wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 07:03 PM EST

PDB ID	:	6MU1
EMDB ID	:	EMD-9243
Title	:	Structure of full-length IP3R1 channel bound with Adenophostin A
Authors	:	Serysheva, I.I.; Fan, G.; Baker, M.R.; Wang, Z.; Seryshev, A.; Ludtke, S.J.; Baker, M.L.
Deposited on	:	2018-10-22
Resolution	:	4.10 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 (1)) were used in the production of this report:

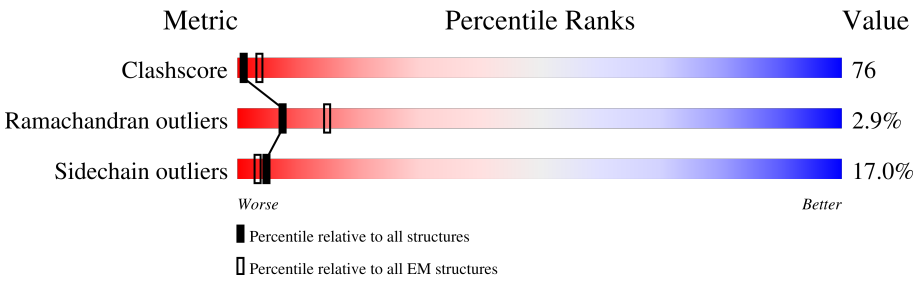
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.10 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	2739	21% 48% 24% 6% • 22%
1	B	2739	21% 47% 24% 6% • 22%
1	C	2739	21% 47% 24% 6% • 22%
1	D	2739	21% 47% 24% 6% • 22%

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
2	JYP	A	2801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JYP	B	2801	-	-	X	-
2	JYP	C	2801	-	-	X	-
2	JYP	D	2801	-	-	X	-

2 Entry composition (i)

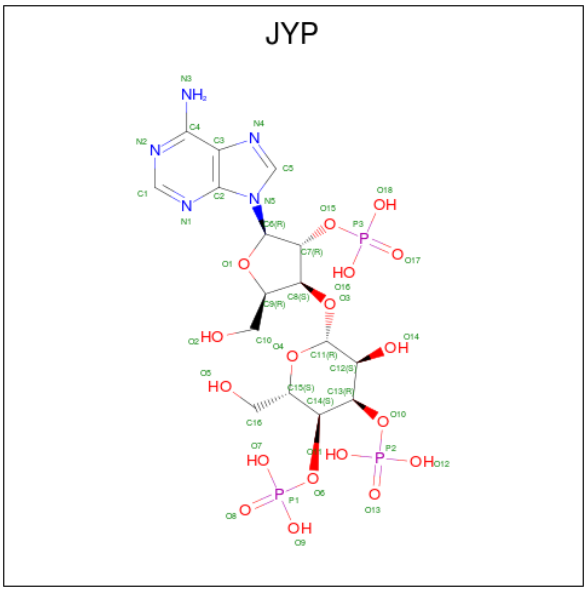
There are 2 unique types of molecules in this entry. The entry contains 50184 atoms, of which 20 are hydrogens and 0 are deuteriums.

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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2149	12499	7356	2487	2612	44	0	0
1	C	2149	12499	7356	2487	2612	44	0	0
1	B	2149	12499	7356	2487	2612	44	0	0
1	D	2149	12499	7356	2487	2612	44	0	0

- Molecule 2 is Adenophostin A (three-letter code: JYP) (formula: $C_{16}H_{26}N_5O_{18}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	A	1	47	16	5	5	18	3	0
2	C	1	47	16	5	5	18	3	0
2	B	1	47	16	5	5	18	3	0

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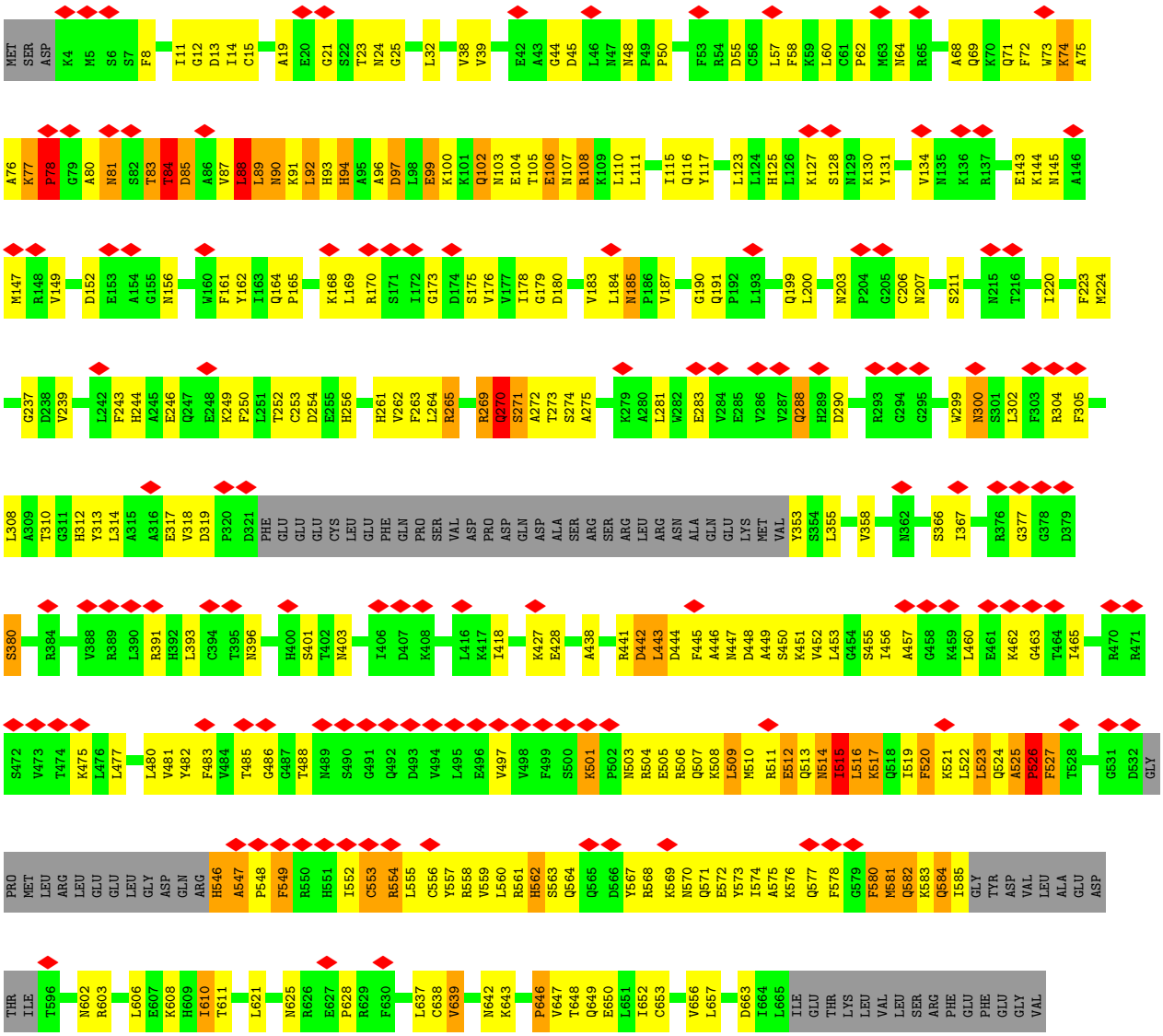
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	D	1	47	16	5	5	18	3	0

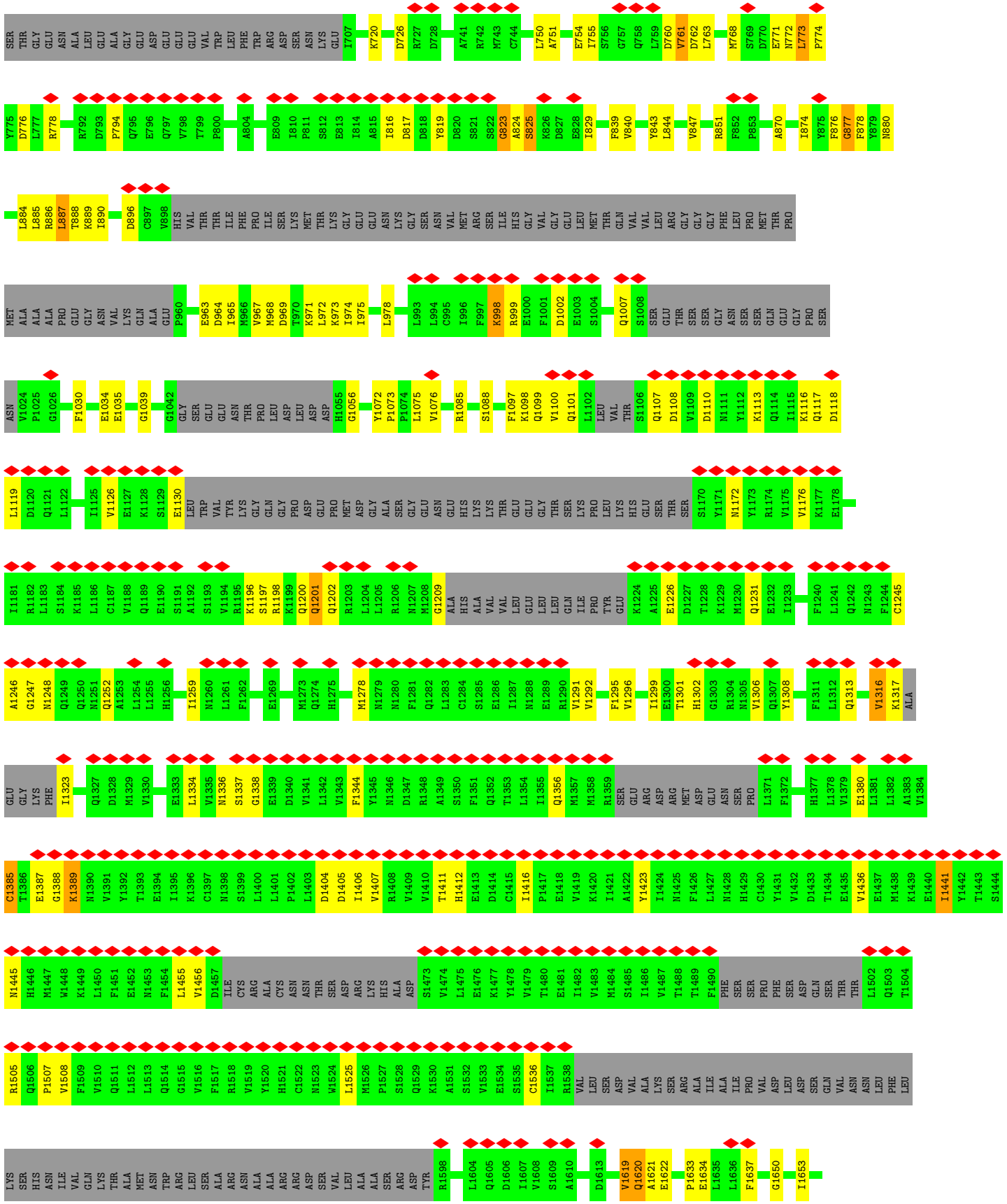
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Inositol 1,4,5-trisphosphate receptor type 1

Chain A:

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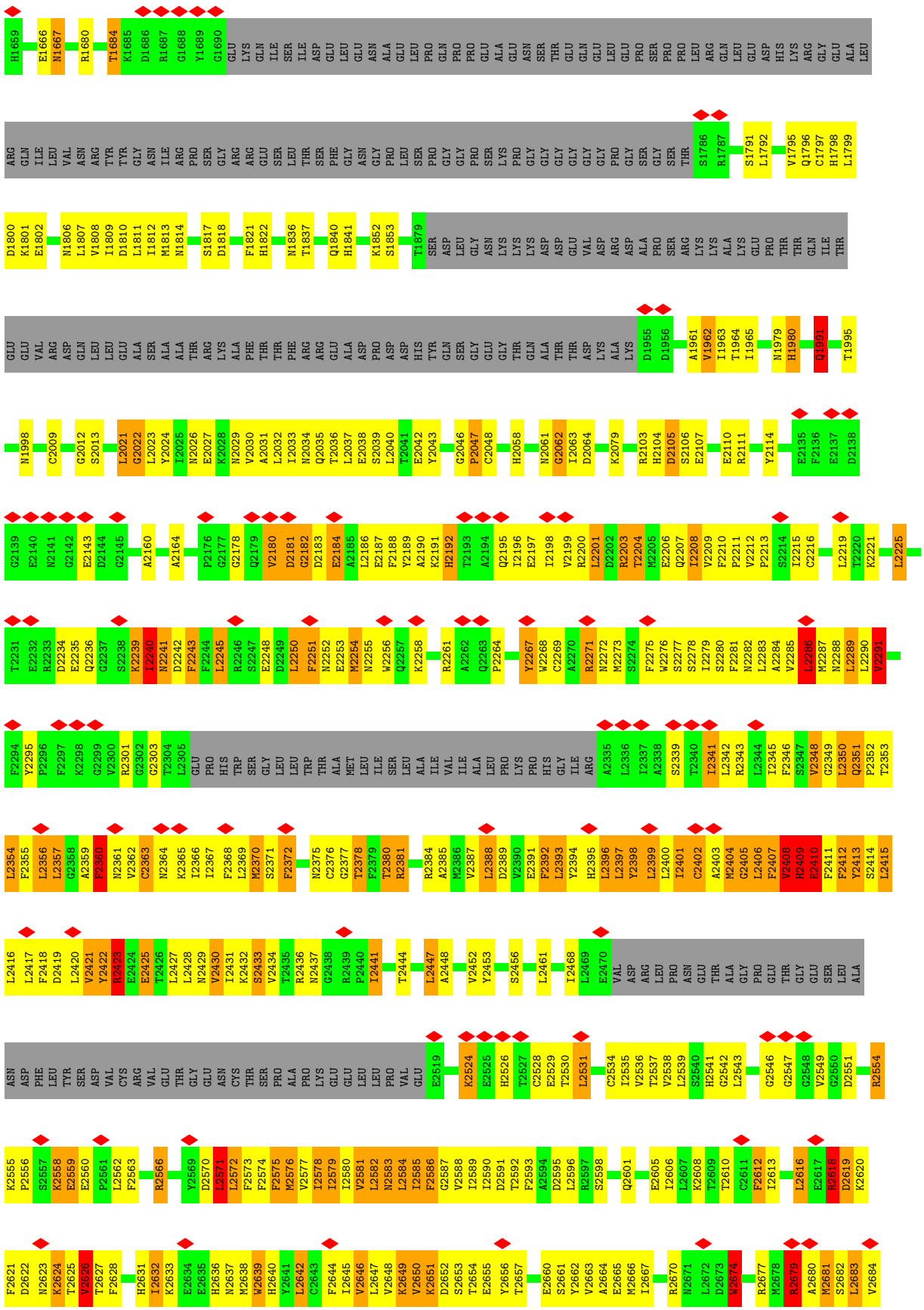
Y775 D776 L777 R778 R792 D793 P794 Q795 E796 Q797 V798 T799 P800 A804 E809 I810 P811 S812 E813 I814 A815 I816 D817 D818 Y819 D820 S821 S822 G823 A824 S825 K826 D827 E828 I829 F839 V840 Y843 L844 V847 R851 F852 P853 A870 I874 Y875 F876 G877 F878 Y879 N880
L884 L885 R886 L887 T888 K889 I890 D896 C897 V898 HIS VAL THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL VAL LEU ARG GLY GLY GLY PHE LEU PRO MET THR PRO
MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E963 D964 I965 M966 V967 M968 D969 T970 K971 L972 K973 I974 I975 L978 L993 L994 C995 I996 F997 K998 R999 E1000 F1001 D1002 E1003 S1004 Q1007 S1008 SER GLU THR SER SER GLY ASN SER SER GLN GLU GLY PRO SER
ASN V1024 P1025 G1026 F1030 E1034 E1035 G1039 G1042 GLY SER GLU GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 G1056 Y1072 P1073 P1074 L1075 V1076 R1085 S1088 F1097 K1098 Q1099 V1100 Q1101 L1102 LEU VAL THR S1106 Q1107 D1108 V1109 D1110 N1111 Y1112 K1113 Q1114 I1115 K1116 Q1117 D1118
L1119 D1120 Q1121 L1122 I1125 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 Y1173 R1174 V1175 V1176 K1177 E1178
I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200 Q1201 Q1202 R1203 L1204 L1205 R1206 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 F1240 L1241 Q1242 N1243 F1244 C1245
A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 L1254 L1255 H1256 I1259 N1260 L1261 F1262 E1269 M1273 Q1274 H1275 M1278 N1279 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291 V1292 F1295 V1296 I1299 E1300 T1301 H1302 G1303 R1304 N1305 V1306 Q1307 Y1308 F1311 L1312 Q1313 V1316 K1317 ALA
GLU GLY LYS PHE I1323 Q1327 D1328 M1329 V1330 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 Y1345 N1346 D1347 R1348 A1349 S1350 F1351 Q1352 T1353 L1354 I1355 Q1356 M1357 M1358 R1359 SER GLU ARG ASP ARG MET ASP GLU ASN SER PRO L1371 F1372 H1377 L1378 V1379 E1380 L1381 L1382 A1383 V1384
C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 Y1423 I1424 N1425 F1426 L1427 N1428 H1429 C1430 Y1431 V1432 D1433 T1434 E1435 V1436 E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444
N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 PHE SER SER PRO PHE SER ASP GLN SER THR THR L1502 Q1503 T1504
R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP SER GLN VAL ASN ASN LEU PHE LEU
LYS SER HIS ASN ILE VAL GLN LYS THR ALA ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 L1604 Q1605 D1606 I1607 V1608 S1609 A1610 D1613 V1619 Q1620 A1621 E1622 P1633 E1634 L1635 L1636 F1637 G1650 I1653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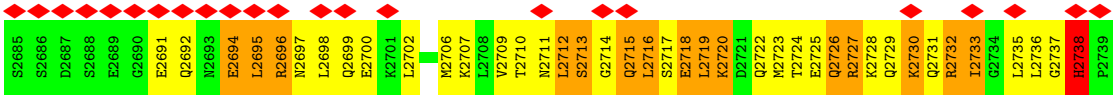
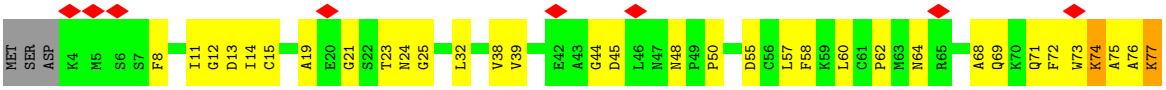
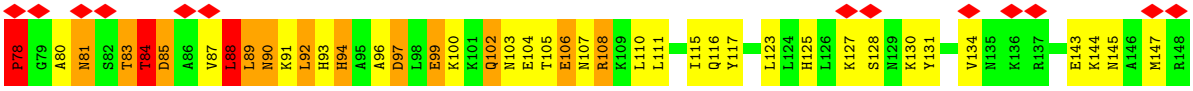
ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY GLY PRO GLY SER GLY SER THR S1786 R1787 S1791 L1792 V1795 Q1796 C1797 H1798 L1799
D1800 K1801 E1802 N1806 L1807 V1808 I1809 D1810 L1811 I1812 M1813 N1814 S1817 D1818 F1821 H1822 N1836 T1837 Q1840 H1841 K1852 S1853 T1879 SER ASP LEU GLY ASN LYS LYS LYS ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR
GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 A1961 V1962 I1963 T1964 I1965 N1979 H1980 Q1991 T1995
N1998 C2009 G2012 S2013 L2021 G2022 L2023 Y2024 I2025 N2026 E2027 K2028 N2029 V2030 A2031 L2032 I2033 N2034 Q2035 T2036 L2037 E2038 S2039 L2040 T2041 E2042 Y2043 G2046 P2047 C2048 H2058 N2061 G2062 I2063 D2064 K2079 R2103 H2104 D2105 S2106 E2107 E2110 R2111 Y2114 E2135 F2136 E2137 D2138
G2139 E2140 N2141 G2142 E2143 D2144 G2145 A2160 A2164 P2176 G2177 G2178 Q2179 V2180 D2181 G2182 D2183 E2184 A2185 L2186 E2187 F2188 Y2189 A2190 K2191 H2192 T2193 A2194 Q2195 I2196 E2197 I2198 V2199 R2200 L2201 D2202 R2203 T2204 M2205 E2206 Q2207 I2208 V2209 F2210 P2211 V2212 P2213 S2214 I2215 C2216 L2219 T2220 K2221 L2225
T2231 E2232 R2233 D2234 E2235 Q2236 G2237 S2238 K2239 I2240 N2241 D2242 F2243 F2244 L2245 R2246 S2247 E2248 D2249 L2250 F2251 N2252 E2253 M2254 N2255 W2256 Q2257 K2258 R2261 A2262 Q2263 P2264 Y2267 W2268 C2269 A2270 R2271 N2272 M2273 S2274 F2275 W2276 S2277 S2278 I2279 S2280 F2281 N2282 L2283 A2284 V2285 L2286 M2287 N2288 L2289 L2290 V2291
F2294 Y2295 P2296 F2297 K2298 G2299 V2300 R2301 G2302 G2303 T2304 L2305 GLU PRO HIS TRP SER GLY LEU LEU TRP THR ALA MET LEU LEU ILE SER LEU ALA ILE VAL ILE ALA LEU PRO LYS PRO HIS GLY ILE ARG A2335 L2336 I2337 A2338 S2339 T2340 I2341 L2342 R2343 L2344 I2345 F2346 S2347 V2348 G2349 L2350 Q2351 P2352 T2353
L2354 F2355 L2356 L2357 G2358 A2359 F2360 N2361 V2362 C2363 N2364 K2365 I2366 I2367 F2368 L2369 M2370 S2371 F2372 N2375 C2376 G2377 T2378 F2379 T2380 R2381 R2384 A2385 M2386 V2387 L2388 D2389 V2390 E2391 F2392 L2393 Y2394 H2395 L2396 L2397 Y2398 L2399 L2400 I2401 C2402 A2403 M2404 G2405 L2406 F2407 V2408 H2409 E2410 F2411 F2412 Y2413 S2414 L2415
L2416 L2417 F2418 D2419 L2420 V2421 Y2422 R2423 E2424 E2425 T2426 L2427 L2428 N2429 V2430 I2431 K2432 S2433 V2434 T2435 R2436 N2437 G2438 R2439 P2440 I2441 T2444 L2447 A2448 V2452 Y2453 S2456 L2461 I2468 L2469 E2470 VAL ASP ARG LEU PRO ASN GLU THR ALA GLY PRO GLU THR GLY GLU SER LEU ALA
ASN ASP PHE LEU TYR SER ASP VAL CYS ARG VAL GLU THR GLY GLU ASN CYS THR SER PRO ALA PRO LYS GLU GLU LEU LEU PRO VAL GLU E2519 K2524 E2525 H2526 T2527 C2528 E2529 T2530 L2531 C2534 I2535 V2536 T2537 V2538 L2539 S2540 H2541 G2542 L2543 G2546 G2547 G2548 V2549 G2550 D2551 R2554
K2555 P2556 S2557 K2558 E2559 E2560 P2561 L2562 F2563 R2566 Y2569 D2570 L2571 L2572 F2573 F2574 F2575 M2576 V2577 I2578 I2579 I2580 V2581 L2582 N2583 L2584 I2585 F2586 G2587 V2588 I2589 I2590 D2591 T2592 F2593 A2594 D2595 L2596 R2597 S2598 Q2601 E2605 I2606 L2607 K2608 T2609 T2610 C2611 F2612 I2613 L2616 E2617 R2618 D2619 K2620
F2621 D2622 N2623 K2624 T2625 V2626 T2627 F2628 H2631 I2632 K2633 E2634 E2635 H2636 N2637 M2638 W2639 H2640 Y2641 L2642 C2643 F2644 I2645 V2646 L2647 V2648 K2649 V2650 K2651 D2652 S2653 T2654 E2655 Y2656 T2657 E2660 S2661 Y2662 V2663 A2664 E2665 M2666 I2667 R2670 N2671 L2672 D2673 W2674 R2677 M2678 R2679 A2680 M2681 S2682 L2683 V2684

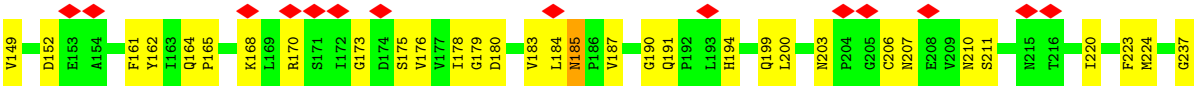


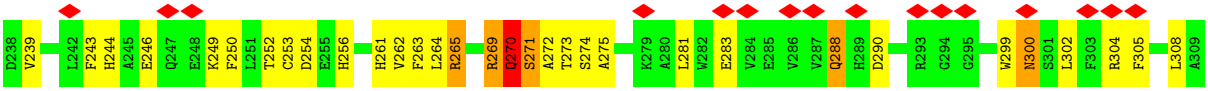
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

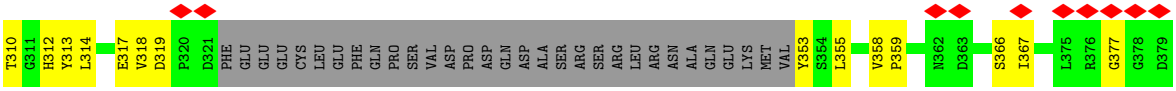
Chain C:

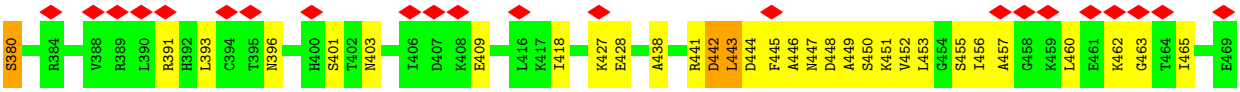


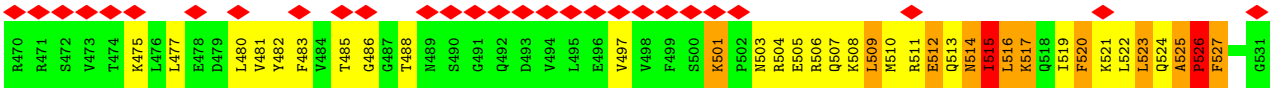


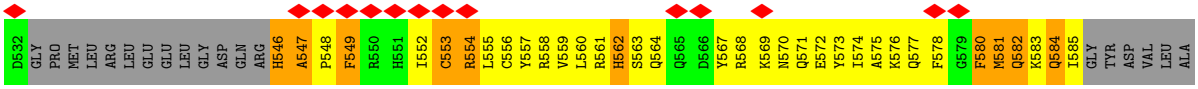


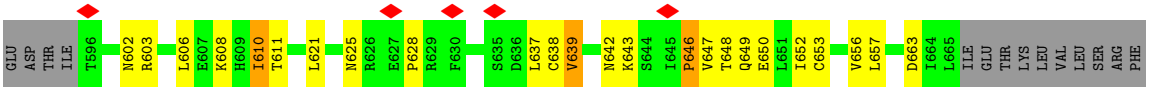


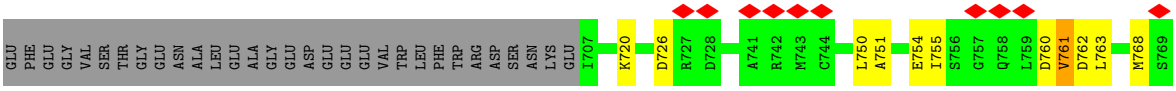


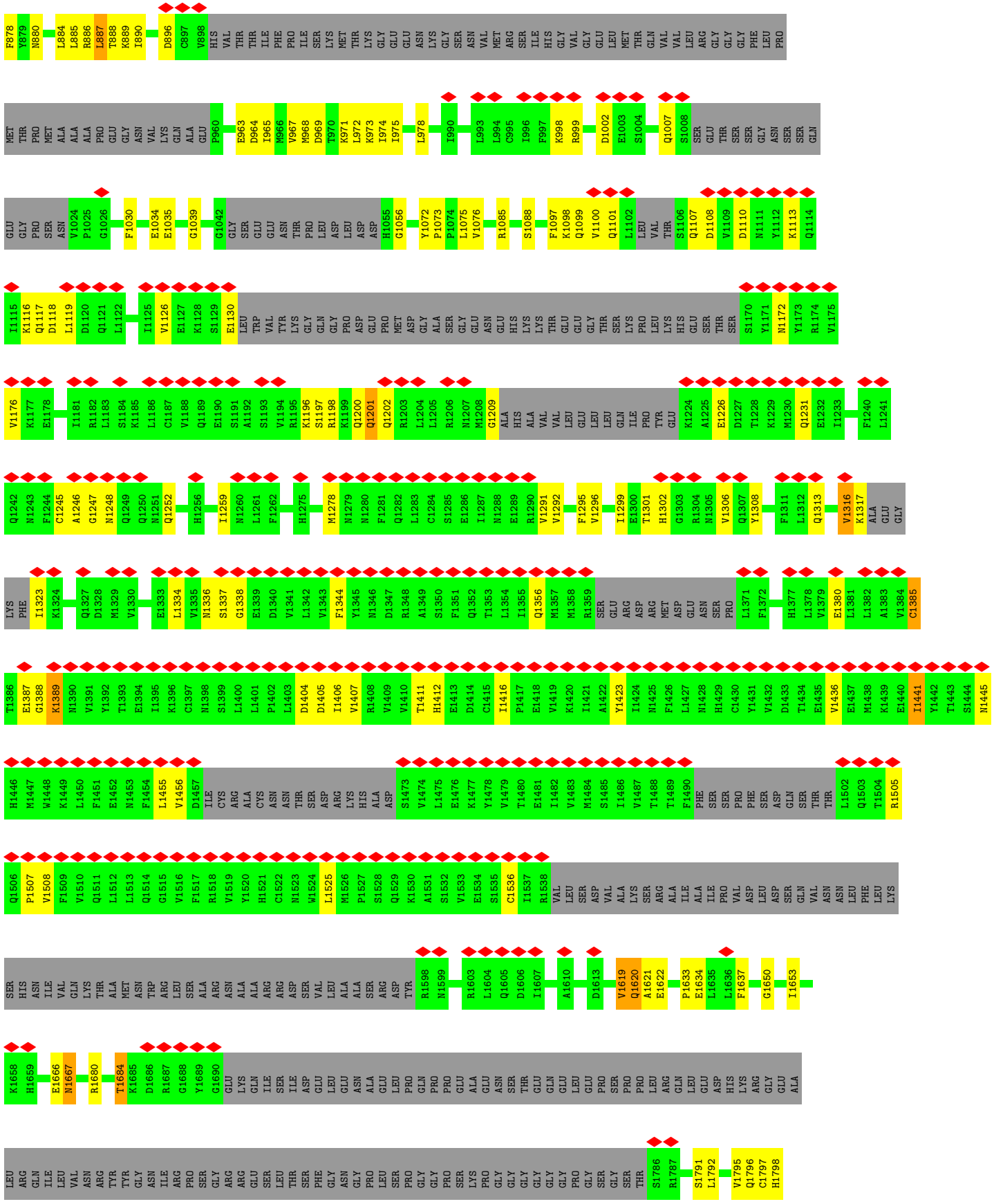








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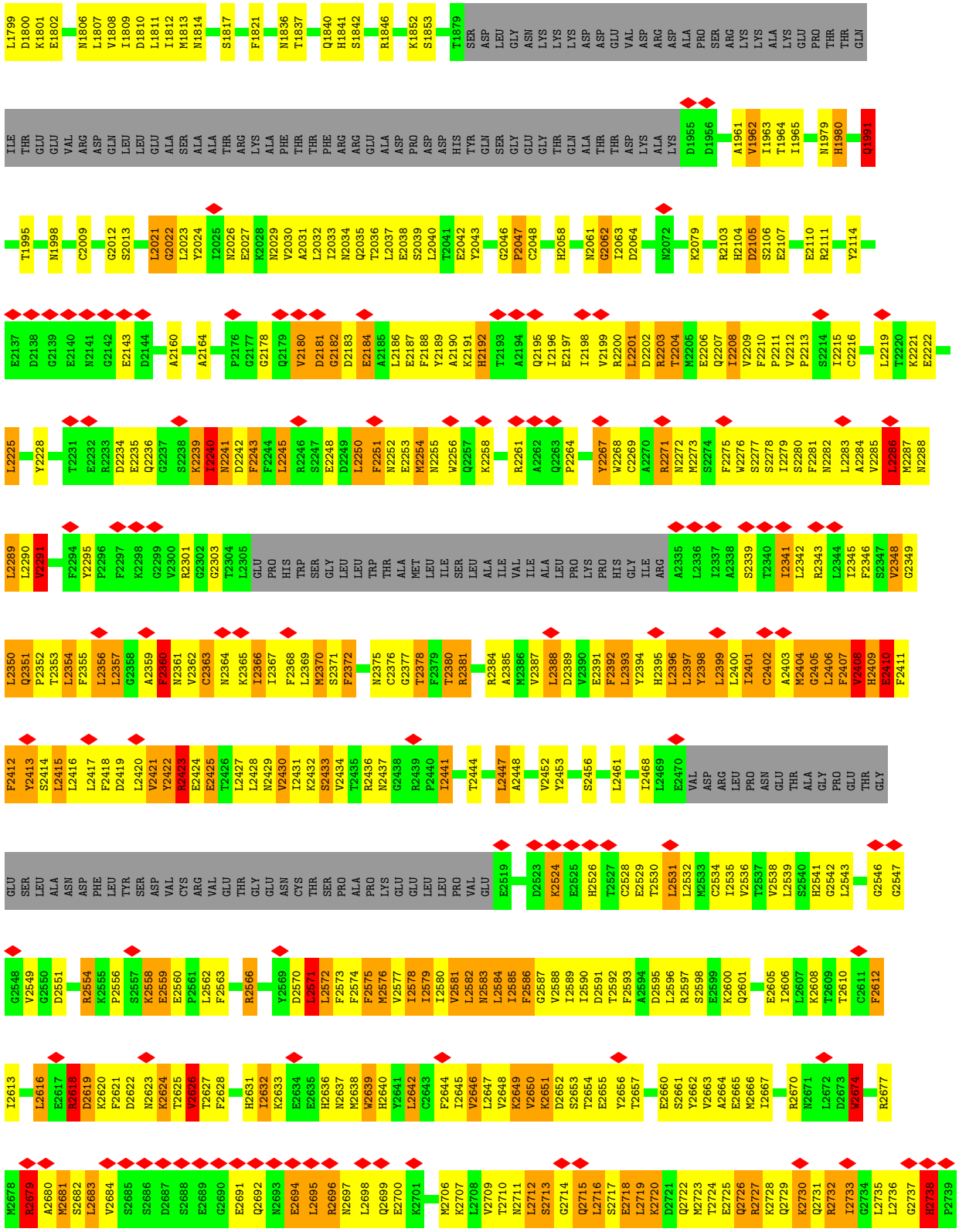
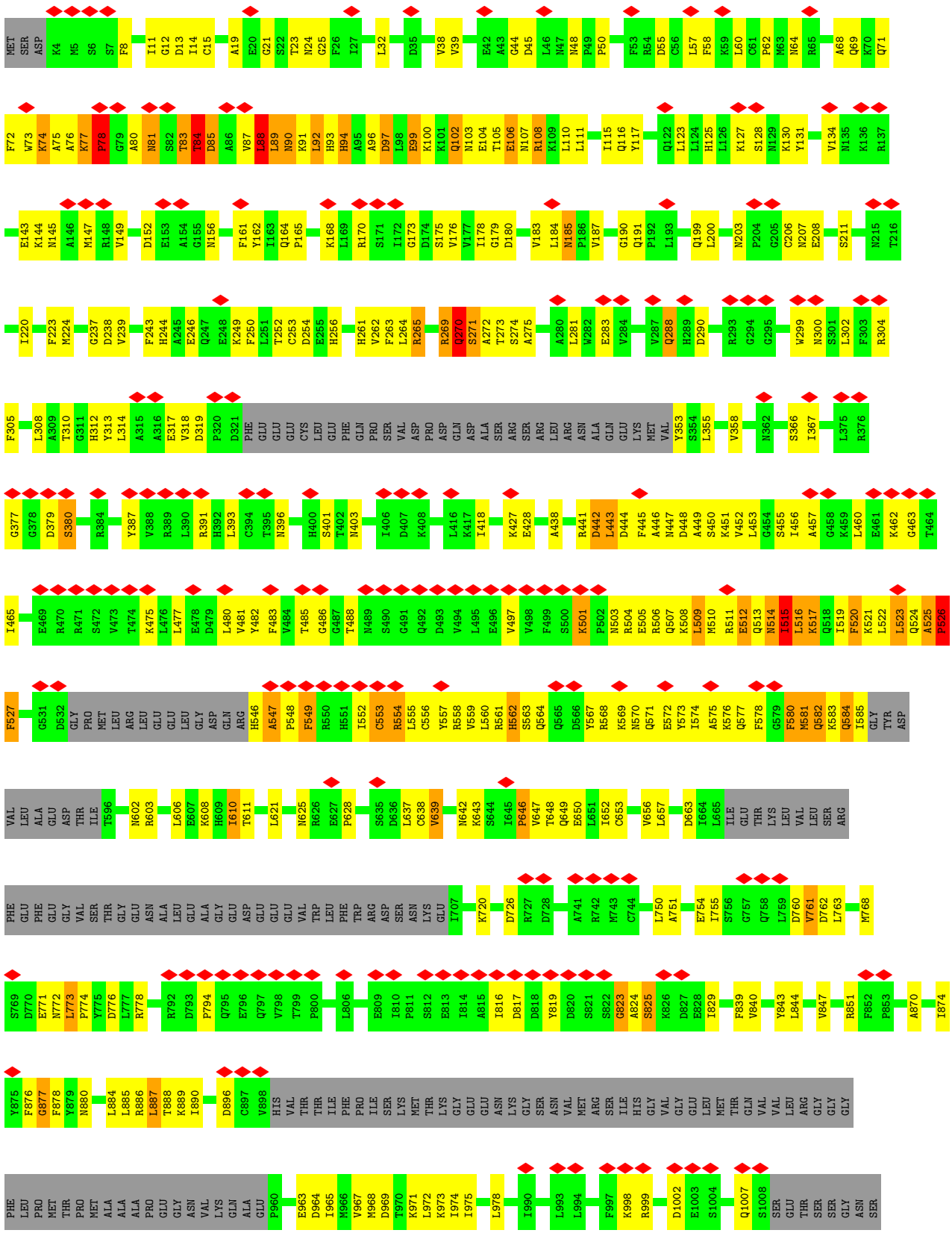
MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E963 D964 I965 M966 V967 M968 D969 T970 K971 L972 K973 I974 I975 L978 I990 L993 L994 C995 I996 F997 K998 R999 D1002 E1003 S1004 Q1007 S1008 SER GLU THR SER SER GLY ASN SER SER GLN
GLU GLY PRO SER ASN V1024 P1025 G1026 F1030 E1034 E1035 G1039 G1042 GLY SER GLU GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 G1056 Y1072 P1073 P1074 L1075 V1076 R1085 S1088 F1097 K1098 Q1099 V1100 Q1101 L1102 LEU VAL THR S1106 Q1107 D1108 V1109 D1110 N1111 Y1112 K1113 Q1114
I1115 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 I1125 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 Y1173 R1174 V1175
V1176 K1177 E1178 I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200 Q1201 Q1202 R1203 L1204 L1205 R1206 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 F1240 L1241
Q1242 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 H1256 I1259 N1260 L1261 F1262 H1275 M1278 N1279 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291 V1292 F1295 V1296 I1299 E1300 T1301 H1302 G1303 R1304 N1305 V1306 Q1307 Y1308 F1311 L1312 Q1313 V1316 K1317 ALA GLU GLY
LYS PHE I1323 K1324 Q1327 D1328 M1329 V1330 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 Y1345 N1346 D1347 R1348 A1349 S1350 F1351 Q1352 T1353 L1354 I1355 Q1356 M1357 M1358 R1359 SER GLU ARG ASP ARG MET ASP GLU ASN SER PRO L1371 F1372 H1377 L1378 V1379 E1380 L1381 L1382 A1383 V1384 C1385
T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 Y1423 I1424 N1425 F1426 L1427 N1428 H1429 C1430 Y1431 V1432 D1433 T1434 E1435 V1436 E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445
H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 PHE SER SER PRO PHE SER ASP GLN SER THR THR L1502 Q1503 T1504 R1505
Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP SER GLN VAL ASN ASN LEU PHE LEU LYS
SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 N1599 R1603 L1604 Q1605 D1606 I1607 A1610 D1613 V1619 Q1620 A1621 E1622 P1633 E1634 L1635 L1636 F1637 G1650 I1653
K1658 H1659 E1666 N1667 R1680 T1684 K1685 D1686 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER PRO PRO LEU ARG GLN LEU GLU ASP HIS LYS ARG GLY GLU ALA
LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY LEU ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY PRO GLY SER GLY SER THR S1786 R1787 S1791 L1792 V1795 Q1796 C1797 H1798



• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain B: 21% 47% 24% 6% • 22%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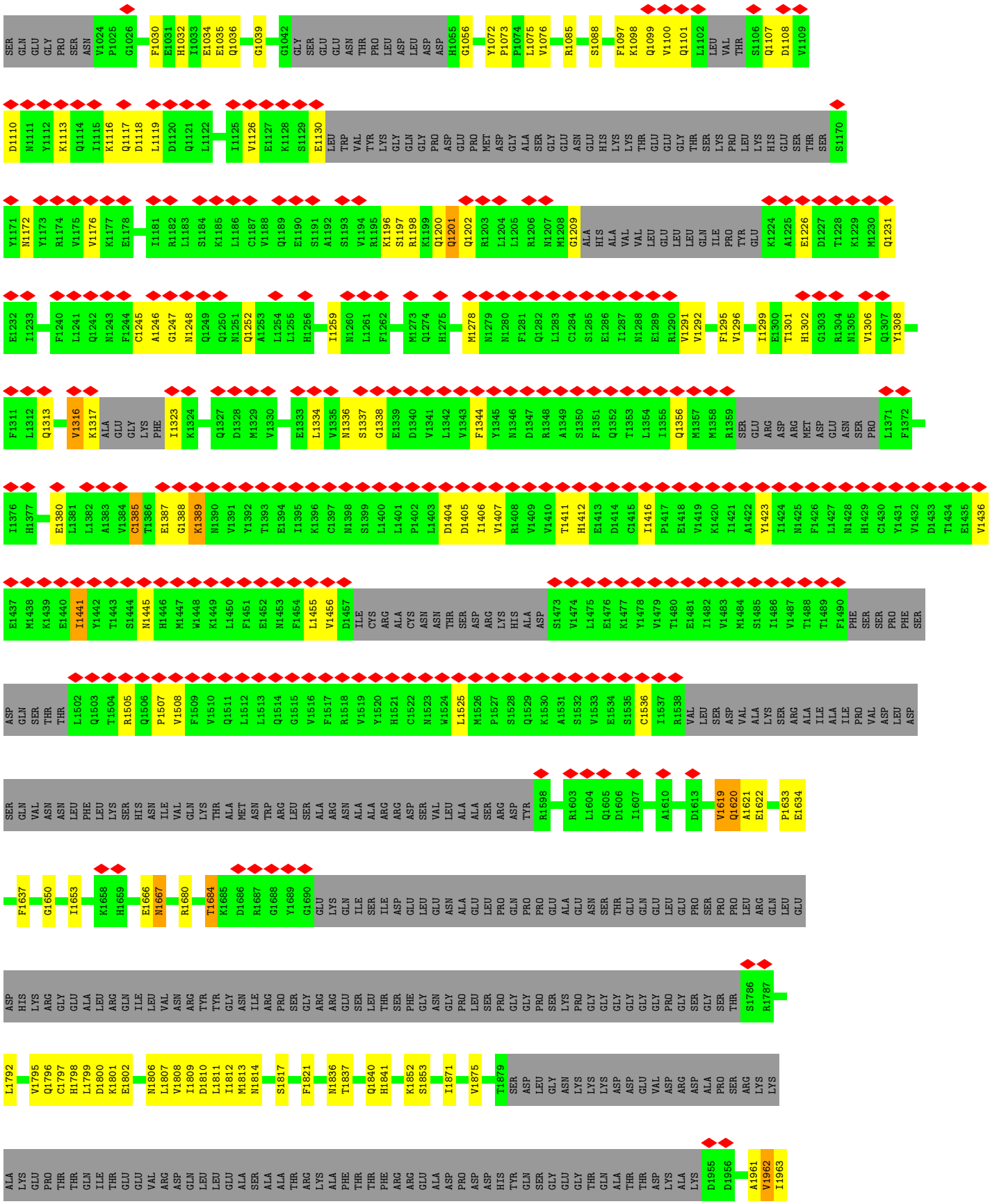
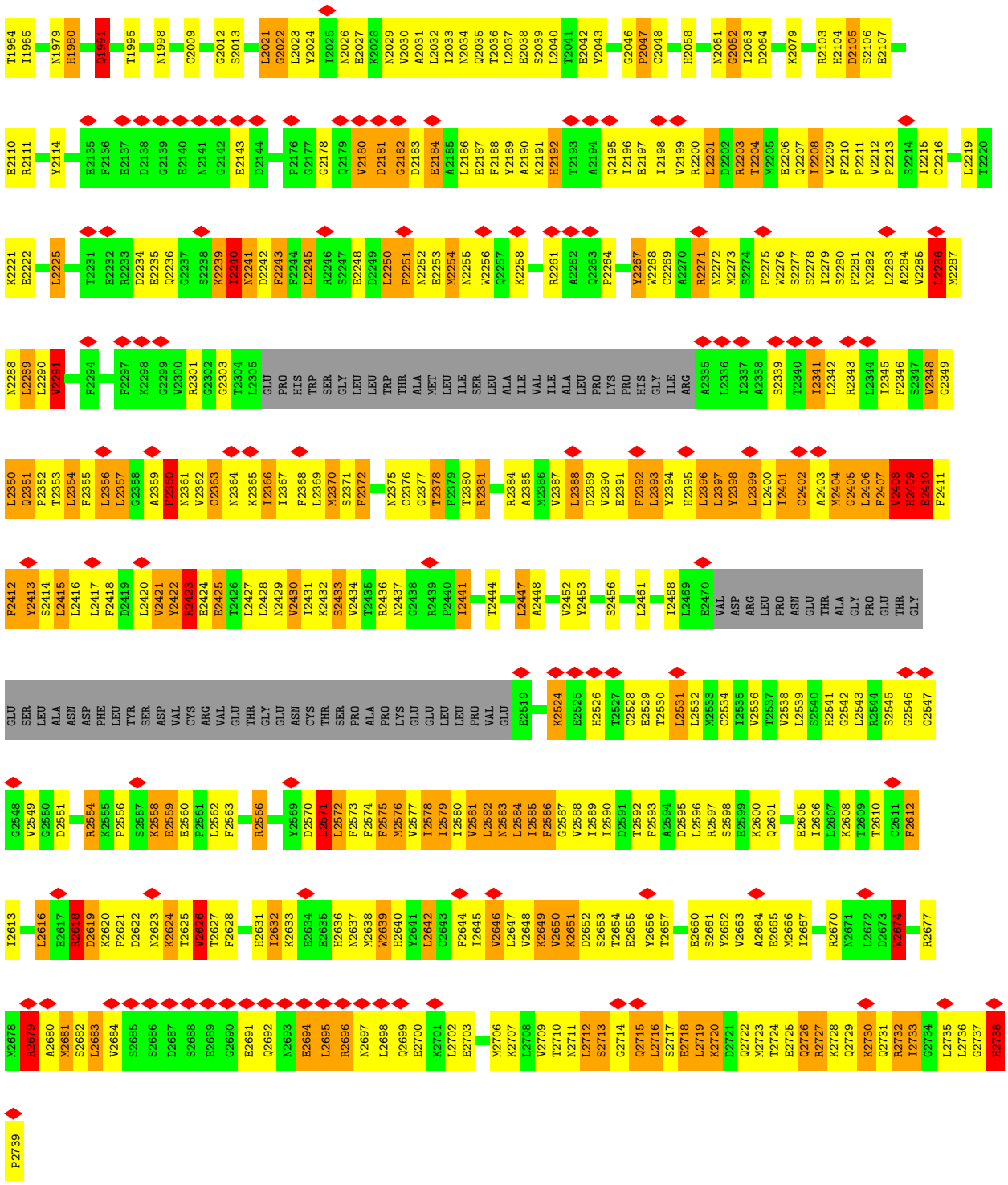
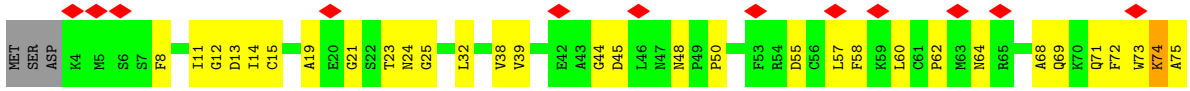
F72 W73 K74 A75 A76 K77 P78 G79 A80 N81 S82 T83 T84 D85 A86 V87 L88 L89 N90 K91 L92 H93 H94 A95 A96 D97 L98 E99 K100 K101 Q102 N103 E104 T105 E106 N107 R108 K109 L110 L111 I115 Q116 Y117 Q122 L123 L124 H125 L126 K127 S128 N129 K130 Y131 V134 N135 K136 R137
E143 K144 N145 A146 M147 R148 V149 D152 E153 A154 G155 N156 F161 Y162 I163 Q164 P165 K168 L169 R170 S171 I172 G173 D174 S175 V176 V177 I178 G179 D180 V183 L184 N185 P186 V187 G190 Q191 P192 L193 Q199 L200 N203 P204 G205 C206 N207 E208 S211 N215 T216
I220 F223 M224 G237 D238 V239 F243 H244 A245 E246 Q247 E248 K249 F250 L251 T252 C253 D254 E255 H256 H261 V262 F263 L264 R265 R269 Q270 S271 A272 T273 S274 A275 A280 L281 W282 E283 V284 V287 Q288 H289 D290 R293 G294 G295 W299 N300 S301 L302 F303 R304
F305 L308 A309 T310 G311 H312 Y313 L314 A315 A316 E317 V318 D319 P320 D321 PHE GLU GLU GLU CYS LEU GLU PHE GLN PRO SER VAL ASP PRO ASP GLN ASP ALA SER ARG SER ARG LEU ARG ASN ALA GLN GLU LYS MET VAL Y353 S354 L355 V358 N362 S366 I367 L375 R376
G377 G378 D379 S380 R384 Y387 V388 R389 L390 R391 H392 L393 C394 T395 N396 H400 S401 T402 N403 I406 D407 K408 L416 K417 I418 K427 E428 A438 R441 D442 L443 D444 F445 A446 N447 D448 A449 S450 K451 V452 L453 G454 S455 I456 A457 G458 K459 L460 E461 K462 G463 T464
I465 E469 R470 R471 S472 V473 T474 K475 L476 L477 E478 D479 L480 V481 Y482 F483 V484 T485 G486 G487 T488 N489 S490 G491 Q492 D493 V494 L495 E496 V497 V498 F499 S500 K501 P502 N503 R504 E505 R506 Q507 K508 L509 M510 R511 E512 Q513 N514 I515 L516 K517 Q518 I519 F520 K521 L522 L523 Q524 A525 P526
F527 G531 D532 GLY PRO MET LEU ARG LEU GLU GLU LEU GLY ASP GLN ARG H546 A547 P548 F549 R550 H551 I552 C553 R554 L555 C556 Y557 R558 V559 L560 R561 H562 S563 Q564 Q565 D566 Y567 R568 K569 N570 Q571 E572 Y573 I574 A575 K576 Q577 F578 G579 F580 M581 Q582 K583 Q584 I585 GLY TYR ASP
VAL LEU ALA GLU ASP THR ILE T596 N602 R603 L606 E607 K608 H609 I610 T611 L621 N625 R626 E627 P628 S635 D636 L637 C638 V639 N642 K643 S644 I645 P646 V647 T648 Q649 E650 L651 I652 C653 V656 L657 D663 I664 L665 ILE GLU THR LYS LEU VAL LEU SER ARG
PHE GLU PHE GLU GLY VAL SER THR GLY GLU ASN ALA LEU GLU ALA GLY GLU ASP GLU GLU GLU VAL TRP LEU PHE TRP ARG ASP SER ASN LYS GLU I707 K720 D726 R727 D728 A741 R742 M743 C744 L750 A751 E754 I755 S756 G757 Q758 L759 D760 V761 D762 L763 M768
S769 D770 E771 N772 L773 P774 Y775 D776 L777 R778 R792 D793 P794 Q795 E796 Q797 V798 T799 P800 L806 E809 I810 P811 S812 E813 I814 A815 I816 D817 D818 Y819 D820 S821 S822 G823 A824 S825 K826 D827 E828 I829 F839 V840 Y843 L844 V847 R851 F852 P853 A870 I874
Y875 F876 G877 F878 Y879 N880 L884 L885 R886 L887 T888 K889 I890 D896 C897 V898 HIS VAL THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN VAL VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL VAL LEU ARG GLY GLY GLY
PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E963 D964 I965 M966 V967 M968 D969 T970 K971 L972 K973 I974 I975 L978 I990 L993 L994 F997 K998 R999 D1002 E1003 S1004 Q1007 S1008 SER GLU THR SER SER GLY ASN SER


SER GLN GLU GLY PRO SER ASN V1024 P1025 G1026 F1030 E1031 H1032 I1033 E1034 E1035 Q1036 G1039 G1042 GLY SER GLU GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 G1056 Y1072 P1073 P1074 L1075 V1076 R1085 S1088 F1097 K1098 Q1099 V1100 Q1101 L1102 LEU VAL THR S1106 Q1107 D1108 V1109
D1110 N1111 Y1112 K1113 Q1114 I1115 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 I1125 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170
Y1171 N1172 Y1173 R1174 V1175 V1176 K1177 E1178 I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200 Q1201 Q1202 R1203 L1204 L1205 R1206 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231
E1232 I1233 F1240 L1241 Q1242 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 L1254 L1255 H1256 I1259 N1260 L1261 F1262 M1273 Q1274 H1275 M1278 N1279 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291 V1292 F1295 V1296 I1299 E1300 T1301 H1302 G1303 R1304 N1305 V1306 Q1307 Y1308
F1311 L1312 Q1313 V1316 K1317 ALA GLU GLY LYS PHE I1323 K1324 Q1327 D1328 M1329 V1330 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 Y1345 N1346 D1347 R1348 A1349 S1350 F1351 Q1352 T1353 L1354 I1355 Q1356 M1357 M1358 R1359 SER GLU ARG ASP ARG MET ASP GLU ASN SER PRO L1371 F1372
I1376 H1377 E1380 L1381 L1382 A1383 V1384 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 Y1423 I1424 N1425 F1426 L1427 N1428 H1429 C1430 Y1431 V1432 D1433 T1434 E1435 V1436
E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 I1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 PHE SER SER PRO PHE SER
ASP GLN SER THR THR L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP
SER GLN VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 R1603 L1604 Q1605 D1606 I1607 A1610 D1613 V1619 Q1620 A1621 E1622 P1633 E1634
F1637 G1650 I1653 K1658 H1659 E1666 N1667 R1680 T1684 K1685 D1686 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER PRO PRO LEU SER GLN LEU GLU
ASP HIS LYS ARG GLY GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY PRO GLY SER GLY SER THR S1786 R1787
L1792 V1795 Q1796 C1797 H1798 L1799 D1800 K1801 E1802 N1806 L1807 V1808 I1809 D1810 L1811 I1812 M1813 N1814 S1817 F1821 N1836 T1837 Q1840 H1841 K1852 S1853 I1871 V1875 T1879 SER ASP LEU GLY ASN LYS LYS LYS ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS
ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 A1961 V1962 I1963



• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain D:



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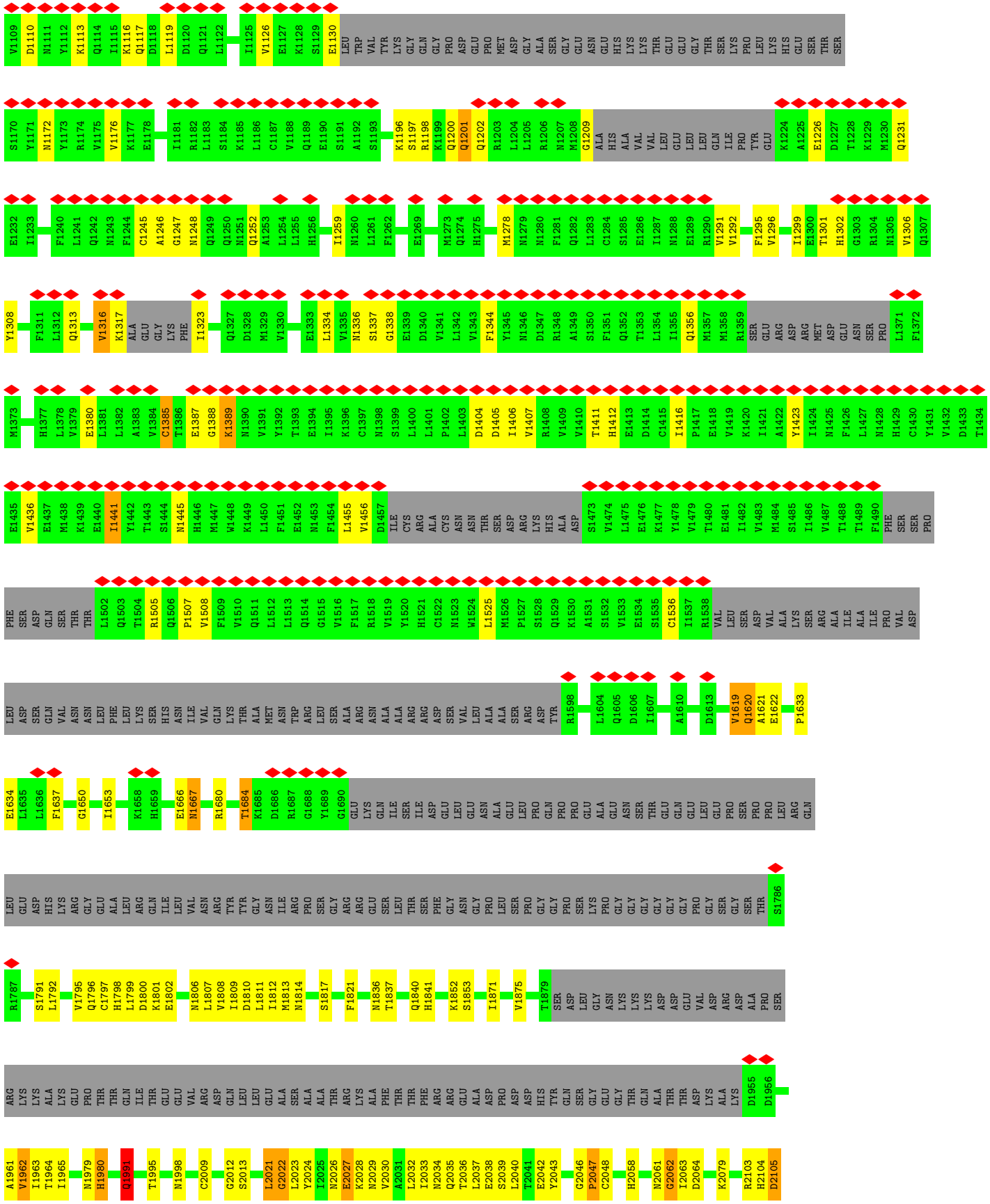
A146 M147 R148 V149 D152 E153 A154 G155 N156 S159 W160 F161 Y162 I163 Q164 P165 K168 L169 R170 S171 I172 G173 D174 S175 V176 V177 I178 G179 D180 V183 L184 N185 P186 V187 G190 Q191 P192 L193 H194 Q199 L200 N203 P204 G205 C206 N207 N210 S211 N215 T216
I220 F223 M224 G237 D238 V239 L242 F243 H244 A245 E246 Q247 E248 K249 F250 L251 T252 C253 D254 E255 H256 H261 V262 F263 L264 R265 R269 Q270 S271 A272 T273 S274 A275 K279 A280 L281 W282 E283 V284 V287 Q288 H289 D290 R293 G294 G295 W299 N300 S301 L302 F303
R304 F305 L308 A309 T310 G311 H312 Y313 L314 A315 A316 E317 V318 D319 P320 D321 PHE GLU GLU GLU CYS LEU GLU PHE GLN PRO SER VAL ASP PRO ASP GLN ASP ALA SER ARG SER ARG LEU ARG ASN ALA GLN GLU LYS MET VAL Y353 S354 L355 V358 N362 D363 S366 I367
L370 R376 G377 G378 D379 S380 R384 V388 R389 L390 R391 H392 L393 C394 T395 N396 H400 S401 T402 N403 I406 D407 K408 L416 K417 I418 K427 E428 A438 R441 D442 L443 D444 F445 A446 N447 D448 A449 S450 K451 V452 L453 G454 S455 I456 A457 G458 K459 L460 E461 K462
G463 T464 I465 E469 R470 R471 S472 V473 T474 K475 L476 L477 E478 D479 L480 V481 Y482 F483 V484 T485 G486 G487 T488 N489 S490 G491 Q492 D493 V494 L495 E496 V497 V498 F499 S500 K501 P502 N503 R504 E505 R506 Q507 K508 L509 M510 R511 E512 Q513 N514 I515 L516 K517 Q518 I519 F520 K521 L522 L523 Q524
A525 P526 F527 G531 D532 GLY PRO MET LEU ARG LEU GLU GLU LEU GLY ASP GLN ARG H546 A547 P548 F549 R550 H551 I552 C553 R554 L555 C556 Y557 R558 V559 L560 R561 H562 S563 Q564 Q565 D566 Y567 R568 K569 N570 Q571 E572 Y573 I574 A575 K576 Q577 F578 G579 F580 M581 Q582 K583 Q584 I585 GLY
TYR ASP VAL LEU ALA GLU ASP THR ILE T596 N602 R603 L606 E607 K608 H609 I610 T611 L621 N625 R626 E627 P628 L637 C638 V639 N642 K643 S644 I645 P646 V647 T648 Q649 E650 L651 I652 C653 V656 L657 D663 I664 L665 ILE GLU THR LYS LEU VAL LEU SER ARG
PHE GLU PHE GLU GLY VAL SER THR GLY GLU ASN ALA LEU GLU ALA GLY GLU ASP GLU GLU GLU VAL TRP LEU PHE TRP ARG ASP SER ASN LYS GLU I707 K720 D726 R727 D728 A741 R742 M743 C744 L750 A751 E754 I755 S756 G757 Q758 L759 D760 V761 D762 L763 M768
S769 D770 E771 N772 L773 P774 Y775 D776 L777 R778 D793 P794 Q795 E796 Q797 V798 T799 P800 A804 E809 S812 E813 I814 A815 I816 D817 D818 Y819 D820 S821 S822 G823 A824 S825 K826 D827 E828 I829 F839 V840 Y843 L844 V847 R851 F852 P853 A870 I874 Y875 F876
G877 F878 Y879 N880 L884 L885 R886 L887 T888 K889 I890 D896 C897 V898 HIS VAL THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL VAL LEU ARG GLY GLY GLY PHE LEU
PRO MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E963 D964 I965 M966 V967 M968 D969 T970 K971 L972 K973 I974 I975 L978 I990 L993 L994 C995 I996 F997 K998 R999 E1000 F1001 D1002 E1003 S1004 Q1007 S1008 SER GLU THR SER SER GLY ASN SER
SER GLN GLU GLY PRO SER ASN V1024 P1025 G1026 F1030 E1031 H1032 I1033 E1034 E1035 Q1036 G1039 G1042 GLY SER GLU GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 G1056 Y1072 P1073 P1074 L1075 V1076 R1085 H1086 F1087 S1088 F1097 K1098 Q1099 V1100 Q1101 L1102 LEU VAL THR S1106 Q1107 D1108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S1170 Y1171 N1172 Y1173 R1174 V1175 V1176 K1177 E1178 I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 K1196 S1197 R1198 K1199 Q1200 Q1201 Q1202 R1203 L1204 L1205 R1206 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231
E1232 I1233 F1240 L1241 Q1242 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 L1254 L1255 H1256 I1259 N1260 L1261 F1262 E1269 M1273 Q1274 H1275 M1278 N1279 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291 V1292 F1295 V1296 I1299 E1300 T1301 H1302 G1303 R1304 N1305 V1306 Q1307
Y1308 F1311 L1312 Q1313 V1316 K1317 ALA GLU GLY LYS PHE I1323 Q1327 D1328 M1329 V1330 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 Y1345 N1346 D1347 R1348 A1349 S1350 F1351 Q1352 T1353 L1354 I1355 Q1356 M1357 M1358 R1359 SER GLU ARG ASP ARG MET ASP GLU ASN SER PRO L1371 F1372
M1373 H1377 L1378 V1379 E1380 L1381 L1382 A1383 V1384 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 Y1423 I1424 N1425 F1426 L1427 N1428 H1429 C1430 Y1431 V1432 D1433 T1434
E1435 V1436 E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 PHE SER SER PRO
PHE SER ASP GLN SER THR THR L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP
LEU ASP SER GLN VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 L1604 Q1605 D1606 I1607 A1610 D1613 V1619 Q1620 A1621 E1622 P1633
E1634 L1635 L1636 F1637 G1650 I1653 K1658 H1659 E1666 N1667 R1680 T1684 K1685 D1686 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER PRO PRO LEU ARG GLN
LEU GLU ASP HIS LYS ARG GLY GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG GLU ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY PRO GLY SER GLY SER THR S1786
R1787 S1791 L1792 V1795 Q1796 C1797 H1798 L1799 D1800 K1801 E1802 N1806 L1807 V1808 I1809 D1810 L1811 I1812 M1813 N1814 S1817 F1821 N1836 T1837 Q1840 H1841 K1852 S1853 I1871 V1875 T1879 SER ASP LEU GLY ASN LYS LYS LYS ASP ASP GLU VAL ASP ARG ASP ALA PRO SER
ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1965 D1966
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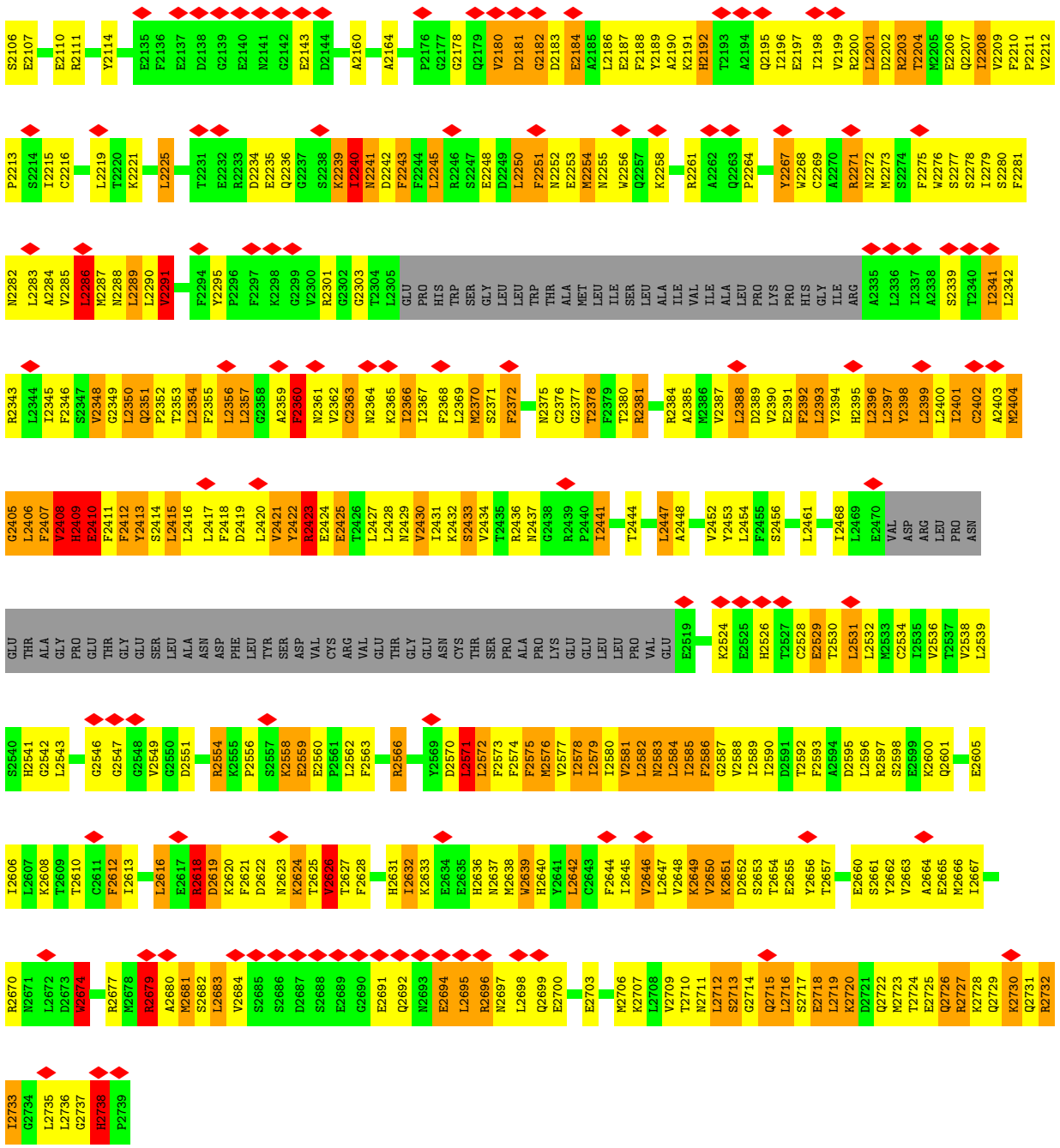
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P2213 S2214 I2215 C2216 L2219 T2220 K2221 L2225 T2231 E2232 R2233 D2234 E2235 Q2236 G2237 S2238 K2239 I2240 N2241 D2242 F2243 F2244 L2245 R2246 S2247 E2248 D2249 L2250 F2251 N2252 E2253 N2254 N2255 W2256 Q2257 K2258 R2261 A2262 Q2263 P2264 Y2267 W2268 C2269 A2270 R2271 N2272 M2273 S2274 F2275 W2276 S2277 S2278 I2279 S2280 F2281
N2282 L2283 A2284 V2285 L2286 M2287 N2288 L2289 L2290 V2291 F2294 Y2295 P2296 F2297 K2298 G2299 V2300 R2301 G2302 G2303 T2304 L2305 GLU PRO HIS TRP SER GLY LEU LEU TRP THR ALA MET LEU ILE SER LEU ALA ILE VAL ILE ALA LEU PRO LYS PRO HIS GLY ILE ARG A2335 L2336 I2337 A2338 S2339 T2340 I2341 L2342
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G2405 L2406 F2407 V2408 H2409 E2410 F2411 F2412 Y2413 S2414 L2415 L2416 L2417 F2418 D2419 L2420 V2421 Y2422 R2423 E2424 E2425 T2426 L2427 L2428 N2429 V2430 I2431 K2432 S2433 V2434 T2435 R2436 N2437 G2438 R2439 P2440 I2441 T2444 L2447 A2448 V2452 Y2453 L2454 F2455 S2456 L2461 I2468 L2469 E2470 VAL ASP ARG LEU PRO ASN
GLU THR ALA GLY PRO GLU THR GLY GLU SER LEU ALA ASN ASP PHE LEU TYR SER ASP VAL CYS ARG VAL GLU THR GLY GLU ASN CYS THR SER PRO ALA PRO LYS GLU GLU LEU LEU PRO VAL GLU E2519 K2524 E2525 H2526 T2527 C2528 E2529 T2530 L2531 L2532 M2533 C2534 I2535 V2536 T2537 V2538 L2539
S2540 H2541 G2542 L2543 G2546 G2547 G2548 V2549 G2550 D2551 R2554 K2555 P2556 S2557 K2558 E2559 E2560 P2561 L2562 F2563 R2566 Y2569 D2570 L2571 L2572 F2573 F2574 F2575 M2576 V2577 I2578 I2579 I2580 V2581 L2582 N2583 L2584 I2585 F2586 G2587 V2588 I2589 I2590 D2591 T2592 F2593 A2594 D2595 L2596 R2597 S2598 E2599 K2600 Q2601 E2605
I2606 L2607 K2608 T2609 T2610 C2611 F2612 I2613 L2616 E2617 R2618 D2619 K2620 F2621 D2622 N2623 K2624 T2625 V2626 T2627 F2628 H2631 I2632 K2633 E2634 E2635 H2636 N2637 M2638 W2639 H2640 Y2641 L2642 C2643 F2644 I2645 V2646 L2647 V2648 K2649 V2650 K2651 D2652 S2653 T2654 E2655 Y2656 T2657 E2660 S2661 Y2662 V2663 A2664 E2665 M2666 I2667
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I2733 G2734 L2735 L2736 G2737 H2738 P2739

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	179760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	16.041	Depositor
Minimum map value	-13.204	Depositor
Average map value	0.092	Depositor
Map value standard deviation	0.632	Depositor
Recommended contour level	1.75	Depositor
Map size (Å)	252.0, 252.0, 252.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.26, 1.26, 1.26	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.62	8/12648 (0.1%)	0.99	63/16640 (0.4%)
1	B	0.62	8/12648 (0.1%)	0.99	61/16640 (0.4%)
1	C	0.62	8/12648 (0.1%)	0.99	62/16640 (0.4%)
1	D	0.62	8/12648 (0.1%)	0.99	63/16640 (0.4%)
All	All	0.62	32/50592 (0.1%)	0.99	249/66560 (0.4%)

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	A	0	17
1	B	0	17
1	C	0	17
1	D	0	17
All	All	0	68

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1201	GLN	C-N	10.45	1.58	1.34
1	C	1201	GLN	C-N	10.42	1.58	1.34
1	A	1201	GLN	C-N	10.41	1.58	1.34
1	D	1201	GLN	C-N	10.40	1.57	1.34
1	A	2583	ASN	CB-CG	7.56	1.68	1.51

The worst 5 of 249 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2738	HIS	C-N-CD	11.36	152.25	128.40
1	A	2738	HIS	C-N-CD	11.35	152.24	128.40
1	C	2738	HIS	C-N-CD	11.35	152.23	128.40
1	D	2738	HIS	C-N-CD	11.34	152.21	128.40
1	D	2584	LEU	CA-CB-CG	-11.29	89.33	115.30

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1323	ILE	Mainchain
1	A	319	ASP	Peptide
1	A	501	LYS	Peptide
1	A	514	ASN	Mainchain
1	A	84	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12499	0	8930	1716	0
1	B	12499	0	8931	1719	0
1	C	12499	0	8931	1699	0
1	D	12499	0	8930	1704	0
2	A	42	5	0	26	0
2	B	42	5	0	25	0
2	C	42	5	0	25	0
2	D	42	5	0	26	0
All	All	50164	20	35722	6549	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 76.

The worst 5 of 6549 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:B:2243:PHE:CE1	1:B:2642:LEU:HD11	1.23	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2243:PHE:CE1	1:D:2642:LEU:HD11	1.23	1.63
1:A:2700:GLU:CG	1:B:2702:LEU:HD12	1.17	1.63
1:A:2696:ARG:HH12	1:D:2696:ARG:CZ	1.09	1.62
1:A:275:ALA:HB2	2:A:2801:JYP:C5	1.15	1.62

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	2109/2739 (77%)	1793 (85%)	255 (12%)	61 (3%)	4 32
1	B	2109/2739 (77%)	1793 (85%)	255 (12%)	61 (3%)	4 32
1	C	2109/2739 (77%)	1792 (85%)	256 (12%)	61 (3%)	4 32
1	D	2109/2739 (77%)	1792 (85%)	256 (12%)	61 (3%)	4 32
All	All	8436/10956 (77%)	7170 (85%)	1022 (12%)	244 (3%)	7 32

5 of 244 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	SER
1	A	646	PRO
1	A	663	ASP
1	A	761	VAL
1	A	772	ASN

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	857/2449 (35%)	711 (83%)	146 (17%)	2 13
1	B	857/2449 (35%)	712 (83%)	145 (17%)	2 14
1	C	857/2449 (35%)	712 (83%)	145 (17%)	2 14
1	D	857/2449 (35%)	710 (83%)	147 (17%)	2 12
All	All	3428/9796 (35%)	2845 (83%)	583 (17%)	5 13

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	516	LEU
1	D	2719	LEU
1	D	581	MET
1	D	515	ILE
1	D	2393	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	ASN
1	B	584	GLN
1	D	2722	GLN
1	D	584	GLN
1	B	185	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)

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	$\#\|Z\| > 2$
2	JYP	B	2801	1	41,45,45	1.95	9 (21%)	53,70,70	1.40	4 (7%)
2	JYP	C	2801	1	41,45,45	1.95	9 (21%)	53,70,70	1.40	4 (7%)
2	JYP	A	2801	1	41,45,45	1.95	9 (21%)	53,70,70	1.40	4 (7%)
2	JYP	D	2801	1	41,45,45	1.95	9 (21%)	53,70,70	1.40	4 (7%)

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	JYP	B	2801	1	-	10/23/63/63	0/4/4/4
2	JYP	C	2801	1	-	10/23/63/63	0/4/4/4
2	JYP	A	2801	1	-	10/23/63/63	0/4/4/4
2	JYP	D	2801	1	-	10/23/63/63	0/4/4/4

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2801	JYP	O1-C6	4.81	1.47	1.41
2	A	2801	JYP	O1-C6	4.75	1.47	1.41
2	B	2801	JYP	O1-C6	4.75	1.47	1.41
2	D	2801	JYP	O1-C6	4.74	1.47	1.41
2	D	2801	JYP	P3-O15	4.62	1.68	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2801	JYP	N1-C1-N2	-5.49	120.09	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2801	JYP	N1-C1-N2	-5.49	120.10	128.68
2	A	2801	JYP	N1-C1-N2	-5.49	120.10	128.68
2	C	2801	JYP	N1-C1-N2	-5.48	120.12	128.68
2	D	2801	JYP	C6-N5-C2	-4.98	117.89	126.64

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2801	JYP	C8-C7-O15-P3
2	A	2801	JYP	C13-O10-P2-O13
2	C	2801	JYP	C8-C7-O15-P3
2	C	2801	JYP	C13-O10-P2-O13
2	B	2801	JYP	C8-C7-O15-P3

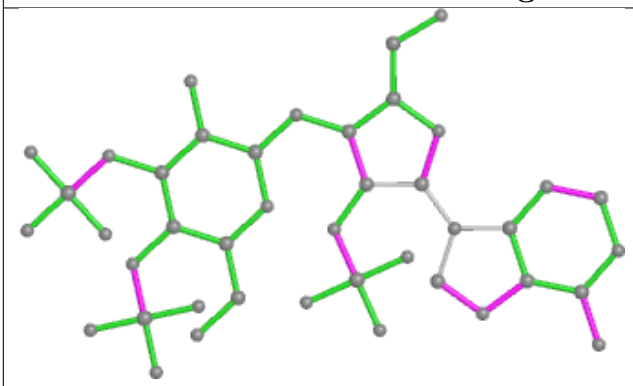
There are no ring outliers.

4 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2801	JYP	25	0
2	C	2801	JYP	25	0
2	A	2801	JYP	26	0
2	D	2801	JYP	26	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.

Ligand JYP B 2801



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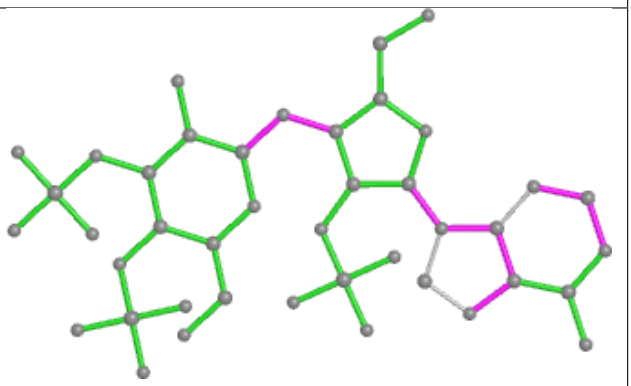
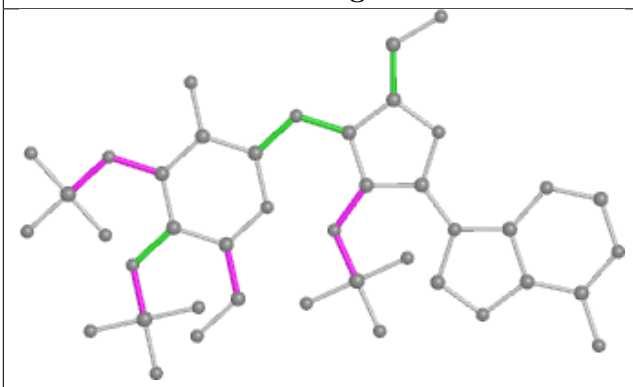
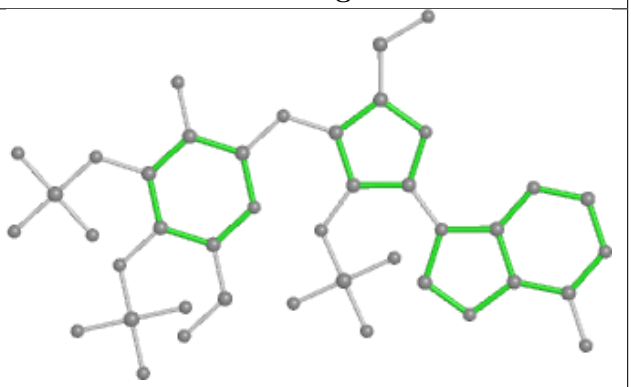


Bond angles

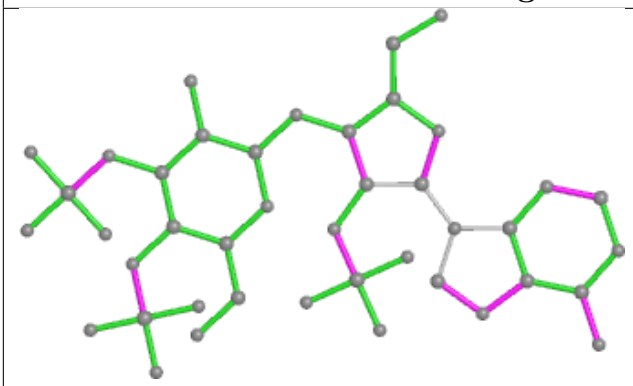


Torsions



Rings

Ligand JYP C 2801



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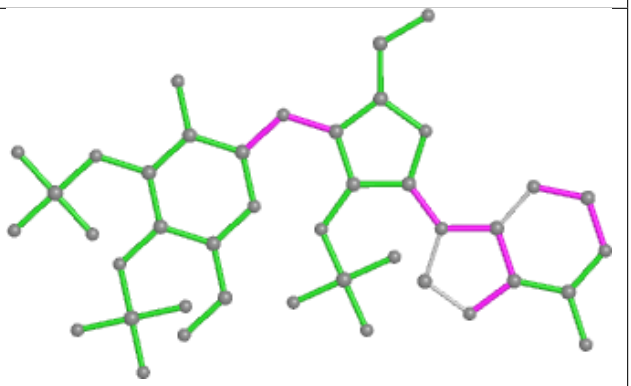
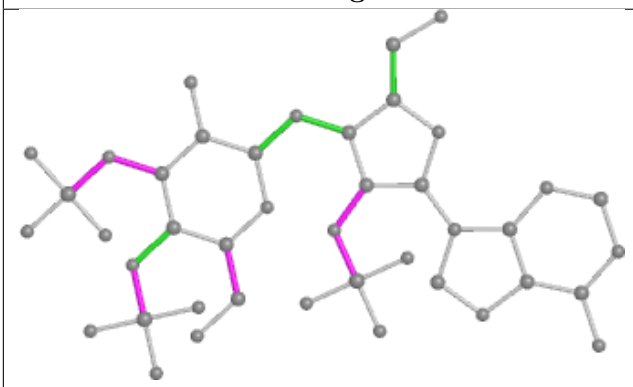
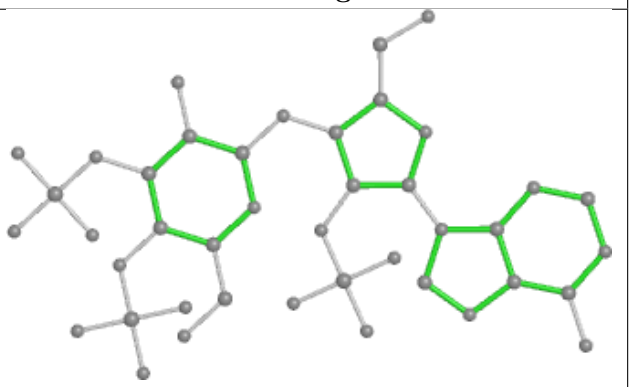


Bond angles

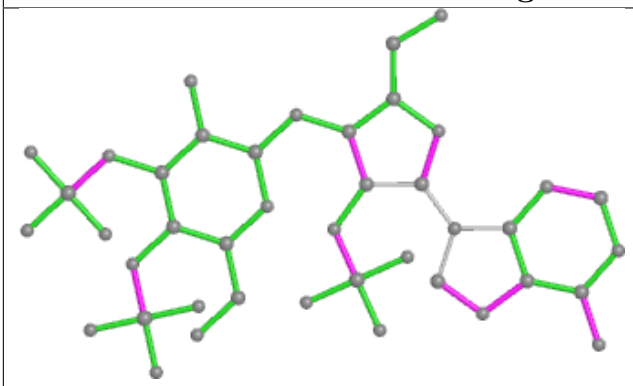


Torsions

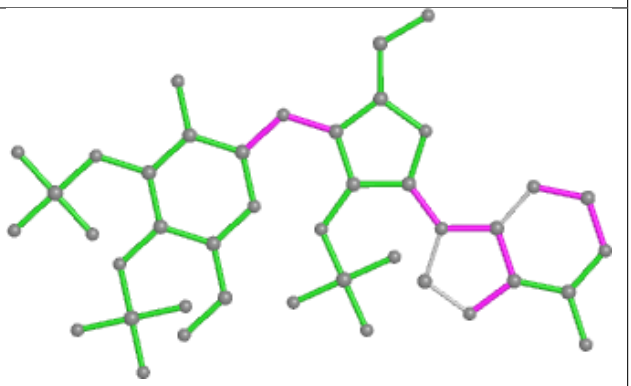


Rings

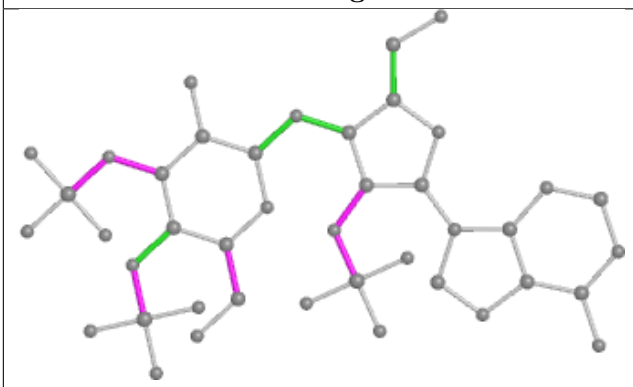
Ligand JYP A 2801



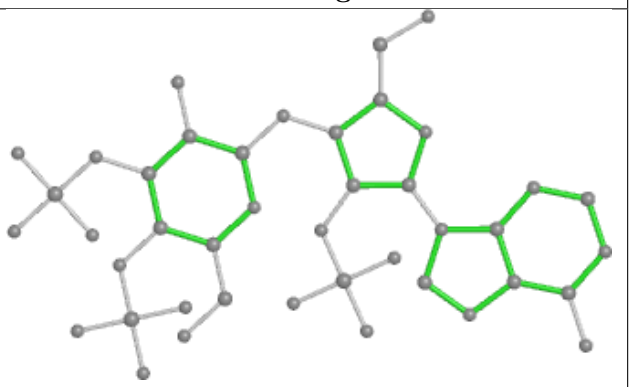
Bond lengths



Bond angles

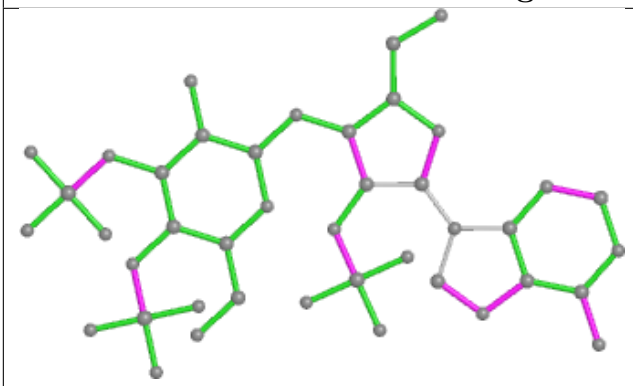


Torsions

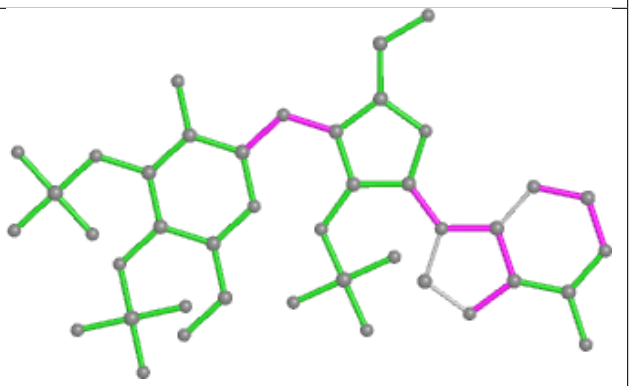


Rings

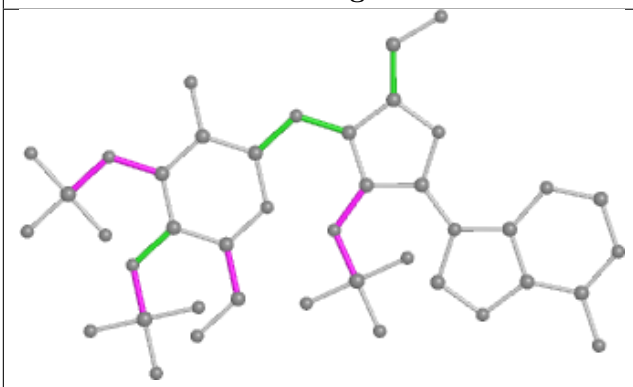
Ligand JYP D 2801



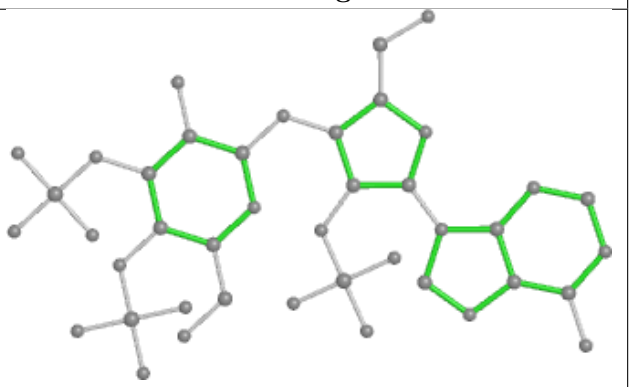
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

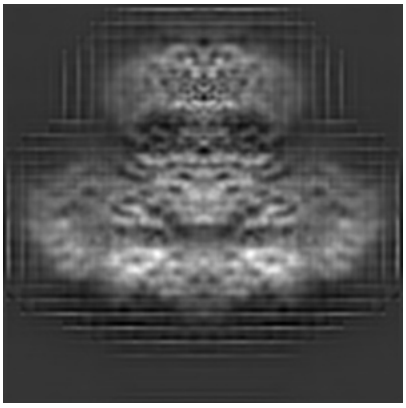
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9243. These allow visual inspection of the internal detail of the map and identification of artifacts.

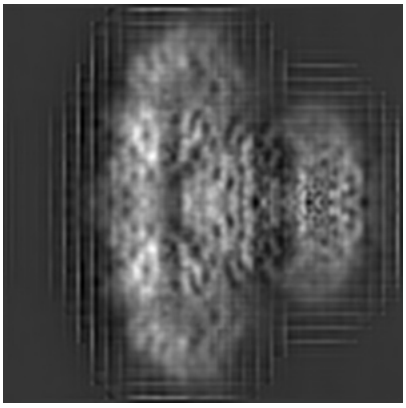
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

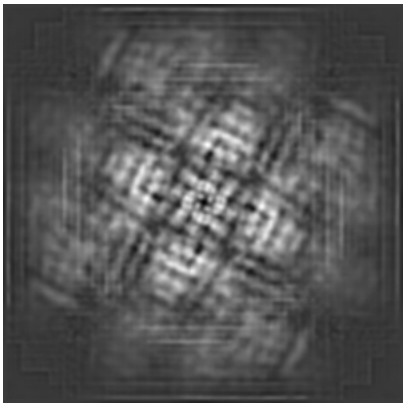
6.1.1 Primary map



X



Y

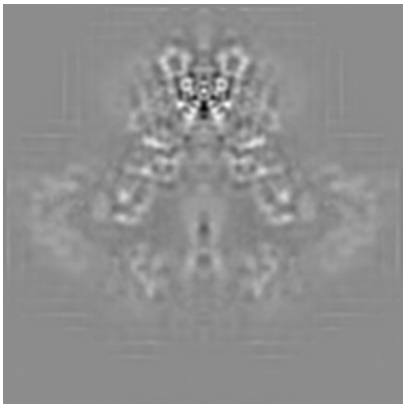


Z

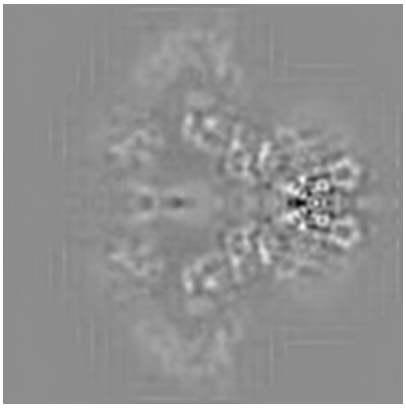
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

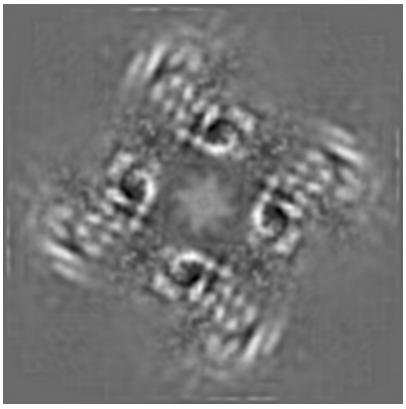
6.2.1 Primary map



X Index: 100



Y Index: 100

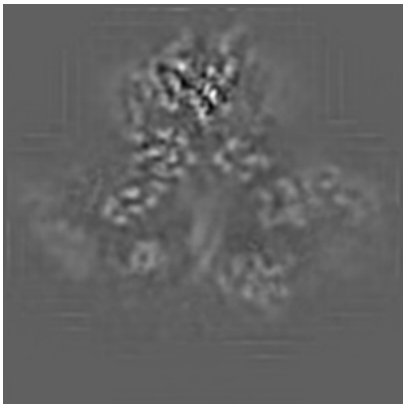


Z Index: 100

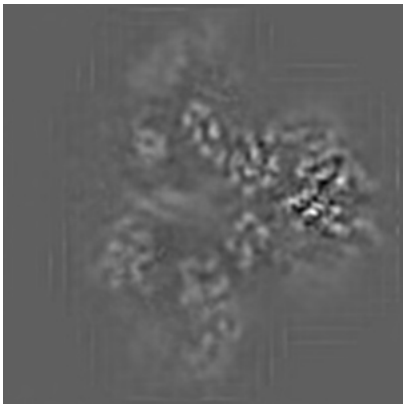
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

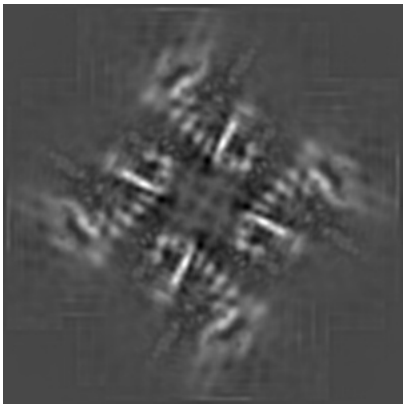
6.3.1 Primary map



X Index: 94



Y Index: 94



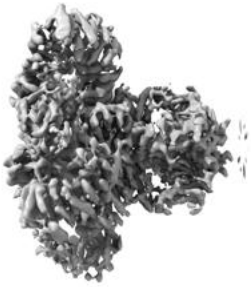
Z Index: 109

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 1.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

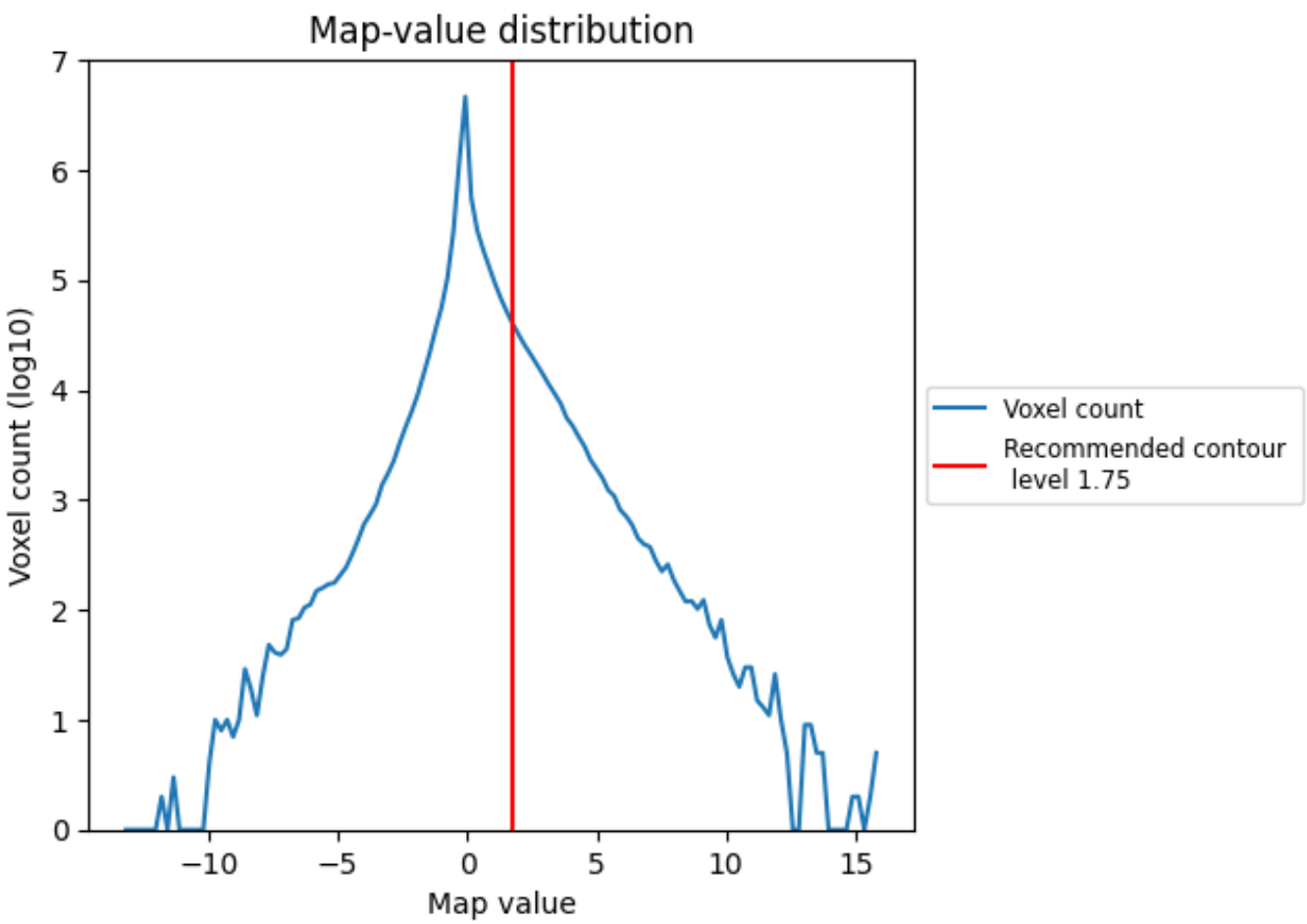
6.5 Mask visualisation (i)

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

7 Map analysis (i)

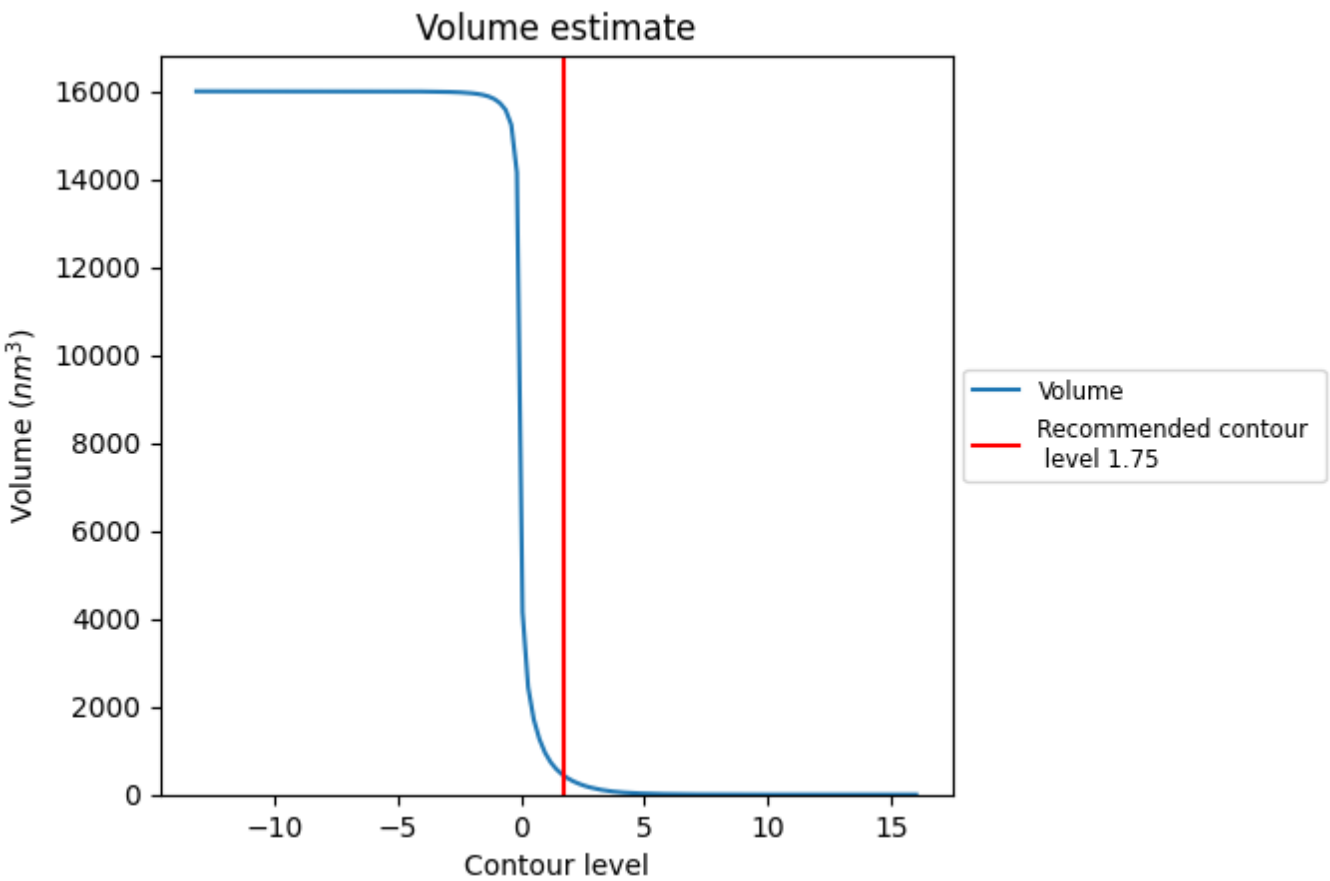
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

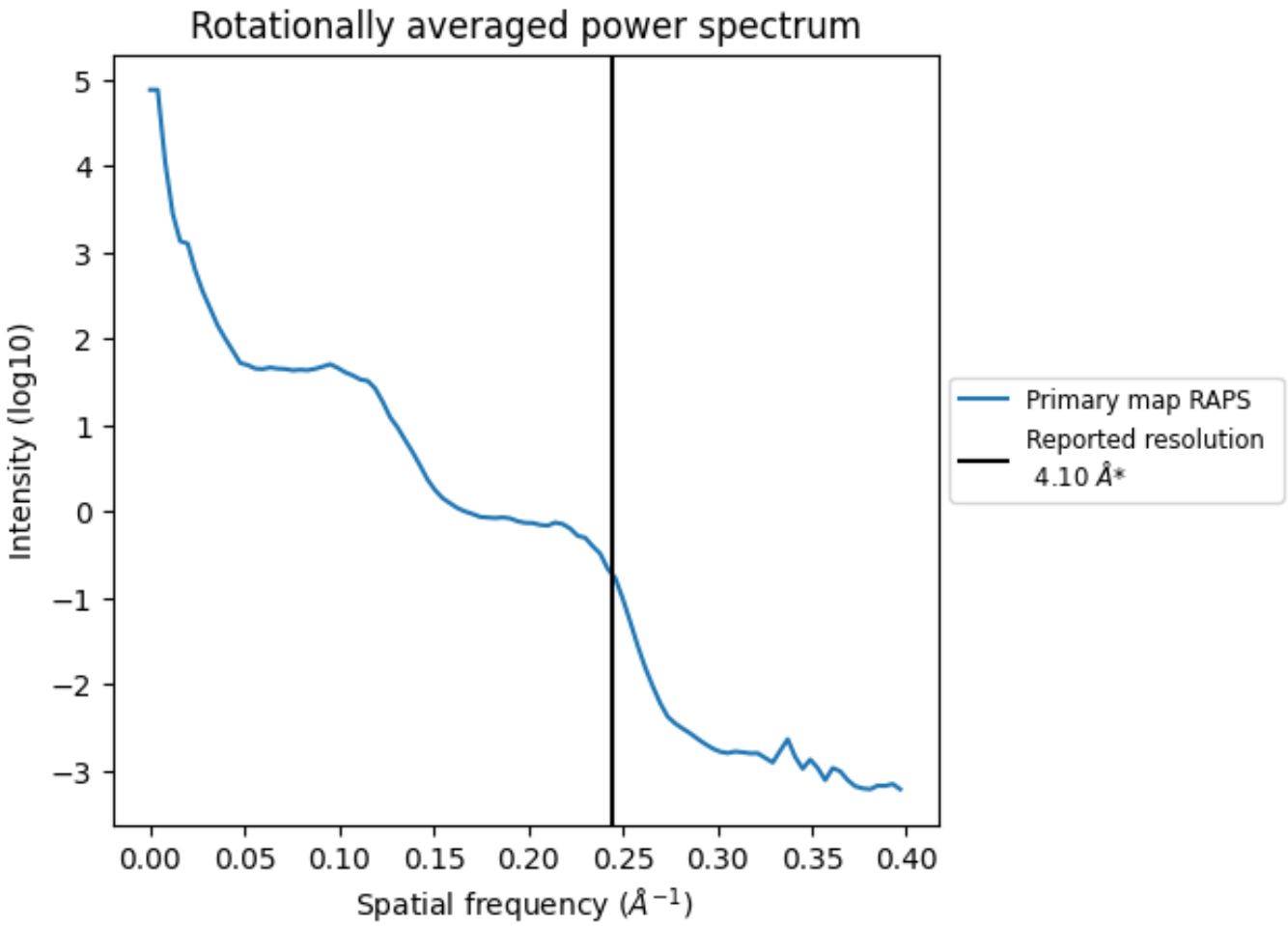
7.2 Volume estimate (i)



The volume at the recommended contour level is 423 nm^3; this corresponds to an approximate mass of 382 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 0.244 Å^{-1}

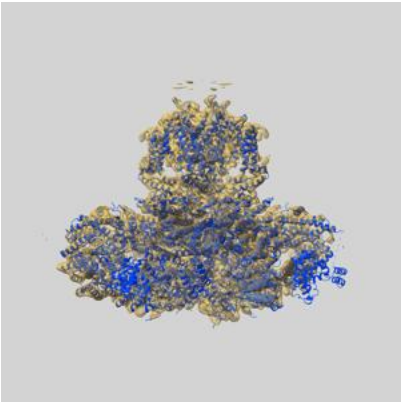
8 Fourier-Shell correlation (i)

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

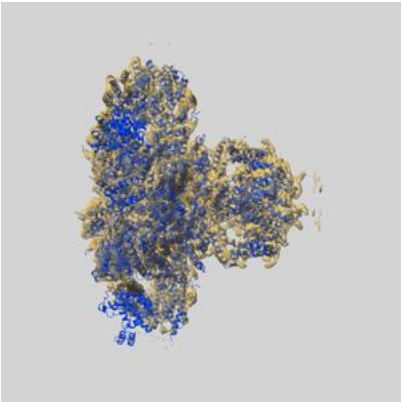
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9243 and PDB model 6MU1. Per-residue inclusion information can be found in section 3 on page 6.

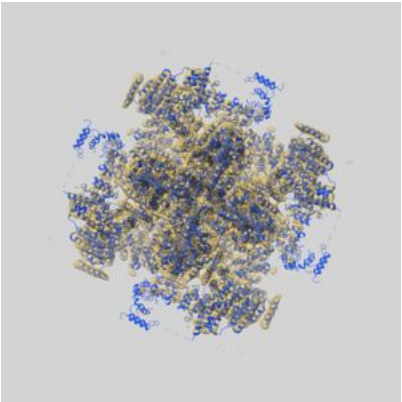
9.1 Map-model overlay (i)



X



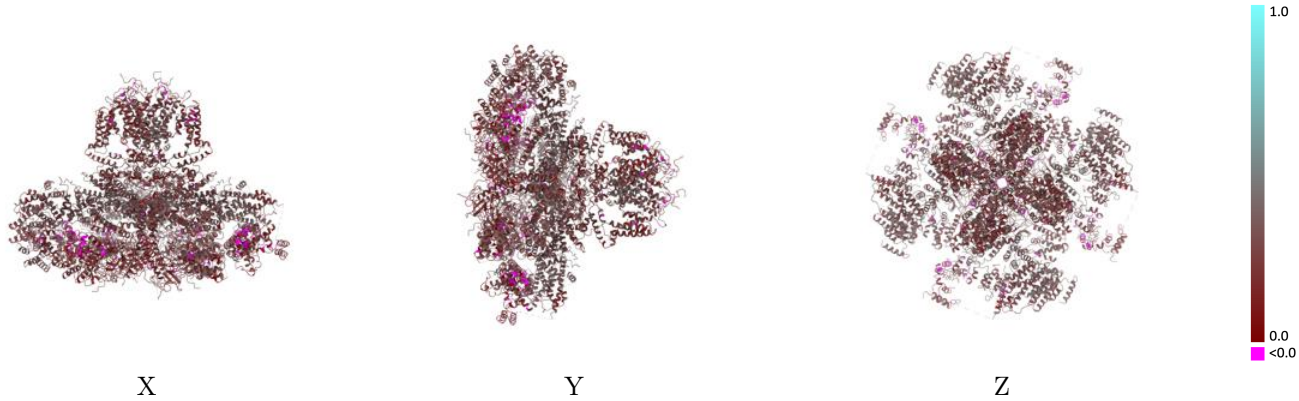
Y



Z

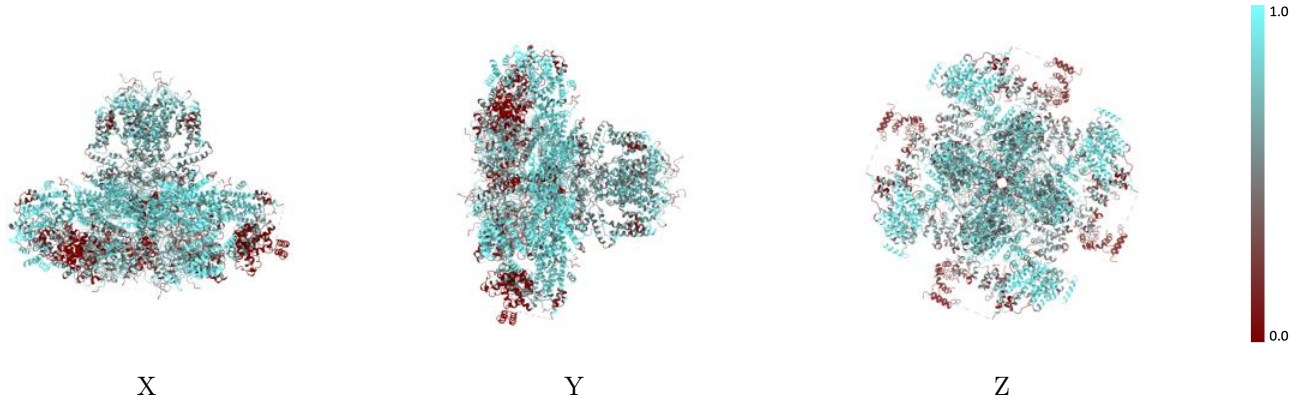
The images above show the 3D surface view of the map at the recommended contour level 1.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



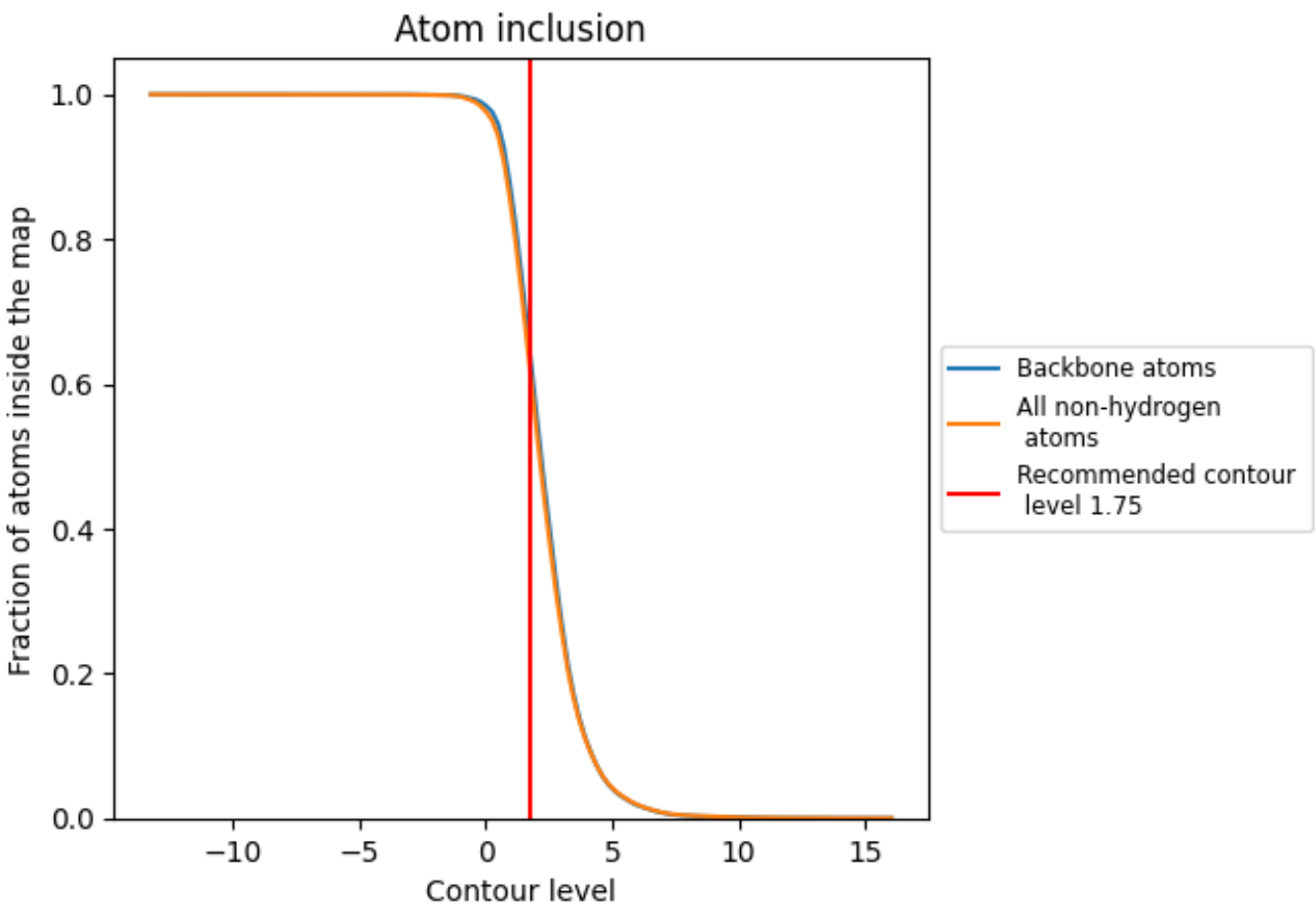
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (1.75).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6226	0.2630
A	0.6275	0.2640
B	0.6250	0.2610
C	0.6244	0.2630
D	0.6263	0.2640