wwPDB EM Validation Summary Report (i)

Jun 20, 2024 – 02:36 AM JST

PDB ID	:	7WLU
EMDB ID	:	EMD-32593
Title	:	The Flattened Structure of mPIEZO1 in Lipid Bilayer
Authors	:	Yang, X.; Lin, C.; Chen, X.; Li, S.; Li, X.; Xiao, B.
Deposited on	:	2022-01-13
Resolution	:	6.81 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

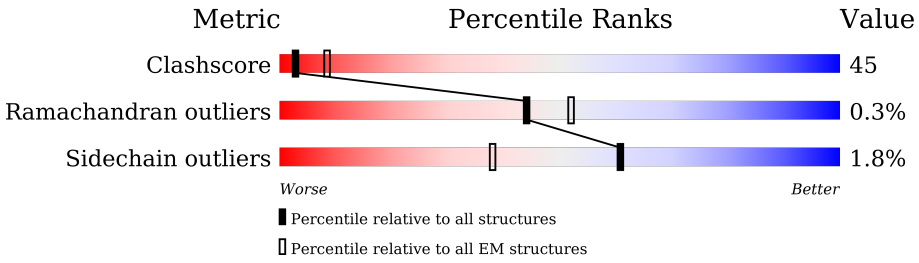
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.81 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2547	15% 27% 31% · 41%
1	C	2547	15% 27% 31% · 41%
1	E	2547	15% 27% 31% · 41%

2 Entry composition (i)

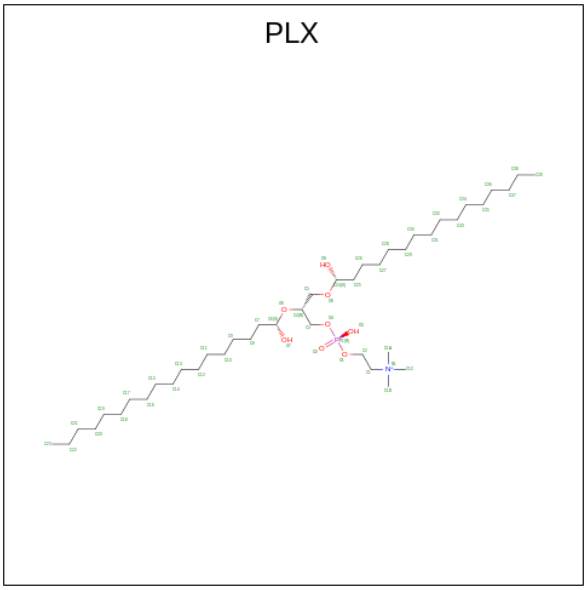
There are 2 unique types of molecules in this entry. The entry contains 34761 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1498	Total	C	N	O	S	0	0
			11535	7496	1973	2005	61		
1	C	1498	Total	C	N	O	S	0	0
			11535	7496	1973	2005	61		
1	E	1498	Total	C	N	O	S	0	0
			11535	7496	1973	2005	61		

- Molecule 2 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

Continued on next page...

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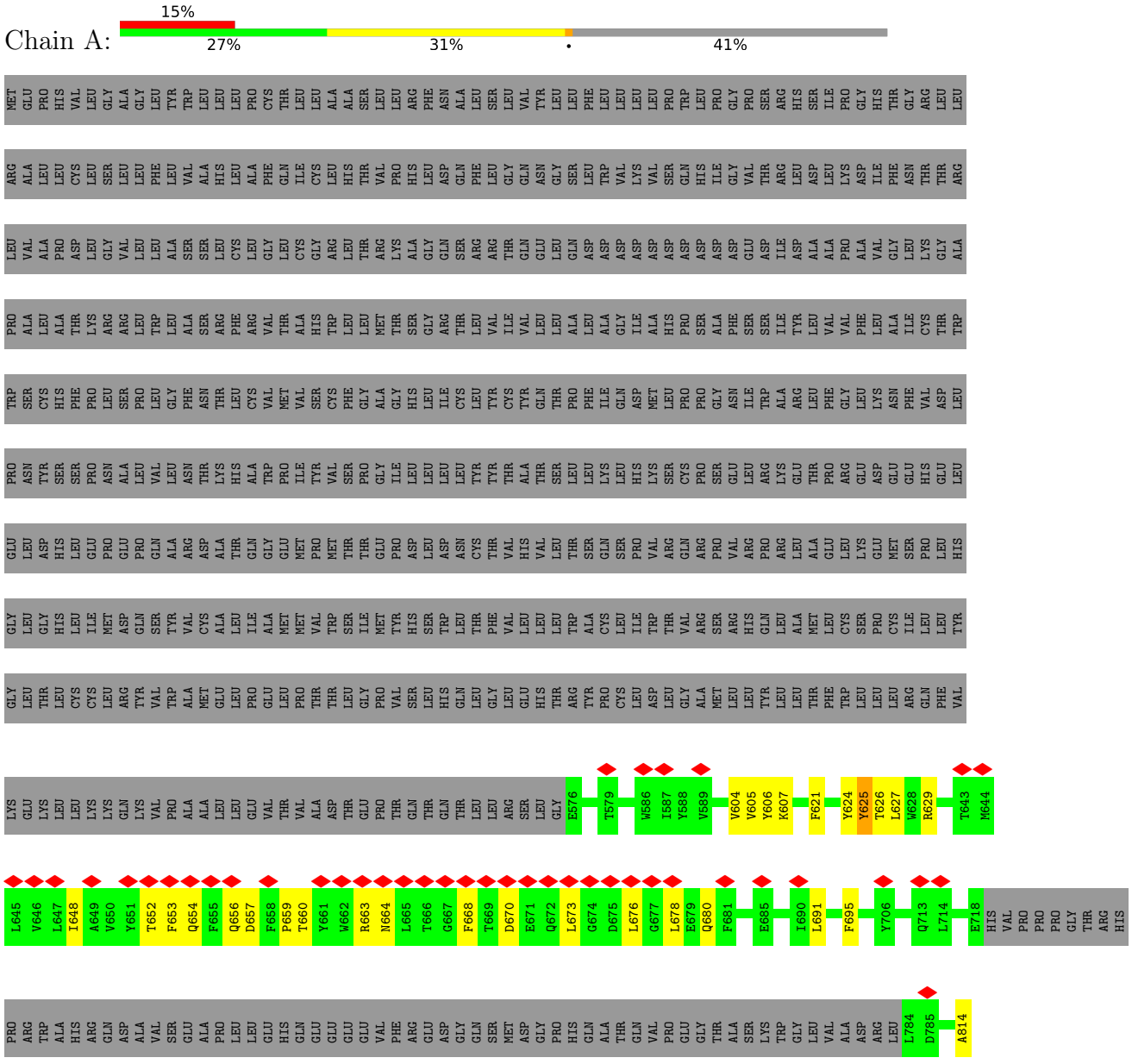
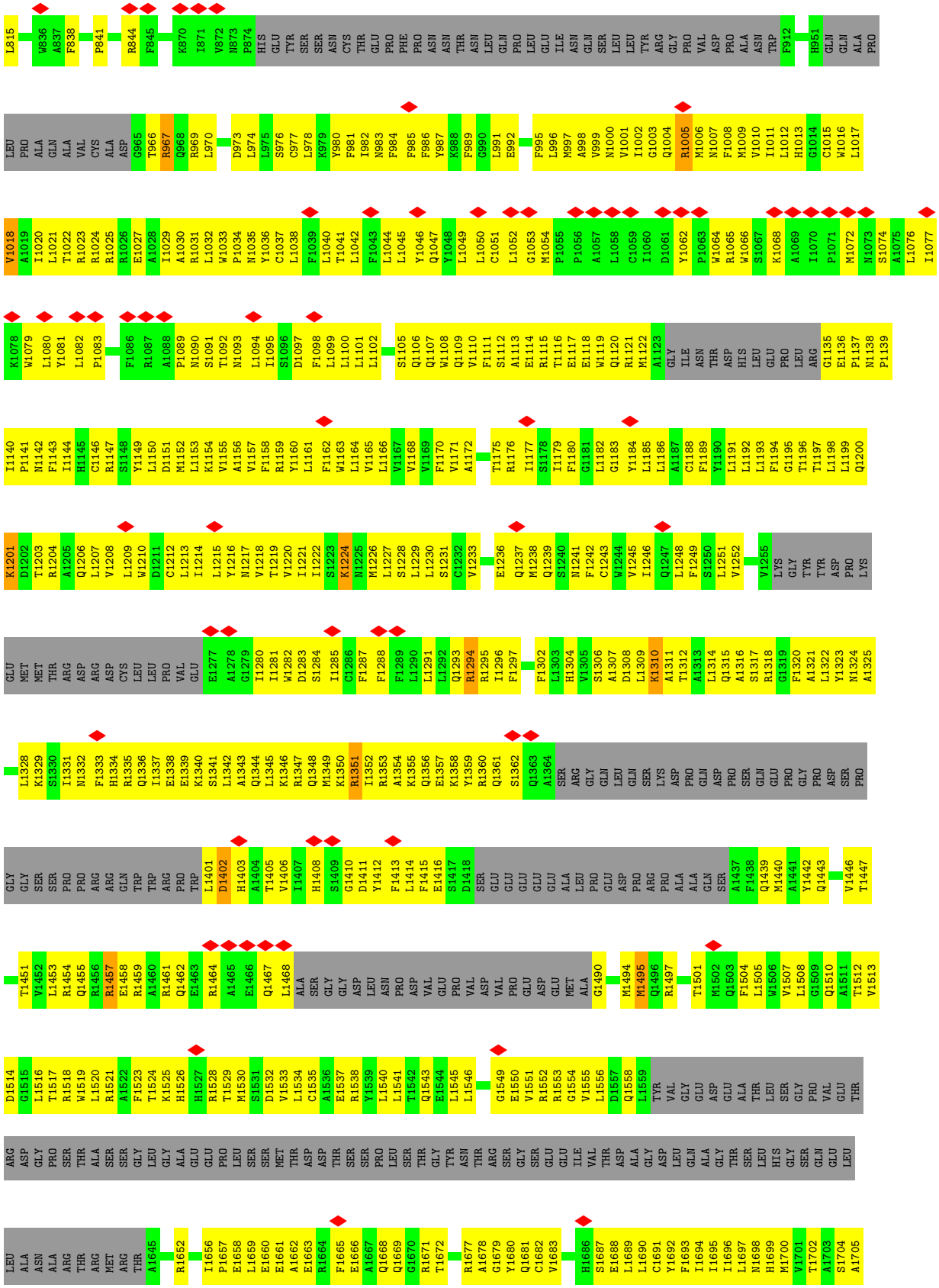
Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Piezo-type mechanosensitive ion channel component 1

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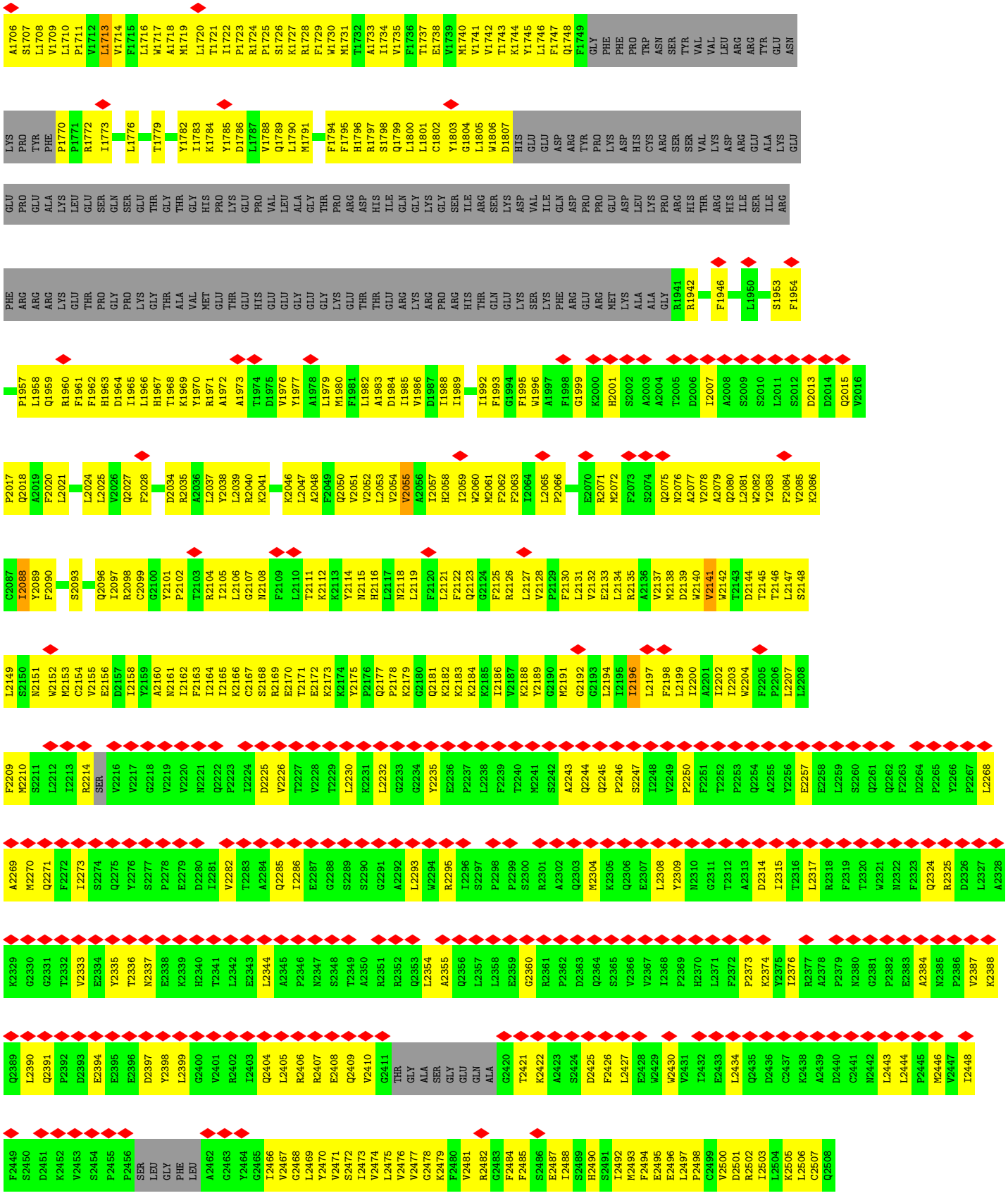
V1018 A1019 I1020 L1021 T1022 R1023 R1024 R1025 R1026 E1027 A1028 I1029 A1030 R1031 L1032 W1033 P1034 N1035 Y1036 C1037 L1038 F1039 L1040 T1041 L1042 F1043 L1044 L1045 Y1046 Q1047 Y1048 L1049 L1050 C1051 L1052 G1053 M1054 P1055 P1056 A1057 L1058 C1059 I1060 D1061 Y1062 P1063 W1064 R1065 W1066 S1067 K1068 A1069 I1070 P1071 M1072 N1073 S1074 A1075 L1076 I1077
K1078 W1079 L1080 Y1081 L1082 P1083 F1086 R1087 A1088 P1089 N1090 S1091 T1092 N1093 L1094 I1095 S1096 D1097 F1098 L1099 L1100 L1101 L1102 S1105 Q1106 Q1107 W1108 Q1109 V1110 F1111 S1112 A1113 E1114 R1115 T1116 E1117 E1118 W1119 Q1120 R1121 M1122 A1123 GLY ILE ASN THR ASP HIS LEU GLU PRO LEU ARG G1135 E1136 P1137 N1138 P1139
I1140 P1141 N1142 F1143 I1144 H1145 C1146 R1147 S1148 Y1149 L1150 D1151 M1152 L1153 K1154 V1155 A1156 V1157 F1158 R1159 Y1160 L1161 F1162 W1163 L1164 V1165 L1166 V1167 V1168 V1169 F1170 V1171 A1172 T1175 R1176 I1177 S1178 I1179 F1180 G1181 L1182 G1183 Y1184 L1185 L1186 A1187 C1188 F1189 Y1190 L1191 L1192 L1193 F1194 G1195 T1196 T1197 L1198 L1199 Q1200
K1201 D1202 T1203 R1204 A1205 Q1206 L1207 V1208 L1209 W1210 D1211 C1212 L1213 I1214 L1215 Y1216 N1217 V1218 T1219 V1220 I1221 I1222 S1223 K1224 N1225 M1226 L1227 S1228 L1229 L1230 S1231 C1232 V1233 E1236 Q1237 M1238 Q1239 S1240 N1241 F1242 C1243 W1244 V1245 I1246 Q1247 L1248 F1249 S1250 L1251 V1252 V1255 LYS GLY TYR TYR ASP PRO LYS
GLU MET MET THR ARG ASP ARG ASP CYS LEU LEU PRO VAL GLU E1277 A1278 G1279 I1280 I1281 W1282 D1283 S1284 I1285 C1286 F1287 F1288 F1289 L1290 L1291 L1292 Q1293 R1294 R1295 I1296 F1297 F1302 L1303 H1304 V1305 S1306 A1307 D1308 L1309 K1310 A1311 T1312 A1313 L1314 Q1315 A1316 S1317 R1318 G1319 F1320 A1321 L1322 Y1323 N1324 A1325
L1328 K1329 S1330 I1331 N1332 F1333 H1334 R1335 Q1336 I1337 E1338 E1339 K1340 S1341 L1342 A1343 Q1344 L1345 K1346 R1347 Q1348 M1349 K1350 R1351 I1352 R1353 A1354 K1355 Q1356 E1357 K1358 Y1359 R1360 Q1361 S1362 Q1363 A1364 SER ARG GLY GLN LEU GLN SER LYS ASP PRO GLN ASP PRO SER GLN GLU PRO GLY PRO ASP SER PRO
GLY GLY SER SER PRO PRO ARG ARG GLN TRP TRP ARG PRO TRP L1401 D1402 H1403 A1404 T1405 V1406 I1407 H1408 S1409 G1410 D1411 Y1412 F1413 L1414 F1415 E1416 S1417 D1418 SER GLU GLU GLU GLU GLU ALA LEU PRO GLU ASP PRO ARG PRO ALA ALA GLN SER A1437 F1438 Q1439 M1440 A1441 Y1442 Q1443 V1446 T1447
T1451 Y1452 L1453 R1454 Q1455 R1456 R1457 E1458 R1459 A1460 R1461 Q1462 E1463 R1464 A1465 E1466 Q1467 L1468 ALA SER GLY GLY ASP LEU ASN PRO ASP VAL GLU PRO VAL ASP VAL PRO GLU ASP GLU MET ALA G1490 M1494 M1495 Q1496 R1497 T1501 M1502 Q1503 F1504 L1505 W1506 V1507 L1508 G1509 Q1510 A1511 T1512 V1513
D1514 G1515 L1516 T1517 R1518 W1519 L1520 R1521 A1522 F1523 T1524 K1525 H1526 H1527 R1528 T1529 M1530 S1531 D1532 V1533 L1534 C1535 A1536 E1537 R1538 Y1539 L1540 L1541 T1542 Q1543 E1544 L1545 L1546 G1549 E1550 V1551 R1552 R1553 G1554 V1555 L1556 D1557 Q1558 L1559 TYR VAL GLY GLU ASP GLU ALA THR LEU SER GLY PRO VAL GLU THR
ARG ASP GLY PRO SER THR ALA SER SER GLY LEU GLY ALA GLU GLU PRO LEU SER SER MET THR ASP ASP THR SER SER PRO LEU SER THR GLY TYR ASN THR ARG SER GLY SER GLU GLU ILE VAL THR ASP ALA GLY ASP LEU GLN ALA GLY THR SER LEU HIS GLY SER GLY PRO GLN GLU LEU
LEU ALA ASN ALA ARG THR ARG MET ARG THR A1645 R1652 I1656 P1657 E1658 L1659 E1660 E1661 A1662 E1663 R1664 F1665 E1666 A1667 Q1668 Q1669 G1670 R1671 T1672 R1677 A1678 G1679 Y1680 Q1681 C1682 V1683 H1686 S1687 E1688 L1689 L1690 C1691 Y1692 F1693 I1694 I1695 I1696 L1697 N1698 H1699 M1700 V1701 T1702 A1703 S1704 A1705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LYS PRO TYR PHE P1770 P1771 R1772 I1773 L1776 T1779 Y1782 I1783 K1784 Y1785 D1786 L1787 V1788 Q1789 L1790 M1791 F1794 F1795 H1796 R1797 S1798 Q1799 L1800 L1801 C1802 Y1803 G1804 L1805 W1806 D1807 HIS GLU GLU ASP ARG TYR PRO LYS ASP HIS CYS ARG SER SER VAL LYS ASP ARG GLU ALA LYS GLU
GLU PRO GLU ALA LYS LEU GLU SER GLN SER GLU THR GLY THR GLY HIS PRO LYS GLU PRO VAL LEU ALA GLY THR PRO ARG ASP HIS ILE GLN GLY LYS GLY SER ILE ARG SER LYS ASP VAL ILE GLN ASP PRO PRO GLU ASP LEU LYS PRO ARG HIS THR ARG HIS ILE SER ILE ARG
PHE ARG ARG ARG LYS GLU THR PRO GLY PRO LYS GLY THR ALA VAL MET GLU THR GLU HIS GLU GLU GLY GLU GLY LYS GLU THR THR GLU ARG LYS ARG PRO ARG HIS THR GLN GLU LYS SER LYS PHE ARG GLU ARG MET LYS ALA ALA GLY R1941 R1942 F1946 L1950 S1953 F1954
P1957 L1958 Q1959 R1960 F1961 F1962 H1963 D1964 I1965 L1966 H1967 T1968 K1969 Y1970 R1971 A1972 A1973 T1974 D1975 V1976 Y1977 A1978 L1979 M1980 F1981 L1982 A1983 D1984 I1985 V1986 D1987 I1988 I1989 I1992 F1993 G1994 F1995 W1996 A1997 F1998 G1999 K2000 H2001 S2002 A2003 A2004 T2005 D2006 I2007 A2008 S2009 S2010 L2011 S2012 D2013 D2014 Q2015 V2016
P2017 Q2018 A2019 F2020 L2021 L2024 L2025 V2026 Q2027 F2028 D2034 R2035 A2036 L2037 Y2038 L2039 R2040 K2041 K2046 L2047 A2048 F2049 Q2050 V2051 V2052 L2053 V2054 V2055 A2056 I2057 H2058 I2059 W2060 M2061 F2062 F2063 I2064 L2065 P2066 E2070 R2071 M2072 F2073 S2074 Q2075 N2076 A2077 V2078 A2079 Q2080 L2081 W2082 Y2083 F2084 V2085 K2086
C2087 I2088 Y2089 F2090 S2093 Q2096 I2097 R2098 C2099 G2100 Y2101 P2102 T2103 R2104 I2105 L2106 G2107 N2108 F2109 L2110 T2111 K2112 K2113 Y2114 N2115 H2116 L2117 N2118 L2119 F2120 L2121 F2122 Q2123 G2124 F2125 R2126 L2127 V2128 P2129 F2130 L2131 V2132 E2133 L2134 R2135 A2136 V2137 M2138 D2139 W2140 V2141 W2142 T2143 D2144 T2145 T2146 L2147 S2148
L2149 S2150 N2151 W2152 M2153 C2154 V2155 E2156 D2157 I2158 Y2159 A2160 N2161 I2162 F2163 I2164 I2165 K2166 C2167 S2168 R2169 E2170 T2171 E2172 K2173 K2174 Y2175 P2176 Q2177 P2178 K2179 G2180 Q2181 K2182 K2183 K2184 K2185 I2186 V2187 K2188 Y2189 G2190 M2191 G2192 G2193 L2194 I2195 I2196 L2197 F2198 L2199 I2200 A2201 I2202 I2203 W2204 P2205 P2206 L2207 L2208
F2209 M2210 S2211 L2212 I2213 R2214 SER V2216 V2217 G2218 V2219 V2220 N2221 Q2222 P2223 I2224 D2225 V2226 T2227 V2228 T2229 L2230 K2231 L2232 G2233 G2234 Y2235 E2236 P2237 L2238 F2239 T2240 M2241 S2242 A2243 Q2244 Q2245 P2246 S2247 I2248 V2249 P2250 F2251 T2252 P2253 Q2254 A2255 Y2256 E2257 E2258 L2259 S2260 Q2261 Q2262 F2263 D2264 P2265 Y2266 P2267 L2268
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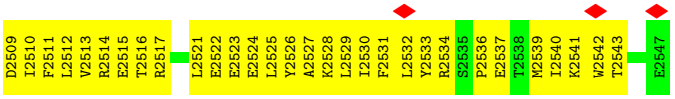
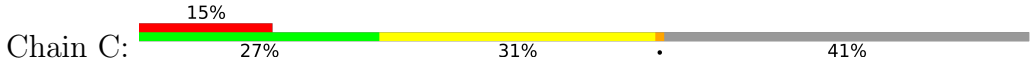
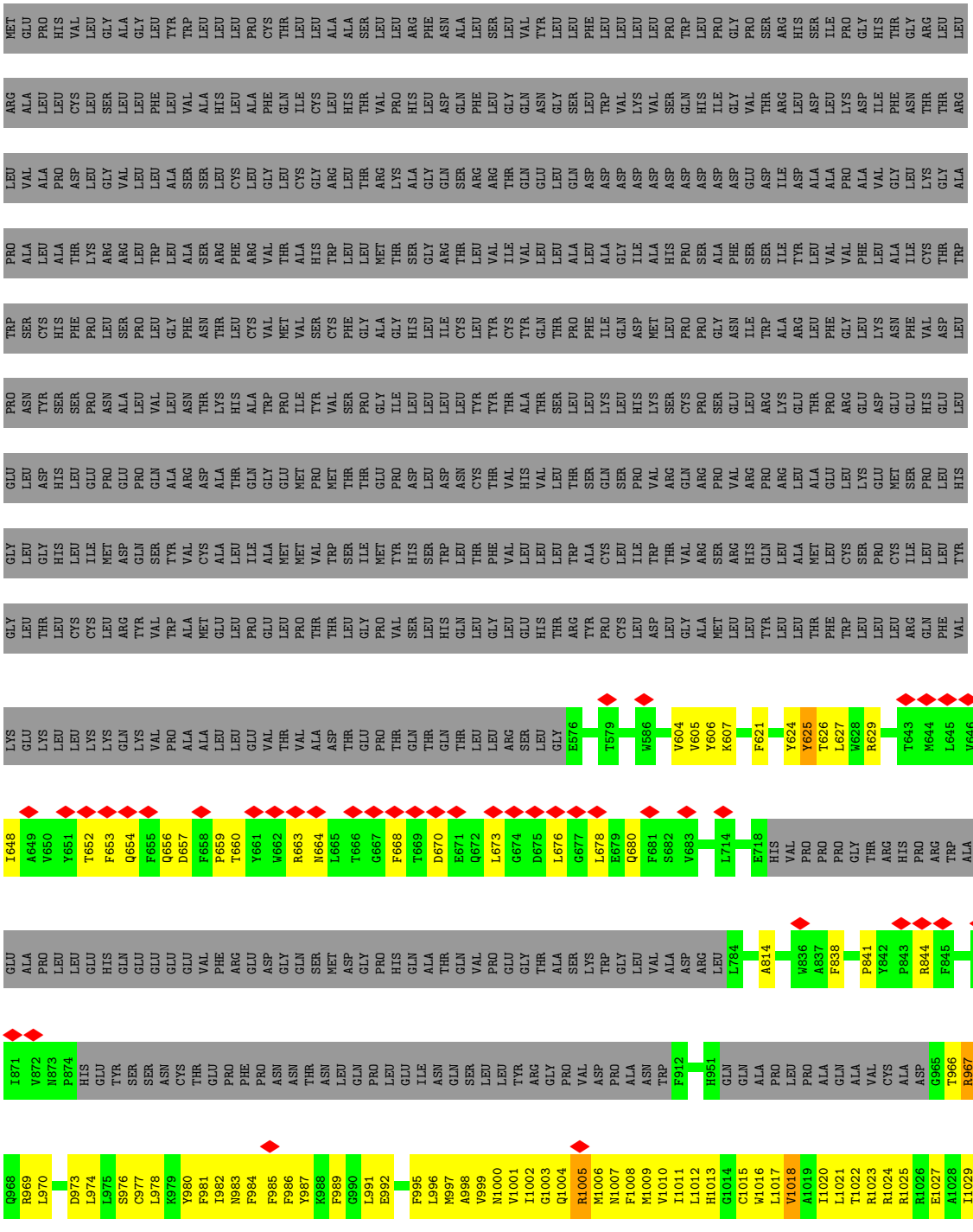
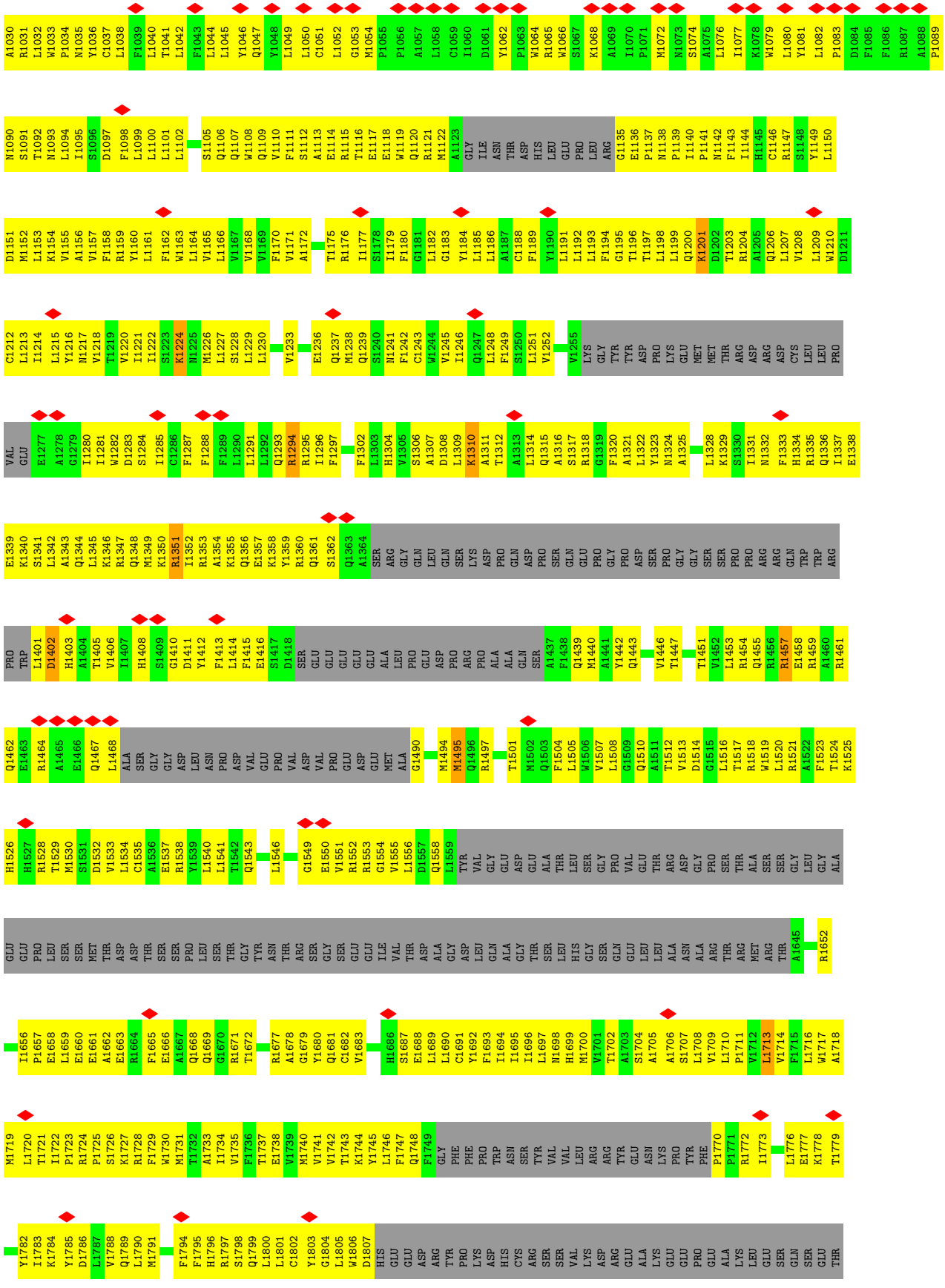
Q2389 L2390 Q2391 P2392 D2393 E2394 E2395 E2396 D2397 Y2398 L2399 G2400 V2401 R2402 I2403 Q2404 L2405 R2406 R2407 E2408 Q2409 V2410 G2411 THR GLY ALA SER GLY GLU GLN ALA G2420 T2421 K2422 A2423 S2424 D2425 F2426 L2427 E2428 W2429 W2430 V2431 I2432 E2433 L2434 Q2435 D2436 C2437 K2438 A2439 D2440 C2441 N2442 L2443 L2444 P2445 M2446 V2447 I2448
F2449 S2450 D2451 K2452 V2453 S2454 P2455 P2456 SER LEU GLY PHE LEU A2462 G2463 Y2464 G2465 I2466 V2467 G2468 L2469 Y2470 V2471 S2472 I2473 V2474 L2475 V2476 V2477 G2478 K2479 F2480 V2481 R2482 G2483 F2484 F2485 S2486 E2487 I2488 S2489 H2490 S2491 I2492 M2493 F2494 E2495 E2496 L2497 P2498 C2499 V2500 D2501 R2502 I2503 L2504 K2505 L2506 C2507 Q2508

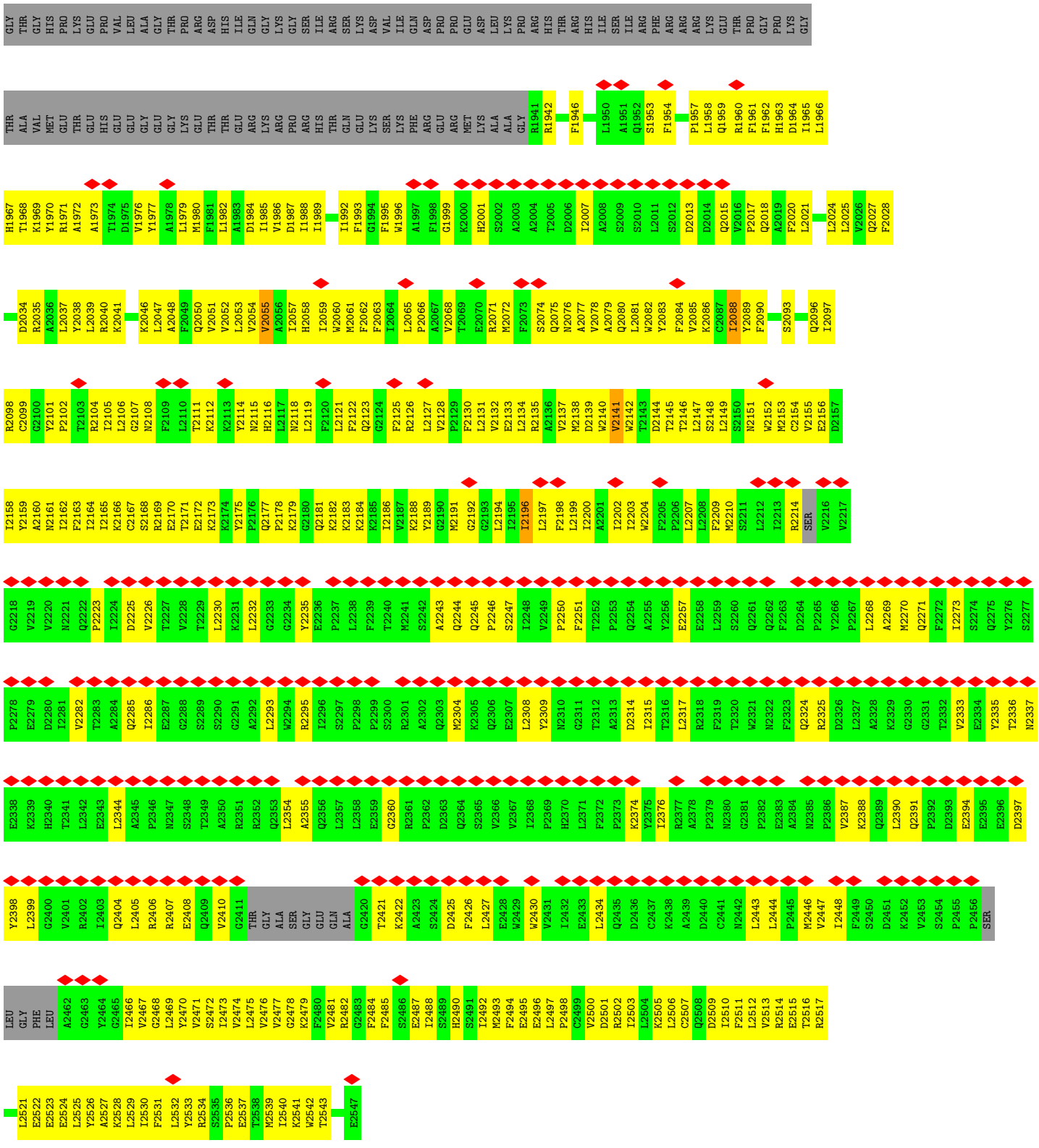


• Molecule 1: Piezo-type mechanosensitive ion channel component 1



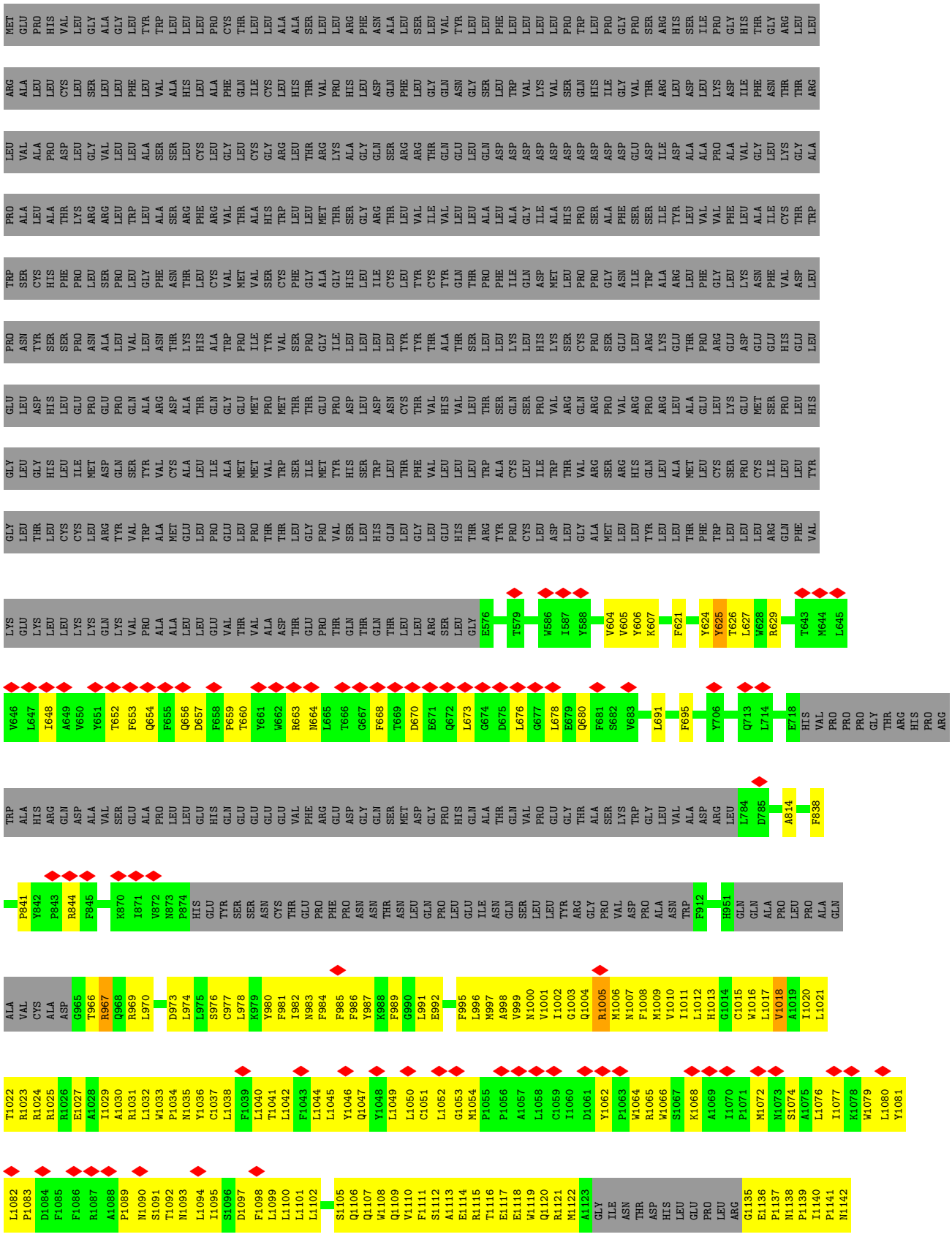


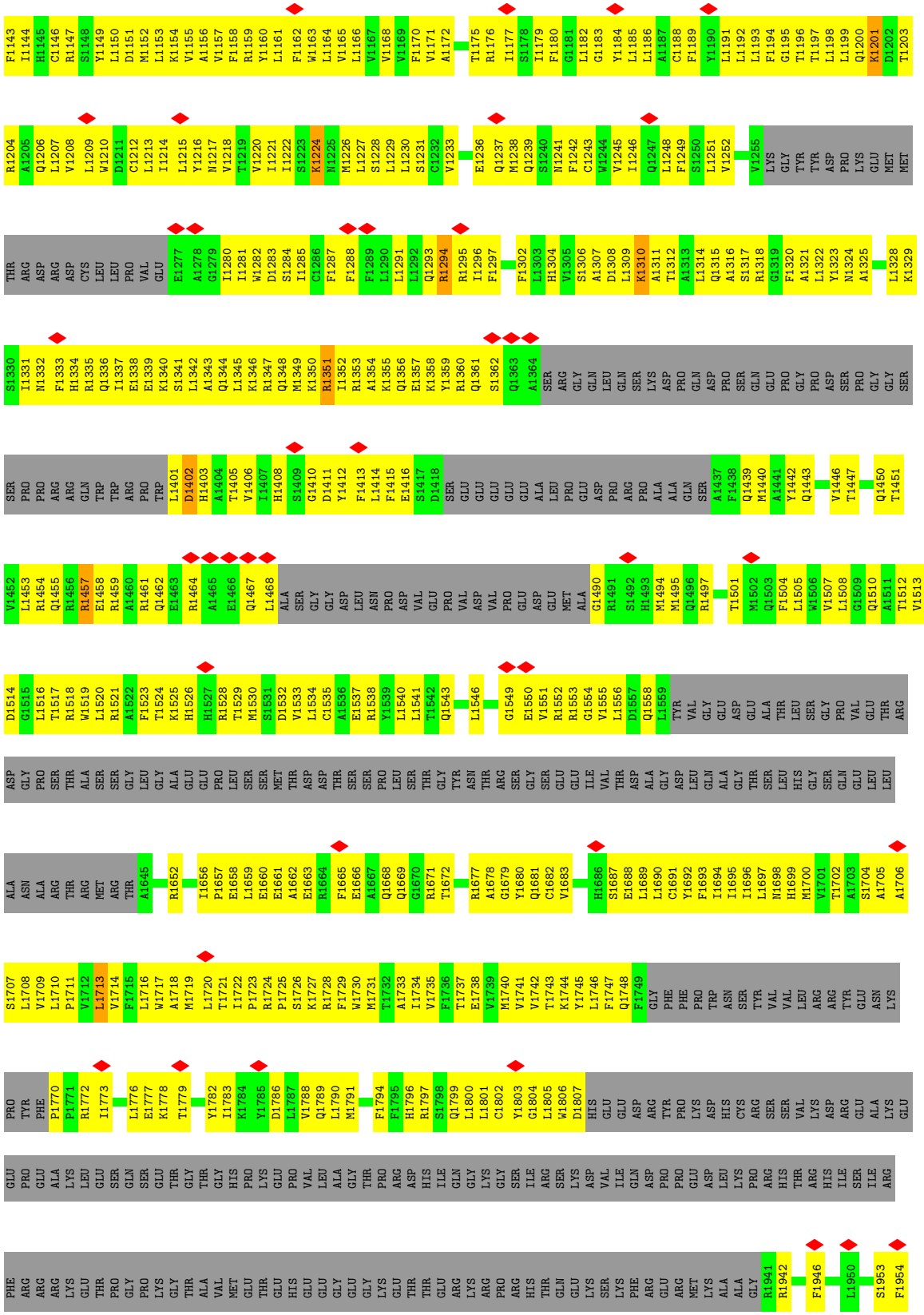




• Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain E:

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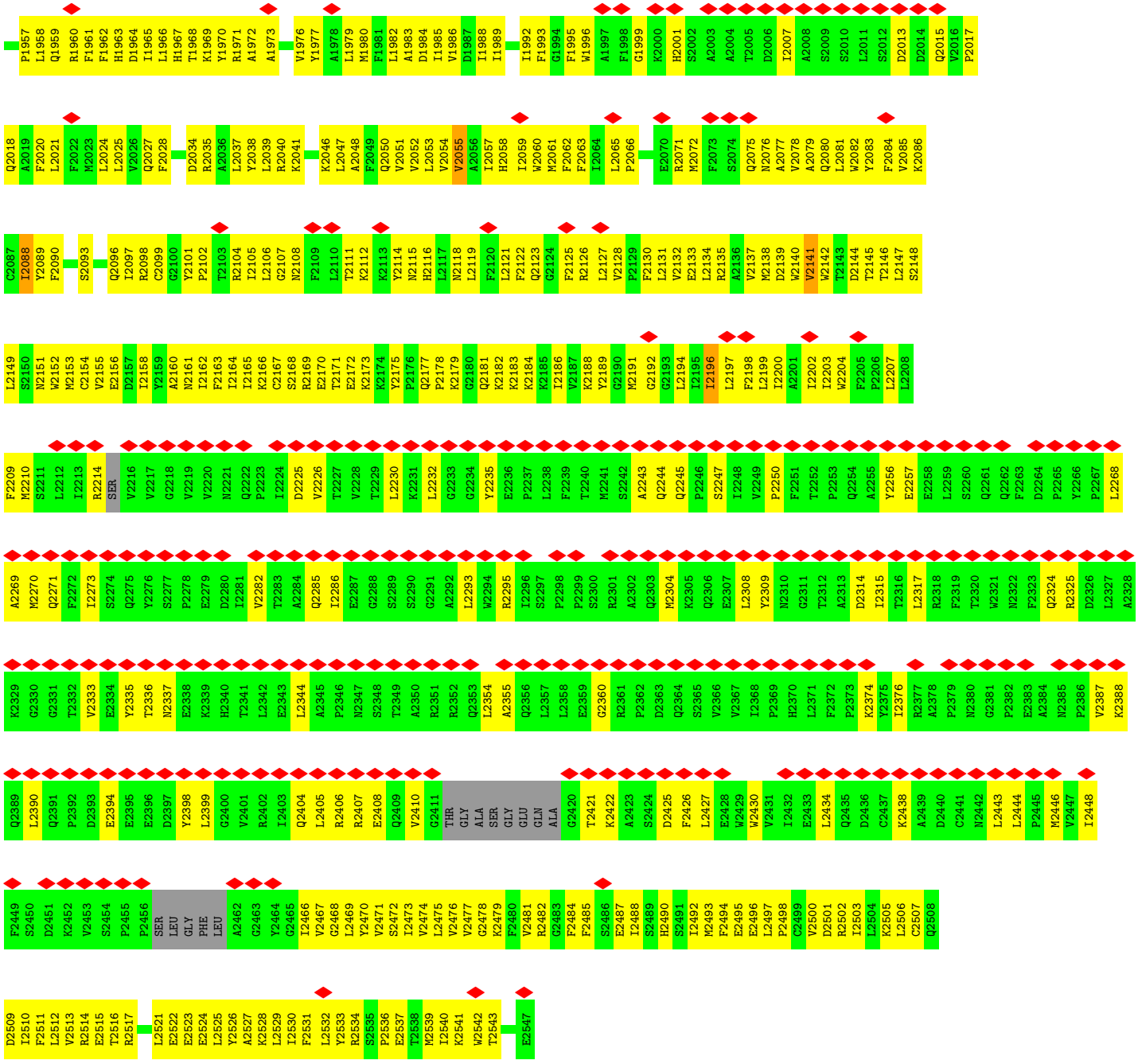
R1204 A1205 Q1206 L1207 V1208 L1209 W1210 D1211 C1212 L1213 I1214 L1215 Y1216 N1217 V1218 T1219 V1220 I1221 I1222 S1223 K1224 N1225 M1226 L1227 S1228 L1229 L1230 S1231 C1232 V1233 E1236 Q1237 M1238 Q1239 S1240 N1241 F1242 C1243 W1244 V1245 I1246 Q1247 L1248 F1249 S1250 L1251 V1252 V1255 LYS GLY TYR TYR ASP PRO LYS GLU MET MET
THR ARG ASP ARG ASP CYS LEU LEU PRO VAL GLU E1277 A1278 G1279 I1280 I1281 W1282 D1283 S1284 I1285 C1286 F1287 F1288 F1289 L1290 L1291 L1292 Q1293 R1294 R1295 I1296 F1297 F1302 L1303 H1304 V1305 S1306 A1307 D1308 L1309 K1310 A1311 T1312 A1313 L1314 Q1315 A1316 S1317 R1318 G1319 F1320 A1321 L1322 Y1323 N1324 A1325 L1328 K1329
S1330 I1331 N1332 F1333 H1334 R1335 Q1336 I1337 E1338 E1339 K1340 S1341 L1342 A1343 Q1344 L1345 K1346 R1347 Q1348 M1349 K1350 R1351 I1352 R1353 A1354 K1355 Q1356 E1357 K1358 Y1359 R1360 Q1361 S1362 Q1363 A1364 SER ARG GLY GLN LEU GLN SER LYS ASP PRO GLN ASP PRO SER GLN GLU PRO GLY PRO ASP SER PRO GLY GLY SER
SER PRO PRO ARG GLN TRP TRP ARG PRO TRP L1401 D1402 H1403 A1404 T1405 V1406 I1407 H1408 S1409 G1410 D1411 Y1412 F1413 L1414 F1415 E1416 S1417 D1418 SER GLU GLU GLU GLU GLU ALA LEU PRO GLU ASP PRO ARG PRO ALA ALA GLN SER A1437 F1438 Q1439 M1440 A1441 Y1442 Q1443 V1446 T1447 Q1450 T1451
V1452 L1453 R1454 Q1455 R1456 R1457 E1458 R1459 A1460 R1461 Q1462 E1463 R1464 A1465 E1466 Q1467 L1468 ALA SER GLY GLY ASP LEU ASN PRO ASP VAL ASP VAL PRO GLU ASP GLU MET ALA G1490 R1491 S1492 H1493 M1494 M1495 Q1496 R1497 T1501 M1502 Q1503 F1504 L1505 W1506 V1507 L1508 G1509 Q1510 A1511 T1512 V1513
D1514 G1515 L1516 T1517 R1518 W1519 L1520 R1521 A1522 F1523 T1524 K1525 H1526 H1527 R1528 T1529 M1530 S1531 D1532 V1533 L1534 C1535 A1536 E1537 R1538 Y1539 L1540 L1541 T1542 Q1543 L1546 G1549 E1550 V1551 R1552 R1553 G1554 V1555 L1556 D1557 Q1558 L1559 TYR VAL GLY GLU ASP GLU ALA THR LEU SER GLY PRO VAL GLU GLY THR ARG
ASP GLY PRO SER THR ALA SER SER GLY LEU GLY ALA GLU GLU PRO LEU SER SER MET THR ASP ASP THR SER SER PRO LEU SER THR GLY TYR ASN THR ARG SER GLY SER GLU GLU ILE VAL THR ASP ALA GLY ASP LEU GLN ALA ALA GLY THR HIS GLY SER GLN GLU LEU LEU
ALA ASN ALA ARG THR ARG MET ARG THR A1645 R1652 I1656 P1657 E1658 L1659 E1660 E1661 A1662 E1663 R1664 F1665 E1666 A1667 Q1668 Q1669 G1670 R1671 T1672 R1677 A1678 G1679 Y1680 Q1681 C1682 V1683 H1686 S1687 E1688 L1689 L1690 C1691 Y1692 F1693 I1694 I1695 I1696 L1697 N1698 H1699 M1700 V1701 T1702 A1703 S1704 A1705 A1706
S1707 L1708 V1709 L1710 P1711 Y1712 L1713 V1714 F1715 L1716 W1717 A1718 M1719 L1720 T1721 I1722 P1723 R1724 P1725 S1726 K1727 R1728 F1729 W1730 M1731 T1732 A1733 I1734 V1735 F1736 T1737 E1738 V1739 M1740 V1741 V1742 T1743 K1744 Y1745 L1746 F1747 Q1748 F1749 GLY PHE PHE PRO TRP ASN SER TYR VAL VAL LEU ARG ARG TYR GLU ASN LYS
PRO TYR PHE P1770 P1771 R1772 I1773 L1776 E1777 K1778 T1779 Y1782 I1783 K1784 Y1785 D1786 L1787 V1788 Q1789 L1790 M1791 F1794 F1795 H1796 R1797 S1798 Q1799 L1800 L1801 C1802 Y1803 G1804 L1805 W1806 D1807 HIS GLU GLU ASP ARG TYR PRO LYS ASP HIS CYS ARG SER VAL LYS ASP ARG GLU ALA LYS GLU
GLU PRO GLU ALA LYS LEU GLU SER GLN SER GLU THR GLY THR HIS GLY PRO LYS GLU PRO VAL LEU ALA GLY THR PRO ARG ASP HIS ILE GLN GLY LYS ARG GLY SER ILE ARG SER LYS ASP VAL ILE GLN ASP PRO PRO GLU ASP LEU LYS PRO ARG HIS THR ARG HIS ILE SER ILE ARG
PHE ARG ARG ARG LYS GLU THR PRO GLY PRO LYS GLY THR ALA VAL MET GLU THR GLU HIS GLU GLU GLY GLU GLY LYS GLU ARG LYS ARG PRO ARG SER HIS THR GLN GLU LYS SER LYS PHE ARG GLU ARG ARG MET LYS ALA ALA GLY R1941 R1942 F1946 L1950 S1953 F1954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Q2018 A2019 F2020 L2021 F2022 M2023 L2024 L2025 V2026 Q2027 F2028 D2034 R2035 A2036 L2037 Y2038 L2039 R2040 K2041 K2046 L2047 A2048 F2049 Q2050 V2051 V2052 L2053 V2054 V2055 A2056 I2057 H2058 I2059 W2060 M2061 F2062 F2063 I2064 L2065 P2066 E2070 R2071 M2072 F2073 S2074 Q2075 N2076 A2077 V2078 A2079 Q2080 L2081 W2082 Y2083 F2084 V2085 K2086
C2087 I2088 Y2089 F2090 S2093 Q2096 I2097 R2098 C2099 G2100 Y2101 P2102 T2103 R2104 I2105 L2106 G2107 N2108 F2109 L2110 T2111 K2112 K2113 Y2114 N2115 H2116 L2117 N2118 L2119 F2120 L2121 F2122 Q2123 G2124 F2125 R2126 L2127 V2128 F2129 F2130 L2131 V2132 E2133 L2134 R2135 A2136 V2137 M2138 D2139 W2140 V2141 W2142 T2143 D2144 T2145 T2146 L2147 S2148
L2149 S2150 N2151 W2152 M2153 C2154 V2155 E2156 D2157 I2158 Y2159 A2160 N2161 I2162 F2163 I2164 I2165 K2166 C2167 S2168 R2169 E2170 T2171 E2172 K2173 K2174 Y2175 P2176 Q2177 P2178 K2179 G2180 Q2181 K2182 K2183 K2184 K2185 I2186 V2187 K2188 Y2189 G2190 M2191 G2192 G2193 L2194 I2195 I2196 L2197 F2198 L2199 I2200 A2201 I2202 I2203 W2204 F2205 P2206 L2207 L2208
F2209 M2210 S2211 L2212 I2213 R2214 SER V2216 V2217 G2218 V2219 V2220 N2221 Q2222 P2223 I2224 D2225 V2226 T2227 V2228 T2229 L2230 K2231 L2232 G2233 G2234 Y2235 E2236 P2237 L2238 F2239 T2240 M2241 S2242 A2243 Q2244 Q2245 P2246 S2247 I2248 V2249 P2250 F2251 T2252 P2253 Q2254 A2255 Y2256 E2257 E2258 L2259 S2260 Q2261 Q2262 F2263 D2264 P2265 Y2266 P2267 L2268
A2269 M2270 Q2271 F2272 I2273 S2274 Q2275 Y2276 S2277 P2278 E2279 D2280 I2281 V2282 T2283 A2284 Q2285 I2286 E2287 G2288 S2289 S2290 G2291 A2292 L2293 W2294 R2295 I2296 S2297 P2298 P2299 S2300 R2301 A2302 Q2303 M2304 K2305 Q2306 E2307 L2308 Y2309 N2310 G2311 T2312 A2313 D2314 I2315 T2316 L2317 R2318 F2319 T2320 W2321 N2322 F2323 Q2324 R2325 D2326 L2327 A2328
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Q2389 L2390 Q2391 P2392 D2393 E2394 E2395 E2396 D2397 Y2398 L2399 G2400 V2401 R2402 I2403 Q2404 L2405 R2406 R2407 E2408 Q2409 V2410 G2411 THR GLY ALA SER GLY GLU GLN ALA G2420 T2421 K2422 A2423 S2424 D2425 F2426 L2427 E2428 W2429 W2430 V2431 I2432 E2433 L2434 Q2435 D2436 C2437 K2438 A2439 D2440 C2441 N2442 L2443 L2444 P2445 M2446 V2447 I2448
F2449 S2450 D2451 K2452 V2453 S2454 P2455 P2456 SER LEU GLY PHE LEU A2462 G2463 Y2464 G2465 I2466 V2467 G2468 L2469 Y2470 V2471 S2472 I2473 V2474 L2475 V2476 V2477 G2478 K2479 F2480 V2481 R2482 G2483 F2484 F2485 S2486 E2487 I2488 S2489 H2490 S2491 I2492 M2493 F2494 E2495 E2496 L2497 P2498 C2499 V2500 D2501 R2502 I2503 L2504 K2505 L2506 C2507 Q2508
D2509 I2510 F2511 L2512 V2513 R2514 E2515 T2516 R2517 L2521 E2522 E2523 E2524 L2525 Y2526 A2527 K2528 L2529 I2530 F2531 L2532 Y2533 R2534 S2535 P2536 E2537 T2538 M2539 I2540 K2541 W2542 T2543 E2547

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	395.28003, 395.28003, 395.28003	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.196, 2.196, 2.196	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLX

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	0.47	0/11796	0.69	0/16031
1	C	0.47	0/11796	0.69	0/16031
1	E	0.47	0/11796	0.69	0/16031
All	All	0.47	0/35388	0.69	0/48093

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	11535	0	10972	1041	0
1	C	11535	0	10972	1046	0
1	E	11535	0	10972	1025	0
2	A	52	0	88	3	0
2	C	52	0	88	3	0
2	E	52	0	88	2	0
All	All	34761	0	33180	3061	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 45.

The worst 5 of 3061 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:1700:MET:SD	1:A:2080:GLN:HB3	1.29	1.69
1:E:1700:MET:SD	1:E:2080:GLN:HB3	1.29	1.68
1:C:1700:MET:SD	1:C:2080:GLN:HB3	1.29	1.66
1:E:1700:MET:SD	1:E:2080:GLN:CB	2.22	1.28
1:A:1700:MET:SD	1:A:2080:GLN:CB	2.22	1.27

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 PDB entries followed by that with respect to all EM entries.

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	1468/2547 (58%)	1376 (94%)	88 (6%)	4 (0%)	41	77
1	C	1468/2547 (58%)	1376 (94%)	88 (6%)	4 (0%)	41	77
1	E	1468/2547 (58%)	1376 (94%)	88 (6%)	4 (0%)	41	77
All	All	4404/7641 (58%)	4128 (94%)	264 (6%)	12 (0%)	44	77

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	TYR
1	C	625	TYR
1	E	625	TYR
1	A	605	VAL
1	C	605	VAL

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 PDB entries followed by that with respect to all EM

entries.

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	1117/2246 (50%)	1097 (98%)	20 (2%)	59	77
1	C	1117/2246 (50%)	1097 (98%)	20 (2%)	59	77
1	E	1117/2246 (50%)	1097 (98%)	20 (2%)	59	77
All	All	3351/6738 (50%)	3291 (98%)	60 (2%)	61	77

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1310	LYS
1	E	2055	VAL
1	C	2055	VAL
1	E	1713	LEU
1	E	2270	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2118	ASN
1	E	1304	HIS
1	C	2391	GLN
1	E	1668	GLN
1	A	2118	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
2	PLX	A	2601	-	51,51,51	1.13	4 (7%)	55,59,59	0.86	1 (1%)
2	PLX	E	2601	-	51,51,51	1.13	4 (7%)	55,59,59	0.86	1 (1%)
2	PLX	C	2601	-	51,51,51	1.14	4 (7%)	55,59,59	0.86	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	A	2601	-	-	12/55/55/55	-
2	PLX	E	2601	-	-	12/55/55/55	-
2	PLX	C	2601	-	-	12/55/55/55	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2601	PLX	O6-C4	-2.64	1.41	1.44
2	E	2601	PLX	O6-C4	-2.64	1.41	1.44
2	A	2601	PLX	O6-C4	-2.61	1.41	1.44
2	C	2601	PLX	C7-C6	2.48	1.56	1.50
2	E	2601	PLX	C7-C6	2.47	1.56	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2601	PLX	C26-C25-C24	-2.42	107.79	113.38
2	A	2601	PLX	C26-C25-C24	-2.41	107.80	113.38
2	C	2601	PLX	C26-C25-C24	-2.41	107.81	113.38

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

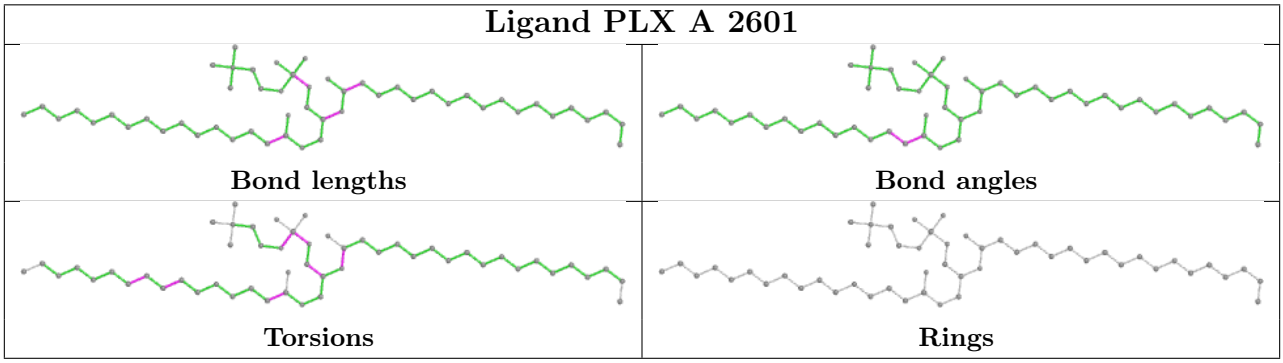
Mol	Chain	Res	Type	Atoms
2	A	2601	PLX	O7-C6-O6-C4
2	A	2601	PLX	C3-O4-P1-O3
2	A	2601	PLX	C2-O1-P1-O2
2	C	2601	PLX	O7-C6-O6-C4
2	C	2601	PLX	C3-O4-P1-O3

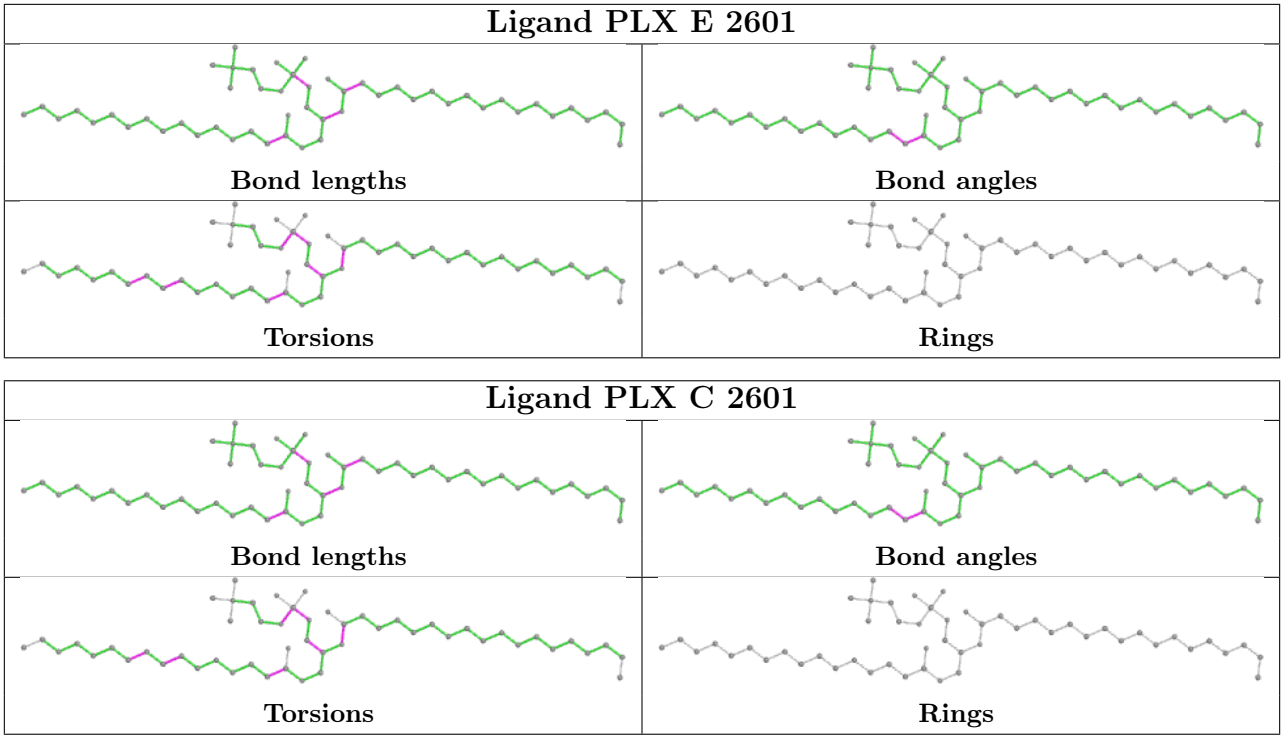
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	PLX	3	0
2	E	2601	PLX	2	0
2	C	2601	PLX	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

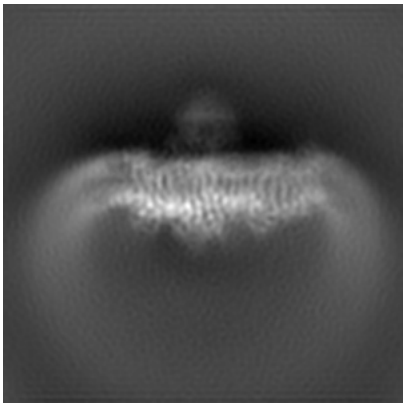
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32593. These allow visual inspection of the internal detail of the map and identification of artifacts.

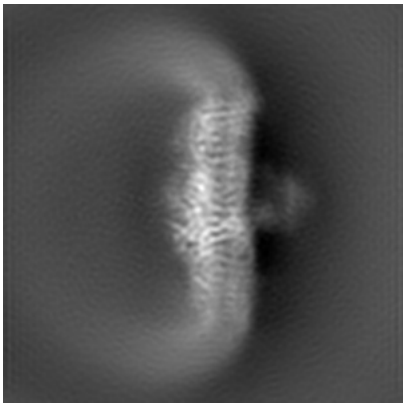
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

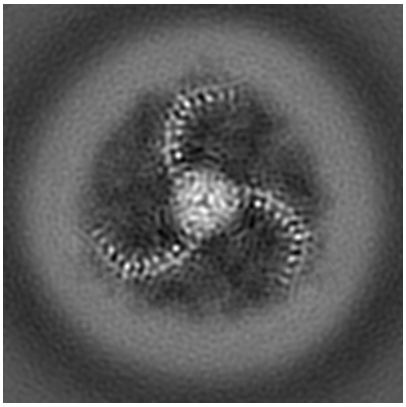
6.1.1 Primary map



X



Y

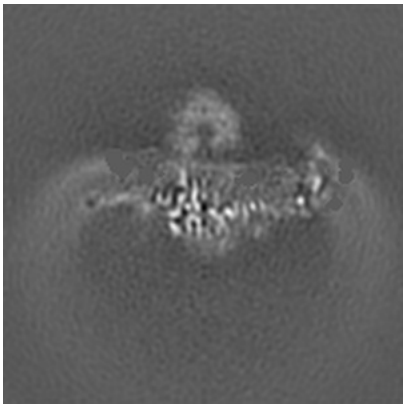


Z

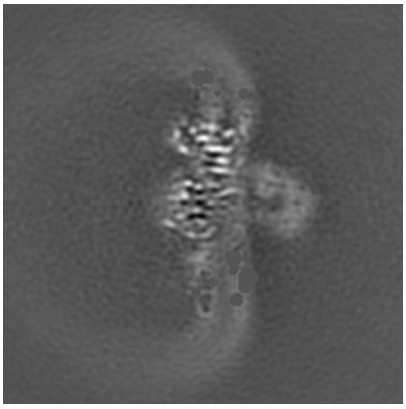
The images above show the map projected in three orthogonal directions.

6.2 Central slices

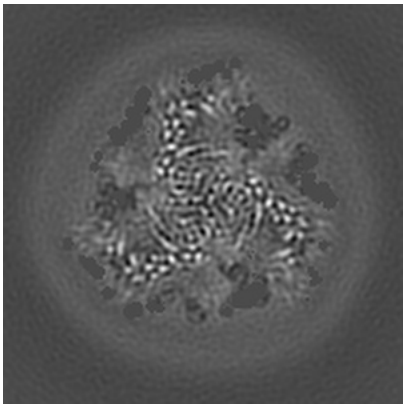
6.2.1 Primary map



X Index: 90



Y Index: 90

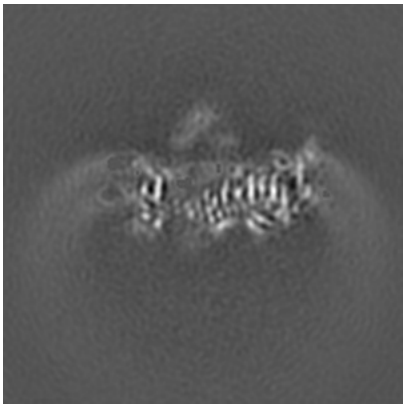


Z Index: 90

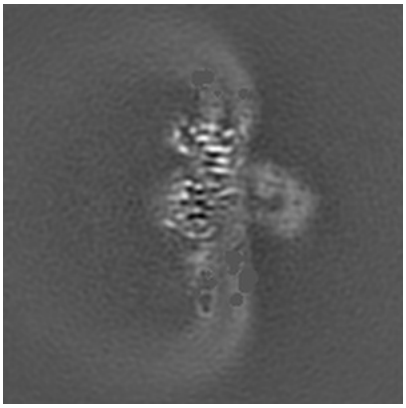
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

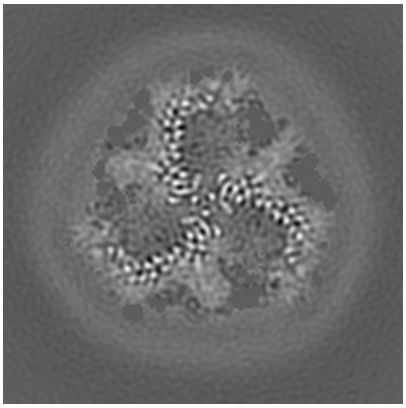
6.3.1 Primary map



X Index: 78



Y Index: 90

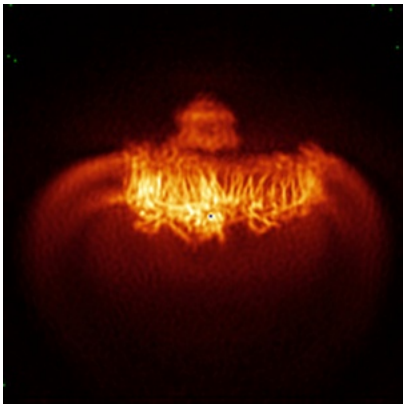


Z Index: 92

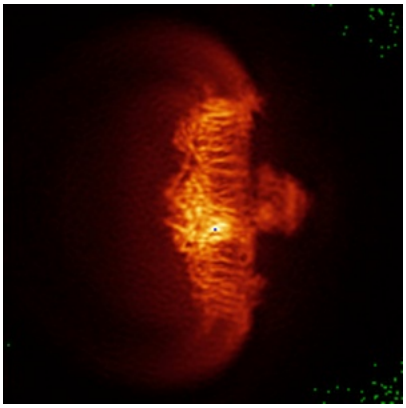
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

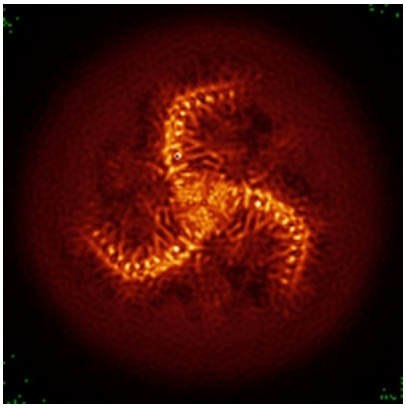
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

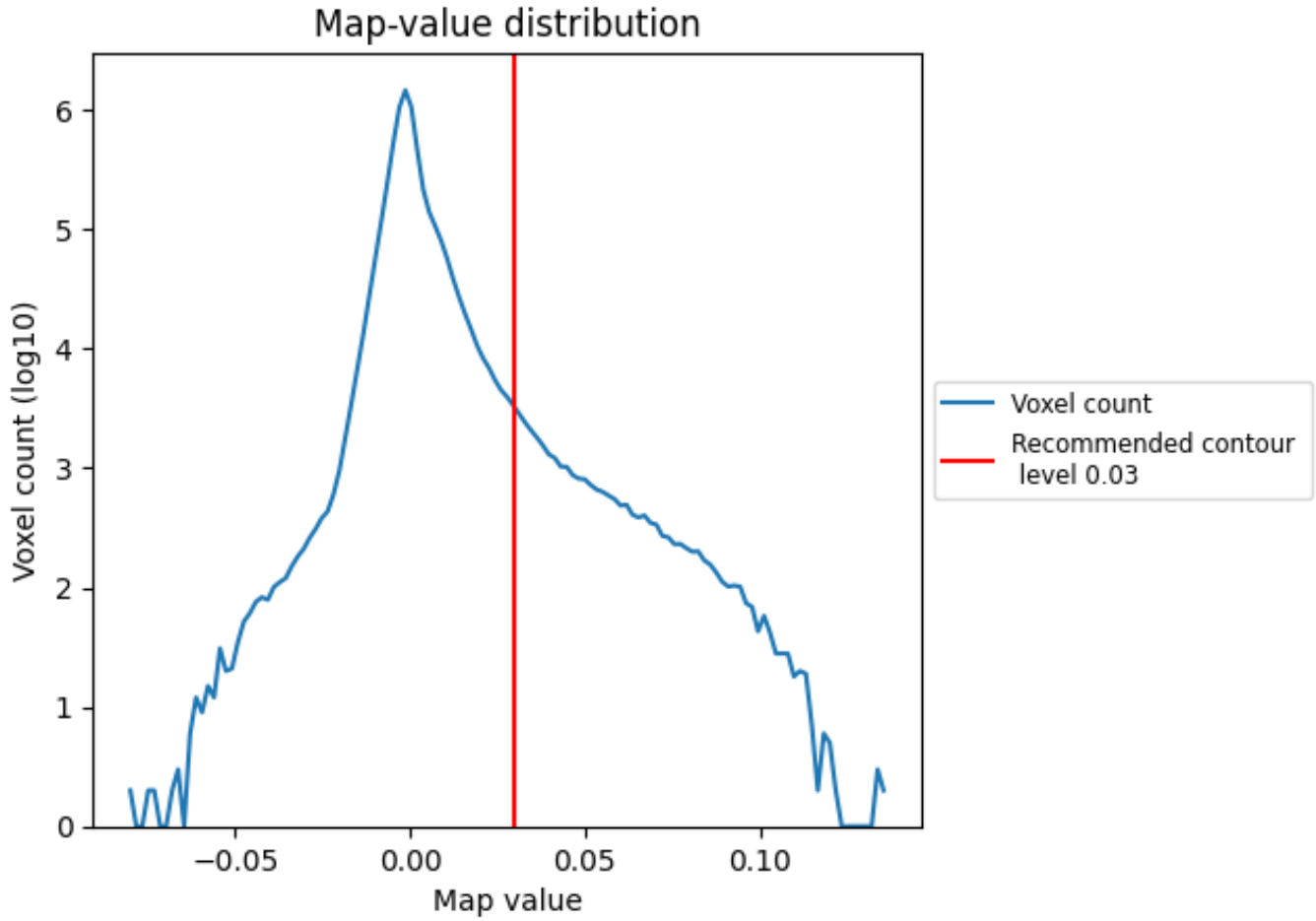
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

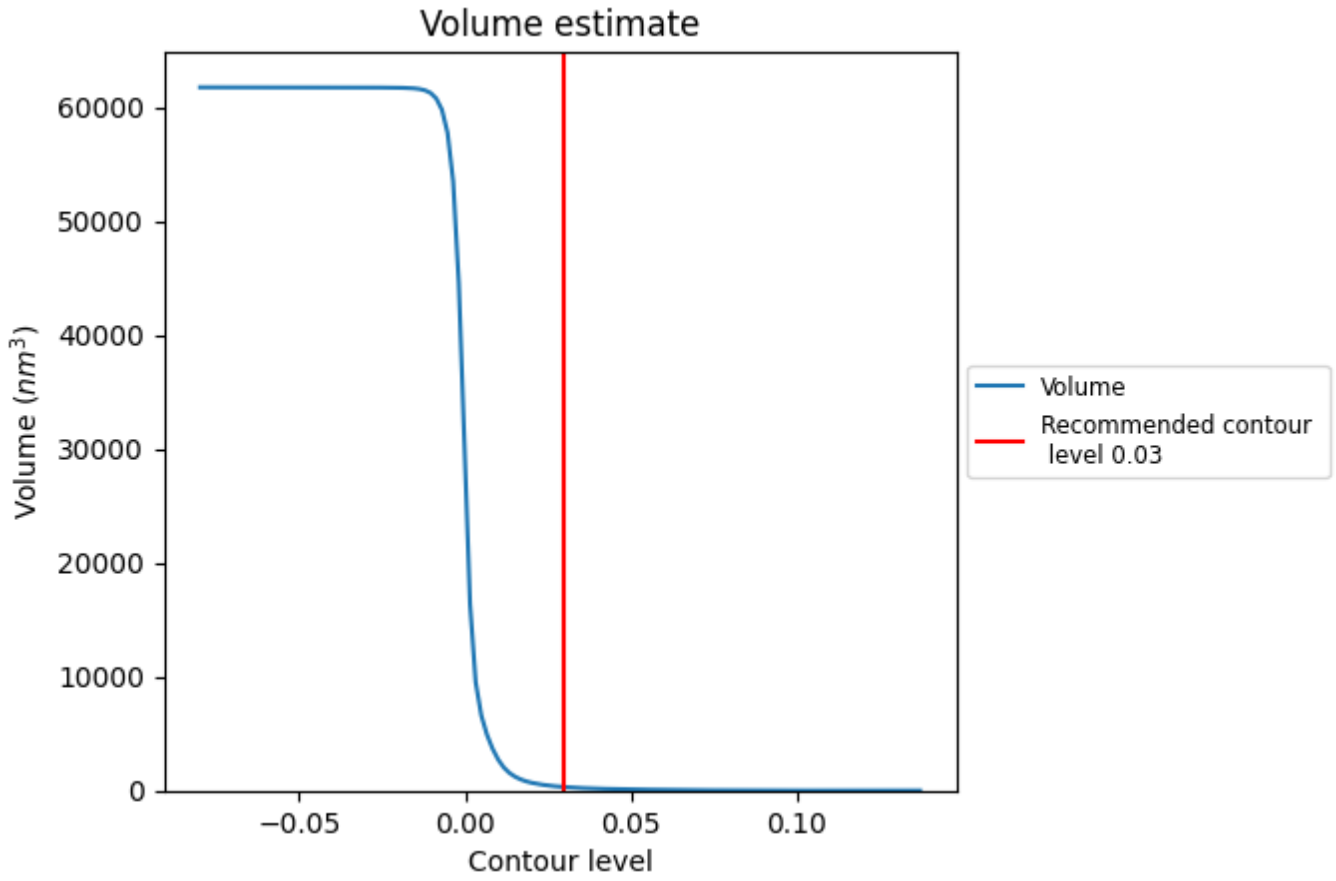
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

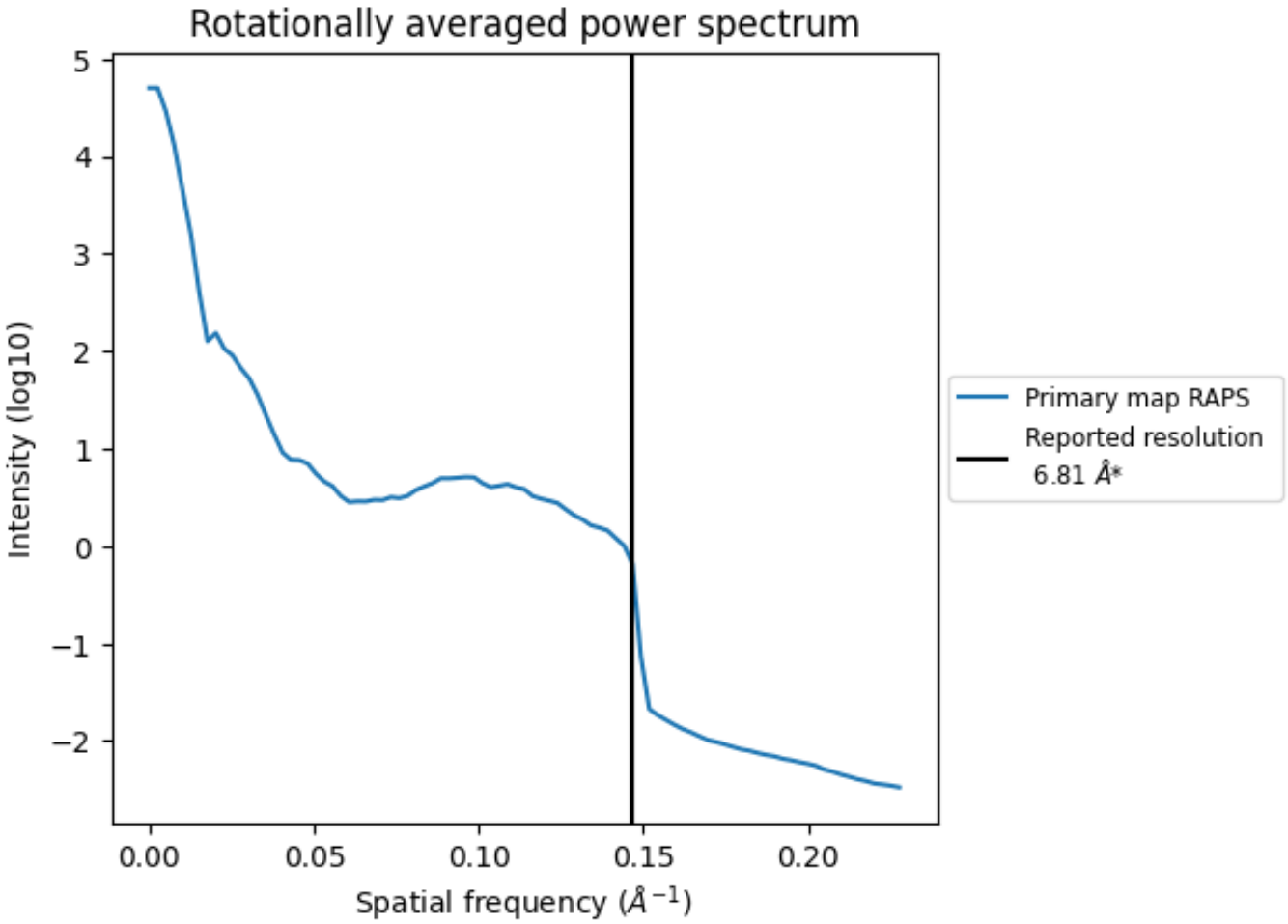
7.2 Volume estimate (i)



The volume at the recommended contour level is 309 nm^3; this corresponds to an approximate mass of 279 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.147 Å^{-1}

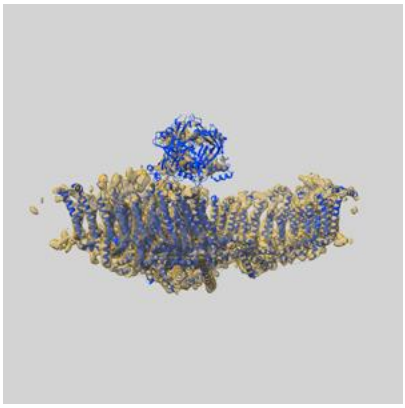
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

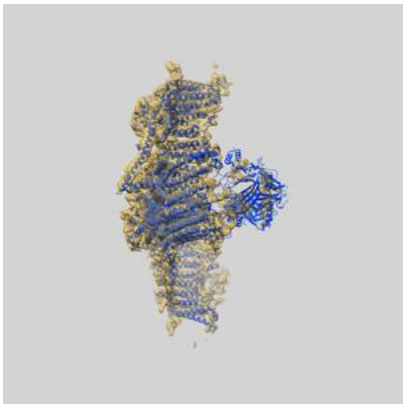
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32593 and PDB model 7WLU. Per-residue inclusion information can be found in section 3 on page 5.

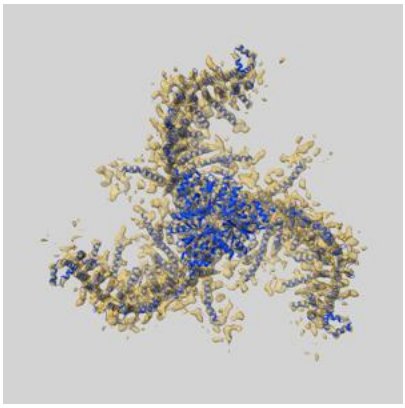
9.1 Map-model overlay



X



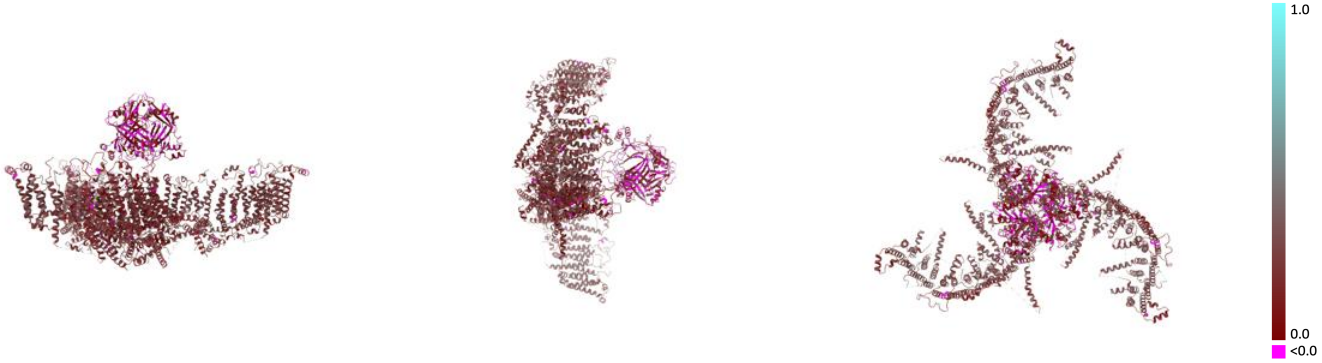
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

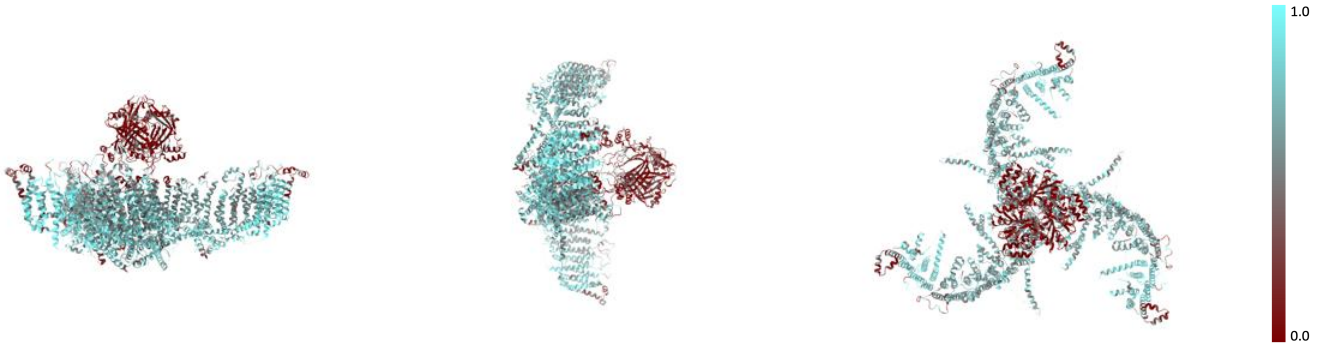
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

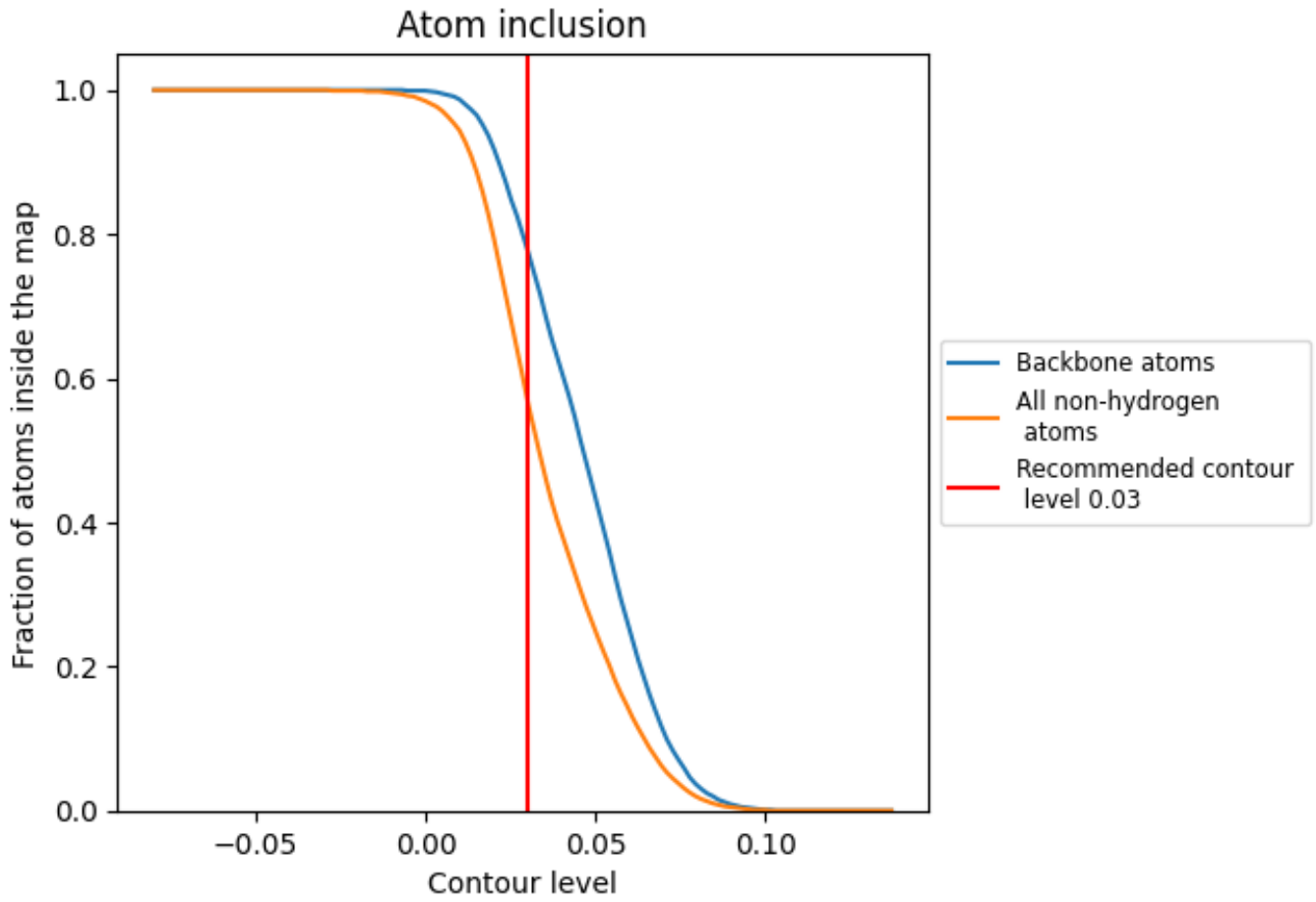
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5690	0.1960
A	0.5690	0.1960
C	0.5720	0.1980
E	0.5680	0.1940