wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 12:28 PM EDT

PDB ID	:	4YLN
Title	:	E. coli Transcription Initiation Complex - 17-bp spacer and 4-nt RNA
Authors	:	Zuo, Y.; Steitz, T.A.
Deposited on	:	2015-03-05
Resolution	:	5.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

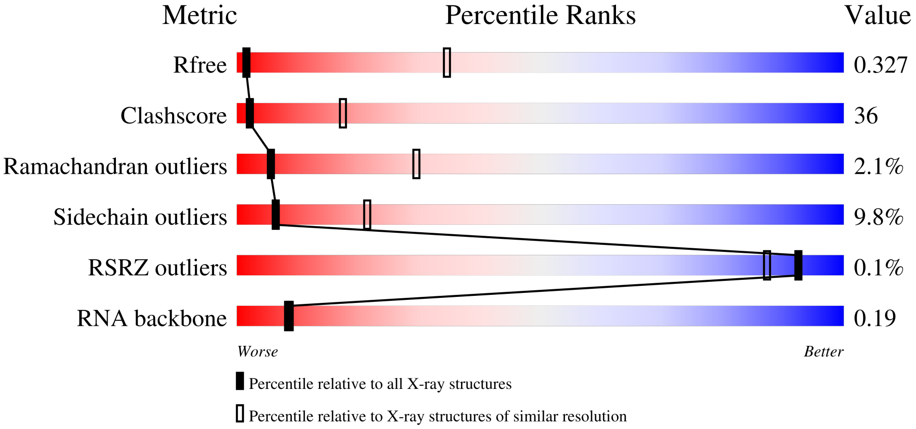
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

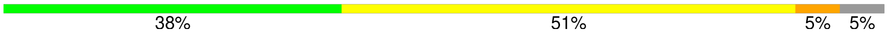
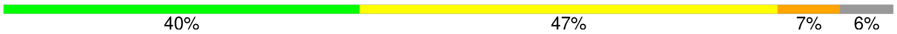
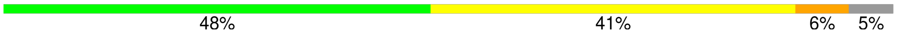
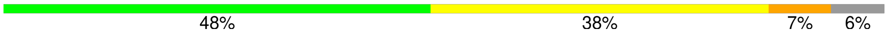
The reported resolution of this entry is 5.50 Å.

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}	164625	1029 (7.00-4.00)
Clashscore	180529	1069 (7.00-4.00)
Ramachandran outliers	177936	1010 (7.04-3.96)
Sidechain outliers	177891	1004 (7.04-3.94)
RSRZ outliers	164620	1023 (7.00-4.00)
RNA backbone	3690	1172 (7.80-3.00)

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	242	
1	B	242	
1	G	242	
1	H	242	

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Mol	Chain	Length	Quality of chain
1	M	242	49% 43% • 5%
1	N	242	48% 40% 6% 6%
2	C	1342	46% 48% 6%
2	I	1342	48% 47% 5%
2	O	1342	50% 45% •
3	D	1407	44% 47% 6% •
3	J	1407	41% 48% 7% •
3	P	1407	45% 45% 7% •
4	E	90	48% 50% •
4	K	90	53% 42% •
4	Q	90	67% 29% •
5	F	628	43% 32% • 21%
5	L	628	43% 31% 5% 21%
5	R	628	41% 32% 6% 21%
6	1	49	29% 71%
6	4	49	31% 69%
6	7	49	31% 69%
7	2	49	37% 63%
7	5	49	41% 59%
7	8	49	35% 65%
8	3	4	25% 50% 25%
8	6	4	50% 50%
8	9	4	75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ZN	J	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94608 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	230	Total C N O S 1787 1112 317 352 6	0	0	0
1	B	228	Total C N O S 1767 1100 312 349 6	0	0	0
1	G	230	Total C N O S 1787 1112 317 352 6	0	0	0
1	H	228	Total C N O S 1767 1100 312 349 6	0	0	0
1	M	230	Total C N O S 1787 1112 317 352 6	0	0	0
1	N	228	Total C N O S 1767 1100 312 349 6	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP A7ZSI4
A	-5	HIS	-	expression tag	UNP A7ZSI4
A	-4	HIS	-	expression tag	UNP A7ZSI4
A	-3	HIS	-	expression tag	UNP A7ZSI4
A	-2	HIS	-	expression tag	UNP A7ZSI4
A	-1	HIS	-	expression tag	UNP A7ZSI4
A	0	HIS	-	expression tag	UNP A7ZSI4
B	-6	ALA	-	expression tag	UNP A7ZSI4
B	-5	HIS	-	expression tag	UNP A7ZSI4
B	-4	HIS	-	expression tag	UNP A7ZSI4
B	-3	HIS	-	expression tag	UNP A7ZSI4
B	-2	HIS	-	expression tag	UNP A7ZSI4
B	-1	HIS	-	expression tag	UNP A7ZSI4
B	0	HIS	-	expression tag	UNP A7ZSI4
G	-6	ALA	-	expression tag	UNP A7ZSI4
G	-5	HIS	-	expression tag	UNP A7ZSI4
G	-4	HIS	-	expression tag	UNP A7ZSI4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	HIS	-	expression tag	UNP A7ZSI4
G	-2	HIS	-	expression tag	UNP A7ZSI4
G	-1	HIS	-	expression tag	UNP A7ZSI4
G	0	HIS	-	expression tag	UNP A7ZSI4
H	-6	ALA	-	expression tag	UNP A7ZSI4
H	-5	HIS	-	expression tag	UNP A7ZSI4
H	-4	HIS	-	expression tag	UNP A7ZSI4
H	-3	HIS	-	expression tag	UNP A7ZSI4
H	-2	HIS	-	expression tag	UNP A7ZSI4
H	-1	HIS	-	expression tag	UNP A7ZSI4
H	0	HIS	-	expression tag	UNP A7ZSI4
M	-6	ALA	-	expression tag	UNP A7ZSI4
M	-5	HIS	-	expression tag	UNP A7ZSI4
M	-4	HIS	-	expression tag	UNP A7ZSI4
M	-3	HIS	-	expression tag	UNP A7ZSI4
M	-2	HIS	-	expression tag	UNP A7ZSI4
M	-1	HIS	-	expression tag	UNP A7ZSI4
M	0	HIS	-	expression tag	UNP A7ZSI4
N	-6	ALA	-	expression tag	UNP A7ZSI4
N	-5	HIS	-	expression tag	UNP A7ZSI4
N	-4	HIS	-	expression tag	UNP A7ZSI4
N	-3	HIS	-	expression tag	UNP A7ZSI4
N	-2	HIS	-	expression tag	UNP A7ZSI4
N	-1	HIS	-	expression tag	UNP A7ZSI4
N	0	HIS	-	expression tag	UNP A7ZSI4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1341	Total 10576	C 6636	N 1842	O 2055	S 43	0	0	0
2	I	1341	Total 10576	C 6636	N 1842	O 2055	S 43	0	0	0
2	O	1341	Total 10576	C 6636	N 1842	O 2055	S 43	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1362	Total 10568	C 6633	N 1887	O 1998	S 50	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	1362	Total 10568	C 6633	N 1887	O 1998	S 50	0	0	0
3	P	1362	Total 10568	C 6633	N 1887	O 1998	S 50	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total 708	C 430	N 136	O 141	S 1	0	0	0
4	K	90	Total 708	C 430	N 136	O 141	S 1	0	0	0
4	Q	90	Total 708	C 430	N 136	O 141	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	497	Total 4022	C 2512	N 719	O 768	S 23	0	0	0
5	L	497	Total 4022	C 2512	N 719	O 768	S 23	0	0	0
5	R	497	Total 4022	C 2512	N 719	O 768	S 23	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	THR	-	expression tag	UNP P00579
L	-14	MET	-	expression tag	UNP P00579
L	-13	ARG	-	expression tag	UNP P00579
L	-12	GLY	-	expression tag	UNP P00579
L	-11	SER	-	expression tag	UNP P00579
L	-10	HIS	-	expression tag	UNP P00579
L	-9	HIS	-	expression tag	UNP P00579
L	-8	HIS	-	expression tag	UNP P00579
L	-7	HIS	-	expression tag	UNP P00579
L	-6	HIS	-	expression tag	UNP P00579
L	-5	HIS	-	expression tag	UNP P00579
L	-4	THR	-	expression tag	UNP P00579
L	-3	ASP	-	expression tag	UNP P00579
L	-2	GLN	-	expression tag	UNP P00579
L	-1	PHE	-	expression tag	UNP P00579
L	0	THR	-	expression tag	UNP P00579
R	-14	MET	-	expression tag	UNP P00579
R	-13	ARG	-	expression tag	UNP P00579
R	-12	GLY	-	expression tag	UNP P00579
R	-11	SER	-	expression tag	UNP P00579
R	-10	HIS	-	expression tag	UNP P00579
R	-9	HIS	-	expression tag	UNP P00579
R	-8	HIS	-	expression tag	UNP P00579
R	-7	HIS	-	expression tag	UNP P00579
R	-6	HIS	-	expression tag	UNP P00579
R	-5	HIS	-	expression tag	UNP P00579
R	-4	THR	-	expression tag	UNP P00579
R	-3	ASP	-	expression tag	UNP P00579
R	-2	GLN	-	expression tag	UNP P00579
R	-1	PHE	-	expression tag	UNP P00579
R	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a DNA chain called NT strand DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	1	49	996	476	178	294	48	0	0	0
6	4	49	996	476	178	294	48	0	0	0
6	7	49	996	476	178	294	48	0	0	0

- Molecule 7 is a DNA chain called T strand DNA (49-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	2	49	Total C N O P 1012 481 191 292 48	0	0	0
7	5	49	Total C N O P 1012 481 191 292 48	0	0	0
7	8	49	Total C N O P 1012 481 191 292 48	0	0	0

- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*AP*GP*U)-3').

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	3	4	Total C N O P 97 39 17 35 6	0	0	0
8	6	4	Total C N O P 97 39 17 35 6	0	0	0
8	9	4	Total C N O P 97 39 17 35 6	0	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Zn 2 2	0	0
9	J	2	Total Zn 2 2	0	0
9	P	2	Total Zn 2 2	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

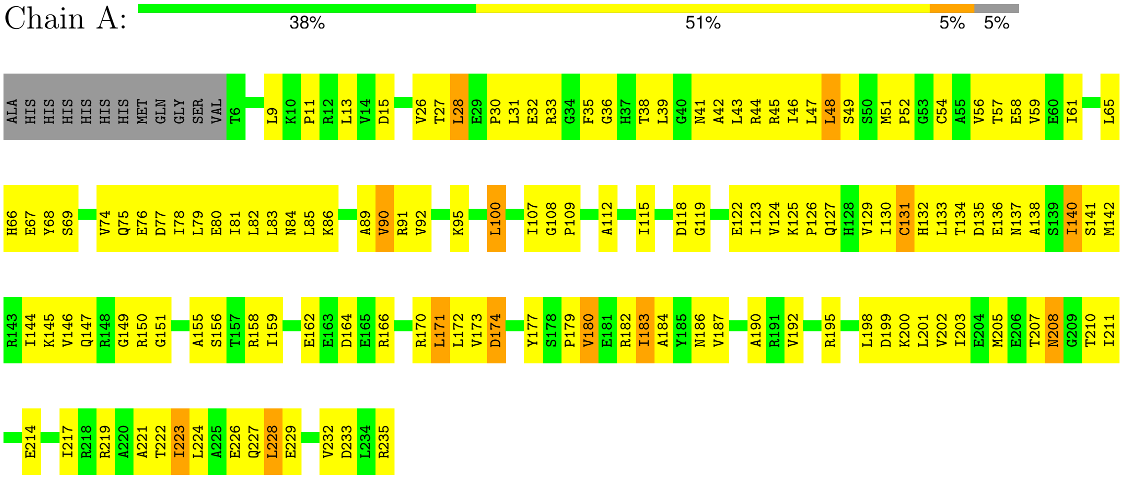
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Mg 1 1	0	0
10	6	1	Total Mg 1 1	0	0
10	P	1	Total Mg 1 1	0	0

3 Residue-property plots ⓘ

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

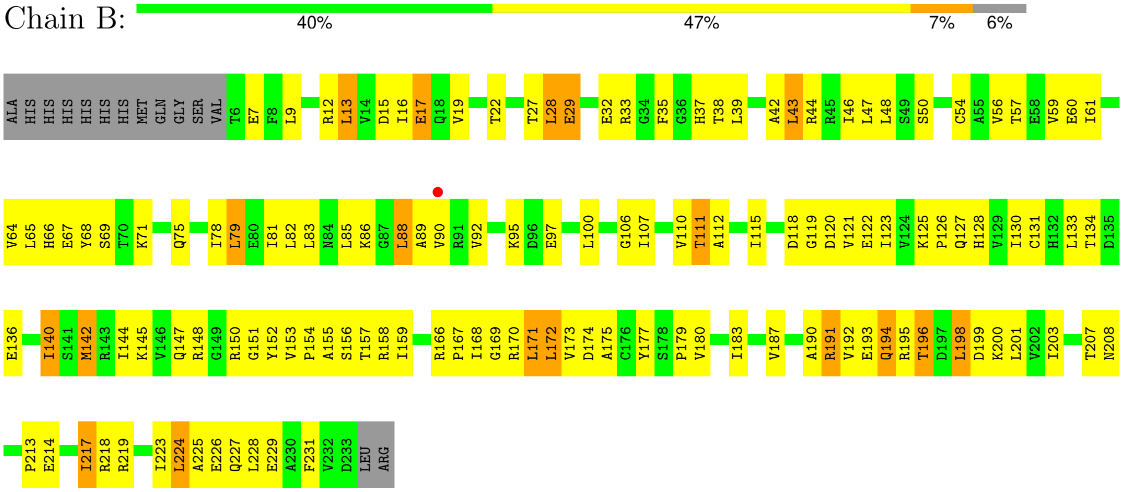
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



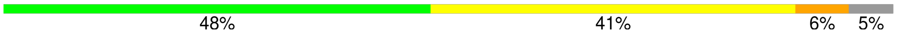
- Molecule 1: DNA-directed RNA polymerase subunit alpha

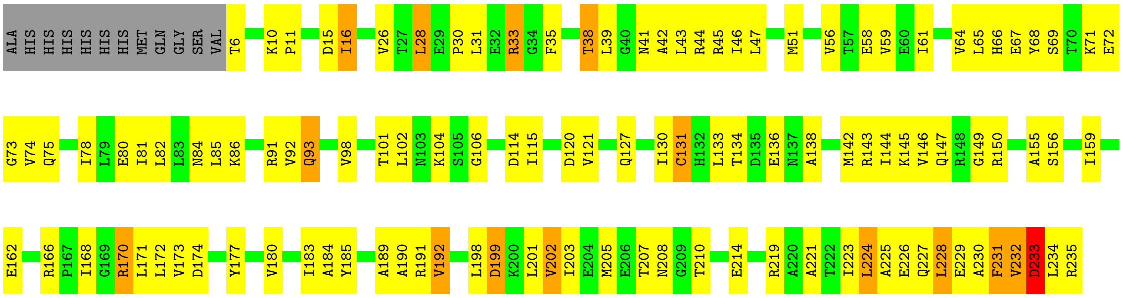
Chain B:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

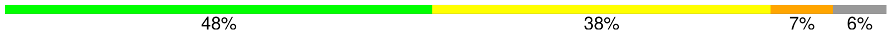
Chain G:

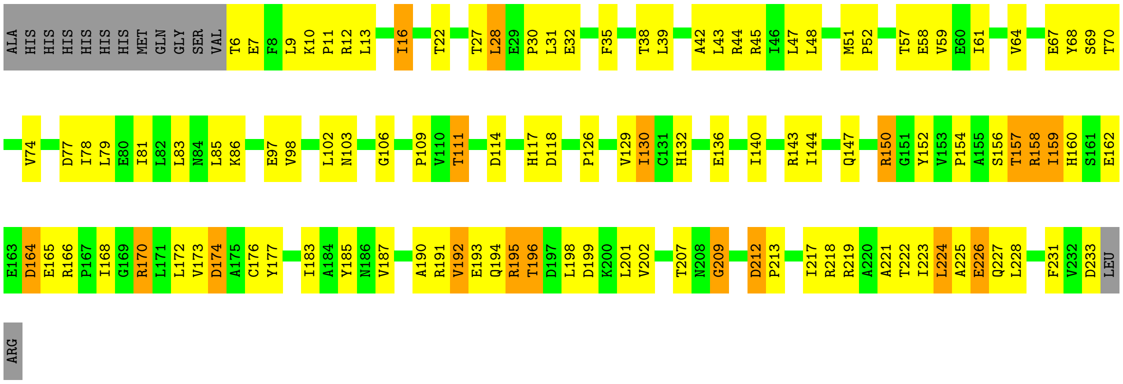




- Molecule 1: DNA-directed RNA polymerase subunit alpha

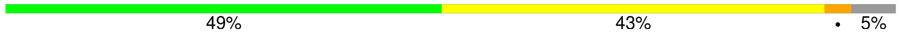
Chain H:

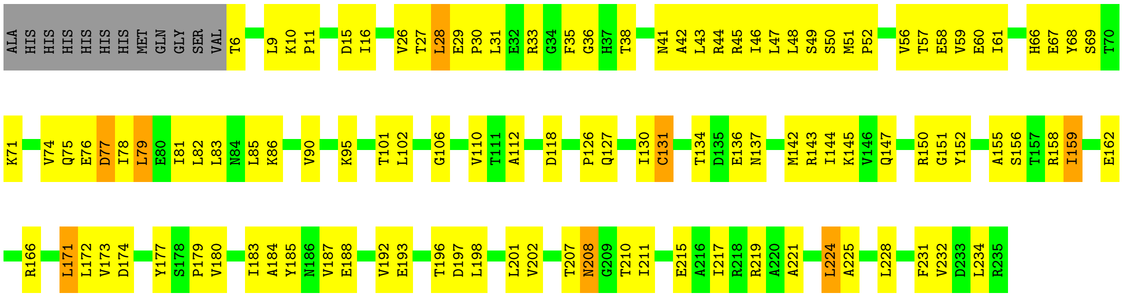




- Molecule 1: DNA-directed RNA polymerase subunit alpha

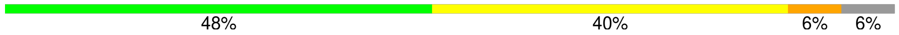
Chain M:

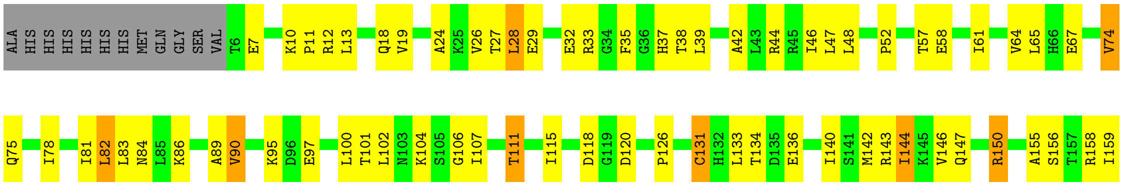


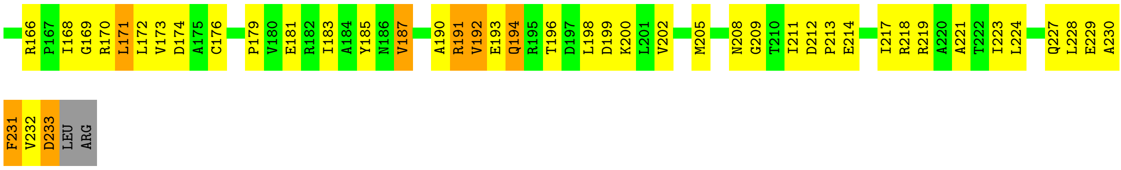


- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain N:

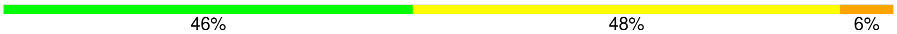


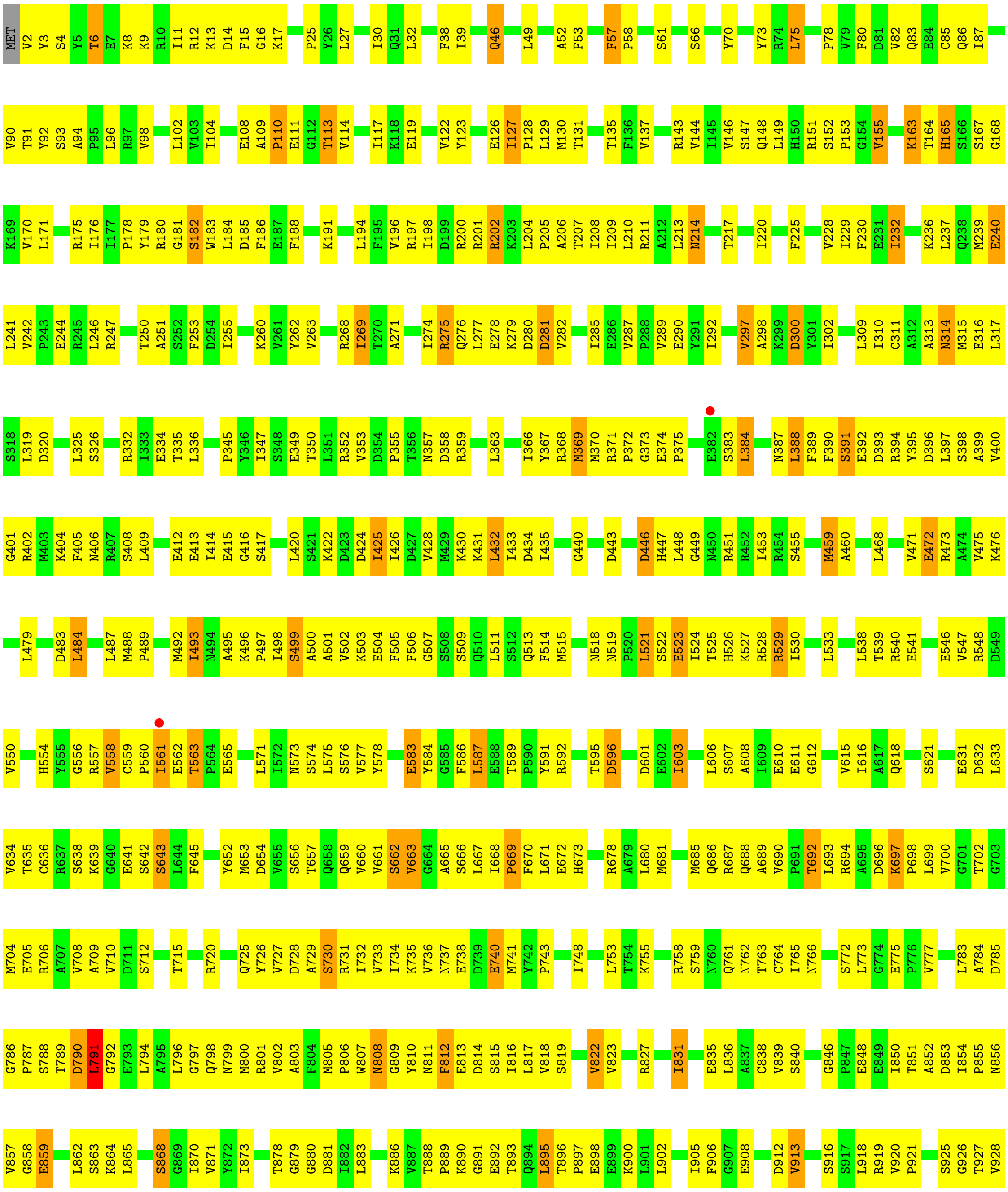


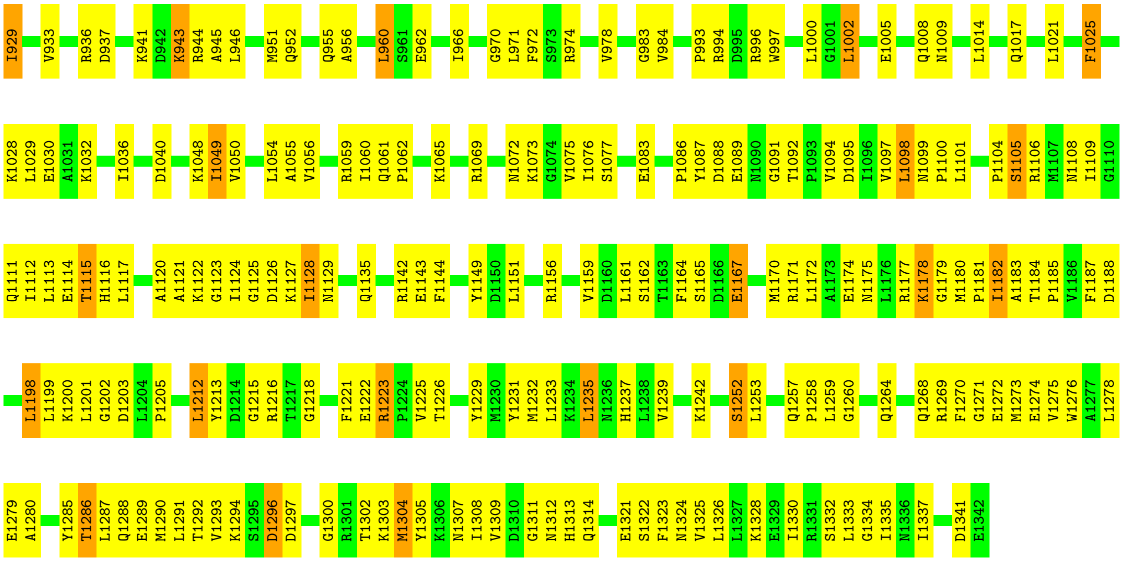

R166 P167 I168 G169 R170 L171 L172 V173 D174 A175 C176 P179 V180 E181 R182 I183 A184 Y185 N186 V187 A190 R191 V192 E193 Q194 R195 T196 D197 L198 D199 K200 L201 V202 M205 N208 G209 T210 I211 D212 P213 E214 I217 R218 R219 A220 A221 T222 I223 L224 Q227 L228 E229 A230
F231 V232 D233 LEU ARG

- Molecule 2: DNA-directed RNA polymerase subunit beta

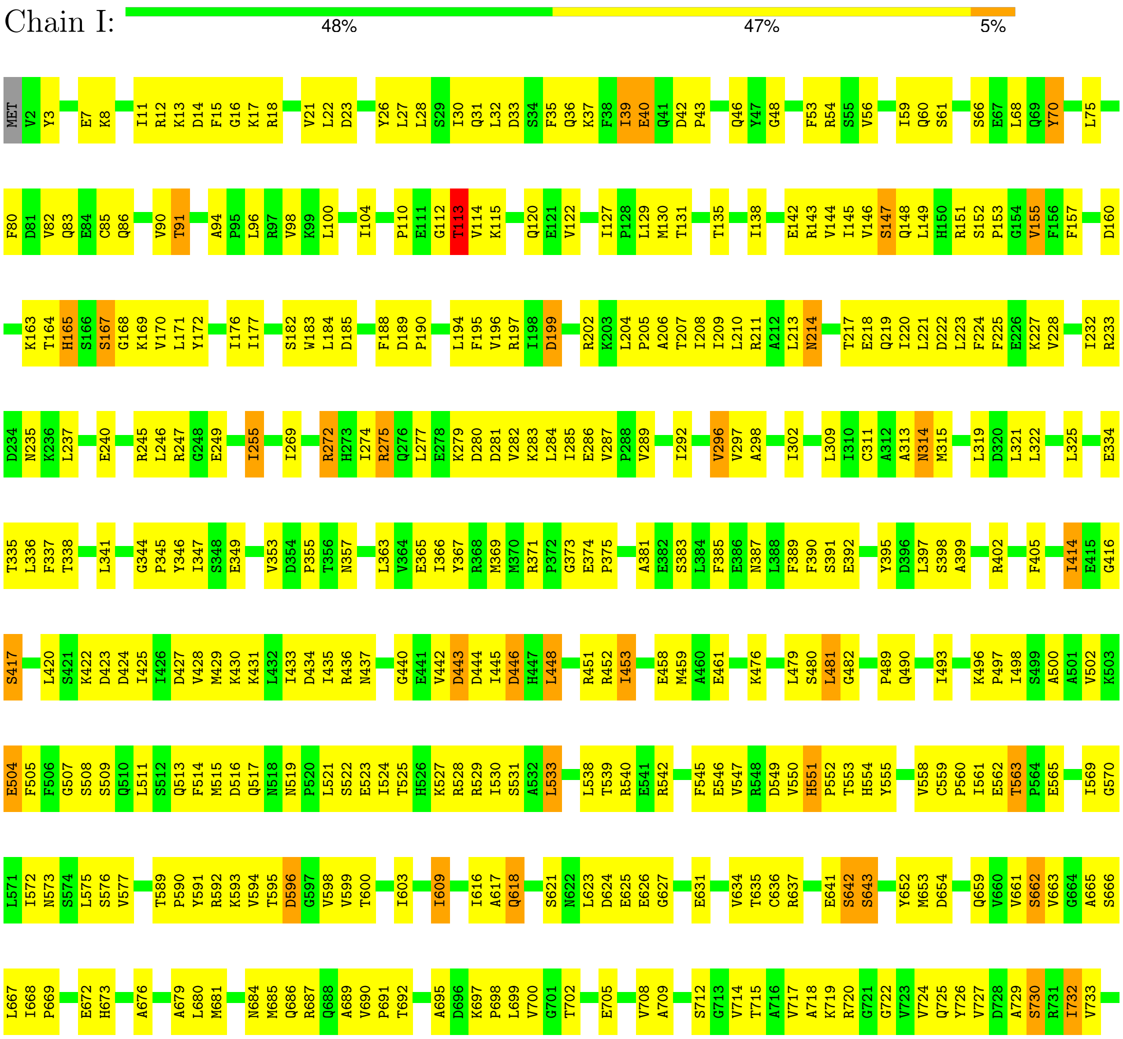
Chain C:

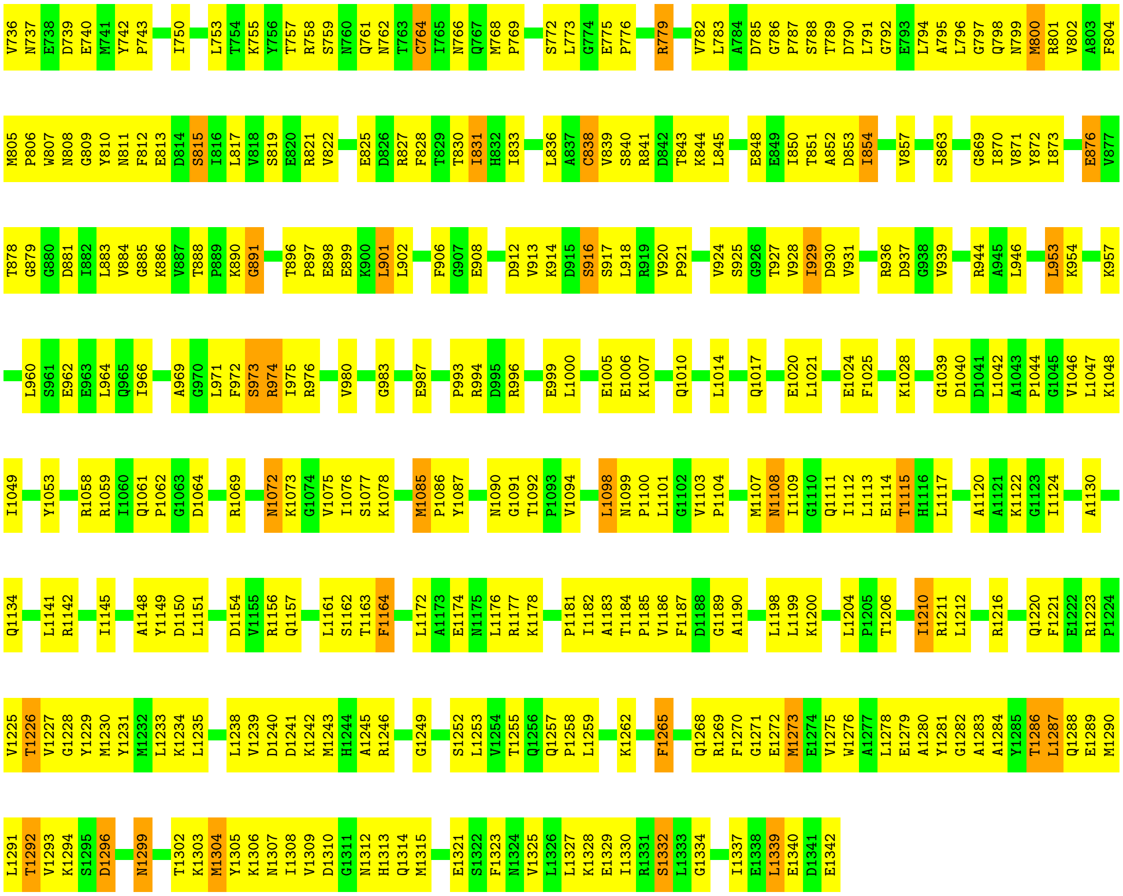



MET V2 Y3 S4 Y5 T6 E7 K8 K9 R10 I11 R12 K13 D14 F15 G16 K17 P25 Y26 L27 I30 Q31 L32 F38 I39 Q46 L49 A52 F53 F57 P58 S61 S66 Y70 Y73 R74 L75 P78 V79 F80 D81 V82 Q83 E84 C85 Q86 I87
V90 T91 Y92 S93 A94 P95 L96 R97 V98 L102 V103 I104 E108 A109 P110 E111 G112 T113 V114 I117 K118 E119 V122 Y123 E126 I127 P128 L129 M130 T131 T135 F136 V137 R143 V144 I145 V146 S147 Q148 L149 H150 R151 S152 P153 G154 V155 K163 T164 H165 S166 S167 G168
K169 V170 L171 R175 I176 I177 P178 Y179 R180 G181 S182 W183 L184 D185 F186 E187 F188 K191 L194 F195 V196 R197 I198 D199 R200 R201 R202 K203 L204 P205 A206 T207 I208 I209 L210 R211 A212 L213 N214 T217 I220 F225 V228 I229 F230 E231 I232 K236 L237 Q238 M239 E240
L241 V242 P243 E244 R245 L246 R247 T250 A251 S252 F253 D254 I255 K260 V261 Y262 V263 R268 I269 T270 A271 I274 R275 Q276 L277 E278 K279 D280 D281 V282 I285 E286 V287 P288 V289 E290 Y291 I292 V297 A298 K299 D300 Y301 I302 L309 I310 C311 A312 A313 N314 M315 E316 L317
S318 L319 D320 L325 S326 R332 I333 E334 T335 L336 P345 Y346 I347 S348 E349 T350 L351 R352 V353 D354 P355 T356 N357 D358 R359 L363 I366 Y367 R368 M369 M370 R371 P372 G373 E374 P375 E382 S383 L384 N387 L388 F389 F390 S391 E392 D393 R394 Y395 D396 L397 S398 A399 V400
G401 R402 M403 K404 F405 N406 R407 S408 L409 E412 E413 I414 E415 G416 S417 L420 S421 K422 D423 D424 I425 I426 D427 V428 M429 K430 K431 L432 I433 D434 I435 G440 D443 D446 H447 L448 G449 N450 R451 R452 I453 R454 S455 M459 A460 L468 V471 E472 R473 A474 V475 K476
L479 D483 L484 L487 M488 P489 M492 I493 N494 A495 K496 P497 I498 S499 A500 A501 V502 K503 E504 F505 F506 G507 S508 S509 Q510 L511 S512 Q513 F514 M515 N518 N519 P520 L521 S522 E523 I524 T525 H526 K527 R528 R529 I530 L533 L538 T539 R540 E541 E546 V547 R548 D549
V550 H554 Y555 G556 R557 V558 C559 P560 I561 E562 T563 P564 E565 L571 I572 N573 S574 L575 S576 V577 Y578 E583 Y584 G585 F586 L587 E588 T589 P590 Y591 R592 T595 D596 D601 E602 I603 L606 S607 A608 I609 E610 E611 G612 V615 I616 A617 Q618 S621 E631 D632 L633
V634 T635 C636 R637 S638 K639 G640 E641 S642 S643 L644 F645 Y652 M653 D654 V655 S656 T657 Q658 Q659 V660 V661 S662 V663 G664 A665 S666 L667 I668 P669 F670 L671 E672 H673 R678 A679 L680 M681 M685 Q686 R687 Q688 A689 V690 P691 T692 L693 R694 A695 D696 K697 P698 L699 V700 G701 T702 G703
M704 E705 R706 A707 V708 A709 V710 D711 S712 T715 R720 Q725 Y726 V727 D728 A729 S730 R731 I732 V733 I734 K735 V736 N737 E738 D739 E740 M741 Y742 P743 I748 L753 T754 K755 R758 S759 N760 Q761 N762 T763 C764 I765 N766 S772 L773 G774 E775 P776 V777 L783 A784 D785
G786 P787 S788 T789 D790 L791 G792 E793 L794 A795 L796 G797 Q798 N799 M800 R801 V802 A803 F804 M805 P806 W807 N808 G809 Y810 N811 F812 E813 D814 S815 I816 L817 V818 S819 V822 V823 R827 I831 E835 L836 A837 C838 V839 S840 G846 P847 E848 E849 I850 T851 A852 D853 I854 P855 N856
V857 G858 E859 L862 S863 K864 L865 S868 G869 I870 V871 Y872 I873 T878 G879 G880 D881 I882 L883 K886 V887 T888 P889 K890 G891 E892 T893 Q894 L895 T896 P897 E898 E899 K900 L901 L902 I905 F906 G907 E908 D912 V913 S916 S917 L918 R919 V920 P921 S925 G926 T927 V928



- Molecule 2: DNA-directed RNA polymerase subunit beta





- Molecule 2: DNA-directed RNA polymerase subunit beta

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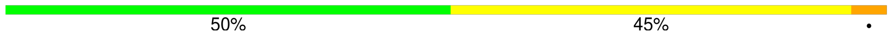

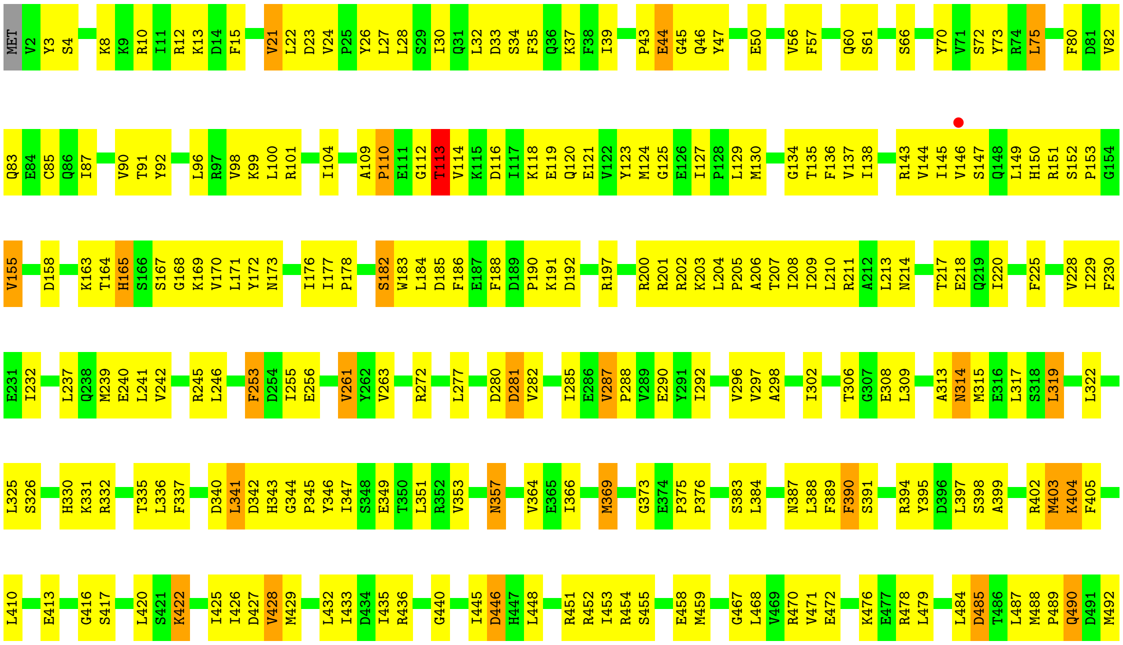

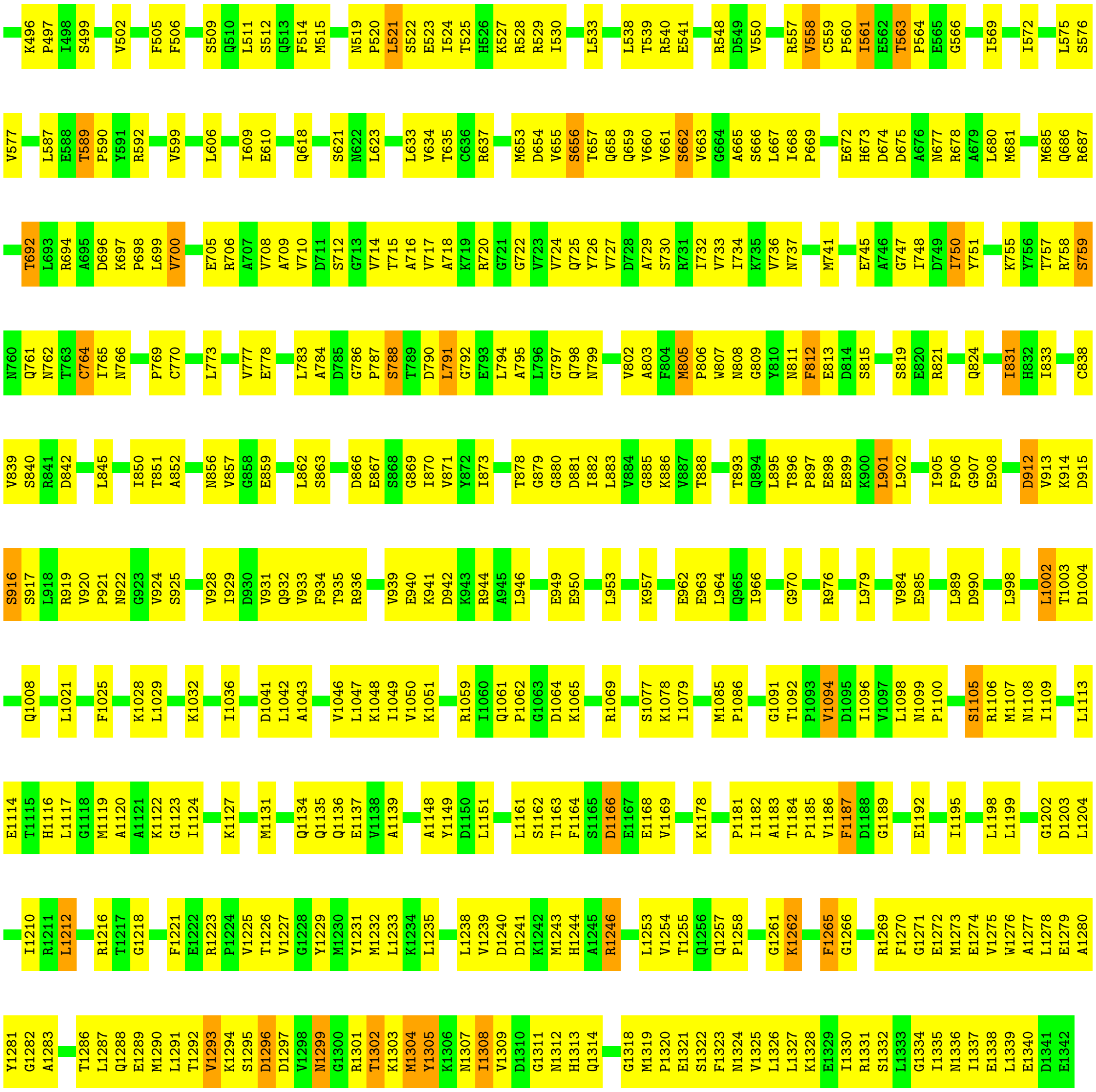

- Molecule 3: DNA-directed RNA polymerase subunit beta'

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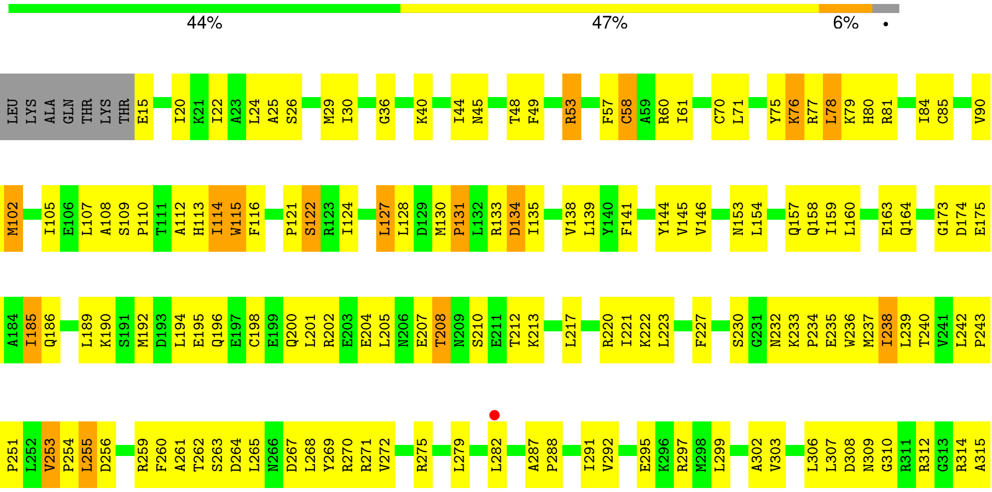
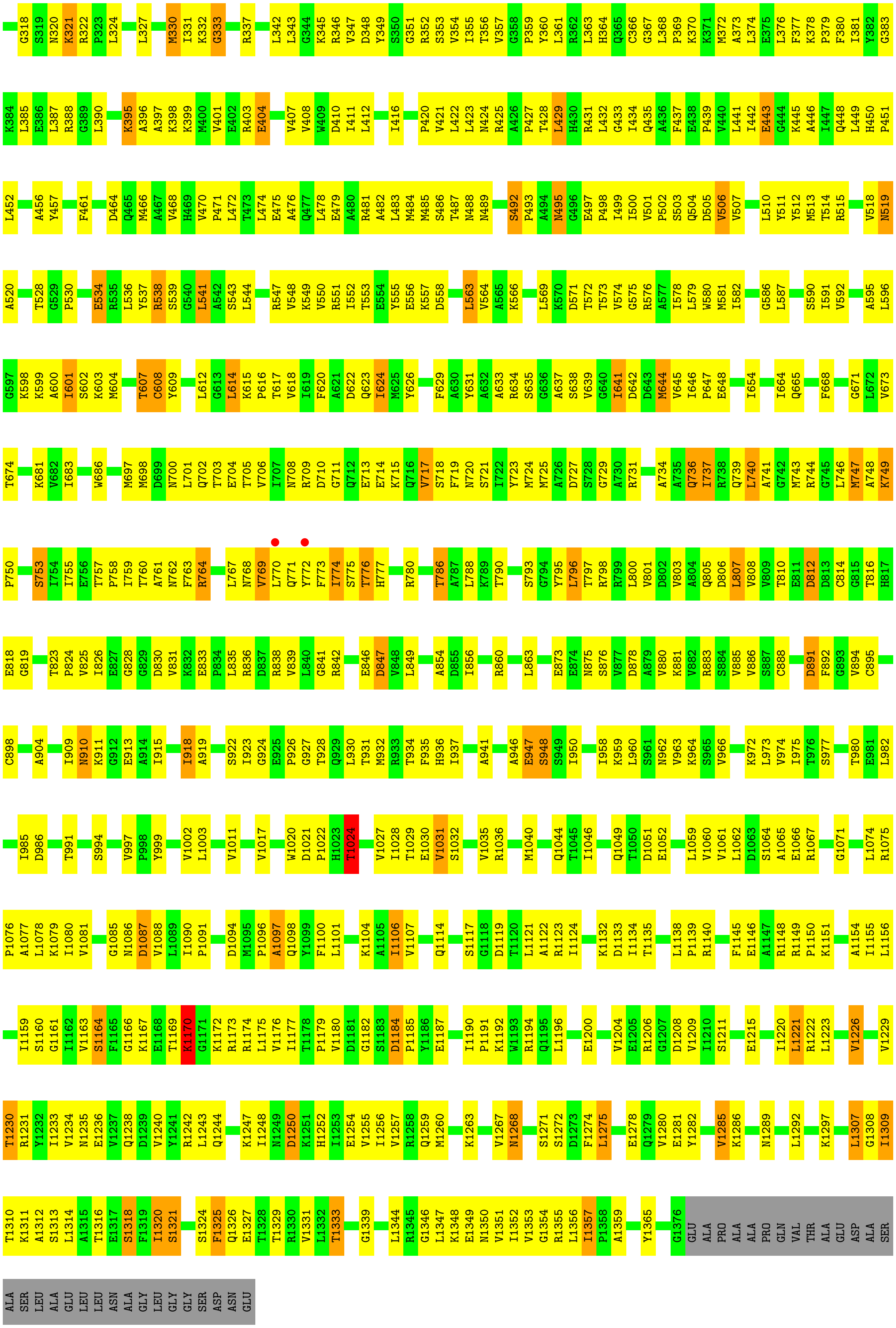
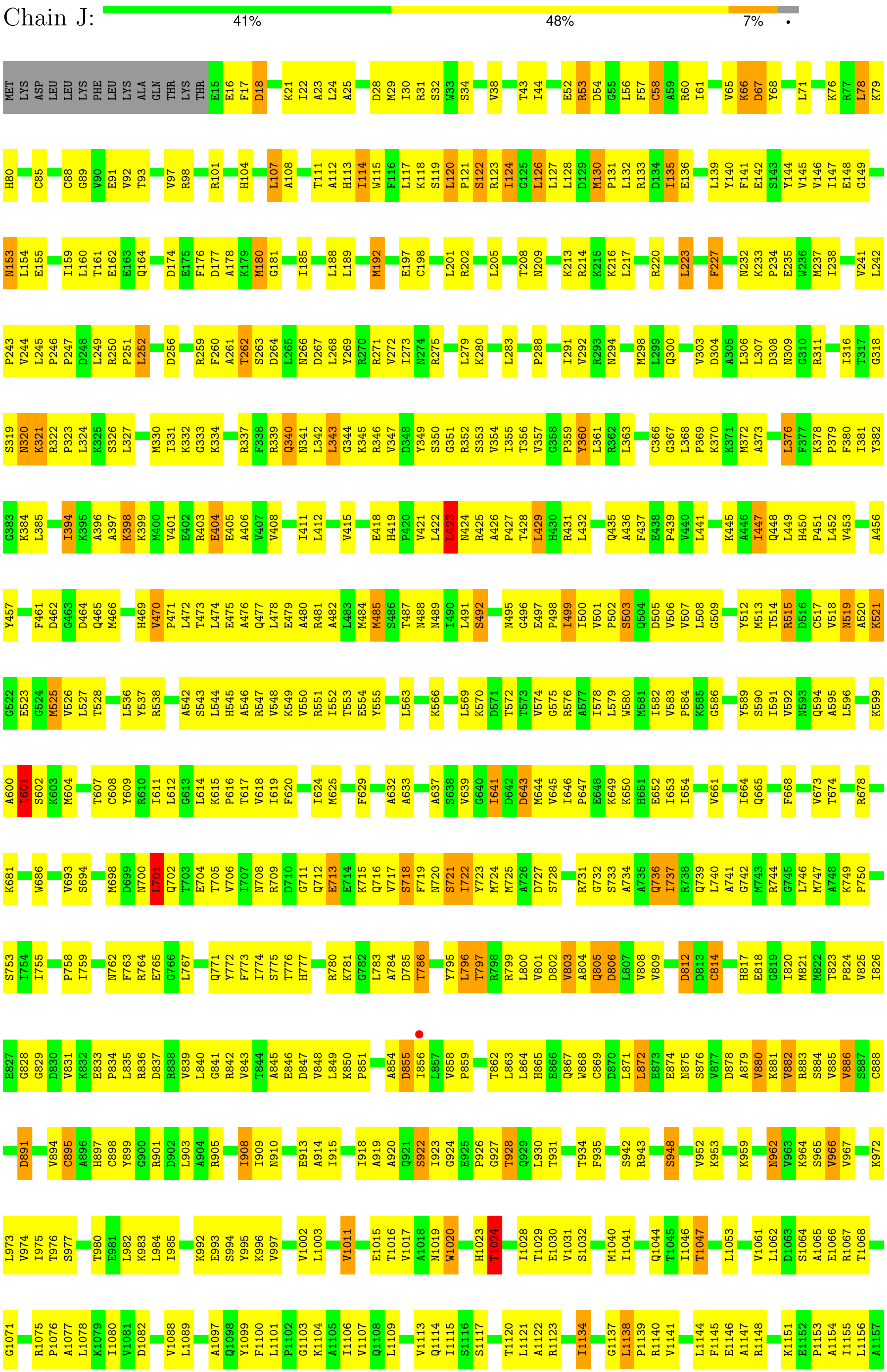




- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:


41%
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S753 I754 I755 P758 I759 N762 F763 R764 E765 G766 L767 Q771 Y772 F773 I774 S775 T776 H777 R780 K781 G782 L783 A784 D785 T786 Y795 L796 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 D812 D813 C814 H817 E818 G819 I820 M821 M822 T823 P824 V825 I826
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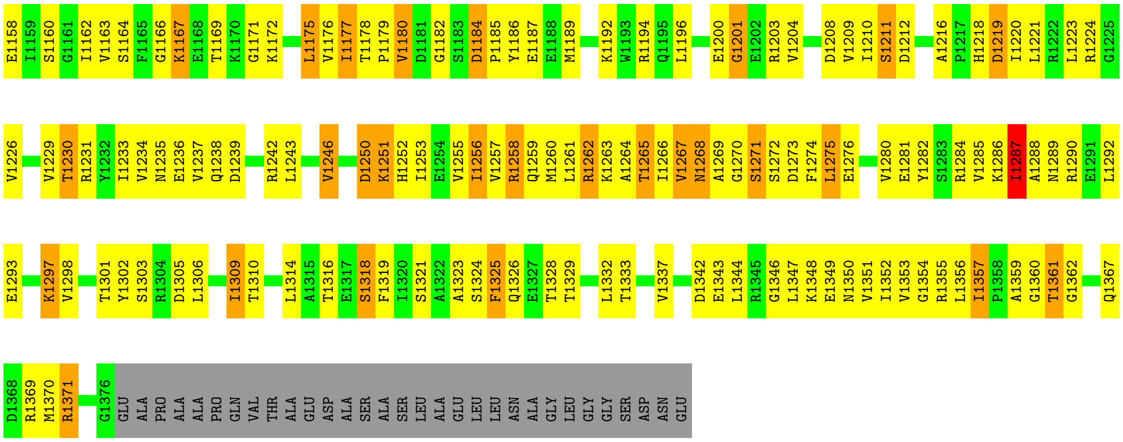
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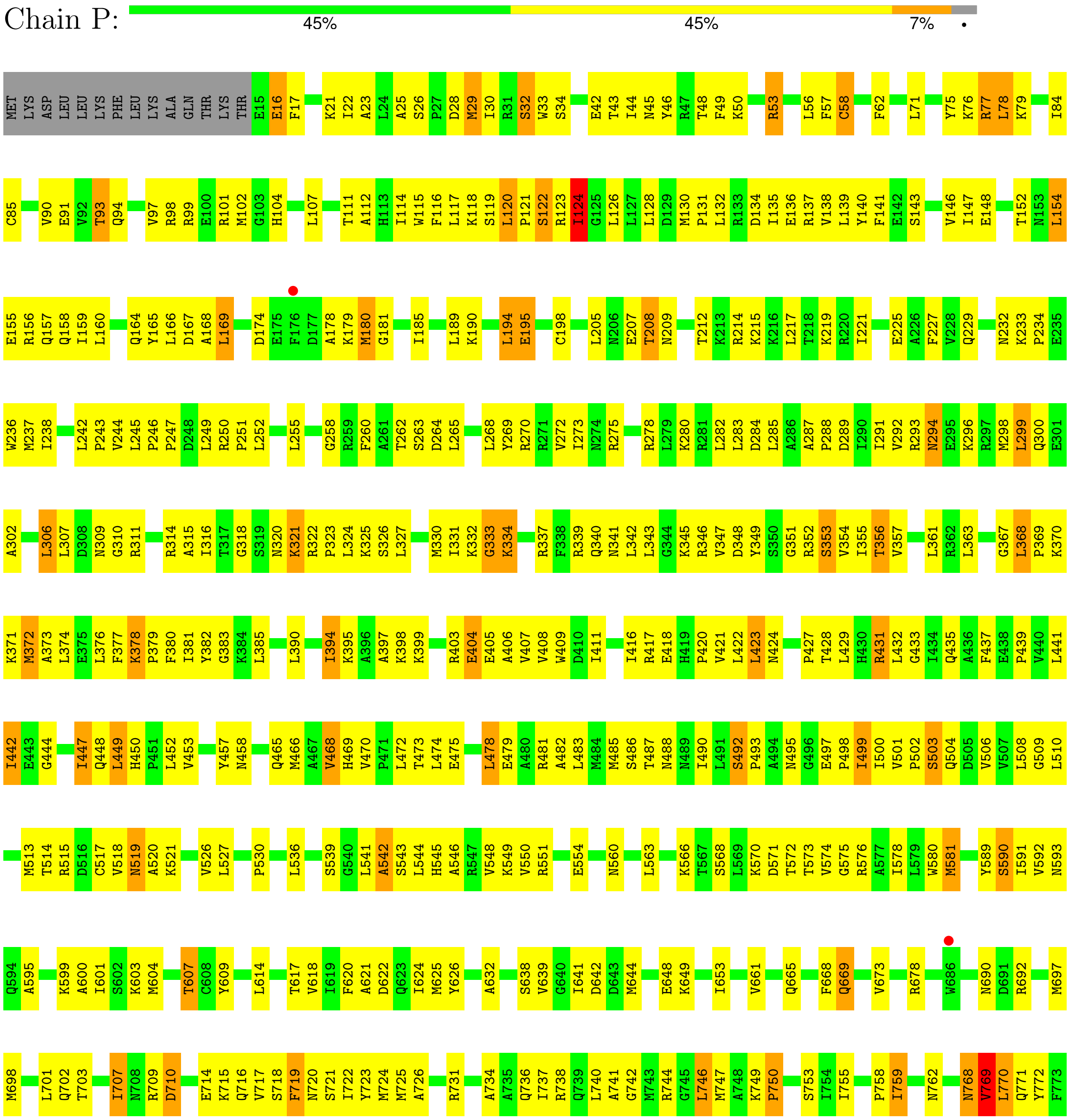
- Molecule 3: DNA-directed RNA polymerase subunit beta'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45%
45%
7%
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C85 V90 E91 V92 T93 Q94 V97 R98 R99 E100 R101 M102 G103 H104 L107 T111 A112 H113 I114 W115 F116 L117 K118 S119 L120 P121 S122 R123 I124 G125 L126 L127 L128 D129 M130 P131 L132 R133 D134 I135 E136 R137 V138 L139 Y140 F141 E142 S143 V146 I147 E148 T152 N153 L154
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A302 L306 L307 D308 N309 G310 R311 R314 A315 I316 T317 G318 S319 N320 K321 R322 P323 L324 K325 S326 L327 M330 I331 K332 G333 K334 R337 F338 R339 Q340 N341 L342 L343 G344 K345 R346 V347 D348 Y349 S350 G351 R352 S353 V354 I355 T356 V357 L361 R362 L363 G367 L368 P369 K370
K371 M372 A373 L374 E375 L376 F377 K378 P379 F380 I381 Y382 G383 K384 L385 L390 I394 K395 A396 A397 K398 K399 R403 E404 E405 A406 V407 V408 W409 D410 I411 I416 R417 E418 H419 P420 V421 L422 L423 N424 P427 T428 L429 H430 R431 L432 G433 I434 Q435 A436 F437 E438 P439 V440 L441
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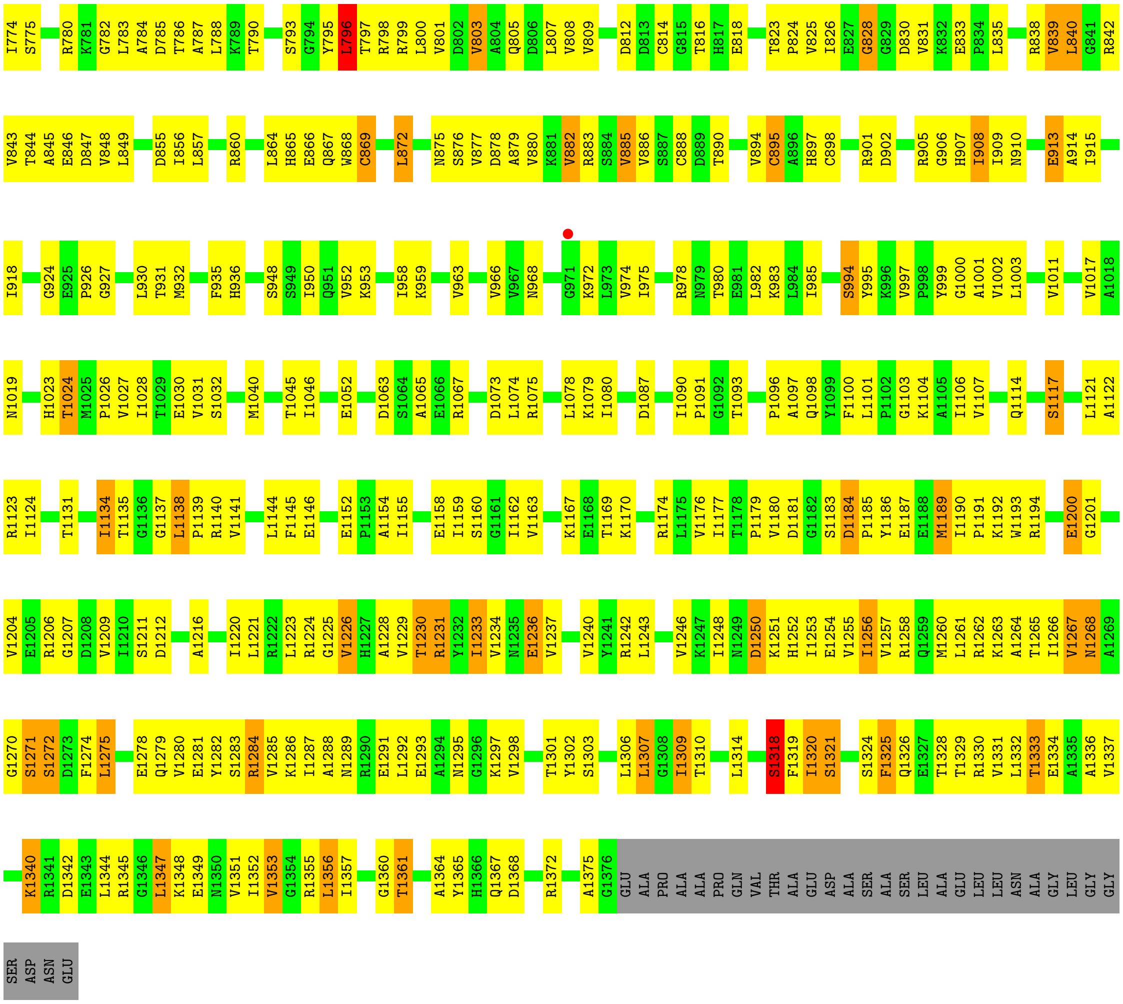

- Molecule 4: DNA-directed RNA polymerase subunit omega

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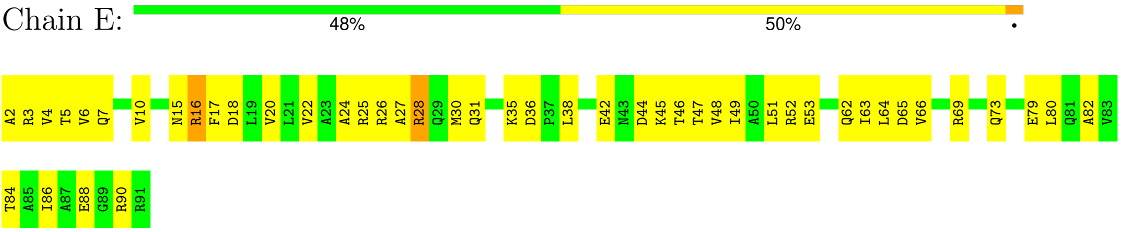

- Molecule 4: DNA-directed RNA polymerase subunit omega

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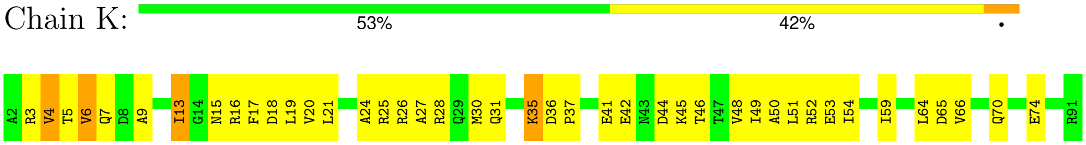
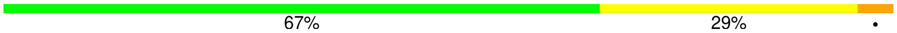
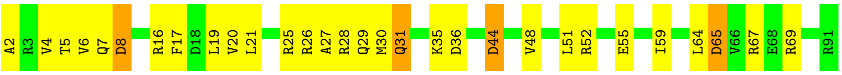


- Molecule 4: DNA-directed RNA polymerase subunit omega

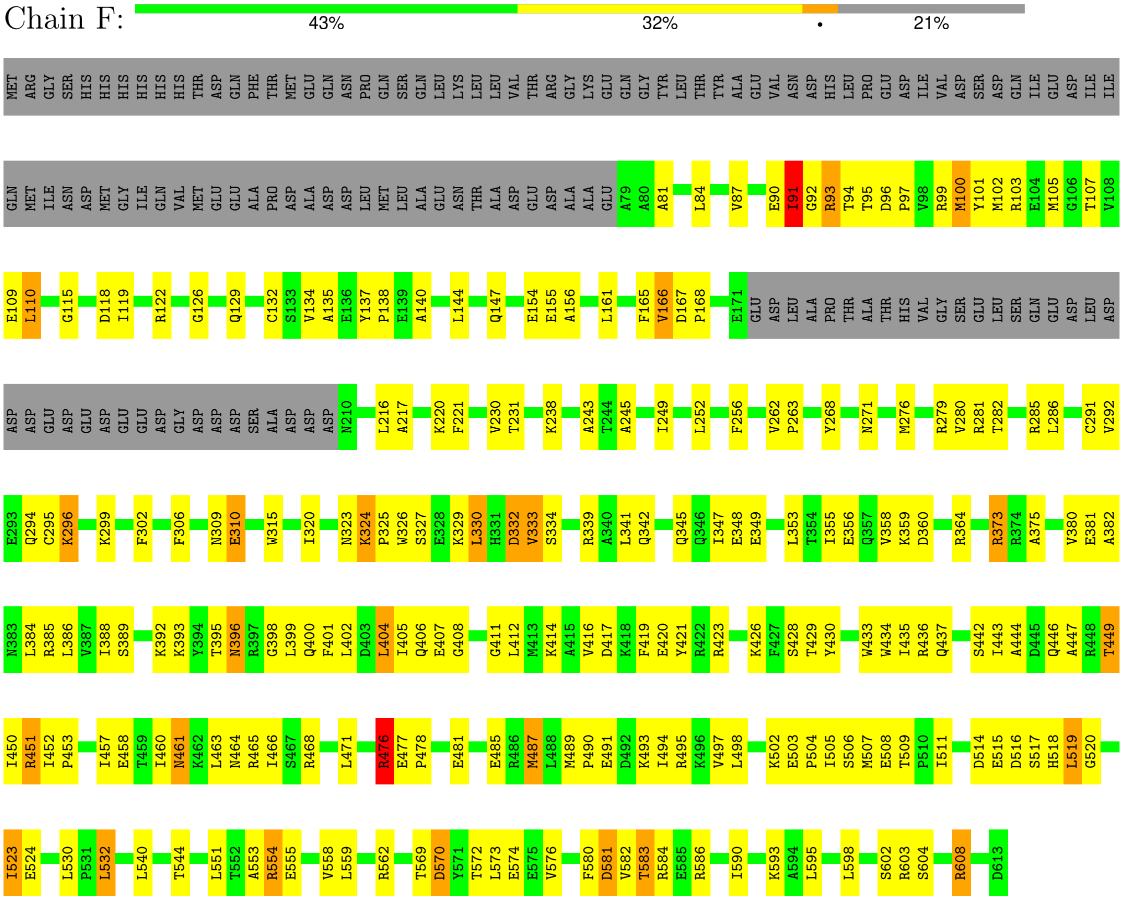
Chain Q:





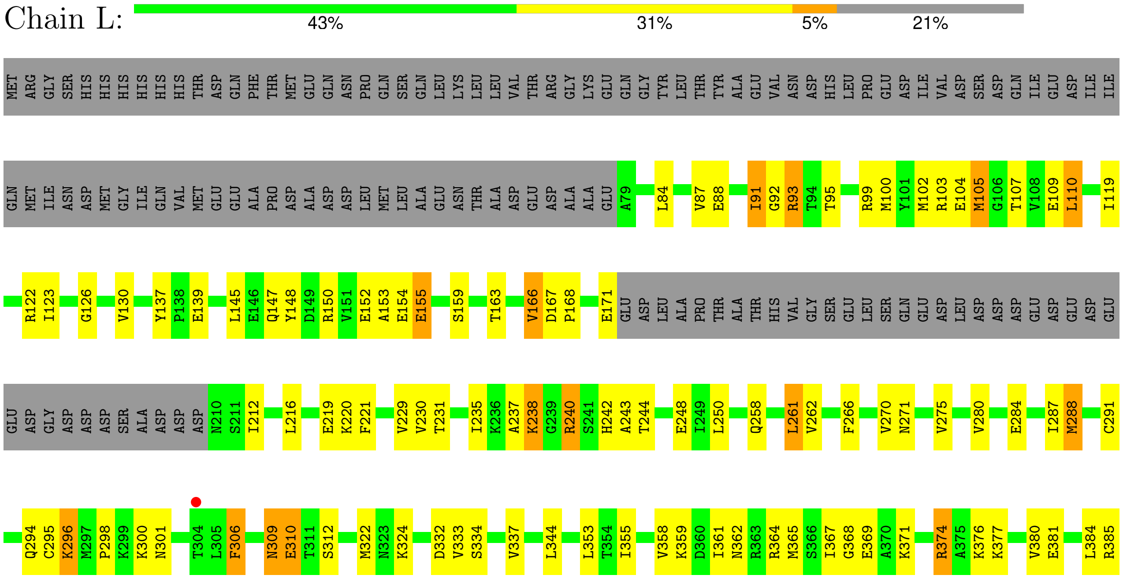
• Molecule 5: RNA polymerase sigma factor RpoD

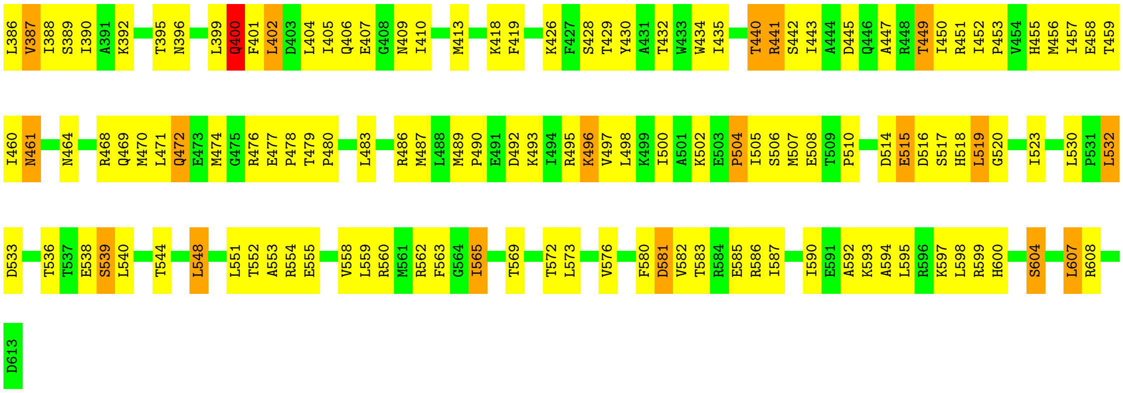
Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

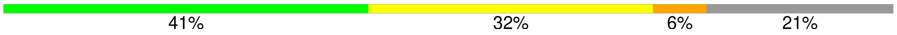
Chain L:

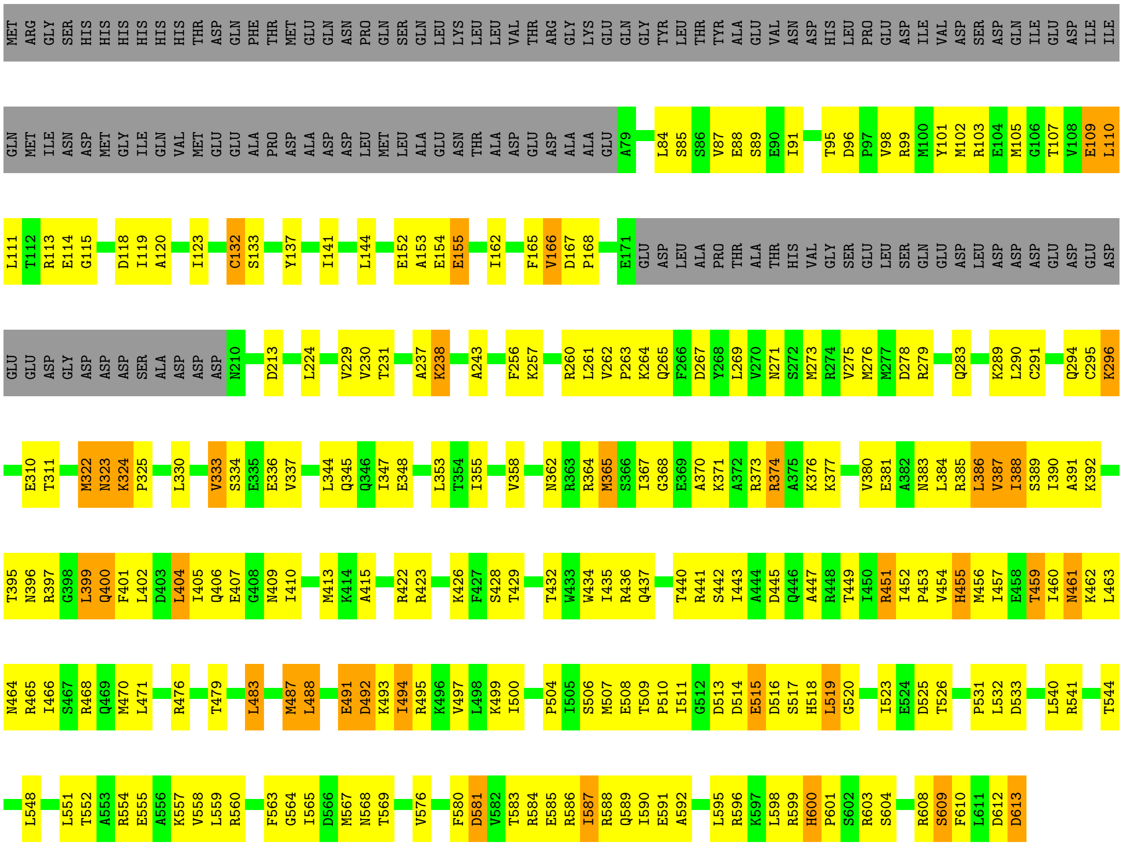




- Molecule 5: RNA polymerase sigma factor RpoD

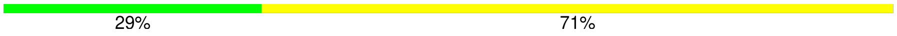
Chain R:

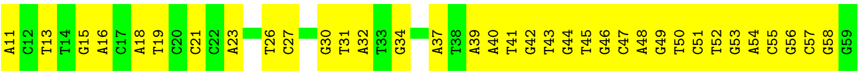




- Molecule 6: NT strand DNA (49-MER)

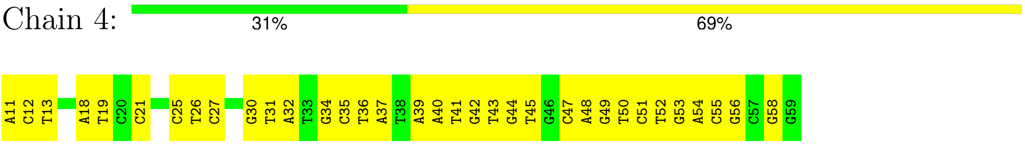
Chain 1:





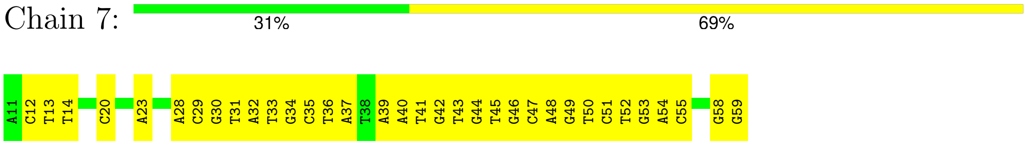
- Molecule 6: NT strand DNA (49-MER)

Chain 4:



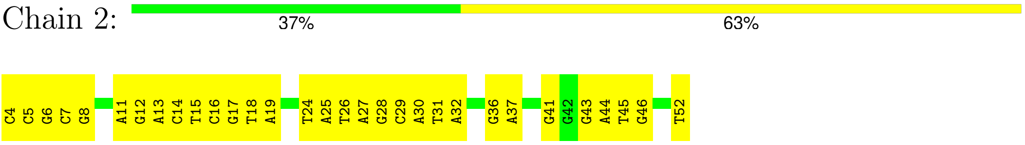
- Molecule 6: NT strand DNA (49-MER)

Chain 7:



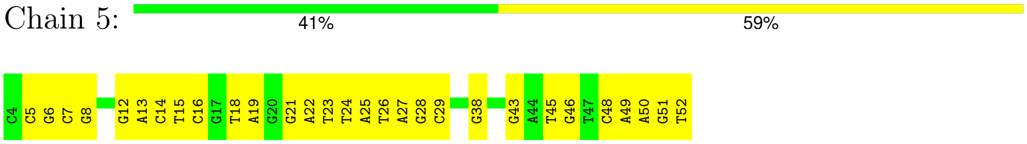
- Molecule 7: T strand DNA (49-MER)

Chain 2:



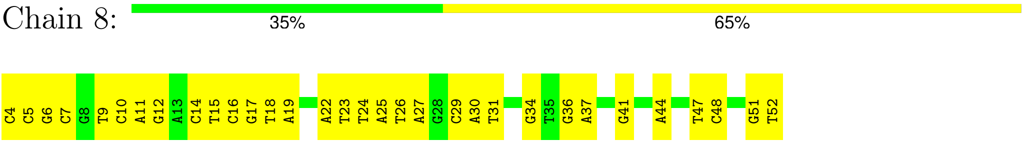
- Molecule 7: T strand DNA (49-MER)

Chain 5:



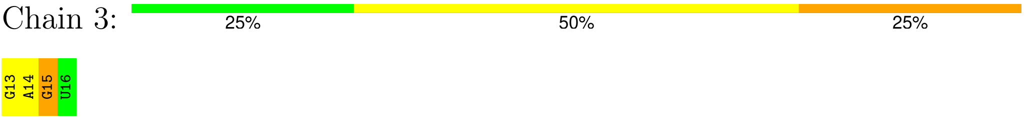
- Molecule 7: T strand DNA (49-MER)

Chain 8:



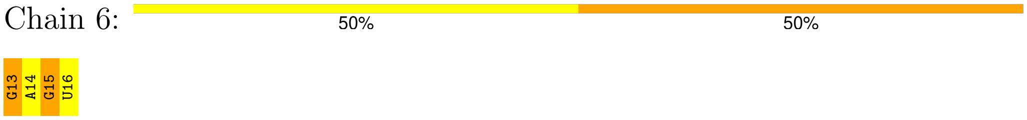
- Molecule 8: RNA (5'-D(*(GTP))-R(P*AP*GP*U)-3')

Chain 3:



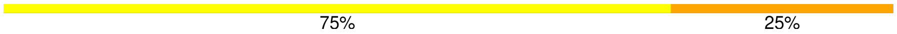
- Molecule 8: RNA (5'-D(*(GTP))-R(P*AP*GP*U)-3')

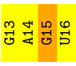
Chain 6:



- Molecule 8: RNA (5'-D(*(GTP))-R(P*AP*GP*U)-3')

Chain 9:




G13
A14
G15
U16

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	237.40Å 206.05Å 248.69Å 90.00° 116.55° 90.00°	Depositor
Resolution (Å)	39.90 – 5.50 39.90 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.90-5.50) 99.3 (39.90-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 5.37Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.245 , 0.328 0.245 , 0.327	Depositor DCC
R_{free} test set	3459 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	268.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 190.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	94608	wwPDB-VP
Average B, all atoms (Å^2)	219.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, GTP, 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	0.59	0/1809	0.84	1/2450 (0.0%)
1	B	0.54	0/1789	0.78	0/2425
1	G	0.56	0/1809	0.76	1/2450 (0.0%)
1	H	0.53	0/1789	0.76	0/2425
1	M	0.53	0/1809	0.74	0/2450
1	N	0.54	0/1789	0.79	2/2425 (0.1%)
2	C	0.54	0/10745	0.78	4/14499 (0.0%)
2	I	0.54	3/10745 (0.0%)	0.77	2/14499 (0.0%)
2	O	0.53	0/10745	0.75	3/14499 (0.0%)
3	D	0.54	0/10729	0.77	4/14487 (0.0%)
3	J	0.58	2/10729 (0.0%)	0.81	10/14487 (0.1%)
3	P	0.55	1/10729 (0.0%)	0.77	6/14487 (0.0%)
4	E	0.54	1/710 (0.1%)	0.72	0/956
4	K	0.53	0/710	0.73	0/956
4	Q	0.52	0/710	0.72	0/956
5	F	0.49	1/4076 (0.0%)	0.69	0/5482
5	L	0.51	0/4076	0.72	0/5482
5	R	0.55	2/4076 (0.0%)	0.74	1/5482 (0.0%)
6	1	0.41	0/1115	0.69	0/1718
6	4	0.33	0/1112	0.66	0/1706
6	7	0.37	0/1114	0.67	0/1714
7	2	0.37	0/1134	0.67	0/1744
7	5	0.35	0/1134	0.65	0/1744
7	8	0.38	0/1136	0.64	0/1752
8	3	0.44	0/72	0.62	0/110
8	6	0.40	0/72	0.61	0/110
8	9	0.36	0/72	0.59	0/110
All	All	0.53	10/96535 (0.0%)	0.76	34/131605 (0.0%)

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	D	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1340	LYS	CB-CG	6.65	1.70	1.52
2	I	626	GLU	CD-OE2	6.62	1.32	1.25
2	I	626	GLU	CD-OE1	5.92	1.32	1.25
5	R	109	GLU	CD-OE1	5.75	1.31	1.25
5	F	491	GLU	CB-CG	5.70	1.62	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	737	ILE	CB-CA-C	-7.98	95.64	111.60
3	J	803	VAL	CB-CA-C	-7.38	97.38	111.40
5	R	488	LEU	CA-CB-CG	7.32	132.12	115.30
3	D	737	ILE	CB-CA-C	-7.15	97.30	111.60
2	O	57	PHE	C-N-CD	-7.09	105.00	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	671	GLY	Peptide

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	1787	0	1813	220	0
1	B	1767	0	1789	175	0
1	G	1787	0	1812	173	0
1	H	1767	0	1789	149	0
1	M	1787	0	1813	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1767	0	1789	142	0
2	C	10576	0	10591	868	0
2	I	10576	0	10591	845	0
2	O	10576	0	10591	771	0
3	D	10568	0	10782	856	3
3	J	10568	0	10780	1069	2
3	P	10568	0	10780	901	0
4	E	708	0	719	42	0
4	K	708	0	719	48	0
4	Q	708	0	719	36	0
5	F	4022	0	4083	243	0
5	L	4022	0	4083	270	0
5	R	4022	0	4083	282	0
6	1	996	0	554	70	1
6	4	996	0	557	76	0
6	7	996	0	555	74	0
7	2	1012	0	556	62	0
7	5	1012	0	556	59	0
7	8	1012	0	554	64	0
8	3	97	0	44	7	0
8	6	97	0	44	8	0
8	9	97	0	44	4	0
9	D	2	0	0	0	0
9	J	2	0	0	2	0
9	P	2	0	0	0	0
10	6	1	0	0	0	0
10	D	1	0	0	0	0
10	P	1	0	0	0	0
All	All	94608	0	92790	6821	3

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 36.

The worst 5 of 6821 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:608:CYS:SG	3:D:617:THR:HG22	1.31	1.67
3:D:501:VAL:CG1	3:D:502:PRO:HD2	1.33	1.55
3:J:349:TYR:O	3:J:470:VAL:HG23	1.24	1.30
3:D:645:VAL:CG2	3:D:701:LEU:HD13	1.59	1.30
5:L:573:LEU:HB2	7:5:46:DG:OP2	1.15	1.28

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1169:THR:OG1	6:1:16:DA:OP1[2_657]	1.85	0.35
3:D:710:ASP:OD2	3:J:1282:TYR:OH[2_547]	1.93	0.27
3:D:710:ASP:CA	3:J:1302:TYR:OH[2_547]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	228/242 (94%)	214 (94%)	11 (5%)	3 (1%)	10	42
1	B	226/242 (93%)	204 (90%)	17 (8%)	5 (2%)	5	29
1	G	228/242 (94%)	209 (92%)	16 (7%)	3 (1%)	10	42
1	H	226/242 (93%)	207 (92%)	13 (6%)	6 (3%)	4	25
1	M	228/242 (94%)	214 (94%)	14 (6%)	0	100	100
1	N	226/242 (93%)	209 (92%)	14 (6%)	3 (1%)	10	42
2	C	1339/1342 (100%)	1218 (91%)	98 (7%)	23 (2%)	7	36
2	I	1339/1342 (100%)	1214 (91%)	105 (8%)	20 (2%)	8	39
2	O	1339/1342 (100%)	1234 (92%)	90 (7%)	15 (1%)	12	46
3	D	1360/1407 (97%)	1220 (90%)	109 (8%)	31 (2%)	5	28
3	J	1360/1407 (97%)	1227 (90%)	99 (7%)	34 (2%)	4	26
3	P	1360/1407 (97%)	1226 (90%)	99 (7%)	35 (3%)	4	25
4	E	88/90 (98%)	83 (94%)	5 (6%)	0	100	100
4	K	88/90 (98%)	84 (96%)	3 (3%)	1 (1%)	12	46
4	Q	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
5	F	493/628 (78%)	444 (90%)	27 (6%)	22 (4%)	2	17
5	L	493/628 (78%)	447 (91%)	28 (6%)	18 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	493/628 (78%)	449 (91%)	30 (6%)	14 (3%)	4	24
All	All	11202/11853 (94%)	10187 (91%)	782 (7%)	233 (2%)	5	29

5 of 233 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	ASP
1	B	118	ASP
2	C	110	PRO
2	C	214	ASN
2	C	247	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/208 (95%)	181 (91%)	17 (9%)	8	26
1	B	196/208 (94%)	172 (88%)	24 (12%)	4	16
1	G	198/208 (95%)	178 (90%)	20 (10%)	6	20
1	H	196/208 (94%)	174 (89%)	22 (11%)	5	17
1	M	198/208 (95%)	178 (90%)	20 (10%)	6	20
1	N	196/208 (94%)	176 (90%)	20 (10%)	6	20
2	C	1156/1157 (100%)	1042 (90%)	114 (10%)	6	21
2	I	1156/1157 (100%)	1052 (91%)	104 (9%)	8	24
2	O	1156/1157 (100%)	1050 (91%)	106 (9%)	7	24
3	D	1135/1168 (97%)	1026 (90%)	109 (10%)	7	22
3	J	1135/1168 (97%)	1014 (89%)	121 (11%)	5	19
3	P	1135/1168 (97%)	1017 (90%)	118 (10%)	5	20
4	E	74/74 (100%)	70 (95%)	4 (5%)	18	40
4	K	74/74 (100%)	67 (90%)	7 (10%)	7	22
4	Q	74/74 (100%)	66 (89%)	8 (11%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	439/554 (79%)	406 (92%)	33 (8%)	11	31
5	L	439/554 (79%)	394 (90%)	45 (10%)	6	20
5	R	439/554 (79%)	393 (90%)	46 (10%)	5	19
All	All	9594/10107 (95%)	8656 (90%)	938 (10%)	6	21

5 of 938 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	153	ASN
4	Q	19	LEU
4	K	65	ASP
3	P	1321	SER
3	P	442	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	113	HIS
5	R	383	ASN
3	P	294	ASN
3	P	736	GLN
1	G	66	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	2/4 (50%)	1 (50%)	0
8	6	3/4 (75%)	1 (33%)	1 (33%)
8	9	3/4 (75%)	1 (33%)	1 (33%)
All	All	8/12 (66%)	3 (37%)	2 (25%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	15	G
8	6	15	G
8	9	15	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	6	13	GTP
8	9	13	GTP

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	4	3
7	2	3
7	5	3
6	7	1
7	8	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	45:DT	O3’	46:DG	P	5.04
1	7	50:DT	O3’	51:DC	P	4.24
1	8	22:DA	O3’	23:DT	P	3.80
1	2	22:DA	O3’	23:DT	P	3.79
1	5	22:DA	O3’	23:DT	P	3.79

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/242 (95%)	-0.83	0	100	100	153, 175, 210, 235	0
1	B	228/242 (94%)	-0.77	1 (0%)	89	79	162, 194, 217, 238	0
1	G	230/242 (95%)	-0.69	0	100	100	157, 185, 216, 248	0
1	H	228/242 (94%)	-0.73	0	100	100	160, 191, 229, 261	0
1	M	230/242 (95%)	-0.77	0	100	100	166, 200, 233, 252	0
1	N	228/242 (94%)	-0.57	0	100	100	186, 233, 258, 273	0
2	C	1341/1342 (99%)	-0.74	2 (0%)	92	87	119, 186, 244, 277	0
2	I	1341/1342 (99%)	-0.76	0	100	100	130, 195, 278, 377	0
2	O	1341/1342 (99%)	-0.74	1 (0%)	92	87	144, 183, 235, 270	0
3	D	1362/1407 (96%)	-0.67	3 (0%)	92	84	128, 214, 296, 349	0
3	J	1362/1407 (96%)	-0.67	1 (0%)	92	87	132, 194, 280, 314	0
3	P	1362/1407 (96%)	-0.67	3 (0%)	92	84	148, 208, 292, 330	0
4	E	90/90 (100%)	-0.54	0	100	100	169, 206, 407, 461	0
4	K	90/90 (100%)	-0.58	0	100	100	144, 199, 394, 442	0
4	Q	90/90 (100%)	-0.70	0	100	100	167, 222, 416, 460	0
5	F	497/628 (79%)	-0.62	0	100	100	182, 294, 404, 418	0
5	L	497/628 (79%)	-0.59	1 (0%)	92	84	168, 262, 400, 406	0
5	R	497/628 (79%)	-0.61	0	100	100	172, 259, 413, 444	0
6	1	49/49 (100%)	-0.39	0	100	100	201, 272, 311, 317	0
6	4	49/49 (100%)	-0.35	0	100	100	209, 264, 308, 350	0
6	7	49/49 (100%)	-0.27	0	100	100	211, 255, 278, 300	0
7	2	49/49 (100%)	-0.38	0	100	100	210, 278, 312, 343	0
7	5	49/49 (100%)	-0.37	0	100	100	195, 270, 339, 341	0
7	8	49/49 (100%)	-0.35	0	100	100	194, 260, 296, 335	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
8	3	3/4 (75%)	-0.83	0	100	100	255, 255, 281, 321	0
8	6	3/4 (75%)	-0.73	0	100	100	263, 263, 272, 282	0
8	9	3/4 (75%)	-0.59	0	100	100	262, 262, 277, 295	0
All	All	11547/12159 (94%)	-0.69	12 (0%)	92	87	119, 203, 358, 461	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	282	LEU	5.4
3	D	772	TYR	4.8
5	L	304	THR	3.1
3	P	971	GLY	3.0
1	B	90	VAL	2.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MG	6	101	1/1	0.96	0.22	189,189,189,189	0
9	ZN	D	1502	1/1	0.99	0.02	212,212,212,212	0
9	ZN	J	1501	1/1	0.99	0.06	200,200,200,200	0
9	ZN	D	1501	1/1	0.99	0.04	228,228,228,228	0
10	MG	P	1503	1/1	0.99	0.03	194,194,194,194	0
9	ZN	P	1502	1/1	1.00	0.06	187,187,187,187	0
10	MG	D	1503	1/1	1.00	0.02	176,176,176,176	0
9	ZN	J	1502	1/1	1.00	0.06	174,174,174,174	0
9	ZN	P	1501	1/1	1.00	0.02	214,214,214,214	0

6.5 Other polymers ⓘ

There are no such residues in this entry.