wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 03:45 am BST

PDB ID	:	3QT1
Title	:	RNA polymerase II variant containing A Chimeric RPB9-C11 subunit
Authors	:	Ruan, W.; Lehmann, E.; Thomm, M.; Kostrewa, D.; Cramer, P.
Deposited on	:	2011-02-22
Resolution	:	4.30 Å(reported)

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

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

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

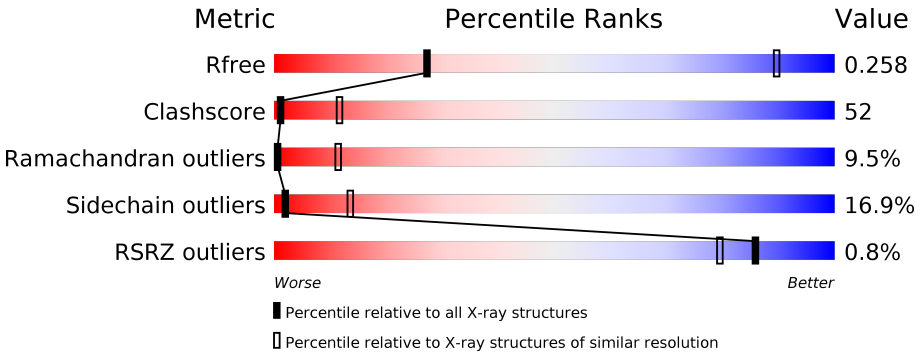
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	1733	% 23% 44% 14% • 18%
2	B	1224	% 26% 49% 15% • 10%
3	C	318	26% 44% 13% 16%
4	D	219	21% 45% 14% • 19%
5	E	215	27% 60% 11% •
6	F	155	13% 34% 9% • 44%

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Mol	Chain	Length	Quality of chain
7	G	171	32% 54% 13%
8	H	146	3% 35% 42% 13% 8%
9	I	133	13% 17% 5% 65%
10	J	70	19% 61% 11% 7%
11	K	120	33% 39% 23% 5%
12	L	70	13% 26% 20% 7% 34%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30535 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
			Total	C	N	O	S			
1	A	1416	11143	7021	1949	2111	62	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1103	8770	5554	1535	1626	55	0	0	0

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

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

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

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

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

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

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

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

- 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			

- 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			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9, DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	47	Total	C	N	O	S	0	0	0
			398	246	72	75	5			

- 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			

- 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			

- 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			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Zn 1 1	0	0
13	I	1	Total Zn 1 1	0	0
13	C	1	Total Zn 1 1	0	0
13	A	2	Total Zn 2 2	0	0
13	L	1	Total Zn 1 1	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

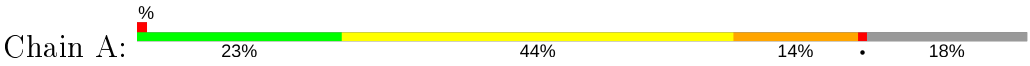
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0

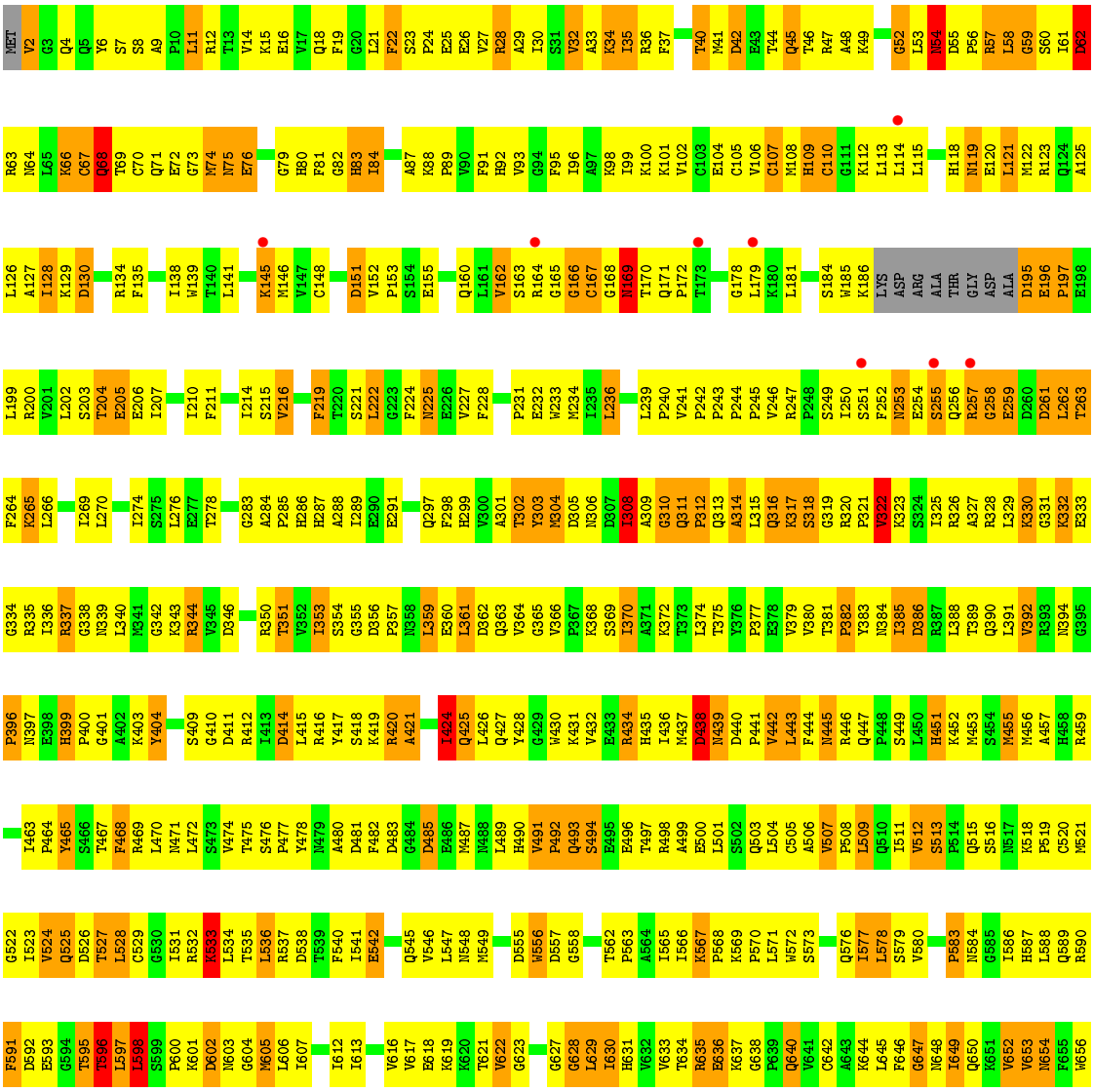
3 Residue-property plots (i)

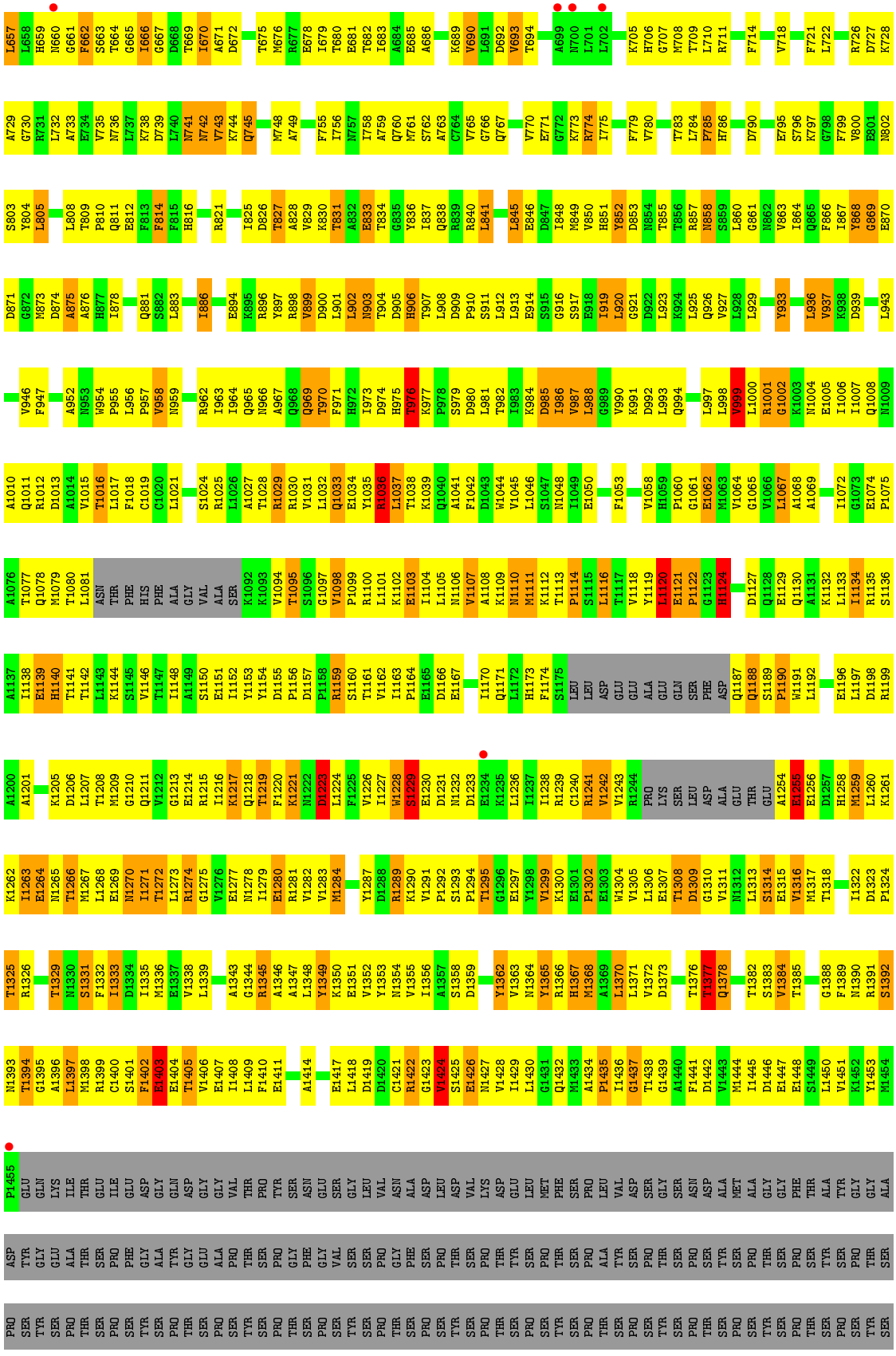
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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

Chain A:



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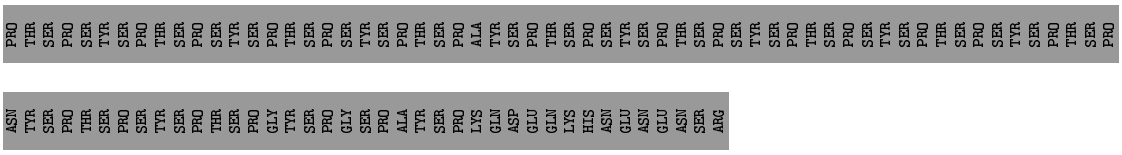
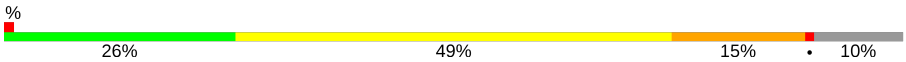
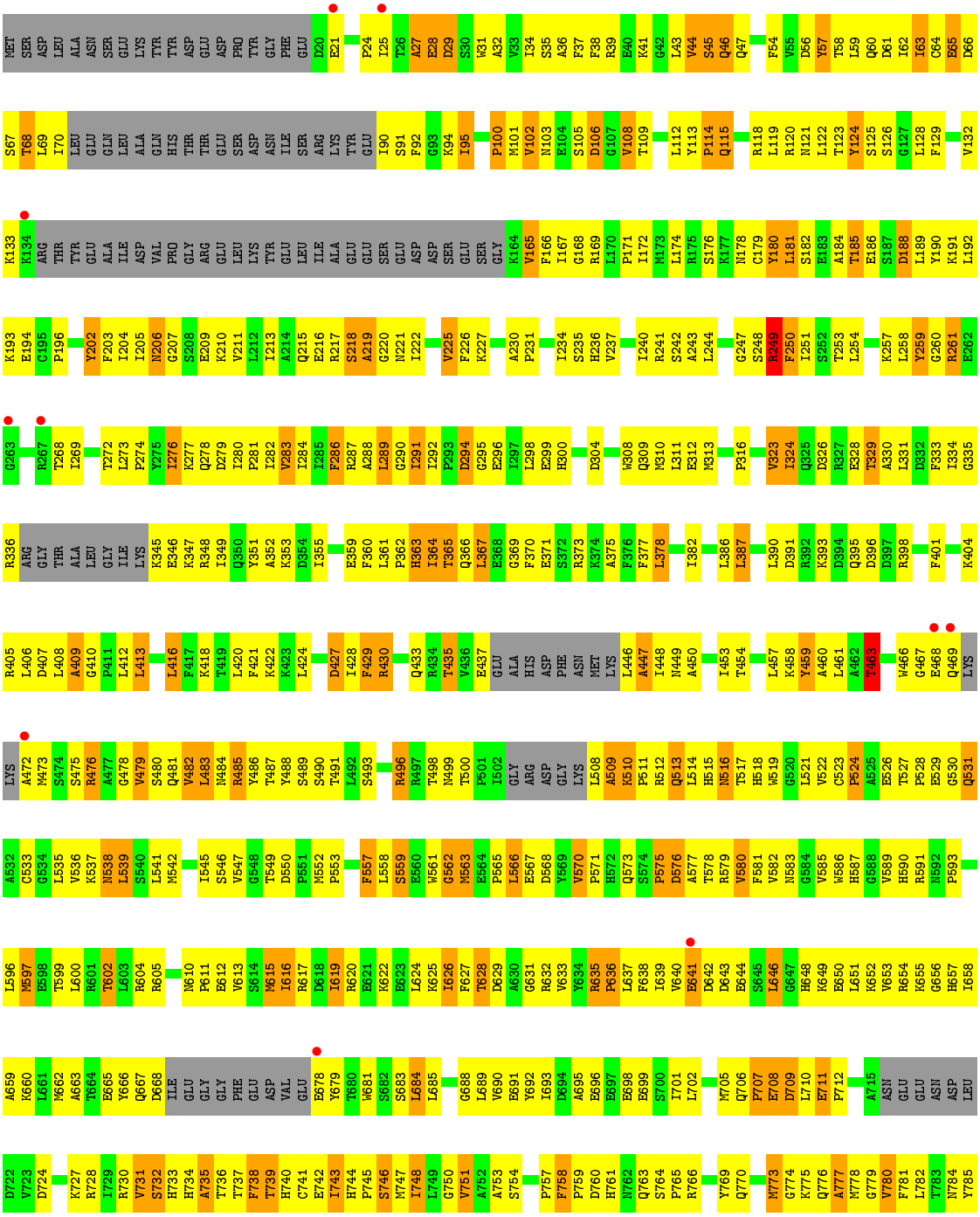
A729 G730 R731 L732 A733 E734 V735 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 M748 A749 F755 I756 N757 I758 A759 Q760 M761 S762 A763 C764 V765 G766 Q767 V770 E771 G772 K773 R774 I775 F779 V780 T783 L784 P785 H786 D790 E795 S796 K797 G798 F799 V800 E801 N802
S803 Y804 L805 L808 T809 P810 Q811 E812 F813 F814 F815 H816 R821 I825 D826 T827 A828 V829 K830 T831 A832 E833 T834 G835 Y836 I837 Q838 R839 R840 L841 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 A876 H877 I878 Q881 S882 L883 I886 E894 K895 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 L923 K924 L925 Q926 V927 L928 L929 Y933 L936 V937 K938 D939 L943
V946 F947 A952 N953 W954 P955 L956 P957 V958 N959 R962 I963 I964 Q965 N966 A967 Q968 Q969 T970 F971 H972 I973 D974 H975 T976 K977 F978 S979 D980 L981 T982 I983 K984 D985 I986 V987 L988 G989 V990 K991 D992 L993 Q994 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 S1024 R1025 L1026 A1027 T1028 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 V1046 S1047 N1048 I1049 E1050 F1053 V1058 H1059 P1060 G1061 E1062 M1063 V1064 G1065 V1066 L1067 A1068 A1069 I1072 G1073 E1074 P1075
A1076 T1077 Q1078 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA GLY VAL ALA SER K1092 K1093 V1094 T1095 S1096 G1097 V1098 P1099 R1100 L1101 K1102 E1103 I1104 L1105 N1106 V1107 A1108 K1109 N1110 M1111 K1112 N1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 E1121 P1122 G1123 H1124 D1127 Q1128 E1129 Q1130 A1131 K1132 L1133 T1134 R1135 S1136
A1137 I1138 E1139 H1140 T1141 T1142 L1143 K1144 S1145 V1146 T1147 I1148 A1149 S1150 E1151 I1152 Y1153 Y1154 D1155 P1156 D1157 P1158 R1159 S1160 T1161 V1162 I1163 P1164 E1165 D1166 E1167 I1170 Q1171 L1172 H1173 F1174 S1175 LEU LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 E1196 L1197 D1198 R1199
A1200 A1201 K1205 D1206 L1207 T1208 M1209 G1210 Q1211 V1212 G1213 E1214 R1215 I1216 K1217 Q1218 T1219 F1220 K1221 M1222 D1223 L1224 F1225 V1226 I1227 W1228 S1229 E1230 D1231 N1232 D1233 E1234 K1235 L1236 I1237 I1238 R1239 C1240 R1241 V1242 V1243 R1244 PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 D1257 H1258 M1259 L1260 K1261
K1262 I1263 E1264 N1265 T1266 M1267 L1268 E1269 N1270 I1271 T1272 L1273 R1274 G1275 V1276 E1277 N1278 I1279 E1280 R1281 V1282 V1283 M1284 Y1287 D1288 R1289 K1290 V1291 P1292 S1293 P1294 T1295 G1296 E1297 Y1298 V1299 K1300 E1301 P1302 E1303 W1304 V1305 L1306 E1307 T1308 D1309 G1310 V1311 N1312 L1313 S1314 E1315 V1316 M1317 T1318 I1322 D1323 P1324
T1325 R1326 T1329 N1330 S1331 F1332 I1333 D1334 I1335 M1336 E1337 V1338 L1339 A1343 G1344 R1345 A1346 A1347 L1348 Y1349 K1350 E1351 V1352 Y1353 N1354 V1355 I1356 G1423 A1357 S1358 D1359 Y1362 V1363 N1364 Y1365 R1366 H1367 M1368 A1369 L1370 L1371 V1372 D1373 T1376 T1377 Q1378 T1382 S1383 V1384 T1385 G1388 F1389 N1390 R1391 S1392
N1393 T1394 G1395 A1396 L1397 M1398 R1399 C1400 S1401 F1402 E1403 E1404 T1405 Q1406 E1407 I1408 L1409 F1410 E1411 A1414 E1417 L1418 D1419 D1420 C1421 R1422 G1423 V1424 S1425 E1426 N1427 V1428 I1429 L1430 G1431 Q1432 M1433 A1434 P1435 I1436 G1437 T1438 G1439 A1440 F1441 D1442 V1443 M1444 I1445 D1446 E1447 E1448 S1449 L1450 V1451 K1452 Y1453 M1454
P1455 GLU GLN LYS ILE THR GLU ILE GLU ASP GLY GLN ASP GLY VAL THR PRO TYR SER ASN GLU SER LEU VAL SER PRO GLY VAL ASN ALA ASP LEU ASP VAL LYS ASP GLU LEU MET PHE SER PRO LEU VAL ASP SER GLY SER ALA ASN ASP ALA MET ALA GLY GLY PHE THR ALA TYR GLY GLY ALA
ASP TYR GLY GLU ALA THR SER PRO PHE GLY ALA TYR GLY GLU ALA PRO THR SER PRO PHE GLY VAL SER SER PRO VAL SER PRO ASN ALA TYR SER PRO THR SER PRO THR SER PRO ALA TYR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER
PRO SER TYR SER PRO THR SER PRO PRO SER PRO TYR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER PRO THR SER

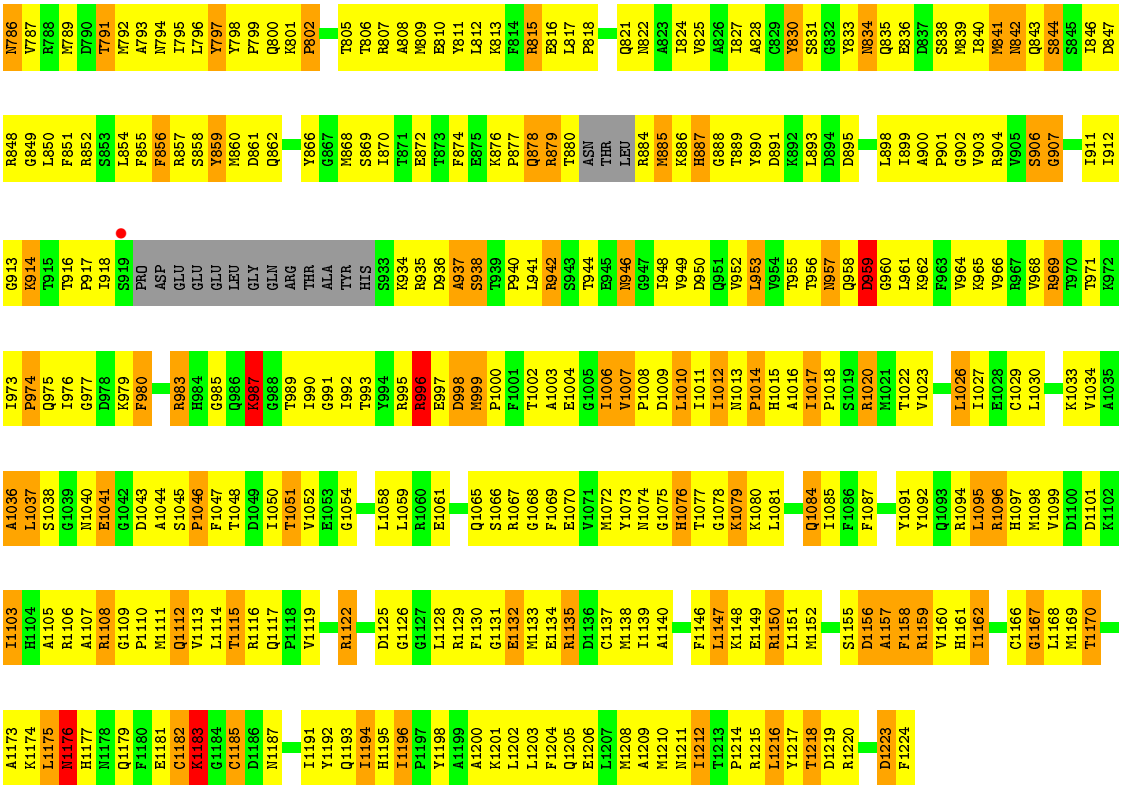


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

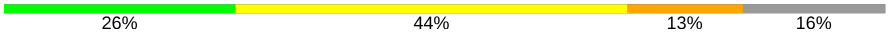


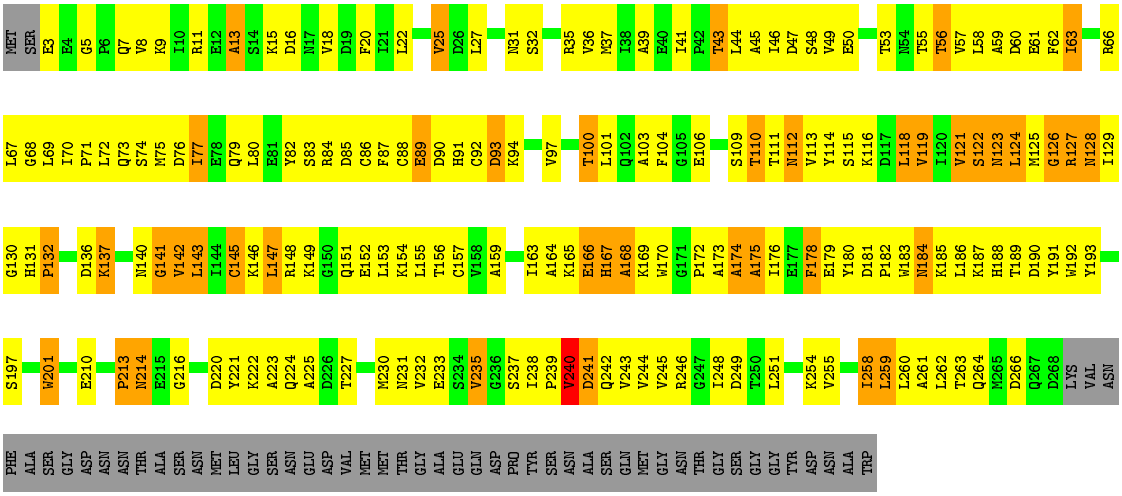




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

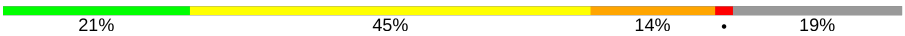
Chain C:

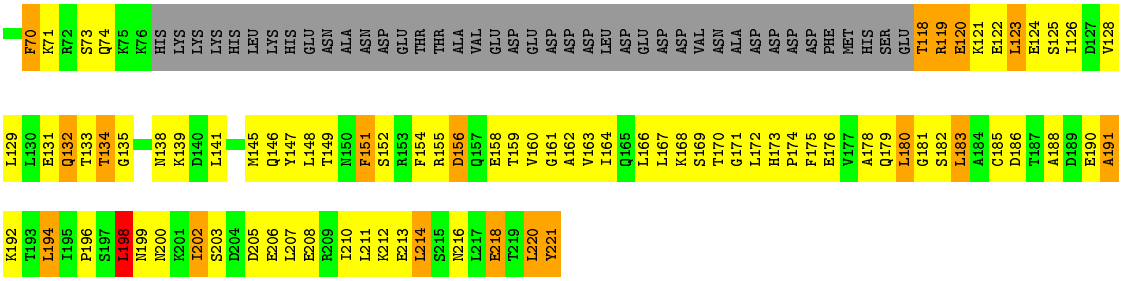




• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

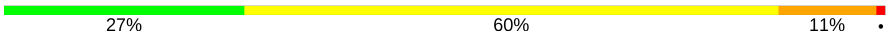
Chain D:

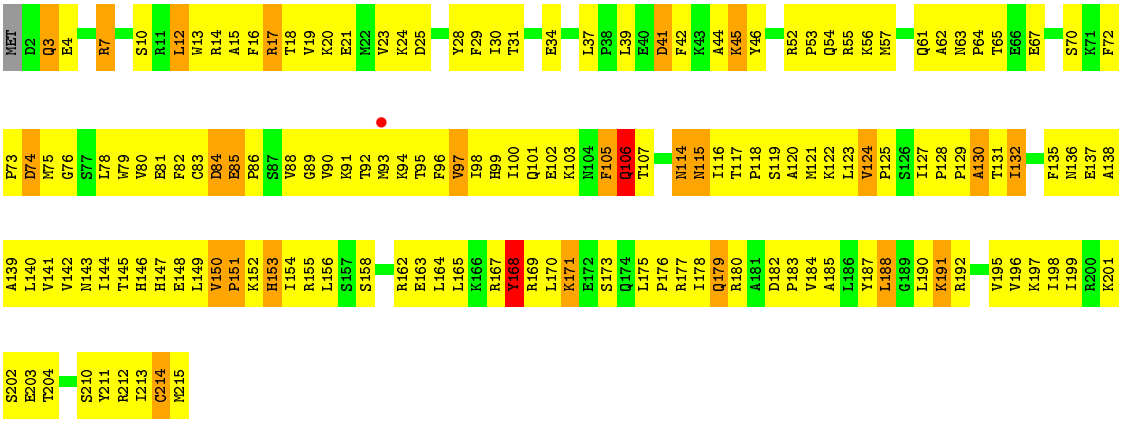




• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

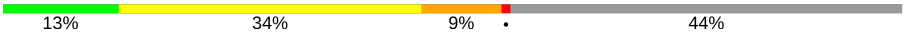
Chain E:

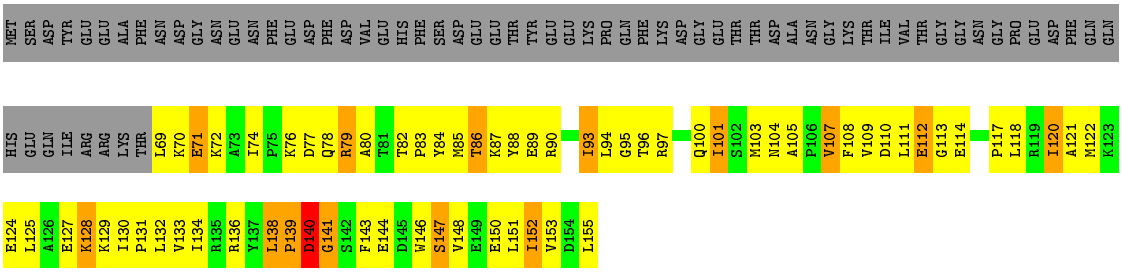




• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

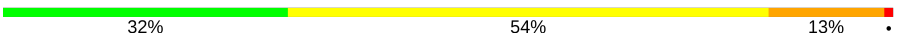
Chain F:

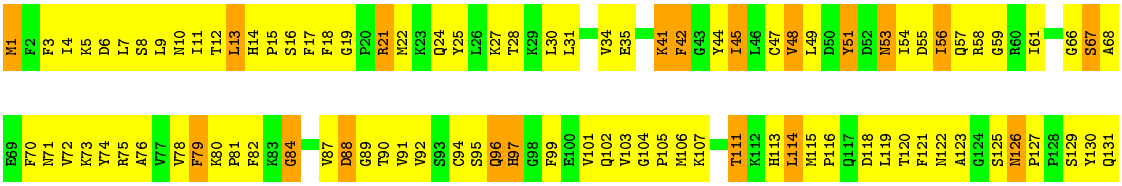


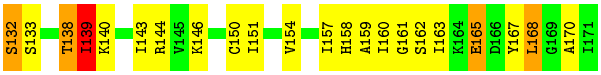


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

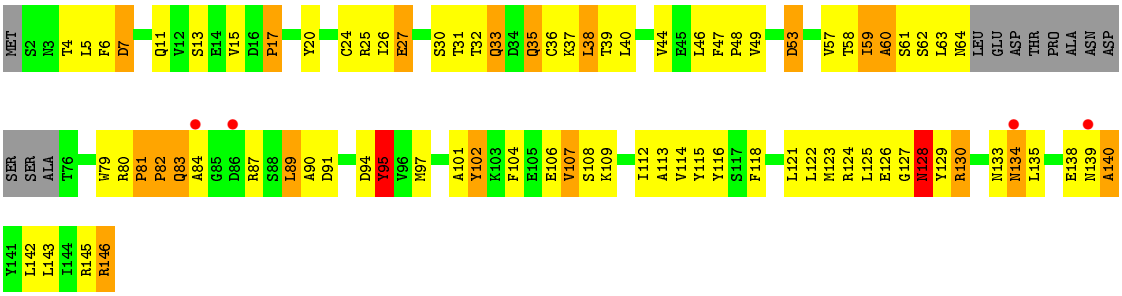






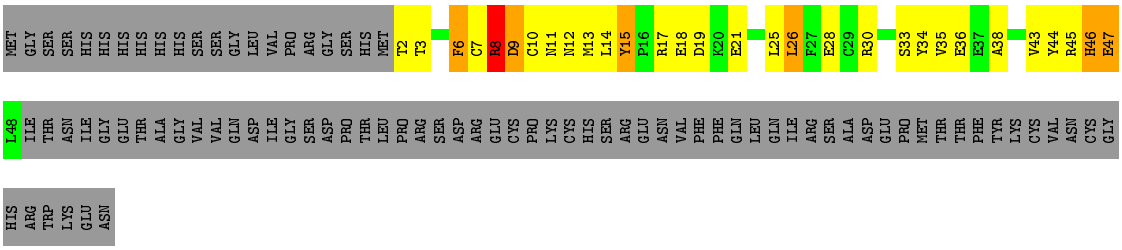
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



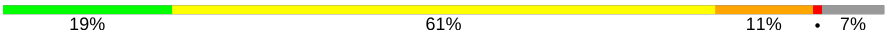
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9, DNA-directed RNA polymerase III subunit RPC10

Chain I:



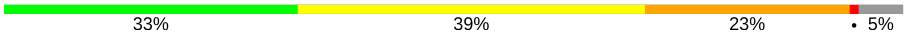
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

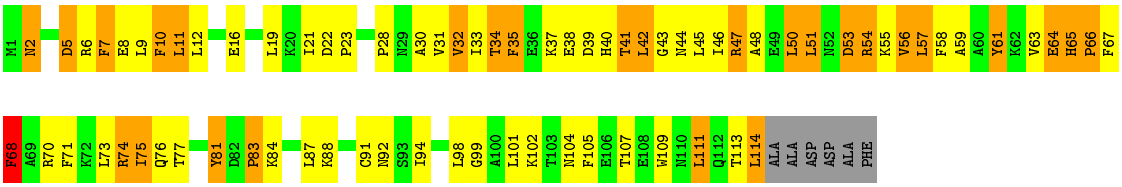
Chain J:



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

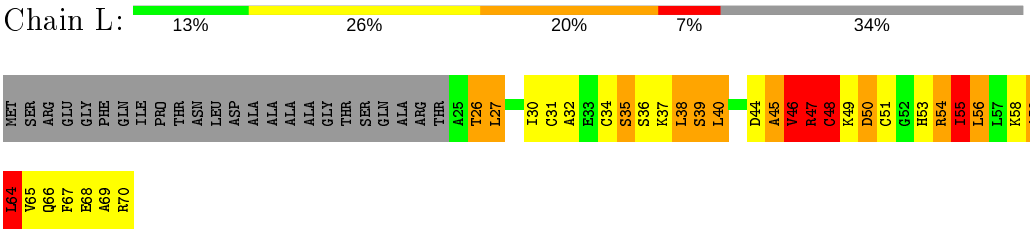
Chain K:





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

Chain L:


13%
26%
20%
7%
34%
MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR A25 T26 L27 I30 C31 A32 E33 C34 S35 S36 K37 L38 S39 L40 D44 A45 V46 R47 C48 K49 D50 C51 G52 H53 R54 I55 L56 L57 K58 A59 R60 T61 K62 R63 L64 V65 Q66 F67 E68 A69 R70

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.38Å 393.38Å 281.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 4.30 48.66 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.60-4.30) 98.5 (48.66-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.235 , 0.281 0.209 , 0.258	Depositor DCC
R_{free} test set	2022 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å^2)	172.3	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 119.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.057 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.067 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	30535	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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

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	0.35	0/11342	0.58	0/15337
2	B	0.34	0/8939	0.56	0/12051
3	C	0.33	0/2133	0.56	0/2891
4	D	0.32	0/1444	0.52	0/1935
5	E	0.32	0/1788	0.54	0/2406
6	F	0.40	0/717	0.63	0/967
7	G	0.33	0/1368	0.55	0/1844
8	H	0.29	0/1094	0.50	0/1481
9	I	0.36	0/406	0.57	0/546
10	J	0.33	0/541	0.57	0/727
11	K	0.38	0/937	0.56	0/1265
12	L	0.36	0/365	0.64	0/485
All	All	0.34	0/31074	0.56	0/41935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1243	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8770	0	8795	984	0
3	C	2095	0	2051	223	0
4	D	1434	0	1460	163	0
5	E	1752	0	1776	172	0
6	F	705	0	731	101	0
7	G	1340	0	1357	153	0
8	H	1076	0	1046	97	0
9	I	398	0	370	37	0
10	J	532	0	542	92	0
11	K	919	0	929	113	0
12	L	363	0	386	65	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	30535	0	30660	3185	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 52.

The worst 5 of 3185 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)
1:A:775:ILE:HB	1:A:797:LYS:O	1.37	1.23
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.21	1.17
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.26	1.15
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.17	1.14
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.30	1.13

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%)	974 (69%)	284 (20%)	148 (10%)	0 8
2	B	1081/1224 (88%)	754 (70%)	232 (22%)	95 (9%)	1 12
3	C	264/318 (83%)	187 (71%)	48 (18%)	29 (11%)	0 8
4	D	174/219 (80%)	116 (67%)	43 (25%)	15 (9%)	1 13
5	E	212/215 (99%)	156 (74%)	41 (19%)	15 (7%)	1 16
6	F	85/155 (55%)	61 (72%)	19 (22%)	5 (6%)	1 20
7	G	169/171 (99%)	120 (71%)	43 (25%)	6 (4%)	3 28
8	H	130/146 (89%)	90 (69%)	29 (22%)	11 (8%)	1 13
9	I	45/133 (34%)	31 (69%)	10 (22%)	4 (9%)	1 12
10	J	63/70 (90%)	43 (68%)	14 (22%)	6 (10%)	0 11
11	K	112/120 (93%)	79 (70%)	24 (21%)	9 (8%)	1 14
12	L	44/70 (63%)	21 (48%)	8 (18%)	15 (34%)	0 0
All	All	3785/4574 (83%)	2632 (70%)	795 (21%)	358 (10%)	0 11

5 of 358 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	42	ASP
1	A	48	ALA
1	A	54	ASN
1	A	57	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%)	1031 (83%)	208 (17%)	2 14
2	B	957/1061 (90%)	800 (84%)	157 (16%)	2 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	234/274 (85%)	200 (86%)	34 (14%)	3 18
4	D	160/198 (81%)	127 (79%)	33 (21%)	1 7
5	E	196/197 (100%)	170 (87%)	26 (13%)	4 20
6	F	77/137 (56%)	65 (84%)	12 (16%)	2 16
7	G	152/152 (100%)	124 (82%)	28 (18%)	1 11
8	H	118/128 (92%)	98 (83%)	20 (17%)	2 13
9	I	45/122 (37%)	35 (78%)	10 (22%)	1 6
10	J	60/65 (92%)	50 (83%)	10 (17%)	2 14
11	K	99/102 (97%)	76 (77%)	23 (23%)	1 5
12	L	40/57 (70%)	29 (72%)	11 (28%)	0 3
All	All	3377/4013 (84%)	2805 (83%)	572 (17%)	2 13

5 of 572 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	496	ARG
2	B	980	PHE
10	J	7	CYS
2	B	559	SER
2	B	748	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	GLN
2	B	761	HIS
7	G	113	HIS
2	B	178	ASN
2	B	516	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1416/1733 (81%)	-0.32	14 (0%) 82 74	31, 133, 223, 314	0
2	B	1103/1224 (90%)	-0.26	11 (0%) 82 74	23, 141, 230, 357	0
3	C	266/318 (83%)	-0.32	0 100 100	58, 139, 209, 281	0
4	D	178/219 (81%)	-0.43	0 100 100	64, 146, 212, 263	0
5	E	214/215 (99%)	-0.35	1 (0%) 91 86	71, 165, 246, 367	0
6	F	87/155 (56%)	-0.36	0 100 100	48, 95, 156, 221	0
7	G	171/171 (100%)	-0.37	0 100 100	43, 121, 199, 230	0
8	H	134/146 (91%)	0.05	4 (2%) 50 39	115, 185, 250, 406	0
9	I	47/133 (35%)	-0.26	0 100 100	93, 163, 204, 221	0
10	J	65/70 (92%)	-0.35	0 100 100	80, 147, 210, 261	0
11	K	114/120 (95%)	-0.36	0 100 100	63, 128, 194, 254	0
12	L	46/70 (65%)	-0.28	0 100 100	93, 159, 240, 306	0
All	All	3841/4574 (83%)	-0.30	30 (0%) 86 79	23, 140, 227, 406	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	134	LYS	3.5
8	H	139	ASN	3.5
1	A	257	ARG	3.4
2	B	472	ALA	3.1
2	B	469	GLN	3.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	MG	A	3009	1/1	0.85	0.97	89,89,89,89	0
13	ZN	A	3006	1/1	0.89	0.07	274,274,274,274	0
13	ZN	A	3008	1/1	0.96	0.13	97,97,97,97	0
13	ZN	L	3005	1/1	0.97	0.08	229,229,229,229	0
13	ZN	C	3002	1/1	0.98	0.11	129,129,129,129	0
13	ZN	J	3001	1/1	0.98	0.29	153,153,153,153	0
13	ZN	B	3007	1/1	0.99	0.20	116,116,116,116	0
13	ZN	I	3003	1/1	1.00	0.12	133,133,133,133	0

6.5 Other polymers (i)

There are no such residues in this entry.