wwPDB X-ray Structure Validation Summary Report (i)

Nov 12, 2024 – 11:59 AM EST

PDB ID	:	2R7Z
Title	:	Cisplatin lesion containing RNA polymerase II elongation complex
Authors	:	Damsma, G.E.; Alt, A.; Brueckner, F.; Carell, T.; Cramer, P.
Deposited on	:	2007-09-10
Resolution	:	3.80 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:

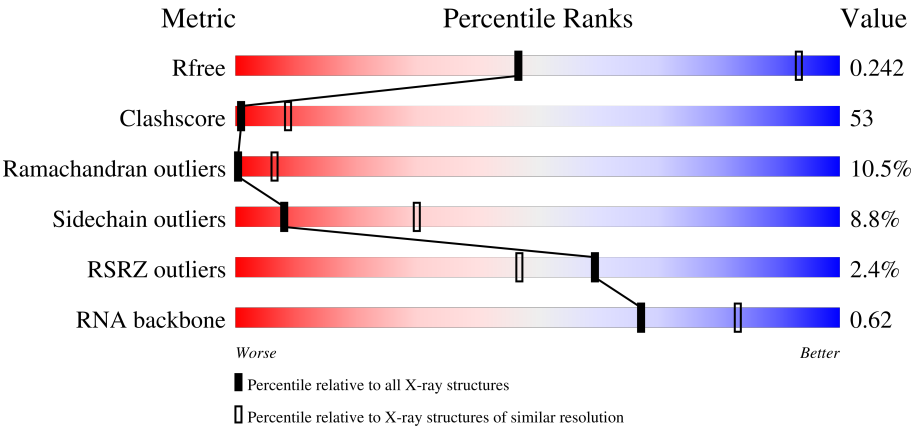
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1025 (3.98-3.62)
Clashscore	180529	1005 (3.96-3.64)
Ramachandran outliers	177936	1044 (3.98-3.62)
Sidechain outliers	177891	1039 (3.98-3.62)
RSRZ outliers	164620	1025 (3.98-3.62)
RNA backbone	3690	1131 (4.60-3.00)

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 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	T	17	6% 65% 29% 6%
2	N	7	14% 71% 29%
3	P	10	10% 20% 70% 10%
4	A	1733	% 26% 45% 10% • 18%

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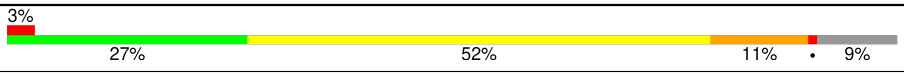
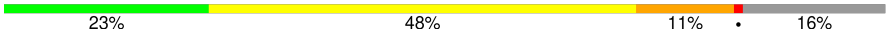
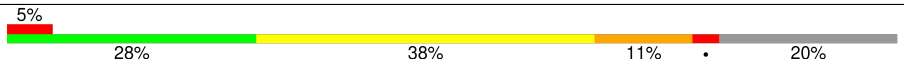
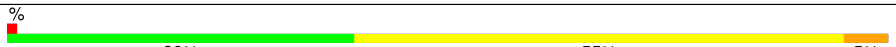
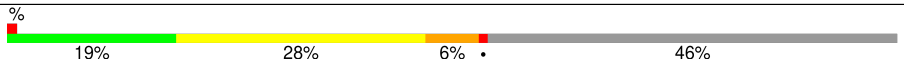
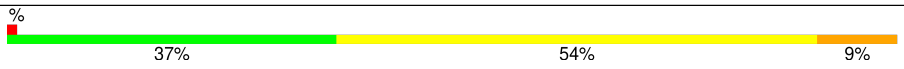
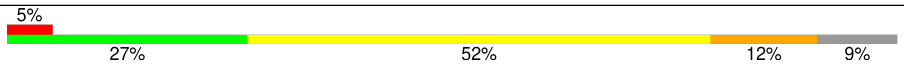
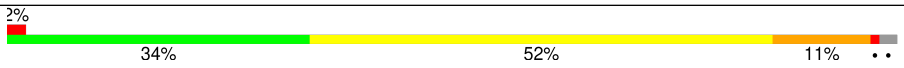
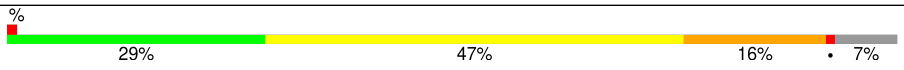
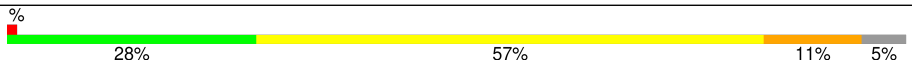
Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 31804 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 DNA chain called 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	17	336	163	53	104	16	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	N	7	143	69	30	38	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	10	216	97	41	69	9	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1416	11140	7021	1946	2111	62	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1108	8810	5580	1541	1634	55	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

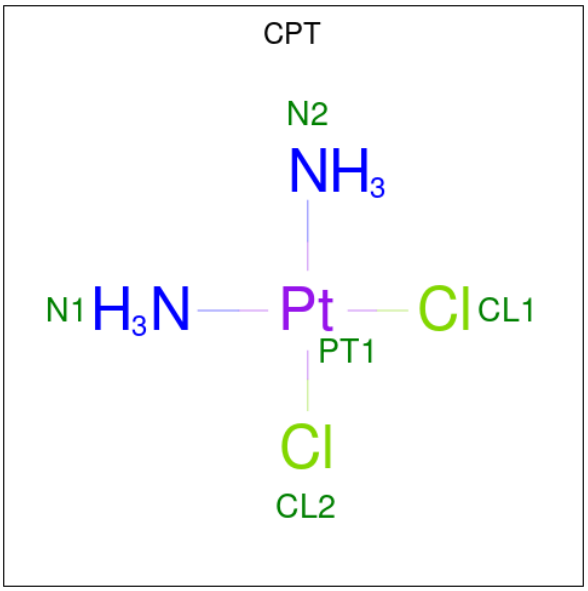
- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 16 is Cisplatin (three-letter code: CPT) (formula: $Cl_2H_6N_2Pt$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	T	1	Total	N	Pt	0	0
			3	2	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total Zn 1 1	0	0
17	C	1	Total Zn 1 1	0	0
17	I	2	Total Zn 2 2	0	0
17	J	1	Total Zn 1 1	0	0
17	L	1	Total Zn 1 1	0	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

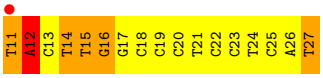
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Mg 1 1	0	0

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: 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3'

Chain T:

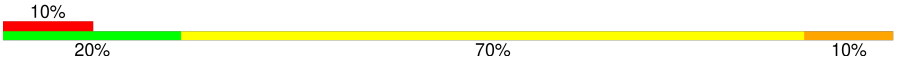


• Molecule 2: 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'

Chain N:

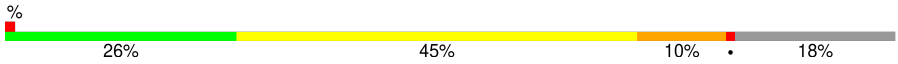
• Molecule 3: 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'

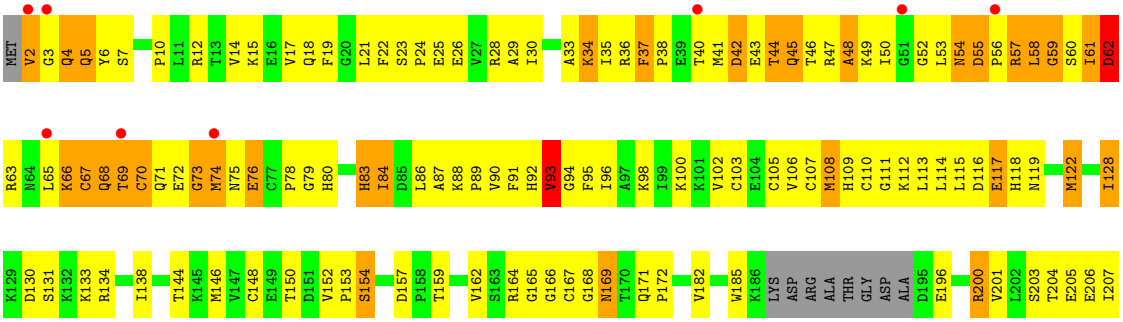
Chain P:

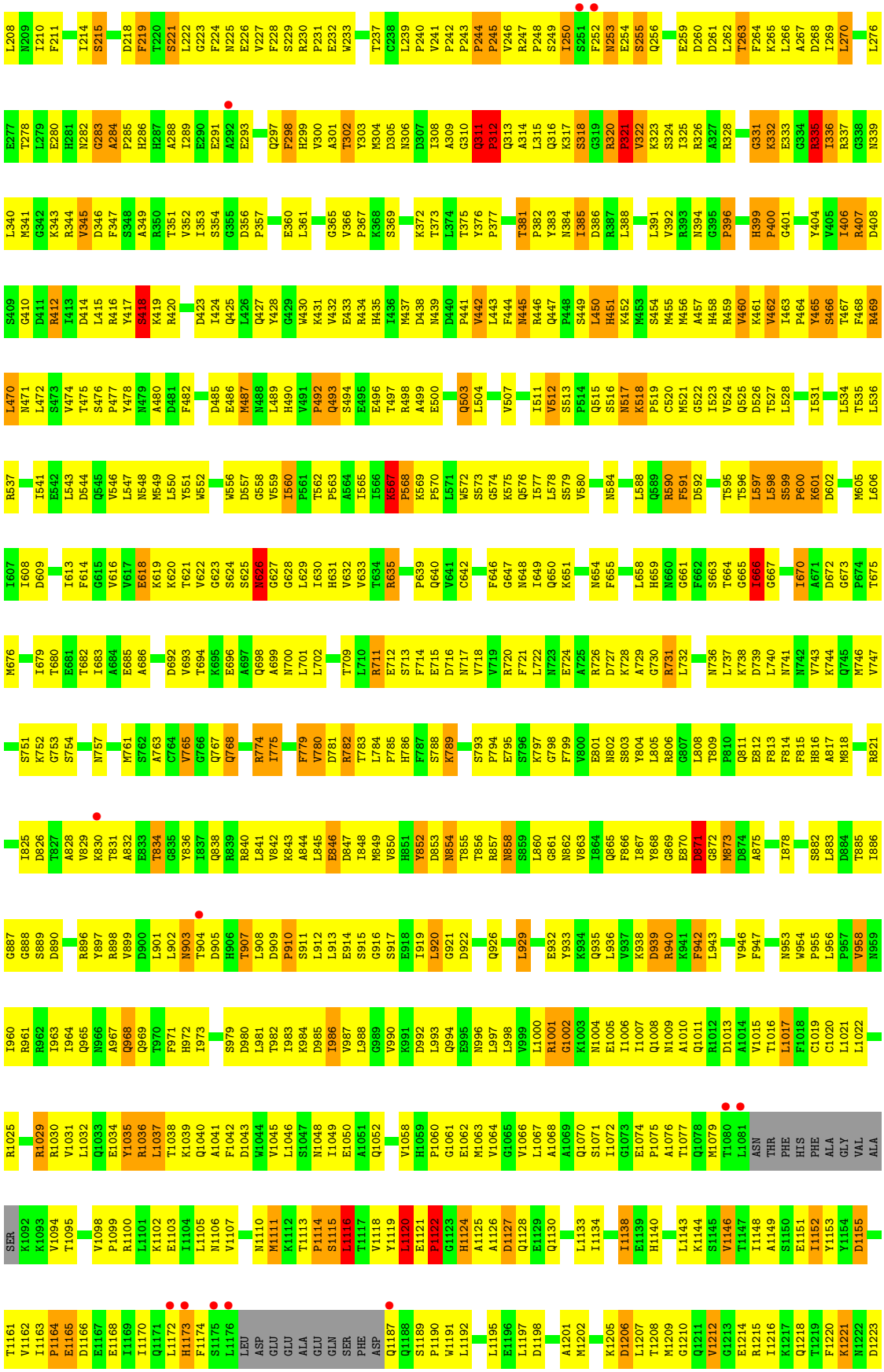


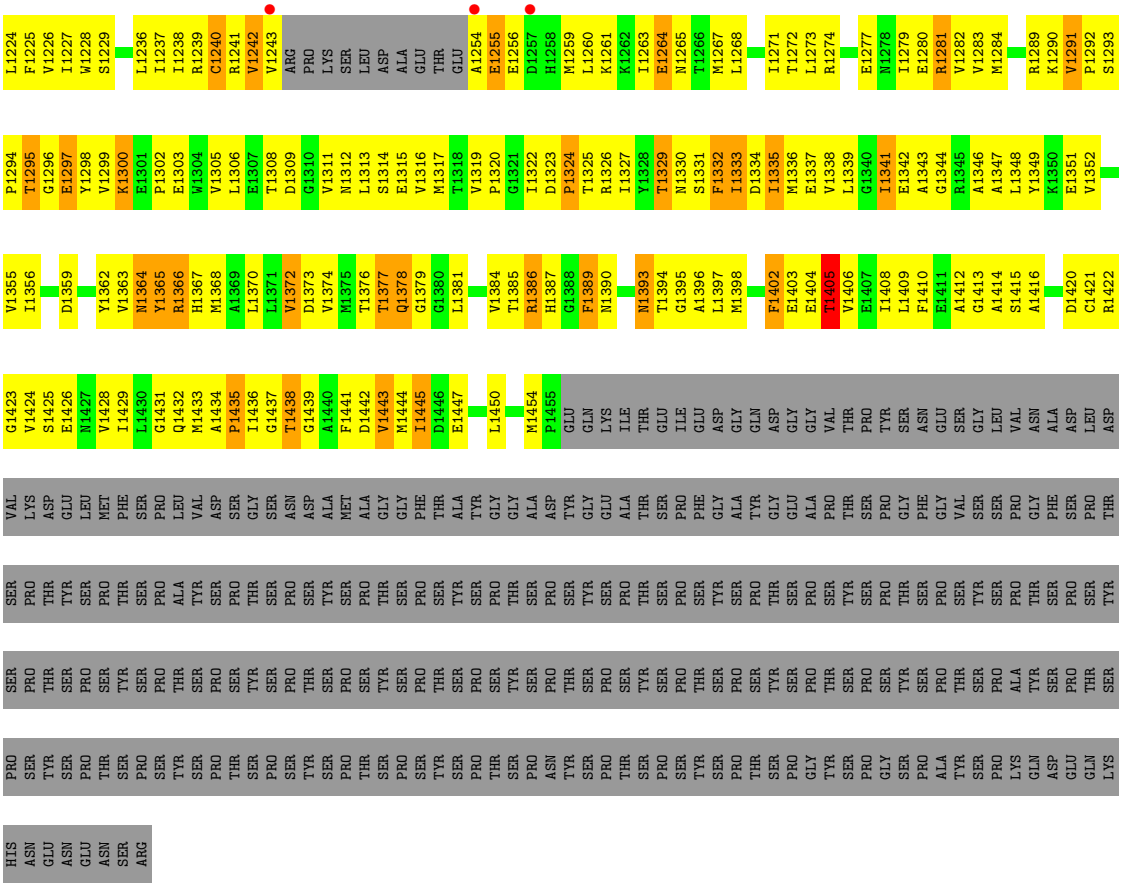
• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A:



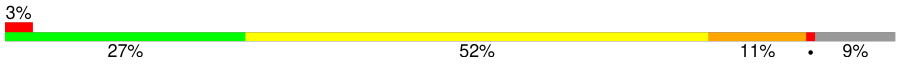


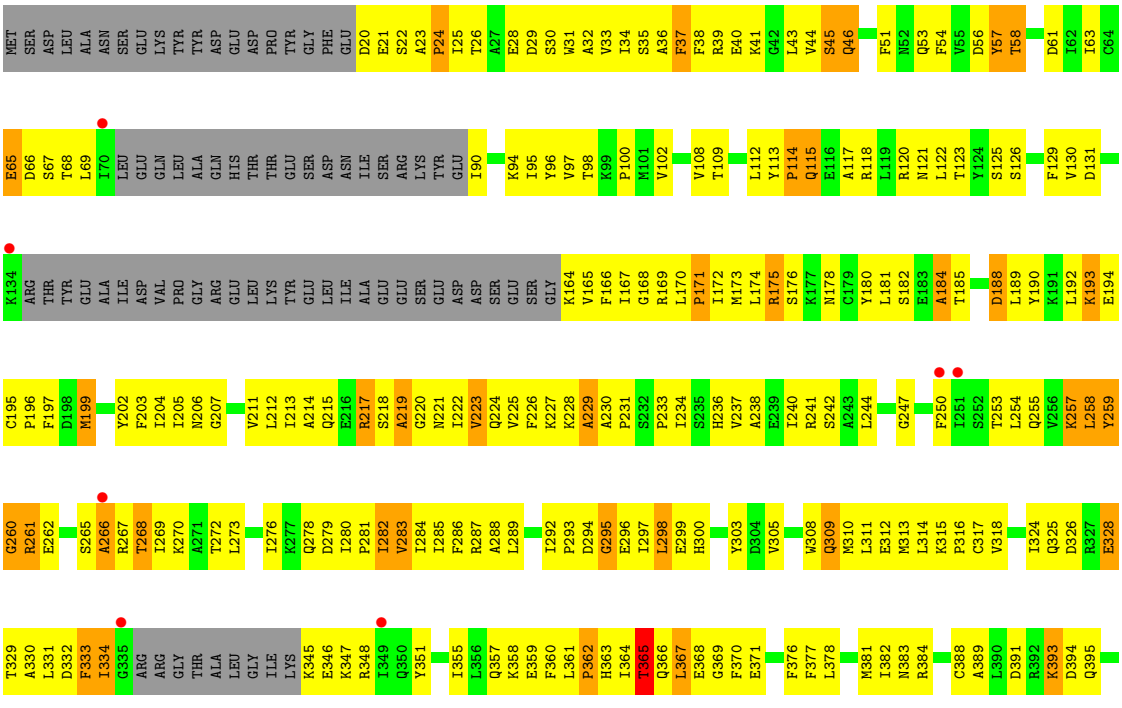

L208 N209 I210 F211 I214 S215 D218 F219 T220 S221 L222 G223 F224 N225 E226 V227 F228 S229 R230 P231 E232 W233 T237 C238 L239 P240 V241 P242 P243 P244 P245 V246 R247 P248 S249 I250 S251 F252 N253 E254 S255 Q256 E259 D260 D261 L262 T263 F264 K265 L266 A267 D268 I269 L270 L276
E277 T278 L279 E280 H281 N282 G283 A284 P285 H286 H287 A288 I289 E290 E291 A292 E293 Q297 F298 H299 V300 A301 T302 Y303 M304 D305 N306 D307 I308 A309 G310 G311 P312 Q313 A314 L315 Q316 K317 S318 G319 R320 P321 V322 K323 S324 I325 R326 A327 R328 G331 K332 E333 G334 R335 I336 R337 G338 N339
L340 M341 G342 K343 R344 V345 D346 F347 S348 A349 R350 T351 V352 I353 S354 G355 D356 P357 E360 L361 G365 V366 P367 K368 S369 K372 T373 L374 T375 Y376 P377 T381 P382 Y383 N384 I385 D386 R387 L388 L391 V392 R393 N394 G395 P396 H399 P400 G401 Y404 V405 I406 R407 D408
S409 G410 D411 R412 I413 D414 L415 R416 Y417 S418 K419 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 S449 L450 H451 K452 M453 S454 M455 M456 A457 H458 R459 V460 K461 V462 I463 P464 Y465 S466 T467 F468 R469
L470 N471 L472 S473 V474 T475 S476 P477 Y478 N479 A480 D481 F482 D485 E486 M487 N488 L489 H490 V491 P492 Q493 S494 E495 E496 T497 R498 A499 E500 Q503 L504 V507 I511 V512 S513 P514 Q515 S516 N517 K518 P519 C520 M521 G522 I523 V524 Q525 D526 T527 L528 I531 L534 T535 L536
R537 I541 E542 L543 D544 Q545 V546 L547 N548 M549 L550 Y551 W552 W556 D557 G558 V559 I560 P561 T562 P563 A564 I565 I566 K567 P568 K569 P570 L571 W572 S573 G574 K575 Q576 I577 L578 S579 V580 N584 L588 Q589 R590 P591 D592 T595 T596 L597 L598 S599 P600 K601 D602 M605 L606
I607 I608 D609 I613 F614 G615 V616 V617 E618 K619 K620 T621 V622 G623 S624 S625 K626 G627 G628 L629 I630 H631 V632 V633 T634 R635 P639 Q640 V641 C642 F646 G647 N648 I649 Q650 K651 N654 F655 L658 H659 N660 G661 F662 S663 T664 G665 I666 G667 I670 A671 D672 G673 P674 T675
M676 I679 T680 E681 T682 I683 A684 E685 A686 D692 V693 T694 K695 E696 A697 Q698 A699 N700 L701 L702 T709 L710 R711 E712 S713 F714 E715 D716 N717 V718 V719 R720 F721 L722 N723 E724 A725 R726 D727 K728 A729 G730 R731 L732 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 M746 V747
S751 K752 G753 S754 N757 M761 S762 A763 C764 V765 G766 Q767 Q768 R774 I775 F779 V780 D781 R782 T783 L784 P785 H786 F787 S788 K789 S793 P794 E795 S796 K797 G798 F799 V800 E801 N802 S803 Y804 L805 R806 G807 L808 T809 P810 Q811 E812 F813 F814 F815 H816 A817 M818 R821
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 N862 V863 I864 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 I878 S882 L883 D884 T885 I886
G887 G888 S889 D890 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908 D909 P910 S911 L912 L913 E914 S915 G916 S917 E918 I919 L920 G921 D922 Q926 L929 E932 Y933 K934 Q935 L936 V937 K938 D939 R940 K941 F942 L943 V946 F947 N953 W954 P955 L956 P957 V958 N959
I960 R961 R962 I963 I964 Q965 N966 A967 Q968 Q969 T970 F971 H972 I973 S979 D980 L981 T982 I983 K984 D985 I986 V987 L988 G989 V990 K991 D992 L993 Q994 E995 N996 L997 L998 V999 L1000 R1001 G1002 K1003 N1004 E1005 I1006 I1007 Q1008 N1009 A1010 Q1011 R1012 D1013 A1014 V1015 T1016 L1017 F1018 C1019 C1020 L1021 L1022
R1025 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 L1046 S1047 N1048 I1049 E1050 A1051 Q1052 V1058 H1059 P1060 G1061 E1062 M1063 V1064 G1065 V1066 L1067 A1068 A1069 Q1070 S1071 I1072 G1073 E1074 P1075 A1076 T1077 Q1078 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA GLY VAL ALA
SER K1092 K1093 V1094 T1095 V1098 P1099 R1100 L1101 K1102 E1103 I1104 L1105 N1106 V1107 N1110 M1111 K1112 T1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 S1189 P1122 G1123 H1124 A1125 A1126 D1127 Q1128 E1129 Q1130 L1133 I1134 I1138 E1139 H1140 L1143 K1144 S1145 V1146 T1147 I1148 A1149 S1150 E1151 I1152 Y1153 Y1154 D1155
T1161 V1162 I1163 P1164 E1165 D1166 E1167 E1168 I1169 I1170 Q1171 L1172 H1173 F1174 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 L1195 E1196 L1197 D1198 A1201 M1202 K1205 D1206 L1207 T1208 M1209 G1210 Q1211 V1212 G1213 E1214 R1215 I1216 K1217 Q1218 T1219 F1220 K1221 N1222 D1223

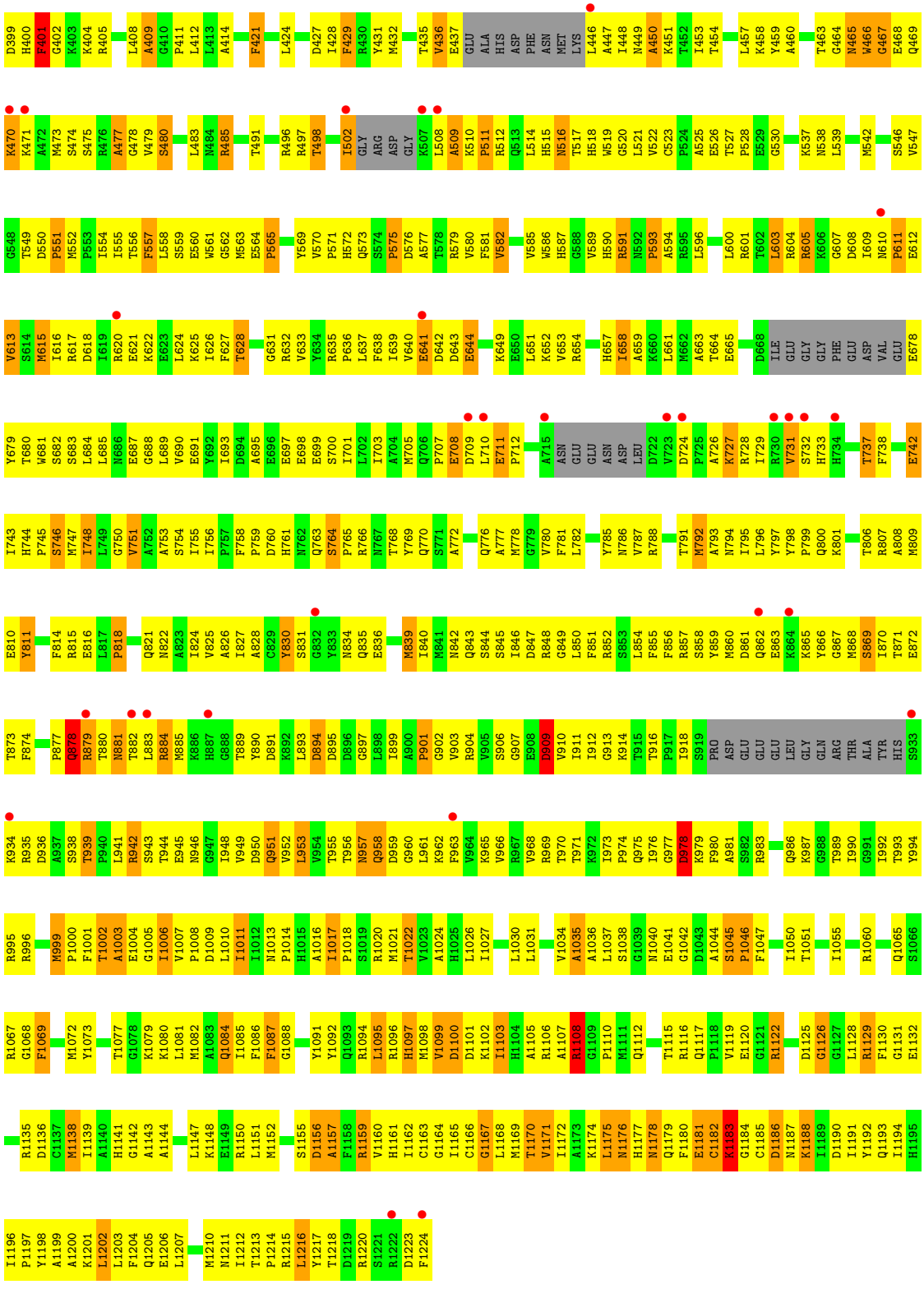


• Molecule 5: DNA-directed RNA polymerase II subunit RPB2

Chain B:

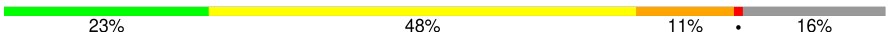


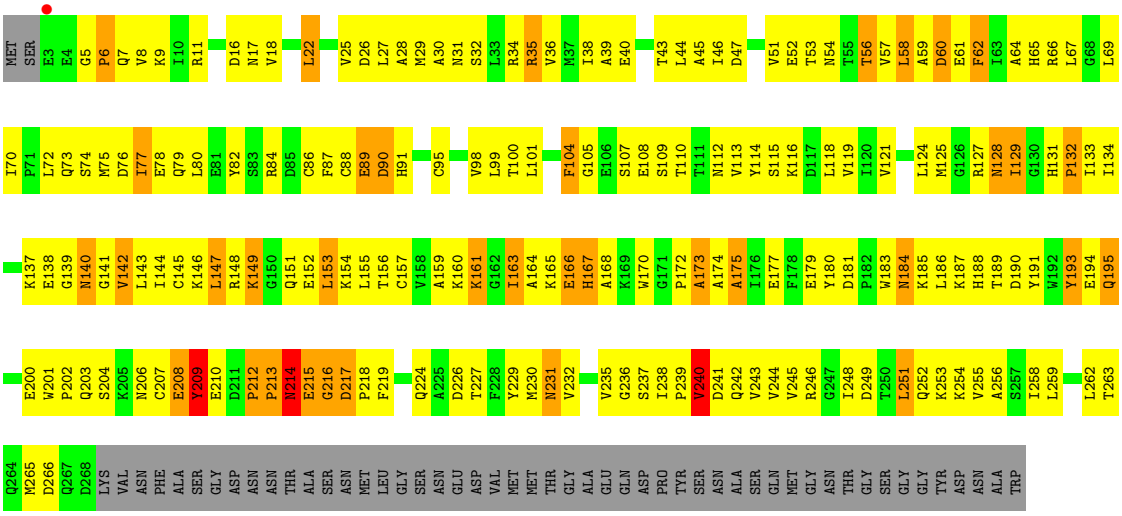




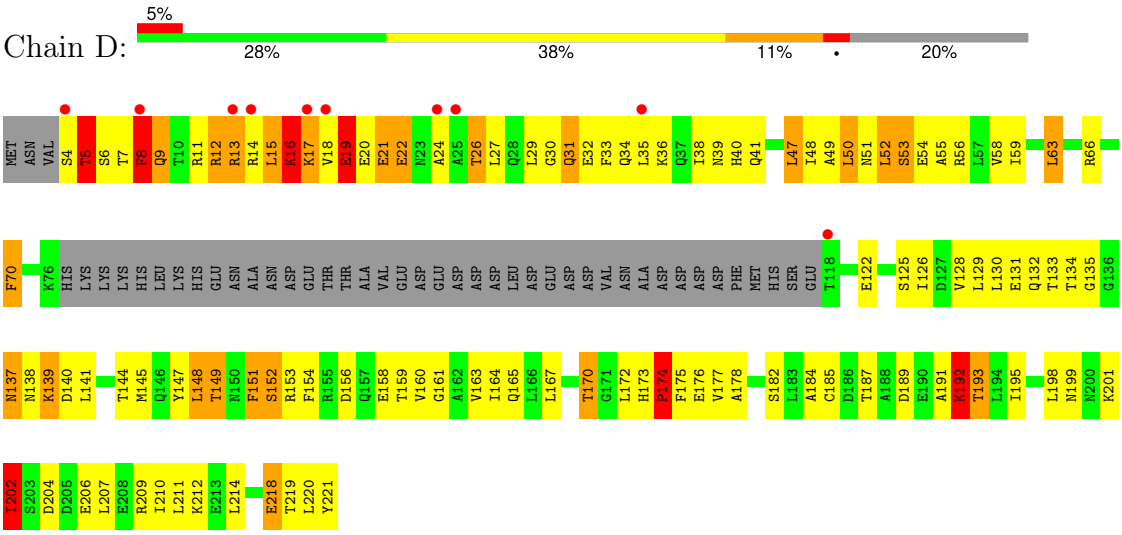
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C:

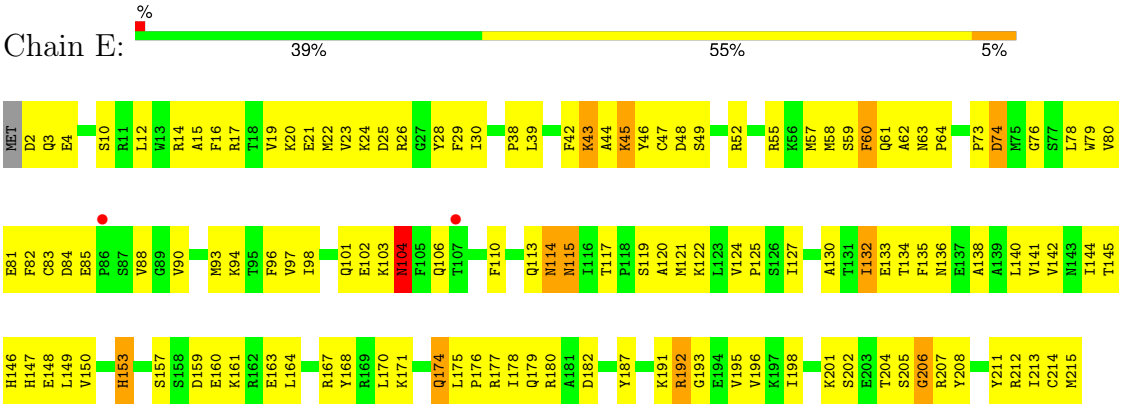




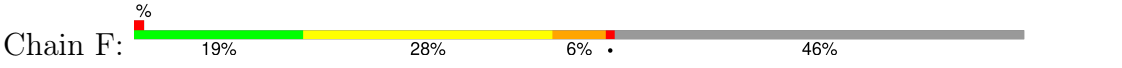
• Molecule 7: DNA-directed RNA polymerase II subunit RPB4

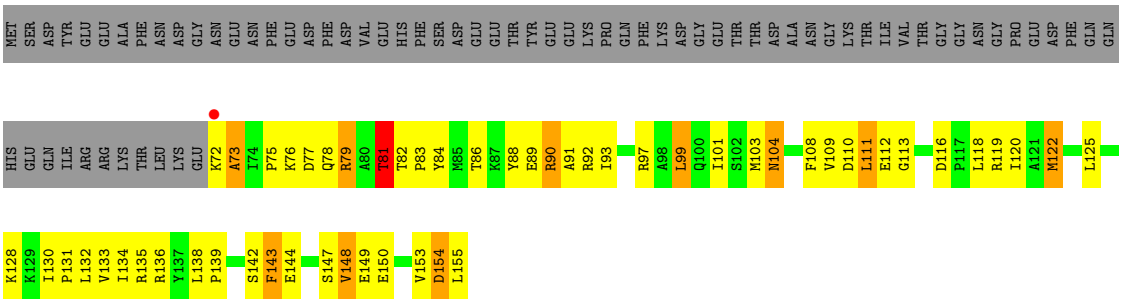


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



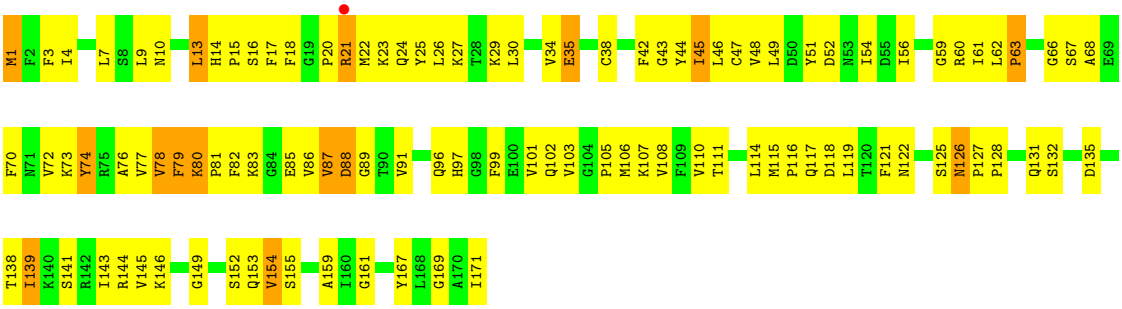
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2





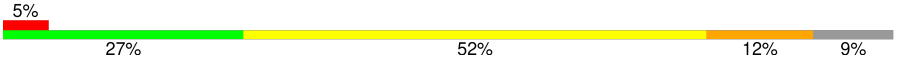
• Molecule 10: DNA-directed RNA polymerase II subunit RPB7

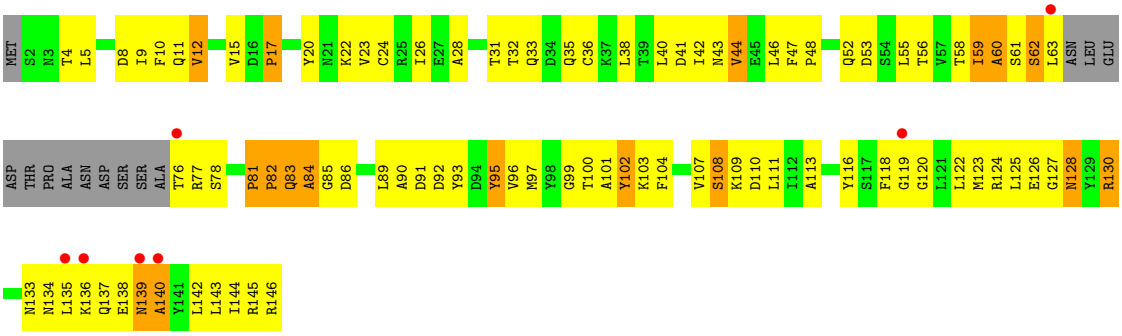
Chain G:



• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

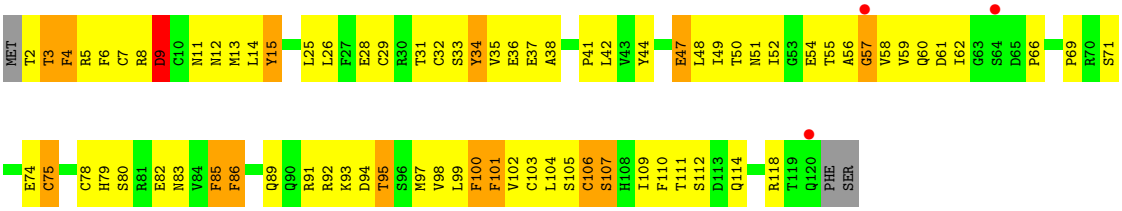
Chain H:





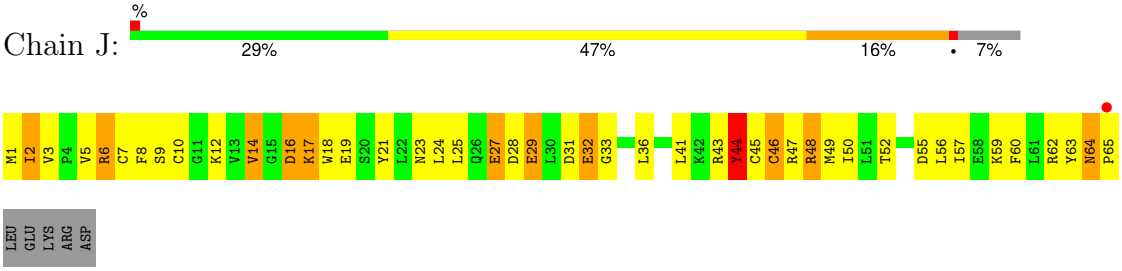
• Molecule 12: DNA-directed RNA polymerase II subunit RPB9

Chain I:



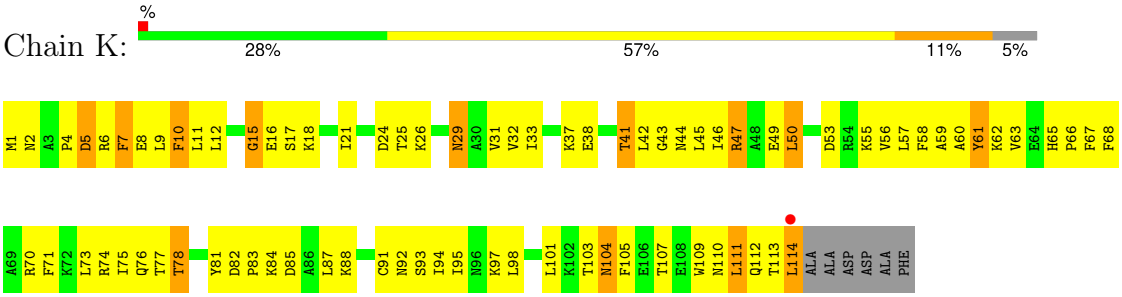
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



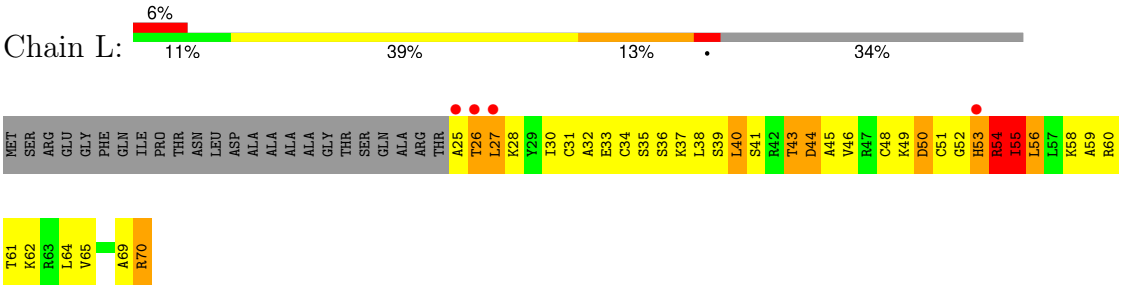
• Molecule 14: DNA-directed RNA polymerase II subunit RPB11

Chain K:



• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.06Å 393.12Å 283.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.7 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.240 0.216 , 0.242	Depositor DCC
R_{free} test set	2410 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	106.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.045 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31804	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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, MG, CPT

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	T	1.41	5/373 (1.3%)	1.79	11/572 (1.9%)
2	N	1.38	0/161	1.10	0/247
3	P	0.95	0/242	0.98	0/377
4	A	0.43	0/11339	0.72	4/15334 (0.0%)
5	B	0.42	0/8981	0.68	0/12108
6	C	0.44	0/2133	0.72	0/2891
7	D	0.42	0/1437	0.69	1/1925 (0.1%)
8	E	0.41	0/1788	0.65	0/2406
9	F	0.49	0/691	0.77	0/933
10	G	0.45	0/1368	0.72	0/1844
11	H	0.38	0/1086	0.65	0/1470
12	I	0.36	0/989	0.65	0/1331
13	J	0.47	0/541	0.74	0/727
14	K	0.45	0/937	0.68	0/1265
15	L	0.47	0/366	0.71	0/485
All	All	0.46	5/32432 (0.0%)	0.73	16/43915 (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
1	T	0	2
2	N	0	2
6	C	0	1
13	J	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	16	DG	N3-C4	8.85	1.41	1.35
1	T	17	DG	N3-C4	7.68	1.40	1.35
1	T	17	DG	C2-N3	6.93	1.38	1.32
1	T	16	DG	N1-C2	5.71	1.42	1.37
1	T	14	DT	O3'-P	5.20	1.67	1.61

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	17	DG	O4'-C1'-N9	11.85	116.29	108.00
1	T	16	DG	O4'-C1'-N9	9.50	114.65	108.00
1	T	17	DG	N3-C2-N2	7.61	125.22	119.90
4	A	567	LYS	C-N-CD	6.05	141.11	128.40
1	T	16	DG	N1-C2-N3	-5.93	120.34	123.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	82	TYR	Sidechain
2	N	5	DT	Sidechain
2	N	6	DA	Sidechain
1	T	11	DT	Sidechain
1	T	12	DA	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	T	336	0	195	46	0
2	N	143	0	80	20	0
3	P	216	0	108	13	0
4	A	11140	0	11217	1294	0
5	B	8810	0	8847	1025	0
6	C	2095	0	2052	253	0
7	D	1427	0	1451	136	0
8	E	1752	0	1776	149	0
9	F	679	0	701	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	G	1340	0	1357	152	0
11	H	1068	0	1040	131	0
12	I	971	0	930	102	0
13	J	532	0	543	106	0
14	K	919	0	929	115	0
15	L	364	0	388	57	0
16	T	3	0	0	1	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	31804	0	31614	3347	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 53.

The worst 5 of 3347 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)
11:H:100:THR:HG23	11:H:138:GLU:HA	1.26	1.16
10:G:138:THR:HG22	10:G:139:ILE:H	1.09	1.12
4:A:53:LEU:HD23	4:A:54:ASN:H	0.99	1.12
4:A:1094:VAL:HG13	4:A:1113:THR:HG21	1.32	1.11
5:B:510:LYS:HG3	5:B:511:PRO:HD3	1.12	1.11

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
4	A	1406/1733 (81%)	988 (70%)	277 (20%)	141 (10%)	0 7
5	B	1090/1224 (89%)	754 (69%)	217 (20%)	119 (11%)	0 6
6	C	264/318 (83%)	181 (69%)	50 (19%)	33 (12%)	0 4
7	D	173/221 (78%)	125 (72%)	28 (16%)	20 (12%)	0 5
8	E	212/215 (99%)	157 (74%)	38 (18%)	17 (8%)	1 11
9	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1 15
10	G	169/171 (99%)	131 (78%)	30 (18%)	8 (5%)	2 18
11	H	129/146 (88%)	90 (70%)	19 (15%)	20 (16%)	0 3
12	I	117/122 (96%)	84 (72%)	23 (20%)	10 (8%)	0 9
13	J	63/70 (90%)	36 (57%)	15 (24%)	12 (19%)	0 2
14	K	112/120 (93%)	86 (77%)	20 (18%)	6 (5%)	1 17
15	L	44/70 (63%)	17 (39%)	14 (32%)	13 (30%)	0 0
All	All	3861/4565 (85%)	2711 (70%)	746 (19%)	404 (10%)	0 6

5 of 404 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	42	ASP
4	A	44	THR
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP

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
4	A	1239/1520 (82%)	1124 (91%)	115 (9%)	7 27
5	B	962/1061 (91%)	887 (92%)	75 (8%)	10 34
6	C	234/274 (85%)	211 (90%)	23 (10%)	6 25
7	D	159/200 (80%)	129 (81%)	30 (19%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	E	196/197 (100%)	190 (97%)	6 (3%)	35 56
9	F	74/137 (54%)	65 (88%)	9 (12%)	4 19
10	G	152/152 (100%)	139 (91%)	13 (9%)	8 31
11	H	117/128 (91%)	112 (96%)	5 (4%)	25 49
12	I	113/116 (97%)	104 (92%)	9 (8%)	10 33
13	J	60/65 (92%)	56 (93%)	4 (7%)	13 38
14	K	99/102 (97%)	89 (90%)	10 (10%)	6 24
15	L	40/57 (70%)	36 (90%)	4 (10%)	6 24
All	All	3445/4009 (86%)	3142 (91%)	303 (9%)	8 30

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	D	149	THR
13	J	44	TYR
7	D	192	LYS
10	G	21	ARG
15	L	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
6	C	24	ASN
8	E	8	ASN
6	C	79	GLN
7	D	39	ASN
8	E	113	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	U

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
16	CPT	T	67	1	0,2,4	-	-	-		

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	67	CPT	1	0

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	T	17/17 (100%)	0.72	1 (5%)	29	27	110, 139, 169, 175	0
2	N	7/7 (100%)	0.99	1 (14%)	7	11	148, 156, 169, 171	0
3	P	10/10 (100%)	0.56	1 (10%)	14	16	118, 128, 165, 172	0
4	A	1416/1733 (81%)	-0.16	23 (1%)	70	54	44, 103, 161, 199	0
5	B	1108/1224 (90%)	0.05	37 (3%)	49	40	47, 116, 176, 199	0
6	C	266/318 (83%)	-0.21	1 (0%)	89	78	64, 100, 144, 162	0
7	D	177/221 (80%)	0.17	10 (5%)	31	28	70, 120, 177, 190	0
8	E	214/215 (99%)	0.09	2 (0%)	81	67	79, 144, 185, 197	0
9	F	84/155 (54%)	-0.45	1 (1%)	76	60	53, 81, 115, 132	0
10	G	171/171 (100%)	-0.09	1 (0%)	85	73	82, 103, 141, 150	0
11	H	133/146 (91%)	0.48	7 (5%)	33	29	119, 149, 180, 188	0
12	I	119/122 (97%)	0.34	3 (2%)	58	46	94, 150, 183, 199	0
13	J	65/70 (92%)	-0.15	1 (1%)	71	56	71, 96, 131, 140	0
14	K	114/120 (95%)	-0.38	1 (0%)	81	67	64, 101, 130, 149	0
15	L	46/70 (65%)	0.44	4 (8%)	17	18	96, 154, 172, 178	0
All	All	3947/4599 (85%)	-0.04	94 (2%)	59	47	44, 111, 175, 199	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	7.8
4	A	1081	LEU	4.6
11	H	63	LEU	4.4
7	D	25	ALA	4.3
5	B	883	LEU	4.2

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 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
16	CPT	T	67	3/5	0.95	0.30	131,131,131,132	0
17	ZN	I	204	1/1	0.95	0.13	196,196,196,196	0
18	MG	A	1736	1/1	0.98	0.10	58,58,58,58	0
17	ZN	L	105	1/1	0.99	0.05	127,127,127,127	0
17	ZN	A	1734	1/1	0.99	0.05	108,108,108,108	0
17	ZN	I	203	1/1	1.00	0.07	113,113,113,113	0
17	ZN	A	1735	1/1	1.00	0.03	65,65,65,65	0
17	ZN	J	101	1/1	1.00	0.03	68,68,68,68	0
17	ZN	B	1307	1/1	1.00	0.04	71,71,71,71	0
17	ZN	C	319	1/1	1.00	0.06	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.