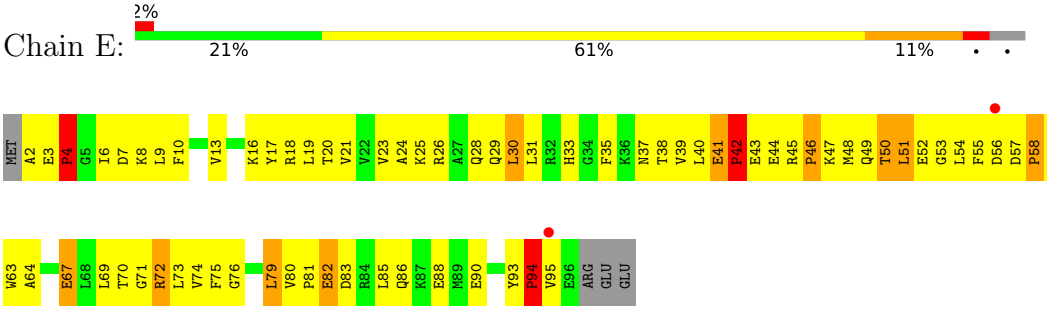


• Molecule 3: DNA-directed RNA polymerase subunit beta'



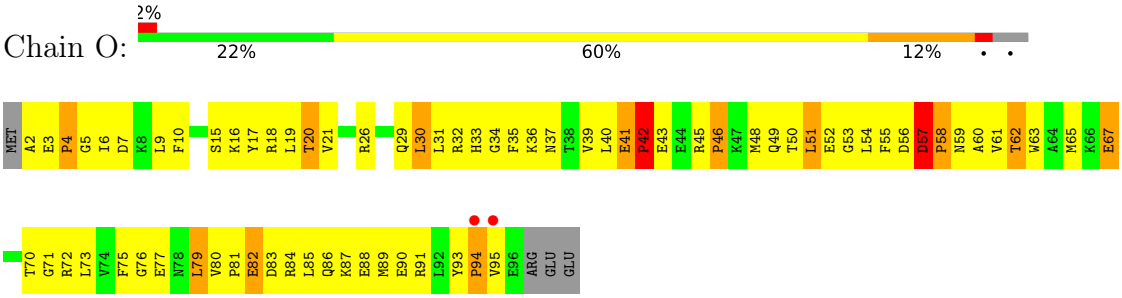


• Molecule 4: DNA-directed RNA polymerase subunit omega



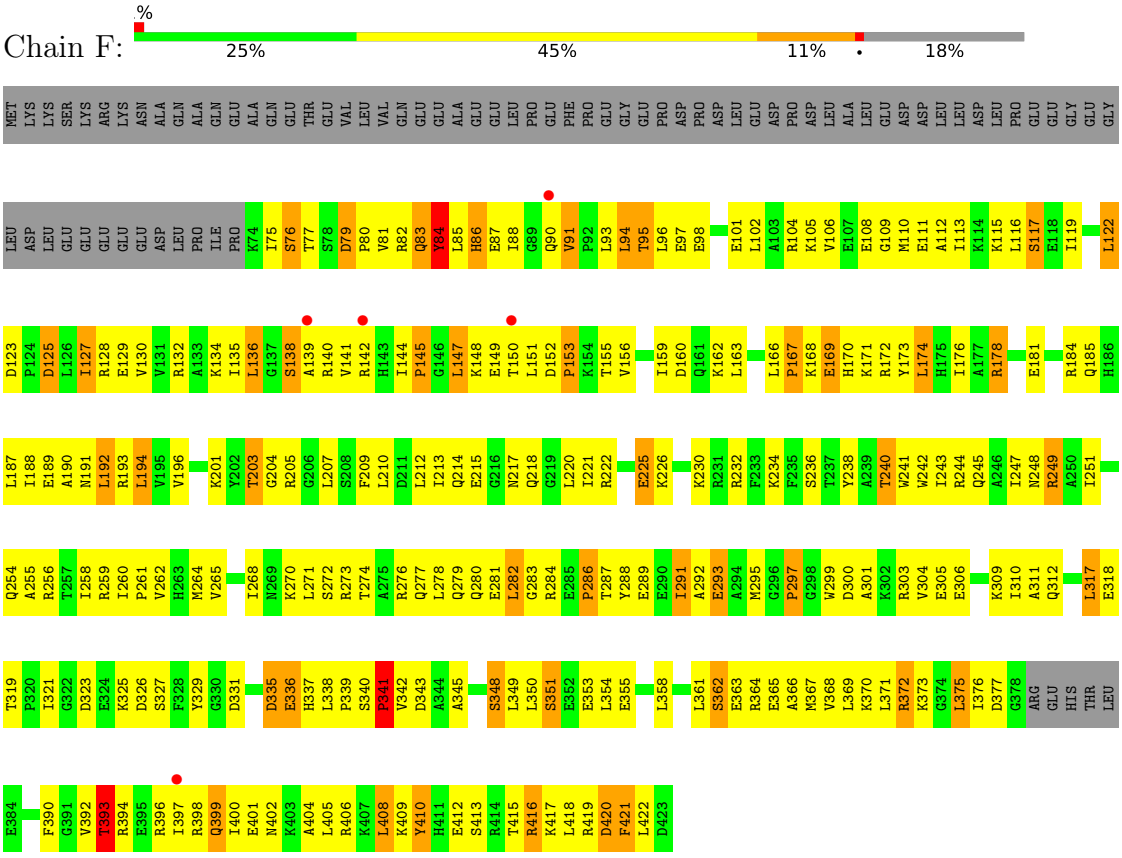
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain O:



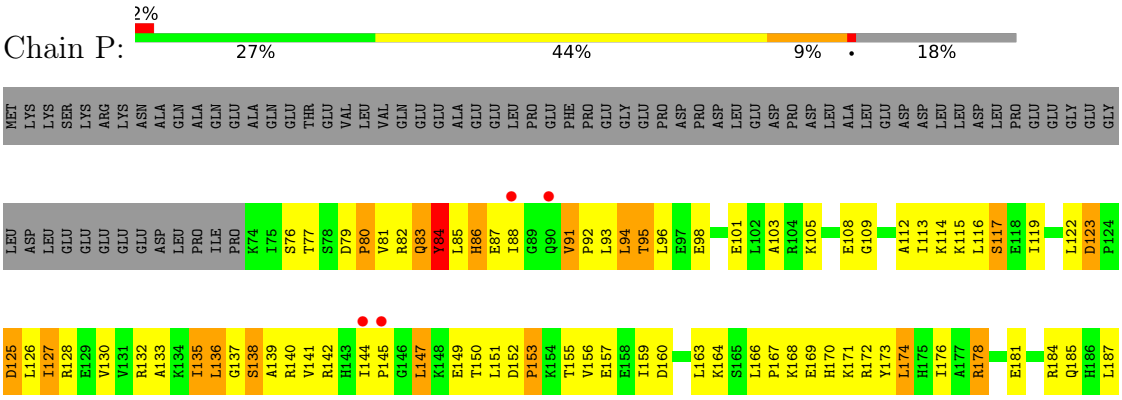
• Molecule 5: RNA polymerase sigma factor rpoD

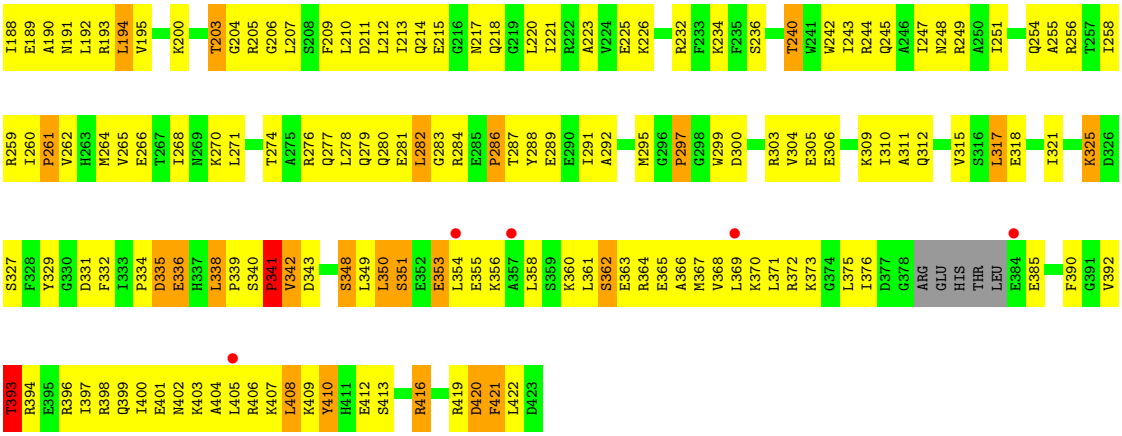
Chain F:



• Molecule 5: RNA polymerase sigma factor rpoD

Chain P:




I188 E189 A190 N191 L192 R193 L194 V195 K200 T203 G204 R205 G206 L207 S208 F209 L210 D211 L212 I213 Q214 E215 G216 N217 Q218 G219 L220 I221 R222 A223 V224 E225 K226 R232 F233 K234 F235 S236 T240 W241 W242 I243 R244 Q245 A246 I247 N248 R249 A250 I251 Q254 A255 R256 T257 I258
R259 I260 P261 V262 H263 M264 V265 E266 T267 I268 N269 K270 L271 T274 A275 R276 Q277 L278 Q279 Q280 E281 L282 G283 R284 E285 P286 T287 Y288 E289 E290 I291 A292 M295 G296 P297 G298 W299 D300 R303 V304 E305 E306 K309 I310 A311 Q312 V315 S316 L317 E318 I321 K325 D326
S327 F328 Y329 G330 D331 F332 I333 P334 D335 E336 H337 L338 P339 S340 P341 V342 D343 S348 L349 L350 S351 E352 E353 L354 E355 K356 A357 L358 S359 K360 L361 S362 E363 R364 E365 A366 M367 V368 L369 K370 L371 R372 K373 G374 L375 I376 D377 G378 ARG GLU HIS THR LEU E384 E385 F390 G391 V392
T393 R394 E395 R396 I397 R398 Q399 I400 E401 N402 K403 A404 L405 R406 K407 L408 K409 Y410 H411 E412 S413 R416 R419 D420 F421 L422 D423

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	235.00Å 235.00Å 254.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.70) 90.4 (39.96-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.270 0.238 , 0.260	Depositor DCC
R_{free} test set	18510 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l 0.048 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	57340	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: MG, ZN, MXP

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	0.84	2/1838 (0.1%)	1.04	9/2498 (0.4%)
1	B	0.74	1/1838 (0.1%)	0.95	9/2498 (0.4%)
1	K	0.81	2/1838 (0.1%)	1.00	8/2498 (0.3%)
1	L	0.75	1/1838 (0.1%)	0.96	10/2498 (0.4%)
2	C	0.73	0/8997	0.94	14/12164 (0.1%)
2	M	0.73	0/8997	0.94	14/12164 (0.1%)
3	D	0.75	2/10582 (0.0%)	0.97	15/14294 (0.1%)
3	N	0.75	1/10582 (0.0%)	0.97	18/14294 (0.1%)
4	E	0.73	0/784	1.23	5/1057 (0.5%)
4	O	0.71	0/784	1.08	3/1057 (0.3%)
5	F	0.65	0/2812	0.85	3/3781 (0.1%)
5	P	0.65	0/2812	0.86	2/3781 (0.1%)
All	All	0.74	9/53702 (0.0%)	0.96	110/72584 (0.2%)

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
3	N	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	C-O	-11.04	1.02	1.23
1	K	26	GLU	C-O	-10.57	1.03	1.23
1	B	26	GLU	C-O	-10.23	1.03	1.23
1	L	26	GLU	C-O	-9.82	1.04	1.23
1	A	16	GLN	CB-CG	5.82	1.68	1.52

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	94	PRO	CA-N-CD	-18.30	85.89	111.50
1	B	138	LEU	CA-CB-CG	12.41	143.84	115.30
1	L	138	LEU	CA-CB-CG	12.19	143.33	115.30
4	O	94	PRO	CA-N-CD	-9.89	97.65	111.50
1	K	26	GLU	CA-C-N	9.51	143.72	117.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	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	1806	0	1861	184	0
1	B	1806	0	1861	197	0
1	K	1806	0	1861	212	0
1	L	1806	0	1861	198	0
2	C	8829	0	8933	1145	0
2	M	8829	0	8933	1073	0
3	D	10407	0	10633	1296	0
3	N	10407	0	10633	1283	0
4	E	770	0	784	121	0
4	O	770	0	784	113	0
5	F	2771	0	2844	316	0
5	P	2771	0	2844	312	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	30	0	31	18	0
7	N	30	0	31	18	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	141	0	0	28	0
9	B	149	0	0	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	704	0	0	215	0
9	D	927	0	0	239	0
9	E	82	0	0	29	0
9	F	305	0	0	77	0
9	K	152	0	0	41	0
9	L	148	0	0	34	0
9	M	680	0	0	180	0
9	N	864	0	0	235	0
9	O	84	0	0	26	0
9	P	260	0	0	71	0
All	All	57340	0	53894	6054	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 57.

The worst 5 of 6054 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:D:610:LYS:HD3	7:D:1527:MXP:C15	1.49	1.41
3:N:610:LYS:HD3	7:N:1527:MXP:C15	1.55	1.37
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.27	1.15
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.27	1.13
3:D:610:LYS:HD3	7:D:1527:MXP:H15B	1.19	1.10

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	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	12 30
1	B	227/315 (72%)	195 (86%)	29 (13%)	3 (1%)	12 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	227/315 (72%)	201 (88%)	22 (10%)	4 (2%)	8 21
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	12 30
2	C	1117/1119 (100%)	905 (81%)	154 (14%)	58 (5%)	2 3
2	M	1117/1119 (100%)	904 (81%)	153 (14%)	60 (5%)	2 3
3	D	1317/1524 (86%)	1098 (83%)	170 (13%)	49 (4%)	3 7
3	N	1317/1524 (86%)	1089 (83%)	176 (13%)	52 (4%)	3 6
4	E	93/99 (94%)	77 (83%)	12 (13%)	4 (4%)	2 5
4	O	93/99 (94%)	77 (83%)	10 (11%)	6 (6%)	1 2
5	F	341/423 (81%)	285 (84%)	37 (11%)	19 (6%)	2 3
5	P	341/423 (81%)	287 (84%)	36 (11%)	18 (5%)	2 3
All	All	6644/7590 (88%)	5517 (83%)	848 (13%)	279 (4%)	3 5

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
2	C	7	GLY
2	C	178	PRO
2	C	231	PRO

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	202/273 (74%)	161 (80%)	41 (20%)	1 3
1	B	202/273 (74%)	163 (81%)	39 (19%)	1 3
1	K	202/273 (74%)	159 (79%)	43 (21%)	1 3
1	L	202/273 (74%)	166 (82%)	36 (18%)	2 4
2	C	941/941 (100%)	755 (80%)	186 (20%)	1 3
2	M	941/941 (100%)	757 (80%)	184 (20%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	1112/1279 (87%)	935 (84%)	177 (16%)	2 6
3	N	1112/1279 (87%)	934 (84%)	178 (16%)	2 6
4	E	84/88 (96%)	68 (81%)	16 (19%)	1 4
4	O	84/88 (96%)	68 (81%)	16 (19%)	1 4
5	F	295/370 (80%)	252 (85%)	43 (15%)	3 7
5	P	295/370 (80%)	254 (86%)	41 (14%)	3 8
All	All	5672/6448 (88%)	4672 (82%)	1000 (18%)	2 4

5 of 1000 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	91	VAL
3	N	1115	THR
1	L	196	THR
3	N	1051	GLU
4	O	30	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	889	HIS
3	N	1334	GLN
3	N	143	ASN
3	N	744	GLN
4	O	37	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MXP	D	1527	-	30,30,30	2.35	13 (43%)	32,38,38	3.46	13 (40%)
7	MXP	N	1527	-	30,30,30	2.62	13 (43%)	32,38,38	3.63	14 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MXP	D	1527	-	-	6/27/28/28	0/1/1/1
7	MXP	N	1527	-	-	7/27/28/28	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	C9-C10	7.23	1.41	1.34
7	D	1527	MXP	C9-C10	6.34	1.40	1.34
7	N	1527	MXP	C1-C5	4.42	1.45	1.34
7	N	1527	MXP	C21-C20	4.32	1.38	1.32
7	D	1527	MXP	O6-C22	4.26	1.29	1.21

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1527	MXP	O4-C6-C7	10.94	138.42	121.07
7	D	1527	MXP	O4-C6-C7	10.20	137.24	121.07
7	D	1527	MXP	O1-C5-C17	7.10	119.05	111.05
7	N	1527	MXP	O1-C5-C1	-7.04	117.16	121.94
7	D	1527	MXP	C8-C9-C10	-6.76	116.93	127.30

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C18-C17-C5-O1
7	N	1527	MXP	C18-C17-C5-O1
7	N	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C18-C17-C5-C1

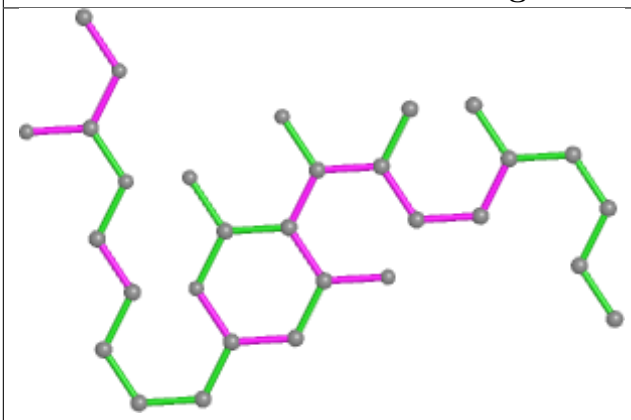
There are no ring outliers.

2 monomers are involved in 36 short contacts:

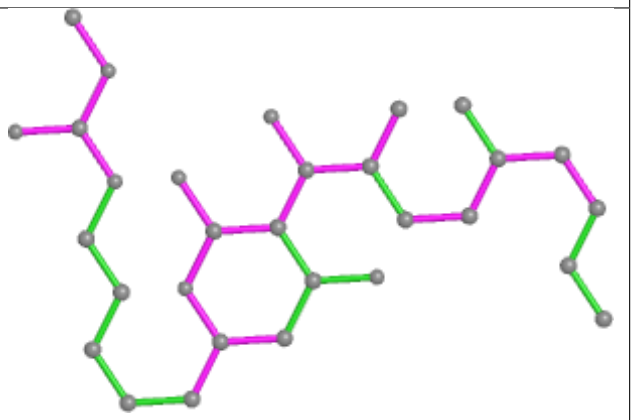
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1527	MXP	18	0
7	N	1527	MXP	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

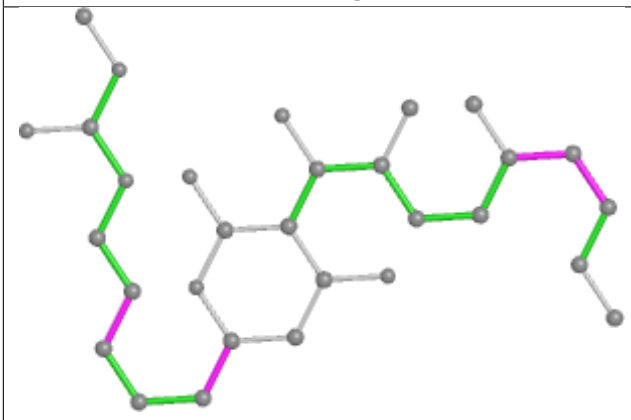
Ligand MXP D 1527



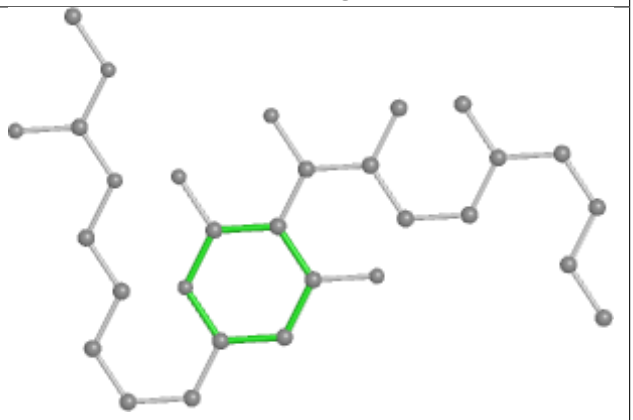
Bond lengths



Bond angles

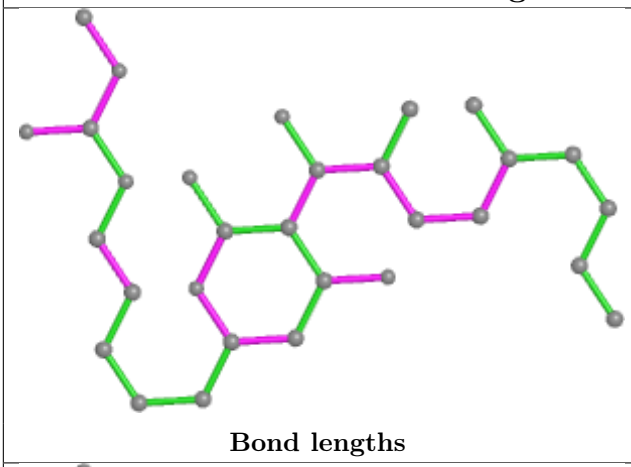


Torsions

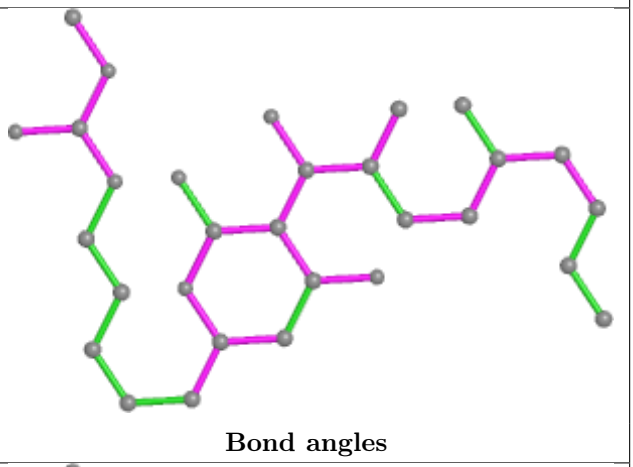


Rings

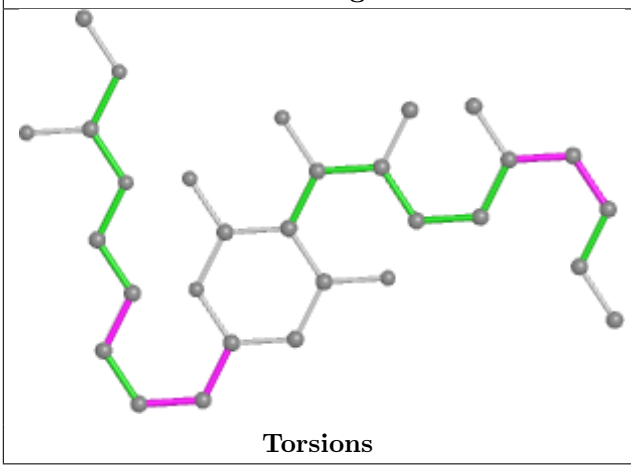
Ligand MXP N 1527



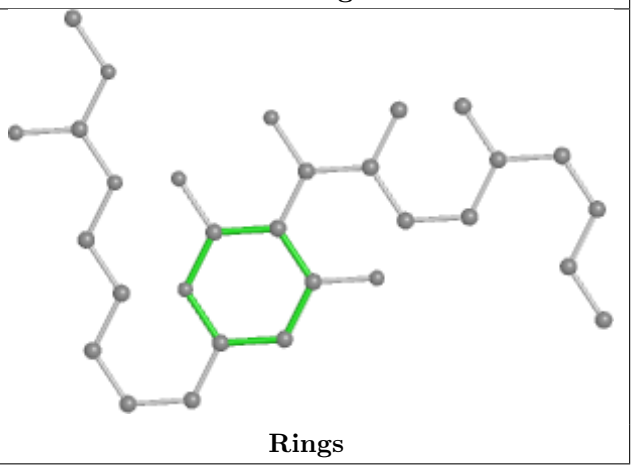
Bond lengths



Bond angles



Torsions



Rings

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, 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	229/315 (72%)	-0.06	3 (1%)	77	78	28, 50, 78, 101	0
1	B	229/315 (72%)	-0.06	8 (3%)	44	44	36, 71, 86, 104	0
1	K	229/315 (72%)	-0.08	2 (0%)	84	85	25, 52, 81, 93	0
1	L	229/315 (72%)	-0.05	6 (2%)	56	57	47, 73, 86, 104	0
2	C	1119/1119 (100%)	-0.06	27 (2%)	59	60	14, 62, 88, 96	0
2	M	1119/1119 (100%)	-0.09	14 (1%)	77	78	11, 60, 86, 101	0
3	D	1321/1524 (86%)	-0.08	20 (1%)	73	76	10, 53, 85, 107	0
3	N	1321/1524 (86%)	-0.10	21 (1%)	72	74	11, 54, 84, 109	0
4	E	95/99 (95%)	-0.13	2 (2%)	63	65	30, 64, 90, 95	0
4	O	95/99 (95%)	-0.19	2 (2%)	63	65	29, 61, 83, 100	0
5	F	345/423 (81%)	-0.10	5 (1%)	75	77	27, 68, 89, 100	0
5	P	345/423 (81%)	-0.07	9 (2%)	56	57	23, 68, 91, 103	0
All	All	6676/7590 (87%)	-0.09	119 (1%)	68	70	10, 59, 87, 109	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1241	PHE	8.6
3	N	1240	THR	6.2
3	N	1243	THR	6.1
2	C	186	VAL	6.0
2	M	186	VAL	5.8

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

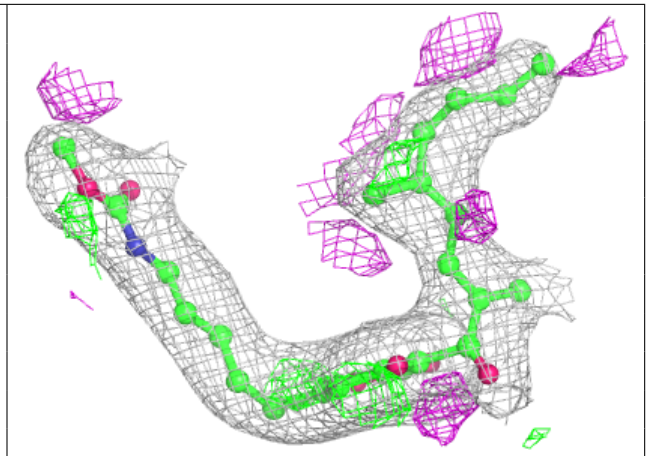
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

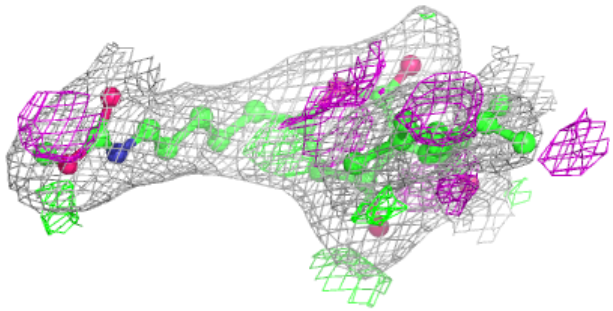
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MXP	D	1527	30/30	0.96	0.19	13,20,27,34	0
7	MXP	N	1527	30/30	0.96	0.17	17,30,38,40	0
6	ZN	D	1525	1/1	0.97	0.14	62,62,62,62	0
6	ZN	N	1526	1/1	0.97	0.18	66,66,66,66	0
8	MG	N	1528	1/1	0.97	0.07	41,41,41,41	0
8	MG	D	1528	1/1	0.98	0.09	35,35,35,35	0
6	ZN	N	1525	1/1	0.99	0.17	58,58,58,58	0
6	ZN	D	1526	1/1	0.99	0.21	48,48,48,48	0

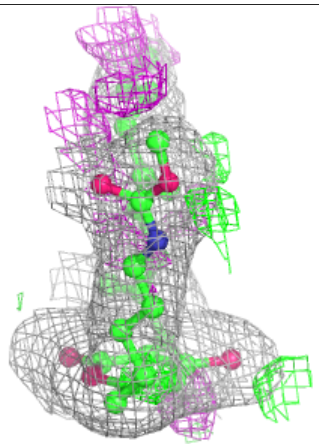
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MXP D 1527:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

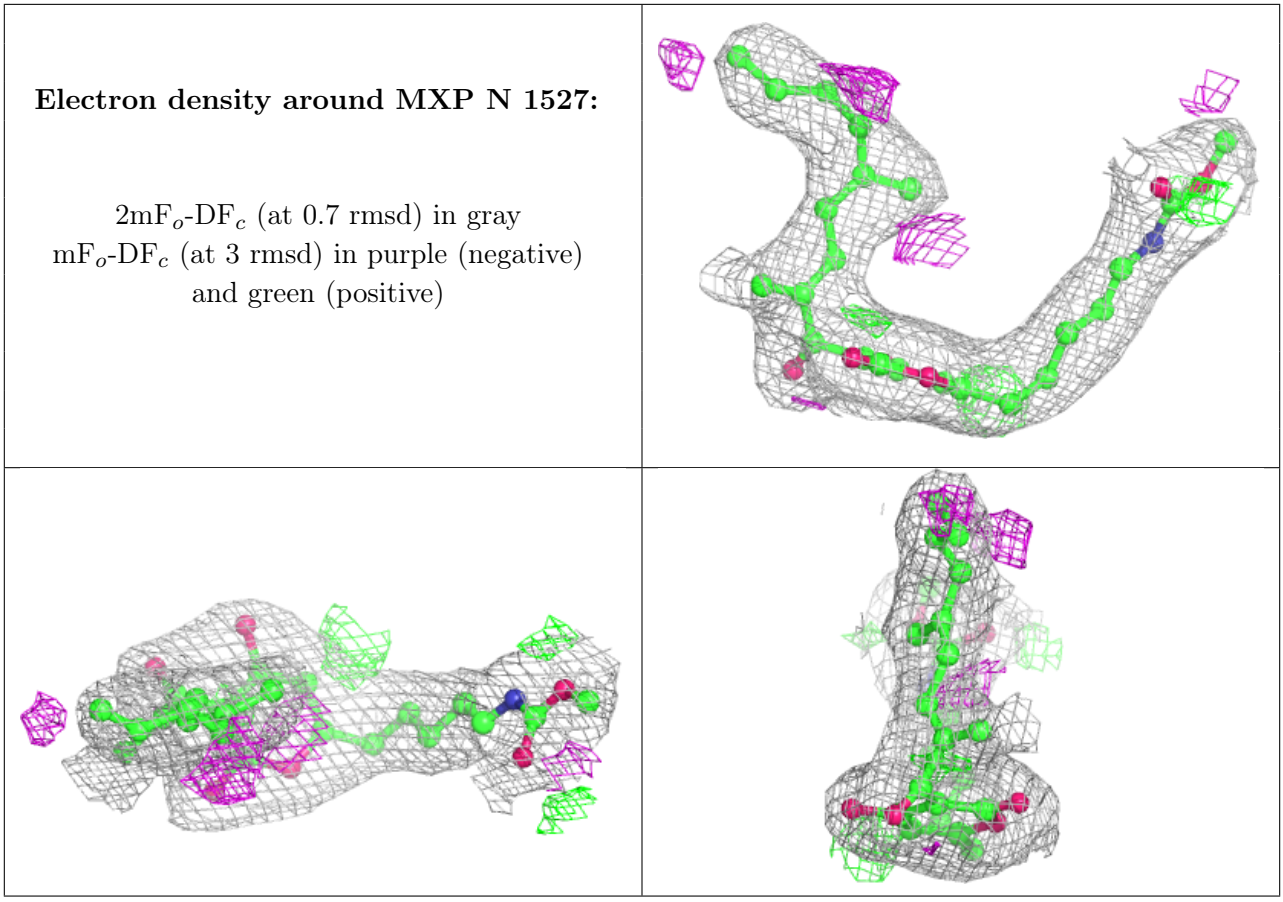






Electron density around MXP N 1527:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.