wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:45 am BST

PDB ID : 5M59
Title : Crystal structure of Chaetomium thermophilum Brr2 helicase core in complex with Prp8 Jab1 domain
Authors : Absmeier, E.; Becke, C.; Wollenhaupt, J.; Santos, K.F.; Wahl, M.C.
Deposited on : 2016-10-20
Resolution : 3.20 Å(reported)

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

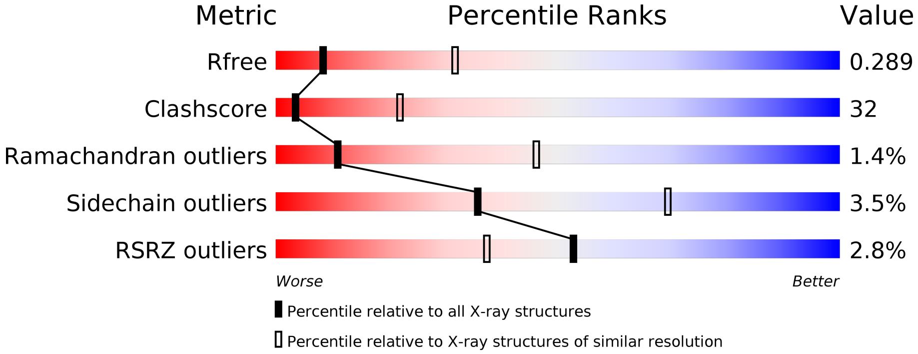
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	B	276	
1	D	276	
1	F	276	
1	H	276	
2	A	1772	
2	C	1772	

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Mol	Chain	Length	Quality of chain
2	E	1772	
2	G	1772	

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
3	ACT	E	2201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 63679 atoms, of which 12 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 Putative pre-mRNA splicing factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	266	Total 2116	C 1352	N 362	O 392	S 10	0	0	0
1	D	263	Total 2093	C 1339	N 359	O 385	S 10	0	0	0
1	F	265	Total 2116	C 1353	N 362	O 391	S 10	0	0	0
1	H	267	Total 2125	C 1358	N 364	O 393	S 10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2034	GLY	-	expression tag	UNP G0SFL3
B	2035	ALA	-	expression tag	UNP G0SFL3
B	2036	MET	-	expression tag	UNP G0SFL3
D	2034	GLY	-	expression tag	UNP G0SFL3
D	2035	ALA	-	expression tag	UNP G0SFL3
D	2036	MET	-	expression tag	UNP G0SFL3
F	2034	GLY	-	expression tag	UNP G0SFL3
F	2035	ALA	-	expression tag	UNP G0SFL3
F	2036	MET	-	expression tag	UNP G0SFL3
H	2034	GLY	-	expression tag	UNP G0SFL3
H	2035	ALA	-	expression tag	UNP G0SFL3
H	2036	MET	-	expression tag	UNP G0SFL3

- Molecule 2 is a protein called Pre-mRNA splicing helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1738	Total 13917	C 8891	N 2369	O 2592	S 65	0	0	0
2	C	1702	Total 13628	C 8709	N 2319	O 2536	S 64	0	0	0

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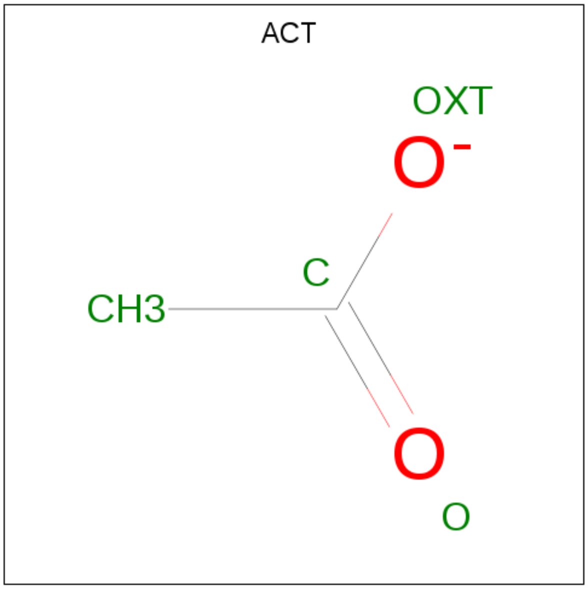
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	1740	Total 13925	C 8896	N 2372	O 2592	S 65	0	0	0
2	G	1710	Total 13701	C 8753	N 2336	O 2547	S 65	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	expression tag	UNP G0S0B9
A	423	ALA	-	expression tag	UNP G0S0B9
A	424	GLU	-	expression tag	UNP G0S0B9
A	425	PHE	-	expression tag	UNP G0S0B9
C	422	GLY	-	expression tag	UNP G0S0B9
C	423	ALA	-	expression tag	UNP G0S0B9
C	424	GLU	-	expression tag	UNP G0S0B9
C	425	PHE	-	expression tag	UNP G0S0B9
E	422	GLY	-	expression tag	UNP G0S0B9
E	423	ALA	-	expression tag	UNP G0S0B9
E	424	GLU	-	expression tag	UNP G0S0B9
E	425	PHE	-	expression tag	UNP G0S0B9
G	422	GLY	-	expression tag	UNP G0S0B9
G	423	ALA	-	expression tag	UNP G0S0B9
G	424	GLU	-	expression tag	UNP G0S0B9
G	425	PHE	-	expression tag	UNP G0S0B9

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 7 2 3 2	0	0
3	C	1	Total C H O 7 2 3 2	0	0
3	E	1	Total C H O 7 2 3 2	0	0
3	G	1	Total C H O 7 2 3 2	0	0

- Molecule 4 is water.

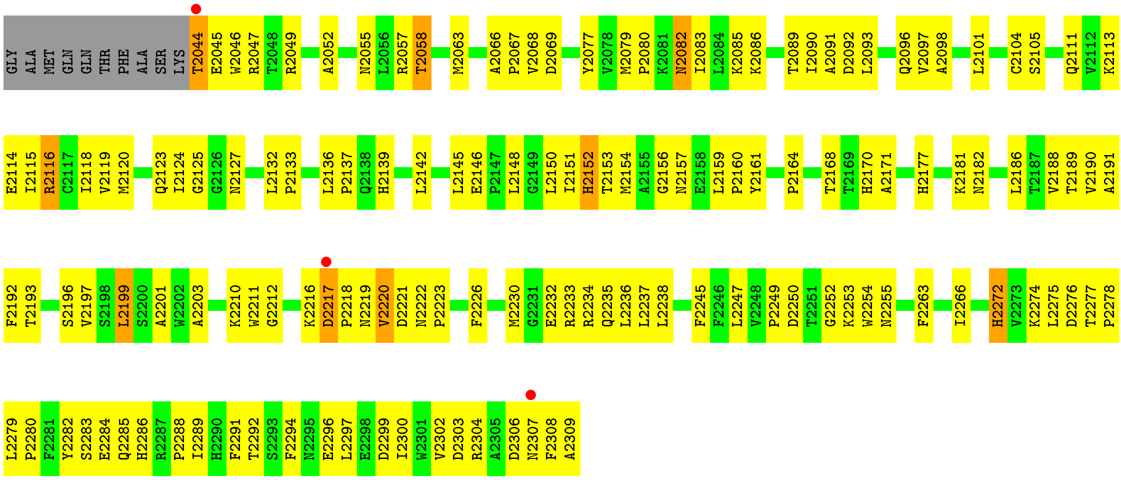
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	D	2	Total O 2 2	0	0
4	C	5	Total O 5 5	0	0
4	F	1	Total O 1 1	0	0
4	E	7	Total O 7 7	0	0
4	G	3	Total O 3 3	0	0

3 Residue-property plots ⓘ

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.

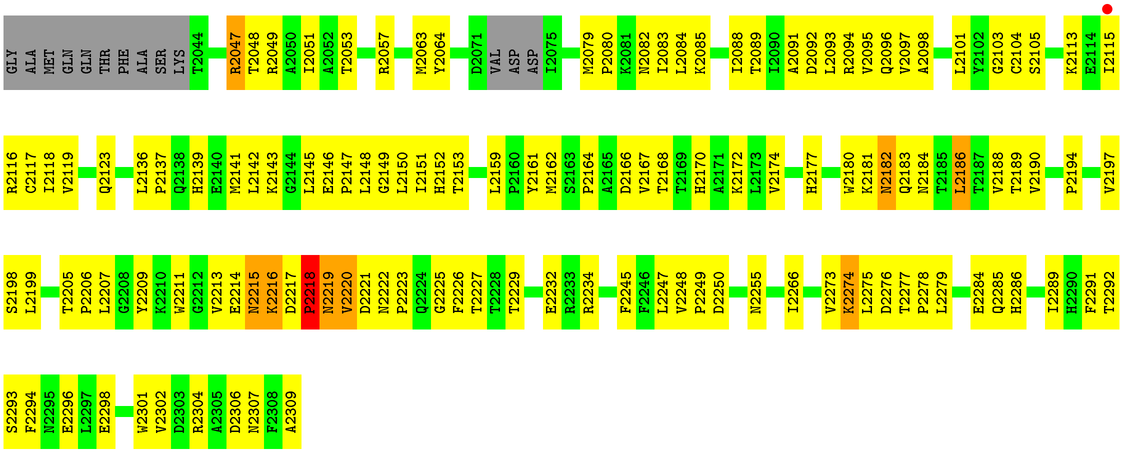
- Molecule 1: Putative pre-mRNA splicing factor

Chain B:

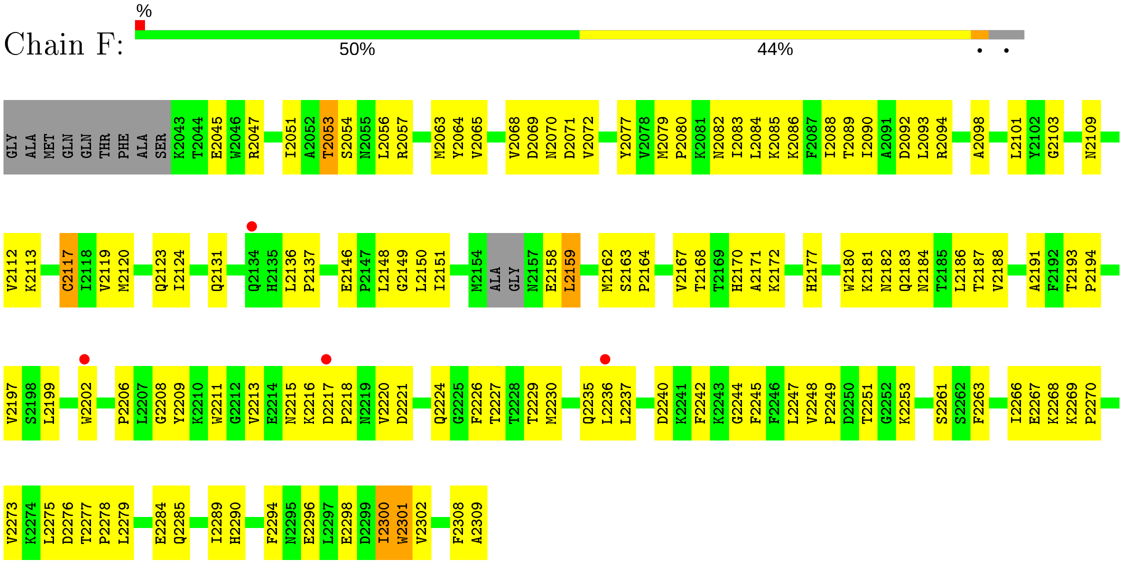


- Molecule 1: Putative pre-mRNA splicing factor

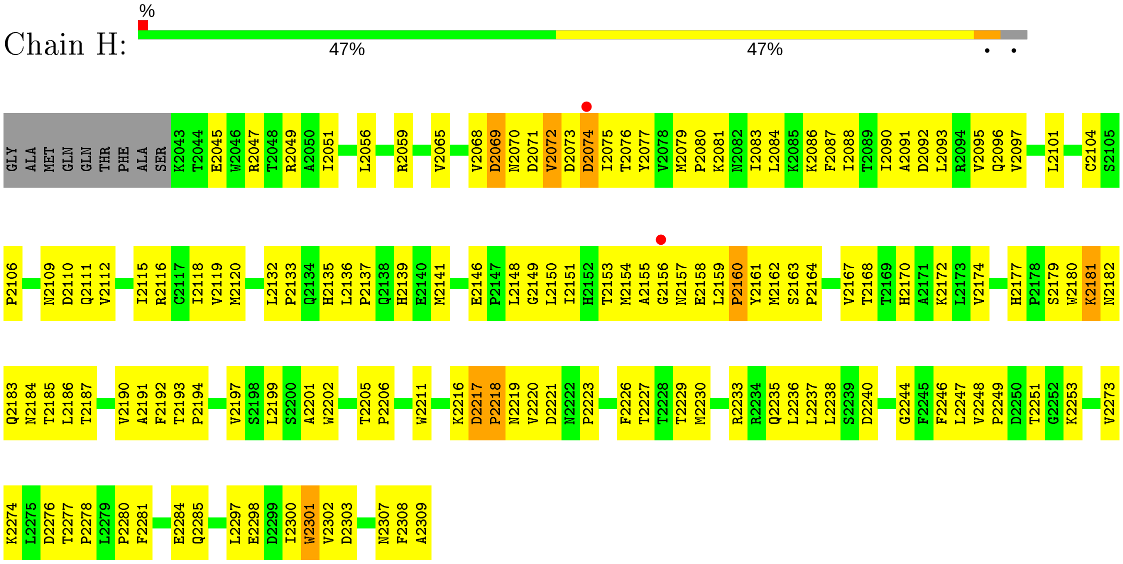
Chain D:



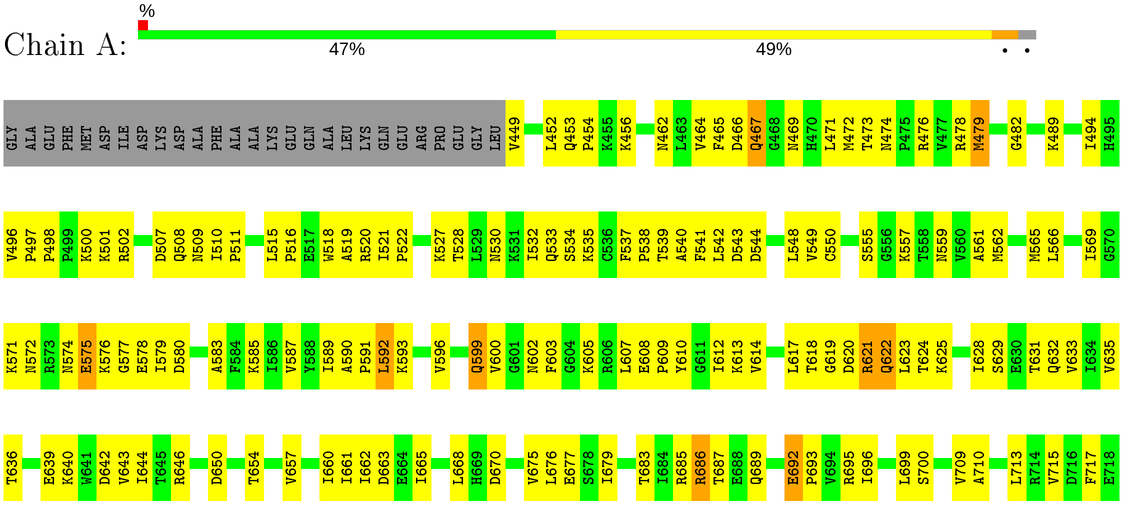
- Molecule 1: Putative pre-mRNA splicing factor

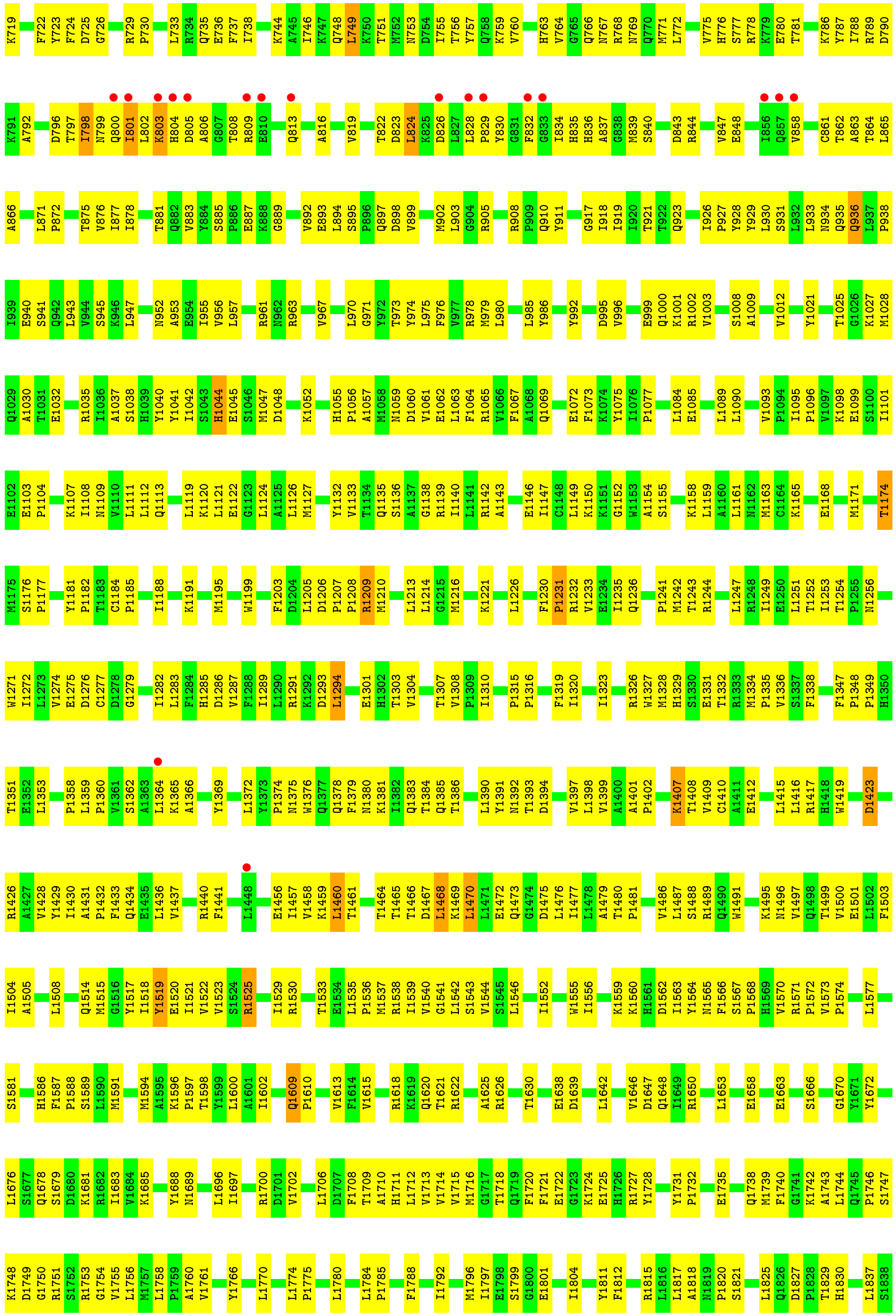


- Molecule 1: Putative pre-mRNA splicing factor



- Molecule 2: Pre-mRNA splicing helicase-like protein

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A866 L871 P872 T875 V876 I877 I878 T881 Q882 V883 Y884 S885 P886 E887 K888 G889 V892 E893 L894 S895 P896 Q897 D898 V899 M902 L903 G904 R905 R908 P909 Q910 Y911 G917 I918 I919 I920 T921 T922 Q923 I926 P927 Y928 Y929 L930 S931 L932 L933 N934 Q935 Q936 L937 P938
I939 E940 S941 Q942 L943 V944 S945 K946 L947 N952 A953 E954 I955 V956 L957 R961 N962 R963 V967 L970 G971 Y972 T973 Y974 L975 F976 V977 R978 M979 L980 L985 Y986 Y992 D995 V996 E999 Q1000 K1001 R1002 V1003 S1008 A1009 V1012 Y1021 T1025 G1026 K1027 M1028
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M1175 S1176 P1177 Y1181 P1182 T1183 C1184 P1185 I1188 K1191 M1195 W1199 F1203 D1204 L1205 D1206 P1207 P1208 R1209 M1210 L1213 L1214 G1215 M1216 K1221 L1226 F1230 P1231 R1232 V1233 E1234 I1235 Q1236 P1241 M1242 T1243 R1244 L1247 R1248 I1249 E1250 L1251 L1252 I1253 T1254 P1255 N1256
W1271 I1272 L1273 V1274 E1275 D1276 C1277 D1278 G1279 I1282 L1283 F1284 H1285 D1286 V1287 F1288 I1289 L1290 R1291 K1292 D1293 L1294 E1301 H1302 T1303 V1304 T1307 V1308 P1309 I1310 P1315 P1316 F1319 I1320 I1323 R1326 W1327 M1328 H1329 S1330 E1331 T1332 R1333 M1334 P1335 V1336 S1337 F1338 F1347 P1348 P1349 H1350
T1351 E1352 L1353 P1358 L1359 P1360 V1361 S1362 A1363 L1364 K1365 A1366 Y1369 L1372 Y1373 P1374 N1375 W1376 Q1377 Q1378 F1379 N1380 K1381 I1382 Q1383 T1384 Q1385 T1386 L1390 Y1391 N1392 T1393 D1394 V1397 L1398 V1399 A1400 A1401 P1402 K1407 T1408 V1409 C1410 A1411 E1412 L1415 L1416 R1417 H1418 W1419 D1423
R1426 A1427 V1428 Y1429 I1430 A1431 P1432 F1433 Q1434 E1435 L1436 V1437 R1440 F1441 L1448 E1456 I1457 V1458 K1459 L1460 T1461 T1464 T1465 T1466 D1467 L1468 K1469 L1470 L1471 E1472 Q1473 G1474 D1475 L1476 I1477 L1478 A1479 T1480 P1481 V1486 L1487 S1488 R1489 Q1490 W1491 K1495 N1496 V1497 Q1498 T1499 V1500 E1501 L1502 F1503
I1504 A1505 L1508 Q1514 M1515 G1516 Y1517 I1518 Y1519 E1520 I1521 V1522 V1523 S1524 R1525 I1529 R1530 T1533 E1534 L1535 P1536 M1537 R1538 I1539 V1540 G1541 L1542 S1543 V1544 S1545 L1546 I1552 W1555 I1556 K1559 K1560 H1561 D1562 I1563 Y1564 N1565 F1566 S1567 P1568 H1569 V1570 R1571 P1572 V1573 P1574 L1577
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L1676 S1677 Q1678 S1679 D1680 K1681 R1682 I1683 V1684 K1685 Y1688 N1689 L1696 I1697 R1700 D1701 V1702 L1706 D1707 F1708 T1709 A1710 H1711 L1712 V1713 V1714 V1715 M1716 G1717 T1718 Q1719 F1720 F1721 E1722 G1723 K1724 E1725 H1726 R1727 Y1728 Y1731 P1732 E1735 Q1738 M1739 F1740 G1741 K1742 A1743 L1744 Q1745 P1746 S1747
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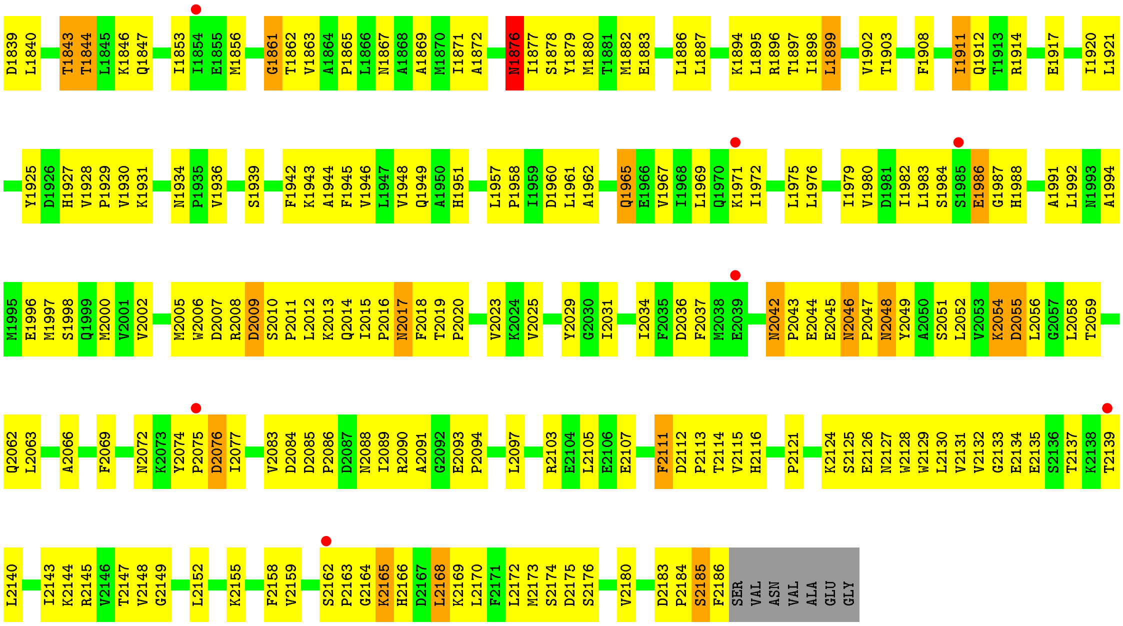
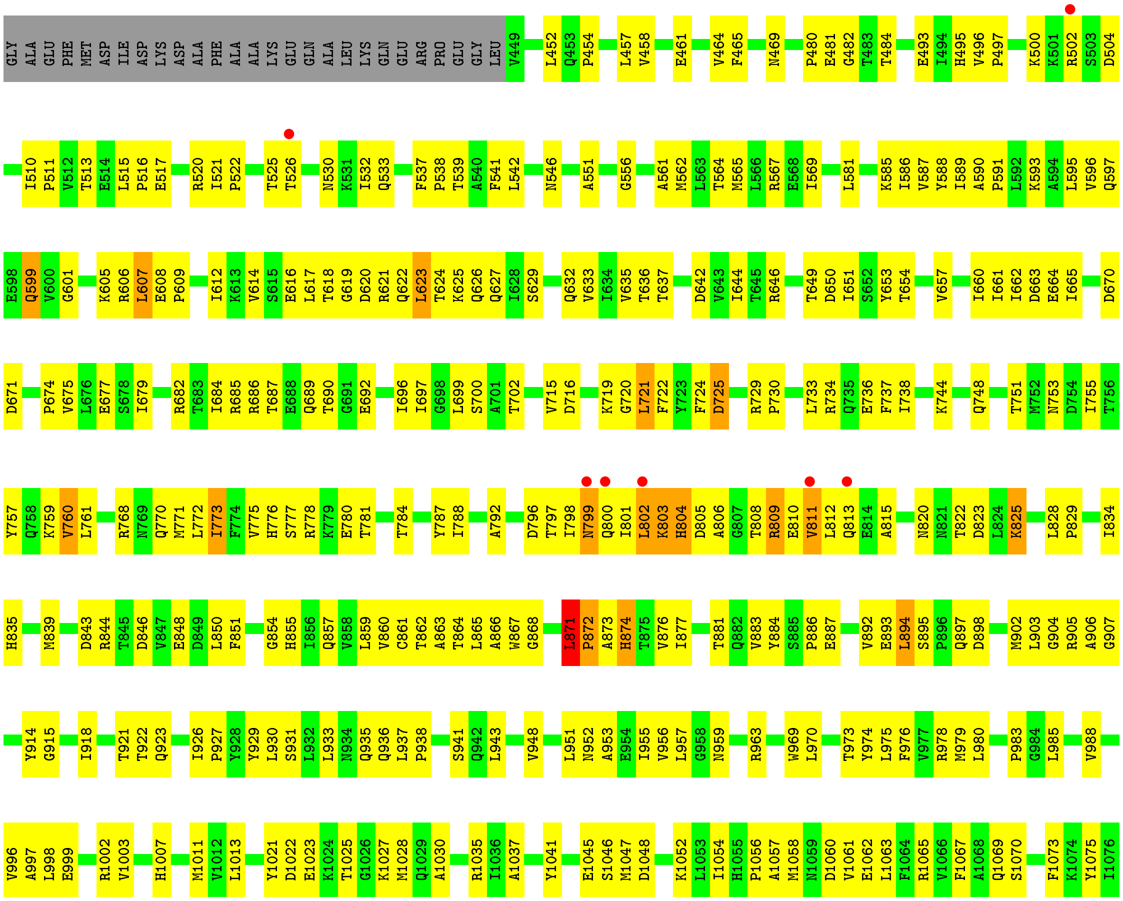
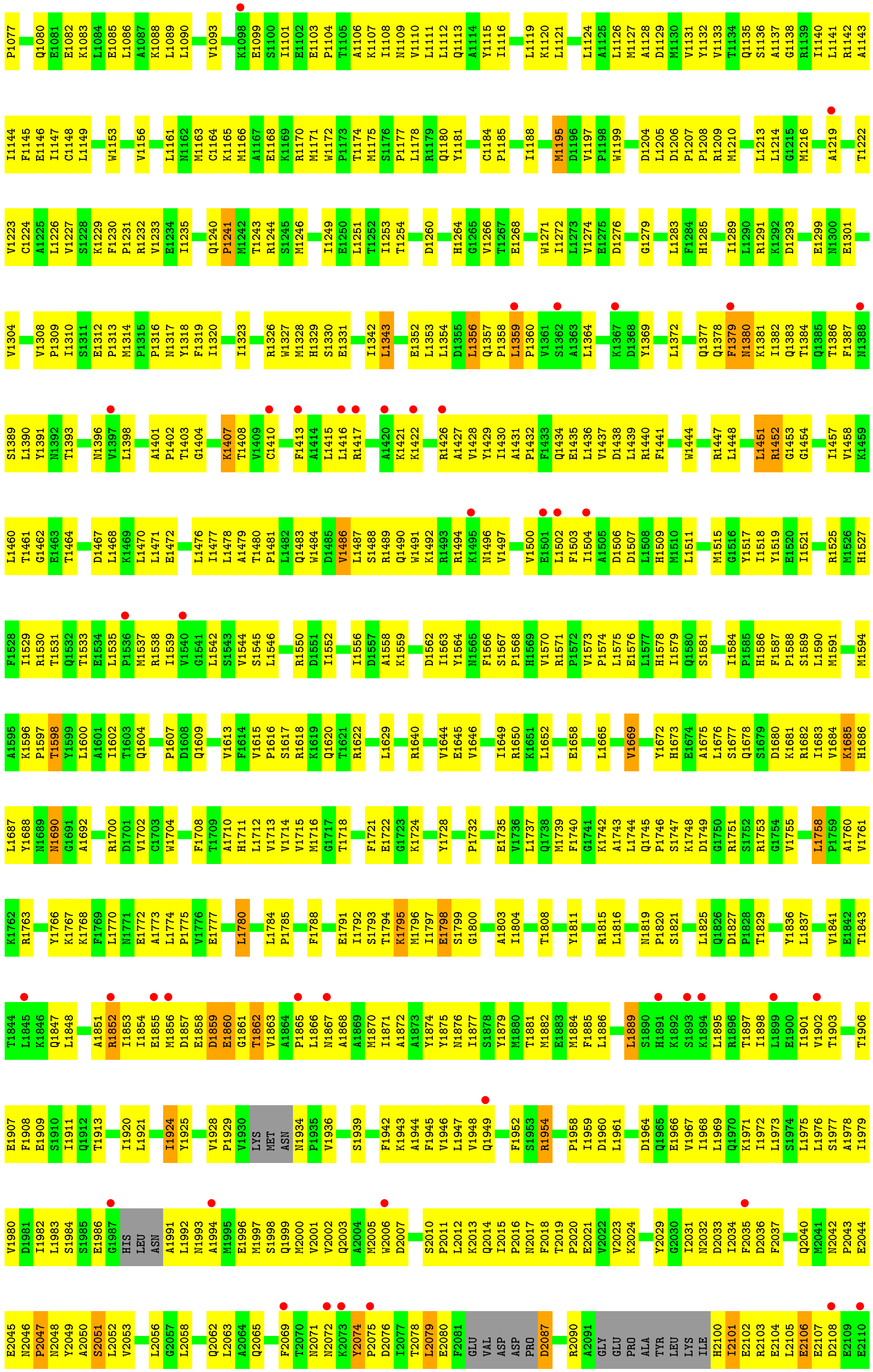


- Molecule 2: Pre-mRNA splicing helicase-like protein

Chain C:

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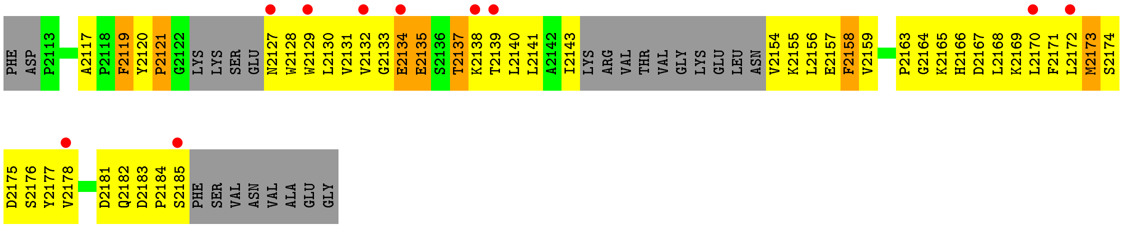
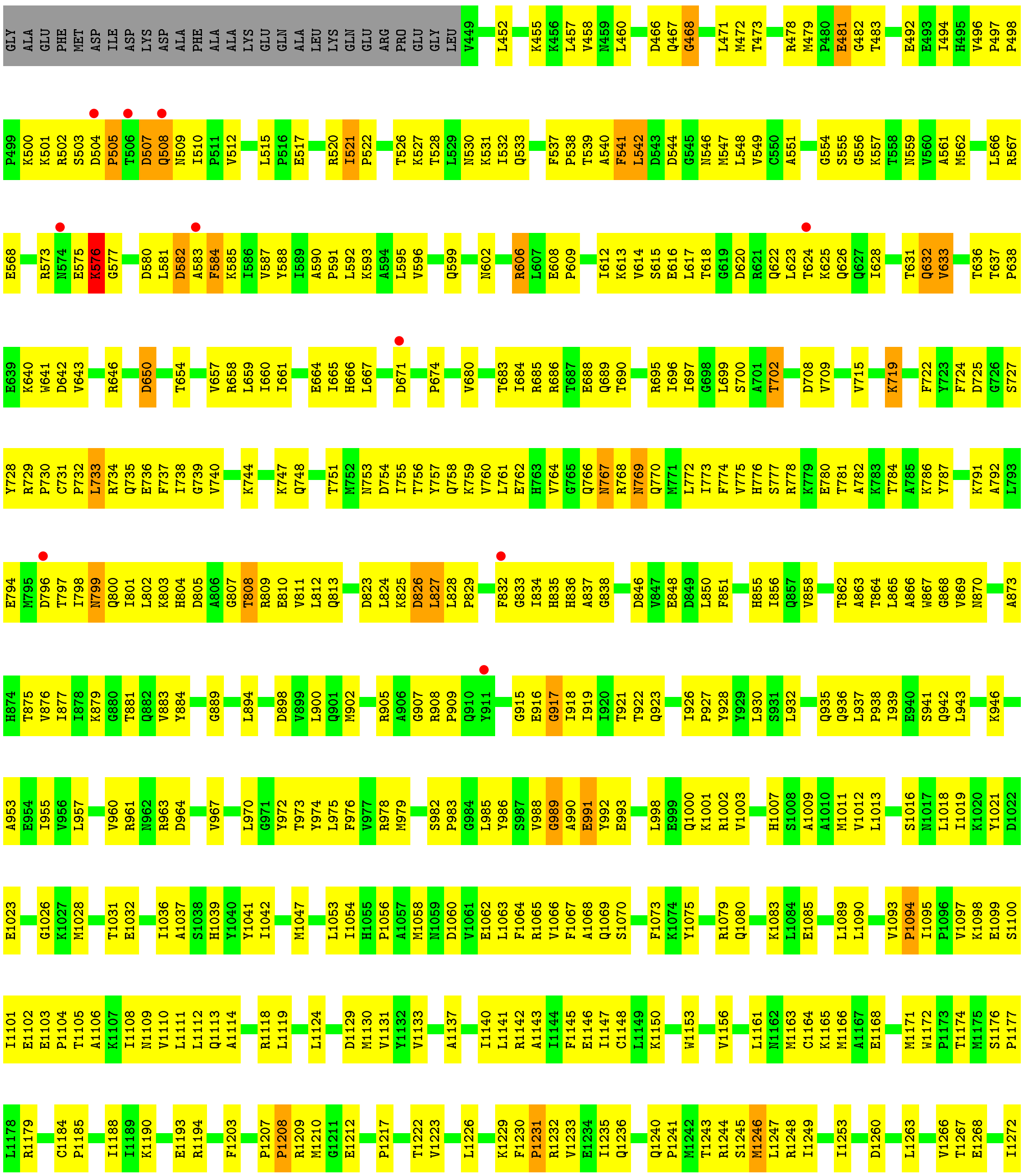
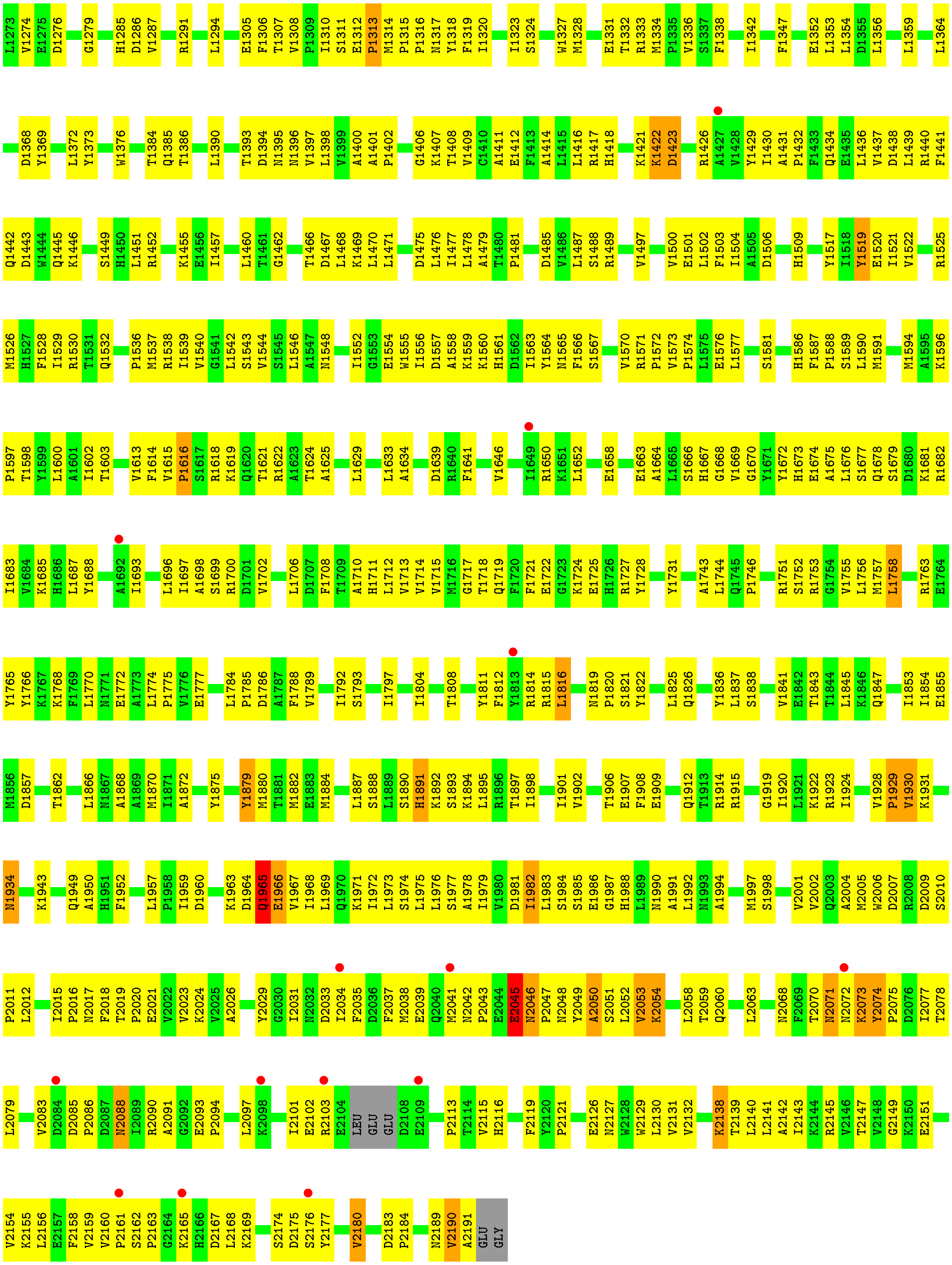


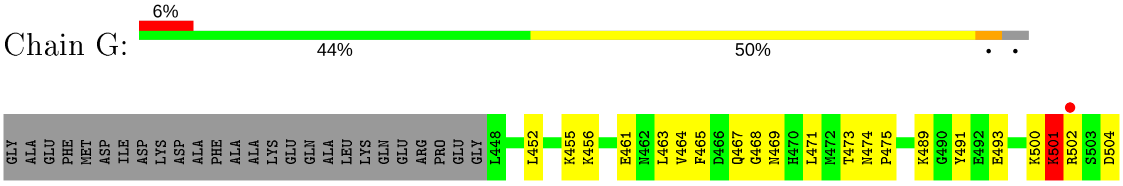
- Molecule 2: Pre-mRNA splicing helicase-like protein

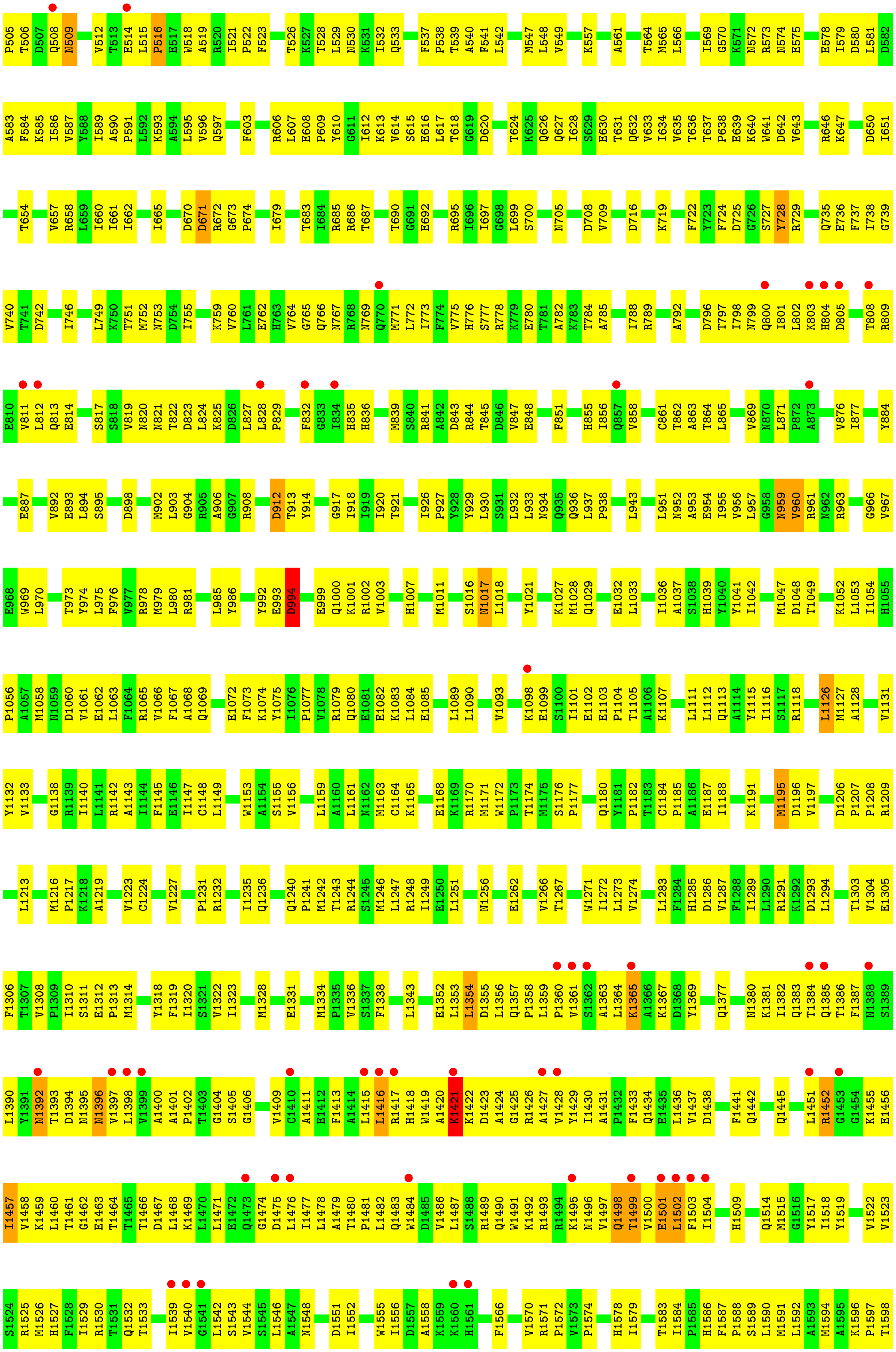
Chain E:

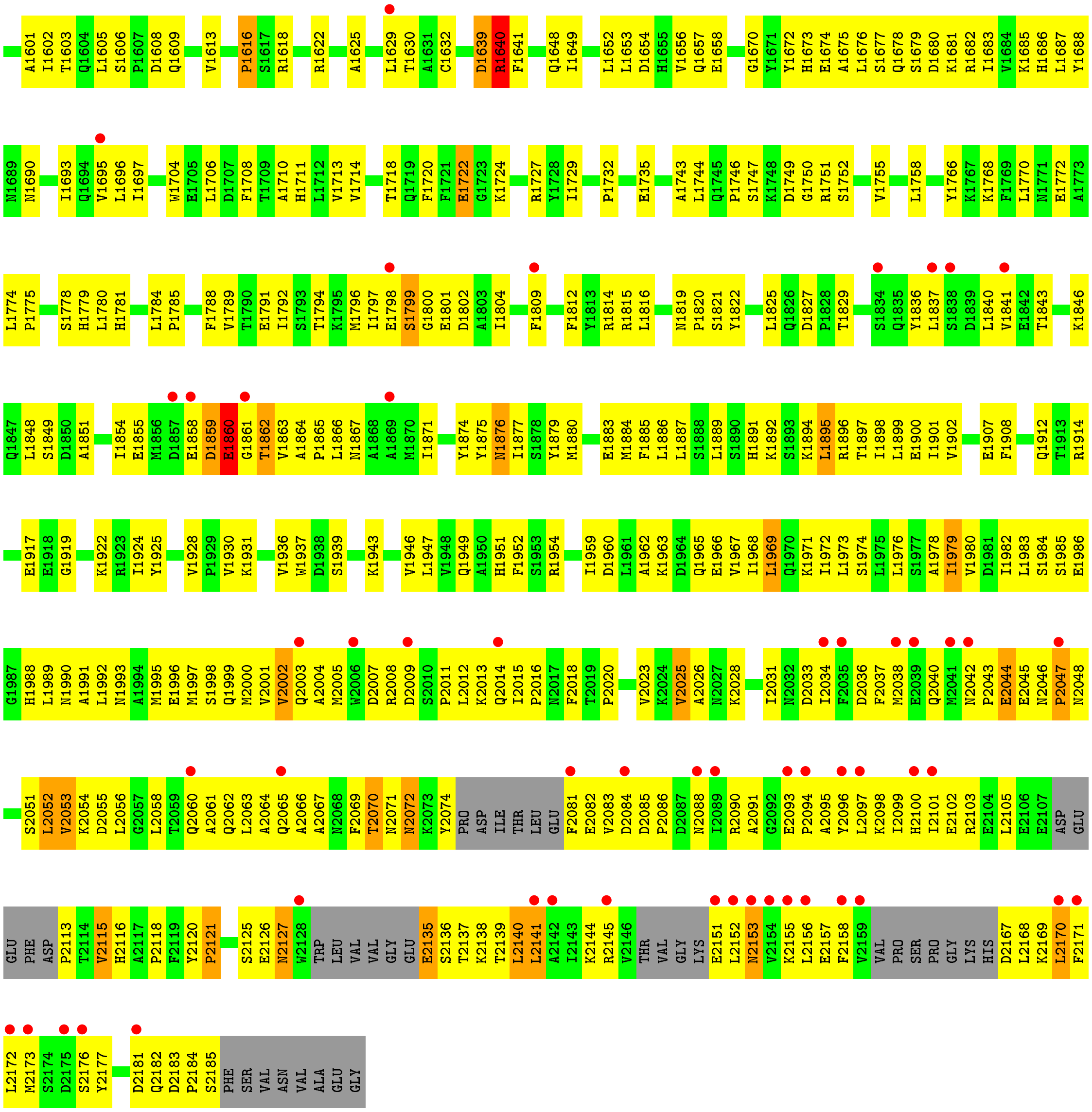




- Molecule 2: Pre-mRNA splicing helicase-like protein




P505 T506 D507 Q508 N509 V512 T513 E514 L515 P516 E517 W518 A519 R520 I521 P522 F523 T526 K527 T528 L529 N530 K531 I532 Q533 F537 P538 T539 A540 F541 L542 M547 L548 V549 K557 A561 T564 M565 L566 I569 G570 K571 N572 R573 N574 E575 E578 I579 D580 L581 D582
A583 F584 K585 I586 V587 Y588 I589 A590 P591 L592 K593 A594 L595 V596 Q597 F603 R606 L607 E608 P609 Y610 G611 I612 K613 V614 S615 E616 L617 T618 G619 D620 T624 K625 Q626 Q627 I628 S629 E630 T631 Q632 V633 I634 V635 T636 T637 P638 E639 K640 W641 D642 V643 R646 K647 D650 I651
T654 V657 R658 L659 I660 I661 I662 I665 D670 D671 R672 G673 P674 I679 T683 I684 R685 R686 T687 T690 G691 E692 R695 I696 I697 G698 L699 S700 N705 D708 V709 D716 K719 F722 Y723 F724 D725 G726 S727 Y728 R729 Q735 E736 F737 I738 G739
V740 T741 D742 I746 L749 K750 T751 M752 N753 D754 I755 K759 V760 L761 E762 H763 V764 G765 Q766 N767 R768 N769 Q770 M771 L772 I773 F774 V775 H776 S777 R778 K779 E780 T781 A782 K783 T784 A785 I788 R789 A792 D796 T797 I798 N799 Q800 I801 L802 K803 H804 D805 T808 R809
E810 V811 L812 Q813 E814 S817 S818 V819 N820 N821 T822 D823 L824 K825 D826 L827 L828 P829 F832 G833 I834 H835 H836 M839 S840 R841 A842 D843 R844 T845 D846 V847 E848 F851 H855 I856 Q857 V858 C861 T862 A863 T864 L865 V869 N870 L871 P872 A873 V876 I877 Y884
E887 V892 E893 L894 S895 D898 M902 L903 G904 R905 A906 G907 R908 D912 T913 Y914 G917 I918 I919 I920 T921 I926 P927 Y928 Y929 L930 S931 L932 L933 N934 Q935 Q936 L937 P938 L943 L951 N952 A953 E954 I955 V956 L957 G958 N959 V960 R961 N962 R963 G966 V967
E968 W969 L970 T973 Y974 L975 F976 V977 R978 M979 L980 R981 L985 Y986 Y992 E993 D994 E999 Q1000 K1001 R1002 V1003 H1007 M1011 S1016 N1017 L1018 Y1021 K1027 M1028 Q1029 E1032 L1033 I1036 A1037 S1038 H1039 Y1040 Y1041 I1042 M1047 D1048 T1049 K1052 L1053 I1054 H1055
P1056 A1057 M1058 N1059 D1060 V1061 E1062 L1063 F1064 R1065 V1066 F1067 A1068 Q1069 E1072 F1073 K1074 Y1075 I1076 P1077 V1078 R1079 Q1080 E1081 E1082 K1083 L1084 E1085 L1089 L1090 V1093 K1098 E1099 S1100 I1101 E1102 E1103 P1104 T1105 A1106 K1107 L1111 L1112 Q1113 A1114 Y1115 I1116 S1117 R1118 L1126 M1127 A1128 V1131
Y1132 V1133 G1138 R1139 I1140 L1141 R1142 A1143 I1144 F1145 E1146 I1147 C1148 L1149 W1153 A1154 S1155 V1156 L1159 A1160 L1161 N1162 M1163 C1164 K1165 E1168 K1169 R1170 M1171 W1172 P1173 T1174 M1175 S1176 P1177 Q1180 Y1181 P1182 T1183 C1184 P1185 A1186 E1187 I1188 K1191 M1195 D1196 V1197 D1206 P1207 P1208 R1209
L1213 M1216 P1217 K1218 A1219 V1223 C1224 V1227 P1231 R1232 I1235 Q1236 Q1240 P1241 M1242 T1243 R1244 S1245 M1246 L1247 R1248 I1249 E1250 L1251 N1256 E1262 V1266 T1267 W1271 I1272 L1273 V1274 L1283 F1284 H1285 D1286 V1287 F1288 I1289 L1290 R1291 K1292 D1293 L1294 T1303 V1304 E1305
F1306 T1307 V1308 P1309 I1310 S1311 E1312 P1313 M1314 Y1318 F1319 I1320 S1321 V1322 I1323 M1328 E1331 M1334 P1335 V1336 S1337 F1338 L1343 E1352 L1353 L1354 D1355 L1356 Q1357 P1358 L1359 P1360 V1361 S1362 A1363 L1364 K1365 A1366 K1367 D1368 Y1369 Q1377 N1380 K1381 I1382 Q1383 T1384 Q1385 T1386 F1387 N1388 S1389
L1390 Y1391 N1392 T1393 D1394 N1395 N1396 V1397 L1398 V1399 A1400 A1401 P1402 T1403 G1404 S1405 G1406 V1409 C1410 A1411 E1412 F1413 A1414 L1415 L1416 R1417 H1418 W1419 A1420 K1421 K1422 D1423 A1424 G1425 R1426 A1427 V1428 Y1429 I1430 A1431 P1432 F1433 Q1434 E1435 L1436 V1437 D1438 F1441 Q1442 Q1445 L1451 R1452 G1453 G1454 K1455 E1456
I1457 V1458 K1459 L1460 T1461 G1462 E1463 T1464 T1465 T1466 D1467 L1468 K1469 L1470 L1471 E1472 Q1473 G1474 D1475 L1476 I1477 L1478 A1479 T1480 P1481 L1482 Q1483 W1484 D1485 V1486 L1487 S1488 R1489 Q1490 W1491 K1492 R1493 R1494 K1495 N1496 V1497 Q1498 T1499 V1500 E1501 L1502 F1503 I1504 H1509 Q1514 M1515 G1516 Y1517 I1518 Y1519 V1522 V1523
S1524 R1525 M1526 H1527 F1528 I1529 R1530 T1531 Q1532 T1533 I1539 V1540 G1541 L1542 S1543 V1544 S1545 L1546 A1547 N1548 D1551 I1552 W1555 I1556 D1557 A1558 K1559 K1560 H1561 F1566 V1570 R1571 P1572 V1573 P1574 H1578 I1579 T1583 I1584 P1585 H1586 F1587 P1588 S1589 L1590 M1591 L1592 A1593 M1594 A1595 K1596 P1597 T1598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N1689 N1690 I1693 Q1694 V1695 L1696 I1697 W1704 E1705 L1706 D1707 F1708 T1709 A1710 H1711 L1712 V1713 V1714 T1718 Q1719 F1720 F1721 E1722 G1723 K1724 R1727 Y1728 I1729 P1732 E1735 A1743 L1744 Q1745 P1746 S1747 K1748 D1749 G1750 R1751 S1752 V1755 L1758 Y1766 K1767 K1768 F1769 L1770 N1771 E1772 A1773
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E1917 E1918 G1919 K1922 R1923 I1924 Y1925 V1928 P1929 V1930 K1931 V1936 W1937 D1938 S1939 K1943 V1946 L1947 V1948 Q1949 A1950 H1951 F1952 S1953 R1954 I1959 D1960 L1961 A1962 K1963 D1964 Q1965 E1966 V1967 I1968 L1969 Q1970 K1971 I1972 L1973 S1974 L1975 L1976 S1977 A1978 I1979 V1980 D1981 I1982 L1983 S1984 S1985 E1986
G1987 H1988 L1989 N1990 A1991 L1992 N1993 A1994 M1995 E1996 M1997 S1998 Q1999 M2000 V2001 V2002 Q2003 A2004 M2005 W2006 D2007 R2008 D2009 S2010 P2011 L2012 K2013 Q2014 I2015 P2016 N2017 F2018 T2019 P2020 V2023 K2024 V2025 A2026 N2027 K2028 I2031 N2032 D2033 I2034 F2035 D2036 F2037 M2038 E2039 Q2040 M2041 N2042 P2043 E2044 E2045 N2046 P2047 N2048
S2051 L2052 V2053 K2054 D2055 L2056 G2057 L2058 T2059 Q2060 A2061 Q2062 L2063 A2064 Q2065 A2066 A2067 N2068 F2069 T2070 N2071 N2072 K2073 Y2074 PRO ASP ILE THR LEU GLU F2081 E2082 V2083 D2084 D2085 P2086 D2087 N2088 I2089 R2090 A2091 G2092 E2093 P2094 A2095 Y2096 L2097 K2098 I2099 H2100 I2101 E2102 R2103 E2104 L2105 E2106 E2107 ASP GLU
GLU PHE ASP P2113 T2114 V2115 H2116 A2117 P2118 F2119 Y2120 P2121 S2125 E2126 N2127 W2128 TRP LEU VAL VAL GLY GLU E2135 S2136 T2137 K2138 T2139 L2140 L2141 A2142 I2143 K2144 R2145 V2146 THR VAL GLY LYS E2151 L2152 N2153 V2154 K2155 L2156 E2157 F2158 V2159 VAL PRO SER PRO GLY LYS HIS D2167 L2168 K2169 L2170 F2171
L2172 M2173 S2174 D2175 S2176 Y2177 D2181 Q2182 D2183 P2184 S2185 PHE SER VAL ASN VAL ALA GLU GLY

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.54Å 269.59Å 231.69Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	49.13 – 3.20 49.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.13-3.20) 99.0 (49.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.287 0.248 , 0.289	Depositor DCC
R_{free} test set	9222 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	93.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	63679	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: ACT

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	B	0.20	0/2175	0.38	0/2962
1	D	0.22	0/2151	0.39	0/2927
1	F	0.21	0/2174	0.39	0/2958
1	H	0.21	0/2184	0.37	0/2973
2	A	0.21	0/14227	0.37	0/19296
2	C	0.21	0/13925	0.38	0/18882
2	E	0.21	0/14234	0.38	0/19306
2	G	0.22	0/13998	0.39	0/18976
All	All	0.21	0/65068	0.38	0/88280

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	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2217	ASP	Peptide
2	E	1965	GLN	Peptide

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	B	2116	0	2075	139	0
1	D	2093	0	2057	120	0
1	F	2116	0	2079	124	0
1	H	2125	0	2088	127	0
2	A	13917	0	13956	862	0
2	C	13628	0	13674	959	0
2	E	13925	0	13970	867	0
2	G	13701	0	13768	973	0
3	A	4	3	3	1	0
3	C	4	3	3	1	0
3	E	4	3	3	4	0
3	G	4	3	3	0	0
4	A	12	0	0	0	0
4	C	5	0	0	0	0
4	D	2	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	G	3	0	0	1	0
All	All	63667	12	63679	4086	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 32.

The worst 5 of 4086 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:521:ILE:HD12	2:E:522:PRO:HD3	1.22	1.21
2:C:874:HIS:HA	2:C:907:GLY:HA2	1.28	1.13
2:G:515:LEU:HB3	2:G:516:PRO:HD2	1.18	1.10
2:A:835:HIS:HA	2:A:839:MET:HE1	1.31	1.10
2:C:2040:GLN:HA	2:C:2046:ASN:HB3	1.29	1.10

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	264/276 (96%)	241 (91%)	19 (7%)	4 (2%)	10	44
1	D	259/276 (94%)	239 (92%)	13 (5%)	7 (3%)	5	30
1	F	261/276 (95%)	237 (91%)	22 (8%)	2 (1%)	19	58
1	H	265/276 (96%)	243 (92%)	13 (5%)	9 (3%)	3	24
2	A	1736/1772 (98%)	1619 (93%)	105 (6%)	12 (1%)	22	61
2	C	1686/1772 (95%)	1537 (91%)	130 (8%)	19 (1%)	14	51
2	E	1736/1772 (98%)	1580 (91%)	127 (7%)	29 (2%)	9	42
2	G	1698/1772 (96%)	1537 (90%)	131 (8%)	30 (2%)	8	41
All	All	7905/8192 (96%)	7233 (92%)	560 (7%)	112 (1%)	11	46

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2217	ASP
1	B	2220	VAL
2	A	575	GLU
2	A	1748	LYS
1	D	2218	PRO

5.3.2 Protein sidechains ⓘ

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	B	234/241 (97%)	225 (96%)	9 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	231/241 (96%)	224 (97%)	7 (3%)	41	73
1	F	235/241 (98%)	227 (97%)	8 (3%)	37	70
1	H	235/241 (98%)	231 (98%)	4 (2%)	60	83
2	A	1534/1562 (98%)	1475 (96%)	59 (4%)	33	67
2	C	1503/1562 (96%)	1439 (96%)	64 (4%)	29	64
2	E	1537/1562 (98%)	1486 (97%)	51 (3%)	38	71
2	G	1511/1562 (97%)	1469 (97%)	42 (3%)	43	74
All	All	7020/7212 (97%)	6776 (96%)	244 (4%)	36	69

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1645	GLU
2	C	2135	GLU
2	G	1639	ASP
2	C	1758	LEU
2	C	1977	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	2184	ASN
2	E	800	GLN
2	G	1988	HIS
1	F	2290	HIS
2	E	769	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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACT	A	2201	-	1,3,3	1.35	0	0,3,3	0.00	-
3	ACT	G	2201	-	1,3,3	1.39	0	0,3,3	0.00	-
3	ACT	E	2201	-	1,3,3	1.33	0	0,3,3	0.00	-
3	ACT	C	2201	-	1,3,3	1.32	0	0,3,3	0.00	-

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2201	ACT	1	0
3	E	2201	ACT	4	0
3	C	2201	ACT	1	0

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, 95th 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	B	266/276 (96%)	-0.05	3 (1%)	80	69	54, 76, 110, 128	0
1	D	263/276 (95%)	-0.06	1 (0%)	92	89	56, 73, 101, 130	0
1	F	265/276 (96%)	-0.02	4 (1%)	73	61	53, 83, 117, 143	0
1	H	267/276 (96%)	-0.01	2 (0%)	87	81	54, 77, 111, 132	0
2	A	1738/1772 (98%)	0.01	25 (1%)	75	63	39, 73, 123, 171	0
2	C	1702/1772 (96%)	0.12	60 (3%)	44	28	49, 86, 159, 209	0
2	E	1740/1772 (98%)	0.06	24 (1%)	75	63	48, 80, 132, 205	0
2	G	1710/1772 (96%)	0.27	106 (6%)	20	11	48, 92, 171, 209	0
All	All	7951/8192 (97%)	0.09	225 (2%)	53	37	39, 81, 154, 209	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	2171	PHE	4.9
2	G	2142	ALA	4.6
2	C	2170	LEU	4.6
2	A	1985	SER	4.5
2	G	2088	ASN	4.5

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

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	C	2201	4/4	0.62	0.36	80,91,97,98	0
3	ACT	E	2201	4/4	0.85	0.27	87,92,111,111	0
3	ACT	G	2201	4/4	0.85	0.24	84,89,104,104	0
3	ACT	A	2201	4/4	0.88	0.20	63,68,81,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.