wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 06:47 am BST

PDB ID	:	4WQS
Title	:	Thermus thermophilus RNA polymerase backtracked complex
Authors	:	Murayama, Y.; Sekine, S.; Yokoyama, S.
Deposited on	:	2014-10-22
Resolution	:	4.31 Å(reported)

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

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

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

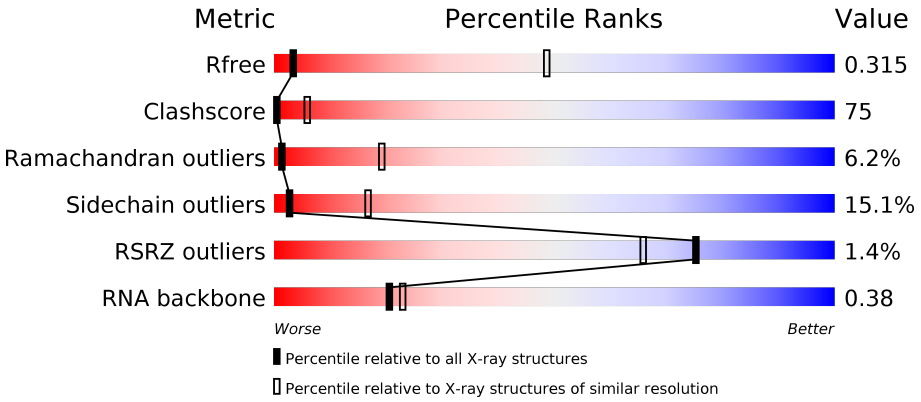
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.31 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)
RNA backbone	3102	1058 (5.60-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	21% 45% 7% 27%
1	B	315	3% 27% 40% • • 27%
1	K	315	% 27% 41% 5% 27%
1	L	315	% 24% 43% 5% 27%

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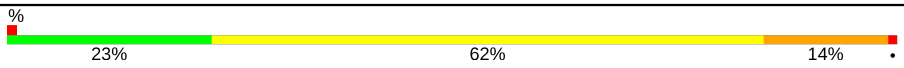
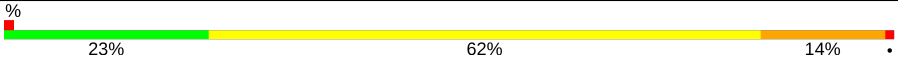
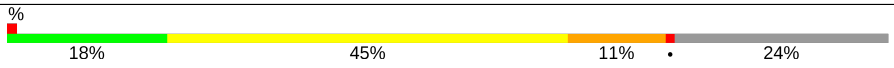
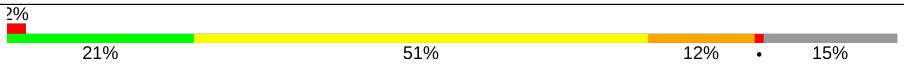
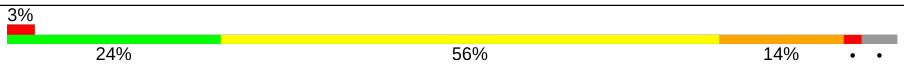
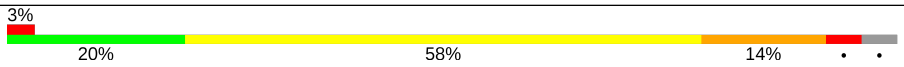
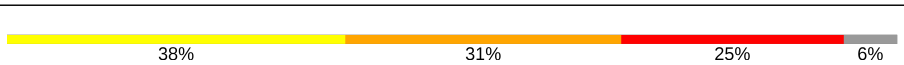
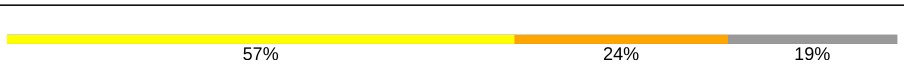
Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	G	28	
5	X	28	
6	H	16	
6	Y	16	
7	I	21	
7	Z	21	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 48166 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	1151	Total	C	N	O	S	0	0	0
			9097	5753	1629	1682	33			
3	N	1288	Total	C	N	O	S	0	0	0
			10175	6441	1804	1899	31			

- 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 DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	27	Total	C	N	O	P	0	0	0
			548	259	104	158	27			
5	X	27	Total	C	N	O	P	0	0	0
			548	259	104	158	27			

- Molecule 6 is a RNA chain called RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP *CP*UP*CP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	16	Total	C	N	O	P	0	0	0
			340	151	61	112	16			
6	Y	15	Total	C	N	O	P	0	0	0
			318	141	56	106	15			

- Molecule 7 is a DNA chain called DNA (5'-D(P*GP*TP*AP*GP*CP*TP*TP*GP*TP*GP *GP*TP*AP*GP*TP*GP*AP*CP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	17	Total	C	N	O	P	0	0	0
			357	169	65	106	17			
7	Z	17	Total	C	N	O	P	0	0	0
			357	169	65	106	17			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

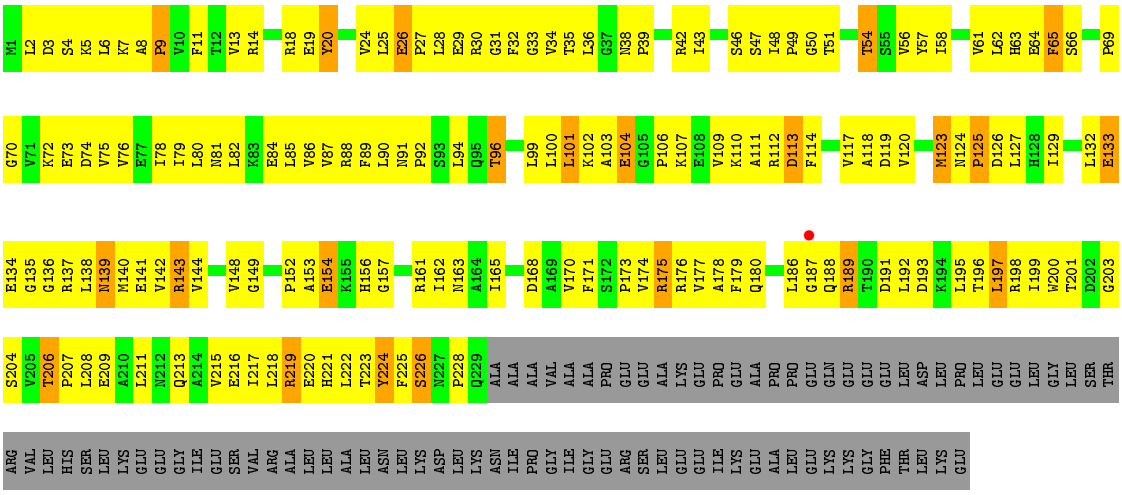
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

3 Residue-property plots (i)

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

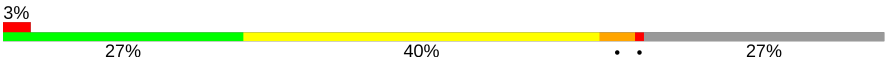
- Molecule 1: DNA-directed RNA polymerase subunit alpha

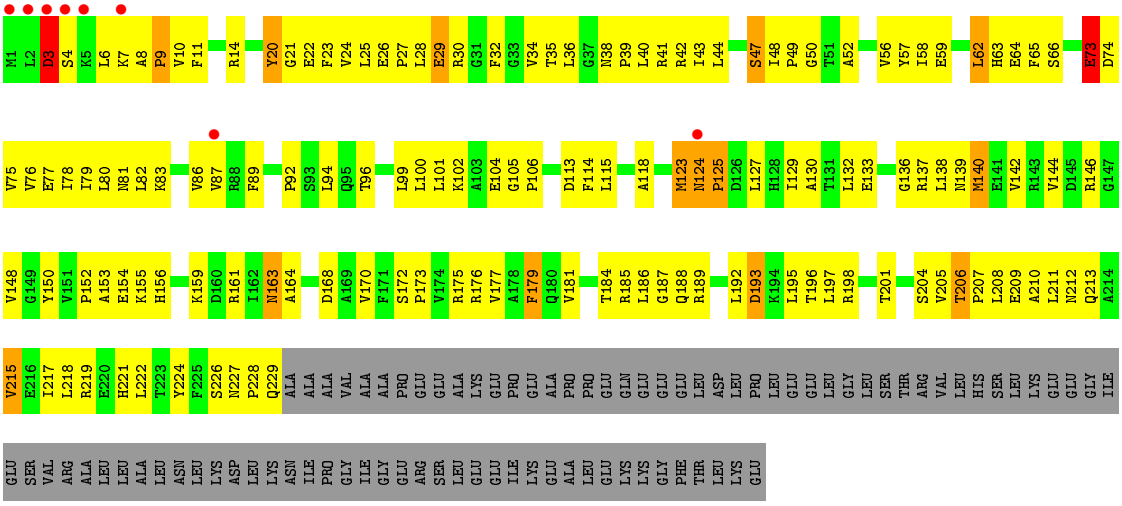
Chain A:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

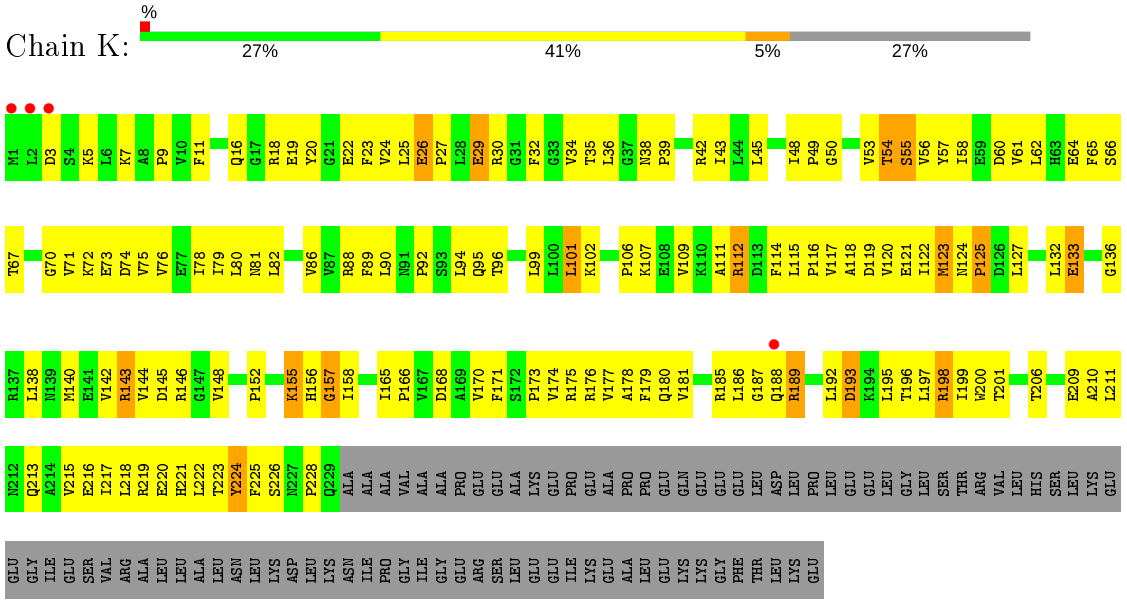
Chain B:





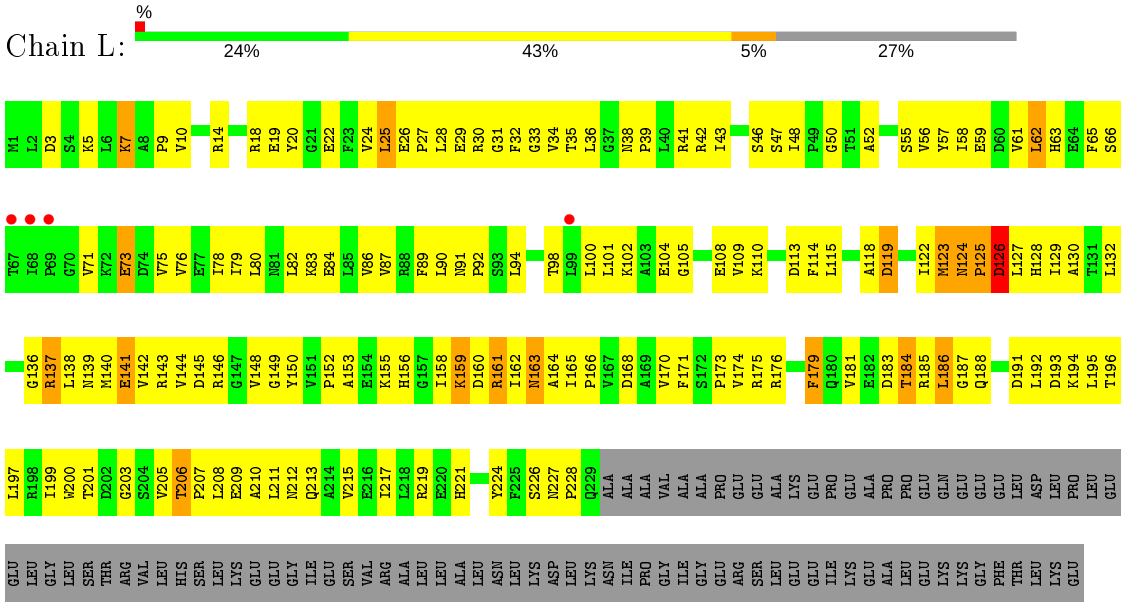
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain K:



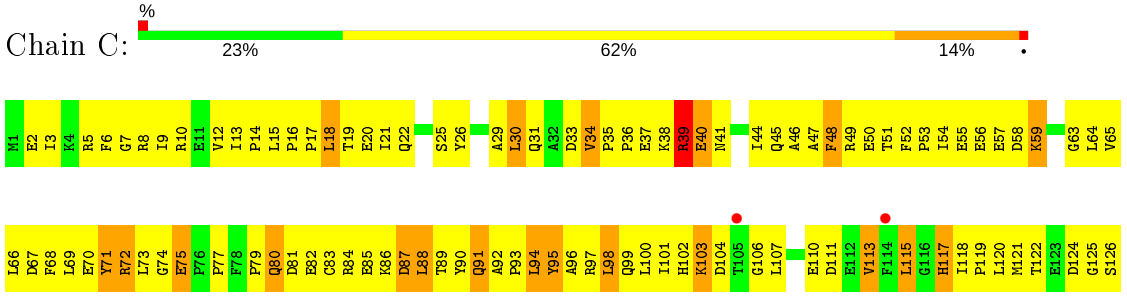
• Molecule 1: DNA-directed RNA polymerase subunit alpha

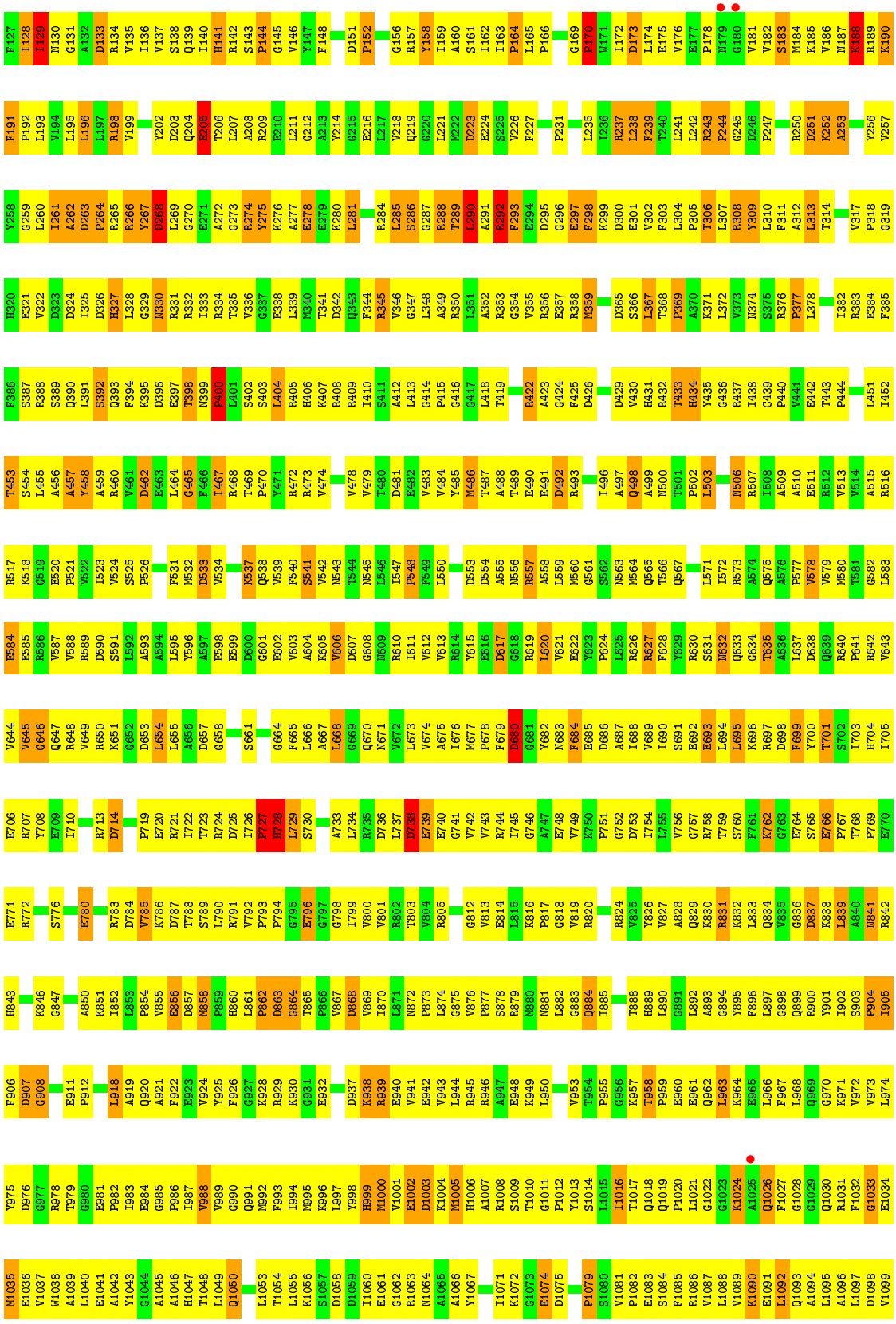
Chain L:



• Molecule 2: DNA-directed RNA polymerase subunit beta

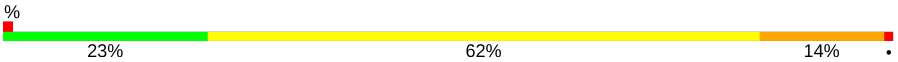
Chain C:

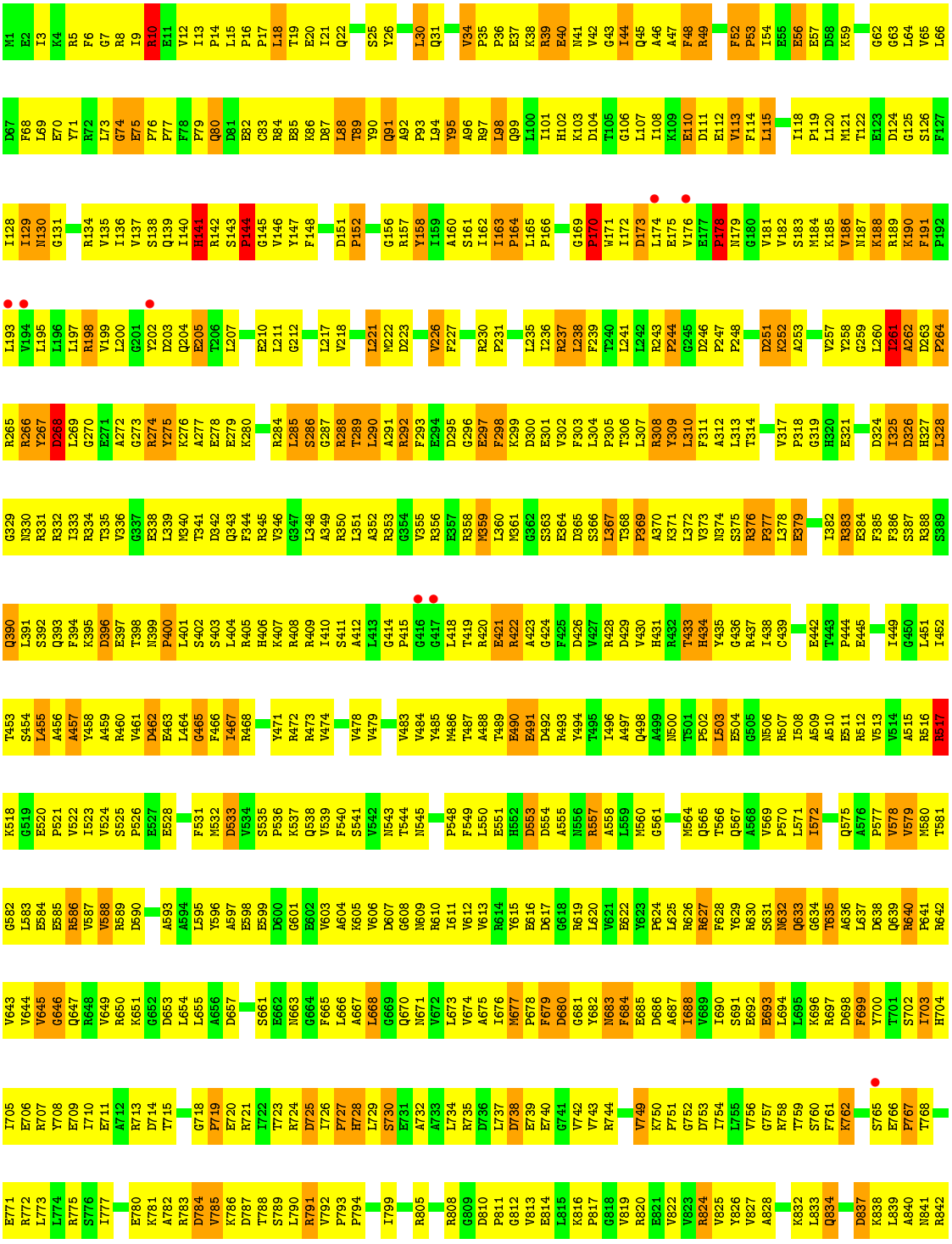


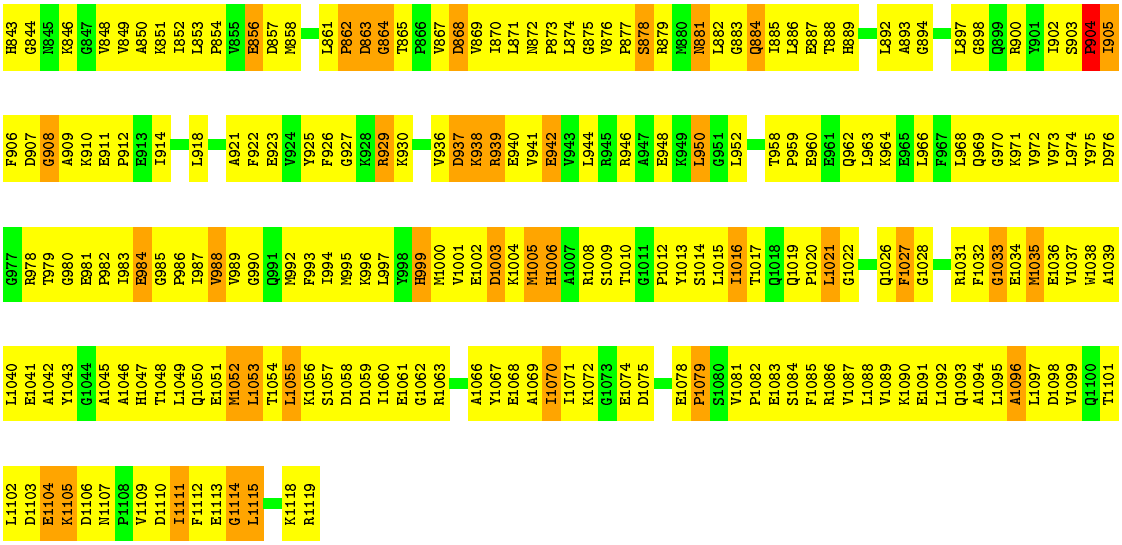

F127 I128 I129 N130 G131 A132 D133 R134 V135 I136 V137 S138 Q139 I140 H141 R142 S143 P144 G145 V146 Y147 F148 D151 P152 G156 R157 Y158 I159 A160 S161 I162 I163 P164 L165 P166 G169 P170 W171 I172 D173 L174 E175 V176 E177 P178 N179 G180 V181 V182 S183 M184 K185 V186 N187 K188 R189 K190
F191 P192 L193 V194 L195 L196 L197 R198 V199 Y202 D203 Q204 E205 T206 L207 A208 R209 E210 L211 G212 A213 Y214 G215 E216 L217 V218 Q219 G220 L221 M222 D223 E224 S225 V226 F227 P231 L235 I236 R237 L238 F239 T240 L241 L242 R243 P244 G245 D246 P247 R250 D251 K252 A253 Y256 V257
Y258 G259 L260 I261 A262 D263 P264 R265 R266 Y267 D268 L269 G270 E271 A272 G273 R274 Y275 K276 A277 E278 E279 K280 L281 R284 L285 S286 G287 R288 T289 L290 A291 R292 F293 E294 D295 G296 E297 F298 K299 D300 E301 V302 F303 L304 P305 T306 L307 R308 Y309 L310 F311 A312 L313 T314 V317 P318 G319
H320 E321 V322 D323 D324 I325 D326 H327 L328 G329 N330 R331 R332 I333 R334 T335 V336 G337 E338 L339 M340 T341 D342 Q343 F344 R345 V346 G347 L348 A349 R350 L351 A352 R353 G354 V355 R356 E357 R358 M359 D365 S366 L367 T368 P369 A370 K371 L372 V373 N374 S375 R376 P377 L378 I382 R383 E384 F385
F386 S387 R388 S389 Q390 L391 S392 Q393 F394 K395 D396 E397 T398 N399 P400 L401 S402 S403 L404 R405 H406 K407 R408 R409 I410 S411 A412 L413 G414 P415 G416 G417 L418 T419 R422 A423 G424 F425 D426 D429 V430 H431 R432 T433 H434 Y435 G436 R437 I438 C439 P440 V441 E442 T443 P444 L451 I452
T453 S454 L455 A456 A457 Y458 A459 R460 V461 D462 E463 L464 G465 F466 I467 R468 T469 P470 Y471 R472 R473 V474 V478 V479 T480 D481 E482 V483 V484 Y485 M486 T487 A488 T489 E490 E491 D492 R493 I496 A497 Q498 A499 N500 T501 P502 L503 N506 R507 I508 A509 A510 E511 R512 V513 V514 A515 R516
R517 K518 G519 E520 P521 V522 I523 V524 S525 P526 F531 M532 D533 V534 K537 Q538 V539 F540 S541 V542 N543 T544 N545 L546 I547 P548 F549 L550 D553 D554 A555 N556 R557 A558 L559 M560 G561 S562 N563 M564 Q565 T566 Q567 L571 I572 R573 A574 Q575 A576 P577 V578 V579 M580 T581 G582 L583
E584 E585 R586 V587 V588 R589 D590 S591 L592 A593 A594 L595 Y596 A597 E598 E599 D600 G601 E602 V603 A604 K605 V606 D607 G608 N609 R610 I611 V612 V613 R614 Y615 E616 D617 G618 R619 L620 V621 E622 Y623 P624 L625 R626 R627 F628 Y629 R630 S631 N632 Q633 G634 T635 A636 L637 D638 Q639 E640 F641 E642 V643
V644 V645 G646 Q647 R648 V649 R650 K651 G652 D653 L654 L655 A656 D657 G658 S661 G664 F665 L666 A667 L668 G669 Q670 N671 V672 L673 V674 A675 I676 M677 P678 F679 D680 G681 Y682 N683 F684 E685 D686 A687 I688 V689 I690 S691 E692 E693 L694 L695 K696 R697 D698 F699 Y700 T701 S702 I703 H704 I705
E706 R707 Y708 E709 I710 R713 D714 P719 E720 R721 I722 T723 R724 D725 I726 F727 R728 L729 S730 A733 L734 R735 D736 L737 D738 E739 E740 G741 V742 V743 R744 I745 G746 A747 E748 V749 K750 P751 G752 D753 I754 L755 V756 G757 R758 T759 S760 F761 K762 G763 E764 S765 E766 F767 T768 E769 E770
E771 R772 S776 E780 R783 D784 V785 K786 D787 T788 S789 L790 R791 V792 P793 P794 G795 E796 G797 G798 I799 V800 V801 R802 T803 V804 R805 G812 V813 E814 L815 K816 P817 G818 V819 R820 R824 V825 Y826 V827 A828 Q829 K830 R831 K832 L833 Q834 V835 G836 D837 K838 L839 A840 N841 R842
H843 K846 G847 A850 K851 I852 L853 P854 Y855 E856 D857 N858 P859 H860 L861 P862 D863 G864 T865 P866 V867 D868 V869 I870 L871 N872 P873 L874 G875 V876 P877 S878 R879 N880 N881 L882 G883 Q884 I885 T888 H889 L890 G891 L892 A893 G894 Y895 F896 L897 G898 Q899 R900 Y901 I902 S903 P904 I905
F906 D907 G908 E911 P912 L918 A919 Q920 A921 F922 E923 Y924 Y925 F926 G927 K928 R929 K930 G931 E932 D937 K938 R939 E940 V941 E942 V943 L944 R945 R946 A947 E948 K949 L950 V953 Y954 P955 G956 K957 T958 P959 E960 E961 Q962 L963 K964 E965 L966 F967 L968 Q969 G970 K971 V972 V973 L974
Y975 D976 G977 R978 T979 G980 E981 P982 I983 E984 G985 P986 I987 V988 V989 G990 Q991 N992 F993 I994 N995 K996 L997 Y998 H999 M1000 V1001 E1002 D1003 K1004 M1005 H1006 A1007 R1008 S1009 T1010 G1011 P1012 Y1013 S1014 L1015 I1016 T1017 Q1018 Q1019 P1020 L1021 G1022 G1023 K1024 A1025 Q1026 F1027 G1028 G1029 Q1030 R1031 F1032 G1033 E1034
M1035 E1036 V1037 W1038 A1039 L1040 E1041 A1042 Y1043 G1044 A1045 A1046 R1047 T1048 L1049 Q1050 L1053 T1054 L1055 K1056 S1057 D1058 D1059 I1060 E1061 G1062 R1063 N1064 A1065 A1066 Y1067 I1071 K1072 G1073 E1074 D1075 P1079 S1080 V1081 P1082 E1083 S1084 F1085 R1086 V1087 L1088 V1089 K1090 E1091 L1092 Q1093 A1094 L1095 A1096 L1097 D1098 V1099

• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain M:

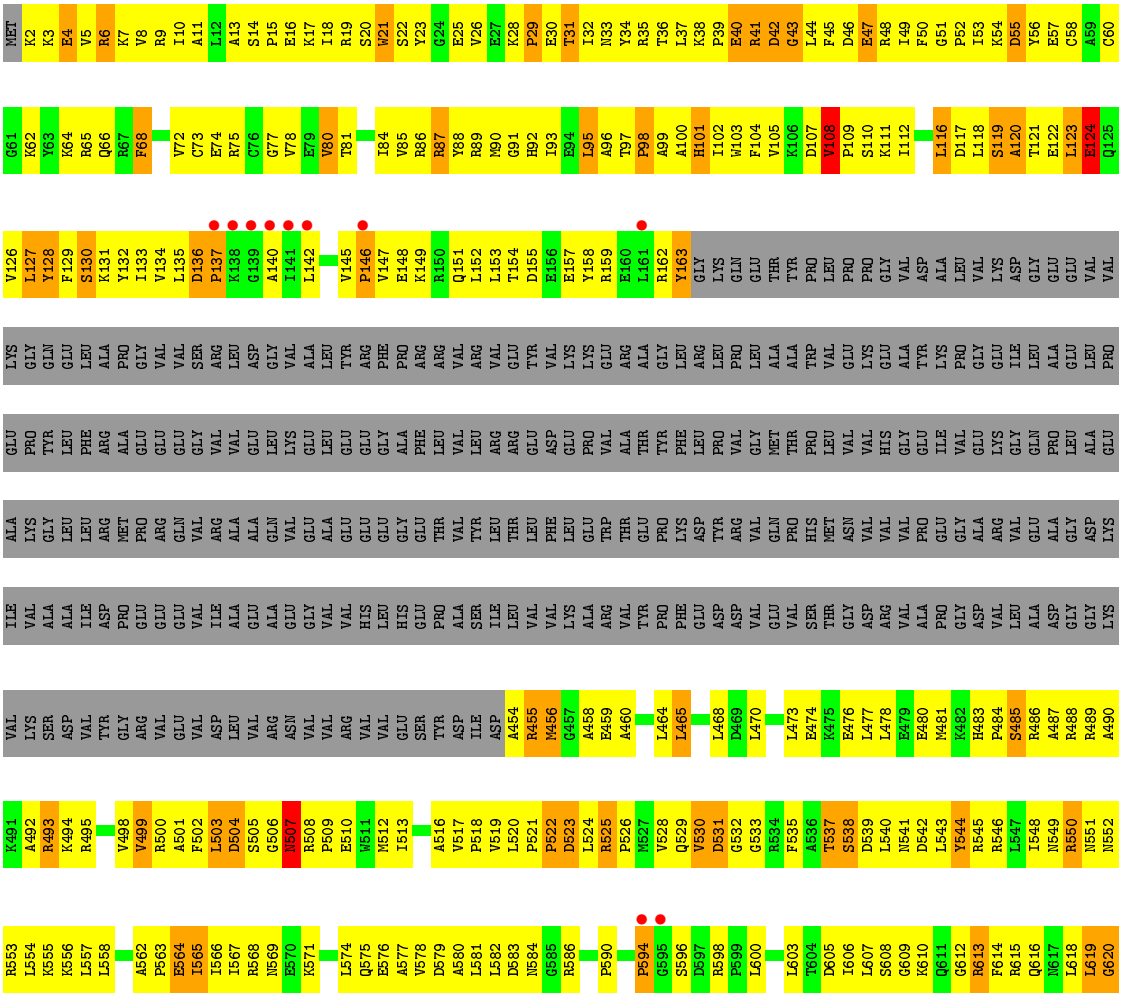


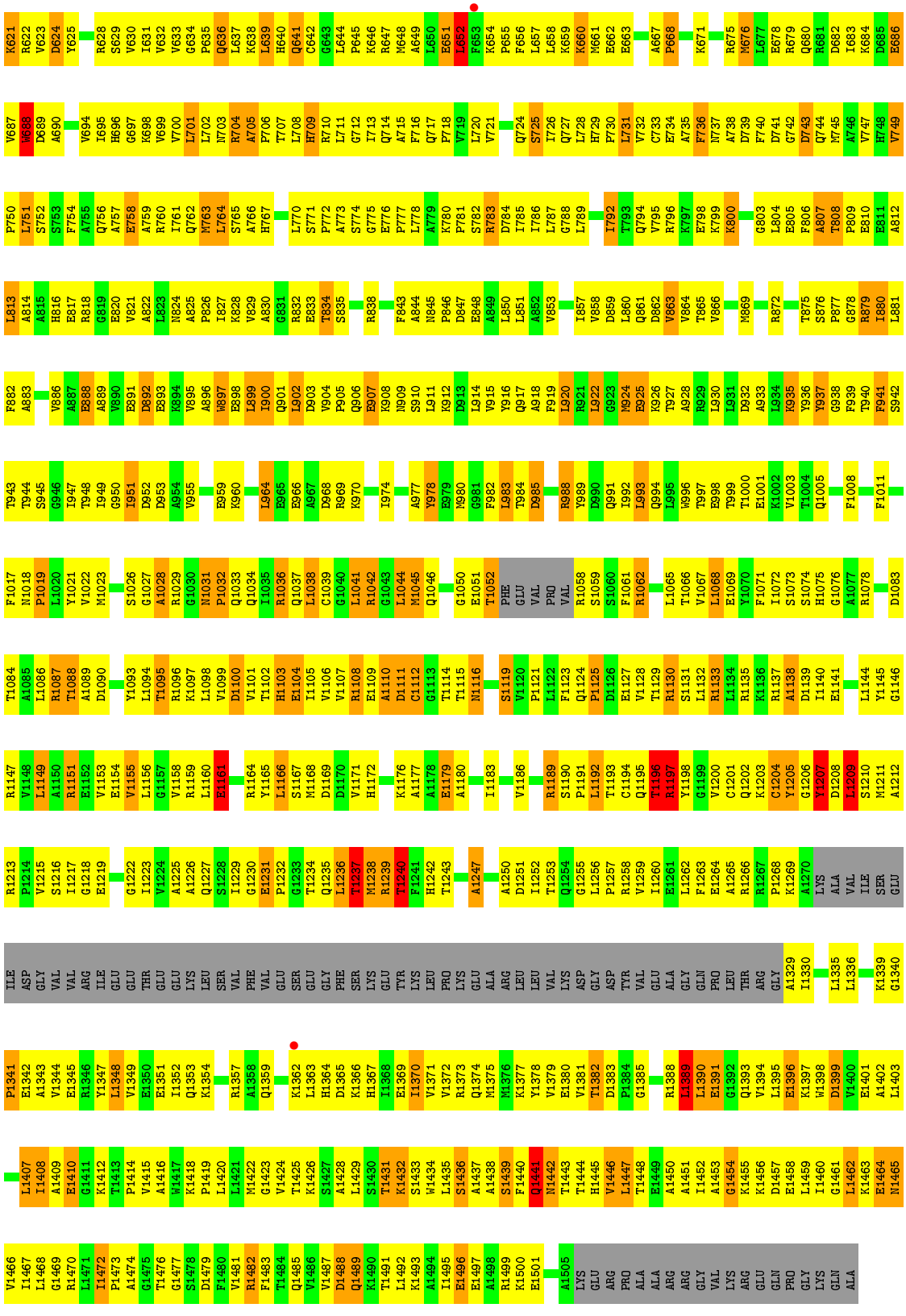




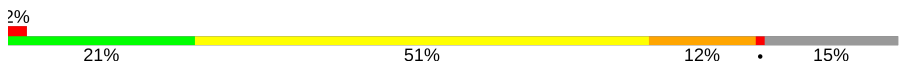
• Molecule 3: DNA-directed RNA polymerase subunit beta'

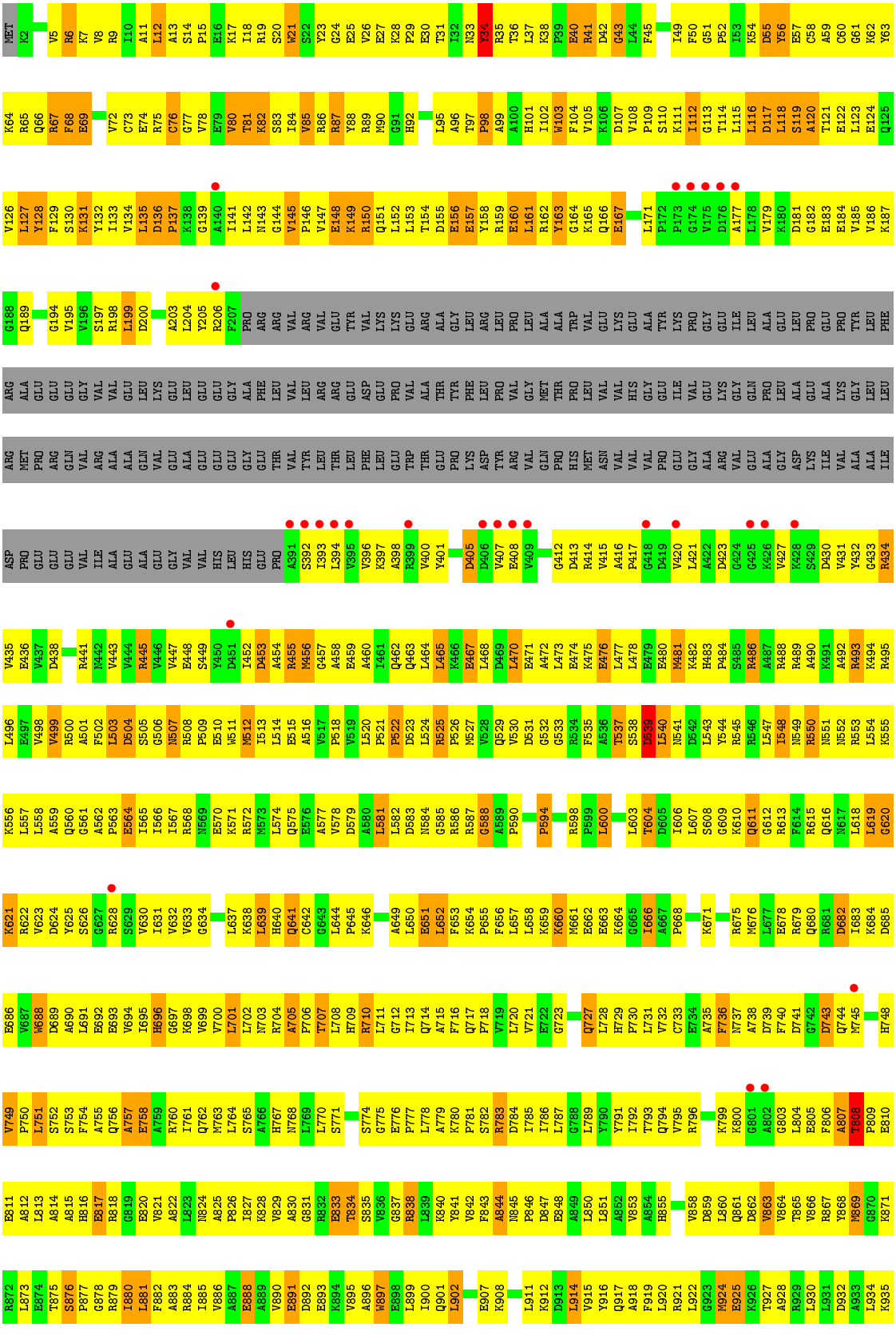
Chain D:

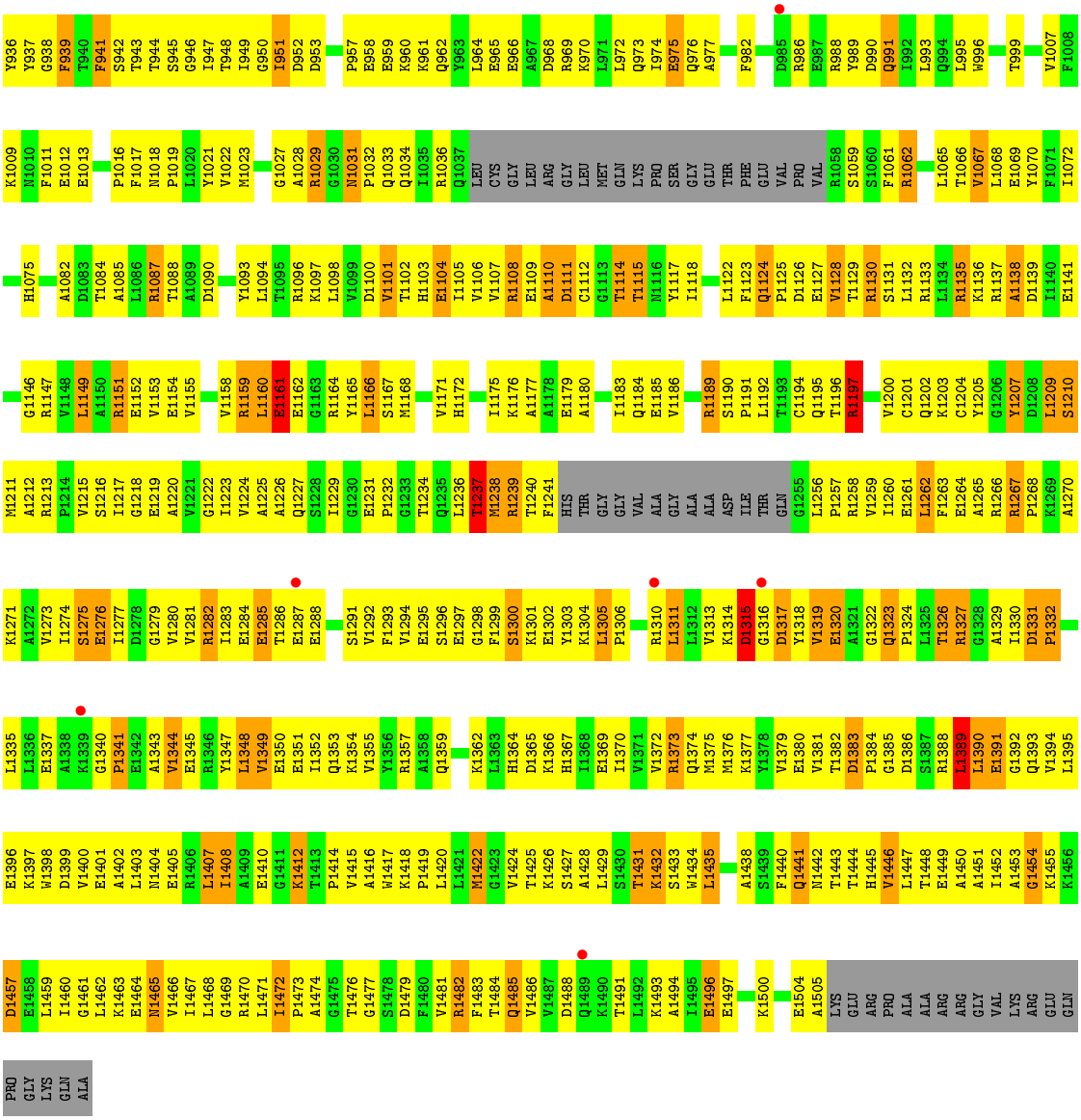




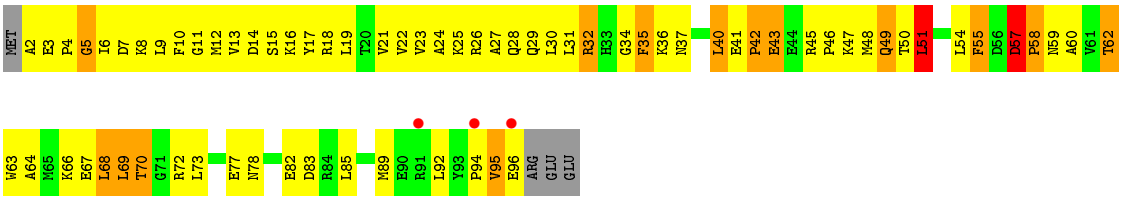
• Molecule 3: DNA-directed RNA polymerase subunit beta'



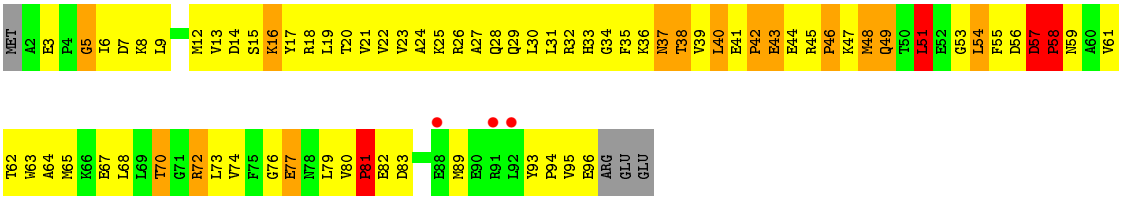




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: DNA (28-MER)

Chain G:

• Molecule 5: DNA (28-MER)

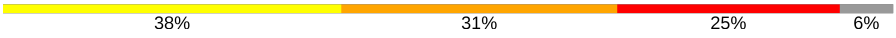
Chain X:

• Molecule 6: RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3')

Chain H:

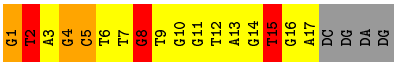
• Molecule 6: RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3')

Chain Y:



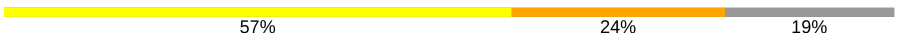
• Molecule 7: DNA (5'-D(P*GP*TP*AP*GP*CP*TP*TP*GP*TP*GP*GP*TP*AP*GP*TP*GP*AP*CP*GP*AP*G)-3')

Chain I:



• Molecule 7: DNA (5'-D(P*GP*TP*AP*GP*CP*TP*TP*GP*TP*GP*GP*TP*AP*GP*TP*GP*AP*CP*GP*AP*G)-3')

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	155.98Å 155.98Å 495.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.15 – 4.31 44.15 – 4.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.15-4.31) 99.4 (44.15-4.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.281 , 0.311 0.285 , 0.315	Depositor DCC
R_{free} test set	3821 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	106.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.15 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.499 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	48166	wwPDB-VP
Average B, all atoms (Å^2)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.38	0/1838	0.69	0/2498
1	B	0.43	0/1838	0.68	0/2498
1	K	0.45	0/1838	0.70	0/2498
1	L	0.42	0/1838	0.67	0/2498
2	C	0.49	0/8997	0.79	3/12164 (0.0%)
2	M	0.48	0/8997	0.78	4/12164 (0.0%)
3	D	0.51	1/9249 (0.0%)	0.83	10/12482 (0.1%)
3	N	0.51	0/10344	0.81	8/13968 (0.1%)
4	E	0.50	0/784	0.87	2/1057 (0.2%)
4	O	0.46	0/784	0.84	2/1057 (0.2%)
5	G	0.99	1/614 (0.2%)	1.41	9/943 (1.0%)
5	X	0.93	0/614	1.43	11/943 (1.2%)
6	H	1.14	3/378 (0.8%)	1.56	6/585 (1.0%)
6	Y	1.15	3/353 (0.8%)	1.45	5/546 (0.9%)
7	I	0.94	1/400 (0.2%)	1.46	7/616 (1.1%)
7	Z	0.90	1/400 (0.2%)	1.28	3/616 (0.5%)
All	All	0.53	10/49266 (0.0%)	0.84	70/67133 (0.1%)

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
5	G	0	10
5	X	0	11
6	H	0	4
6	Y	0	5
7	I	0	6
7	Z	0	4
All	All	0	40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	1	DG	OP3-P	-7.99	1.51	1.61
7	I	1	DG	OP3-P	-7.84	1.51	1.61
6	Y	11	C	N1-C2	-7.40	1.32	1.40
6	H	11	C	N1-C2	-7.38	1.32	1.40
6	H	1	C	OP3-P	-7.06	1.52	1.61

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	1	DG	O5'-P-OP1	-18.71	88.24	110.70
7	Z	1	DG	O5'-P-OP1	-16.85	90.48	110.70
6	H	5	C	N1-C1'-C2'	-15.07	94.41	114.00
6	Y	5	C	N1-C1'-C2'	-9.98	101.02	112.00
7	I	1	DG	O5'-P-OP2	9.33	121.90	110.70

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	10	DA	Sidechain
5	G	2	DT	Sidechain
5	G	3	DC	Sidechain
5	G	4	DA	Sidechain
5	G	9	DC	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	257	0
1	B	1806	0	1861	180	0
1	K	1806	0	1861	189	0
1	L	1806	0	1861	203	0
2	C	8829	0	8933	1430	0
2	M	8829	0	8933	1425	0
3	D	9097	0	9316	1626	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	10175	0	10401	1763	0
4	E	770	0	784	124	0
4	O	770	0	784	151	0
5	G	548	0	301	113	0
5	X	548	0	301	93	0
6	H	340	0	176	76	0
6	Y	318	0	165	56	0
7	I	357	0	194	68	0
7	Z	357	0	194	71	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
All	All	48166	0	47926	7162	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 75.

The worst 5 of 7162 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:C:52:PHE:CZ	2:C:68:PHE:HB2	1.22	1.67
3:D:897:TRP:HA	3:D:900:ILE:CG1	1.33	1.56
3:D:1041:LEU:HD11	3:D:1045:MET:SD	1.55	1.44
3:D:705:ALA:HB1	6:H:14:G:N2	1.24	1.40
3:D:705:ALA:CB	6:H:14:G:H21	1.40	1.32

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%)	194 (86%)	24 (11%)	9 (4%)	3 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	227/315 (72%)	195 (86%)	23 (10%)	9 (4%)	3 26
1	K	227/315 (72%)	193 (85%)	26 (12%)	8 (4%)	3 29
1	L	227/315 (72%)	201 (88%)	17 (8%)	9 (4%)	3 26
2	C	1117/1119 (100%)	893 (80%)	151 (14%)	73 (6%)	1 18
2	M	1117/1119 (100%)	889 (80%)	153 (14%)	75 (7%)	1 18
3	D	1143/1524 (75%)	903 (79%)	167 (15%)	73 (6%)	1 19
3	N	1280/1524 (84%)	1011 (79%)	190 (15%)	79 (6%)	1 19
4	E	93/99 (94%)	67 (72%)	15 (16%)	11 (12%)	0 6
4	O	93/99 (94%)	69 (74%)	13 (14%)	11 (12%)	0 6
All	All	5751/6744 (85%)	4615 (80%)	779 (14%)	357 (6%)	1 19

5 of 357 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	29	GLU
1	A	118	ALA
1	A	133	GLU
1	A	187	GLY

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%)	178 (88%)	24 (12%)	5 23
1	B	202/273 (74%)	182 (90%)	20 (10%)	8 29
1	K	202/273 (74%)	182 (90%)	20 (10%)	8 29
1	L	202/273 (74%)	182 (90%)	20 (10%)	8 29
2	C	941/941 (100%)	790 (84%)	151 (16%)	2 15
2	M	941/941 (100%)	794 (84%)	147 (16%)	2 16
3	D	968/1279 (76%)	806 (83%)	162 (17%)	2 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	N	1088/1279 (85%)	919 (84%)	169 (16%)	2 16
4	E	84/88 (96%)	70 (83%)	14 (17%)	2 14
4	O	84/88 (96%)	70 (83%)	14 (17%)	2 14
All	All	4914/5708 (86%)	4173 (85%)	741 (15%)	3 17

5 of 741 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1269	LYS
2	M	34	VAL
3	N	1210	SER
3	D	1441	GLN
1	K	54	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	406	HIS
2	M	567	GLN
3	N	1031	ASN
2	M	393	GLN
3	N	714	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	H	15/16 (93%)	5 (33%)	1 (6%)
6	Y	14/16 (87%)	3 (21%)	1 (7%)
All	All	29/32 (90%)	8 (27%)	2 (6%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	H	4	G
6	H	5	C
6	H	6	C
6	H	15	C
6	H	16	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	H	5	C
6	Y	5	C

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	229/315 (72%)	-0.77	1 (0%) 92 87	154, 243, 347, 433	0
1	B	229/315 (72%)	-0.48	8 (3%) 44 35	202, 343, 460, 525	0
1	K	229/315 (72%)	-0.59	4 (1%) 70 61	157, 255, 375, 500	0
1	L	229/315 (72%)	-0.49	4 (1%) 70 61	193, 363, 452, 538	0
2	C	1119/1119 (100%)	-0.75	6 (0%) 91 86	12, 213, 336, 454	0
2	M	1119/1119 (100%)	-0.72	8 (0%) 87 82	60, 238, 426, 549	0
3	D	1151/1524 (75%)	-0.73	12 (1%) 82 74	8, 205, 382, 548	0
3	N	1288/1524 (84%)	-0.59	33 (2%) 56 46	81, 249, 452, 545	0
4	E	95/99 (95%)	-0.53	3 (3%) 47 37	156, 217, 337, 395	0
4	O	95/99 (95%)	-0.62	3 (3%) 47 37	205, 297, 426, 451	0
5	G	27/28 (96%)	-0.76	0 100 100	152, 210, 372, 381	0
5	X	27/28 (96%)	-0.67	0 100 100	238, 279, 353, 374	0
6	H	16/16 (100%)	0.21	1 (6%) 20 16	97, 189, 363, 385	0
6	Y	15/16 (93%)	-0.24	0 100 100	208, 249, 351, 378	0
7	I	17/21 (80%)	-0.65	0 100 100	215, 276, 418, 428	0
7	Z	17/21 (80%)	-0.72	0 100 100	264, 305, 348, 352	0
All	All	5902/6874 (85%)	-0.67	83 (1%) 75 66	8, 240, 416, 549	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	140	ALA	12.4
3	N	175	VAL	12.4
3	D	141	ILE	9.5
1	B	3	ASP	8.7
1	L	68	ILE	7.5

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	ZN	N	1601	1/1	0.97	0.13	72,72,72,72	0
8	ZN	D	1601	1/1	0.98	0.05	72,72,72,72	0
8	ZN	N	1602	1/1	0.98	0.11	72,72,72,72	0
8	ZN	D	1602	1/1	0.99	0.14	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.