# wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 10:51 PM EST

| | | |
|---|---|---|
| PDB ID | : | 6DR0 |
| EMDB ID | : | EMD-7987 |
| Title | : | Class 5 IP3-bound human type 3 1,4,5-inositol trisphosphate receptor |
| Authors | : | Hite, R.K.; Paknejad, N. |
| Deposited on | : | 2018-06-11 |
| Resolution | : | 4.47 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:

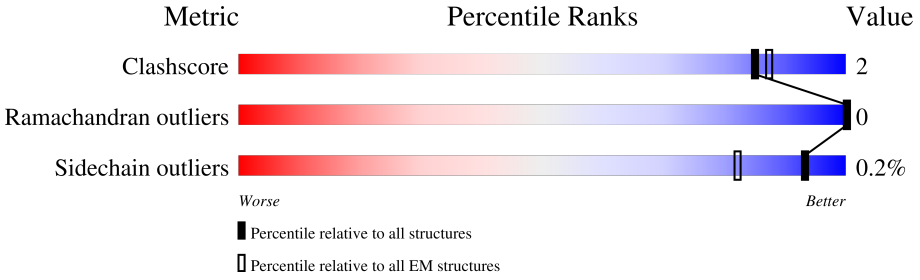
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| 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 4.47 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 | 2671 | 31% 76% 6% 18% |
| 1 | B | 2671 | 39% 76% 6% 18% |
| 1 | C | 2671 | 51% 76% 6% 18% |
| 1 | D | 2671 | 45% 76% 5% 18% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 140024 atoms, of which 70049 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.

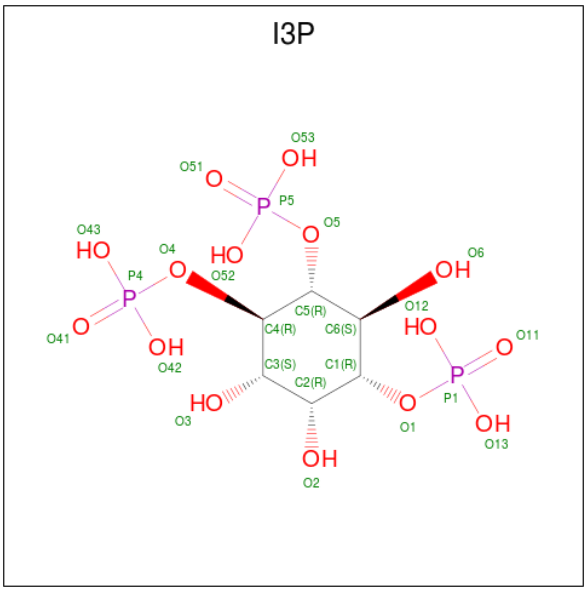
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | A | 2188 | 35063 | 11176 | 17553 | 3000 | 3228 | 106 | 0 | 0 |
| 1 | B | 2188 | 35065 | 11176 | 17555 | 3000 | 3228 | 106 | 0 | 0 |
| 1 | C | 2193 | 35140 | 11199 | 17593 | 3006 | 3236 | 106 | 0 | 0 |
| 1 | D | 2181 | 34620 | 11035 | 17312 | 2979 | 3191 | 103 | 0 | 0 |

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 2 | A | 1 | 1 | 1 | 0 |
| 2 | B | 1 | 1 | 1 | 0 |
| 2 | C | 1 | 1 | 1 | 0 |
| 2 | D | 1 | 1 | 1 | 0 |

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).



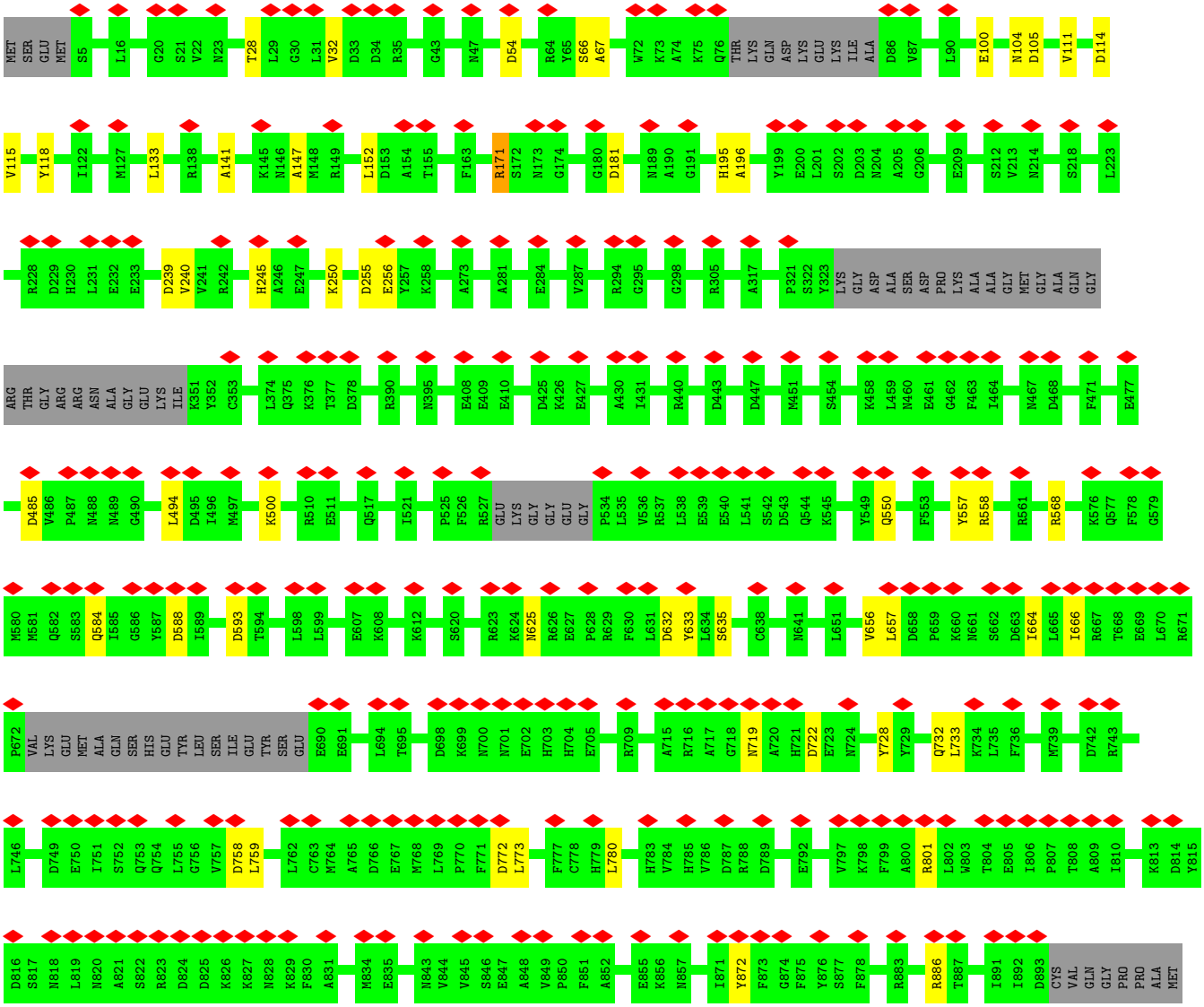

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | H | O | P | 0 |
| | | | 33 | 6 | 9 | 15 | 3 | |
| 3 | B | 1 | Total | C | H | O | P | 0 |
| | | | 33 | 6 | 9 | 15 | 3 | |
| 3 | C | 1 | Total | C | H | O | P | 0 |
| | | | 33 | 6 | 9 | 15 | 3 | |
| 3 | D | 1 | Total | C | H | O | P | 0 |
| | | | 33 | 6 | 9 | 15 | 3 | |

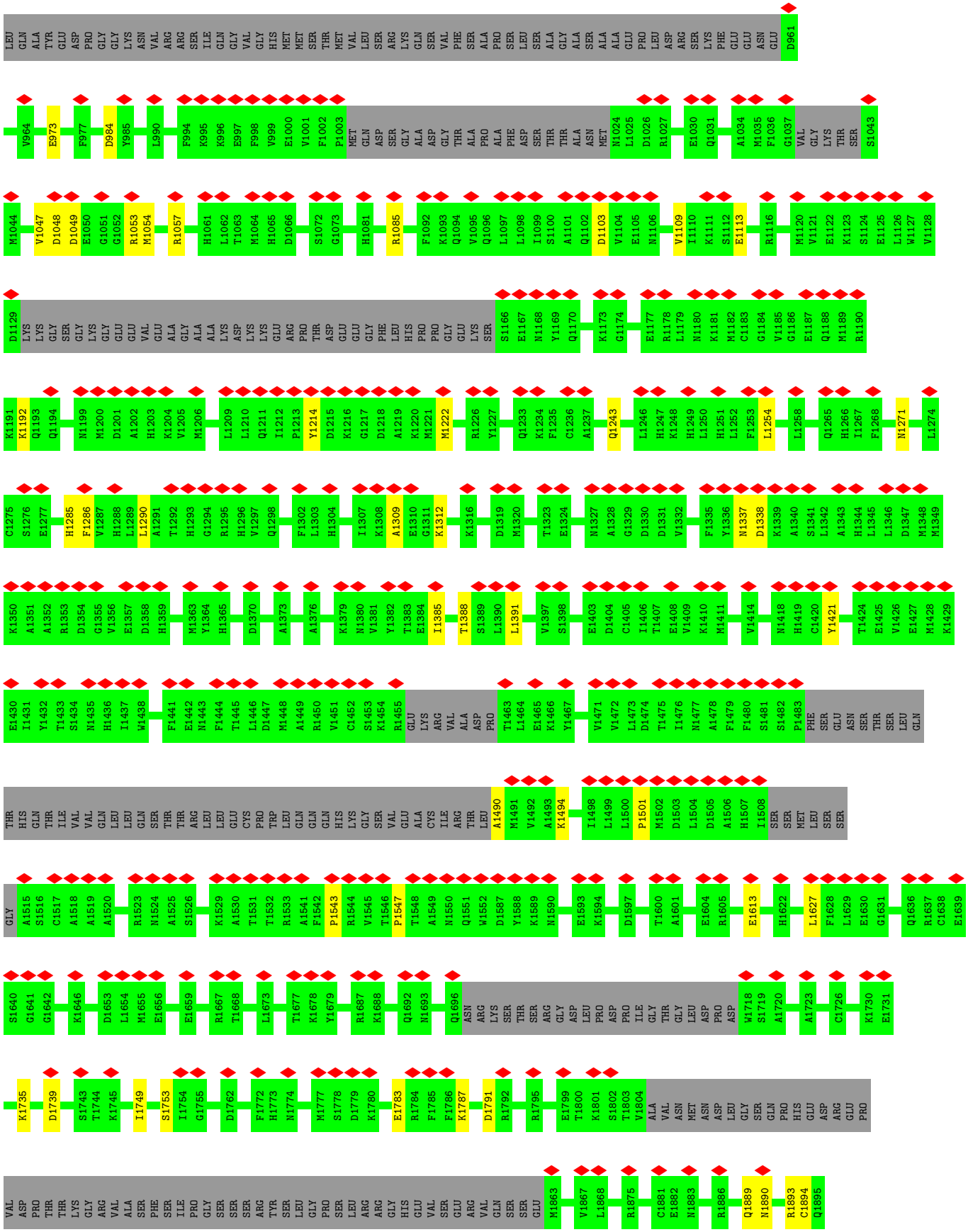
# 3 Residue-property plots (i)

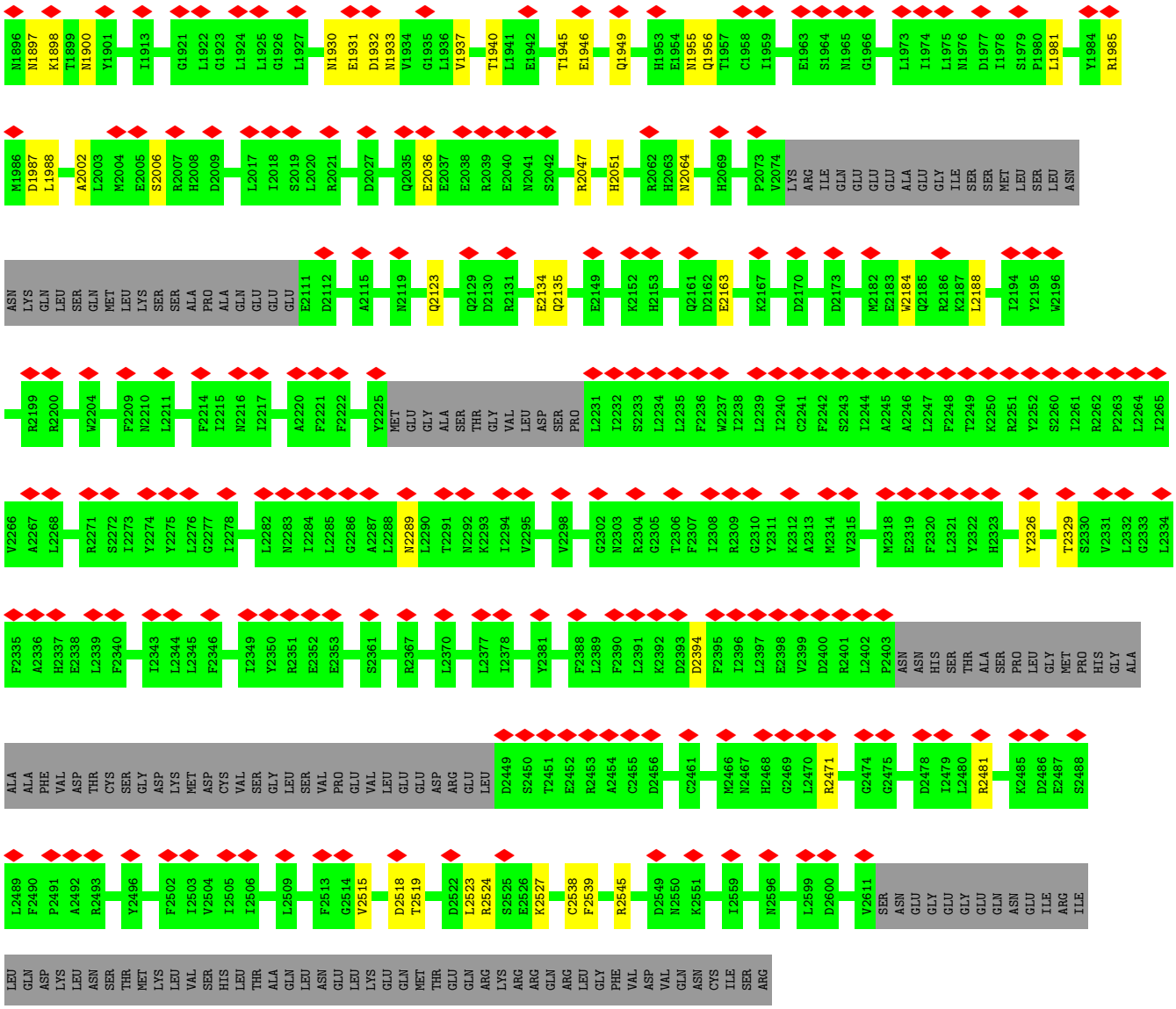
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 3

Chain A:

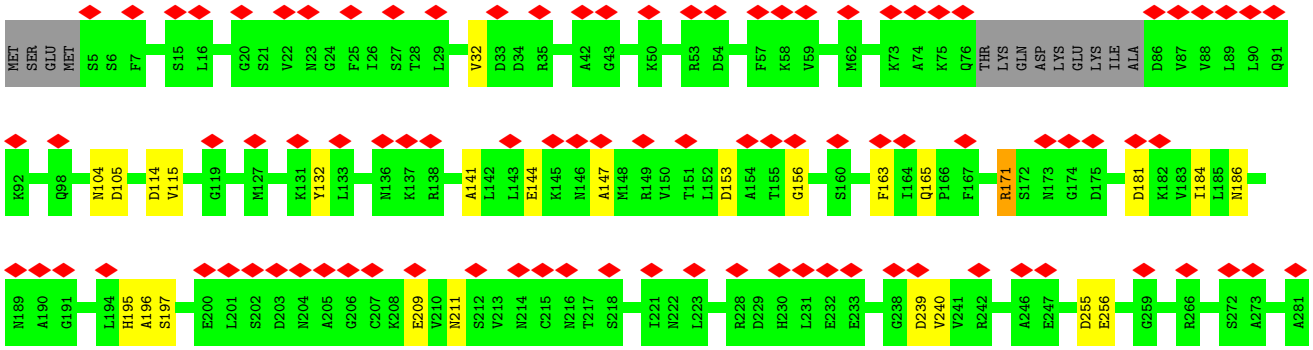


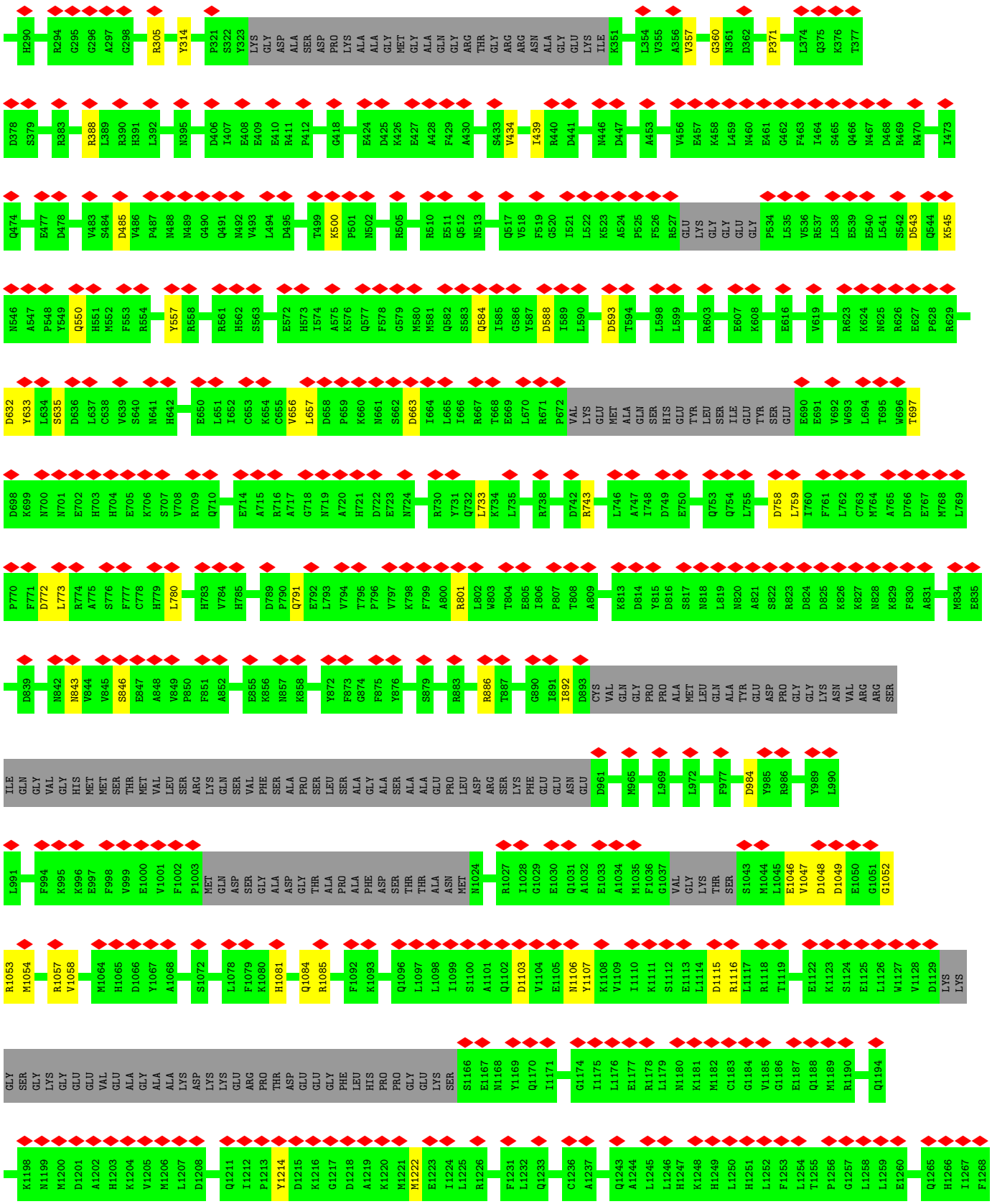

LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961
V964 E973 F977 D984 Y985 L990 F994 K995 K996 E997 F998 V999 E1000 V1001 F1002 P1003 MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA ASN MET N1024 L1025 D1026 R1027 E1030 Q1031 A1034 M1035 F1036 G1037 VAL GLY LYS THR SER S1043
M1044 V1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 R1057 H1061 L1062 T1063 M1064 H1065 D1066 S1072 G1073 H1081 R1085 F1092 K1093 Q1094 V1095 Q1096 L1097 L1098 I1099 S1100 A1101 Q1102 D1103 V1104 E1105 N1106 V1109 I1110 K1111 S1112 E1113 R1116 M1120 V1121 E1122 K1123 S1124 E1125 L1126 W1127 V1128
D1129 LYS LYS GLY SER GLY LYS LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 K1173 G1174 E1177 R1178 L1179 N1180 K1181 M1182 C1183 G1184 V1185 G1186 E1187 Q1188 M1189 R1190
K1191 K1192 Q1193 Q1194 N1199 M1200 D1201 A1202 H1203 K1204 V1205 M1206 L1209 L1210 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222 R1226 Y1227 Q1233 K1234 F1235 C1236 A1237 Q1243 L1246 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 L1258 Q1265 H1266 I1267 F1268 N1271 L1274
C1275 S1276 E1277 H1285 F1286 V1287 H1288 L1289 L1290 A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 F1302 L1303 H1304 I1307 K1308 A1309 E1310 G1311 K1312 K1316 D1319 M1320 T1323 E1324 N1327 A1328 G1329 D1330 D1331 V1332 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 M1348 M1349
K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 M1363 Y1364 H1365 D1370 A1373 A1376 K1379 N1380 V1381 Y1382 T1383 E1384 I1385 T1388 S1389 L1390 L1391 V1397 S1398 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 V1414 N1418 H1419 C1420 Y1421 T1424 E1425 V1426 E1427 M1428 K1429
E1430 I1431 Y1432 T1433 S1434 N1435 H1436 I1437 W1438 F1441 E1442 N1443 F1444 T1445 L1446 D1447 M1448 A1449 R1450 V1451 C1452 S1453 K1454 R1455 GLU LYS ARG VAL ALA ASP PRO T1463 L1464 E1465 K1466 Y1467 V1471 V1472 L1473 D1474 T1475 I1476 N1477 A1478 F1479 F1480 S1481 S1482 P1483 PHE SER GLU ASN SER THR SER LEU GLN
THR HIS GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO TRP LEU GLN GLN GLN HIS LYS GLY SER VAL GLU ALA CYS ILE ARG THR LEU A1490 M1491 V1492 A1493 K1494 I1498 L1499 L1500 P1501 M1502 D1503 L1504 D1505 A1506 H1507 I1508 SER SER MET LEU SER SER
GLY A1515 S1516 C1517 A1518 A1519 A1520 R1523 N1524 A1525 S1526 K1529 A1530 T1531 T1532 R1533 A1541 F1542 P1543 R1544 V1545 T1546 P1547 T1548 A1549 N1550 Q1551 W1552 D1587 Y1588 K1589 N1590 E1593 K1594 D1597 T1600 A1601 E1604 R1605 E1613 H1622 L1627 F1628 L1629 E1630 G1631 Q1636 R1637 C1638 E1639
S1640 G1641 G1642 K1646 D1653 L1654 M1655 E1656 E1659 R1667 T1668 L1673 T1677 K1678 Y1679 R1687 K1688 Q1692 N1693 Q1696 ASN ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP W1718 S1719 A1720 A1723 C1726 K1730 E1731
K1735 D1739 S1743 T1744 K1745 I1749 S1753 I1754 G1755 D1762 F1772 H1773 N1774 M1777 S1778 D1779 K1780 E1783 R1784 F1785 F1786 K1787 D1791 R1792 R1795 E1799 T1800 K1801 S1802 T1803 V1804 ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO
VAL ASP PRO THR THR LYS GLY ARG VAL ALA SER PHE SER ILE PRO GLY SER SER SER ARG TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS GLU VAL SER GLU ARG VAL GLN SER SER GLU M1863 V1867 L1868 R1875 C1881 E1882 N1883 R1886 Q1889 N1890 R1893 C1894 Q1895

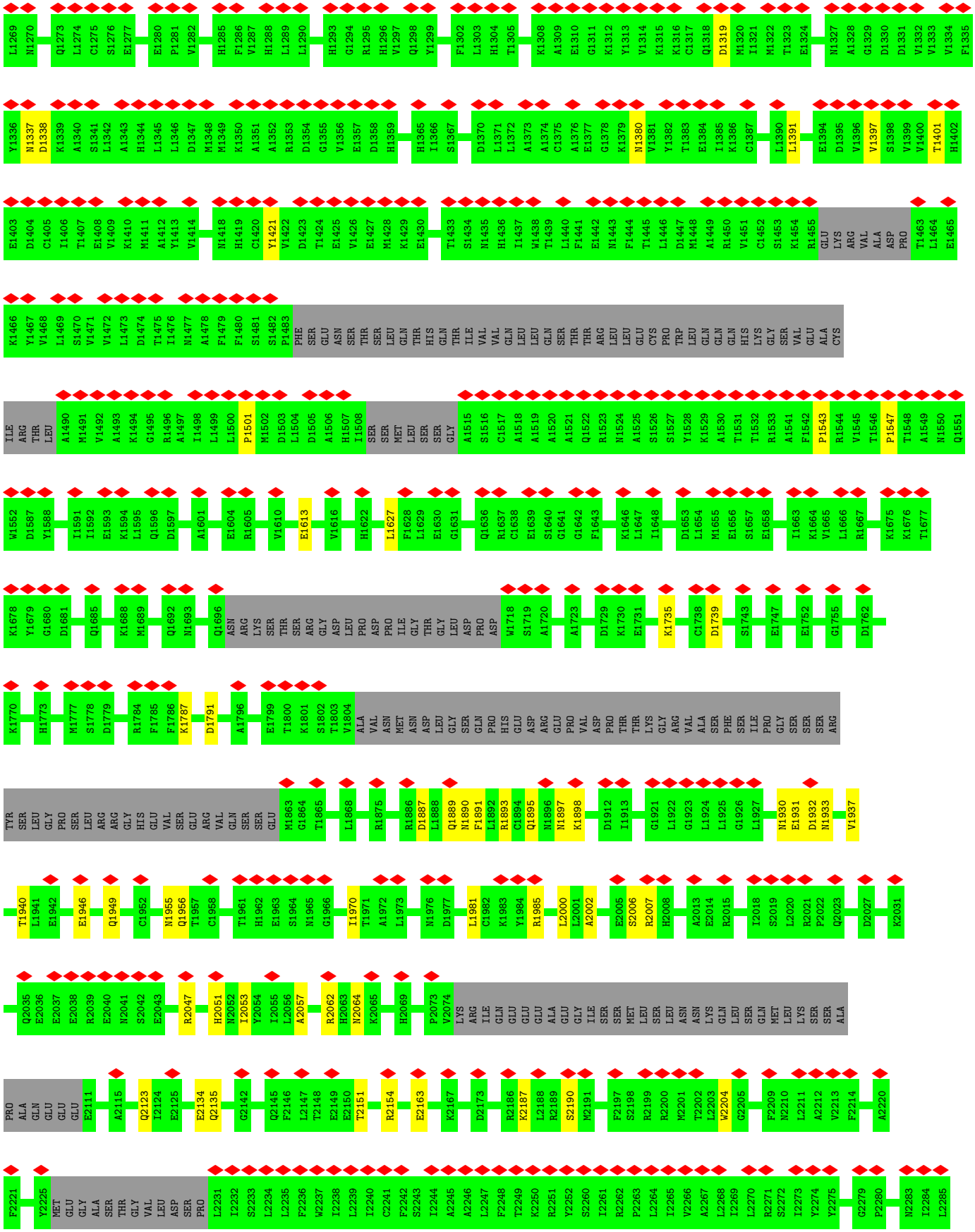


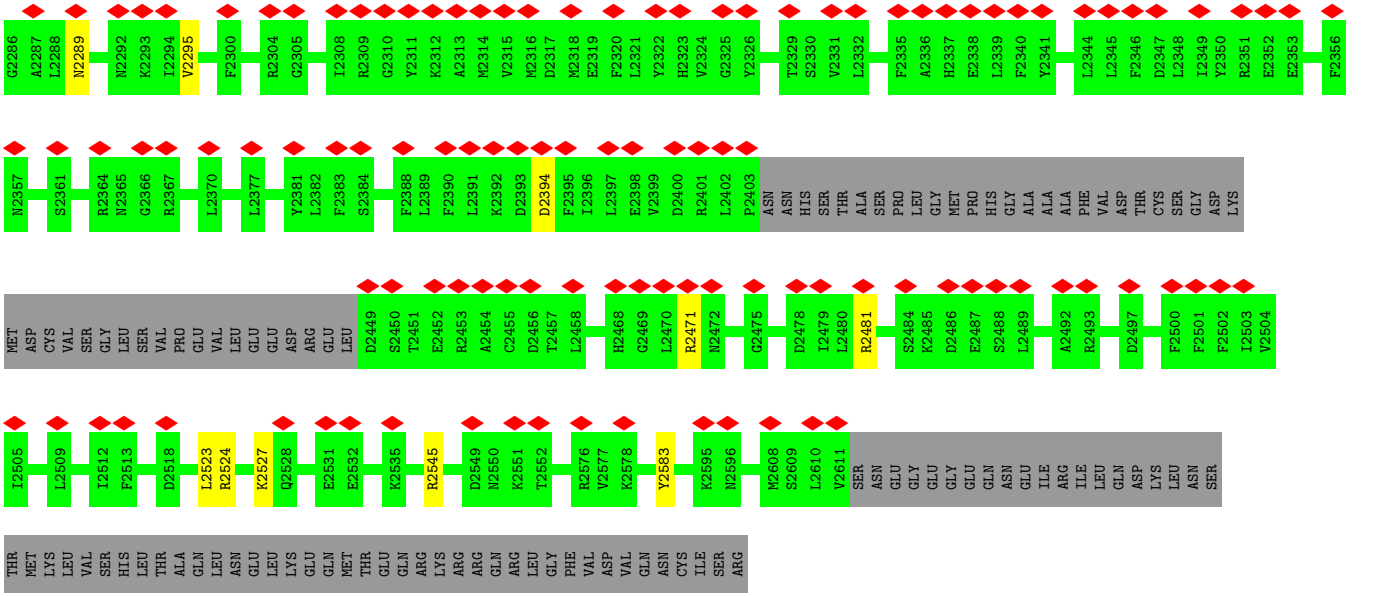

- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain B:



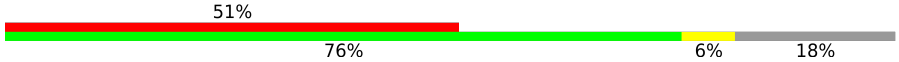

H290
R294 G295 G296 A297 G298
R305
Y314
P321 S322 Y323 LYS GLY ASP ALA SER ASP PRO LYS ALA ALA GLY MET GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA GLY GLU LYS ILE K351
L354 V355 A356 V357
G360 N361 D362
P371
L374 Q375 K376 T377
D378 S379
R383
R388 L389 R390 H391 L392
N395
D406 I407 E408 E409 E410 R411 P412
G418
E424 D425 K426 E427 A428 F429 A430
S433 V434
I439
R440 D441
N446 D447
A453
V456 E457 K458 L459 N460 E461 G462 F463 I464 S465 Q466 N467 D468 R469 R470
I473
Q474
E477 D478
V483 S484 D485 V486 P487 N488 N489 G490 Q491 N492 V493 L494 D495
T499 K500 P501 N502
R505
R510 E511 Q512 N513
Q517 V518 F519 G520 I521 L522 K523 A524 P525 F526 R527 GLU LYS GLY GLY GLU GLY P534 L535 V536 R537 L538 E539 E540 L541 S542 D543 Q544 K545
N546 A547 P548 Y549
Q550
H551 M552 F553 R554
Y557 R558
R561 H562 S563
E572 H573 I574 A575 K576 Q577 F578 G579 M580 M581 Q582 S583 Q584 I585 G586 Y587
D588 I589 L590
D593 T594
L598 L599
R603
E607 K608
E616
V619
R623 K624 N625 R626 E627 P628 R629
D632 Y633
L634 S635
D636 L637 C638 V639 S640 N641 H642
E650 L651 I652 C653 K654 C655 V656 L657 D658 P659 K660 N661 S662 D663 I664 L665 I666 R667 T668 E669 L670 R671 P672 VAL LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER GLU E690 E691 V692 W693 L694 T695 W696 T697
D698 K699 N700 N701 E702 H703 H704 E705 K706 S707 V708 R709 Q710
E714 A715 R716 A717 G718 N719 A720 H721 D722 E723 N724
R730 Y731 Q732 L733 K734 L735
R738
D742 R743
L746 A747 I748 D749 E750
Q753 Q754 L755
D758 L759 I760 F761 L762 C763 M764 A765 D766 E767 M768 L769
P770 F771 D772 L773
R774 A775 S776 F777 C778 H779 L780
H783 V784 H785
D789 P790 Q791
E792 L793 V794 T795 P796 V797 K798 F799 A800
R801 L802 W803 T804 E805 I806 P807 T808 A809
K813 D814 Y815 D816 S817 N818 L819 N820 A821 S822 R823 D824 D825 K826 K827 N828 K829 F830 A831
M834 E835
D839
M842 N843 V844 V845 S846 E847 A848 V849 P850 F851 A852
E855 K856 N857 K858
Y872 F873 G874 F875 Y876
S879
R883
R886 T887
G890 I891 I892 D893 CYS VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER
ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU
D961
M965
L969
L972
F977
D984
Y985 R986
Y989 L990
L991
F994 K995 K996 E997 F998 V999 E1000 V1001 F1002 P1003 MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA ASN MET N1024
R1027 I1028 G1029 E1030 Q1031 A1032 E1033 A1034 M1035 F1036 G1037 VAL GLY LYS THR SER
S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052
R1053 M1054
R1057 V1058
M1064 H1065 D1066 Y1067 A1068
S1072
L1078 F1079 K1080
H1081
Q1084 R1085
F1092 K1093
Q1096 L1097 L1098 I1099 S1100 A1101 Q1102
D1103 V1104 E1105
N1106 Y1107
K1108 V1109 I1110 K1111 S1112 E1113 L1114
D1115 R1116
L1117 R1118 T1119
E1122 K1123 S1124 E1125 L1126 W1127 V1128 D1129 LYS LYS
GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 I1171
G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 M1182 C1183 G1184 V1185 G1186 E1187 Q1188 M1189 R1190
Q1194
K1198 N1199 M1200 D1201 A1202 H1203 K1204 V1205 M1206 L1207 D1208
Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222
E1223 I1224 L1225 R1226
F1231 L1232 Q1233
C1236 A1237
Q1243 A1244 L1245 L1246 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1260
Q1265 H1266 I1267 F1268

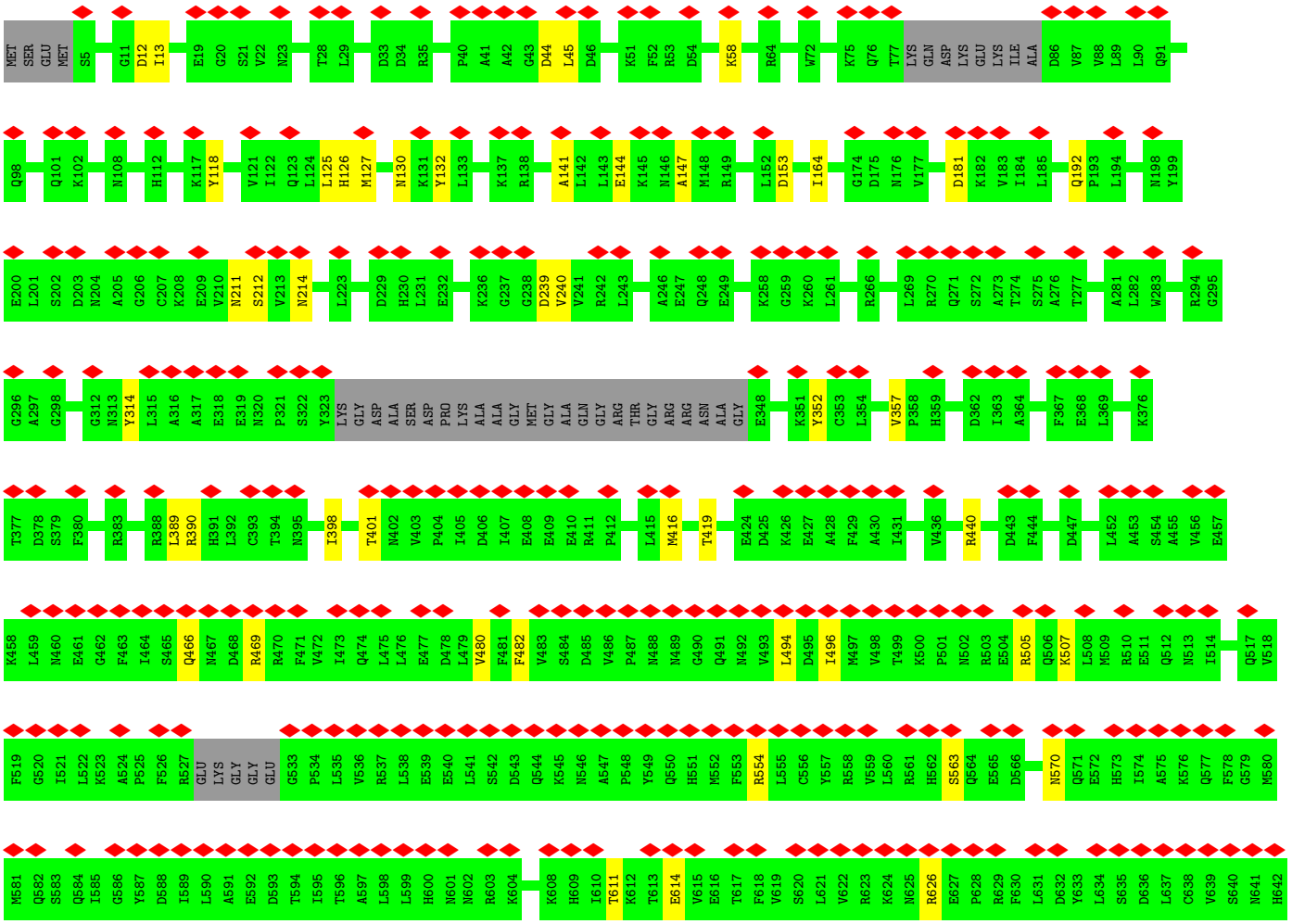

L1269 N1270 Q1273 L1274 C1275 S1276 E1277 E1280 P1281 V1282 H1285 F1286 V1287 H1288 L1289 L1290 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 F1302 L1303 H1304 T1305 K1308 A1309 E1310 G1311 K1312 Y1313 V1314 K1315 K1316 C1317 Q1318 D1319 M1320 I1321 M1322 T1323 E1324 M1327 A1328 G1329 D1330 D1331 V1332 V1333 V1334 F1335
Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 M1348 M1349 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 H1365 I1366 S1367 D1370 L1371 L1372 A1373 A1374 C1375 A1376 E1377 G1378 K1379 N1380 V1381 Y1382 T1383 E1384 I1385 K1386 C1387 L1390 L1391 E1394 D1395 V1396 V1397 S1398 V1399 V1400 T1401 H1402
E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412 Y1413 V1414 N1418 H1419 C1420 Y1421 V1422 D1423 T1424 E1425 V1426 E1427 M1428 K1429 E1430 T1433 S1434 N1435 H1436 I1437 W1438 T1439 L1440 F1441 E1442 N1443 F1444 T1445 L1446 D1447 M1448 A1449 R1450 V1451 C1452 S1453 K1454 R1455 GLU LYS ARG VAL ALA ASP PRO T1463 L1464 E1465
K1466 Y1467 V1468 L1469 S1470 V1471 V1472 L1473 D1474 T1475 I1476 N1477 A1478 F1479 F1480 S1481 S1482 P1483 PHE SER GLU ASN SER THR SER LEU GLN THR HIS GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO TRP LEU GLN GLN GLN HIS LYS GLY SER VAL GLU ALA CYS
ILE ARG THR LEU A1490 M1491 V1492 A1493 K1494 L1595 G1596 R1496 A1497 I1498 L1499 L1500 P1501 M1502 D1503 L1504 D1505 A1506 H1507 I1508 SER SER MET LEU SER SER GLY A1515 S1516 C1517 A1518 A1519 A1520 A1521 Q1522 R1523 N1524 A1525 S1526 S1527 Y1528 K1529 A1530 T1531 T1532 R1533 A1541 F1542 P1543 R1544 V1545 T1546 P1547 T1548 A1549 N1550 Q1551
W1552 D1587 Y1588 I1591 I1592 E1593 K1594 L1595 Q1596 D1597 A1601 E1604 R1605 V1610 E1613 V1616 H1622 L1627 F1628 L1629 E1630 G1631 Q1636 R1637 C1638 E1639 S1640 G1641 G1642 F1643 K1646 L1647 I1648 D1653 L1654 M1655 E1656 S1657 E1658 I1663 K1664 V1665 L1666 R1667 K1675 K1676 T1677
K1678 Y1679 G1680 D1681 Q1685 K1688 M1689 Q1692 N1693 Q1696 ASN ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP W1718 S1719 A1720 A1723 D1729 K1730 E1731 K1735 C1738 D1739 S1743 E1747 E1752 G1755 D1762
K1770 H1773 M1777 S1778 D1779 R1784 F1785 F1786 K1787 D1791 A1796 E1799 T1800 K1801 S1802 T1803 V1804 ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG VAL ALA SER PHE SER ILE PRO GLY SER SER SER SER ARG
TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS GLU VAL SER GLU ARG VAL GLN SER SER GLU M1863 G1864 T1865 L1868 R1875 R1886 D1887 L1888 Q1889 N1890 F1891 L1892 R1893 C1894 Q1895 N1896 N1897 K1898 D1912 I1913 G1921 L1922 G1923 L1924 L1925 G1926 L1927 N1930 E1931 D1932 N1933 V1937
T1940 L1941 E1942 E1946 Q1949 C1952 N1955 Q1956 T1957 C1958 T1961 H1962 E1963 S1964 N1965 G1966 I1970 T1971 A1972 L1973 N1976 D1977 L1981 C1982 K1983 Y1984 R1985 L2000 L2001 A2002 E2005 S2006 R2007 H2008 A2013 E2014 R2015 I2018 S2019 L2020 R2021 P2022 Q2023 D2027 K2031
Q2035 E2036 E2037 E2038 R2039 E2040 N2041 S2042 E2043 R2047 H2051 N2052 I2053 Y2054 I2055 L2056 A2057 R2062 H2063 N2064 K2065 H2069 P2073 V2074 LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU SER LEU ASN ASN LYS GLN LEU SER GLN MET LEU LYS SER SER ALA
PRO ALA GLN GLU GLU GLU E2111 A2115 Q2123 I2124 E2125 E2134 Q2135 G2142 Q2145 F2146 L2147 T2148 E2149 E2150 T2151 R2154 E2163 K2167 D2173 R2186 K2187 L2188 R2189 S2190 M2191 F2197 S2198 R2199 R2200 M2201 T2202 L2203 W2204 G2205 F2209 N2210 L2211 A2212 V2213 F2214 A2220
F2221 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO L2231 I2232 S2233 L2234 L2235 F2236 W2237 I2238 L2239 I2240 C2241 F2242 S2243 I2244 A2245 A2246 L2247 F2248 T2249 K2250 R2251 Y2252 S2260 I2261 R2262 P2263 L2264 I2265 V2266 A2267 L2268 I2269 L2270 R2271 S2272 I2273 Y2274 Y2275 G2279 P2280 N2283 I2284 L2285

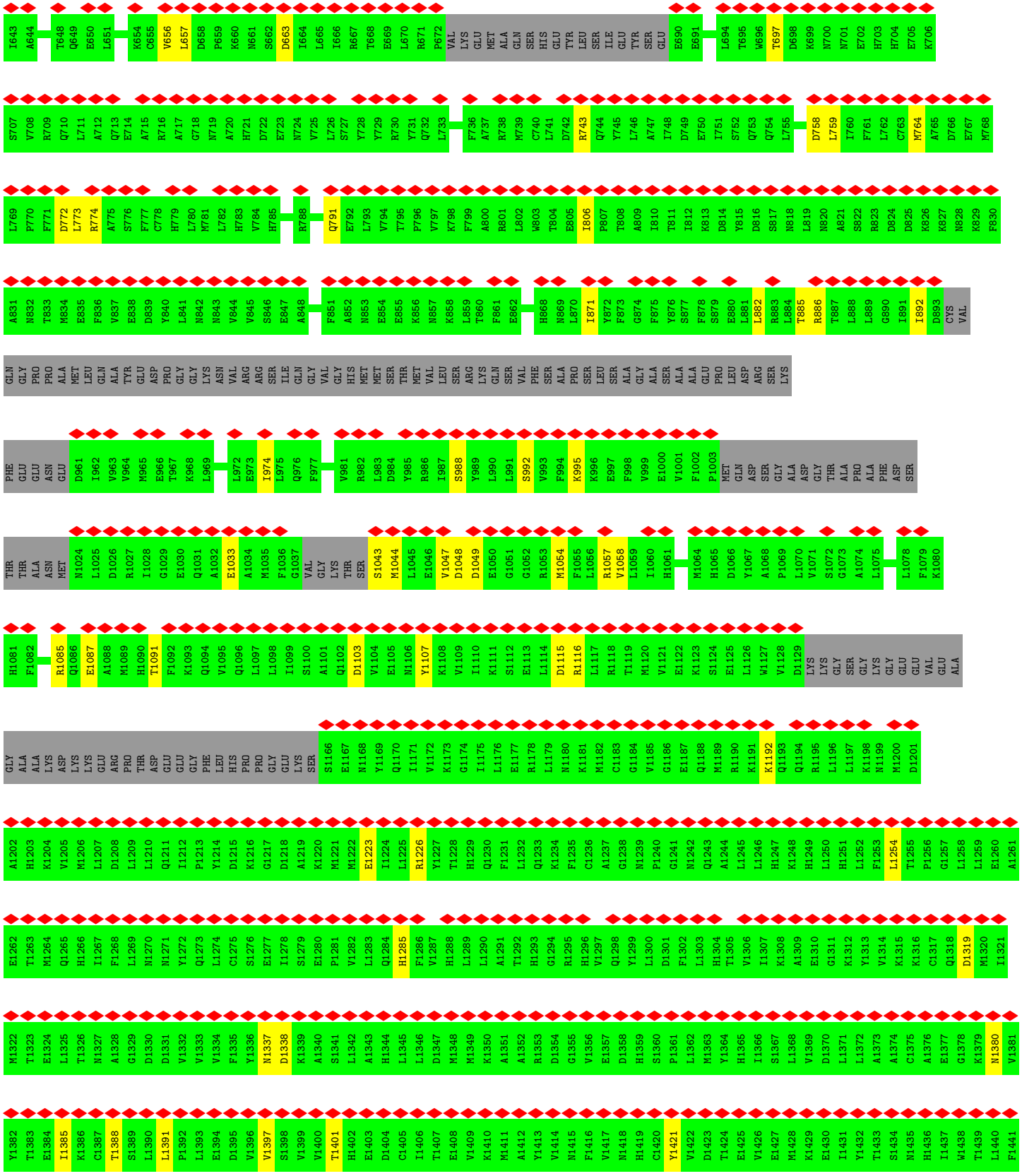


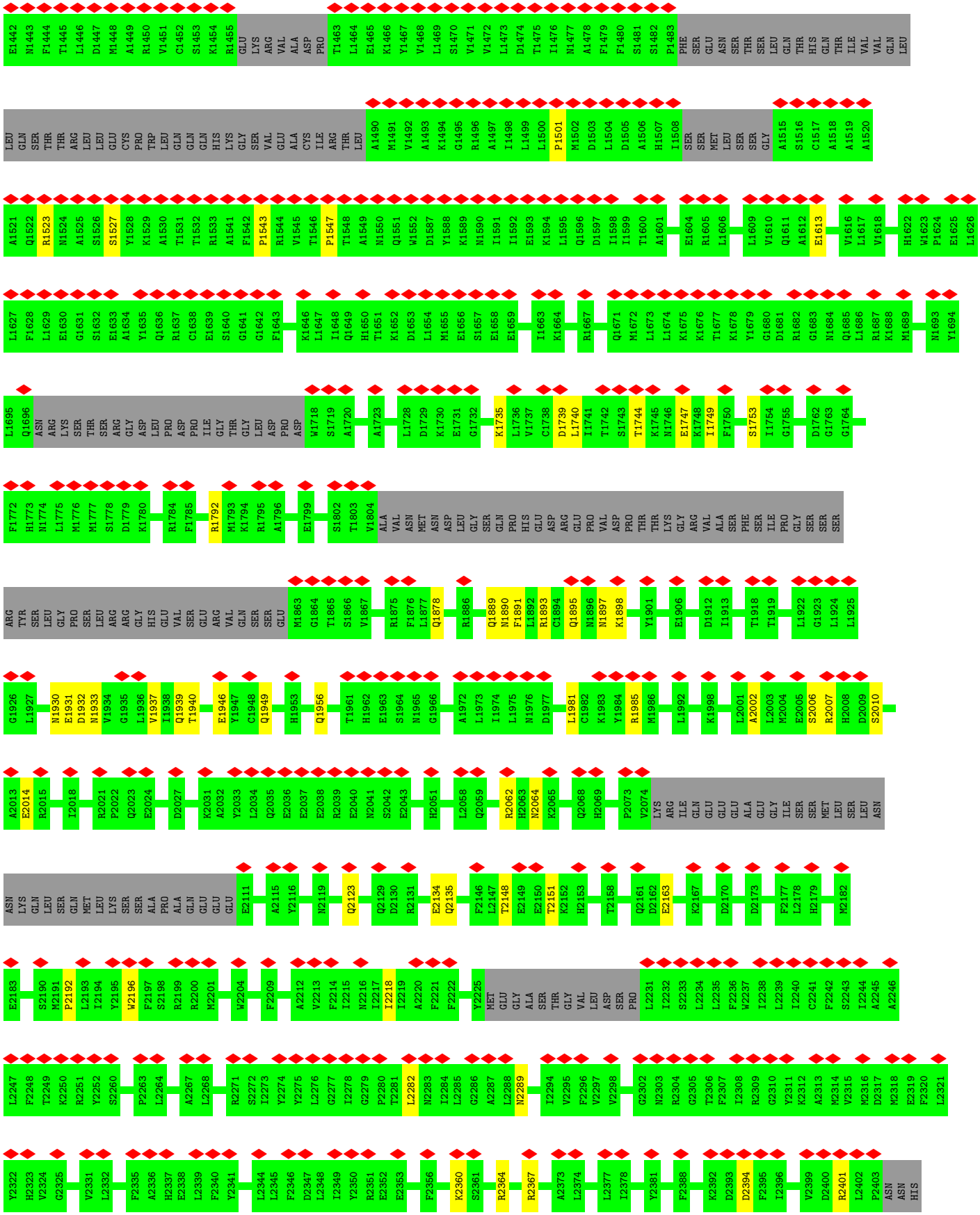

- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

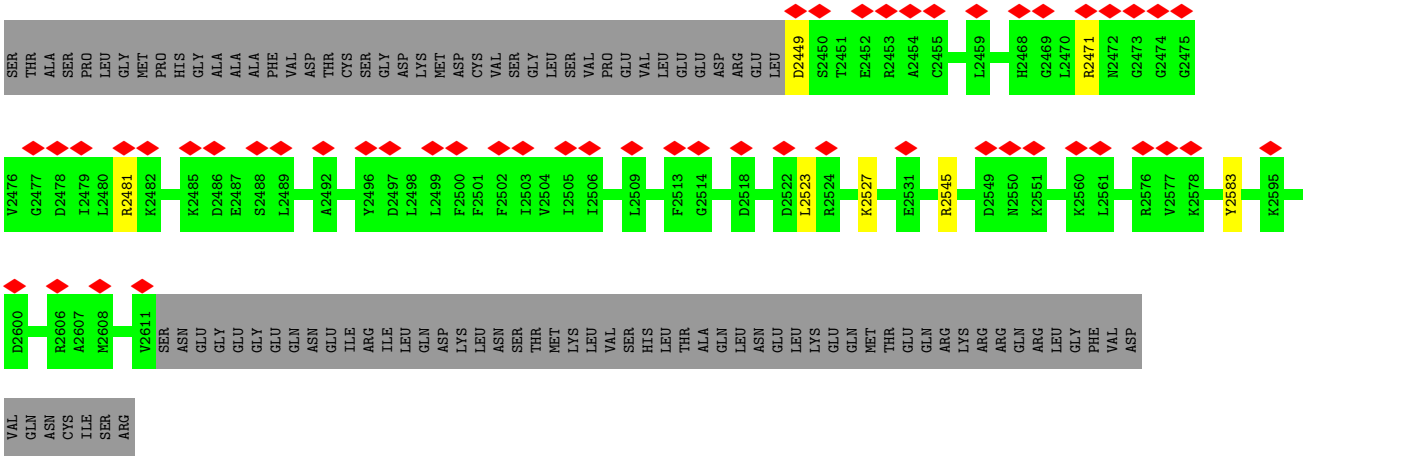
Chain C:



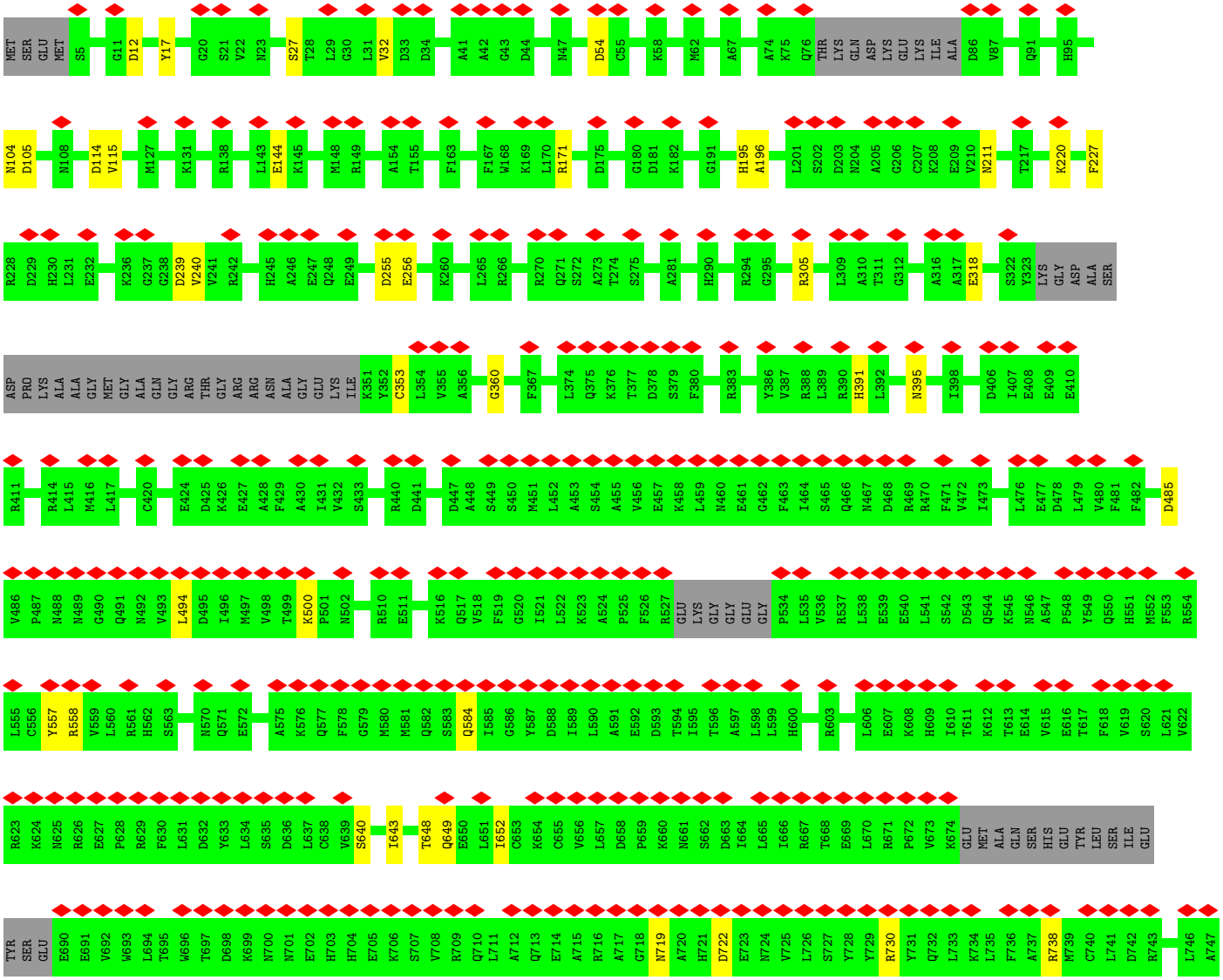

I643 A644 T648 Q649 E650 L651 K654 C655 V656 L657 D658 P659 K660 N661 S662 D663 I664 L665 I666 R667 T668 E669 L670 R671 P672 VAL LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER GLU E690 E691 L694 T695 W696 T697 D698 K699 N700 N701 E702 H703 H704 E705 K706
S707 V708 R709 Q710 L711 A712 Q713 E714 A715 R716 A717 G718 N719 A720 H721 D722 E723 N724 V725 L726 S727 Y728 Y729 R730 Y731 Q732 L733 F736 A737 R738 W739 C740 L741 D742 R743 Q744 Y745 L746 A747 T748 D749 E750 T751 S752 Q753 Q754 L755 D758 L759 I760 F761 L762 C763 M764 A765 D766 E767 M768
L769 P770 F771 D772 L773 R774 A775 S776 F777 C778 H779 L780 M781 L782 H783 V784 H785 R788 Q791 E792 L793 V794 T795 P796 V797 K798 F799 A800 R801 L802 W803 T804 E805 I806 P807 T808 A809 I810 T811 I812 K813 D814 Y815 D816 S817 N818 L819 N820 A821 S822 R823 D824 D825 K826 K827 N828 K829 F830
A831 N832 T833 M834 E835 F836 V837 E838 D839 Y840 L841 N842 N843 V844 V845 S846 E847 A848 F851 A852 N853 E854 E855 K856 N857 K858 L859 T860 F861 E862 H868 N869 L870 I871 Y872 F873 G874 F875 Y876 S877 F878 S879 E880 L881 L882 R883 L884 T885 R886 T887 L888 L889 G890 I891 I892 D893 CYS VAL
GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS
PHE GLU GLU ASN GLU D961 I962 V963 V964 M965 E966 T967 K968 L969 L972 E973 I974 L975 Q976 F977 V981 R982 L983 D984 Y985 R986 I987 S988 Y989 L990 L991 S992 V993 F994 K995 K996 E997 F998 V999 E1000 V1001 F1002 P1003 MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER
THR THR ALA ASN MET N1024 L1025 D1026 R1027 I1028 G1029 E1030 Q1031 A1032 E1033 A1034 M1035 F1036 G1037 VAL GLY LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 F1055 L1056 R1057 V1058 L1059 I1060 H1061 M1064 H1065 D1066 Y1067 A1068 P1069 L1070 V1071 S1072 G1073 A1074 L1075 L1078 F1079 K1080
H1081 F1082 R1085 Q1086 E1087 A1088 M1089 H1090 T1091 F1092 K1093 Q1094 V1095 Q1096 L1097 L1098 I1099 S1100 A1101 Q1102 D1103 V1104 E1105 N1106 Y1107 K1108 V1109 I1110 K1111 S1112 E1113 L1114 D1115 R1116 L1117 R1118 T1119 M1120 V1121 E1122 K1123 S1124 E1125 L1126 W1127 V1128 D1129 LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA
GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 I1171 V1172 K1173 G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 M1182 C1183 G1184 V1185 G1186 E1187 Q1188 M1189 R1190 K1191 K1192 Q1193 Q1194 R1195 L1196 L1197 K1198 N1199 M1200 D1201
A1202 H1203 K1204 V1205 M1206 L1207 D1208 L1209 L1210 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222 E1223 I1224 L1225 R1226 Y1227 T1228 H1229 Q1230 F1231 L1232 Q1233 K1234 F1235 C1236 A1237 G1238 G1184 N1239 P1240 G1241 N1242 Q1243 A1244 L1245 L1246 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1260 A1261
E1262 T1263 M1264 Q1265 H1266 I1267 F1268 L1269 N1270 N1271 Y1272 Q1273 L1274 C1275 S1276 E1277 I1278 S1279 E1280 P1281 V1282 L1283 Q1284 H1285 F1286 V1287 H1288 L1289 L1290 A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 T1305 V1306 I1307 K1308 A1309 E1310 G1311 K1312 Y1313 V1314 K1315 K1316 C1317 Q1318 D1319 M1320 I1321
M1322 T1323 E1324 L1325 T1326 N1327 A1328 G1329 D1330 D1331 V1332 V1333 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 M1348 M1349 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 S1360 P1361 L1362 M1363 Y1364 H1365 I1366 S1367 L1368 V1369 D1370 L1371 L1372 A1373 A1374 C1375 A1376 E1377 G1378 K1379 N1380 V1381
Y1382 T1383 E1384 I1385 K1386 C1387 T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 V1396 V1397 S1398 V1399 V1400 T1401 H1402 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412 Y1413 V1414 N1415 F1416 V1417 N1418 H1419 C1420 Y1421 V1422 D1423 T1424 E1425 V1426 E1427 M1428 K1429 E1430 I1431 Y1432 T1433 S1434 N1435 H1436 I1437 W1438 T1439 L1440 F1441

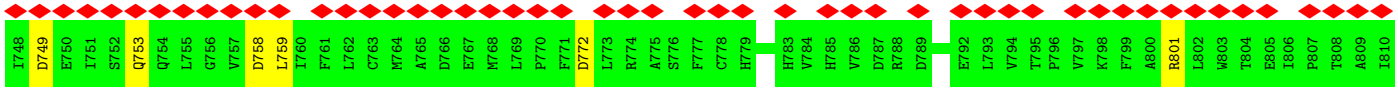

E1442 N1443 F1444 T1445 L1446 D1447 M1448 A1449 R1450 V1451 C1452 S1453 K1454 R1455 GLU LYS ARG VAL ALA ASP PRO T1463 L1464 E1465 K1466 Y1467 V1468 L1469 S1470 V1471 V1472 L1473 D1474 T1475 I1476 N1477 A1478 F1479 F1480 S1481 S1482 P1483 PHE SER GLU ASN SER THR SER LEU GLN THR HIS GLN THR ILE VAL VAL GLN LEU
LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO TRP LEU GLN GLN GLN HIS LYS GLY SER VAL GLU ALA CYS ILE ARG THR LEU A1490 M1491 V1492 A1493 K1494 G1495 R1496 A1497 I1498 L1499 L1500 P1501 M1502 D1503 L1504 D1505 A1506 H1507 I1508 SER SER MET LEU SER SER GLY A1515 S1516 C1517 A1518 A1519 A1520
A1521 Q1522 R1523 N1524 A1525 S1526 S1527 Y1528 K1529 A1530 T1531 T1532 R1533 A1541 F1542 P1543 R1544 V1545 T1546 P1547 T1548 A1549 N1550 Q1551 W1552 D1587 Y1588 K1589 N1590 I1591 I1592 E1593 K1594 L1595 Q1596 D1597 I1598 I1599 T1600 A1601 E1604 R1605 L1606 L1609 V1610 Q1611 A1612 E1613 V1616 L1617 V1618 H1622 W1623 P1624 E1625 L1626
L1627 F1628 L1629 E1630 G1631 S1632 E1633 A1634 Y1635 Q1636 R1637 C1638 E1639 S1640 G1641 G1642 F1643 K1646 L1647 I1648 Q1649 H1650 T1651 K1652 D1653 L1654 M1655 E1656 S1657 E1658 E1659 I1663 K1664 R1667 Q1671 M1672 L1673 L1674 K1675 K1676 T1677 K1678 Y1679 G1680 D1681 R1682 G1683 N1684 Q1685 L1686 R1687 K1688 M1689 N1693 Y1694
L1695 Q1696 ASN ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP W1718 S1719 A1720 A1723 L1728 D1729 K1730 E1731 G1732 K1735 L1736 V1737 C1738 D1739 L1740 I1741 T1742 S1743 T1744 K1745 N1746 E1747 K1748 I1749 F1750 S1753 I1754 G1755 D1762 G1763 G1764
F1772 H1773 N1774 L1775 M1776 M1777 S1778 D1779 K1780 R1784 F1785 R1792 M1793 K1794 R1795 A1796 E1799 S1802 T1803 V1804 ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG VAL ALA SER PHE SER ILE PRO GLY SER SER SER
ARG TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS GLU VAL SER GLU ARG VAL GLN SER SER GLU M1863 G1864 T1865 S1866 V1867 R1875 F1876 L1877 Q1878 R1886 Q1889 N1890 F1891 L1892 R1893 C1894 Q1895 N1896 N1897 K1898 Y1901 E1906 D1912 I1913 T1918 T1919 L1922 G1923 L1924 L1925
G1926 L1927 N1930 E1931 D1932 N1933 V1934 G1935 L1936 V1937 I1938 Q1939 T1940 E1946 Y1947 C1948 Q1949 H1953 Q1956 T1961 H1962 E1963 S1964 N1965 G1966 A1972 L1973 I1974 L1975 N1976 D1977 L1981 C1982 K1983 Y1984 R1985 M1986 L1992 K1998 L2001 A2002 L2003 M2004 E2005 S2006 R2007 H2008 D2009 S2010
A2013 E2014 R2015 I2018 R2021 P2022 Q2023 E2024 D2027 K2031 A2032 Y2033 L2034 Q2035 E2036 E2037 E2038 R2039 E2040 N2041 S2042 E2043 H2051 L2058 Q2059 R2062 H2063 N2064 K2065 Q2068 H2069 P2073 V2074 LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU SER LEU ASN
ASN LYS GLN LEU SER GLN MET LEU LYS SER SER ALA PRO ALA GLN GLU GLU GLU E2111 A2115 Y2116 N2119 Q2123 Q2129 D2130 R2131 E2134 Q2135 F2146 L2147 T2148 E2149 E2150 T2151 K2152 H2153 T2158 Q2161 D2162 E2163 K2167 D2170 D2173 F2177 L2178 H2179 M2182
E2183 S2190 M2191 P2192 L2193 I2194 Y2195 W2196 F2197 S2198 R2199 R2200 M2201 W2204 F2209 A2212 V2213 F2214 I2215 N2216 I2217 I2218 I2219 A2220 F2221 F2222 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO L2231 I2232 S2233 L2234 L2235 F2236 W2237 I2238 L2239 I2240 C2241 F2242 S2243 I2244 A2245 A2246
L2247 F2248 T2249 K2250 R2251 Y2252 S2260 P2263 L2264 A2267 L2268 R2271 S2272 I2273 Y2274 Y2275 L2276 G2277 I2278 G2279 P2280 T2281 L2282 M2283 I2284 L2285 G2286 A2287 L2288 N2289 I2294 V2295 F2296 V2297 V2298 G2302 N2303 R2304 G2305 T2306 F2307 I2308 R2309 G2310 Y2311 K2312 A2313 M2314 V2315 M2316 D2317 M2318 E2319 F2320 L2321
Y2322 H2323 Y2324 G2325 V2331 L2332 F2335 A2336 H2337 E2338 L2339 F2340 Y2341 L2344 L2345 F2346 D2347 L2348 I2349 Y2350 R2351 E2352 E2353 F2356 K2360 S2361 R2364 R2367 A2373 L2374 L2377 I2378 Y2381 F2388 K2392 D2393 D2394 F2395 I2396 V2399 D2400 R2401 L2402 F2403 ASN ASN HIS

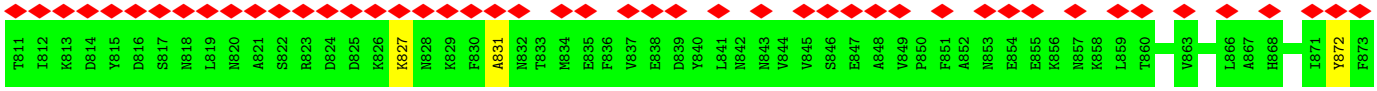


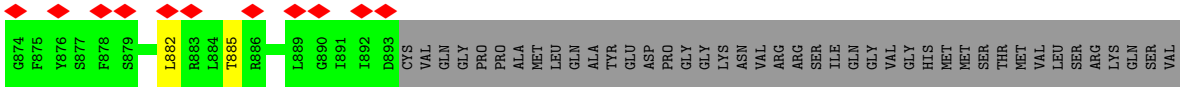

- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

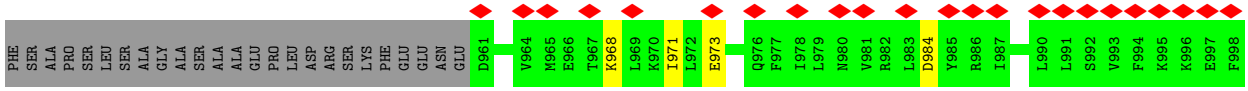
Chain D:

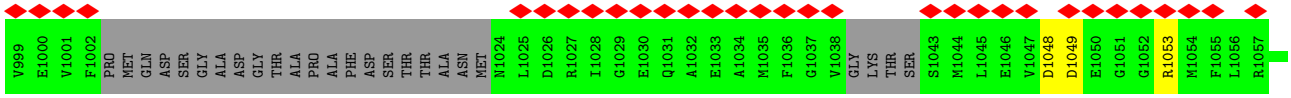


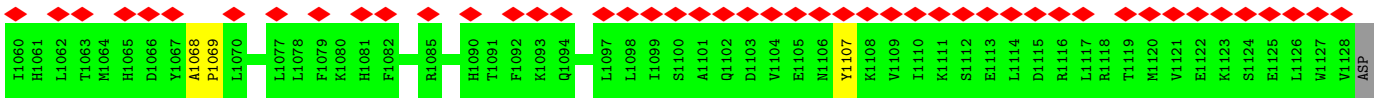

I748 D749 E750 I751 S752 Q753 Q754 L755 G756 V757 D758 L759 I760 F761 L762 C763 M764 A765 D766 E767 M768 L769 P770 F771 D772 L773 R774 A775 S776 F777 C778 H779 H783 V784 H785 V786 D787 R788 D789 E792 L793 V794 T795 P796 V797 K798 F799 A800 R801 L802 W803 T804 E805 I806 P807 T808 A809 I810

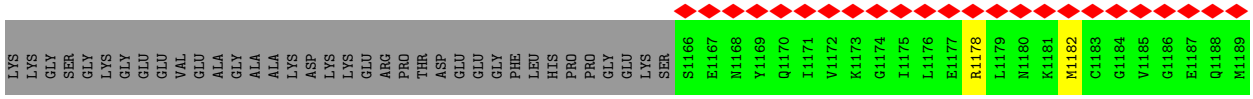

T811 I812 K813 D814 Y815 D816 S817 N818 L819 N820 A821 S822 R823 D824 D825 K826 K827 N828 K829 F830 A831 N832 T833 M834 E835 F836 V837 E838 D839 Y840 L841 N842 N843 V844 V845 S846 E847 A848 V849 P850 F851 A852 N853 E854 E855 K856 N857 K858 L859 T860 V863 L866 A867 H868 I871 Y872 F873

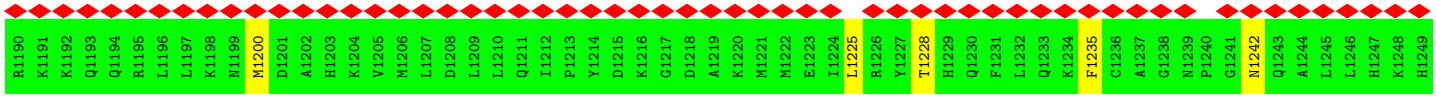

G874 F875 Y876 S877 F878 S879 L882 R883 L884 T885 R886 L889 G890 I891 I892 D893 CYS VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL

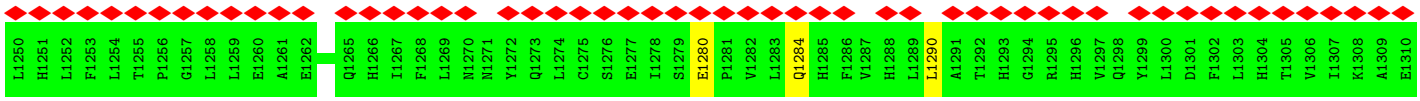

PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 V964 M965 E966 T967 K968 L969 K970 I971 L972 E973 Q976 F977 I978 L979 N980 V981 R982 L983 D984 Y985 R986 I987 L990 L991 S992 V993 F994 K995 K996 E997 F998

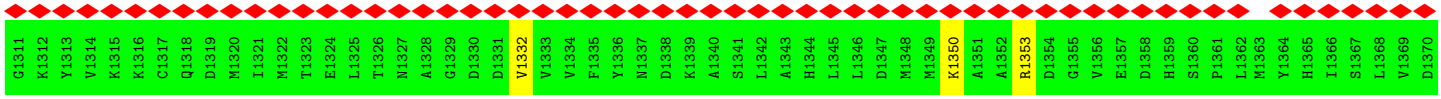

V999 E1000 V1001 F1002 PRO MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA ASN MET N1024 L1025 D1026 R1027 I1028 G1029 E1030 Q1031 A1032 E1033 A1034 M1035 F1036 G1037 V1038 GLY LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 F1055 L1056 R1057

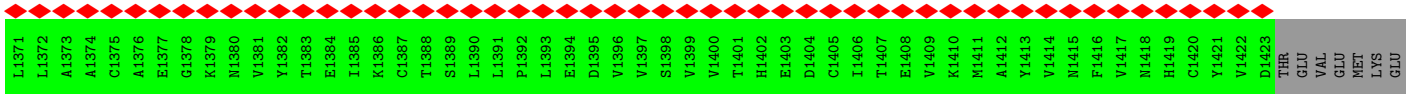

I1060 H1061 L1062 T1063 M1064 H1065 D1066 Y1067 A1068 P1069 L1070 L1077 L1078 F1079 K1080 H1081 F1082 R1085 H1090 T1091 F1092 K1093 Q1094 L1097 L1098 I1099 S1100 A1101 Q1102 D1103 V1104 E1105 N1106 Y1107 K1108 V1109 I1110 K1111 S1112 E1113 L1114 D1115 R1116 L1117 R1118 T1119 M1120 V1121 E1122 K1123 S1124 E1125 L1126 W1127 V1128 ASP

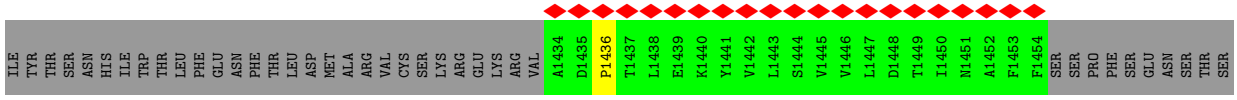

LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 I1171 V1172 K1173 G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 M1182 C1183 G1184 V1185 G1186 E1187 Q1188 M1189

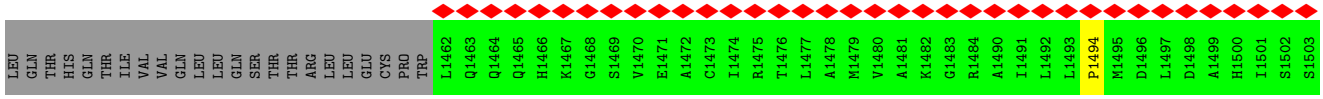

R1190 K1191 K1192 Q1193 Q1194 R1195 L1196 L1197 K1198 N1199 M1200 D1201 A1202 H1203 K1204 V1205 M1206 L1207 D1208 L1209 L1210 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222 E1223 I1224 L1225 R1226 Y1227 T1228 H1229 Q1230 F1231 L1232 Q1233 K1234 F1235 C1236 A1237 G1238 N1239 P1240 G1241 N1242 Q1243 A1244 L1245 L1246 H1247 K1248 H1249

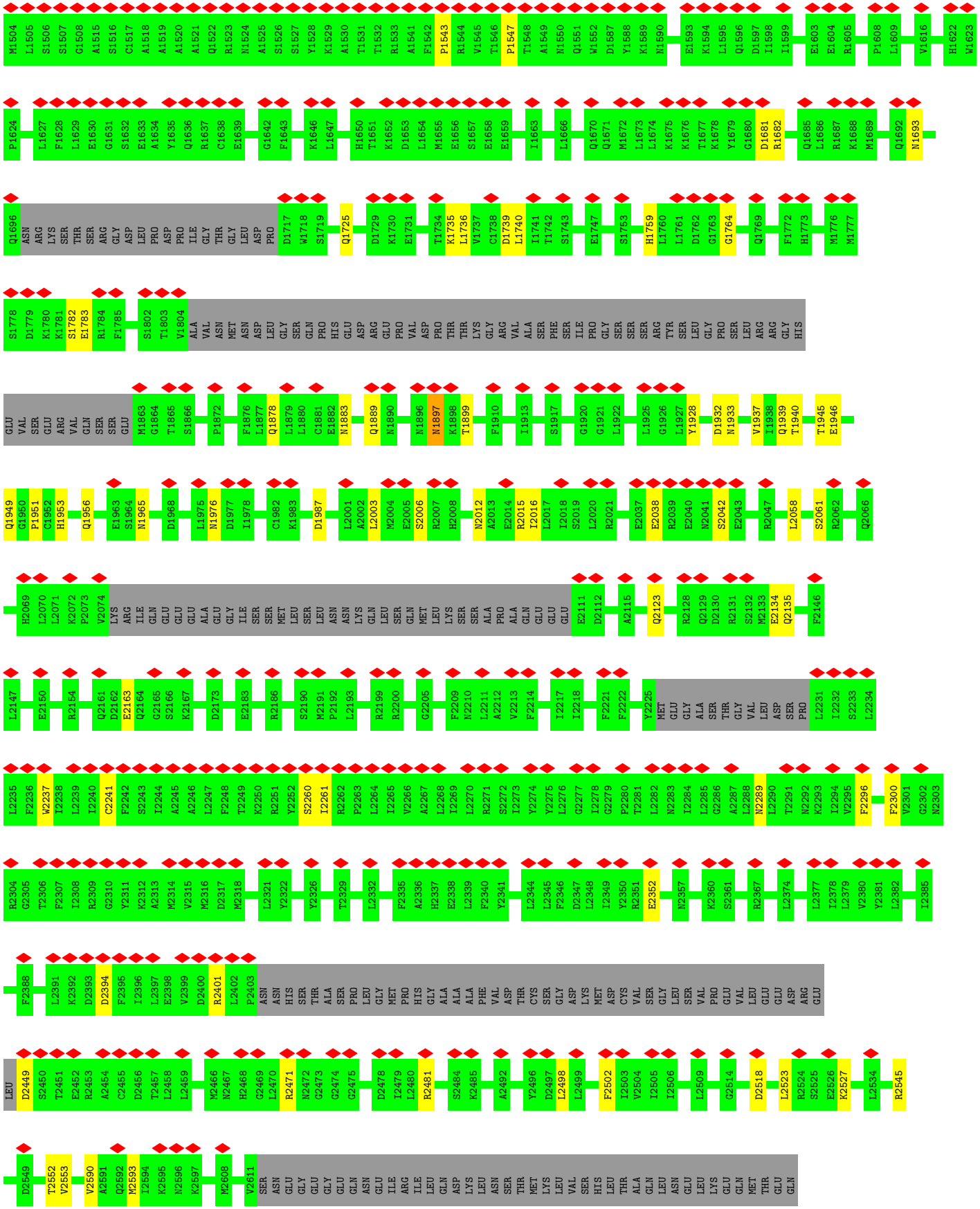

L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1260 A1261 E1262 Q1265 H1266 I1267 F1268 L1269 N1270 N1271 Y1272 Q1273 L1274 C1275 S1276 E1277 I1278 S1279 E1280 P1281 V1282 L1283 Q1284 H1285 F1286 V1287 H1288 L1289 L1290 A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 T1305 V1306 I1307 K1308 A1309 E1310


G1311 K1312 Y1313 V1314 K1315 K1316 C1317 Q1318 D1319 M1320 I1321 M1322 T1323 E1324 L1325 T1326 N1327 A1328 G1329 D1330 D1331 V1332 V1333 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 M1348 M1349 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 S1360 P1361 L1362 M1363 Y1364 H1365 I1366 S1367 L1368 V1369 D1370


L1371 L1372 A1373 A1374 C1375 A1376 E1377 G1378 K1379 N1380 V1381 Y1382 T1383 E1384 I1385 K1386 C1387 T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 V1396 V1397 S1398 V1399 V1400 T1401 H1402 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412 Y1413 V1414 N1415 F1416 V1417 M1418 H1419 C1420 Y1421 V1422 D1423 THR GLU VAL GLU MET LYS GLU


ILE TYR THR SER ASN HIS ILE TRP THR LEU PHE GLU ASN PHE THR LEU ASP MET ALA ARG VAL CYS SER LYS ARG GLU LYS ARG VAL A1434 D1435 P1436 T1437 L1438 E1439 K1440 Y1441 V1442 L1443 S1444 V1445 V1446 L1447 D1448 T1449 I1450 N1451 A1452 F1453 F1454 SER SER PRO PHE SER GLU ASN SER THR SER


LEU GLN THR HIS GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO TRP L1462 Q1463 Q1464 Q1465 H1466 K1467 G1468 S1469 V1470 E1471 A1472 C1473 I1474 R1475 T1476 L1477 A1478 M1479 V1480 A1481 K1482 G1483 R1484 A1490 I1491 L1492 L1493 P1494 M1495 D1496 L1497 D1498 A1499 H1500 I1501 S1502 S1503


M1504 L1505 S1506 S1507 G1508 A1515 S1516 C1517 A1518 A1519 A1520 A1521 Q1522 R1523 N1524 A1525 S1526 S1527 Y1528 K1529 A1530 T1531 T1532 R1533 A1541 F1542 P1543 R1544 V1545 T1546 P1547 T1548 A1549 N1550 Q1551 W1552 D1587 Y1588 K1589 N1590 E1593 K1594 L1595 Q1596 D1597 I1598 I1599 E1603 E1604 R1605 P1608 L1609 V1616 H1622 W1623
P1624 L1627 F1628 L1629 E1630 G1631 S1632 E1633 A1634 Y1635 Q1636 R1637 C1638 E1639 G1642 F1643 K1646 L1647 H1650 T1651 K1652 D1653 L1654 M1655 E1656 S1657 E1658 E1659 I1663 L1666 Q1670 Q1671 M1672 L1673 L1674 K1675 K1676 T1677 K1678 Y1679 G1680 D1681 R1682 Q1685 L1686 R1687 K1688 M1689 Q1692 N1693
Q1696 ASN ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO D1717 W1718 S1719 Q1725 D1729 K1730 E1731 T1734 K1735 L1736 V1737 C1738 D1739 L1740 I1741 T1742 S1743 E1747 S1753 H1759 L1760 L1761 D1762 G1763 G1764 Q1769 F1772 H1773 M1776 M1777
S1778 D1779 K1780 K1781 S1782 E1783 R1784 F1785 S1802 T1803 V1804 ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG VAL ALA SER PHE SER ILE PRO GLY SER SER SER ARG TYR SER LEU GLY PRO SER LEU ARG ARG GLY HIS
GLU VAL SER GLU ARG VAL GLN SER SER GLU M1863 G1864 T1865 S1866 P1872 F1876 L1877 Q1878 L1879 L1880 C1881 E1882 N1883 Q1889 N1890 N1896 N1897 K1898 T1899 F1910 I1913 S1917 G1920 G1921 L1922 L1925 G1926 L1927 Y1928 D1932 N1933 V1937 I1938 Q1939 T1940 T1945 E1946
Q1949 G1950 P1951 C1952 H1953 Q1956 E1963 S1964 N1965 D1968 L1975 N1976 D1977 I1978 C1982 K1983 D1987 L2001 A2002 L2003 M2004 E2005 S2006 R2007 H2008 N2012 A2013 E2014 R2015 I2016 L2017 I2018 S2019 L2020 R2021 E2037 E2038 R2039 E2040 N2041 S2042 E2043 R2047 L2058 S2061 R2062 Q2066
H2069 L2070 L2071 K2072 P2073 V2074 LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU SER LEU ASN ASN LYS GLN GLU SER GLN MET LEU LYS SER SER ALA PRO ALA GLN GLU GLU GLU E2111 D2112 A2115 Q2123 R2128 Q2129 D2130 R2131 S2132 M2133 E2134 Q2135 F2146
L2147 E2150 R2154 Q2161 D2162 E2163 Q2164 G2165 S2166 K2167 D2173 E2183 R2186 S2190 M2191 P2192 L2193 R2199 R2200 G2205 F2209 N2210 L2211 A2212 V2213 F2214 I2217 I2218 F2221 F2222 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO L2231 I2232 S2233 L2234
L2235 F2236 W2237 I2238 L2239 I2240 C2241 F2242 S2243 I2244 A2245 A2246 L2247 F2248 T2249 K2250 R2251 Y2252 S2260 I2261 R2262 P2263 L2264 I2265 V2266 A2267 L2268 I2269 L2270 R2271 S2272 I2273 Y2274 Y2275 L2276 G2277 I2278 G2279 P2280 T2281 L2282 N2283 I2284 L2285 G2286 A2287 L2288 N2289 L2290 T2291 N2292 K2293 I2294 Y2295 F2296 F2300 V2301 G2302 N2303
R2304 G2305 T2306 F2307 I2308 R2309 G2310 Y2311 K2312 A2313 M2314 V2315 M2316 D2317 M2318 L2321 Y2322 Y2326 T2329 L2332 F2335 A2336 H2337 E2338 L2339 F2340 Y2341 L2344 L2345 F2346 D2347 L2348 I2349 Y2350 R2351 E2352 N2357 K2360 S2361 R2367 L2374 L2377 I2378 L2379 V2380 Y2381 L2382 I2385
F2388 L2391 K2392 D2393 D2394 F2395 I2396 L2397 E2398 V2399 D2400 R2401 L2402 P2403 ASN ASN HIS SER THR ALA SER PRO LEU GLY MET PRO HIS GLY ALA ALA ALA PHE VAL ASP THR CYS SER GLY ASP LYS MET ASP CYS VAL SER GLY LEU SER VAL PRO GLU VAL LEU GLU GLU ASP ARG GLU
LEU D2449 S2450 T2451 E2452 R2453 A2454 C2455 D2456 T2457 L2458 L2459 M2466 N2467 H2468 G2469 L2470 R2471 N2472 G2473 G2474 G2475 D2478 I2479 L2480 R2481 S2484 K2485 A2492 Y2496 D2497 L2498 L2499 F2502 I2503 V2504 I2505 I2506 L2509 G2514 D2518 L2523 R2524 S2525 E2526 K2527 L2534 R2545
D2549 T2552 V2553 V2590 A2591 Q2592 M2593 I2594 K2595 N2596 K2597 M2608 V2611 SER ASN GLU GLU GLY GLU GLN ASN GLU ILE ARG ILE LEU GLN ASP LYS LEU ASN SER THR MET LYS LEU VAL SER HIS LEU THR ALA GLN LEU ASN GLU LEU LYS GLU GLN MET THR GLU GLN

ARG
LYS
ARG
ARG
GLN
ARG
LEU
GLY
PHE
VAL
ASP
VAL
GLN
ASN
CYS
ILE
SER
ARG

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 27334 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 61 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | Not provided | |
| Magnification | 22500 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 11.858 | Depositor |
| Minimum map value | -6.272 | Depositor |
| Average map value | -0.006 | Depositor |
| Map value standard deviation | 0.551 | Depositor |
| Recommended contour level | 3.06 | Depositor |
| Map size (Å) | 417.79202, 417.79202, 417.79202 | wwPDB |
| Map dimensions | 384, 384, 384 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.088, 1.088, 1.088 | 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: I3P, ZN

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 | 0.26 | 0/17827 | 0.47 | 3/24087 (0.0%) |
| 1 | B | 0.25 | 0/17827 | 0.47 | 3/24087 (0.0%) |
| 1 | C | 0.25 | 0/17864 | 0.46 | 3/24137 (0.0%) |
| 1 | D | 0.25 | 0/17613 | 0.47 | 4/23801 (0.0%) |
| All | All | 0.25 | 0/71131 | 0.47 | 13/96112 (0.0%) |

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 1547 | PRO | N-CA-CB | 5.71 | 110.15 | 103.30 |
| 1 | C | 1547 | PRO | N-CA-CB | 5.66 | 110.09 | 103.30 |
| 1 | C | 1501 | PRO | N-CA-CB | 5.61 | 110.04 | 103.30 |
| 1 | C | 1543 | PRO | N-CA-CB | 5.61 | 110.03 | 103.30 |
| 1 | B | 1547 | PRO | N-CA-CB | 5.61 | 110.03 | 103.30 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 17510 | 17553 | 17452 | 77 | 0 |
| 1 | B | 17510 | 17555 | 17453 | 75 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | C | 17547 | 17593 | 17492 | 85 | 0 |
| 1 | D | 17308 | 17312 | 17141 | 74 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 24 | 9 | 9 | 1 | 0 |
| 3 | B | 24 | 9 | 9 | 0 | 0 |
| 3 | C | 24 | 9 | 9 | 1 | 0 |
| 3 | D | 24 | 9 | 9 | 0 | 0 |
| All | All | 69975 | 70049 | 69574 | 304 | 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 2.

The worst 5 of 304 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:1054:MET:SD | 1:A:1057:ARG:NH2 | 2.59 | 0.75 |
| 1:C:2163:GLU:O | 1:D:2545:ARG:NH1 | 2.21 | 0.74 |
| 1:A:1085:ARG:NH1 | 1:A:1613:GLU:OE2 | 2.20 | 0.74 |
| 1:A:2545:ARG:NH1 | 1:D:2163:GLU:O | 2.22 | 0.73 |
| 1:D:749:ASP:O | 1:D:753:GLN:NE2 | 2.22 | 0.73 |

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 | 2148/2671 (80%) | 2067 (96%) | 81 (4%) | 0 | 100 100 |
| 1 | B | 2148/2671 (80%) | 2067 (96%) | 81 (4%) | 0 | 100 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | C | 2153/2671 (81%) | 2070 (96%) | 83 (4%) | 0 | 100 | 100 |
| 1 | D | 2139/2671 (80%) | 2063 (96%) | 76 (4%) | 0 | 100 | 100 |
| All | All | 8588/10684 (80%) | 8267 (96%) | 321 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 1924/2385 (81%) | 1919 (100%) | 5 (0%) | 92 | 95 |
| 1 | B | 1924/2385 (81%) | 1919 (100%) | 5 (0%) | 92 | 95 |
| 1 | C | 1928/2385 (81%) | 1924 (100%) | 4 (0%) | 93 | 96 |
| 1 | D | 1875/2385 (79%) | 1870 (100%) | 5 (0%) | 92 | 95 |
| All | All | 7651/9540 (80%) | 7632 (100%) | 19 (0%) | 93 | 96 |

5 of 19 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 171 | ARG |
| 1 | D | 2289 | ASN |
| 1 | D | 2471 | ARG |
| 1 | D | 1976 | ASN |
| 1 | B | 2289 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | I3P | B | 2702 | - | 24,24,24 | 1.28 | 3 (12%) | 36,39,39 | 0.57 | 0 |
| 3 | I3P | D | 2702 | - | 24,24,24 | 1.29 | 3 (12%) | 36,39,39 | 0.64 | 0 |
| 3 | I3P | A | 2702 | - | 24,24,24 | 1.26 | 3 (12%) | 36,39,39 | 0.59 | 0 |
| 3 | I3P | C | 2702 | - | 24,24,24 | 1.29 | 3 (12%) | 36,39,39 | 0.70 | 1 (2%) |

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 |
|---|---|---|---|---|---|---|---|
| 3 | I3P | B | 2702 | - | - | 2/15/39/39 | 0/1/1/1 |
| 3 | I3P | D | 2702 | - | - | 2/15/39/39 | 0/1/1/1 |
| 3 | I3P | A | 2702 | - | - | 0/15/39/39 | 0/1/1/1 |
| 3 | I3P | C | 2702 | - | - | 0/15/39/39 | 0/1/1/1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | D | 2702 | I3P | P4-O4 | 3.21 | 1.65 | 1.59 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | D | 2702 | I3P | P1-O1 | 3.15 | 1.65 | 1.59 |
| 3 | C | 2702 | I3P | P1-O1 | 3.14 | 1.65 | 1.59 |
| 3 | C | 2702 | I3P | P4-O4 | 3.11 | 1.65 | 1.59 |
| 3 | A | 2702 | I3P | P1-O1 | 3.10 | 1.65 | 1.59 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 2702 | I3P | C5-C6-C1 | 2.20 | 113.53 | 108.96 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | B | 2702 | I3P | C1-O1-P1-O11 |
| 3 | B | 2702 | I3P | C1-O1-P1-O12 |
| 3 | D | 2702 | I3P | C3-C4-O4-P4 |
| 3 | D | 2702 | I3P | C4-O4-P4-O43 |

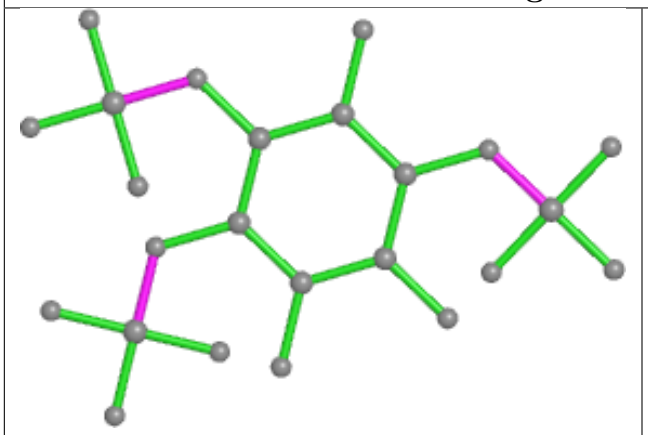
There are no ring outliers.

2 monomers are involved in 2 short contacts:

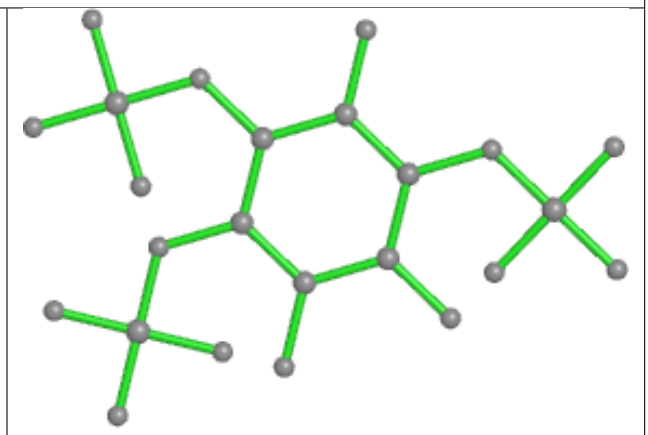
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 2702 | I3P | 1 | 0 |
| 3 | C | 2702 | I3P | 1 | 0 |

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.

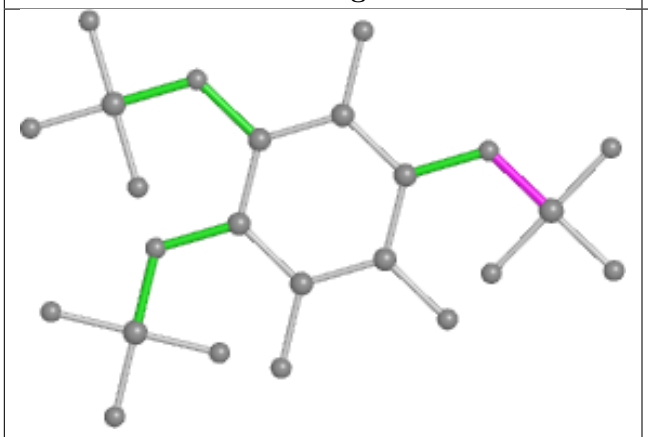
**Ligand I3P B 2702**



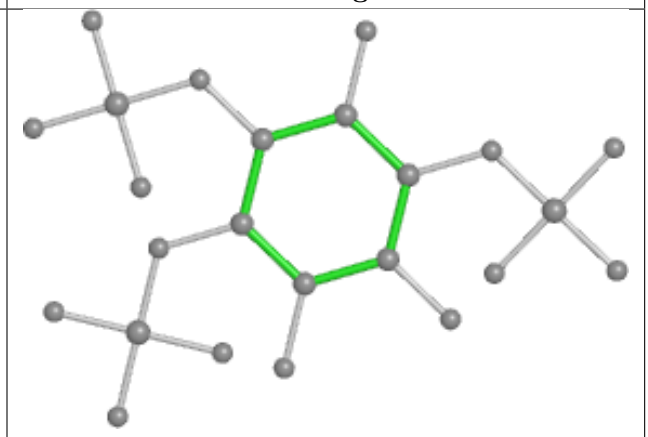
**Bond lengths**



**Bond angles**

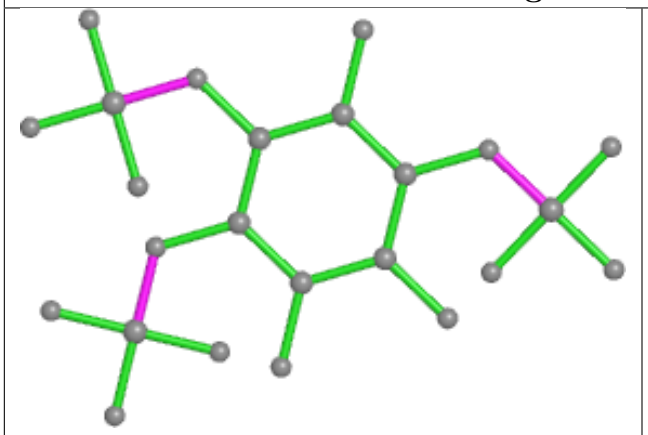


**Torsions**

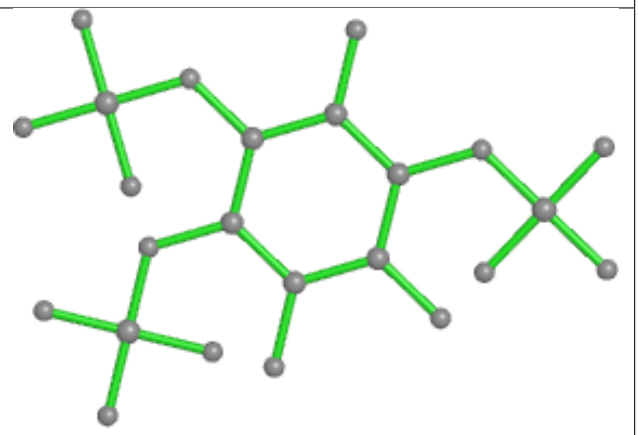


**Rings**

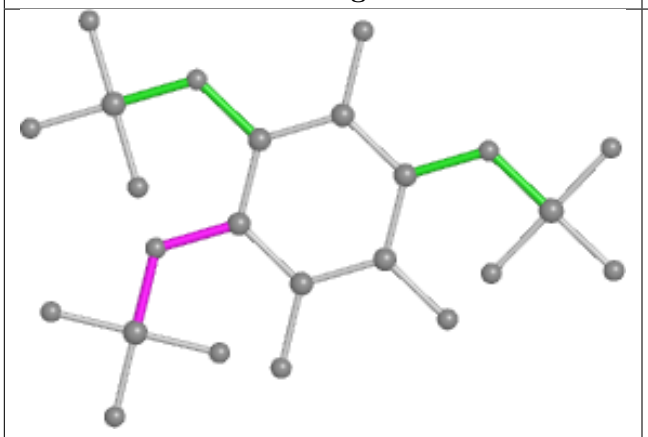
**Ligand I3P D 2702**



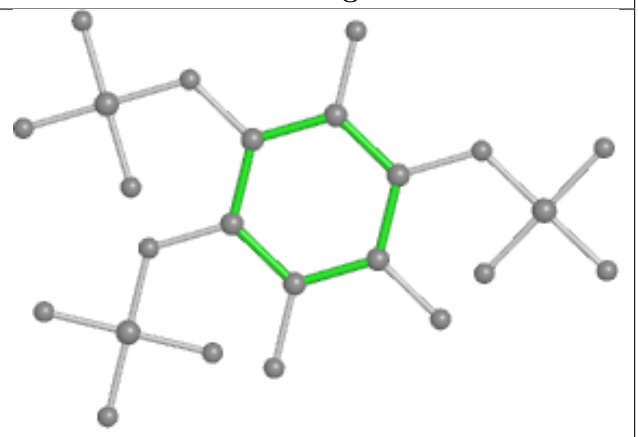
**Bond lengths**



**Bond angles**

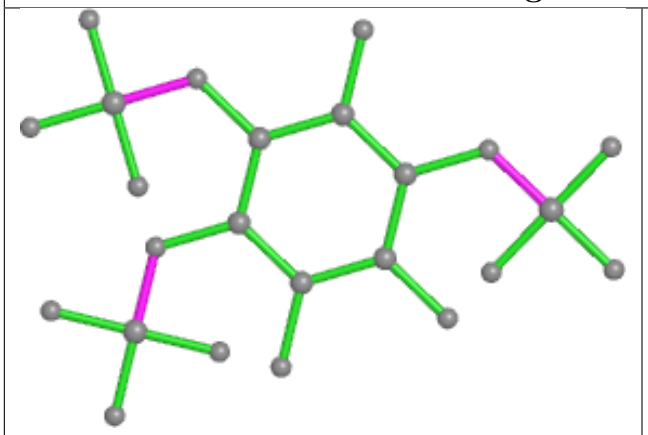


**Torsions**

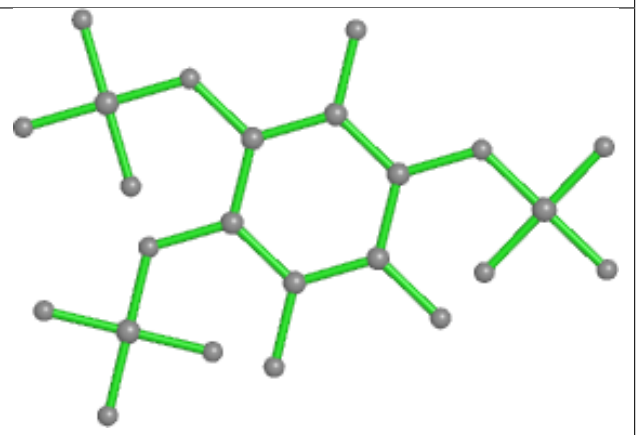


**Rings**

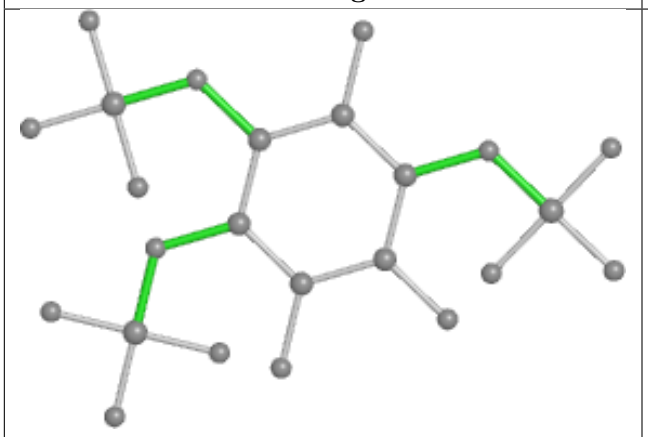
**Ligand I3P A 2702**



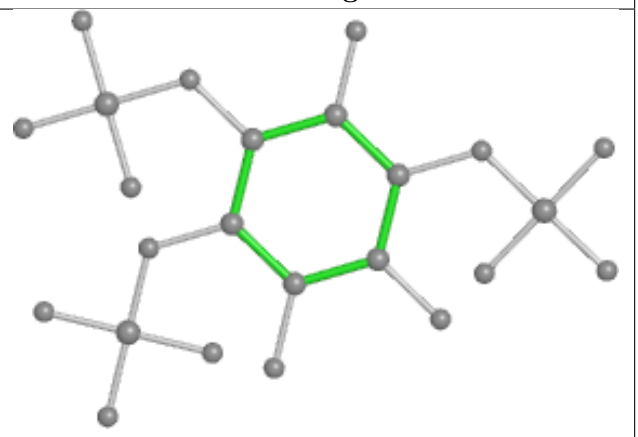
**Bond lengths**



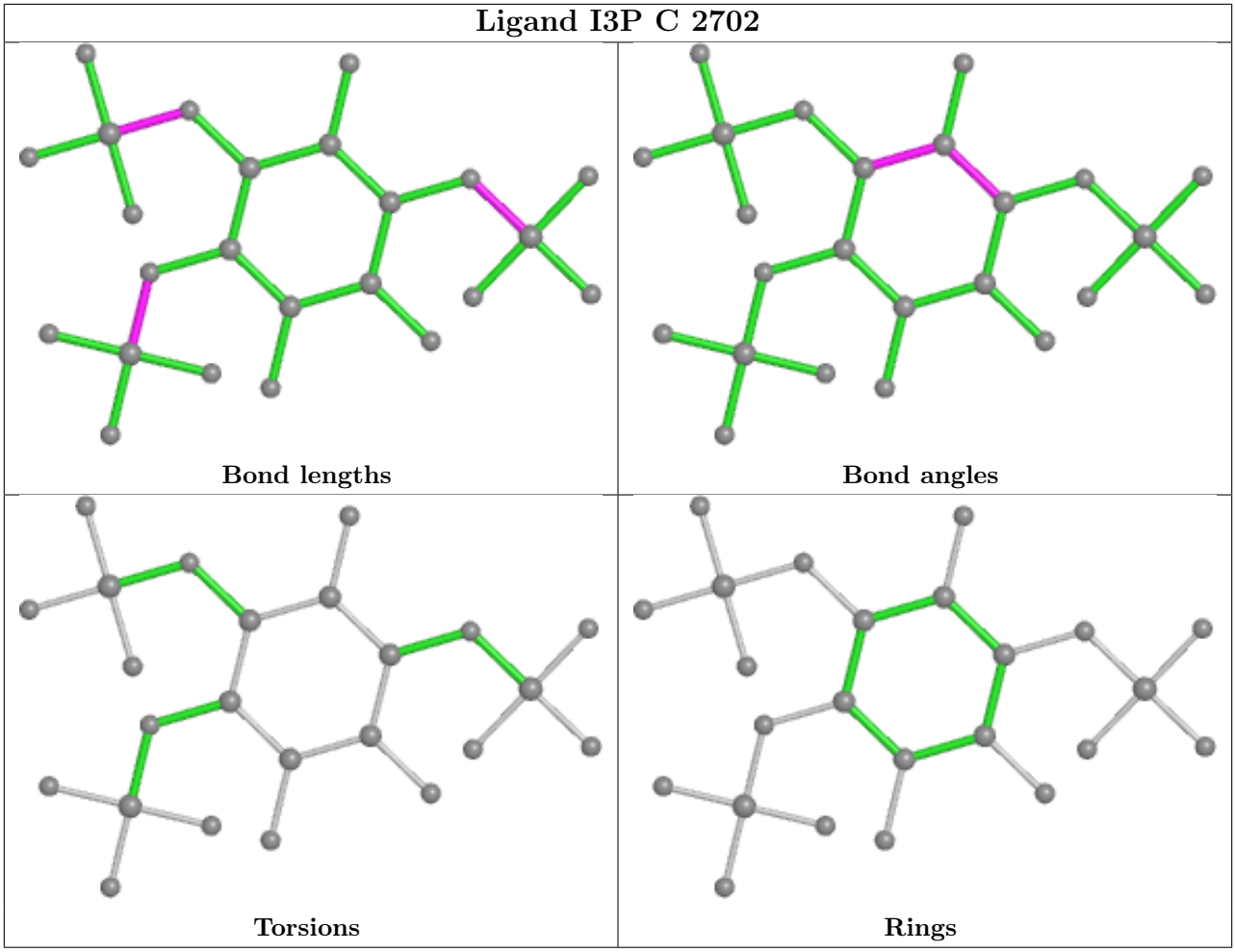
**Bond angles**



**Torsions**



**Rings**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | D | 5 |
| 1 | A | 3 |
| 1 | C | 3 |
| 1 | B | 3 |

The worst 5 of 14 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 1552:TRP | C | 1587:ASP | N | 50.16 |

*Continued on next page...*

*Continued from previous page...*

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | D | 1552:TRP | C | 1587:ASP | N | 50.02 |
| 1 | C | 1552:TRP | C | 1587:ASP | N | 48.78 |
| 1 | B | 1552:TRP | C | 1587:ASP | N | 48.53 |
| 1 | D | 1484:ARG | C | 1490:ALA | N | 15.83 |

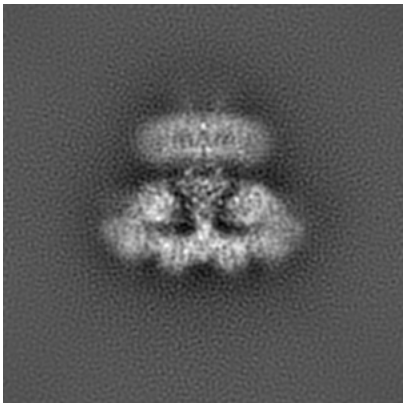
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7987. These allow visual inspection of the internal detail of the map and identification of artifacts.

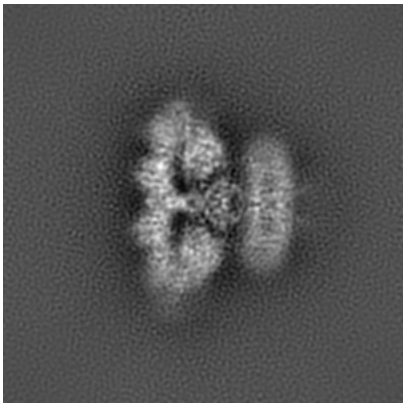
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

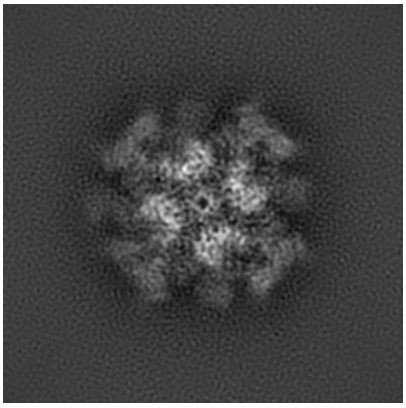
### 6.1.1 Primary map



X



Y

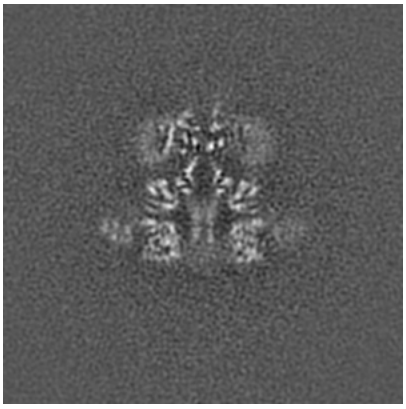


Z

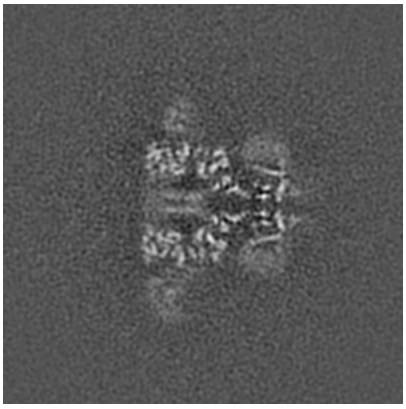
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

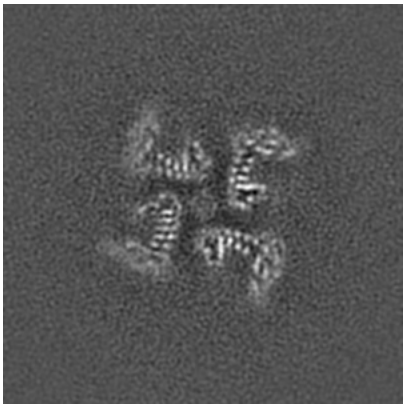
### 6.2.1 Primary map



X Index: 192



Y Index: 192

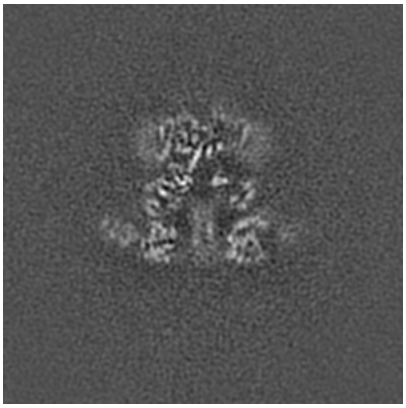


Z Index: 192

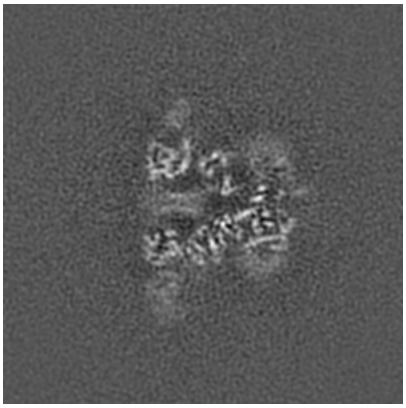
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

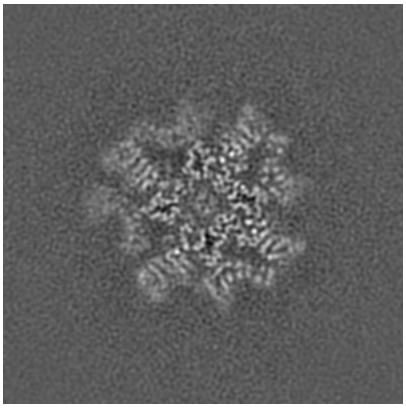
### 6.3.1 Primary map



X Index: 195



Y Index: 189

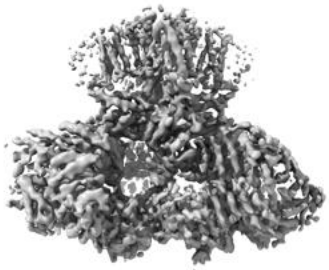


Z Index: 155

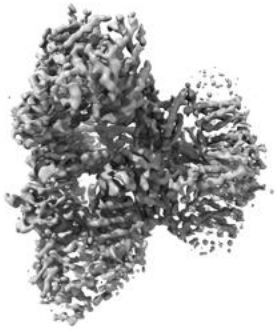
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

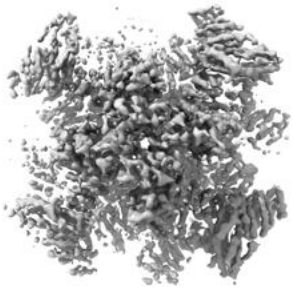
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

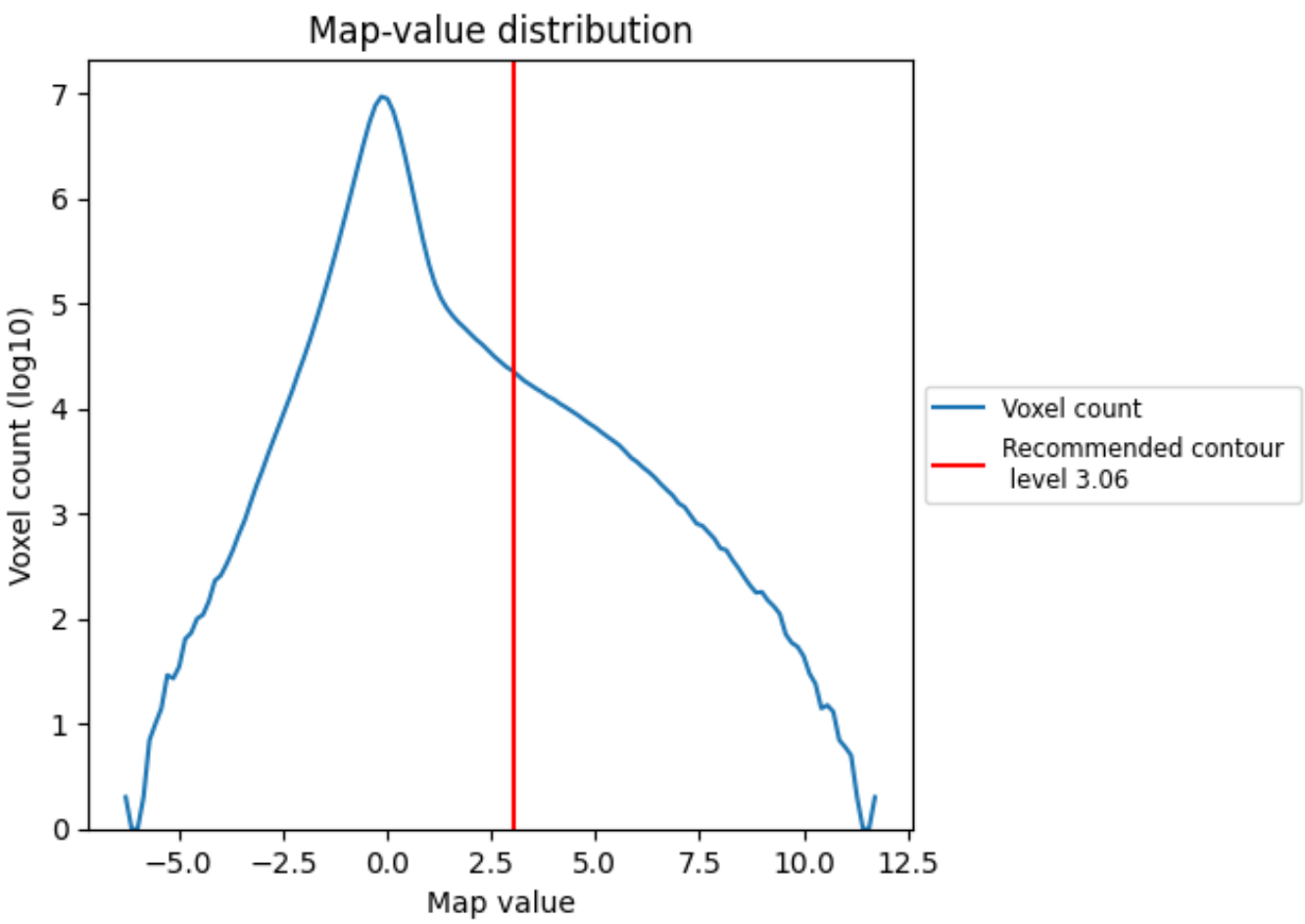
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

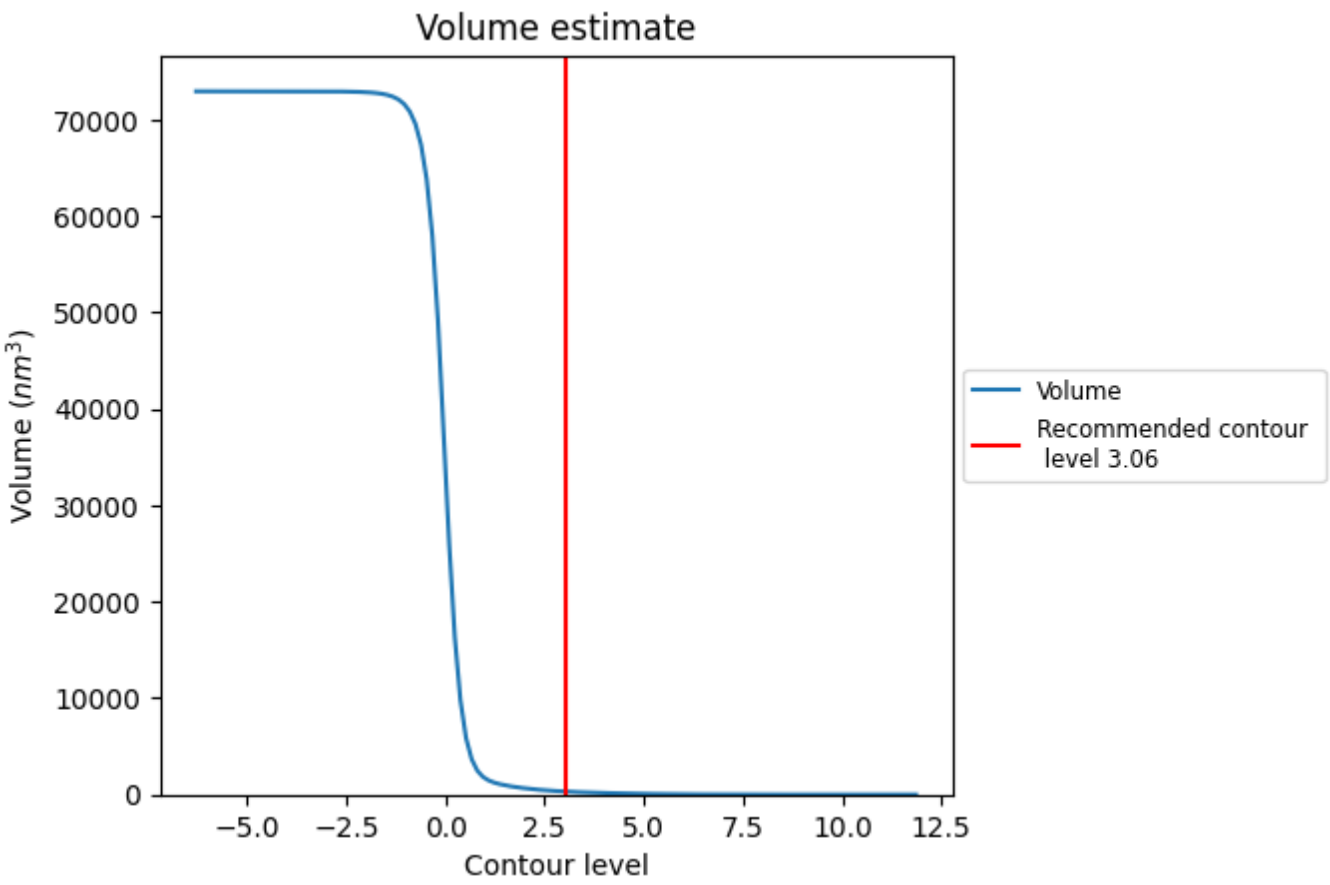
This section contains the results of statistical analysis of the map.

## 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.

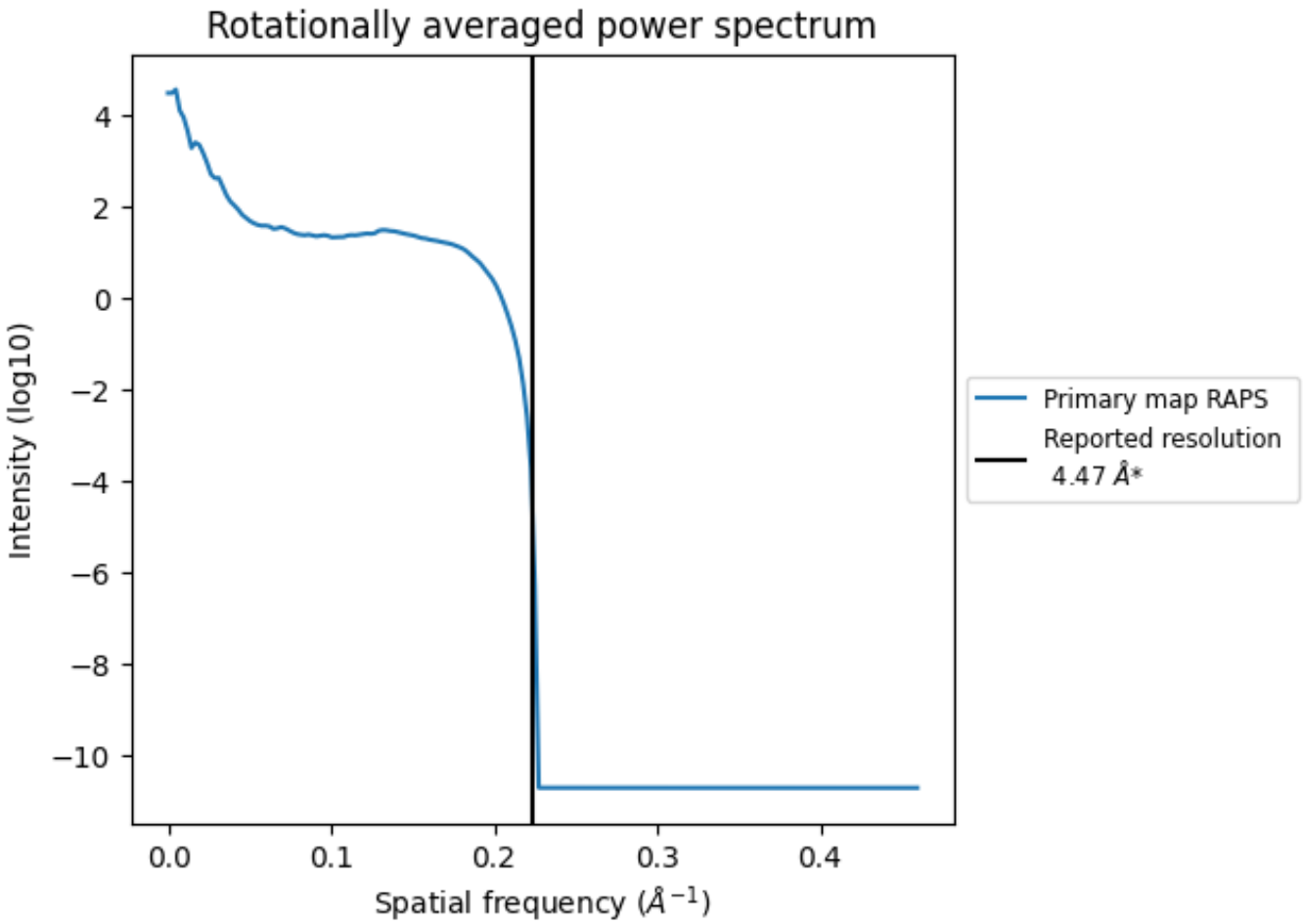
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 308 $nm^3$; this corresponds to an approximate mass of 278 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 0.224 Å$^{-1}$

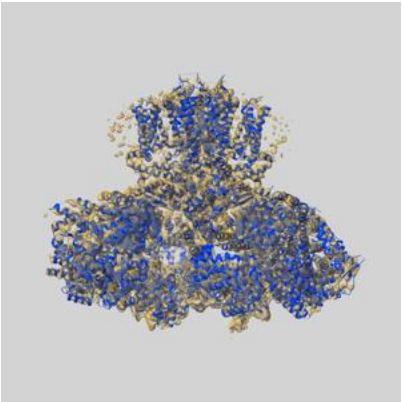
# 8 Fourier-Shell correlation (i)

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

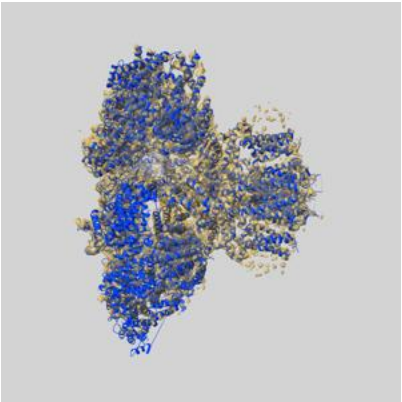
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7987 and PDB model 6DR0. Per-residue inclusion information can be found in section 3 on page 5.

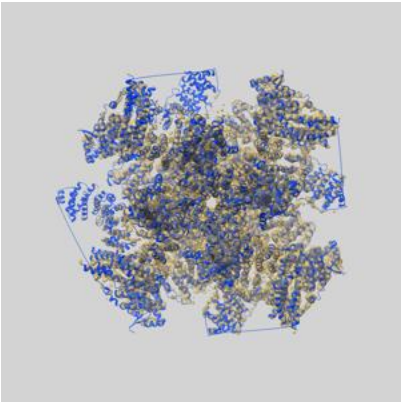
## 9.1 Map-model overlay (i)



X



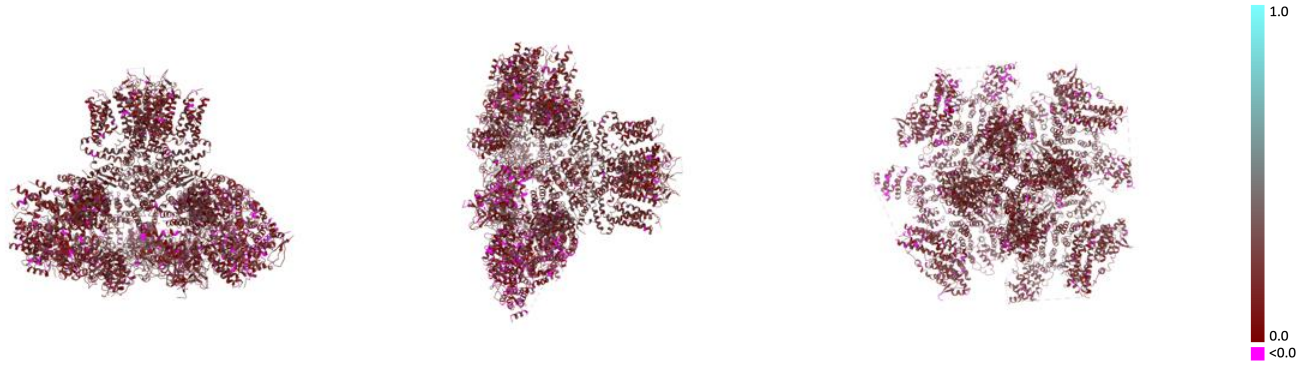
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.06 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.

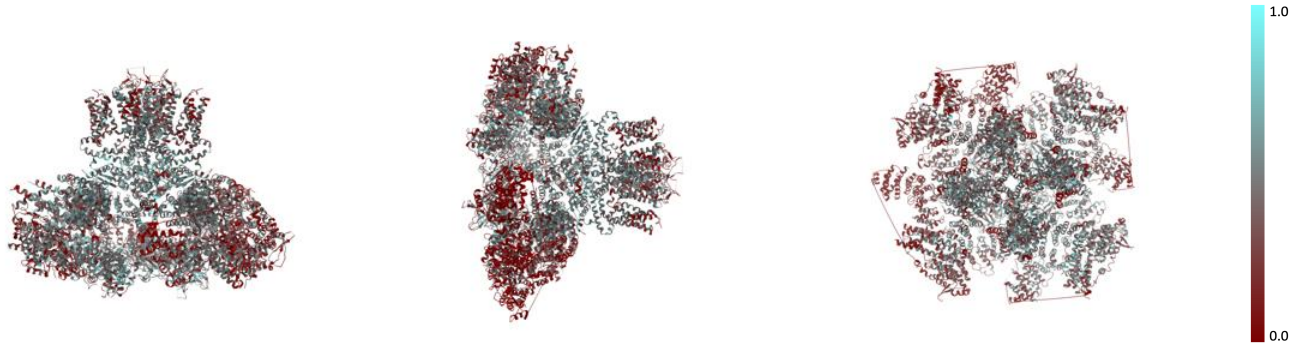
## 9.2 Q-score mapped to coordinate model (i)




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.

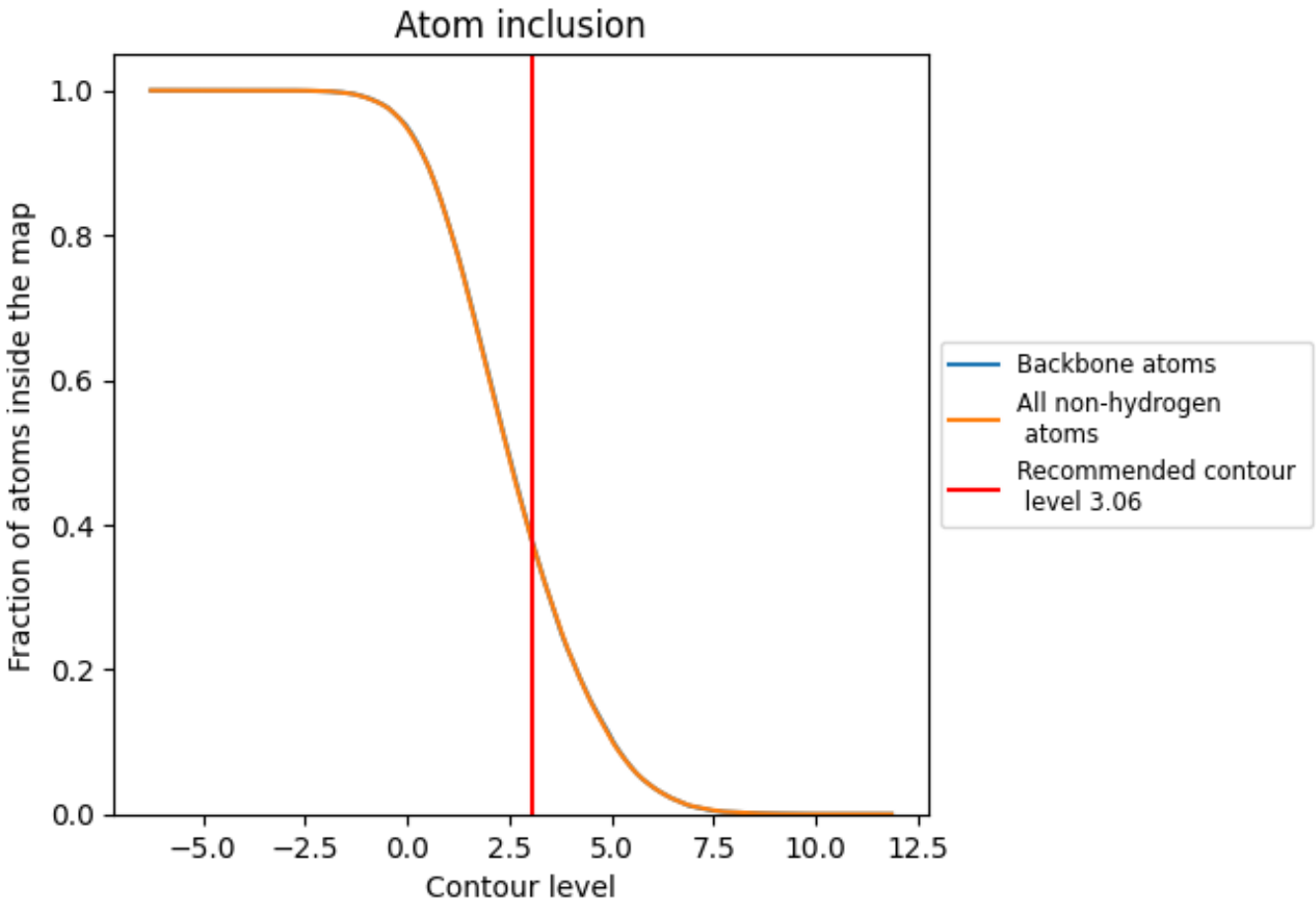
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (3.06).

## 9.4 Atom inclusion (i)




At the recommended contour level, 38% of all backbone atoms, 38% 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 (3.06) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.3759 | 0.1920 |
| A | 0.4514 | 0.2070 |
| B | 0.4068 | 0.2020 |
| C | 0.3124 | 0.1760 |
| D | 0.3518 | 0.1850 |