wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 07:16 PM EDT

PDB ID	:	2BE5
Title	:	Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with inhibitor tagetitoxin
Authors	:	Vassylyev, D.G.; Svetlov, V.; Vassylyeva, M.N.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Artsimovitch, I.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-10-22
Resolution	:	2.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

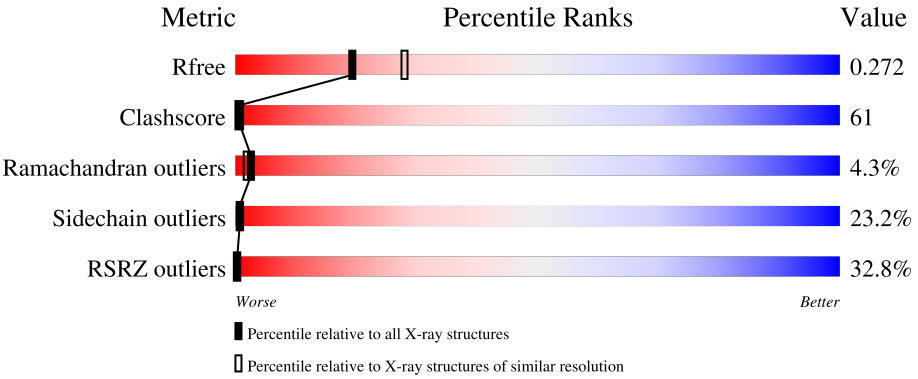
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	22% 14% 45% 12% • 27%
1	B	315	25% 18% 44% 10% • 27%
1	K	315	22% 18% 43% 11% • 27%
1	L	315	22% 15% 45% 12% 27%
2	C	1119	37% 23% 58% 18% •

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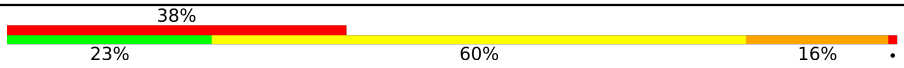
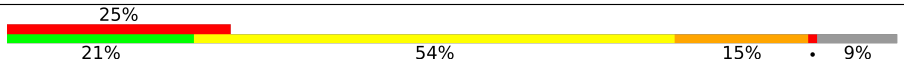
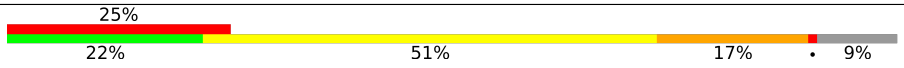
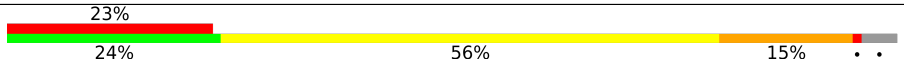
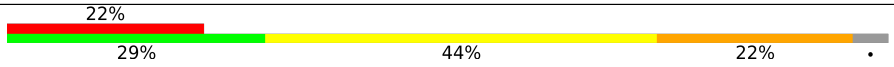
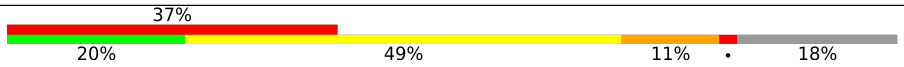
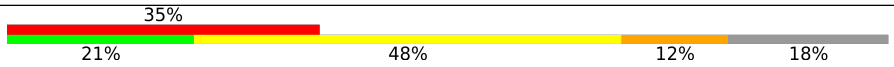
Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 61800 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 alpha chain.

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 beta chain.

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 beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	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			

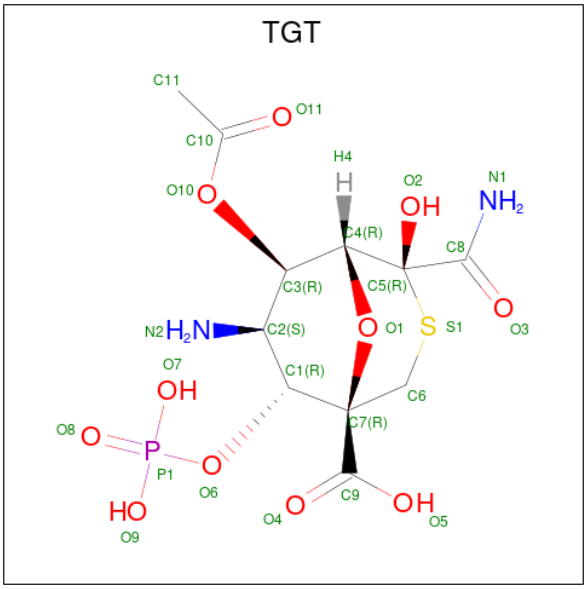
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	N	2	Total	Mg	0	0
			2	2		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is TAGETITOXIN (three-letter code: TGT) (formula: $C_{11}H_{17}N_2O_{11}PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total	C	N	O	P	S	0	0
			26	11	2	11	1	1		
8	N	1	Total	C	N	O	P	S	0	0
			26	11	2	11	1	1		

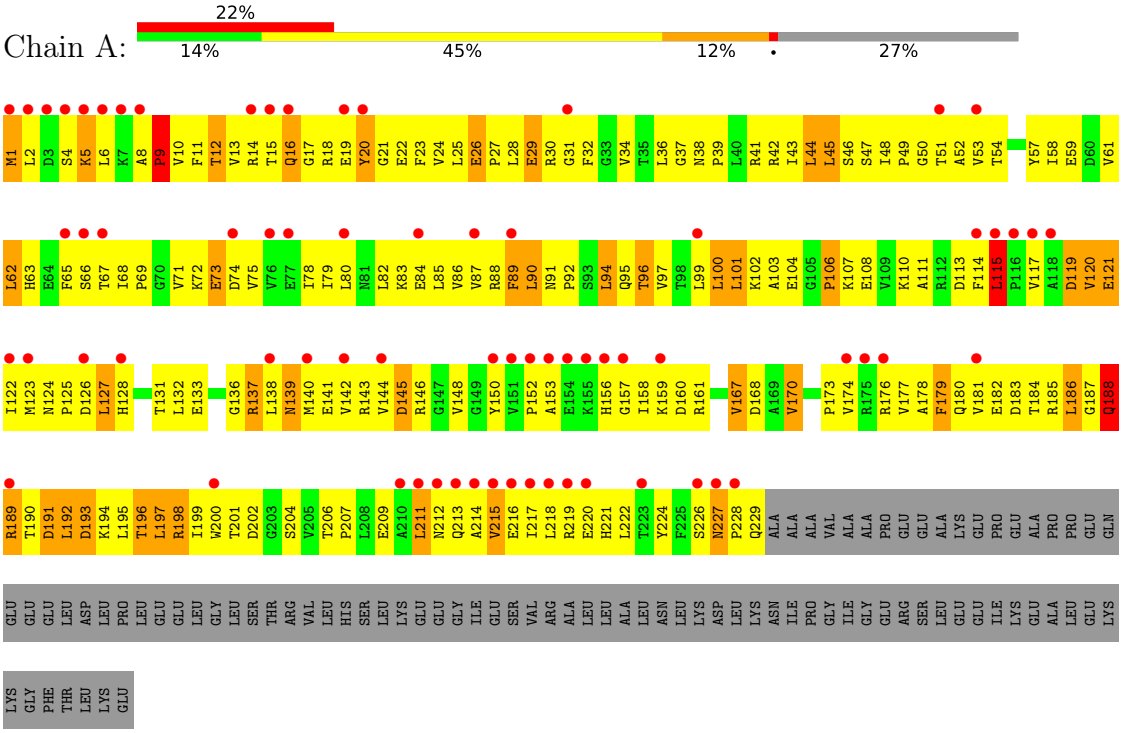
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	250	Total	O	0	0
			250	250		
9	B	329	Total	O	0	0
			329	329		
9	C	1321	Total	O	0	0
			1321	1321		
9	D	1655	Total	O	0	0
			1655	1655		
9	E	176	Total	O	0	0
			176	176		
9	F	519	Total	O	0	0
			519	519		
9	K	278	Total	O	0	0
			278	278		
9	L	309	Total	O	0	0
			309	309		
9	M	1236	Total	O	0	0
			1236	1236		
9	N	1552	Total	O	0	0
			1552	1552		
9	O	137	Total	O	0	0
			137	137		
9	P	422	Total	O	0	0
			422	422		

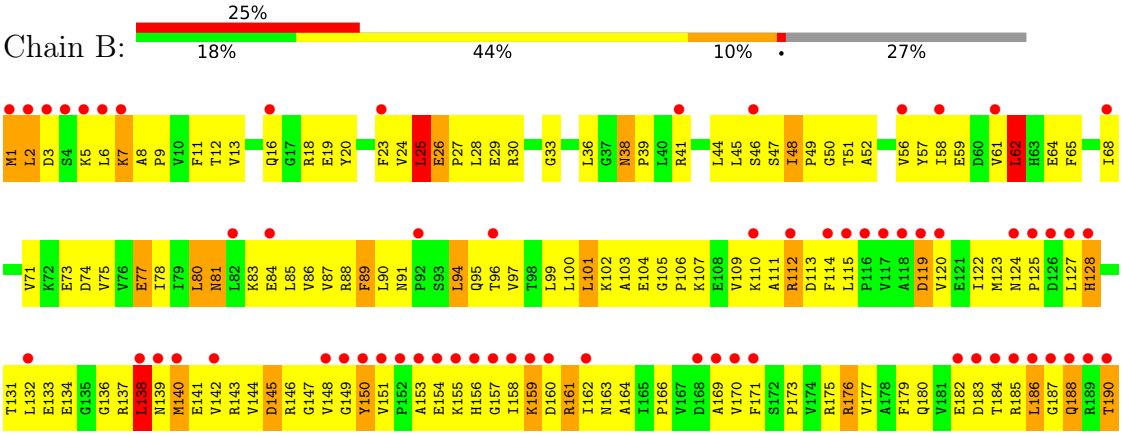
3 Residue-property plots (i)

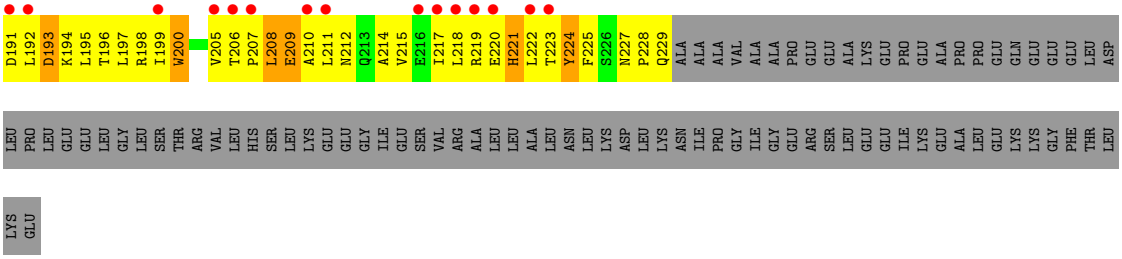
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 alpha chain

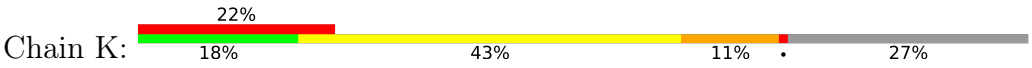


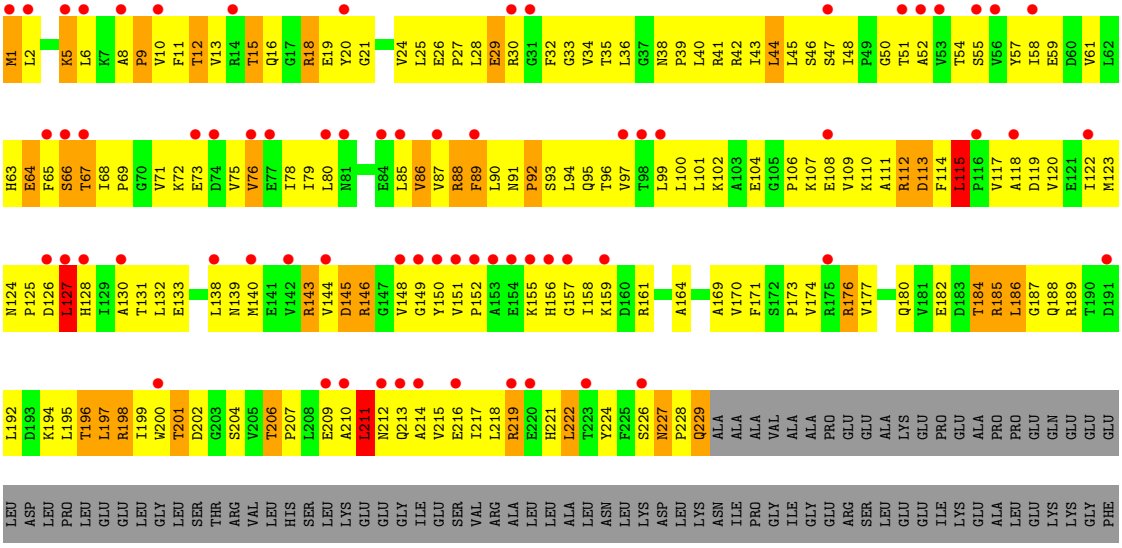
• Molecule 1: DNA-directed RNA polymerase alpha chain



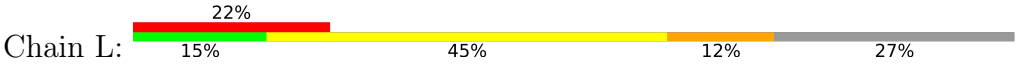


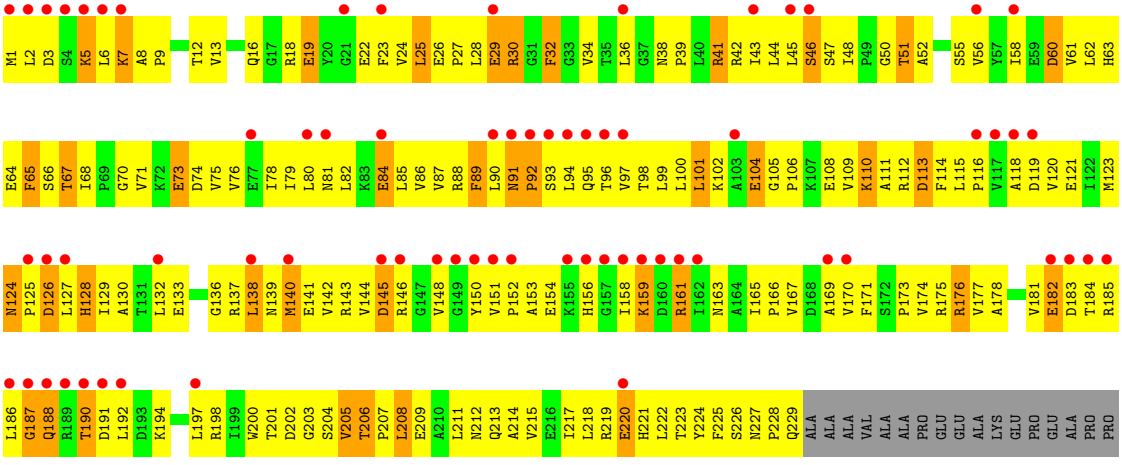
• Molecule 1: DNA-directed RNA polymerase alpha chain

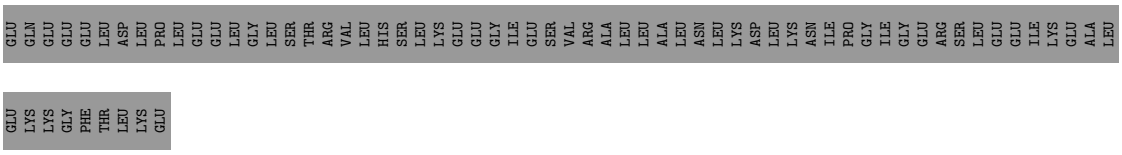




• Molecule 1: DNA-directed RNA polymerase alpha chain

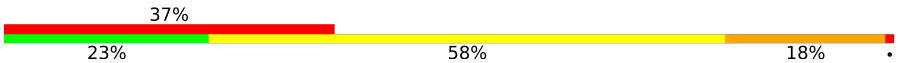


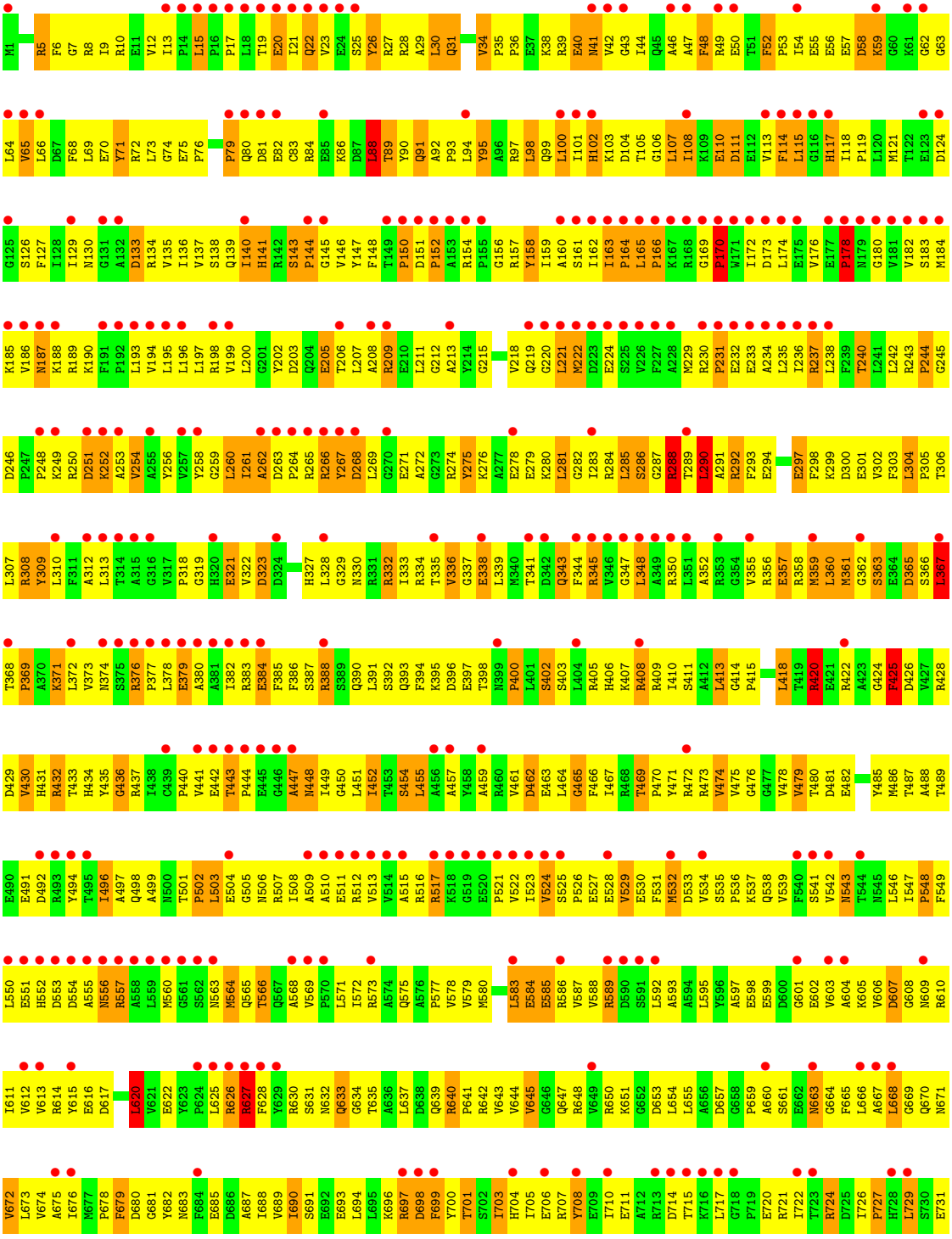


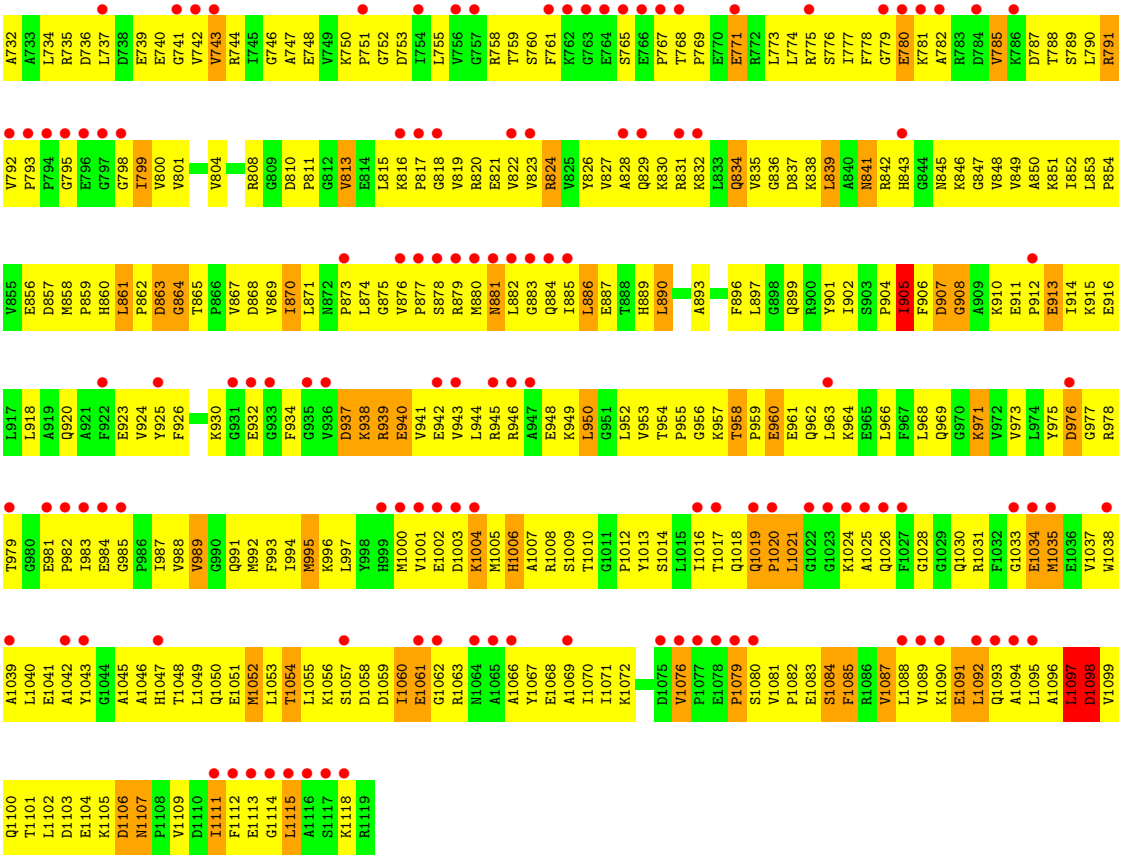


• Molecule 2: DNA-directed RNA polymerase beta chain

Chain C:

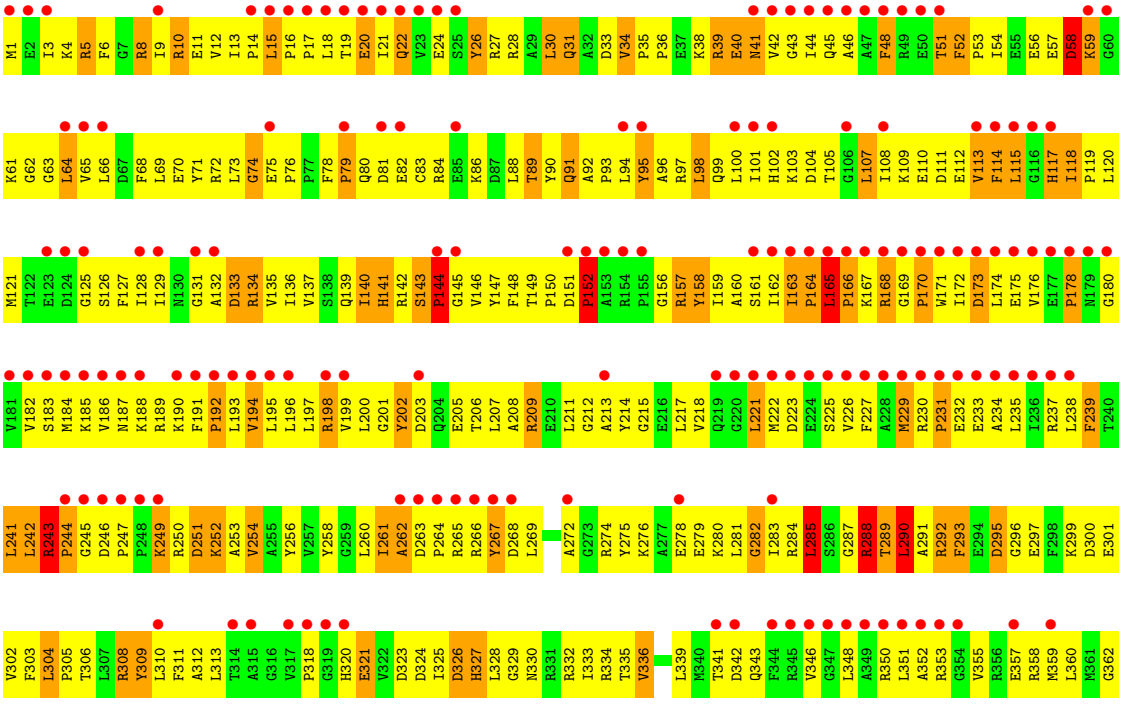


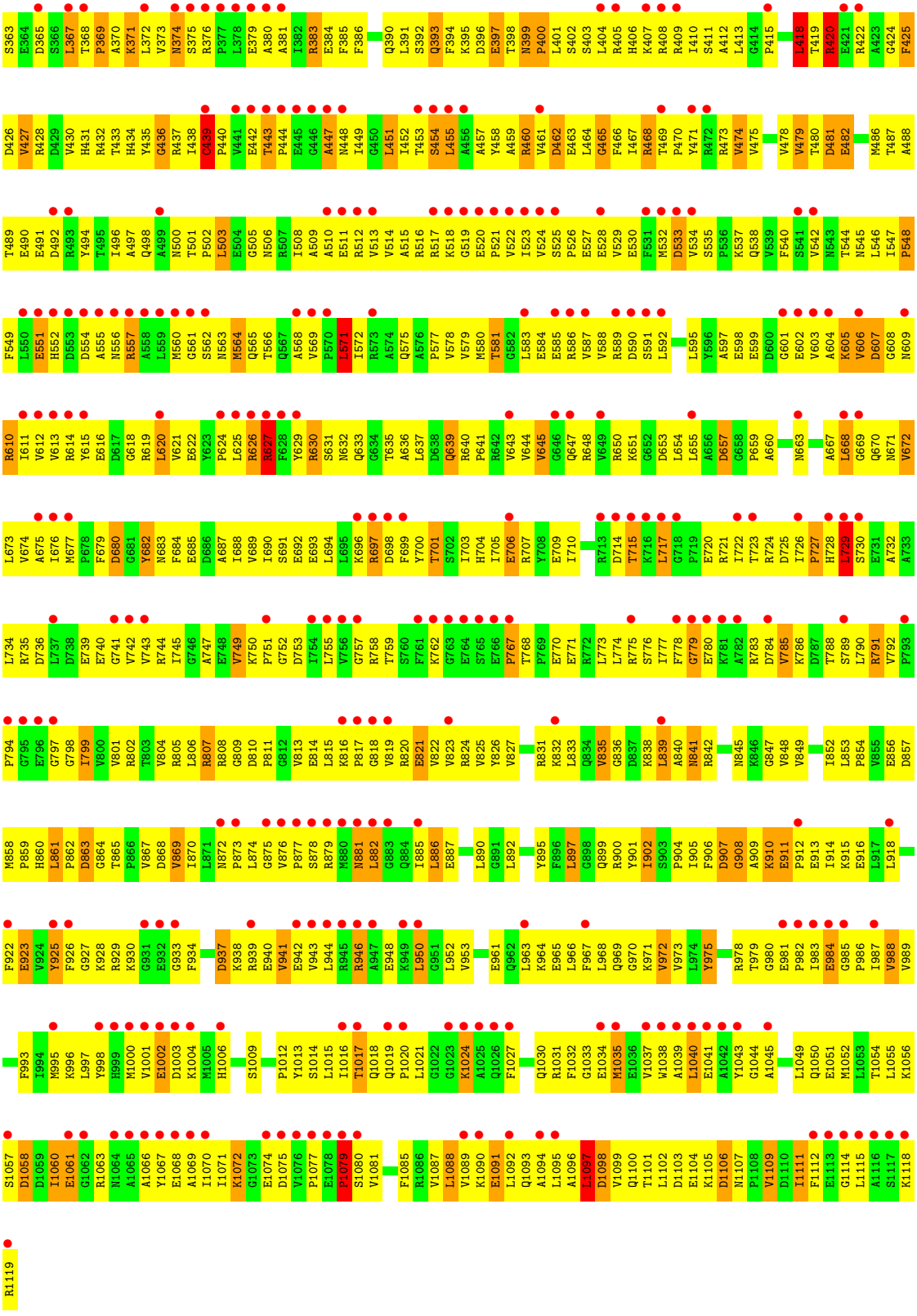




• Molecule 2: DNA-directed RNA polymerase beta chain

Chain M:





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

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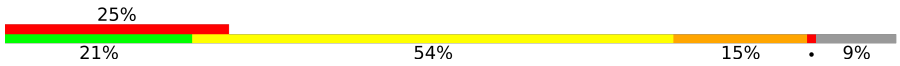

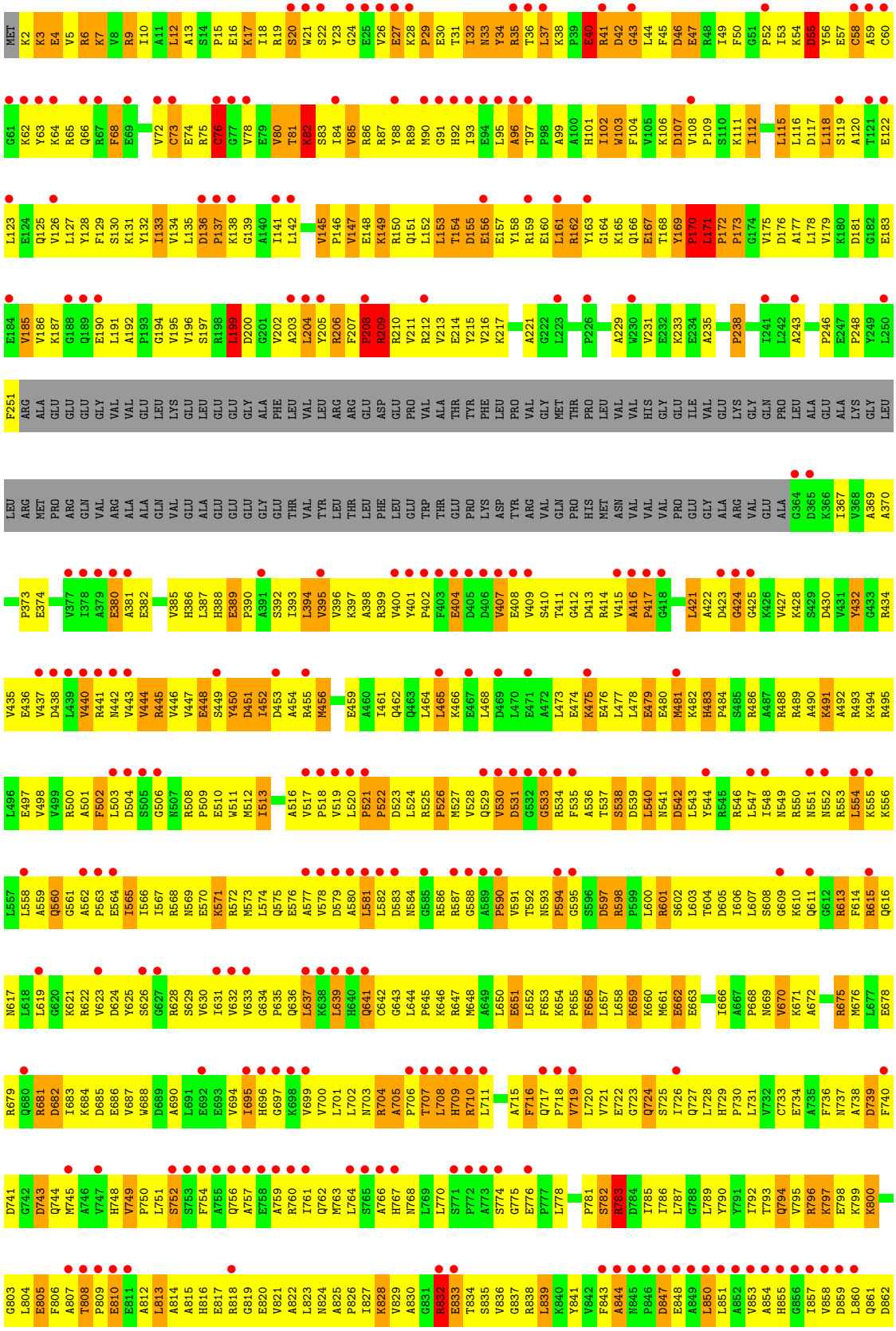
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G61 K62 Y63 K64 R65 Q66 R67 F68 E69 V72 C73 E74 R75 C76 G77 V78 E79 V80 T81 K82 S83 I84 V85 R86 R87 Y88 R89 M90 G91 H92 I93 E94 L95 A96 T97 P98 A99 A100 H101 I102 W103 F104 V105 K106 D107 V108 P109 S110 K111 I112 L115 L116 D117 L118 S119 A120 T121 E122
L123 E124 Q125 V126 L127 Y128 F129 S130 K131 Y132 I133 V134 L135 D136 P137 K138 G139 A140 I141 L142 V145 P146 V147 E148 K149 R150 Q151 L152 L153 T154 D155 E156 E157 Y158 R159 E160 L161 R162 Y163 G164 K165 Q166 E167 T168 Y169 P170 L171 P172 P173 G174 V175 D176 A177 L178 V179 K180 D181 G182 E183
E184 V185 V186 K187 G188 Q189 E190 L191 A192 P193 G194 V195 V196 S197 R198 L199 D200 G201 V202 A203 L204 Y205 R206 F207 P208 R209 R210 V211 R212 V213 E214 Y215 V216 K217 A221 G222 L223 P226 A229 W230 V231 E232 K233 E234 A235 P238 I241 L242 A243 P246 E247 P248 Y249 L250
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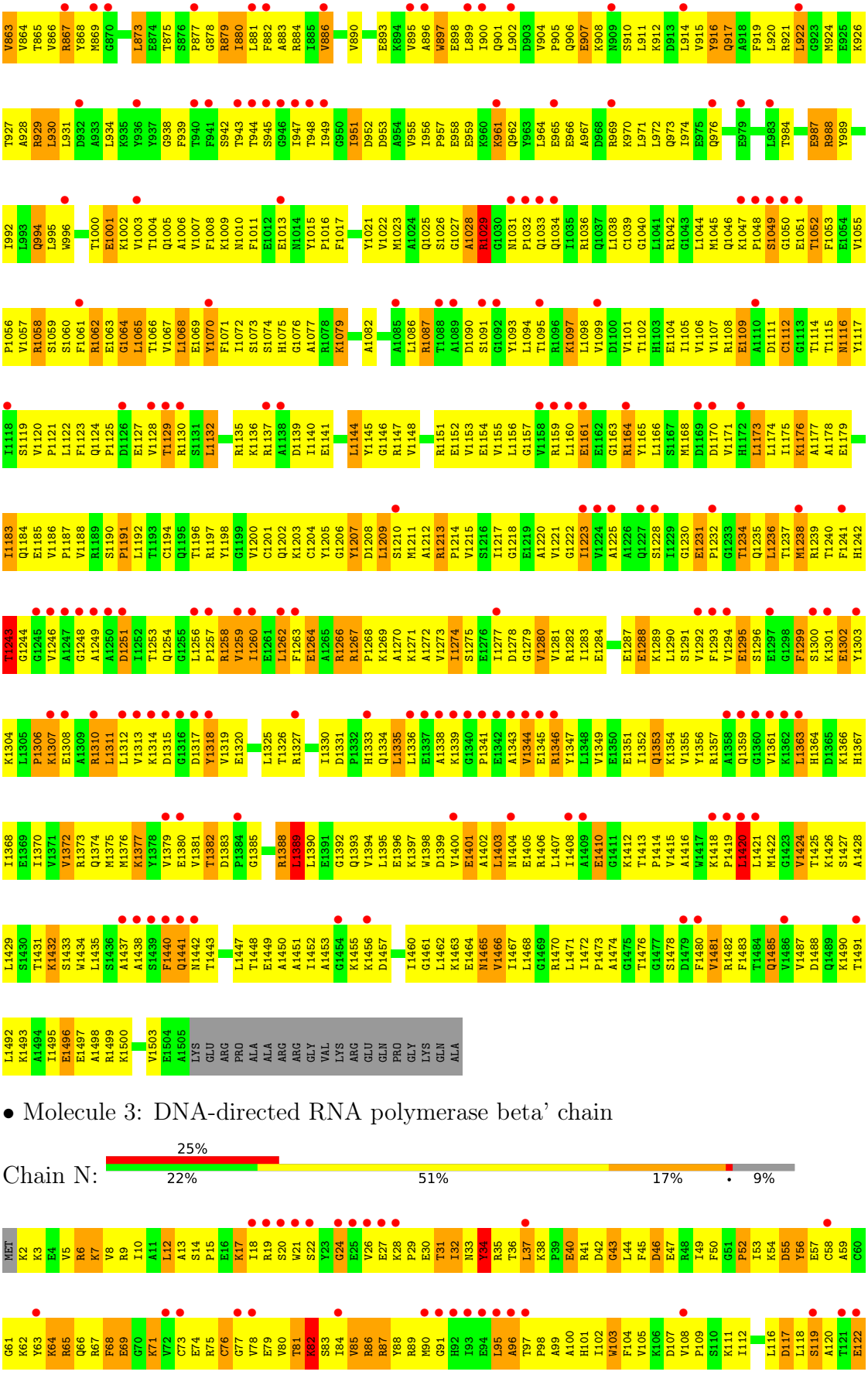
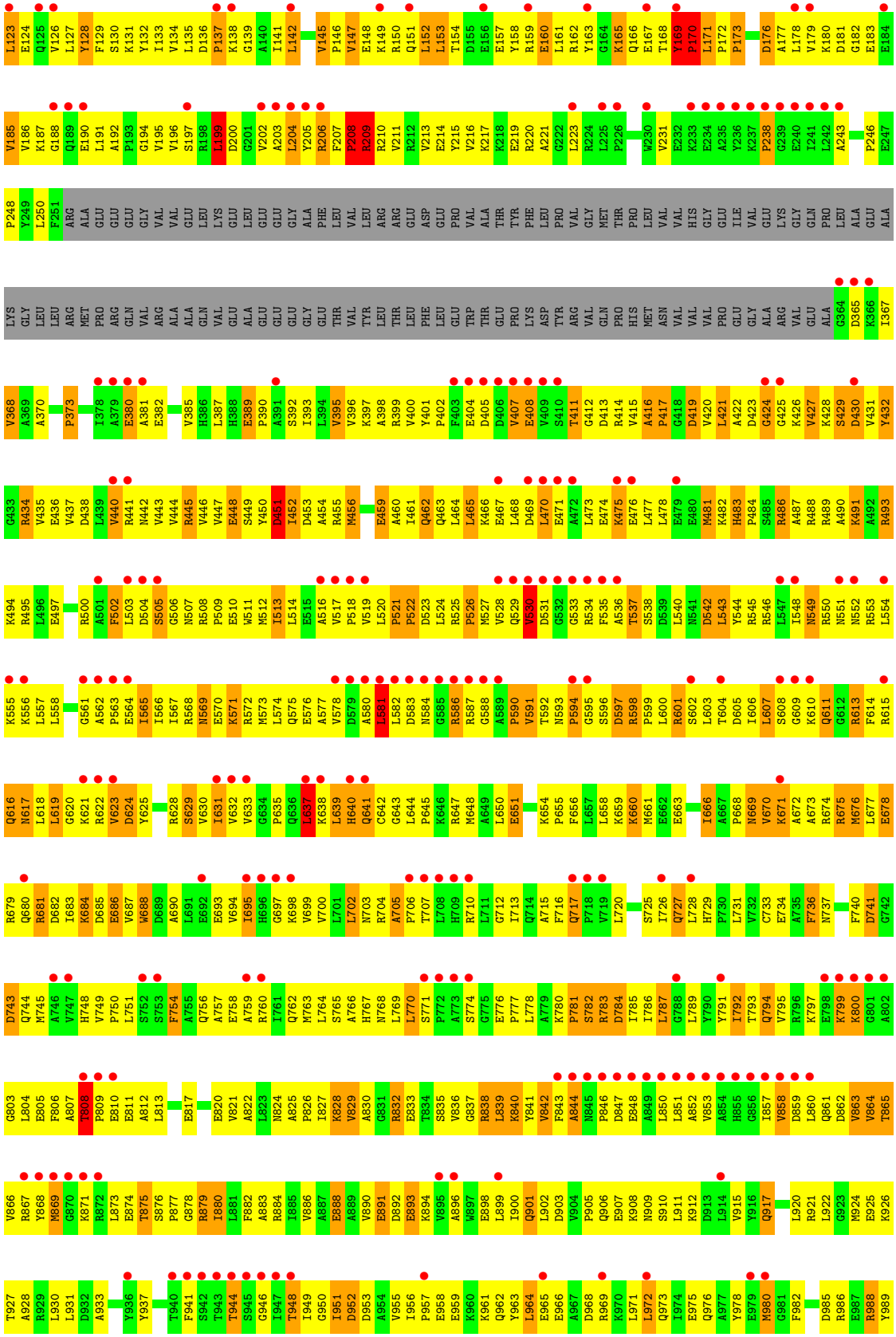
R679 Q680 R681 D682 I683 K684 D685 E686 V687 W688 D689 A690 L691 E692 E693 V694 I695 H696 G697 K698 V699 V700 L701 L702 N703 R704 A705 P706 T707 L708 H709 R710 L711 A715 F716 Q717 P718 V719 L720 V721 E722 G723 Q724 S725 I726 Q727 L728 H729 P730 L731 V732 C733 E734 A735 F736 N737 A738 D739 F740
D741 G742 D743 Q744 M745 A746 V747 H748 V749 P750 L751 S752 S753 F754 A755 Q756 A757 E758 A759 R760 I761 Q762 M763 L764 S765 A766 H767 N768 L769 L770 S771 P772 A773 S774 G775 E776 P777 L778 P781 S782 R783 D784 I785 I786 L787 G788 L789 Y790 Y791 I792 T793 Q794 V795 R796 K797 E798 K799 K800
G803 L804 E805 F806 A807 T808 P809 E810 E811 A812 L813 A814 A815 H816 E817 R818 G819 E820 V821 A822 L823 N824 A825 P826 I827 K828 V829 A830 G831 R832 E833 T834 S835 V836 G837 R838 L839 K840 Y841 V842 F843 A844 N845 P846 D847 E848 A849 L850 L851 A852 V853 A854 H855 G856 I857 V858 D859 L860 Q861 D862



• Molecule 3: DNA-directed RNA polymerase beta' chain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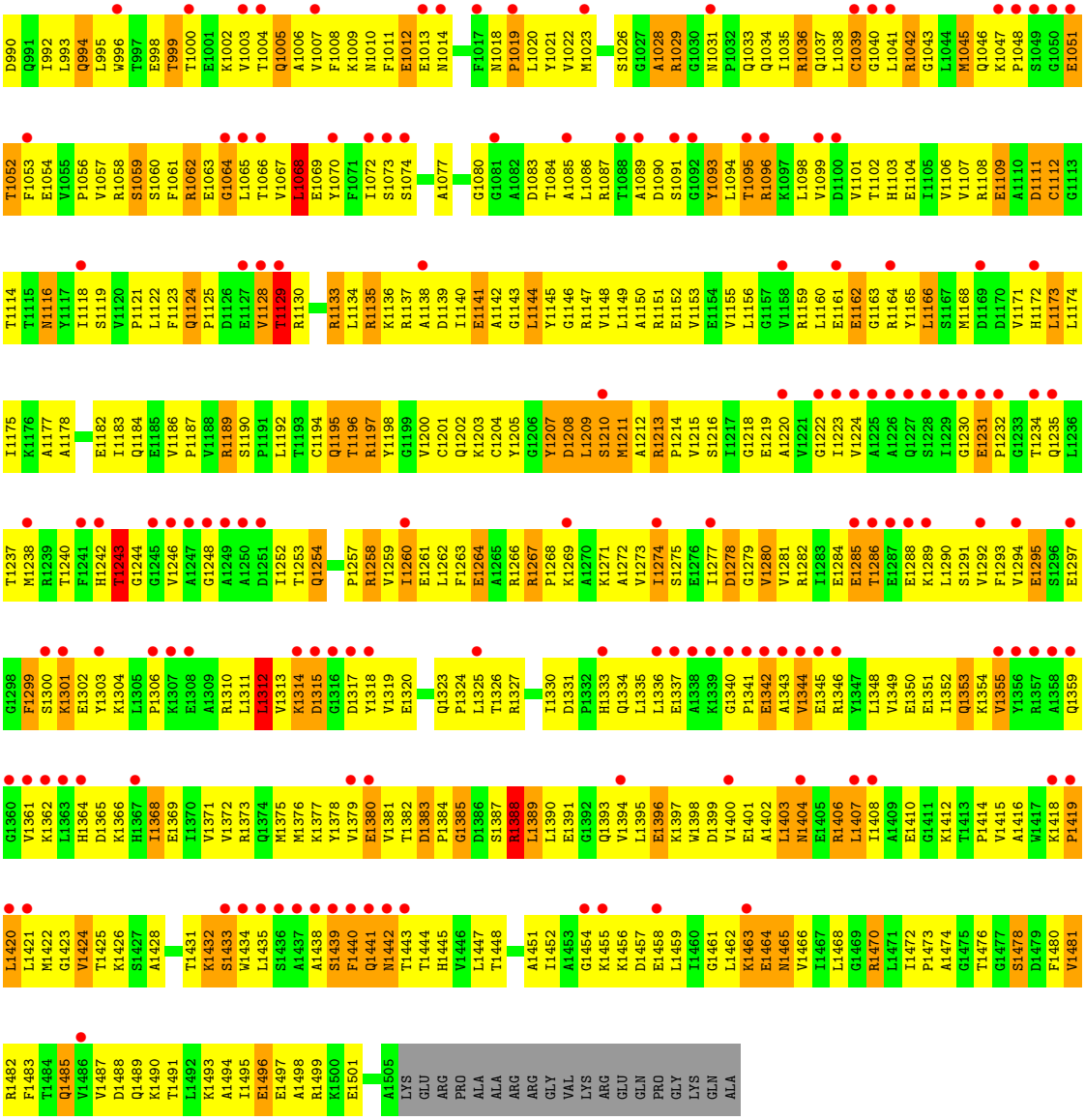
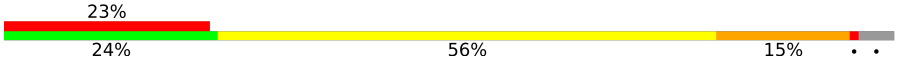
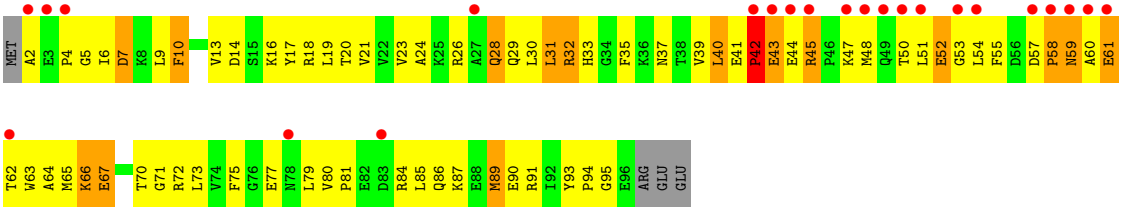
V186 V186 K187 G188 Q189 E190 L191 A192 P193 G194 V195 V196 S197 R198 L199 D200 G201 V202 A203 L204 Y205 R206 F207 P208 R209 R210 V211 R212 V213 E214 Y215 V216 K217 K218 E219 R220 A221 G222 L223 R224 L225 P226 W230 V231 E232 K233 E234 A235 Y236 K237 P238 G239 E240 I241 L242 A243 P246 E247
P248 Y249 L250 F251 ARG ALA GLU GLU GLU GLY VAL VAL GLU LEU LYS GLU LEU GLU GLU GLU ALA PHE LEU VAL LEU ARG ARG GLU ASP GLU PRO VAL ALA THR TYR PHE LEU PRO VAL GLY MET THR PRO LEU VAL VAL HIS GLY GLU ILE VAL GLU LYS GLY GLN PRO LEU ALA GLU ALA
LYS GLY LEU LEU ARG MET PRO ARG GLN VAL ARG ALA ALA GLN VAL GLU ALA GLU GLU GLU GLY GLU THR VAL TYR LEU THR LEU PHE LEU GLU TRP THR GLU PRO LYS ASP TYR ARG VAL GLN PRO HIS MET ASN VAL VAL VAL PRO GLU GLY ALA ARG VAL GLU ALA G364 D365 K366 I367
V368 A369 A370 P373 I378 A379 E380 A381 E382 V385 H386 L387 H388 E389 P390 A391 S392 I393 L394 V395 V396 K397 A398 R399 V400 Q401 P402 F403 E404 D405 D406 V407 E408 V409 S410 T411 G412 D413 R414 V415 A416 P417 G418 D419 V420 L421 A422 D423 G424 G425 K426 V427 K428 S429 D430 V431 Y432
G433 R434 V435 E436 V437 D438 L439 V440 R441 N442 V443 V444 R445 V446 V447 E448 S449 Y450 D451 I452 D453 A454 R455 M456 E459 A460 I461 Q462 Q463 L464 L465 K466 E467 L468 D469 L470 E471 A472 L473 E474 K475 E476 L477 L478 E479 E480 M481 K482 H483 P484 S485 R486 A487 R488 R489 A490 K491 A492 R493
K494 R495 L496 E497 R500 A501 F502 L503 D504 S505 G506 N507 R508 P509 E510 W511 M512 I513 L514 E515 A516 V517 P518 V519 L520 P521 P522 D523 L524 R525 P526 M527 V528 Q529 V530 D531 G532 G533 R534 F535 A536 T537 S538 D539 L540 N541 D542 L543 Y544 R545 R546 L547 I548 N549 R550 N551 N552 R553 L554
K555 K556 L557 L558 G561 A562 P563 E564 I565 I566 I567 R568 N569 E570 K571 R572 M573 L574 Q575 E576 A577 V578 D579 A580 L581 L582 D583 N584 G585 R586 R587 G588 A589 P590 V591 T592 N593 P594 G595 S596 D597 R598 P599 L600 R601 S602 L603 T604 D605 I606 L607 S608 G609 K610 Q611 G612 R613 F614 R615
Q616 N617 L618 L619 G620 K621 R622 V623 D624 Y625 R628 S629 V630 I631 V632 V633 G634 P635 Q636 L637 K638 L639 H640 Q641 C642 G643 L644 P645 K646 R647 M648 A649 L650 E651 K654 P655 F656 L657 L658 K659 K660 M661 E662 E663 I666 A667 P668 N669 V670 K671 A672 A673 R674 R675 M676 L677 E678
R679 Q680 R681 D682 I683 K684 D685 E686 V687 W688 D689 A690 L691 E692 E693 V694 I695 H696 G697 K698 V699 V700 L701 L702 N703 R704 A705 P706 T707 L708 H709 R710 L711 G712 I713 Q714 A715 F716 Q717 P718 V719 L720 S725 I726 Q727 L728 H729 P730 L731 V732 C733 E734 A735 F736 N737 F740 D741 G742
D743 Q744 M745 A746 V747 H748 V749 P750 L751 S752 S753 F754 A755 Q756 A757 E758 A759 R760 I761 Q762 M763 L764 S765 A766 H767 N768 L769 L770 S771 P772 A773 S774 G775 E776 P777 L778 A779 K780 P781 S782 R783 D784 I785 I786 L787 G788 L789 V790 Y791 I792 T793 Q794 V795 R796 K797 E798 K799 K800 G801 A802
G803 L804 E805 F806 A807 T808 P809 E810 E811 A812 L813 E817 E820 V821 A822 L823 N824 A825 P826 I827 K828 V829 A830 G831 R832 E833 T834 S835 V836 G837 R838 L839 K840 Y841 V842 F843 A844 N845 P846 D847 E848 A849 L850 L851 A852 V853 A854 H855 G856 I857 V858 D859 L860 Q861 D862 V863 V864 T865
V866 R867 Y868 M869 G870 K871 R872 L873 E874 T875 S876 P877 G878 R879 I880 L881 F882 A883 R884 I885 V886 A887 E888 A889 V890 E891 D892 E893 K894 V895 A896 W897 E898 L899 I900 Q901 L902 D903 V904 P905 Q906 E907 K908 N909 S910 L911 K912 D913 L914 V915 Y916 Q917 L920 R921 L922 G923 M924 E925 K926
T927 A928 R929 L930 L931 D932 A933 Y936 Y937 T940 F941 S942 T943 T944 S945 G946 I947 T948 I949 G950 I951 D952 D953 A954 V955 I956 P957 E958 E959 K960 K961 Q962 Y963 L964 E965 E966 A967 D968 R969 K970 L971 L972 Q973 I974 E975 Q976 A977 Y978 E979 M980 G981 F982 D985 R986 E987 R988 Y989



• Molecule 4: RNA polymerase omega chain

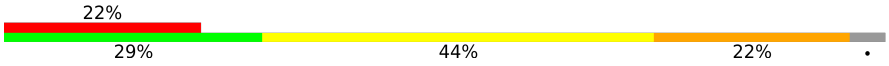
Chain E:

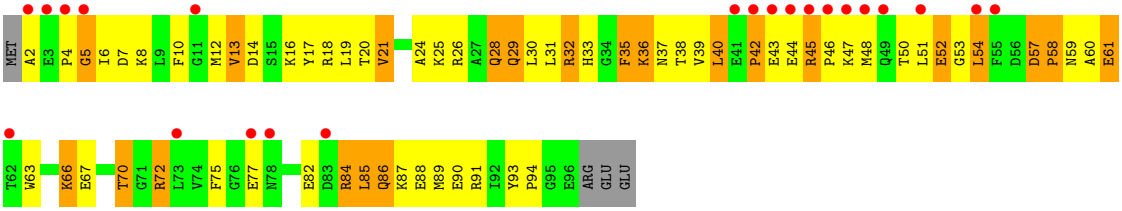




• Molecule 4: RNA polymerase omega chain

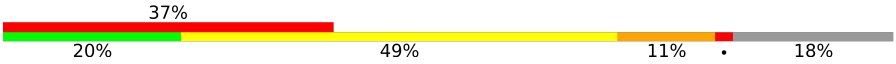
Chain O:

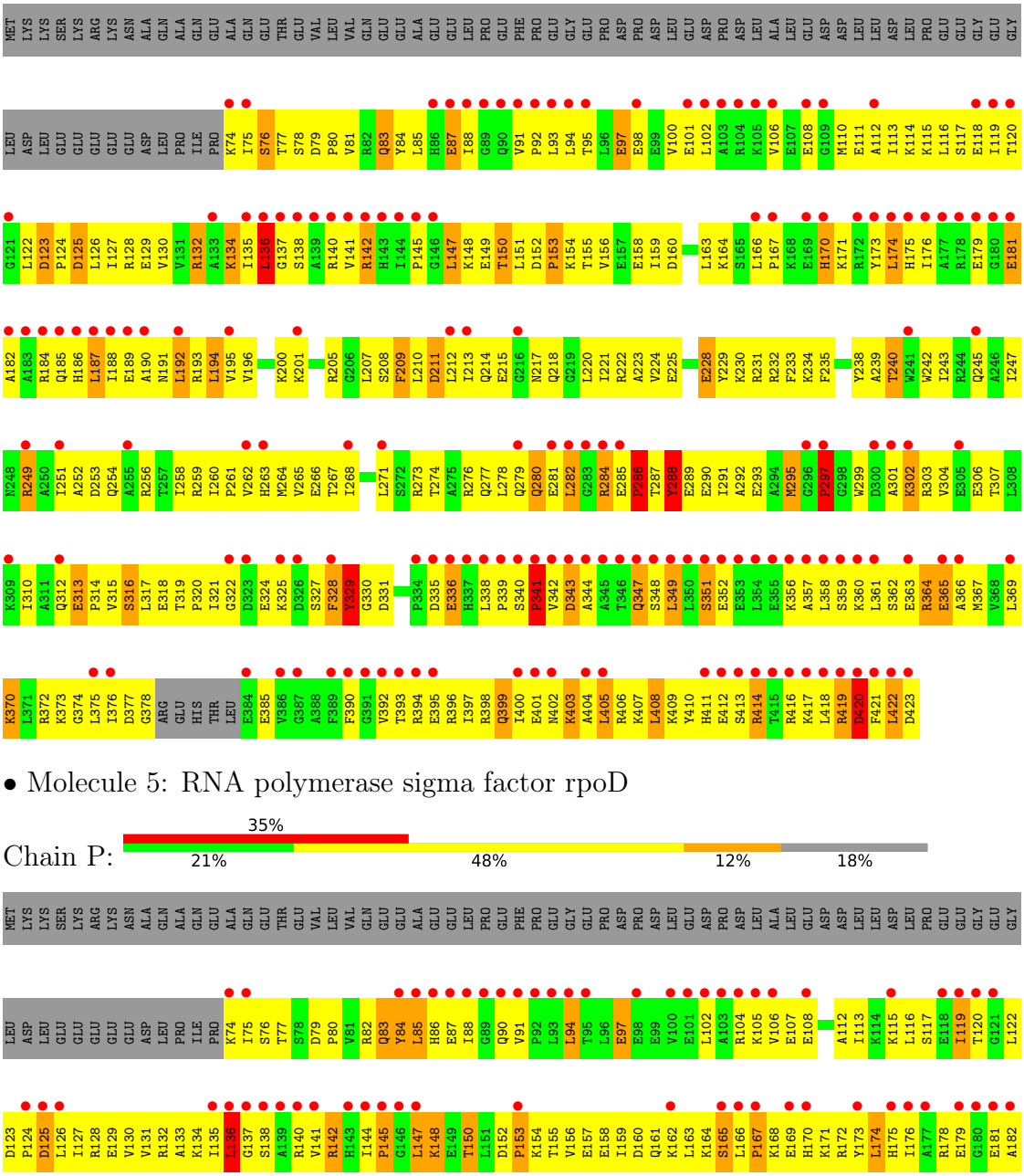




• Molecule 5: RNA polymerase sigma factor rpoD

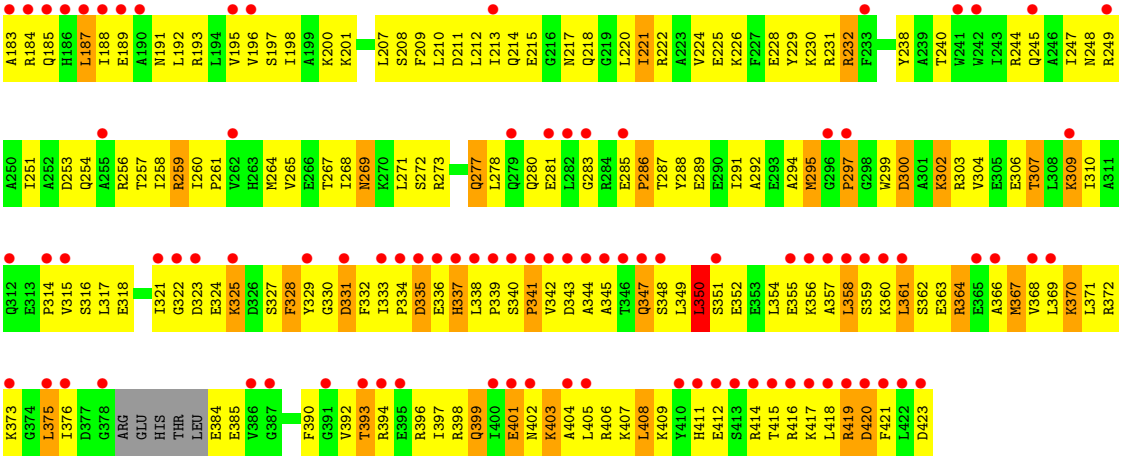
Chain F:





• Molecule 5: RNA polymerase sigma factor rpoD

Chain P: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A250 I251 A252 D253 Q254 A255 R256 T257 I258 R259 I260 P261 V262 H263 M264 V265 E266 T267 I268 N269 K270 L271 S272 R273 Q277 L278 Q279 Q280 E281 L282 G283 R284 E285 P286 T287 Y288 E289 E290 I291 A292 E293 A294 M295 G296 P297 G298 W299 D300 A301 K302 R303 V304 E305 E306 T307 L308 K309 I310 A311
Q312 E313 P314 V315 S316 L317 E318 I321 G322 D323 E324 K325 D326 S327 F328 Y329 G330 D331 F332 I333 P334 D335 E336 H337 L338 P339 S340 P341 V342 D343 A344 A345 T346 Q347 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 V386 G387 F390 G391 V392 T393 R394 E395 R396 I397 R398 Q399 I400 E401 N402 K403 A404 L405 R406 K407 L408 K409 Y410 H411 E412 S413 R414 T415 R416 K417 L418 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	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 36.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 95.2 (36.81-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.65 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.274 0.235 , 0.272	Depositor DCC
R_{free} test set	34795 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.065 for h,-h-k,-l 0.065 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for -h,-k,l	Depositor
Outliers	0 of 604645 reflections	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	61800	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: TGT, 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	0.77	0/1838	0.86	3/2498 (0.1%)
1	B	0.70	0/1838	0.83	4/2498 (0.2%)
1	K	0.76	0/1838	0.85	4/2498 (0.2%)
1	L	0.73	0/1838	0.76	0/2498
2	C	0.81	0/8997	0.89	8/12164 (0.1%)
2	M	0.80	2/8997 (0.0%)	0.89	12/12164 (0.1%)
3	D	0.82	0/10975	0.92	21/14836 (0.1%)
3	N	0.80	1/10975 (0.0%)	0.92	17/14836 (0.1%)
4	E	0.80	0/783	0.94	0/1054
4	O	0.81	0/783	0.92	0/1054
5	F	0.71	0/2812	0.81	1/3781 (0.0%)
5	P	0.72	0/2812	0.78	2/3781 (0.1%)
All	All	0.79	3/54486 (0.0%)	0.89	72/73662 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	733	CYS	CB-SG	-5.54	1.72	1.81
2	M	202	TYR	CD2-CE2	5.05	1.47	1.39
2	M	682	TYR	CD2-CE2	5.02	1.46	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	LEU	CA-CB-CG	10.11	138.56	115.30
3	N	199	LEU	CA-CB-CG	-8.78	95.11	115.30
2	M	557	ARG	NE-CZ-NH2	7.73	124.17	120.30
3	D	199	LEU	CA-CB-CG	-7.64	97.72	115.30
3	N	1389	LEU	CA-CB-CG	7.54	132.65	115.30

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	1806	0	1861	232	0
1	B	1806	0	1861	217	0
1	K	1806	0	1861	195	0
1	L	1806	0	1861	216	0
2	C	8829	0	8933	1248	0
2	M	8829	0	8933	1139	0
3	D	10797	0	10873	1481	0
3	N	10797	0	10873	1398	0
4	E	769	0	775	101	0
4	O	769	0	775	98	0
5	F	2771	0	2844	350	0
5	P	2771	0	2844	345	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	N	2	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	D	26	0	15	3	0
8	N	26	0	14	1	0
9	A	250	0	0	46	0
9	B	329	0	0	67	0
9	C	1321	0	0	266	0
9	D	1655	0	0	324	0
9	E	176	0	0	32	0
9	F	519	0	0	103	0
9	K	278	0	0	43	0
9	L	309	0	0	68	0
9	M	1236	0	0	259	0
9	N	1552	0	0	306	0
9	O	137	0	0	23	0
9	P	422	0	0	84	0
All	All	61800	0	54323	6611	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 61.

The worst 5 of 6611 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)
2:M:409:ARG:HA	2:M:454:SER:HA	1.20	1.15
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.33	1.10
3:D:119:SER:HB2	3:D:123:LEU:H	1.23	1.04
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.41	1.02
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.43	1.01

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%)	22 (10%)	5 (2%)	6	7
1	B	227/315 (72%)	200 (88%)	22 (10%)	5 (2%)	6	7
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	8	10
1	L	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	8	10
2	C	1117/1119 (100%)	927 (83%)	138 (12%)	52 (5%)	2	1
2	M	1117/1119 (100%)	926 (83%)	142 (13%)	49 (4%)	2	2
3	D	1388/1524 (91%)	1155 (83%)	168 (12%)	65 (5%)	2	1
3	N	1388/1524 (91%)	1133 (82%)	187 (14%)	68 (5%)	2	1
4	E	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	2
4	O	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	2
5	F	341/423 (81%)	290 (85%)	35 (10%)	16 (5%)	2	1
5	P	341/423 (81%)	288 (84%)	38 (11%)	15 (4%)	2	2
All	All	6786/7590 (89%)	5671 (84%)	824 (12%)	291 (4%)	2	2

5 of 291 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	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%)	149 (74%)	53 (26%)	0	0
1	B	202/273 (74%)	167 (83%)	35 (17%)	2	2
1	K	202/273 (74%)	154 (76%)	48 (24%)	0	0
1	L	202/273 (74%)	152 (75%)	50 (25%)	0	0
2	C	941/941 (100%)	722 (77%)	219 (23%)	1	1
2	M	941/941 (100%)	731 (78%)	210 (22%)	1	1
3	D	1123/1279 (88%)	861 (77%)	262 (23%)	1	1
3	N	1123/1279 (88%)	832 (74%)	291 (26%)	0	0
4	E	83/87 (95%)	65 (78%)	18 (22%)	1	1
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	0
5	F	295/370 (80%)	234 (79%)	61 (21%)	1	1
5	P	295/370 (80%)	242 (82%)	53 (18%)	1	2
All	All	5692/6446 (88%)	4370 (77%)	1322 (23%)	1	1

5 of 1322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	925	TYR
3	N	1019	PRO
2	M	1111	ILE
2	M	923	GLU

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Mol	Chain	Res	Type
3	N	542	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	565	GLN
3	N	901	GLN
2	M	671	ASN
3	N	166	GLN
3	N	1334	GLN

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 10 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
8	TGT	N	9002	6	21,27,27	4.52	15 (71%)	21,44,44	2.64	6 (28%)
8	TGT	D	9001	6	21,27,27	4.19	17 (80%)	21,44,44	2.60	7 (33%)

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
8	TGT	N	9002	6	-	7/14/57/57	0/2/2/2
8	TGT	D	9001	6	-	6/14/57/57	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	9001	TGT	O11-C10	9.53	1.55	1.20
8	N	9002	TGT	O11-C10	8.80	1.53	1.20
8	N	9002	TGT	O3-C8	8.54	1.41	1.23
8	N	9002	TGT	C1-C2	5.90	1.63	1.53
8	D	9001	TGT	C3-C4	5.77	1.64	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	9001	TGT	O10-C10-C11	7.11	124.18	111.09
8	N	9002	TGT	C3-O10-C10	6.95	128.47	117.72
8	N	9002	TGT	O10-C10-C11	6.89	123.76	111.09
8	D	9001	TGT	C3-O10-C10	5.92	126.88	117.72
8	D	9001	TGT	O9-P1-O6	3.42	121.31	105.99

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	9001	TGT	O1-C7-C9-O5
8	D	9001	TGT	C11-C10-O10-C3
8	D	9001	TGT	O11-C10-O10-C3
8	N	9002	TGT	O1-C7-C9-O5
8	N	9002	TGT	C11-C10-O10-C3

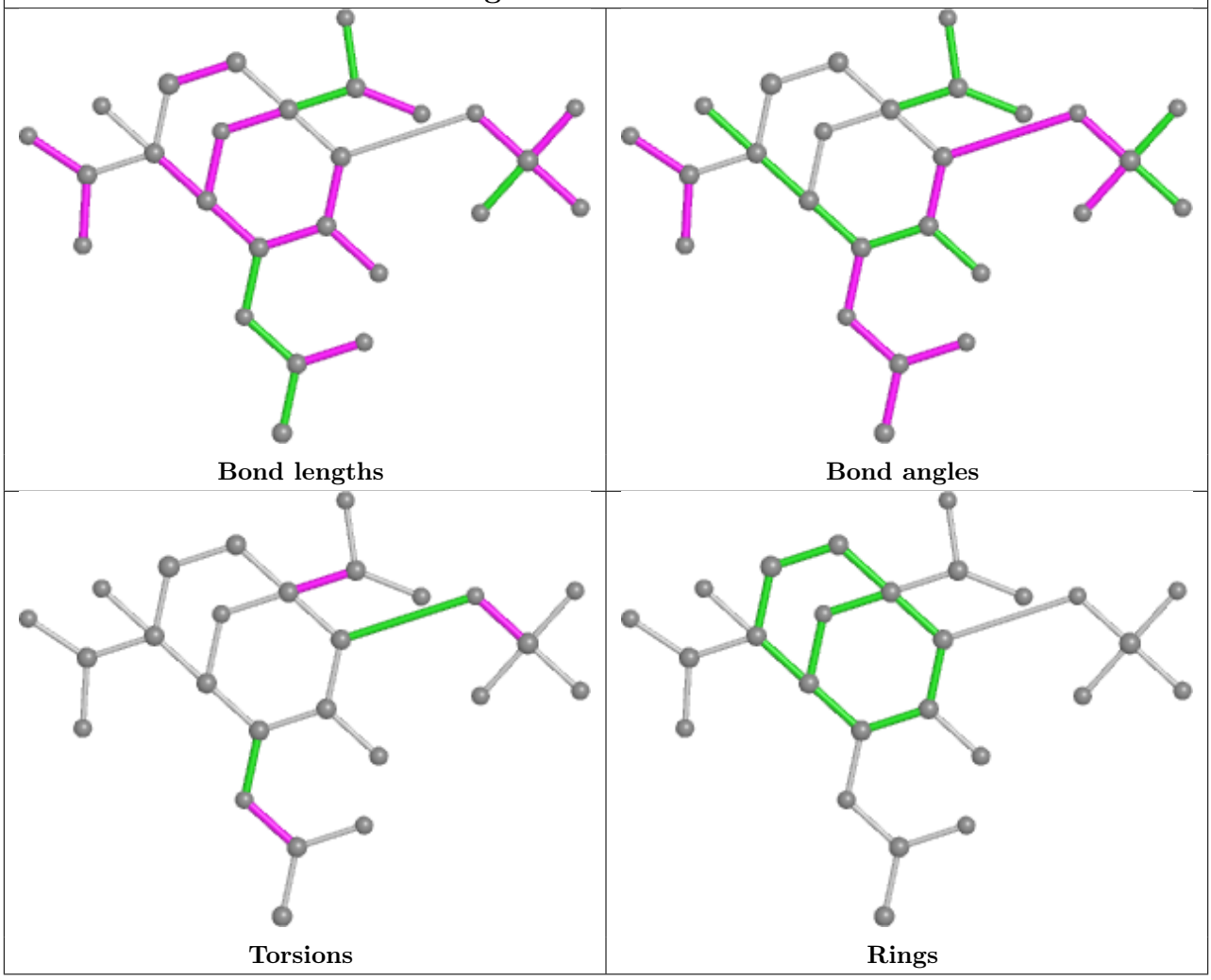
There are no ring outliers.

2 monomers are involved in 4 short contacts:

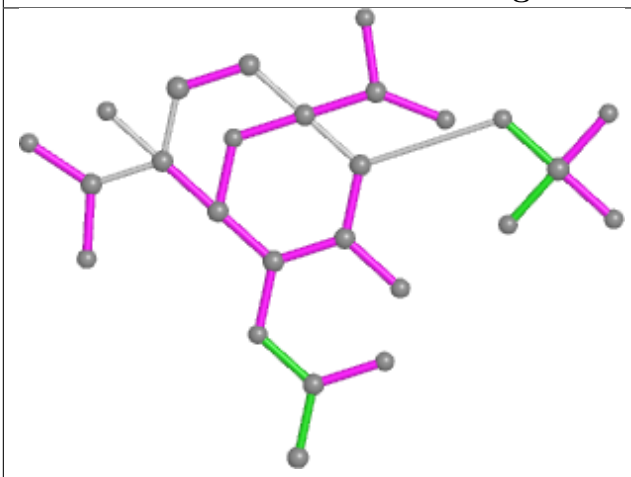
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	9002	TGT	1	0
8	D	9001	TGT	3	0

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.

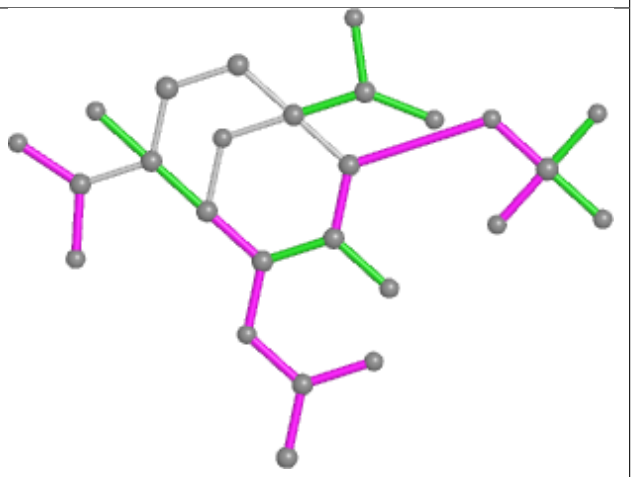
Ligand TGT N 9002



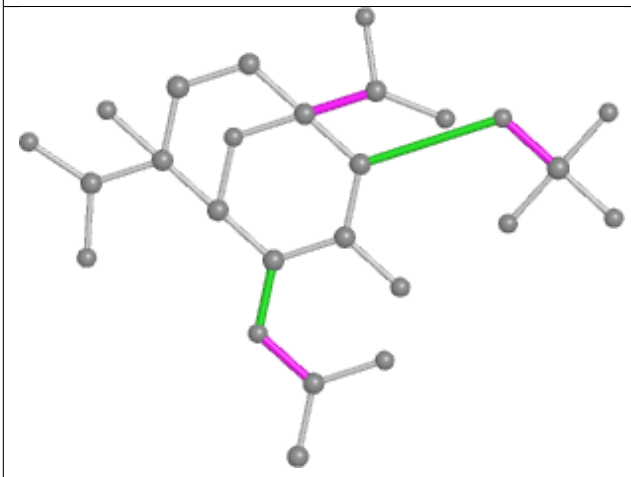
Ligand TGT D 9001



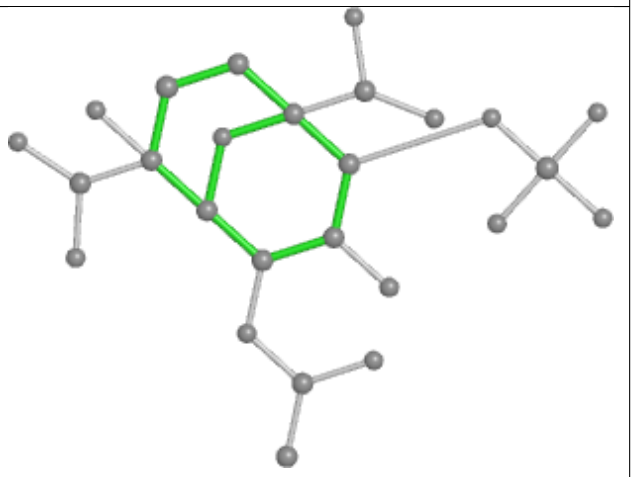
Bond lengths



Bond angles



Torsions



Rings

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	229/315 (72%)	2.02	70 (30%)	0	0	18, 47, 72, 88	0
1	B	229/315 (72%)	2.74	80 (34%)	0	0	34, 66, 82, 88	0
1	K	229/315 (72%)	1.39	69 (30%)	0	0	21, 43, 70, 92	0
1	L	229/315 (72%)	2.07	69 (30%)	0	0	34, 62, 82, 95	0
2	C	1119/1119 (100%)	3.02	409 (36%)	0	0	15, 58, 81, 94	0
2	M	1119/1119 (100%)	3.12	422 (37%)	0	0	15, 55, 81, 97	0
3	D	1392/1524 (91%)	1.93	383 (27%)	0	0	15, 49, 82, 97	0
3	N	1392/1524 (91%)	1.97	384 (27%)	0	0	16, 48, 83, 105	0
4	E	95/99 (95%)	1.35	23 (24%)	0	0	30, 59, 82, 103	0
4	O	95/99 (95%)	1.69	22 (23%)	0	0	22, 59, 77, 87	0
5	F	345/423 (81%)	3.86	158 (45%)	0	0	38, 63, 83, 97	0
5	P	345/423 (81%)	3.90	150 (43%)	0	0	41, 64, 85, 92	0
All	All	6818/7590 (89%)	2.51	2239 (32%)	0	0	15, 54, 82, 105	0

The worst 5 of 2239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	854	ALA	66.8
3	N	1246	VAL	60.6
3	N	532	GLY	59.3
3	N	533	GLY	56.7
3	N	1248	GLY	56.6

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)

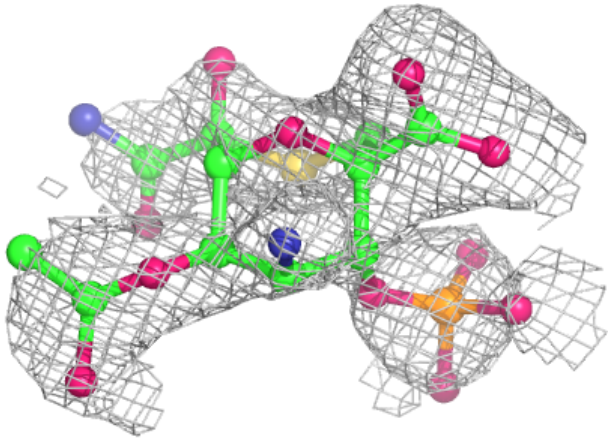
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

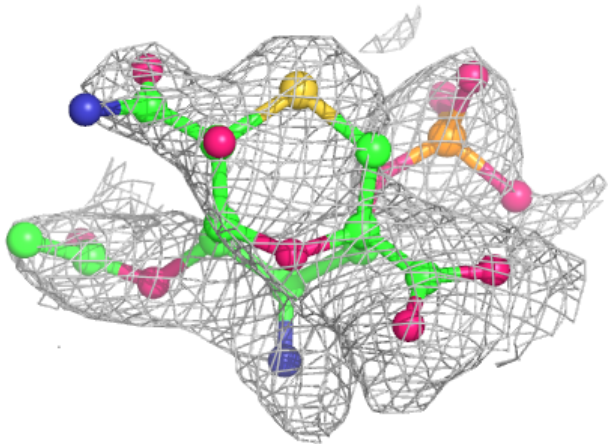
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	TGT	D	9001	26/26	0.81	0.43	44,47,50,52	0
8	TGT	N	9002	26/26	0.81	0.61	41,47,51,52	0
6	MG	C	9004	1/1	0.97	0.06	17,17,17,17	0
6	MG	D	9003	1/1	0.98	0.06	17,17,17,17	0
6	MG	N	9005	1/1	0.98	0.03	13,13,13,13	0
7	ZN	N	9059	1/1	0.99	0.06	42,42,42,42	0
7	ZN	N	9113	1/1	0.99	0.10	41,41,41,41	0
6	MG	N	9006	1/1	0.99	0.04	4,4,4,4	0
7	ZN	D	9112	1/1	0.99	0.05	50,50,50,50	0
7	ZN	D	9058	1/1	1.00	0.17	56,56,56,56	0

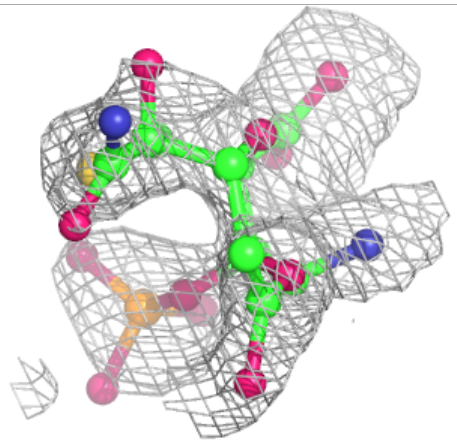
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TGT D 9001:

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

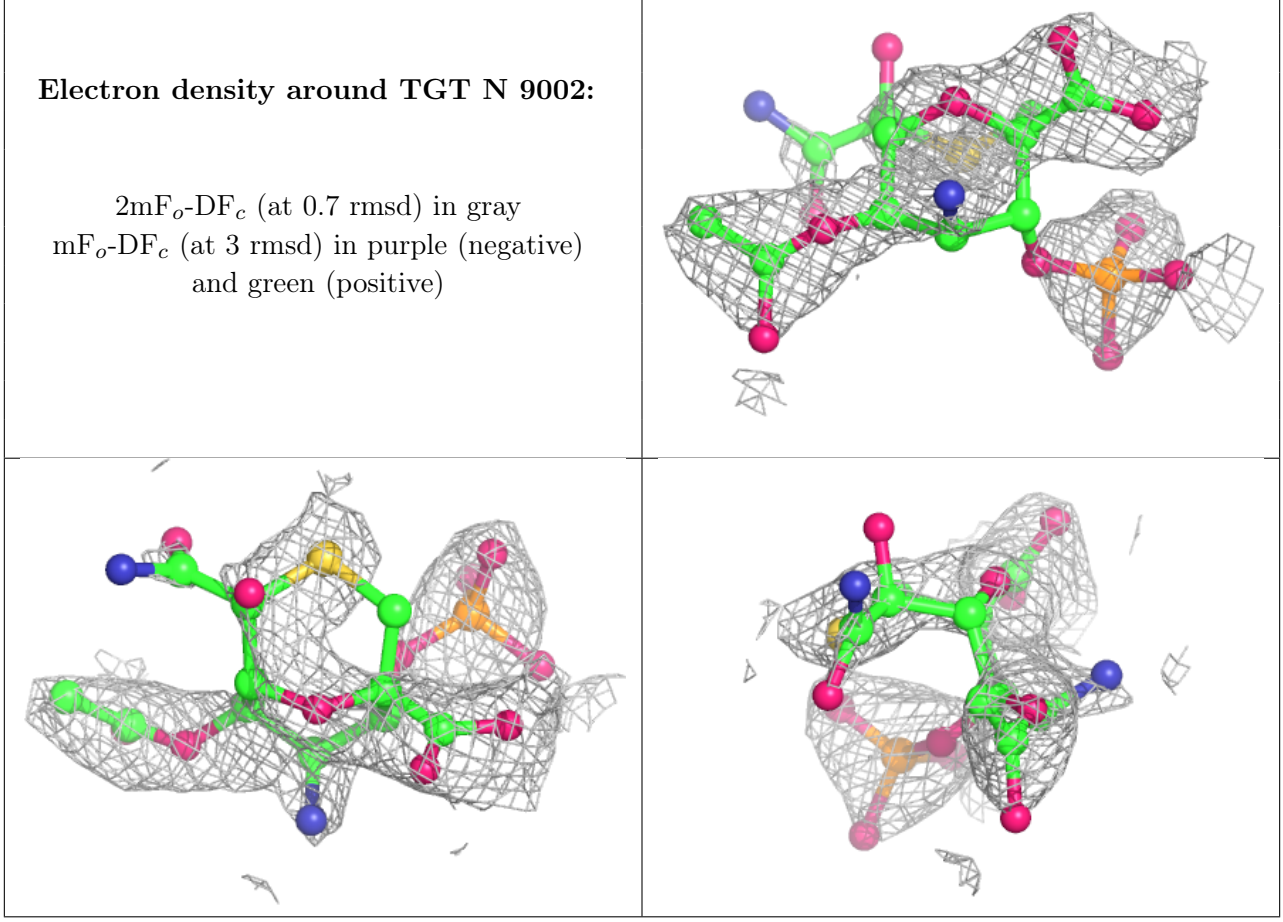






Electron density around TGT N 9002:

$2mF_o$-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.