wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:48 PM GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

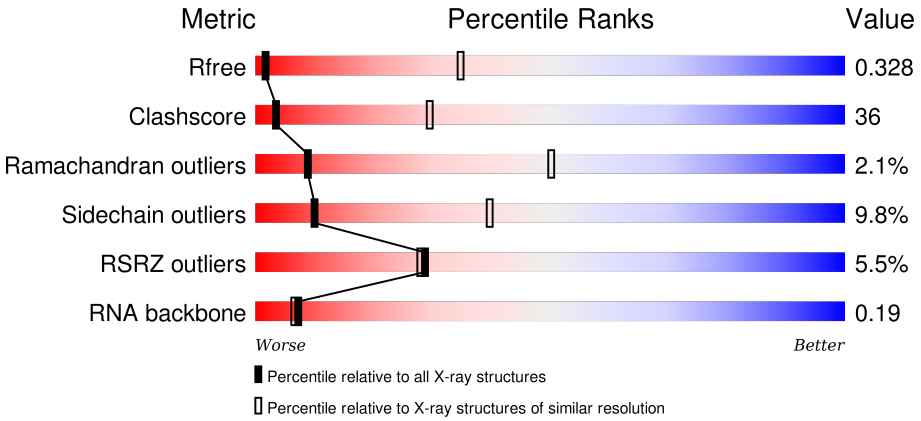
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

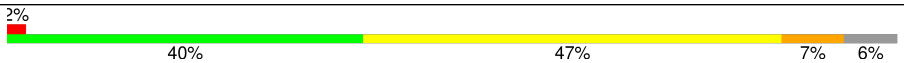
The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)
RNA backbone	2183	1101 (7.80-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	242	
1	B	242	
1	G	242	
1	H	242	

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Mol	Chain	Length	Quality of chain
1	M	242	2% 49% 43% 5%
1	N	242	6% 48% 40% 6% 6%
2	C	1342	% 46% 48% 6%
2	I	1342	2% 48% 47% 5%
2	O	1342	% 50% 45%
3	D	1407	7% 44% 47% 6%
3	J	1407	5% 41% 48% 7%
3	P	1407	9% 45% 45% 7%
4	E	90	31% 48% 50%
4	K	90	13% 53% 42%
4	Q	90	14% 67% 29%
5	F	628	11% 43% 32% 21%
5	L	628	9% 43% 31% 5% 21%
5	R	628	8% 41% 32% 6% 21%
6	1	49	10% 29% 71%
6	4	49	10% 31% 69%
6	7	49	4% 31% 69%
7	2	49	4% 37% 63%
7	5	49	10% 41% 59%
7	8	49	35% 65%
8	3	4	25% 50% 25%
8	6	4	50% 50%
8	9	4	75% 25%

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

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

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94608 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	B	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	G	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	H	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	M	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	N	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 42 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There are 45 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

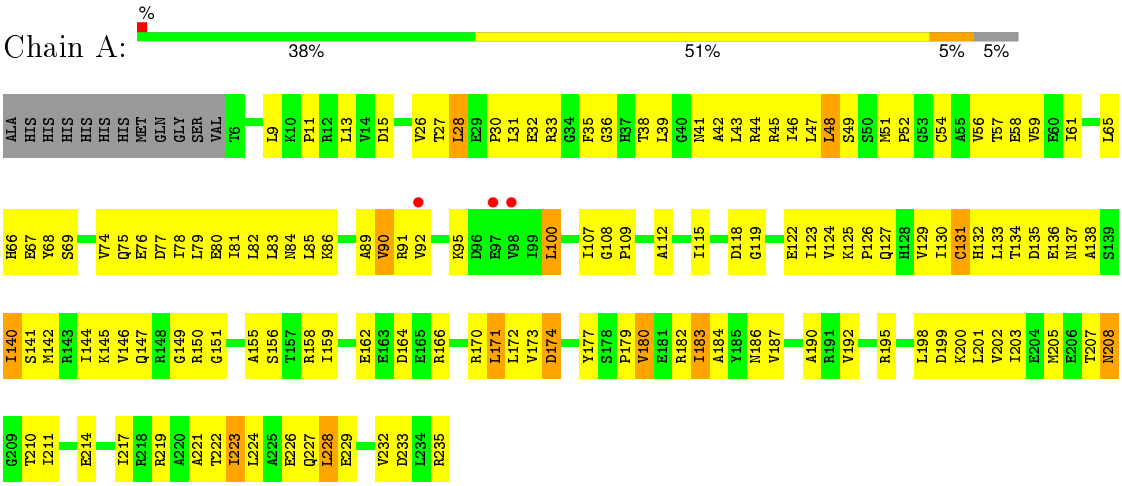
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		
10	6	1	Total	Mg	0	0
			1	1		

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

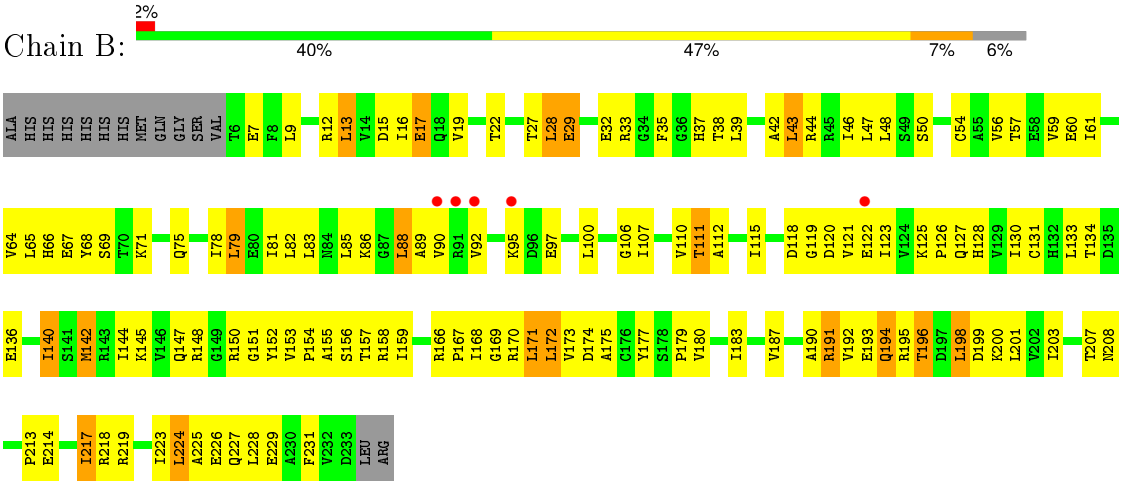
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



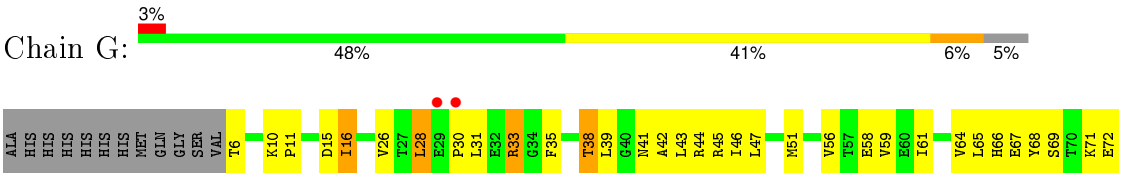
- Molecule 1: DNA-directed RNA polymerase subunit alpha

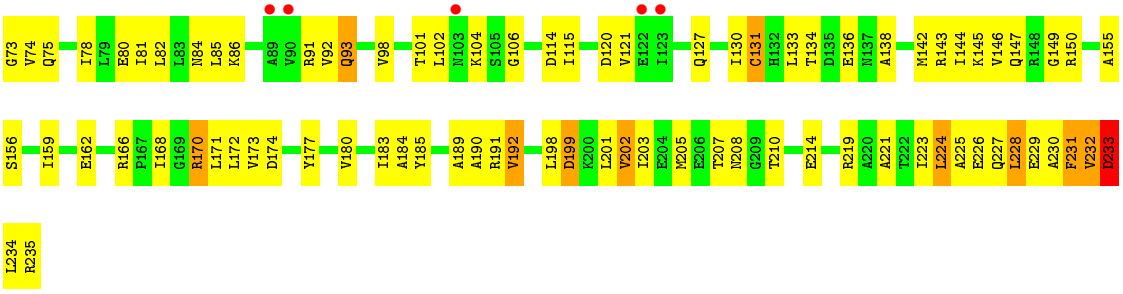
Chain B:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

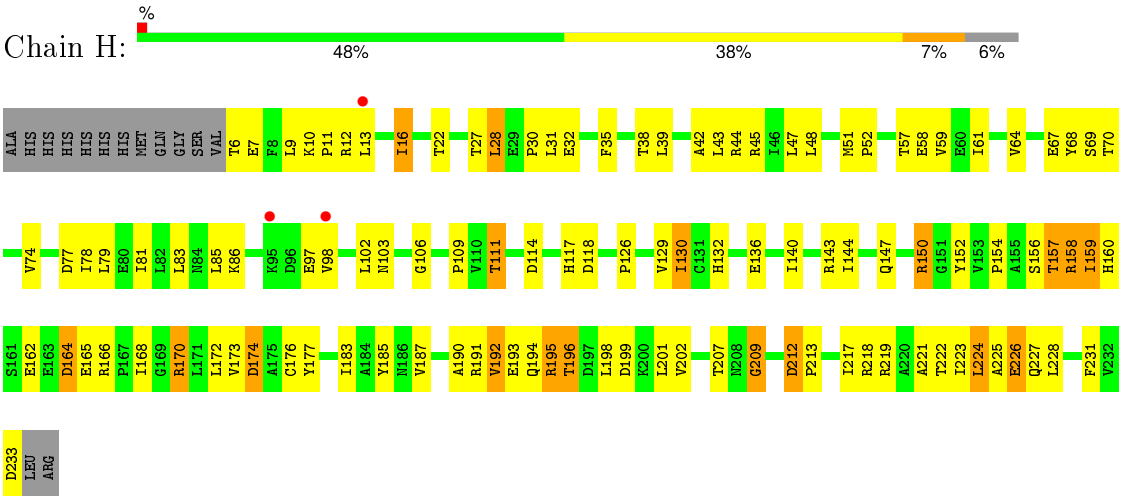
Chain G:





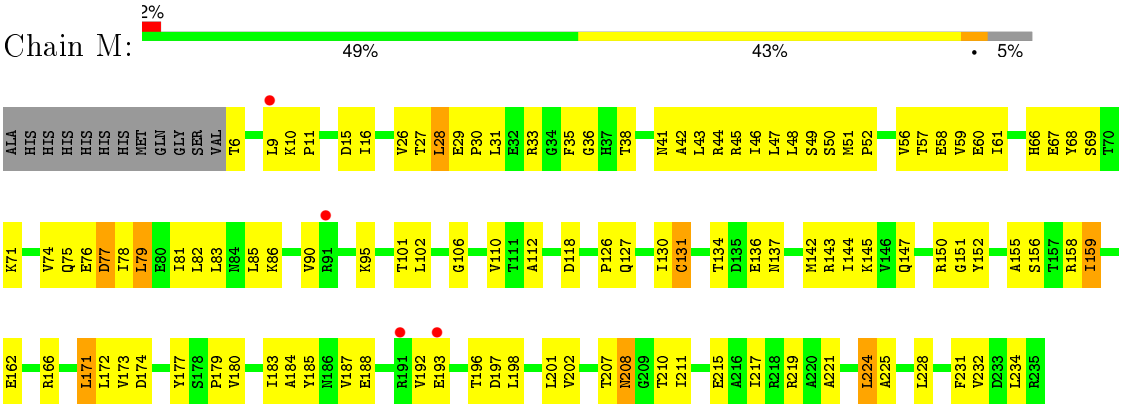
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H:



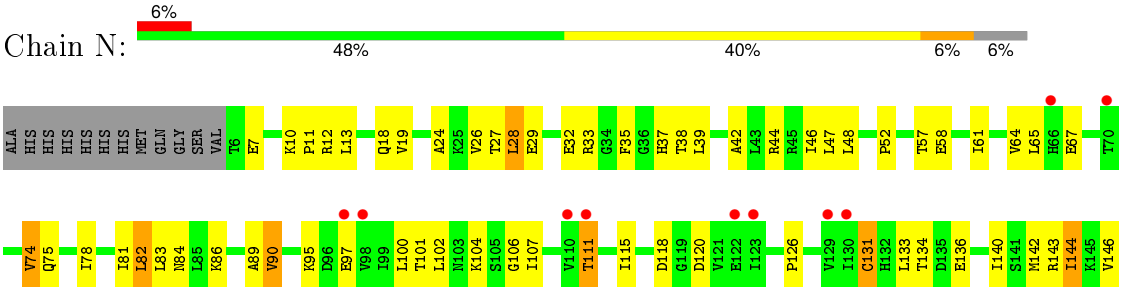
• Molecule 1: DNA-directed RNA polymerase subunit alpha

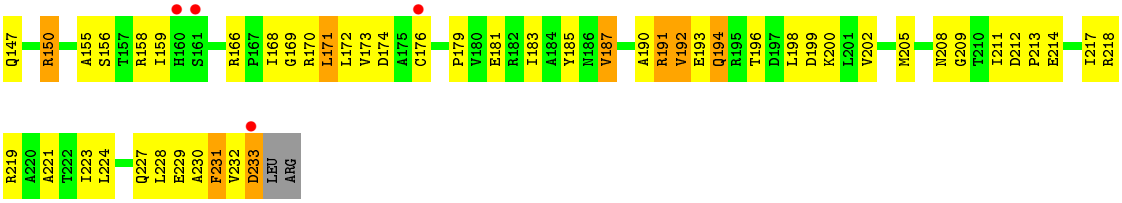
Chain M:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

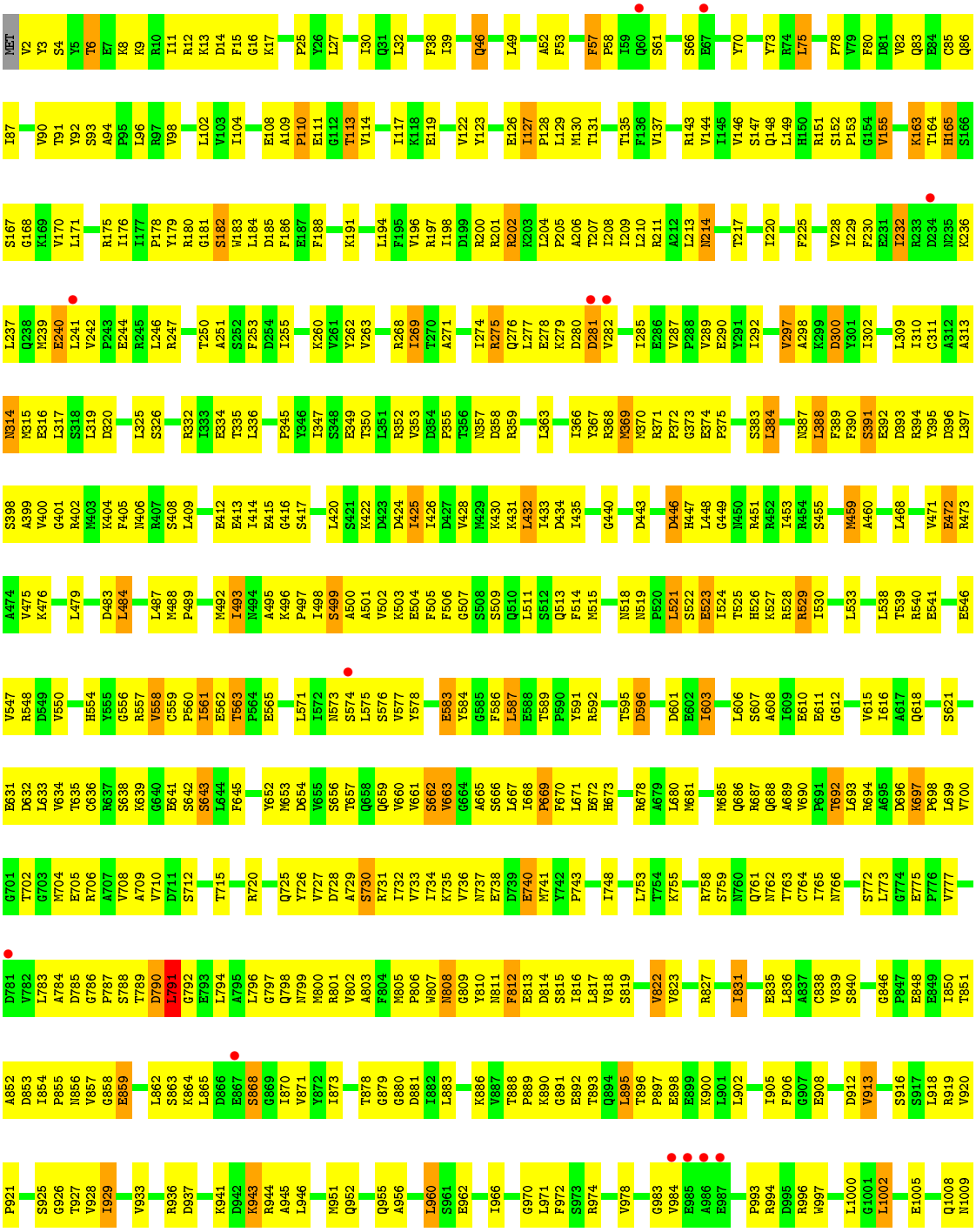
Chain N:

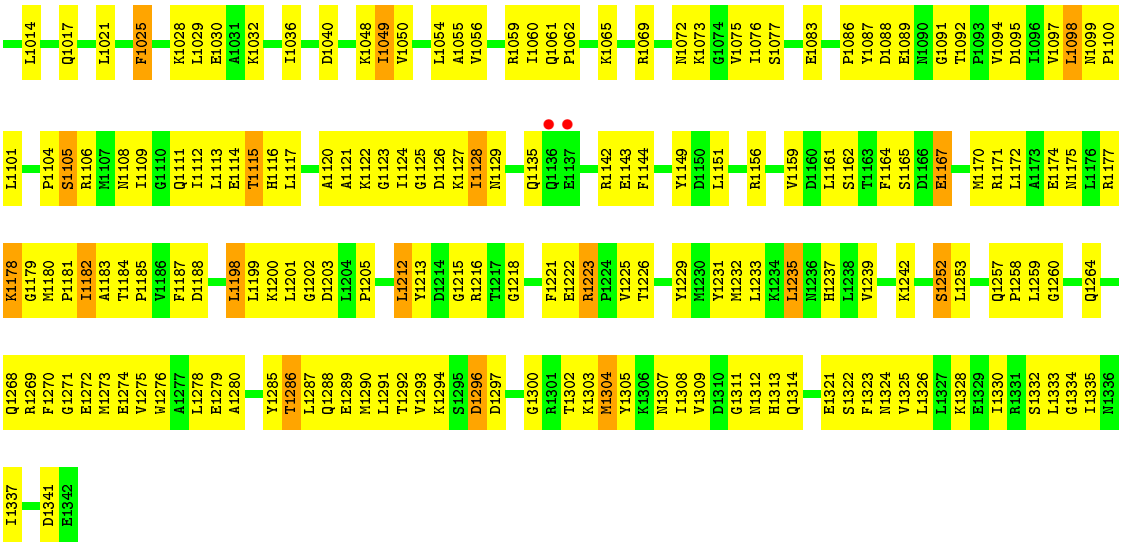




• Molecule 2: DNA-directed RNA polymerase subunit beta

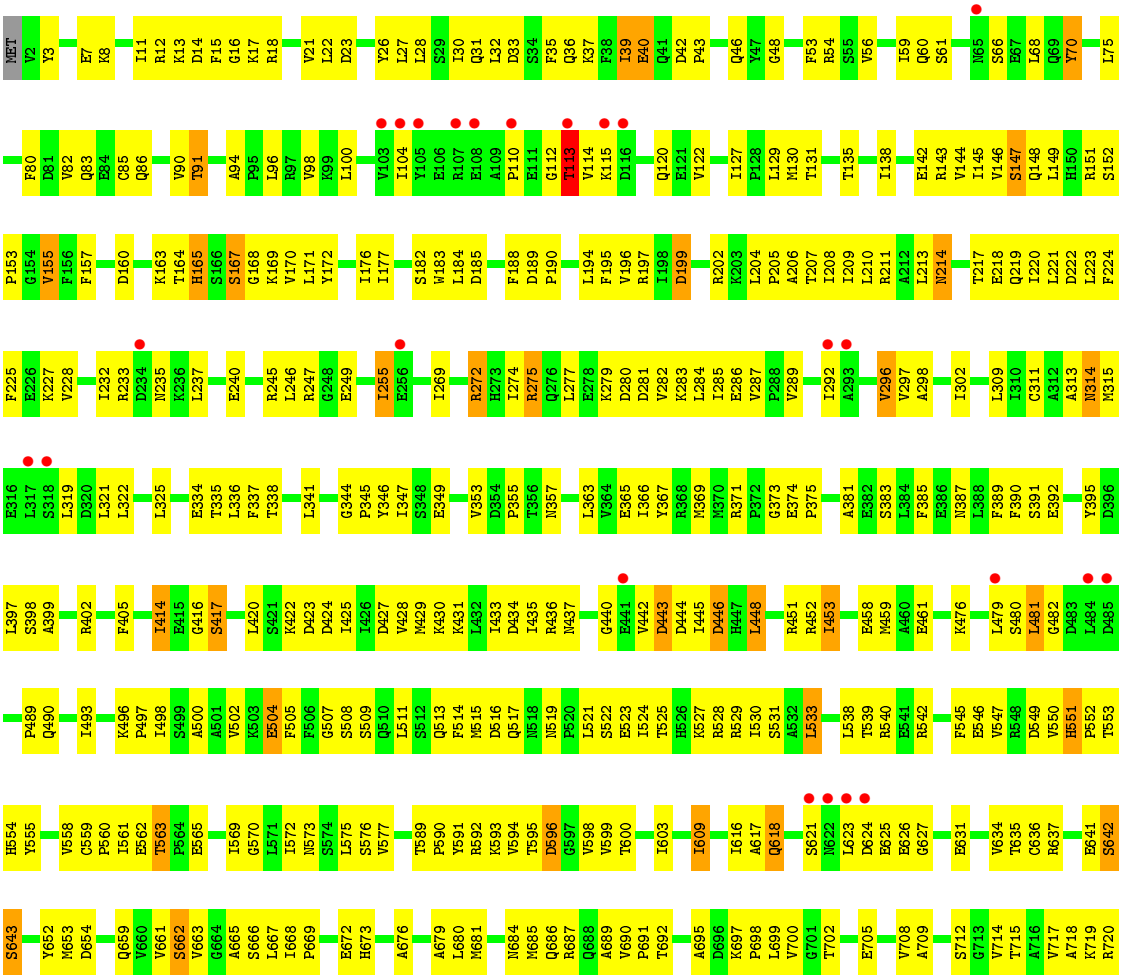
Chain C:

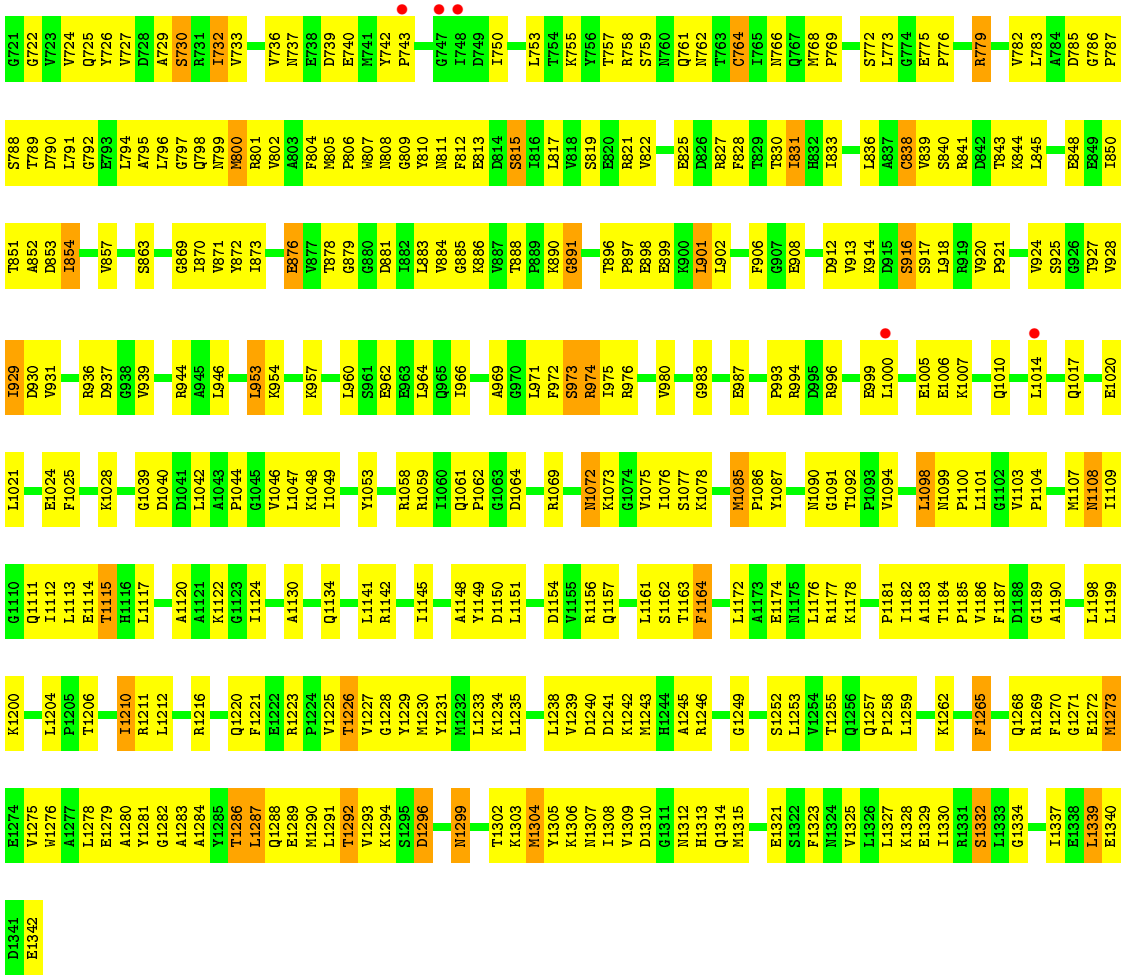




• Molecule 2: DNA-directed RNA polymerase subunit beta

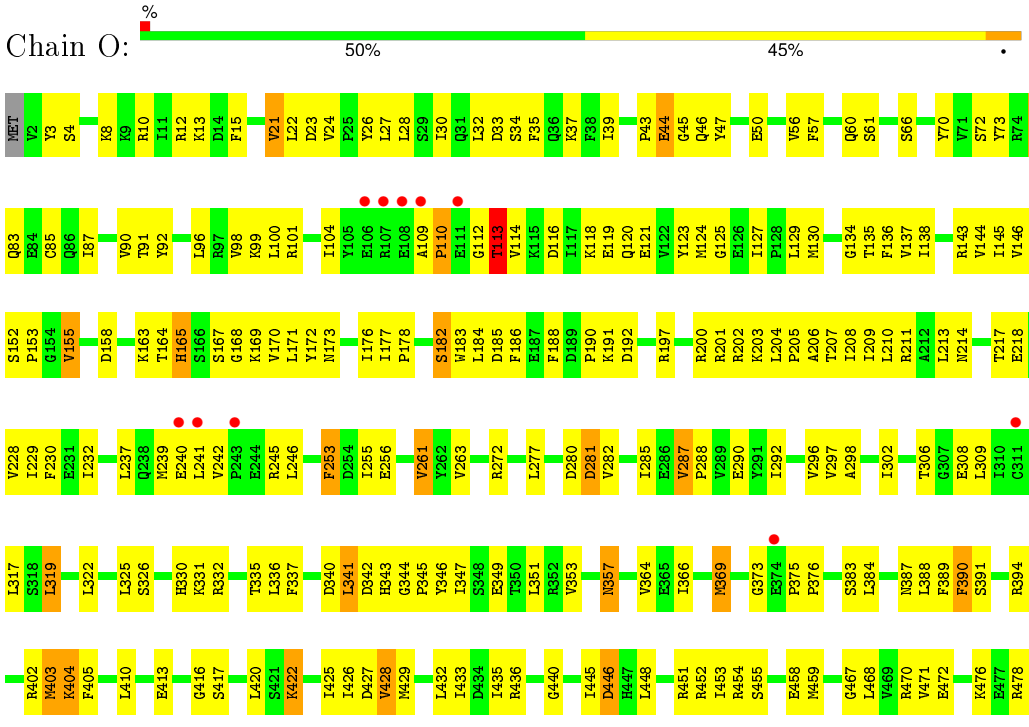
Chain I:

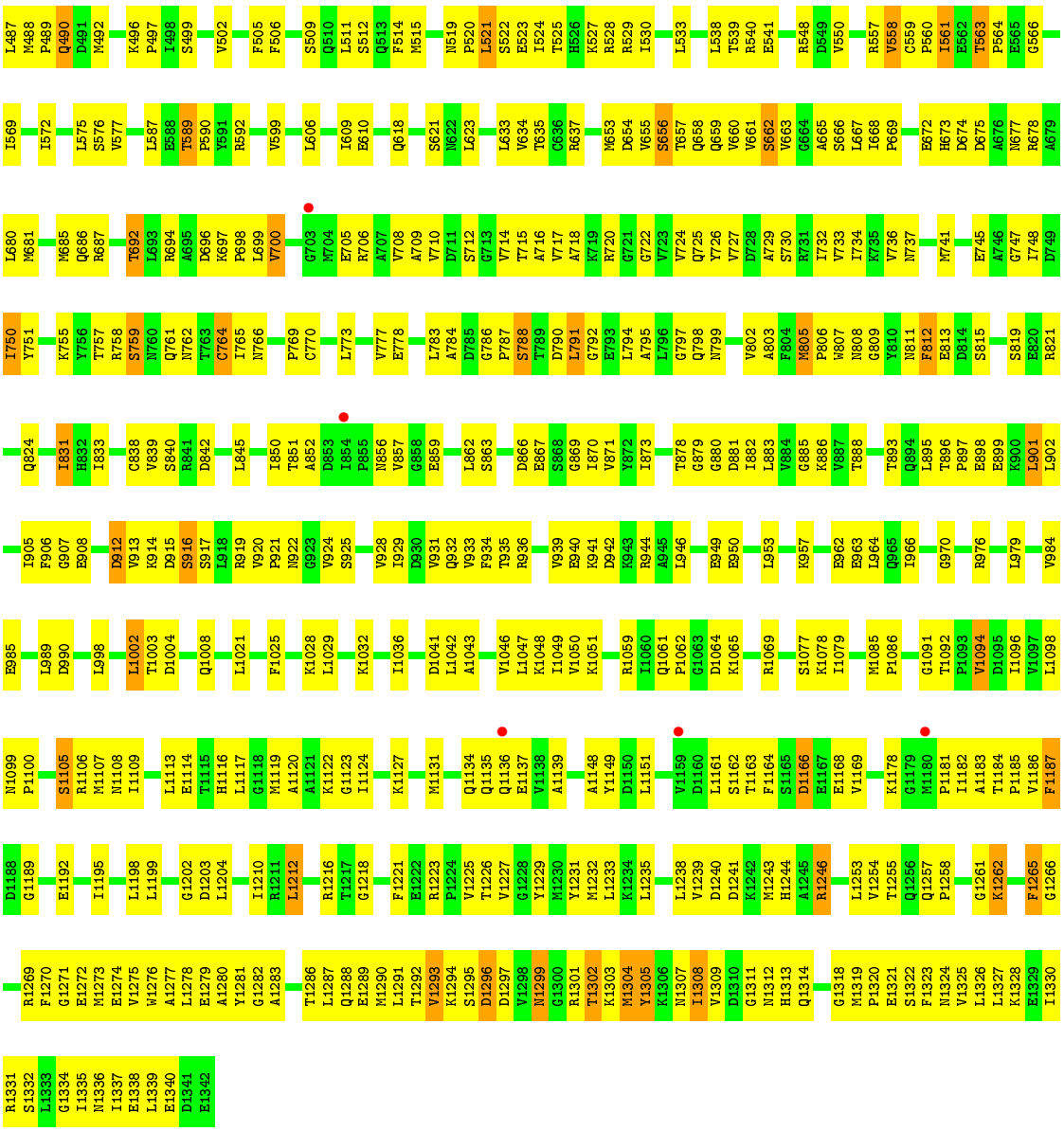




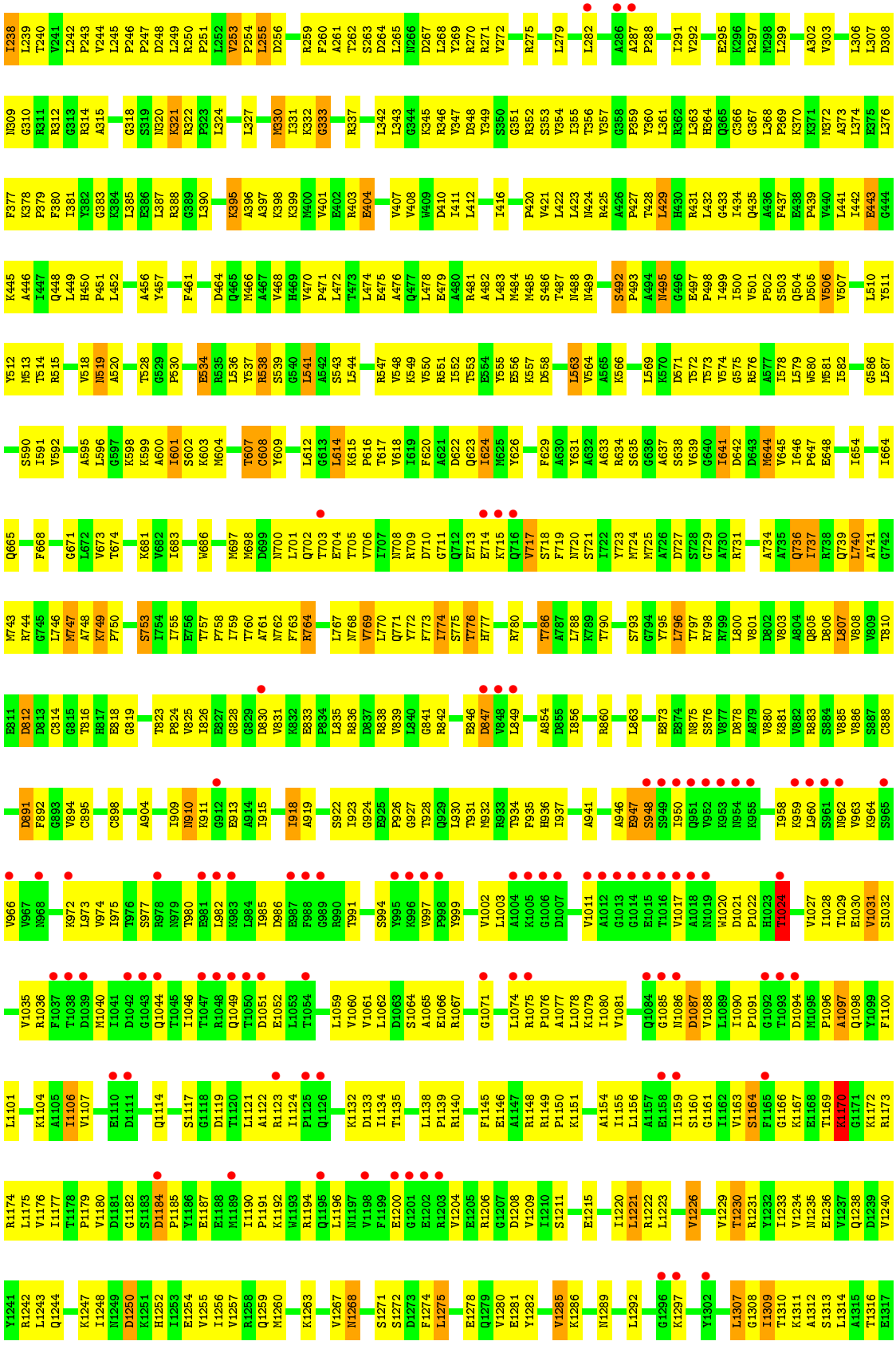
• Molecule 2: DNA-directed RNA polymerase subunit beta

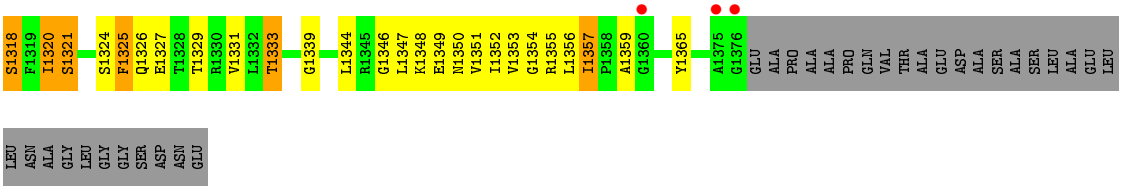
Chain O:





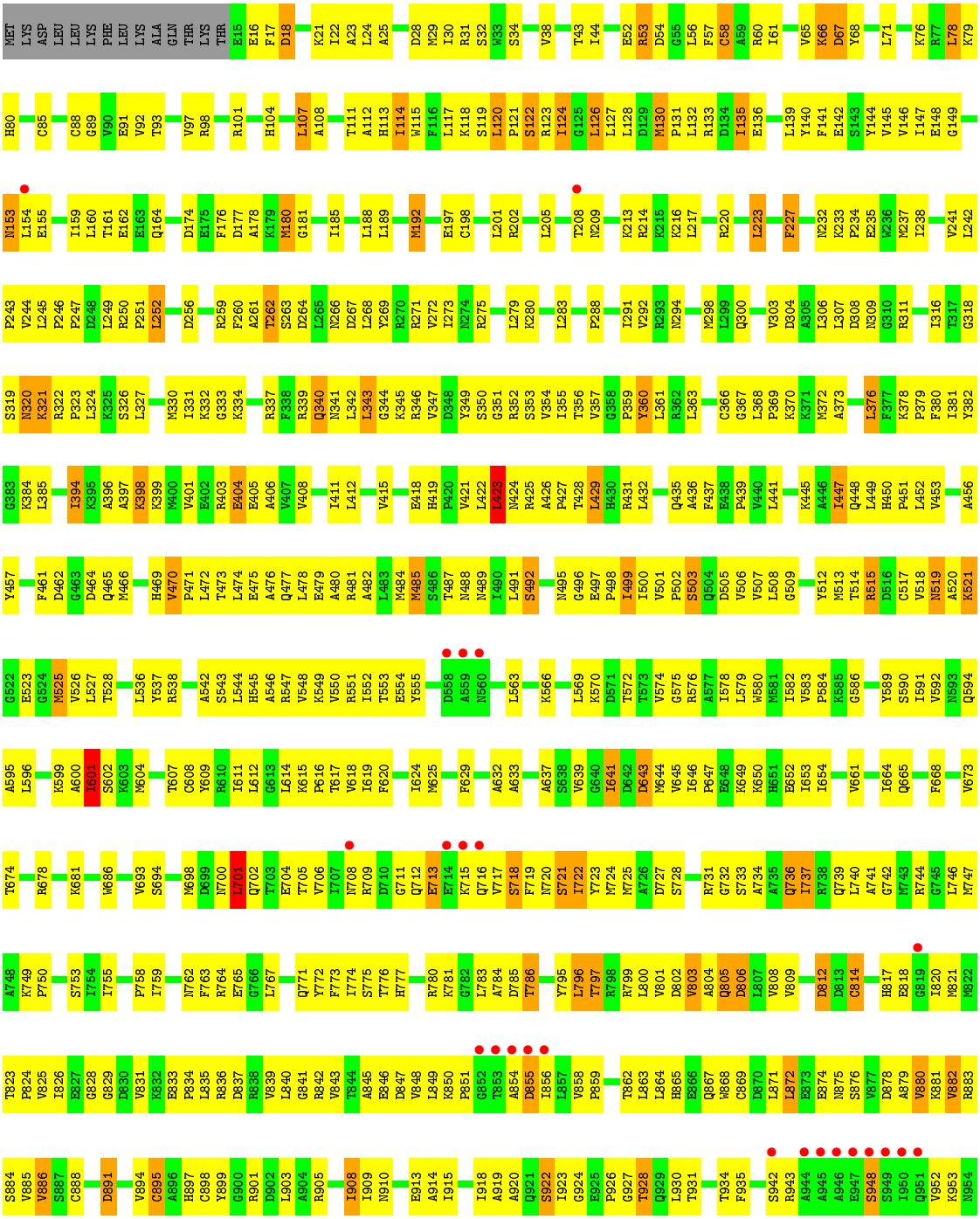
• Molecule 3: DNA-directed RNA polymerase subunit beta'

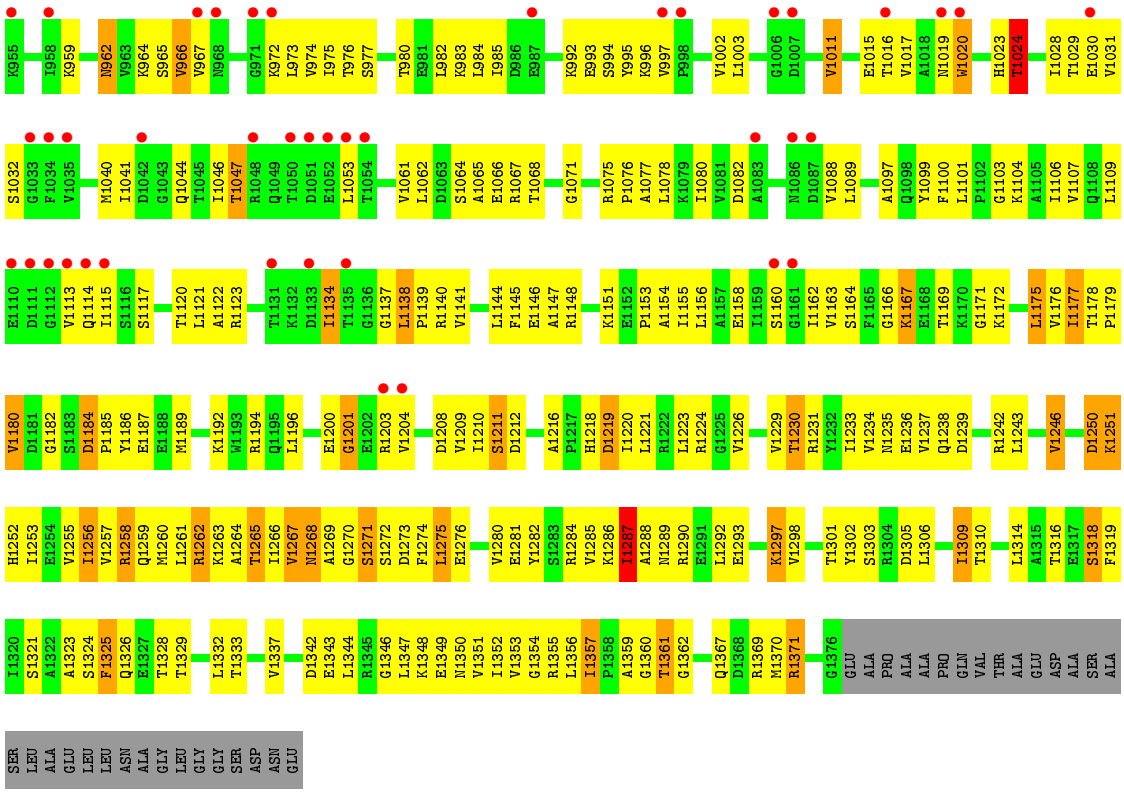

I238 L239 T240 V241 L242 P243 V244 L245 P246 P247 D248 L249 R250 P251 L252 V253 P254 L255 D256 R259 F260 A261 T262 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 R275 L279 L282 A286 A287 P288 I291 V292 E295 K296 R297 W298 L299 A302 V303 L306 L307 D308
N309 G310 R311 R312 G313 R314 A315 G318 S319 N320 K321 R322 P323 L324 L327 M330 I331 K332 G333 R337 L342 L343 G344 K345 R346 V347 D348 Y349 S350 G351 R352 S353 V354 I355 T356 V357 G358 P359 Y360 L361 R362 L363 H364 Q365 C366 G367 L368 P369 K370 K371 M372 A373 L374 E375 L376
F377 K378 P379 F380 I381 Y382 G383 K384 L385 E386 I387 R388 G389 I390 K395 A396 A397 K398 K399 W400 V401 E402 R403 E404 V407 V408 W409 D410 I411 L412 I416 P420 V421 L422 L423 M424 R425 A426 P427 T428 L429 H430 R431 L432 G433 I434 Q435 A436 F437 E438 P439 V440 L441 I442 E443 G444
K445 A446 Y447 Q448 L449 H450 P451 L452 A456 Y457 F461 D464 Q465 M466 A467 V468 H469 V470 P471 L472 T473 L474 E475 A476 Q477 L478 E479 A480 R481 A482 L483 M484 M485 S486 T487 N488 N489 S492 P493 A494 N495 G496 E497 P498 I499 I500 V501 P502 S503 Q504 D505 V506 V507 L510 Y511
Y512 M513 T514 R515 V518 N519 A520 T528 G529 P530 E534 R535 L536 Y537 R538 S539 G540 L541 A542 S543 L544 R547 V548 K549 V550 R551 I552 T553 E554 Y555 E556 K557 D558 L563 V564 A565 K566 L569 K570 D571 T572 T573 V574 G575 R576 A577 I578 L579 W580 M581 I582 G586 L587
S590 I591 V592 A595 L596 G597 K598 K599 A600 I601 S602 K603 M604 T607 C608 Y609 L612 G613 L614 K615 P616 T617 V618 I619 F620 A621 D622 Q623 I624 M625 Y626 F629 A630 Y631 A632 A633 R634 S635 G636 A637 S638 V639 G640 I641 D642 D643 M644 V645 I646 P647 E648 I654 I664
Q665 F668 G671 L672 V673 T674 K681 V682 I683 W686 M697 M698 D699 N700 L701 Q702 T703 E704 T705 V706 I707 N708 R709 D710 G711 Q712 E713 E714 K715 Q716 V717 S718 F719 N720 S721 I722 Y723 M724 M725 A726 D727 S728 G729 A730 R731 A734 A735 Q736 I737 R738 Q739 L740 A741 G742
M743 R744 G745 L746 M747 A748 K749 P750 S753 I754 I755 E756 T757 F758 I759 T760 A761 M762 F763 R764 L767 N768 V769 L770 Q771 Y772 F773 I774 S775 T776 H777 R780 T786 A787 L788 K789 T790 S793 G794 Y795 L796 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 T810
E811 D812 D813 C814 G815 T816 H817 E818 G819 T823 P824 V825 I826 E827 G828 G829 D830 V831 K832 E833 P834 L835 R836 D837 R838 V839 L840 G841 R842 E846 D847 Y848 L849 A854 D855 I856 R860 L863 E873 E874 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 V886 S887 C888
D891 F892 G893 V894 C895 C898 A904 I909 N910 K911 G912 E913 A914 I915 I918 A919 S922 I923 G924 E925 P926 G927 T928 Q929 L930 T931 M932 R933 T934 F935 H936 I937 A941 A946 E947 S948 S949 I950 Q951 V952 K953 N954 K955 I958 K959 L960 S961 N962 V963 K964 S965
V966 V967 N968 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 T991 S994 Y995 K996 V997 P998 Y999 V1002 L1003 A1004 K1005 G1006 D1007 V1011 A1012 G1013 G1014 E1015 T1016 V1017 A1018 N1019 W1020 D1021 P1022 H1023 T1024 V1027 I1028 T1029 E1030 V1031 S1032
V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 G1071 L1074 R1075 P1076 A1077 L1078 K1079 I1080 V1081 Q1084 G1085 N1086 D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 Q1098 Y1099 F1100
L1101 K1104 A1105 I1106 V1107 E1110 D1111 Q1114 S1117 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 Q1126 K1132 D1133 I1134 T1135 L1138 P1139 R1140 F1145 E1146 A1147 R1148 R1149 P1150 K1151 A1154 I1155 L1156 A1157 E1158 I1159 S1160 G1161 I1162 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170 G1171 K1172 R1173
R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 G1182 S1183 D1184 P1185 Y1186 E1187 E1188 M1189 I1190 P1191 K1192 W1193 R1194 Q1195 L1196 N1197 V1198 F1199 E1200 G1201 E1202 R1203 V1204 E1205 R1206 G1207 D1208 V1209 I1210 S1211 E1215 I1220 L1221 R1222 L1223 V1226 V1229 T1230 R1231 Y1232 I1233 V1234 N1235 E1236 V1237 Q1238 D1239 V1240
Y1241 R1242 L1243 Q1244 K1247 I1248 N1249 D1250 K1251 H1252 Y1253 E1254 V1255 I1256 V1257 R1258 Q1259 M1260 K1263 V1267 N1268 S1271 S1272 D1273 F1274 L1275 E1278 Q1279 V1280 E1281 Y1282 V1285 K1286 N1289 L1292 G1296 K1297 Y1302 L1307 G1308 I1309 T1310 K1311 A1312 S1313 L1314 A1315 T1316 E1317



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

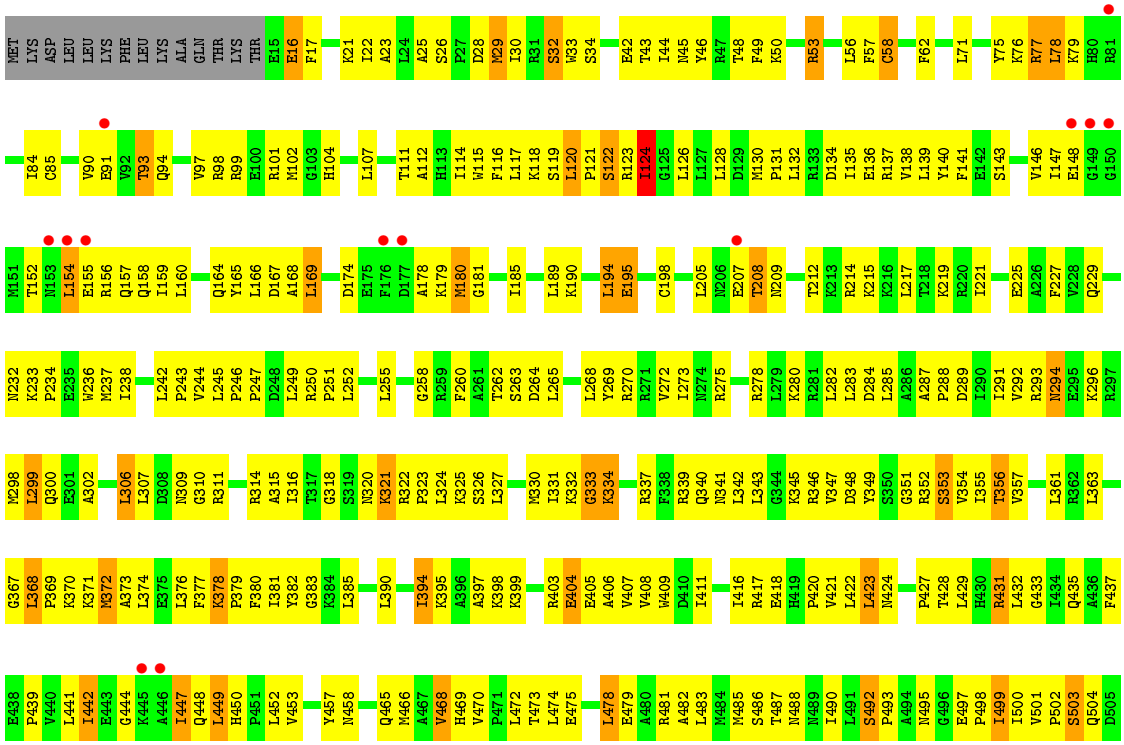
Chain J:

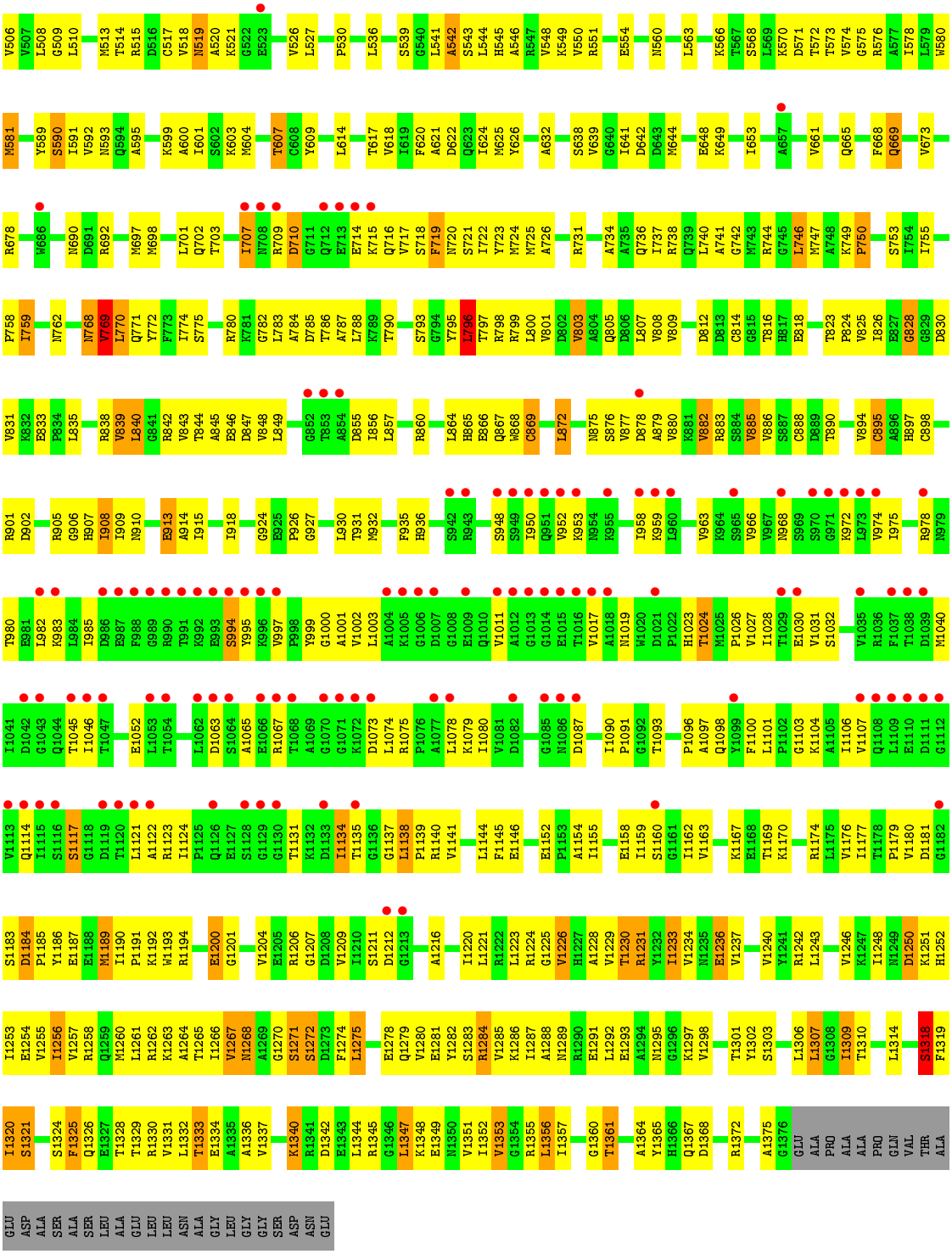




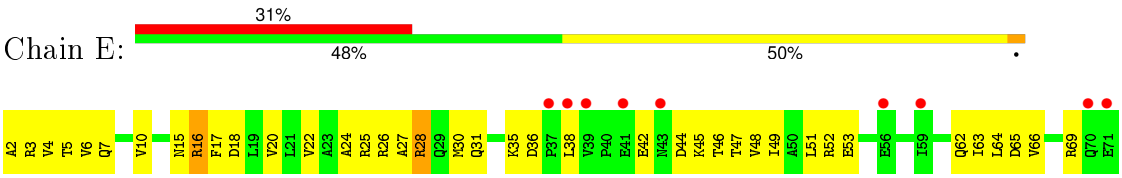
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain P:

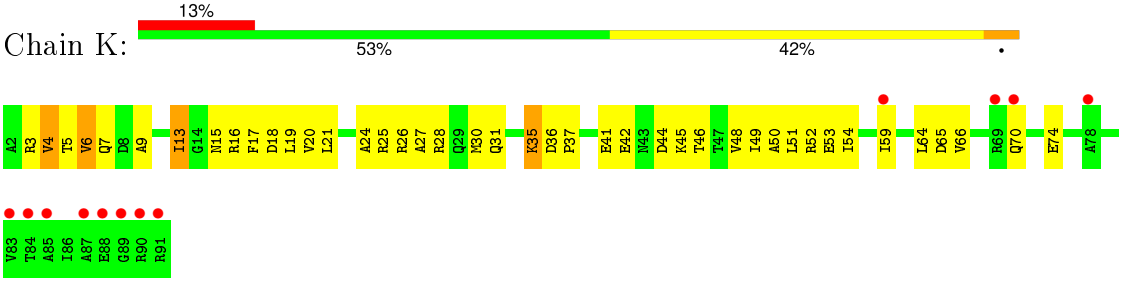




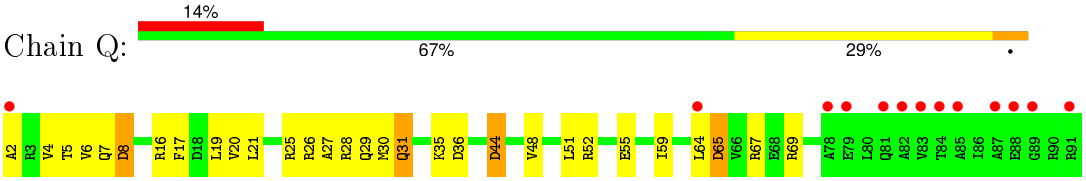
• Molecule 4: DNA-directed RNA polymerase subunit omega



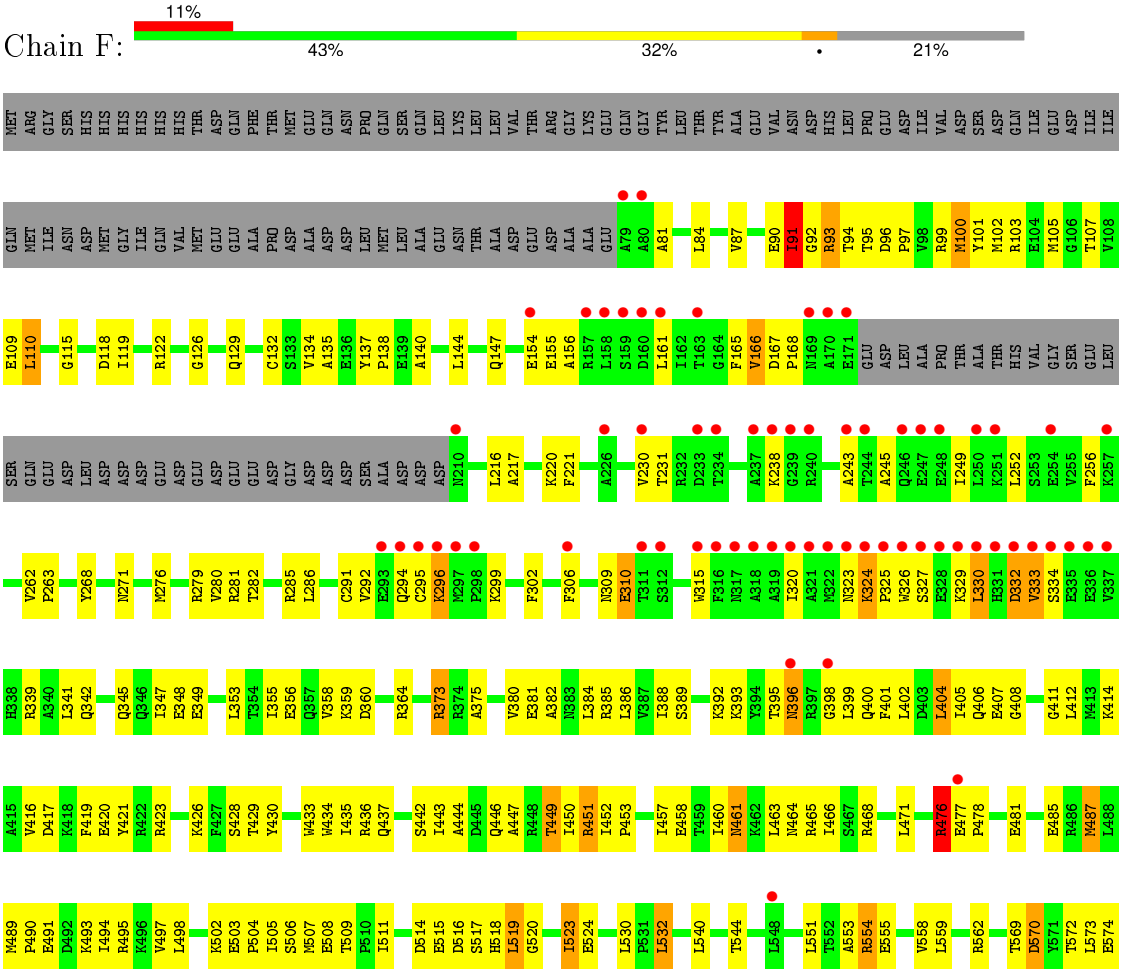
• Molecule 4: DNA-directed RNA polymerase subunit omega

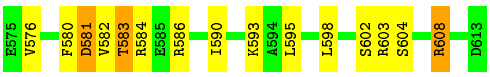


• Molecule 4: DNA-directed RNA polymerase subunit omega



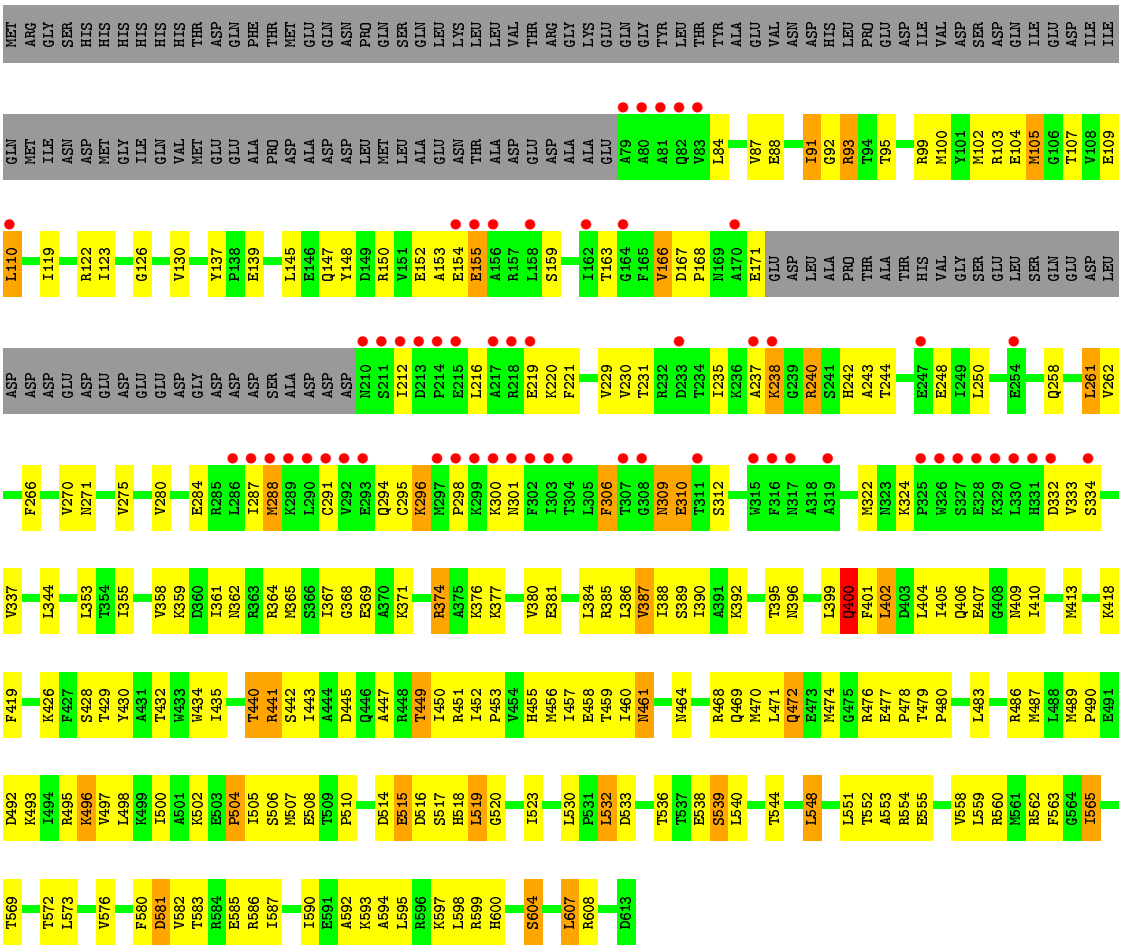
• Molecule 5: RNA polymerase sigma factor RpoD





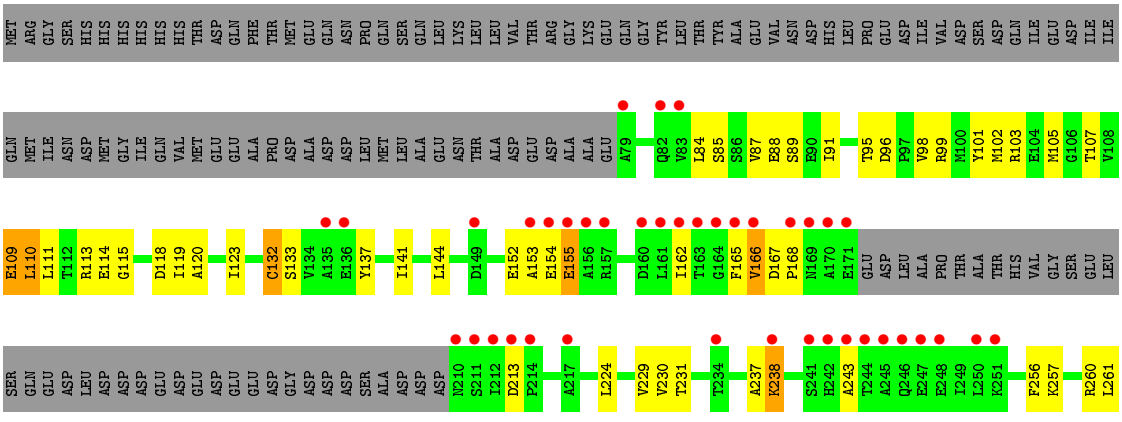
• Molecule 5: RNA polymerase sigma factor RpoD

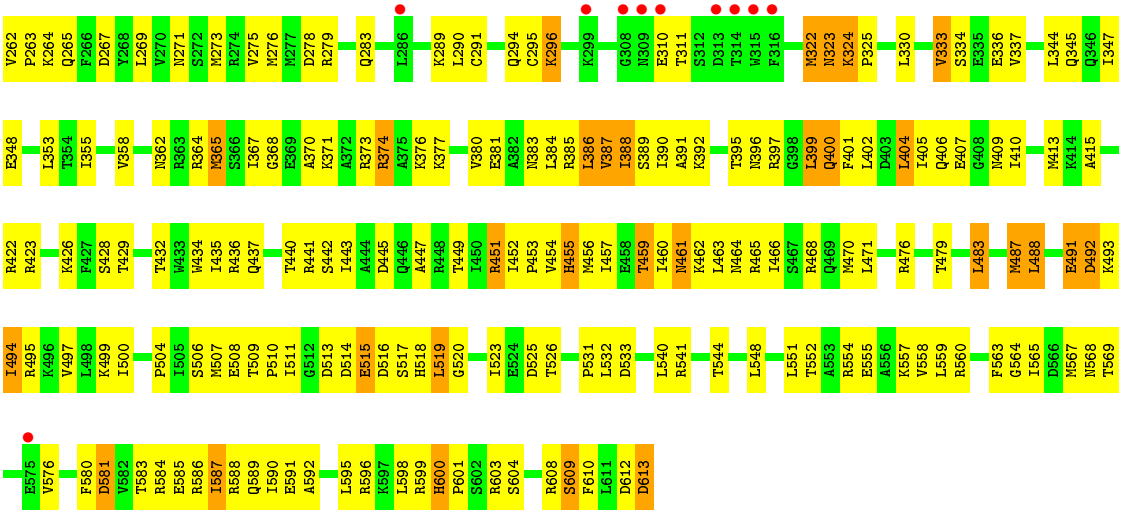
Chain L:



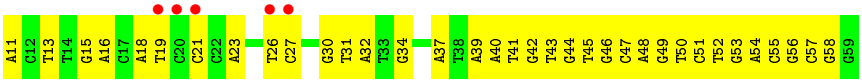
• Molecule 5: RNA polymerase sigma factor RpoD

Chain R:

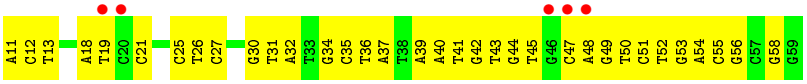




- Molecule 6: NT strand DNA (49-MER)

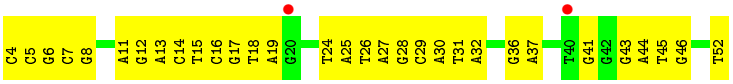


- Molecule 6: NT strand DNA (49-MER)

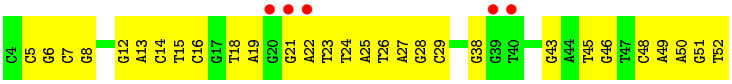


- Molecule 6: NT strand DNA (49-MER)

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

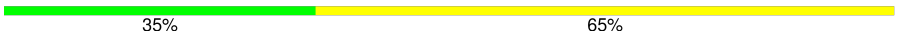


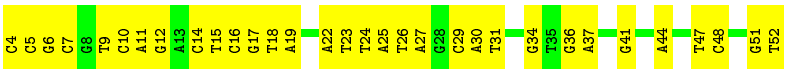
- Molecule 7: T strand DNA (49-MER)



• Molecule 7: T strand DNA (49-MER)

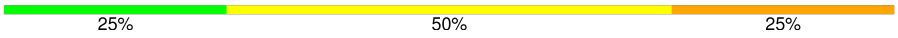
Chain 8:





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

Chain 3:

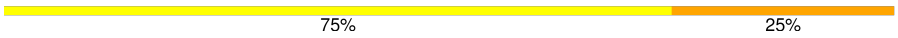


• Molecule 8: RNA (5'-D(*(GTP))-R(P*AP*GP*U)-3')

Chain 6:

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

Chain 9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	237.40Å 206.05Å 248.69Å 90.00° 116.55° 90.00°	Depositor
Resolution (Å)	39.90 – 5.50 39.90 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.90-5.50) 99.6 (39.90-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 5.37Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.245 , 0.328 0.244 , 0.328	Depositor DCC
R_{free} test set	3459 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	268.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 203.9	EDS
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 69425 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	94608	wwPDB-VP
Average B, all atoms (Å^2)	219.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

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

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

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

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	671	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1813	220	0
1	B	1767	0	1789	175	0
1	G	1787	0	1812	173	0
1	H	1767	0	1789	149	0
1	M	1787	0	1813	178	0

Continued on next page...

Continued from previous page...

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

The worst 5 of 6821 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:608:CYS:SG	3:D:617:THR:HG22	1.31	1.67
3:D:501:VAL:CG1	3:D:502:PRO:HD2	1.33	1.55
3:J:349:TYR:O	3:J:470:VAL:HG23	1.24	1.30
3:D:645:VAL:CG2	3:D:701:LEU:HD13	1.59	1.30
5:L:573:LEU:HB2	7:5:46:DG:OP2	1.15	1.28

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

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

5.3 Torsion angles (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	228/242 (94%)	214 (94%)	11 (5%)	3 (1%)	15 59
1	B	226/242 (93%)	204 (90%)	17 (8%)	5 (2%)	8 49
1	G	228/242 (94%)	209 (92%)	16 (7%)	3 (1%)	15 59
1	H	226/242 (93%)	207 (92%)	13 (6%)	6 (3%)	6 44
1	M	228/242 (94%)	214 (94%)	14 (6%)	0	100 100
1	N	226/242 (93%)	209 (92%)	14 (6%)	3 (1%)	15 59
2	C	1339/1342 (100%)	1218 (91%)	98 (7%)	23 (2%)	11 55
2	I	1339/1342 (100%)	1214 (91%)	105 (8%)	20 (2%)	13 57
2	O	1339/1342 (100%)	1234 (92%)	90 (7%)	15 (1%)	17 63
3	D	1360/1407 (97%)	1220 (90%)	109 (8%)	31 (2%)	8 48
3	J	1360/1407 (97%)	1227 (90%)	99 (7%)	34 (2%)	7 46
3	P	1360/1407 (97%)	1226 (90%)	99 (7%)	35 (3%)	7 45
4	E	88/90 (98%)	83 (94%)	5 (6%)	0	100 100
4	K	88/90 (98%)	84 (96%)	3 (3%)	1 (1%)	17 63
4	Q	88/90 (98%)	84 (96%)	4 (4%)	0	100 100
5	F	493/628 (78%)	444 (90%)	27 (6%)	22 (4%)	3 33
5	L	493/628 (78%)	447 (91%)	28 (6%)	18 (4%)	4 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	R	493/628 (78%)	449 (91%)	30 (6%)	14 (3%)	6 44
All	All	11202/11853 (94%)	10187 (91%)	782 (7%)	233 (2%)	9 50

5 of 233 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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	198/208 (95%)	181 (91%)	17 (9%)	13 47
1	B	196/208 (94%)	172 (88%)	24 (12%)	6 31
1	G	198/208 (95%)	178 (90%)	20 (10%)	9 38
1	H	196/208 (94%)	174 (89%)	22 (11%)	7 34
1	M	198/208 (95%)	178 (90%)	20 (10%)	9 38
1	N	196/208 (94%)	176 (90%)	20 (10%)	9 38
2	C	1156/1157 (100%)	1042 (90%)	114 (10%)	10 39
2	I	1156/1157 (100%)	1052 (91%)	104 (9%)	12 44
2	O	1156/1157 (100%)	1050 (91%)	106 (9%)	11 43
3	D	1135/1168 (97%)	1026 (90%)	109 (10%)	10 41
3	J	1135/1168 (97%)	1014 (89%)	121 (11%)	8 36
3	P	1135/1168 (97%)	1017 (90%)	118 (10%)	9 37
4	E	74/74 (100%)	70 (95%)	4 (5%)	27 64
4	K	74/74 (100%)	67 (90%)	7 (10%)	11 41
4	Q	74/74 (100%)	66 (89%)	8 (11%)	8 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	F	439/554 (79%)	406 (92%)	33 (8%)	17 54
5	L	439/554 (79%)	394 (90%)	45 (10%)	9 37
5	R	439/554 (79%)	393 (90%)	46 (10%)	8 37
All	All	9594/10107 (95%)	8656 (90%)	938 (10%)	10 40

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

Mol	Chain	Res	Type
2	I	1085	MET
3	J	882	VAL
3	P	1250	ASP
2	I	1255	THR
3	J	321	LYS

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

Mol	Chain	Res	Type
3	J	419	HIS
3	J	979	ASN
3	P	1259	GLN
3	J	465	GLN
3	J	700	ASN

5.3.3 RNA (i)

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

All (3) RNA backbone outliers are listed below:

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

All (2) RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

The worst 5 of 11 chain breaks are listed below:

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

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	230/242 (95%)	-0.10	3 (1%) 79 73	153, 175, 210, 235	0
1	B	228/242 (94%)	-0.14	5 (2%) 65 60	162, 194, 217, 238	0
1	G	230/242 (95%)	0.09	7 (3%) 54 47	157, 185, 217, 248	0
1	H	228/242 (94%)	-0.10	3 (1%) 79 73	160, 191, 229, 261	0
1	M	230/242 (95%)	0.10	4 (1%) 73 67	166, 200, 233, 252	0
1	N	228/242 (94%)	0.31	14 (6%) 25 23	186, 233, 258, 273	0
2	C	1341/1342 (99%)	-0.06	15 (1%) 82 78	119, 186, 244, 277	0
2	I	1341/1342 (99%)	-0.06	29 (2%) 65 60	130, 195, 278, 377	0
2	O	1341/1342 (99%)	-0.06	15 (1%) 82 78	144, 183, 235, 270	0
3	D	1362/1407 (96%)	0.22	102 (7%) 17 19	128, 214, 296, 349	0
3	J	1362/1407 (96%)	0.13	65 (4%) 34 31	132, 194, 280, 314	0
3	P	1362/1407 (96%)	0.35	129 (9%) 10 13	148, 208, 292, 330	0
4	E	90/90 (100%)	1.21	28 (31%) 1 4	169, 206, 407, 461	0
4	K	90/90 (100%)	0.48	12 (13%) 4 8	144, 199, 394, 442	0
4	Q	90/90 (100%)	0.74	13 (14%) 3 7	167, 222, 416, 460	0
5	F	497/628 (79%)	0.44	66 (13%) 4 8	182, 294, 404, 418	0
5	L	497/628 (79%)	0.38	59 (11%) 6 10	169, 262, 400, 406	0
5	R	497/628 (79%)	0.31	50 (10%) 9 12	172, 259, 413, 444	0
6	1	49/49 (100%)	0.58	5 (10%) 9 12	201, 272, 311, 317	0
6	4	49/49 (100%)	0.38	5 (10%) 9 12	209, 264, 308, 350	0
6	7	49/49 (100%)	0.44	2 (4%) 41 37	211, 255, 278, 300	0
7	2	49/49 (100%)	0.44	2 (4%) 41 37	215, 278, 312, 343	0
7	5	49/49 (100%)	0.63	5 (10%) 9 12	198, 270, 339, 341	0
7	8	49/49 (100%)	0.44	0 100 100	195, 260, 296, 335	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
8	3	3/4 (75%)	0.67	0	100	100	255, 255, 281, 321	0
8	6	3/4 (75%)	0.50	0	100	100	263, 263, 272, 282	0
8	9	3/4 (75%)	0.89	0	100	100	262, 262, 277, 295	0
All	All	11547/12159 (94%)	0.14	638 (5%)	29	28	119, 203, 358, 461	0

The worst 5 of 638 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	210	ASN	8.9
3	P	1068	THR	8.9
3	P	1006	GLY	8.5
5	L	211	SER	8.3
3	D	961	SER	7.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
9	ZN	P	1502	1/1	0.98	0.17	-0.01	187,187,187,187	0
9	ZN	J	1501	1/1	0.88	0.15	-0.87	200,200,200,200	0
9	ZN	D	1502	1/1	0.94	0.11	-0.98	212,212,212,212	0
9	ZN	J	1502	1/1	0.98	0.12	-1.02	174,174,174,174	0
10	MG	D	1503	1/1	0.95	0.16	-1.22	176,176,176,176	0
9	ZN	D	1501	1/1	0.97	0.09	-1.41	228,228,228,228	0
9	ZN	P	1501	1/1	0.95	0.10	-2.02	214,214,214,214	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	MG	P	1503	1/1	0.91	0.15	-2.25	194,194,194,194	0
10	MG	6	101	1/1	0.88	0.34	-	189,189,189,189	0

6.5 Other polymers (i)

There are no such residues in this entry.