wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2023 – 06:37 AM EDT

PDB ID	:	3HOU
Title	:	Complete RNA polymerase II elongation complex I with a T-U mismatch
Authors	:	Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.
Deposited on	:	2009-06-03
Resolution	:	3.20 Å(reported)

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

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

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

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

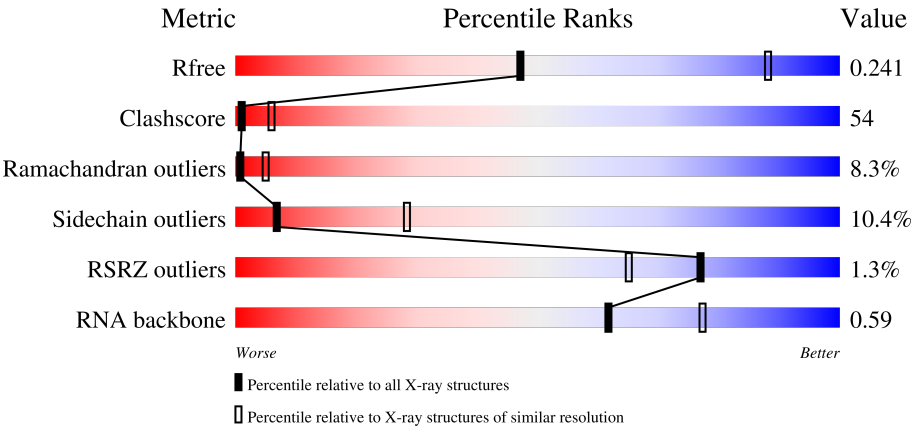
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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	1733	31% 41% 9% • 18%
1	M	1733	% 31% 40% 9% • 18%
2	B	1224	27% 51% 12% 10%
2	N	1224	% 26% 53% 11% • 10%

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Mol	Chain	Length	Quality of chain
3	C	318	29% 44% 11% 16%
3	O	318	28% 44% 11% 16%
4	D	221	26% 41% 12% 19%
4	P	221	10% 15% 47% 17% 19%
5	E	215	26% 64% 9%
5	Q	215	26% 65% 8%
6	F	155	19% 32% 5% 44%
6	R	155	22% 30% 44%
7	G	171	40% 53% 8%
7	S	171	10% 26% 63% 9%
8	H	146	2% 17% 54% 20% 8%
8	T	146	19% 57% 14% 8%
9	I	122	2% 33% 51% 11%
9	U	122	2% 25% 58% 13%
10	J	70	24% 47% 17% 7%
10	V	70	26% 44% 23% 7%
11	K	120	46% 42% 7% 5%
11	W	120	39% 48% 8% 5%
12	L	70	6% 6% 40% 17% 34%
12	X	70	3% 7% 37% 20% 34%
13	1	26	4% 50% 15% 31%
13	4	26	50% 15% 31%
14	2	13	46% 54%
14	5	13	46% 54%
15	3	17	6% 29% 35% 35%

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Mol	Chain	Length	Quality of chain
15	6	17	6% 29% 35% 35%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 63664 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			
1	M	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			
2	N	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			
3	O	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			
4	P	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			
5	Q	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			
6	R	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			
7	S	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			
8	T	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			
9	U	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	V	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			
11	W	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			
12	X	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP *TP*AP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	1	18	Total	Br	C	N	O	P	0	0	0
			368	1	176	66	108	17			
13	4	18	Total	Br	C	N	O	P	0	0	0
			368	1	176	66	108	17			

- Molecule 14 is a DNA chain called 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP *T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	6	Total	C	N	O	P	0	0	0
			117	58	20	34	5			
14	5	6	Total	C	N	O	P	0	0	0
			117	58	20	34	5			

- Molecule 15 is a RNA chain called 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP *AP*GP*GP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	11	Total 230	C 104	N 41	O 75	P 10	0	0	0
15	6	11	Total 230	C 104	N 41	O 75	P 10	0	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

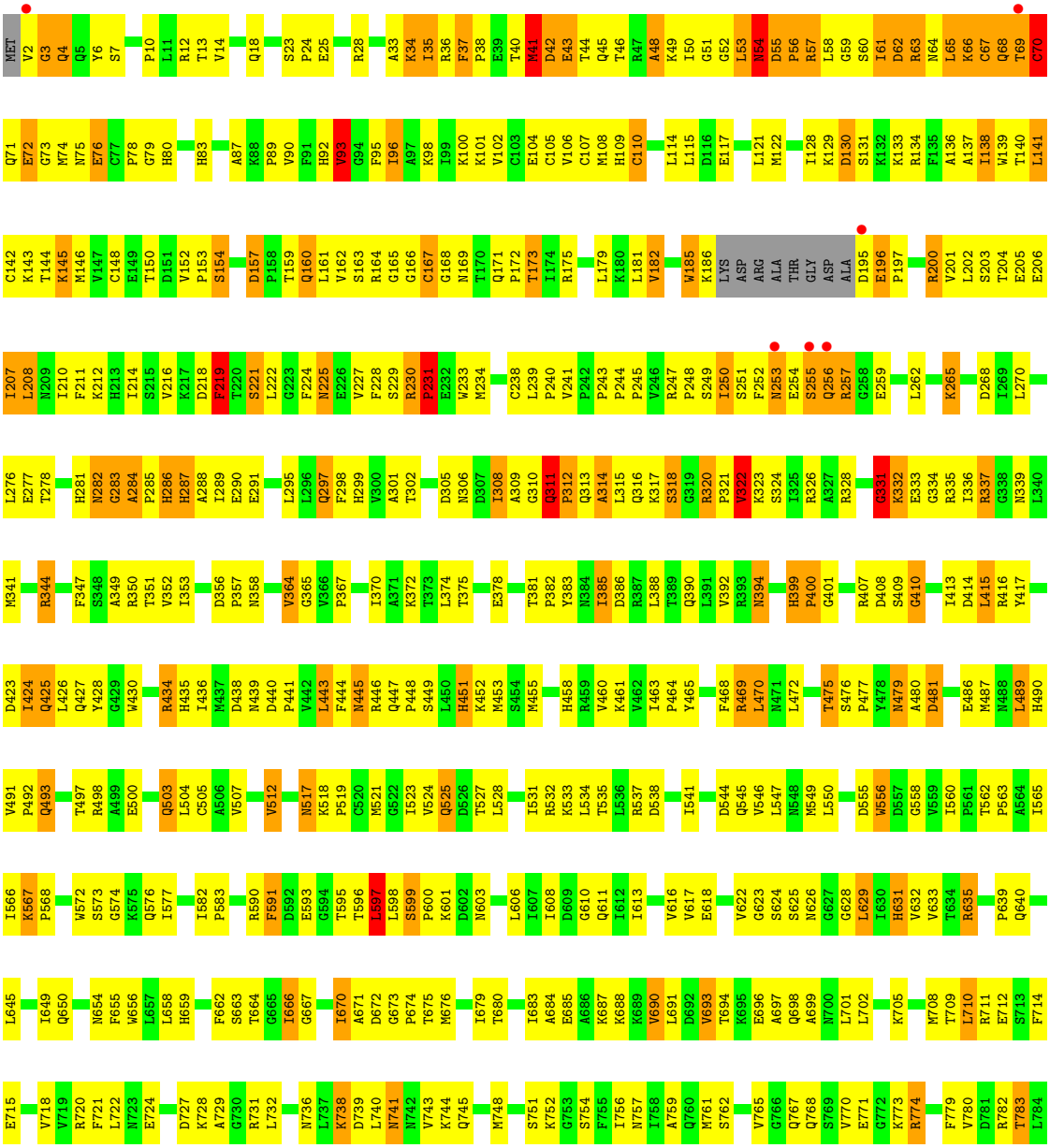
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total 2	Zn 2	0	0
16	B	1	Total 1	Zn 1	0	0
16	C	1	Total 1	Zn 1	0	0
16	I	2	Total 2	Zn 2	0	0
16	J	1	Total 1	Zn 1	0	0
16	L	1	Total 1	Zn 1	0	0
16	M	2	Total 2	Zn 2	0	0
16	N	1	Total 1	Zn 1	0	0
16	O	1	Total 1	Zn 1	0	0
16	U	2	Total 2	Zn 2	0	0
16	V	1	Total 1	Zn 1	0	0
16	X	1	Total 1	Zn 1	0	0

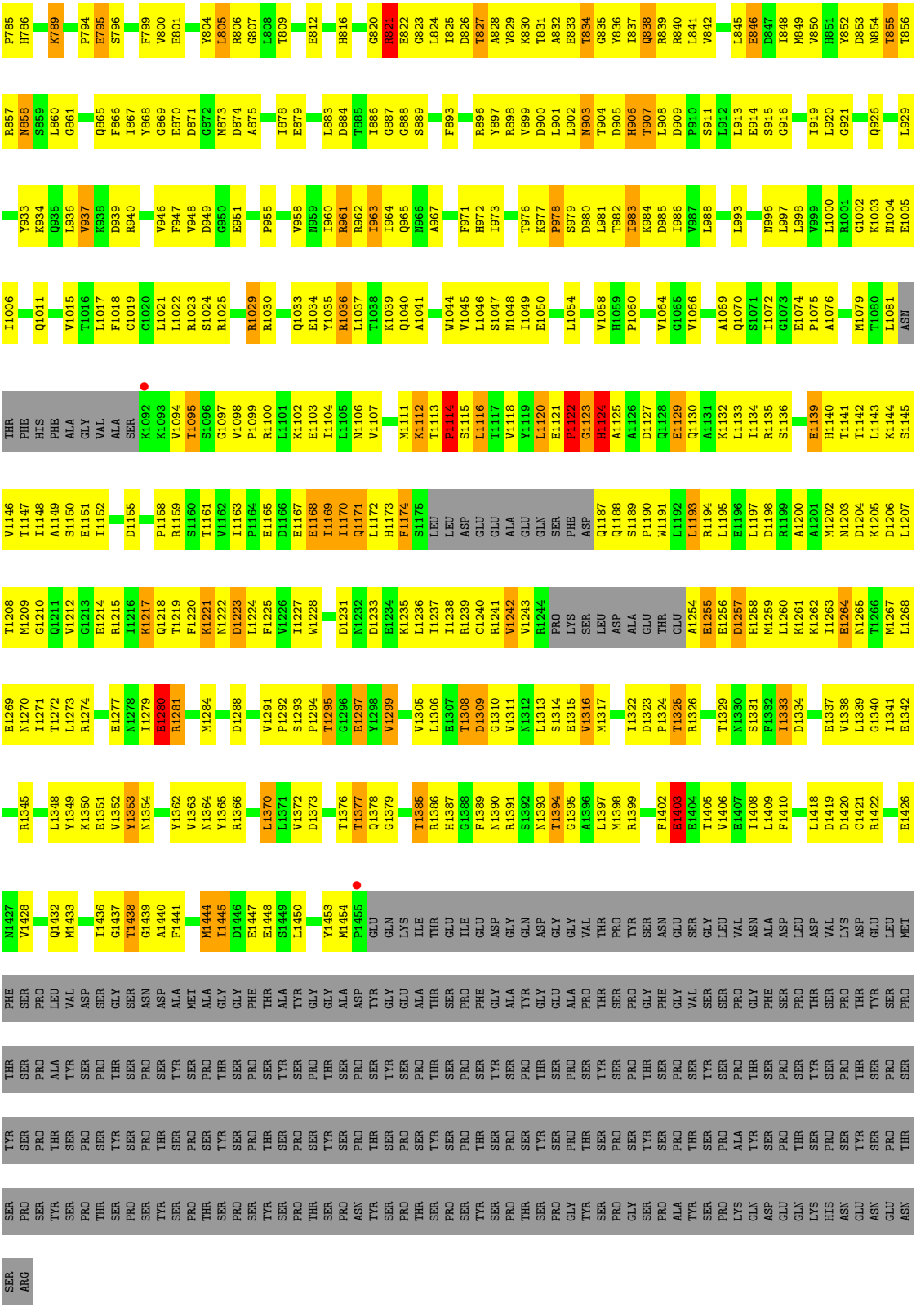
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

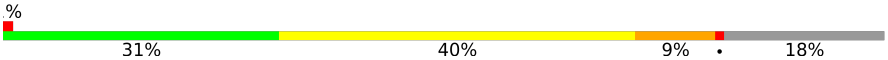
Chain A:

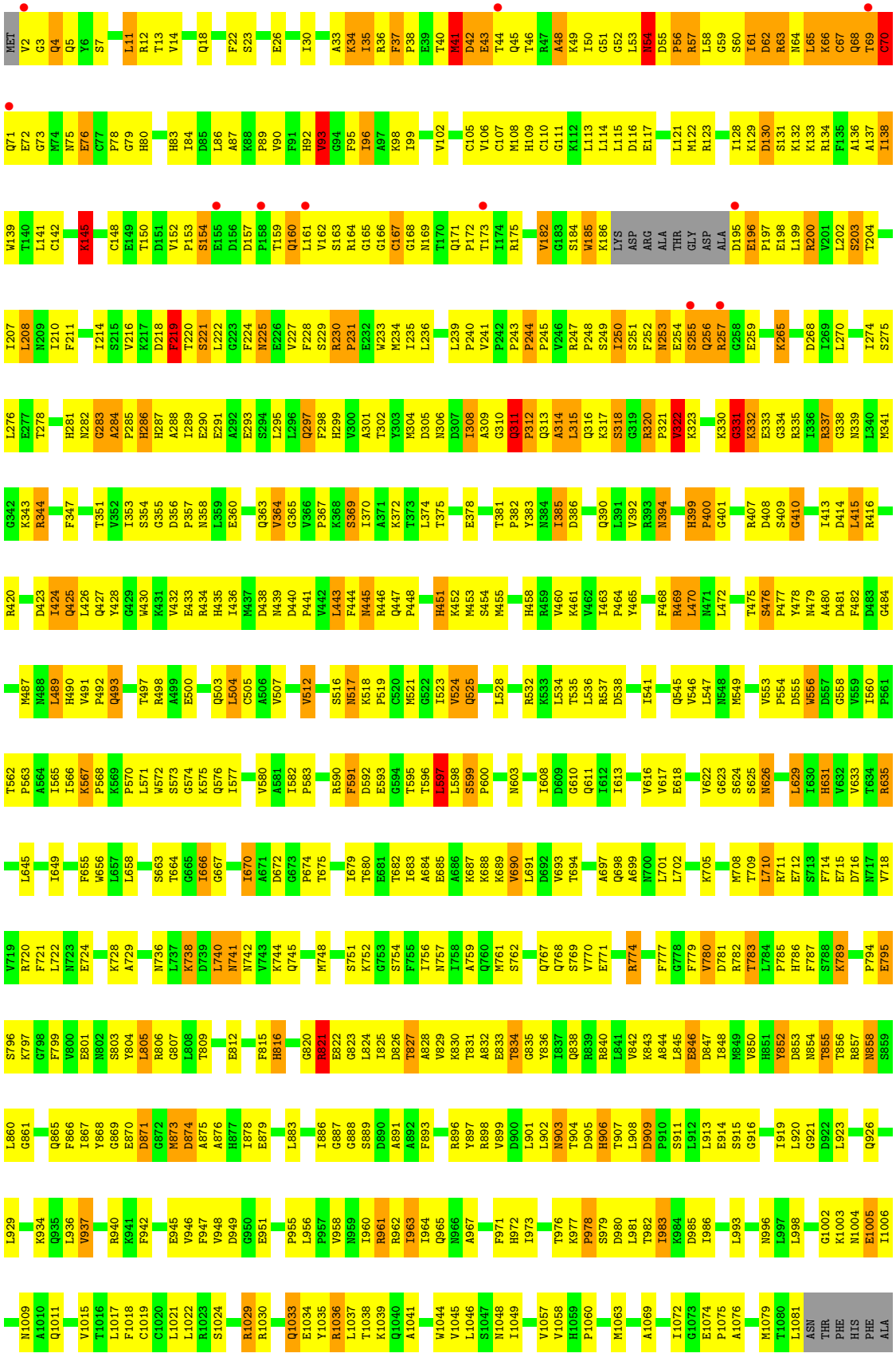




• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain M:

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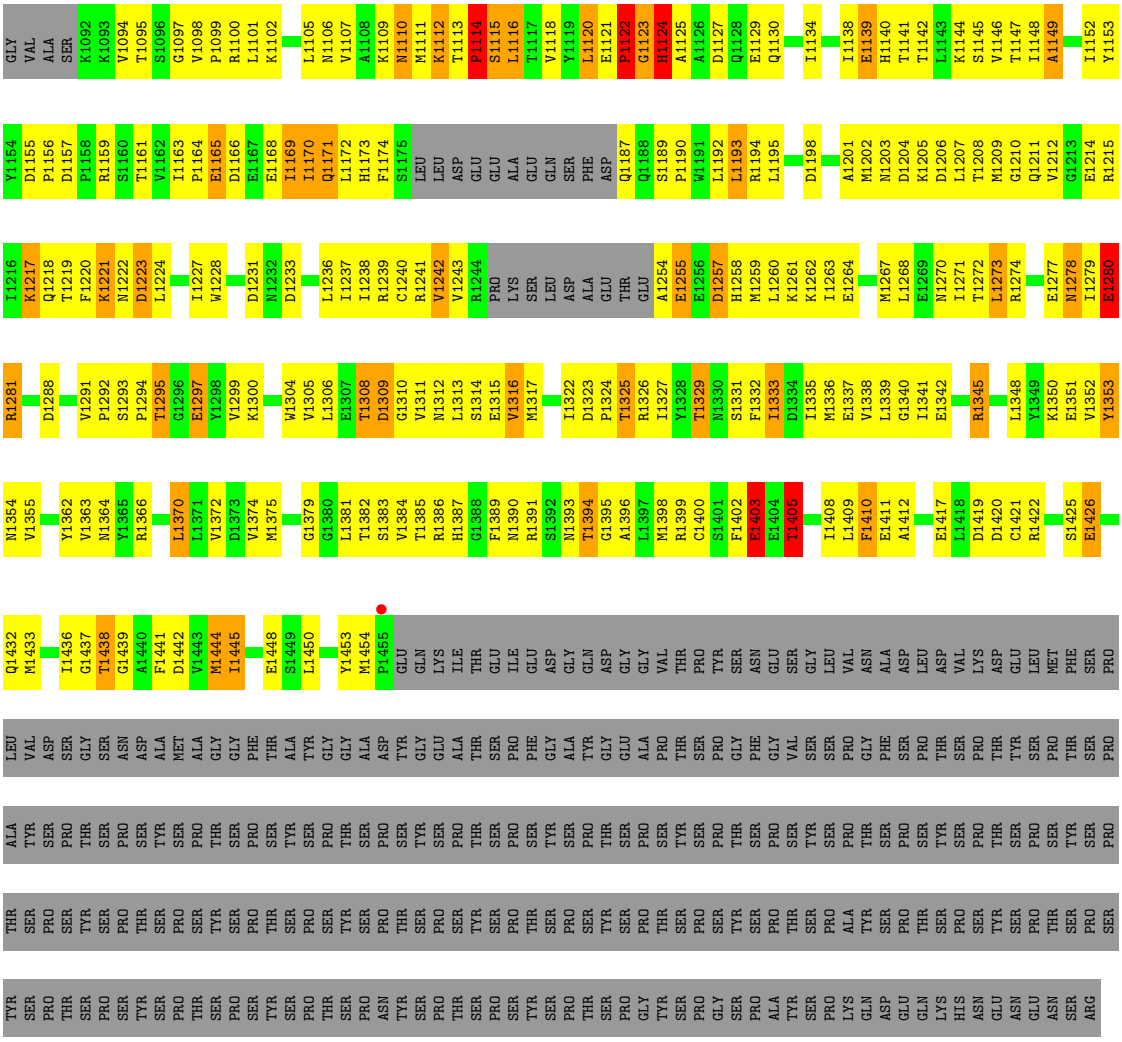
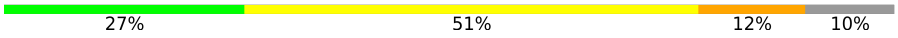
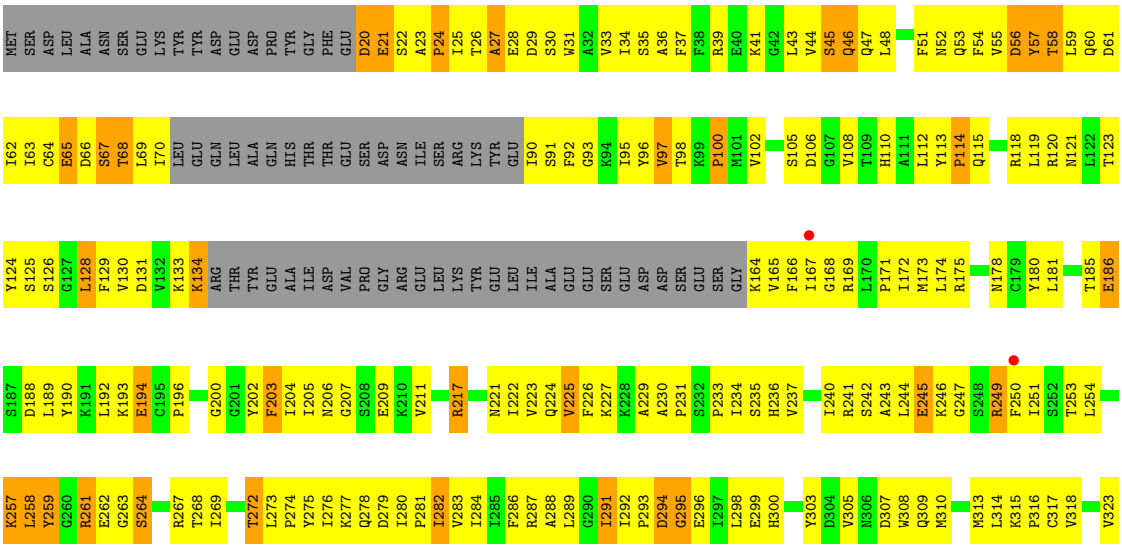
Q71 E72 G73 M74 N75 E76 C77 P78 G79 H80 H83 I84 D85 L86 A87 K88 P89 V90 F91 H92 V93 G94 F95 I96 A97 K98 I99 V102 C105 V106 C107 M108 H109 C110 G111 K112 L113 L114 L115 D116 E117 L121 M122 R123 I128 K129 D130 S131 K132 K133 R134 F135 A136 A137 I138
W139 T140 L141 C142 K145 C148 E149 T150 D151 V152 P153 S154 E155 D156 D157 P158 T159 Q160 L161 V162 S163 R164 G165 G166 C167 G168 N169 T170 Q171 P172 T173 I174 R175 V182 G183 S184 W185 K186 LYS ASP ARG ALA THR GLY ASP ALA D195 E196 P197 E198 L199 R200 V201 L202 S203 T204
I207 L208 N209 I210 F211 I214 S215 V216 K217 D218 F219 T220 S221 L222 G223 F224 N225 E226 V227 F228 S229 R230 P231 E232 W233 M234 I235 L236 L239 P240 V241 P242 P243 P244 P245 V246 R247 P248 S249 I250 S251 F252 N253 E254 S255 Q256 R257 G258 E259 K265 D268 I269 L270 I274 S275
L276 E277 T278 H281 N282 G283 A284 P285 H286 H287 A288 I289 E290 E291 A292 E293 S294 L295 L296 Q297 F298 H299 V300 A301 T302 Y303 M304 D305 N306 D307 I308 A309 G310 Q311 P312 Q313 A314 L315 Q316 K317 S318 G319 R320 P321 V322 K323 K330 Q331 K332 E333 G334 R335 I336 R337 G338 N339 L340 M341
G342 K343 R344 F347 T351 V352 I353 S354 G355 D356 P357 N358 L359 E360 Q363 V364 G365 V366 P367 K368 S369 I370 A371 K372 T373 L374 T375 E378 T381 P382 Y383 N384 I385 D386 Q390 L391 V392 R393 N394 H399 P400 G401 R407 D408 S409 G410 I413 D414 L415 R416
R420 D423 I424 Q425 L426 Q427 Y428 G429 W430 K431 V432 E433 R434 H435 I436 M437 D438 N439 D440 P441 V442 L443 F444 N445 R446 Q447 P448 H451 K452 M453 S454 M455 H458 R459 V460 K461 V462 I463 P464 Y465 F468 R469 L470 N471 L472 T475 S476 P477 Y478 N479 A480 D481 F482 D483 G484
M487 N488 L489 H490 V491 P492 Q493 T497 R498 A499 E500 Q503 L504 C505 A506 V507 V512 S516 N517 K518 P519 C520 M521 G522 I523 V524 Q525 L528 R532 K533 L534 T535 L536 R537 D538 I541 Q545 V546 L547 N548 M549 V553 P554 D555 M556 D557 G558 V559 I560 P561
T562 P563 A564 I565 I566 K567 P568 K569 P570 L571 W572 S573 G574 K575 Q576 I577 V580 A581 I582 P583 R590 F591 D592 E593 G594 T595 T596 L597 L598 S599 P600 N603 I608 D609 G610 Q611 I612 I613 V616 V617 E618 V622 G623 S624 S625 N626 L629 I630 H631 V632 V633 T634 R635
L645 I649 F655 W656 L657 L658 S663 T664 G665 I666 G667 I670 A671 D672 G673 P674 T675 I679 T680 E681 T682 I683 A684 E685 A686 K687 K688 K689 V690 L691 D692 V693 T694 A697 Q698 A699 N700 L701 L702 K705 W708 T709 L710 R711 E712 S713 F714 E715 D716 N717 V718
V719 R720 F721 L722 N723 E724 K728 A729 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 M748 S751 K752 G753 S754 F755 I756 N757 I758 A759 Q760 M761 S762 Q767 Q768 S769 V770 E771 R774 F777 G778 F779 V780 D781 R782 T783 L784 P785 H786 F787 S788 K789 P794 E795
S796 K797 G798 E799 V800 E801 N802 S803 Y804 L805 R806 G807 L808 T809 E812 F815 H816 G820 R821 E822 G823 L824 I825 D826 T827 A828 V829 K830 T831 A832 E833 T834 G835 Y836 I837 Q838 R839 R840 L841 V842 K843 A844 L845 E846 D847 I848 M849 V850 H851 Y852 D853 N854 T855 T856 R857 N858 S859
L860 G861 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 A876 H877 I878 E879 L883 I886 G887 G888 S889 D890 A891 A892 F893 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908 D909 P910 S911 L912 L913 E914 S915 G916 I919 L920 G921 D922 L923 Q926
L929 K934 Q935 L936 V937 R940 K941 F942 E945 V946 F947 V948 D949 G950 E951 P955 L956 P957 V958 N959 I960 R961 R962 I963 I964 Q965 N966 A967 F971 H972 I973 T976 K977 P978 S979 D980 L981 T982 I983 K984 D985 I986 L993 N996 L997 L998 G1002 K1003 N1004 E1005 I1006
N1009 A1010 Q1011 V1015 T1016 L1017 F1018 C1019 C1020 L1021 L1022 R1023 S1024 R1029 R1030 Q1033 E1034 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 W1044 V1045 L1046 S1047 N1048 I1049 V1057 V1058 H1059 P1060 M1063 A1069 I1072 G1073 E1074 P1075 A1076 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA

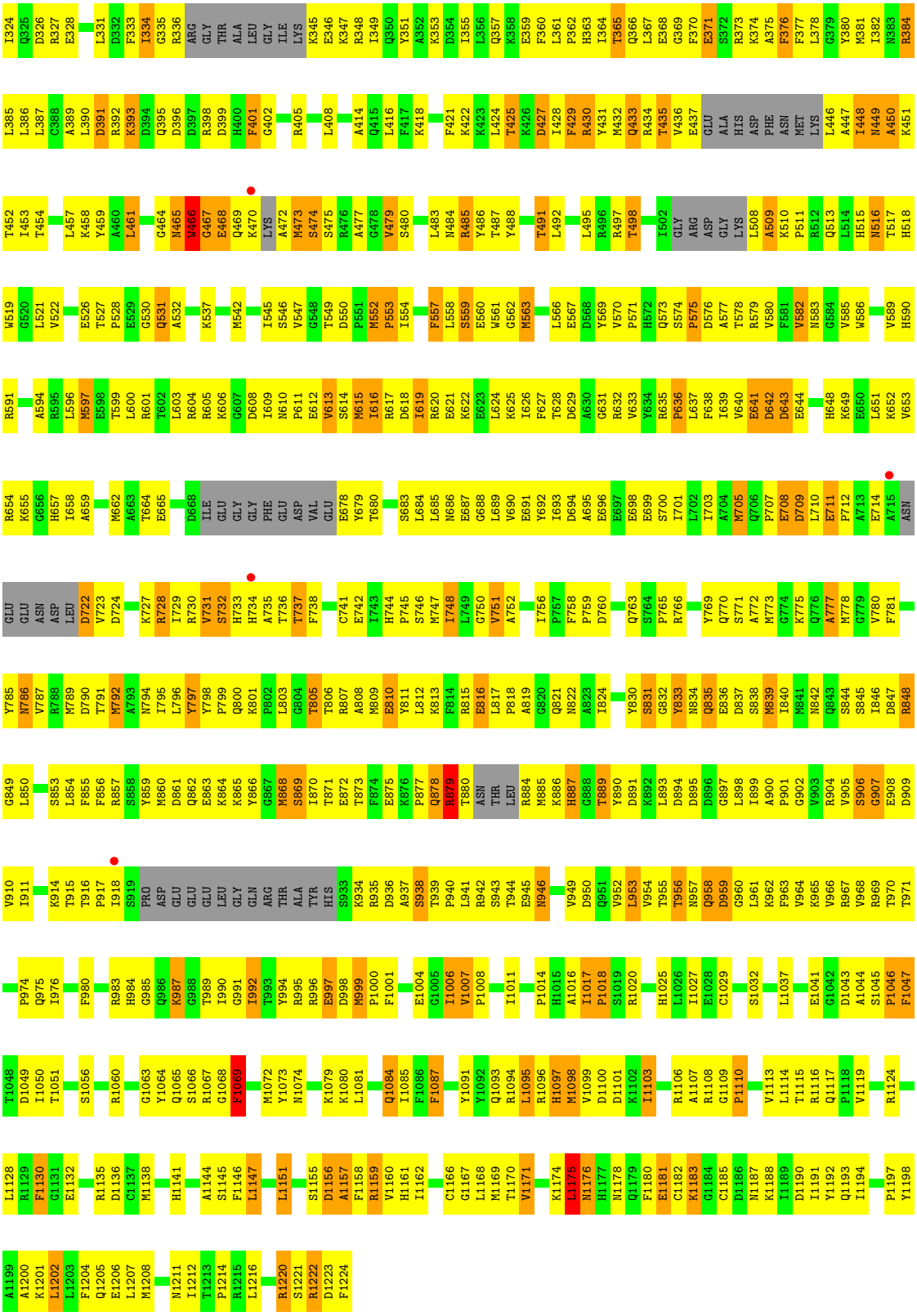


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

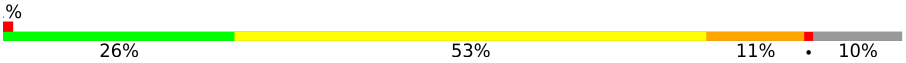
Chain B:

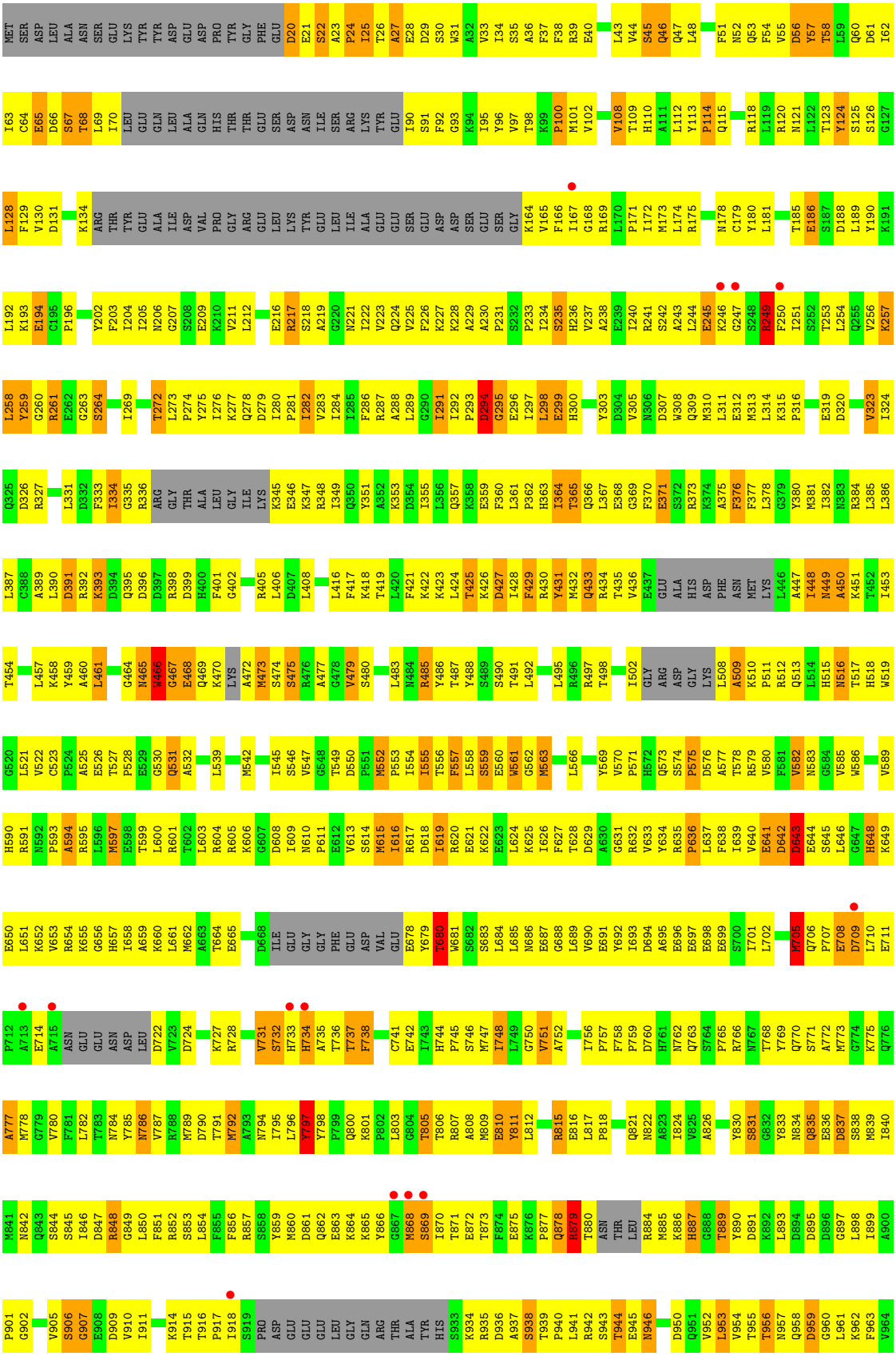


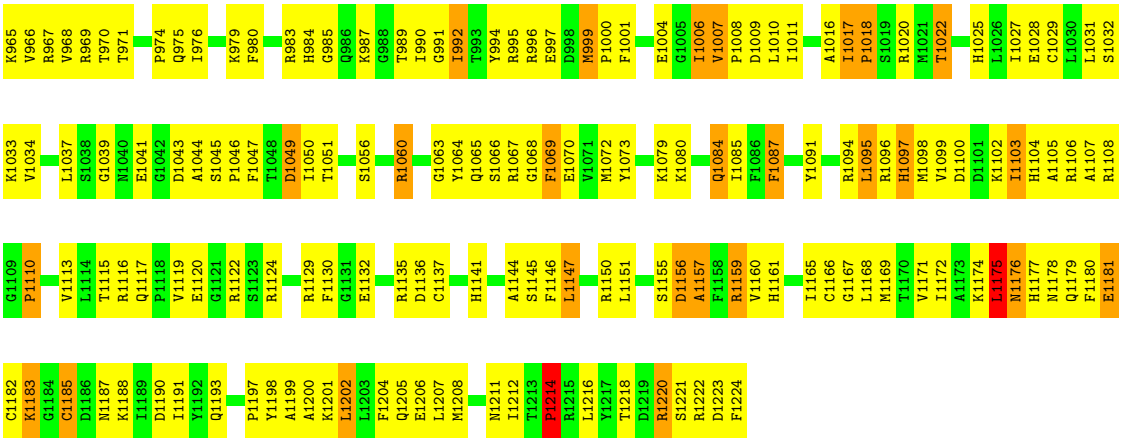




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

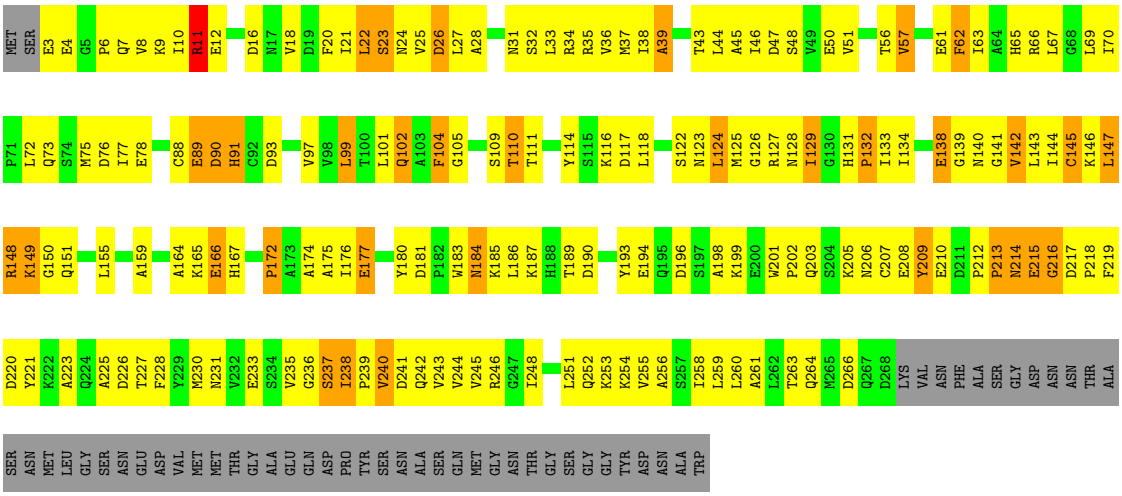






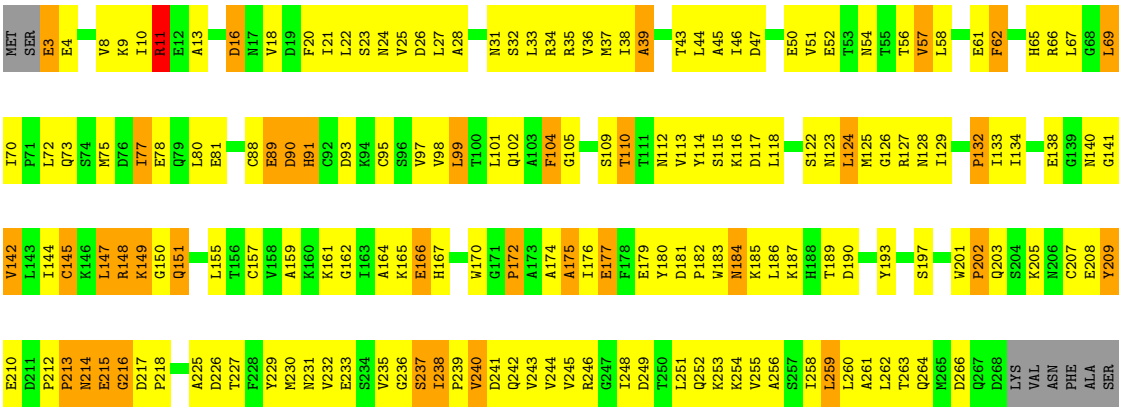
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



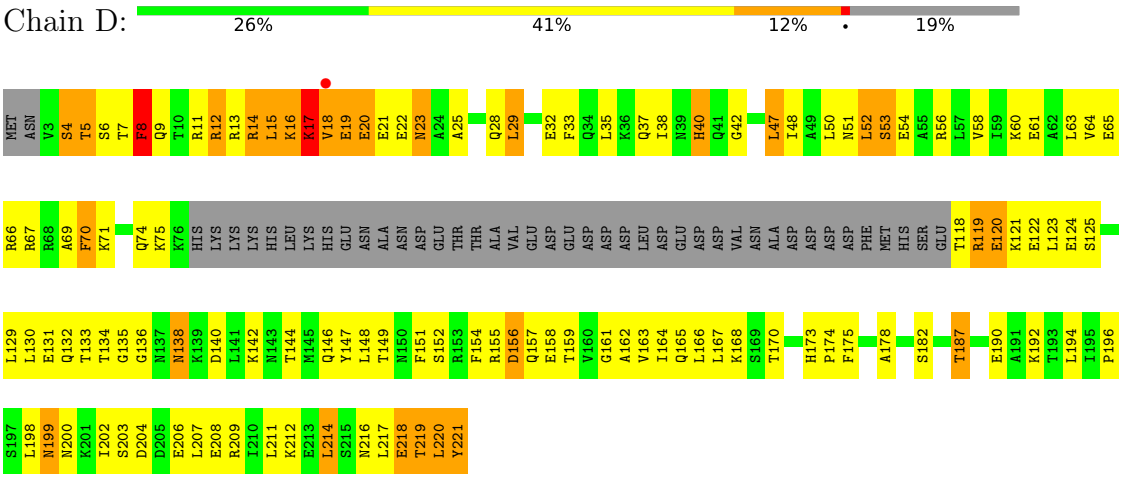
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain O:



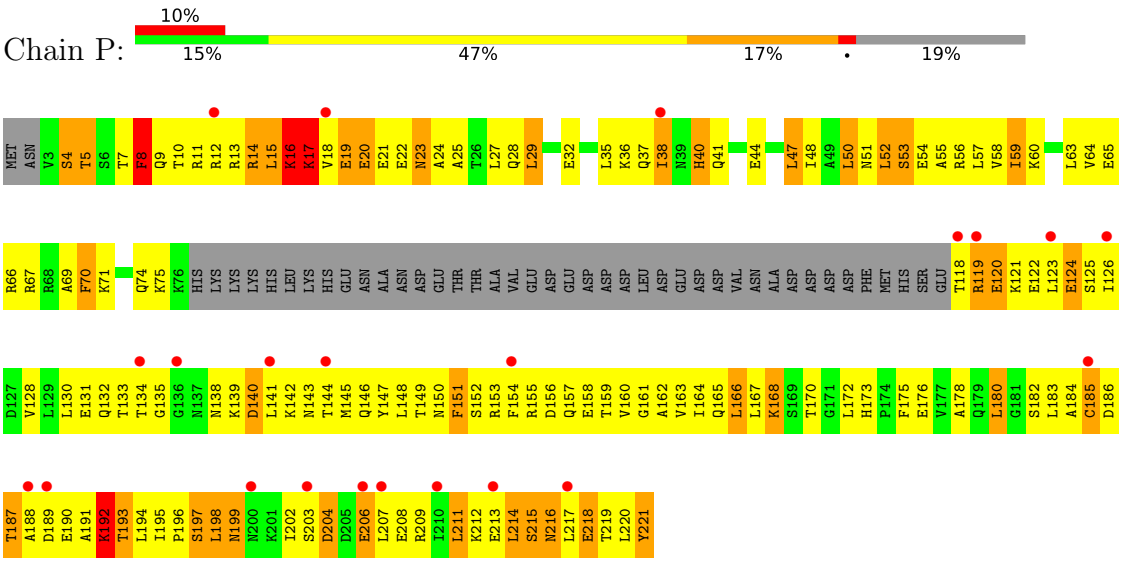
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



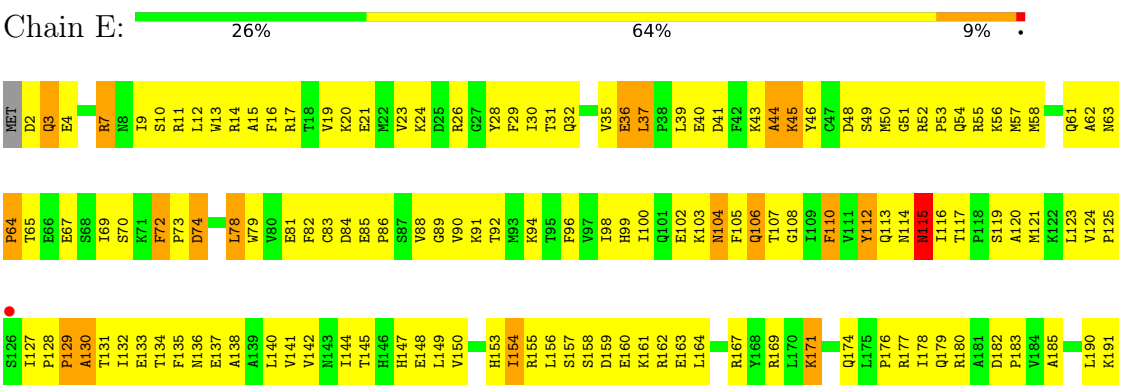
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain P:



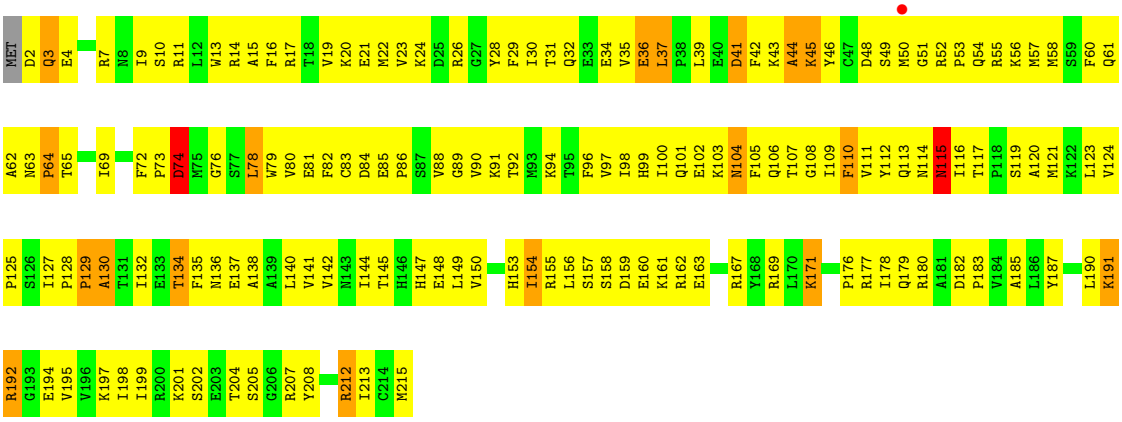
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



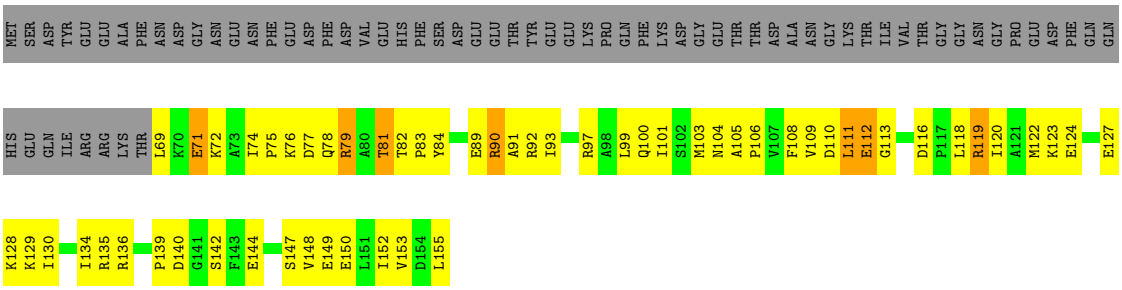
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain Q:



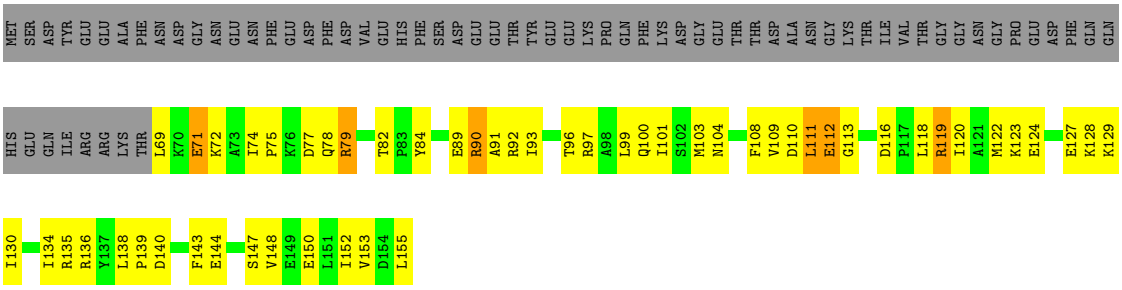
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



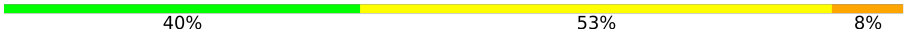
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

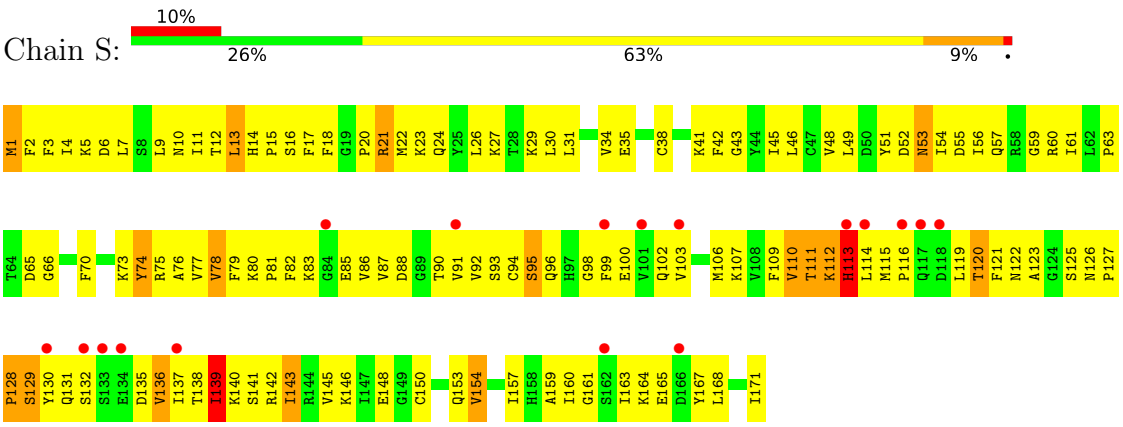
Chain R:



• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



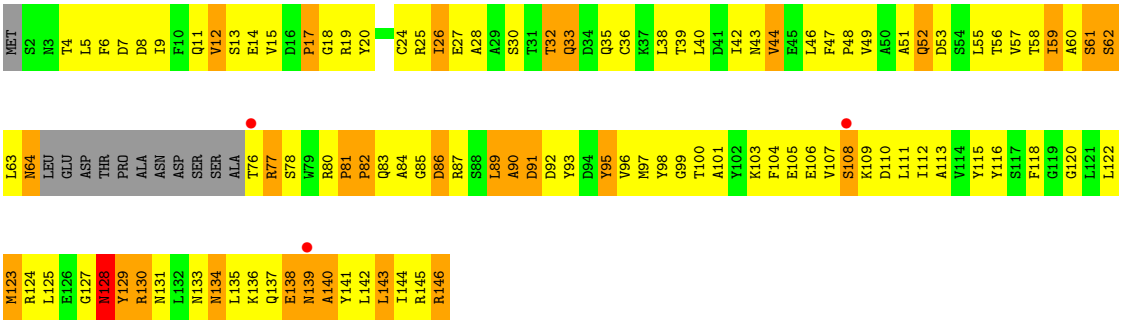


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain S:

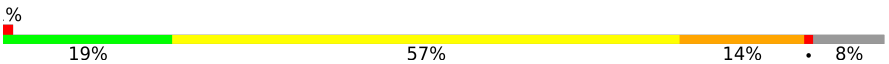
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

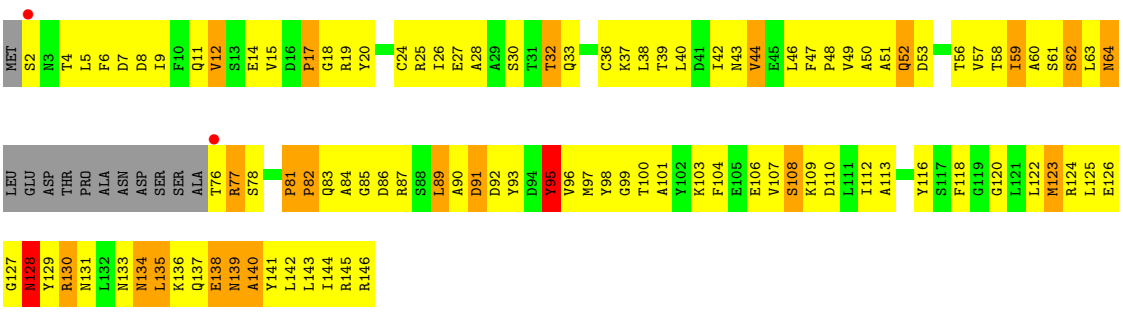
Chain H:



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

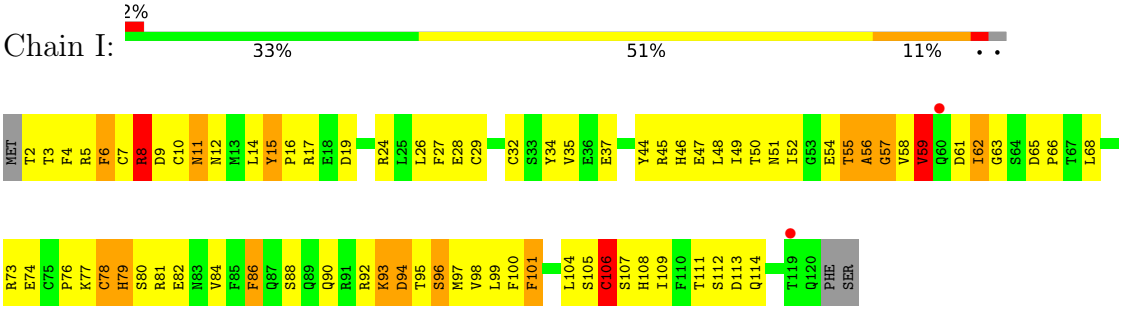
Chain T:





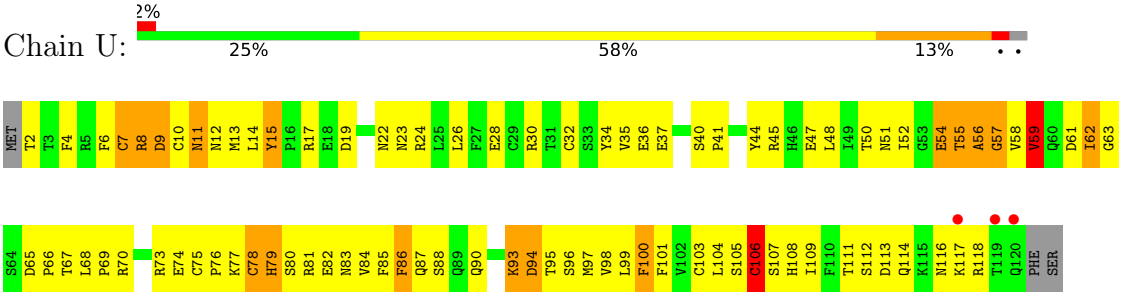
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



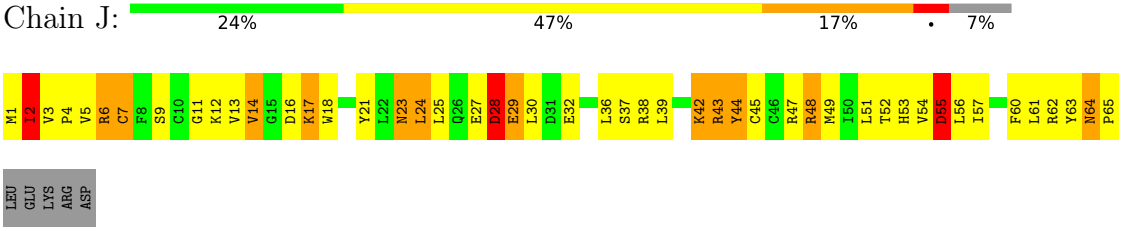
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain U:



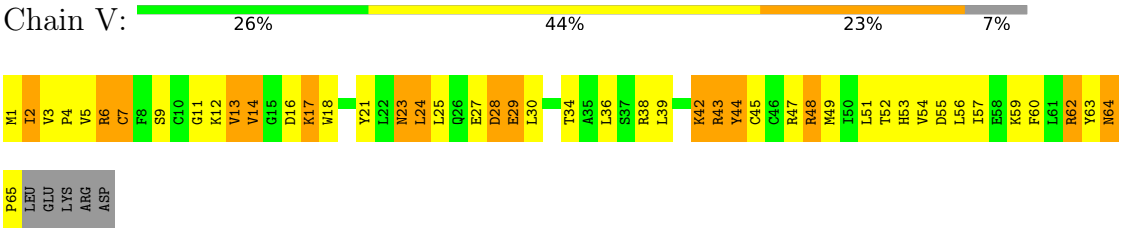
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



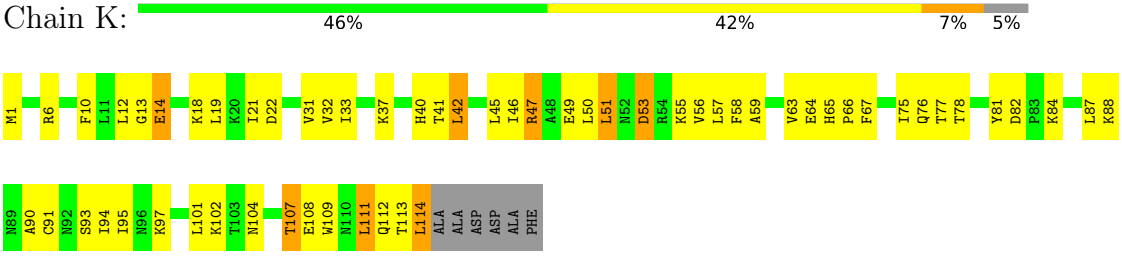
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain V:



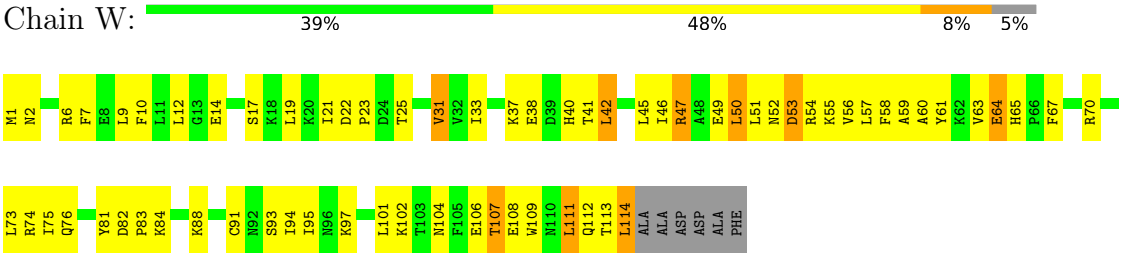
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



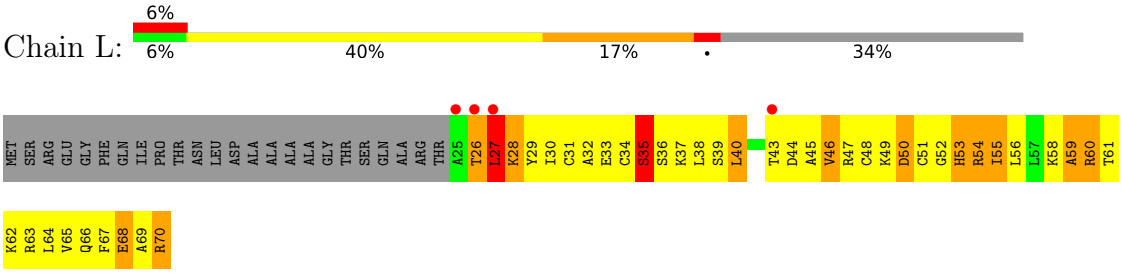
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain W:



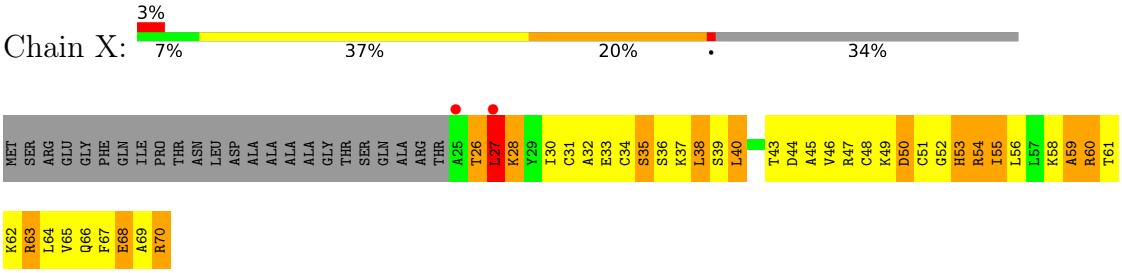
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



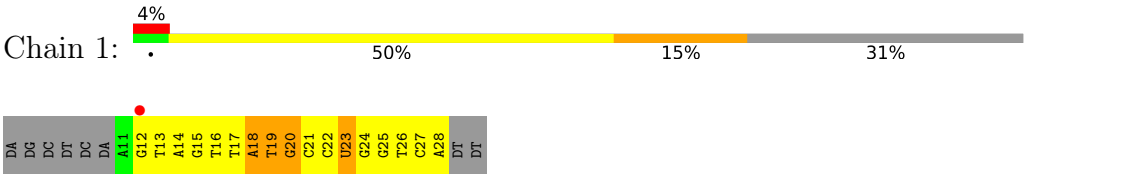
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain X:



• Molecule 13: 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*C P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'

Chain 1:



• Molecule 13: 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*C P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'

Chain 4:

• Molecule 14: 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'

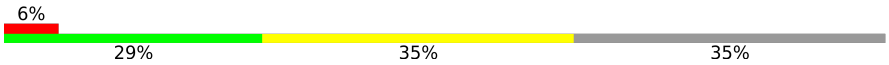
Chain 2:

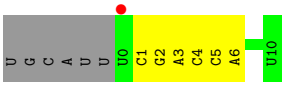
• Molecule 14: 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'

Chain 5:

• Molecule 15: 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*U)-3
'

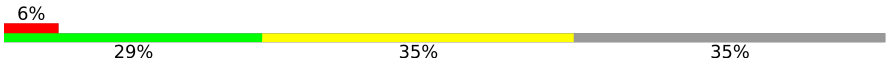
Chain 3:

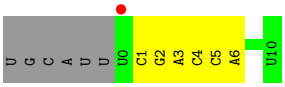




• Molecule 15: 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*U)-3
'

Chain 6:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	394.26Å 221.61Å 283.45Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 38.25 – 3.02	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.00-3.20) 85.7 (38.25-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.233 , 0.252 0.235 , 0.241	Depositor DCC
R_{free} test set	20910 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.018 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.017 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.017 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.257 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	63664	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BRU, 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	0.50	0/11342	0.77	8/15337 (0.1%)
1	M	0.50	0/11342	0.78	8/15337 (0.1%)
2	B	0.48	0/8948	0.74	1/12062 (0.0%)
2	N	0.48	1/8948 (0.0%)	0.74	1/12062 (0.0%)
3	C	0.49	0/2133	0.73	1/2891 (0.0%)
3	O	0.48	0/2133	0.74	1/2891 (0.0%)
4	D	0.44	0/1444	0.72	1/1935 (0.1%)
4	P	0.53	0/1444	0.85	5/1935 (0.3%)
5	E	0.46	0/1788	0.69	1/2406 (0.0%)
5	Q	0.46	0/1788	0.70	1/2406 (0.0%)
6	F	0.57	0/717	0.82	1/967 (0.1%)
6	R	0.56	0/717	0.82	1/967 (0.1%)
7	G	0.46	0/1368	0.75	1/1844 (0.1%)
7	S	0.57	0/1368	0.86	1/1844 (0.1%)
8	H	0.43	0/1094	0.71	0/1481
8	T	0.42	0/1094	0.72	0/1481
9	I	0.42	0/989	0.71	0/1331
9	U	0.45	0/989	0.71	0/1331
10	J	0.51	0/541	0.83	0/727
10	V	0.48	0/541	0.80	0/727
11	K	0.46	0/937	0.67	0/1265
11	W	0.48	0/937	0.68	0/1265
12	L	0.58	0/365	0.84	0/485
12	X	0.57	0/365	0.84	0/485
13	1	0.60	0/389	0.96	0/597
13	4	0.60	0/389	0.94	0/597
14	2	0.61	0/130	0.78	0/198
14	5	0.60	0/130	0.78	0/198
15	3	0.56	0/256	0.74	0/397
15	6	0.54	0/256	0.74	0/397
All	All	0.49	1/64882 (0.0%)	0.76	32/87846 (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
2	B	0	1
2	N	0	2
13	1	0	4
13	4	0	4
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1137	CYS	CB-SG	-5.78	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	180	LEU	CA-CB-CG	-7.93	97.05	115.30
4	P	166	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	56	PRO	N-CA-C	-6.37	95.55	112.10
1	M	56	PRO	N-CA-C	-6.35	95.59	112.10
3	C	39	ALA	N-CA-C	5.97	127.11	111.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1	18	DA	Sidechain
13	1	19	DT	Sidechain
13	1	20	DG	Sidechain
13	1	21	DC	Sidechain
2	B	833	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11143	0	11217	1159	0
1	M	11143	0	11217	1163	0
2	B	8779	0	8808	1066	0
2	N	8779	0	8808	1078	0
3	C	2095	0	2051	226	0
3	O	2095	0	2051	227	0
4	D	1434	0	1460	152	0
4	P	1434	0	1460	273	0
5	E	1752	0	1776	187	0
5	Q	1752	0	1776	202	0
6	F	705	0	731	85	0
6	R	705	0	731	75	0
7	G	1340	0	1357	145	0
7	S	1340	0	1357	205	0
8	H	1076	0	1046	171	0
8	T	1076	0	1046	154	0
9	I	971	0	929	117	0
9	U	971	0	929	126	0
10	J	532	0	542	97	0
10	V	532	0	542	95	0
11	K	919	0	929	81	0
11	W	919	0	929	84	0
12	L	363	0	387	87	0
12	X	363	0	387	84	0
13	1	368	0	203	27	0
13	4	368	0	203	27	0
14	2	117	0	70	13	0
14	5	117	0	70	11	0
15	3	230	0	121	8	0
15	6	230	0	121	8	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
16	M	2	0	0	0	0
16	N	1	0	0	0	0
16	O	1	0	0	0	0
16	U	2	0	0	0	0
16	V	1	0	0	0	0
16	X	1	0	0	0	0
All	All	63664	0	63254	6846	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 54.

The worst 5 of 6846 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:N:510:LYS:HG3	2:N:511:PRO:HD3	1.21	1.17
1:A:855:THR:HG21	1:A:857:ARG:HE	1.08	1.16
9:U:111:THR:HG22	9:U:113:ASP:H	1.05	1.15
5:Q:124:VAL:HG13	5:Q:132:ILE:HB	1.28	1.15
8:H:4:THR:HA	8:H:60:ALA:HB2	1.26	1.14

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	1406/1733 (81%)	1075 (76%)	225 (16%)	106 (8%)	1	7
1	M	1406/1733 (81%)	1073 (76%)	228 (16%)	105 (8%)	1	7
2	B	1082/1224 (88%)	800 (74%)	186 (17%)	96 (9%)	1	4
2	N	1082/1224 (88%)	798 (74%)	186 (17%)	98 (9%)	1	3
3	C	264/318 (83%)	202 (76%)	41 (16%)	21 (8%)	1	6
3	O	264/318 (83%)	203 (77%)	42 (16%)	19 (7%)	1	7
4	D	174/221 (79%)	120 (69%)	37 (21%)	17 (10%)	0	3
4	P	174/221 (79%)	122 (70%)	34 (20%)	18 (10%)	0	3
5	E	212/215 (99%)	155 (73%)	41 (19%)	16 (8%)	1	7
5	Q	212/215 (99%)	159 (75%)	37 (18%)	16 (8%)	1	7
6	F	85/155 (55%)	72 (85%)	11 (13%)	2 (2%)	6	34
6	R	85/155 (55%)	72 (85%)	11 (13%)	2 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	169/171 (99%)	141 (83%)	23 (14%)	5 (3%)	4 28
7	S	169/171 (99%)	139 (82%)	23 (14%)	7 (4%)	3 21
8	H	130/146 (89%)	85 (65%)	25 (19%)	20 (15%)	0 1
8	T	130/146 (89%)	85 (65%)	25 (19%)	20 (15%)	0 1
9	I	117/122 (96%)	77 (66%)	28 (24%)	12 (10%)	0 3
9	U	117/122 (96%)	78 (67%)	28 (24%)	11 (9%)	0 3
10	J	63/70 (90%)	43 (68%)	9 (14%)	11 (18%)	0 0
10	V	63/70 (90%)	42 (67%)	10 (16%)	11 (18%)	0 0
11	K	112/120 (93%)	89 (80%)	20 (18%)	3 (3%)	5 30
11	W	112/120 (93%)	89 (80%)	19 (17%)	4 (4%)	3 23
12	L	44/70 (63%)	19 (43%)	15 (34%)	10 (23%)	0 0
12	X	44/70 (63%)	19 (43%)	15 (34%)	10 (23%)	0 0
All	All	7716/9130 (84%)	5757 (75%)	1319 (17%)	640 (8%)	1 5

5 of 640 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	43	GLU
1	A	57	ARG
1	A	62	ASP
1	A	63	ARG

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	1239/1520 (82%)	1116 (90%)	123 (10%)	8 30
1	M	1239/1520 (82%)	1107 (89%)	132 (11%)	6 27
2	B	958/1061 (90%)	860 (90%)	98 (10%)	7 29
2	N	958/1061 (90%)	853 (89%)	105 (11%)	6 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	234/274 (85%)	212 (91%)	22 (9%)	8 33
3	O	234/274 (85%)	207 (88%)	27 (12%)	5 24
4	D	160/200 (80%)	136 (85%)	24 (15%)	3 14
4	P	160/200 (80%)	127 (79%)	33 (21%)	1 6
5	E	196/197 (100%)	183 (93%)	13 (7%)	16 51
5	Q	196/197 (100%)	184 (94%)	12 (6%)	18 54
6	F	77/137 (56%)	71 (92%)	6 (8%)	12 43
6	R	77/137 (56%)	72 (94%)	5 (6%)	17 51
7	G	152/152 (100%)	140 (92%)	12 (8%)	12 43
7	S	152/152 (100%)	134 (88%)	18 (12%)	5 23
8	H	118/128 (92%)	105 (89%)	13 (11%)	6 26
8	T	118/128 (92%)	108 (92%)	10 (8%)	10 38
9	I	113/116 (97%)	101 (89%)	12 (11%)	6 27
9	U	113/116 (97%)	103 (91%)	10 (9%)	10 36
10	J	60/65 (92%)	51 (85%)	9 (15%)	3 14
10	V	60/65 (92%)	53 (88%)	7 (12%)	5 23
11	K	99/102 (97%)	94 (95%)	5 (5%)	24 60
11	W	99/102 (97%)	90 (91%)	9 (9%)	9 34
12	L	40/57 (70%)	34 (85%)	6 (15%)	3 14
12	X	40/57 (70%)	33 (82%)	7 (18%)	2 9
All	All	6892/8018 (86%)	6174 (90%)	718 (10%)	7 28

5 of 718 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	1333	ILE
2	N	1175	LEU
2	N	22	SER
1	M	1329	THR
2	N	597	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 226 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	65	HIS
9	U	108	HIS
1	M	858	ASN
9	U	83	ASN
4	P	51	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	3	10/17 (58%)	0	0
15	6	10/17 (58%)	0	0
All	All	20/34 (58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
13	BRU	4	23	13,15	18,21,22	3.89	1 (5%)	26,30,33	0.98	1 (3%)
13	BRU	1	23	13,15	18,21,22	3.87	1 (5%)	26,30,33	0.98	1 (3%)

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
13	BRU	4	23	13,15	-	1/7/21/22	0/2/2/2
13	BRU	1	23	13,15	-	1/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	23	BRU	BR-C5	-16.39	1.50	1.88
13	1	23	BRU	BR-C5	-16.29	1.50	1.88

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	4	23	BRU	C6-C5-C4	-2.99	117.64	120.67
13	1	23	BRU	C6-C5-C4	-2.99	117.64	120.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	1	23	BRU	O4'-C4'-C5'-O5'
13	4	23	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	4	23	BRU	6	0
13	1	23	BRU	6	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1416/1733 (81%)	-0.10	8 (0%) 89 83	12, 52, 93, 119	0
1	M	1416/1733 (81%)	-0.08	12 (0%) 86 78	10, 53, 94, 123	0
2	B	1104/1224 (90%)	-0.04	6 (0%) 91 86	12, 62, 103, 120	0
2	N	1104/1224 (90%)	0.02	13 (1%) 79 67	16, 65, 104, 121	0
3	C	266/318 (83%)	-0.13	0 100 100	24, 52, 83, 100	0
3	O	266/318 (83%)	-0.14	0 100 100	25, 54, 85, 106	0
4	D	178/221 (80%)	-0.07	1 (0%) 89 83	36, 68, 100, 108	0
4	P	178/221 (80%)	0.76	22 (12%) 4 2	55, 85, 105, 113	0
5	E	214/215 (99%)	-0.03	1 (0%) 91 86	35, 80, 106, 114	0
5	Q	214/215 (99%)	0.08	1 (0%) 91 86	35, 82, 107, 119	0
6	F	87/155 (56%)	-0.30	0 100 100	13, 34, 62, 78	0
6	R	87/155 (56%)	-0.23	0 100 100	15, 34, 63, 76	0
7	G	171/171 (100%)	-0.10	0 100 100	37, 55, 85, 99	0
7	S	171/171 (100%)	0.71	17 (9%) 7 4	37, 69, 110, 116	0
8	H	134/146 (91%)	0.18	3 (2%) 62 48	60, 88, 105, 114	0
8	T	134/146 (91%)	0.16	2 (1%) 73 61	66, 89, 104, 116	0
9	I	119/122 (97%)	0.08	2 (1%) 70 57	47, 81, 102, 117	0
9	U	119/122 (97%)	0.08	3 (2%) 57 43	45, 84, 102, 119	0
10	J	65/70 (92%)	-0.18	0 100 100	23, 52, 74, 91	0
10	V	65/70 (92%)	-0.17	0 100 100	28, 53, 78, 91	0
11	K	114/120 (95%)	-0.28	0 100 100	23, 54, 72, 83	0
11	W	114/120 (95%)	-0.22	0 100 100	21, 54, 74, 84	0
12	L	46/70 (65%)	0.25	4 (8%) 10 5	37, 89, 107, 107	0
12	X	46/70 (65%)	0.26	2 (4%) 35 22	42, 93, 107, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	17/26 (65%)	0.16	1 (5%) 22 13	47, 101, 140, 144	0
13	4	17/26 (65%)	0.21	0 100 100	50, 102, 139, 142	0
14	2	6/13 (46%)	0.27	0 100 100	114, 121, 127, 133	0
14	5	6/13 (46%)	0.30	0 100 100	114, 121, 129, 136	0
15	3	11/17 (64%)	0.14	1 (9%) 9 5	88, 93, 131, 133	0
15	6	11/17 (64%)	0.08	1 (9%) 9 5	88, 96, 130, 133	0
All	All	7896/9242 (85%)	-0.02	100 (1%) 77 65	10, 61, 102, 144	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	734	HIS	5.0
4	P	188	ALA	4.9
7	S	137	ILE	4.8
4	P	185	CYS	4.5
7	S	116	PRO	4.3

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
13	BRU	1	23	20/21	0.70	0.21	85,89,94,97	0
13	BRU	4	23	20/21	0.75	0.19	83,89,95,98	0

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, 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
16	ZN	I	9989	1/1	0.90	0.17	117,117,117,117	0
16	ZN	M	9992	1/1	0.95	0.22	74,74,74,74	0
16	ZN	A	9984	1/1	0.96	0.19	70,70,70,70	0
16	ZN	J	9990	1/1	0.97	0.23	52,52,52,52	0
16	ZN	U	9997	1/1	0.97	0.18	119,119,119,119	0
16	ZN	X	9999	1/1	0.97	0.17	103,103,103,103	0
16	ZN	N	9994	1/1	0.98	0.22	38,38,38,38	0
16	ZN	O	9995	1/1	0.98	0.23	43,43,43,43	0
16	ZN	I	9988	1/1	0.98	0.23	65,65,65,65	0
16	ZN	A	9985	1/1	0.98	0.22	40,40,40,40	0
16	ZN	B	9986	1/1	0.99	0.24	33,33,33,33	0
16	ZN	L	9991	1/1	0.99	0.15	90,90,90,90	0
16	ZN	U	9996	1/1	0.99	0.22	71,71,71,71	0
16	ZN	C	9987	1/1	0.99	0.22	28,28,28,28	0
16	ZN	V	9998	1/1	0.99	0.25	52,52,52,52	0
16	ZN	M	9993	1/1	0.99	0.23	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.