# Full wwPDB EM Validation Report (i)

Nov 8, 2022 – 12:57 AM EST

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|---|---|---|
| PDB ID | : | 6DRA |
| EMDB ID | : | EMD-7991 |
| Title | : | Low IP3 Ca2+ human type 3 1,4,5-inositol trisphosphate receptor |
| Authors | : | Hite, R.K.; Paknejad, N. |
| Deposited on | : | 2018-06-11 |
| Resolution | : | 3.96 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

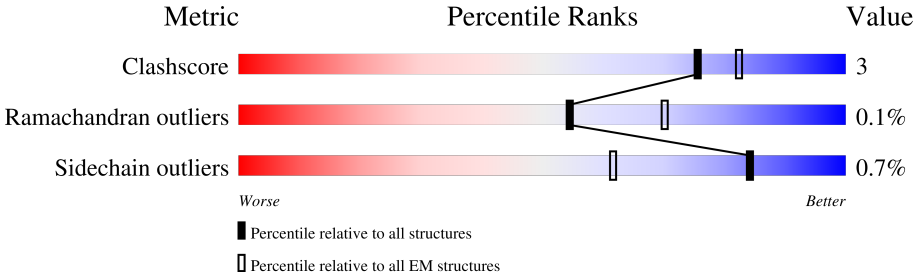
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 3.96 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 | 51% 75% 7% 18% |
| 1 | B | 2671 | 51% 75% 7% 18% |
| 1 | C | 2671 | 51% 74% 7% 18% |
| 1 | D | 2671 | 51% 74% 7% 18% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 139084 atoms, of which 69544 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 | 2191 | 34768 | 11084 | 17386 | 2990 | 3202 | 106 | 0 | 0 |
| 1 | B | 2191 | 34768 | 11084 | 17386 | 2990 | 3202 | 106 | 0 | 0 |
| 1 | C | 2191 | 34768 | 11084 | 17386 | 2990 | 3202 | 106 | 0 | 0 |
| 1 | D | 2191 | 34768 | 11084 | 17386 | 2990 | 3202 | 106 | 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 CALCIUM ION (three-letter code: CA) (formula: Ca).

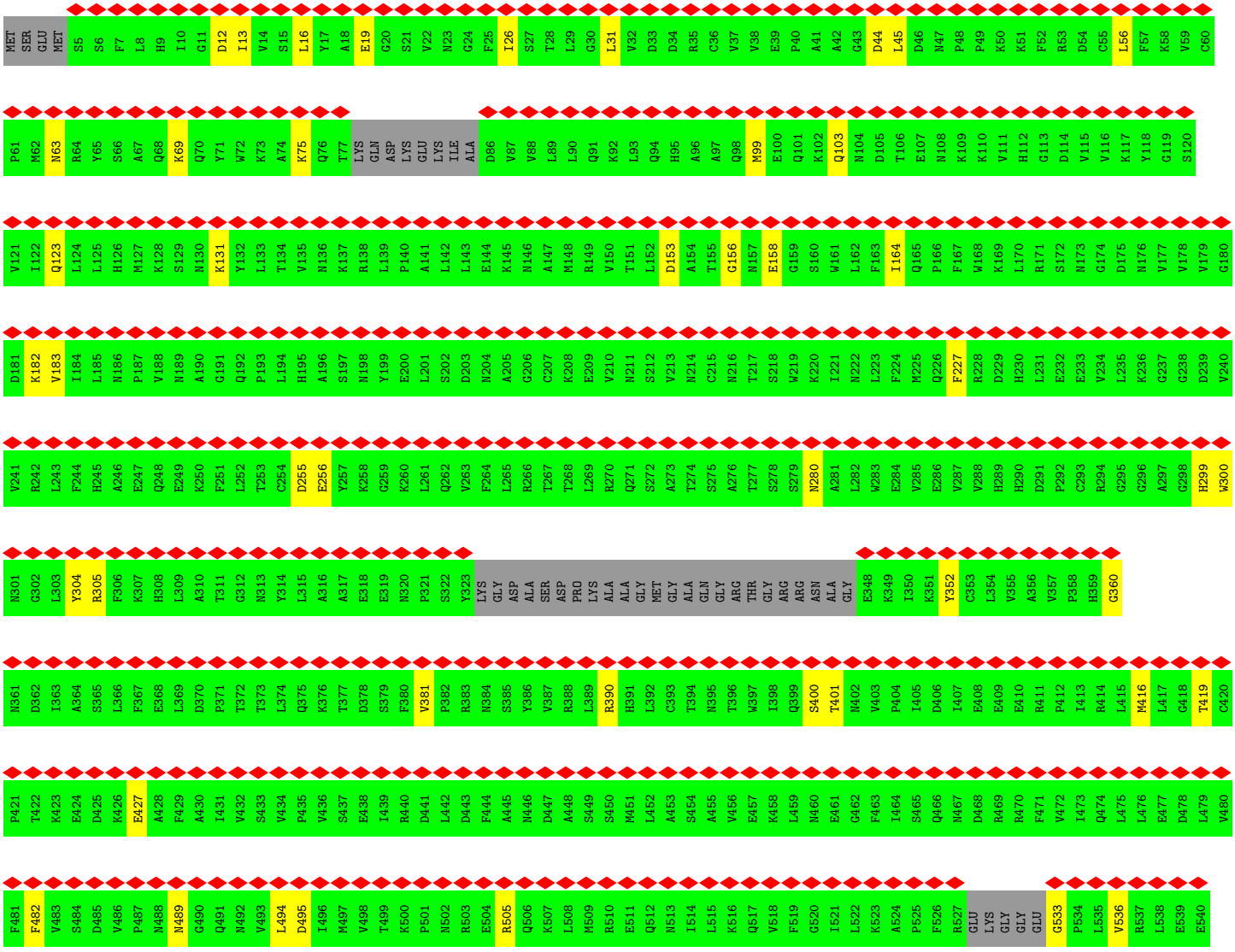
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Ca | |
| 3 | A | 2 | 2 | 2 | 0 |
| 3 | B | 2 | 2 | 2 | 0 |
| 3 | C | 2 | 2 | 2 | 0 |
| 3 | D | 2 | 2 | 2 | 0 |

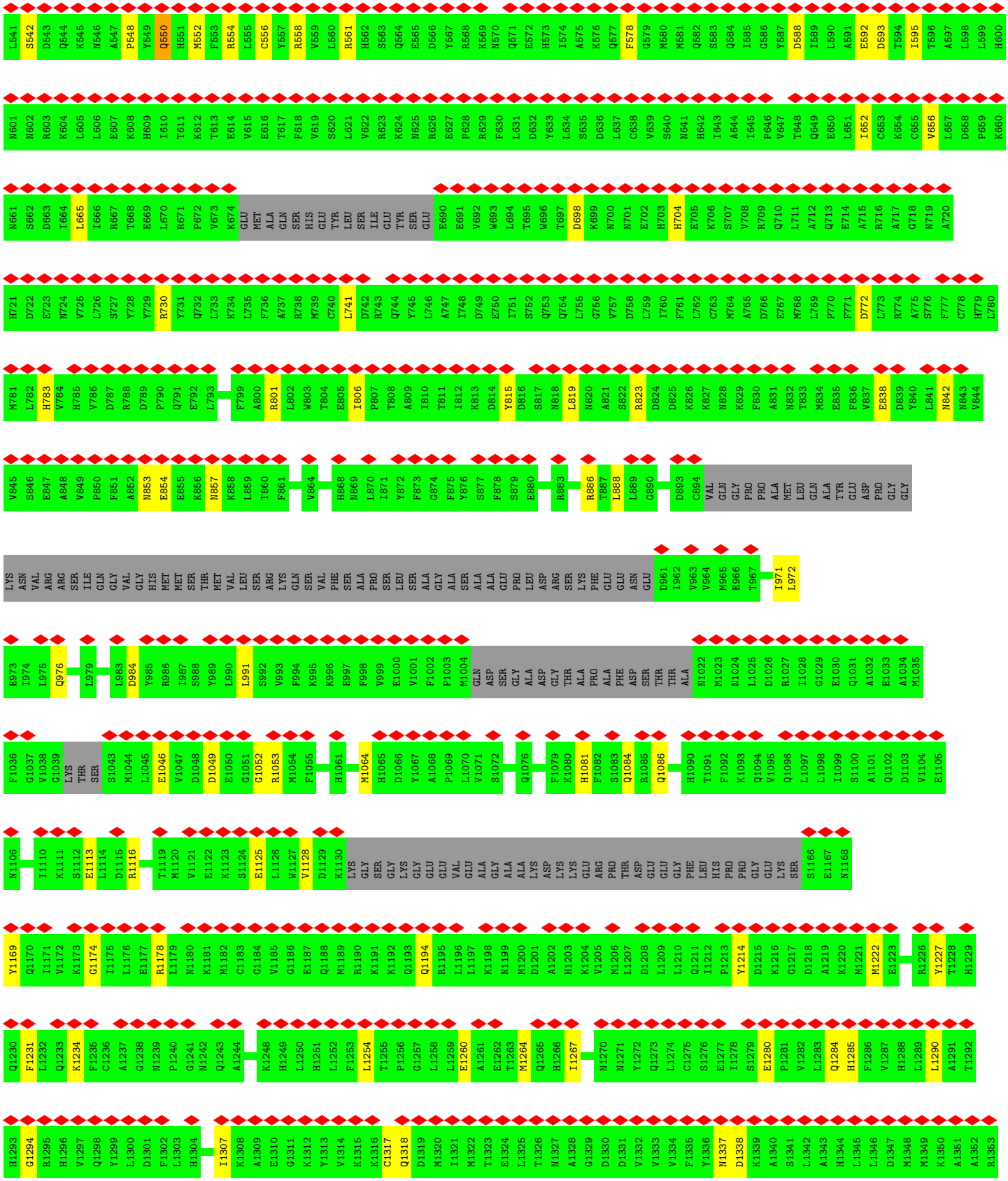
# 3 Residue-property plots (i)

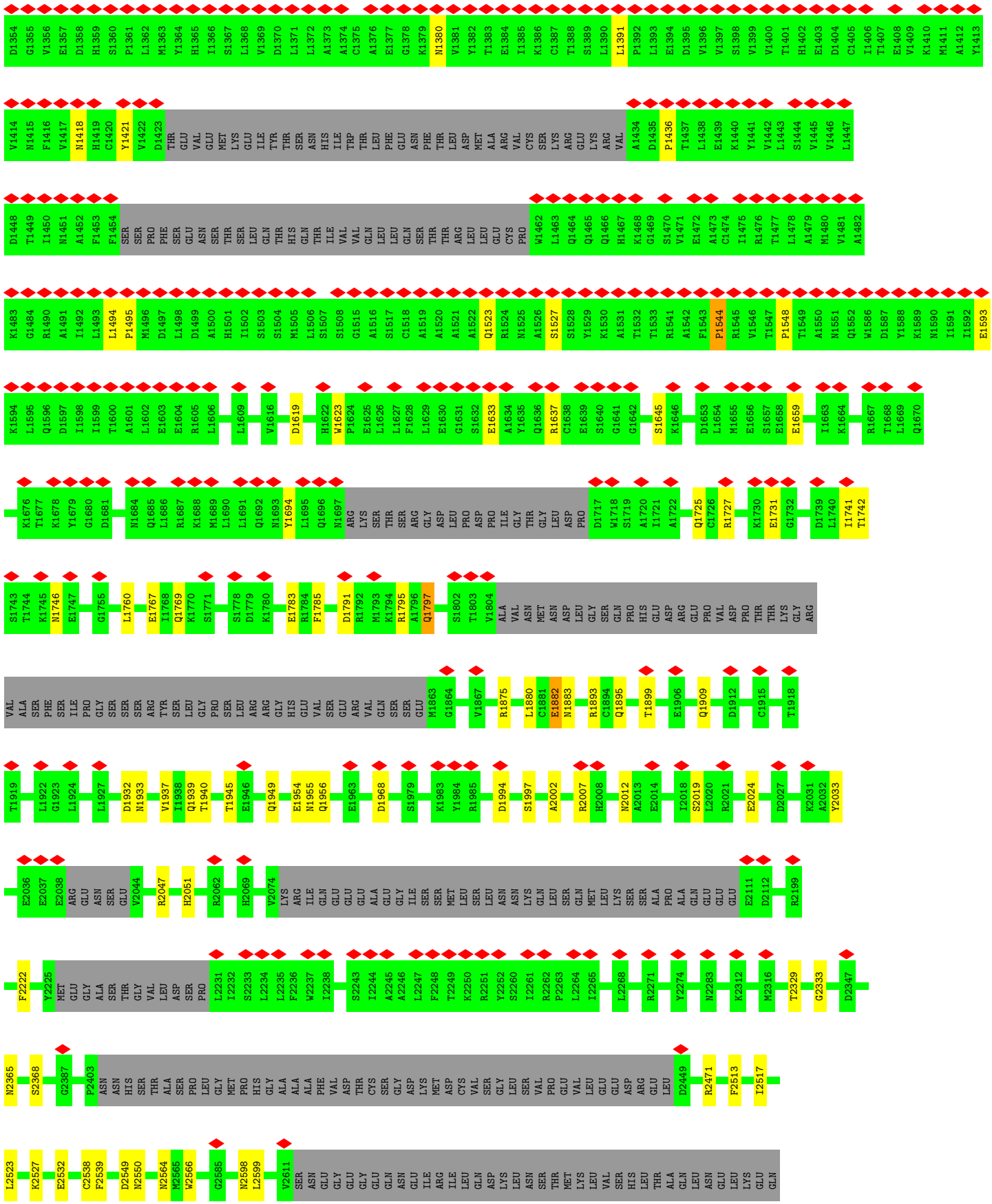
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:




L541 S542 D543 Q544 K545 N546 A547 P548 Y549 Q550 H551 M552 F553 R554 L555 C556 Y557 R558 V559 L560 R561 H562 S563 Q564 E565 D566 Y567 R568 K569 N570 Q571 E572 H573 I574 A575 K576 Q577 F578 G579 M580 M581 Q582 S583 Q584 I585 G586 Y587 D588 I589 L590 A591 E592 D593 T594 I595 T596 A597 L598 L599 H600
N601 N602 R603 K604 K605 L606 E607 K608 H609 I610 T611 K612 T613 E614 V615 E616 T617 F618 V619 S620 L621 V622 R623 K624 N625 R626 E627 P628 R629 F630 L631 D632 Y633 L634 S635 D636 L637 C638 V639 S640 N641 H642 I643 A644 I645 P646 V647 T648 Q649 E650 L651 I652 C653 K654 C655 V656 L657 D658 P659 K660
N661 S662 D663 I664 L665 I666 R667 T668 E669 L670 R671 P672 V673 K674 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 L711 A712 Q713 E714 A715 R716 A717 G718 N719 A720
H721 D722 E723 N724 V725 L726 S727 Y728 Y729 R730 Y731 Q732 L733 K734 L735 F736 A737 R738 M739 C740 L741 D742 R743 Q744 Y745 L746 A747 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 L780
M781 L782 H783 V784 H785 V786 D787 R788 D789 P790 Q791 E792 L793 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 F861 V864 H868 N869 L870 I871 Y872 F873 G874 F875 Y876 S877 F878 S879 E880 R883 R886 T887 L888 L889 G890 D893 C894 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 I971 L972
E973 I974 L975 Q976 L979 L983 D984 Y985 R986 I987 S988 Y989 L990 L991 S992 V993 F994 K995 K996 E997 F998 V999 E1000 V1001 F1002 P1003 M1004 GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 M1023 N1024 L1025 D1026 R1027 I1028 G1029 E1030 Q1031 A1032 E1033 A1034 M1035
F1036 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 F1055 H1061 M1064 H1065 D1066 Y1067 A1068 P1069 L1070 V1071 S1072 Q1076 F1079 K1080 H1081 F1082 S1083 Q1084 R1085 Q1086 H1090 T1091 F1092 K1093 Q1094 V1095 Q1096 L1097 L1098 I1099 S1100 A1101 Q1102 D1103 V1104 E1105
N1106 I1110 K1111 S1112 E1113 L1114 D1115 R1116 T1119 M1120 V1121 E1122 K1123 S1124 E1125 L1126 W1127 V1128 D1129 K1130 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 R1226 Y1227 T1228 H1229
Q1230 F1231 L1232 Q1233 K1234 F1235 C1236 A1237 G1238 N1239 P1240 G1241 N1242 Q1243 A1244 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1260 A1261 E1262 T1263 M1264 Q1265 H1266 I1267 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 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 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 GLN SER THR THR ARG LEU LEU GLU CYS PRO W1462 L1463 Q1464 Q1465 Q1466 H1467 K1468 G1469 S1470 V1471 E1472 A1473 C1474 I1475 R1476 T1477 L1478 A1479 M1480 V1481 A1482
K1483 G1484 R1490 A1491 I1492 L1493 L1494 P1495 M1496 D1497 L1498 D1499 A1500 H1501 I1502 S1503 S1504 M1505 L1506 S1507 S1508 G1515 A1516 S1517 C1518 A1519 A1520 A1521 A1522 Q1523 R1524 N1525 A1526 S1527 S1528 Y1529 K1530 A1531 T1532 T1533 R1541 A1542 F1543 P1544 R1545 V1546 T1547 P1548 T1549 A1550 N1551 Q1552 W1586 D1587 Y1588 K1589 N1590 I1591 I1592 E1593
K1594 L1595 Q1596 D1597 I1598 I1599 T1600 A1601 L1602 E1603 E1604 R1605 L1606 L1609 V1616 D1619 H1622 W1623 P1624 E1625 L1626 L1627 F1628 L1629 E1630 G1631 S1632 E1633 A1634 Y1635 Q1636 R1637 C1638 E1639 S1640 G1641 G1642 S1645 K1646 D1653 L1654 M1655 E1656 S1657 E1658 E1659 I1663 K1664 R1667 T1668 L1669 Q1670
K1676 T1677 K1678 Y1679 G1680 D1681 N1684 Q1685 L1686 R1687 K1688 M1689 L1690 L1691 Q1692 N1693 Y1694 L1695 Q1696 N1697 ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO D1717 W1718 S1719 A1720 I1721 A1722 Q1725 C1726 R1727 K1730 E1731 G1732 D1739 L1740 I1741 T1742
S1743 T1744 K1745 N1746 E1747 G1755 L1760 E1767 I1768 Q1769 K1770 S1771 S1778 D1779 K1780 E1783 R1784 F1785 D1791 R1792 M1793 K1794 R1795 A1796 Q1797 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 V1867 R1875 L1880 C1881 E1882 N1883 R1893 C1894 Q1895 T1899 E1906 Q1909 D1912 C1915 T1918
T1919 L1922 G1923 L1924 L1927 D1932 N1933 V1937 T1938 Q1939 T1940 T1945 E1946 Q1949 E1954 N1955 Q1956 E1963 D1968 S1979 K1983 Y1984 R1985 D1994 S1997 A2002 R2007 H2008 N2012 A2013 E2014 I2018 S2019 L2020 R2021 E2024 D2027 K2031 A2032 Y2033
E2036 E2037 E2038 ARG GLU ASN SER GLU V2044 R2047 H2051 R2062 H2069 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 D2112 R2199
F2222 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO L2231 I2232 S2233 L2234 L2235 F2236 W2237 I2238 S2243 I2244 A2245 A2246 L2247 F2248 T2249 K2250 R2251 Y2252 S2260 I2261 R2262 P2263 L2264 I2265 L2268 R2271 Y2274 N2283 K2312 M2316 T2329 G2333 D2347
N2365 S2368 G2387 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 R2471 F2513 I2517
L2523 K2527 E2532 C2538 F2539 D2549 N2550 N2564 M2565 W2566 G2585 N2598 L2599 V2611 SER ASN GLU GLY 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

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

Chain B: 51% 75% 7% 18%

MET SER GLU MET S5 S6 F7 L8 H9 I10 G11 D12 I13 V14 S15 L16 Y17 A18 E19 G20 S21 V22 N23 G24 F25 I26 S27 T28 L29 G30 L31 V32 D33 D34 R35 C36 V37 V38 E39 P40 A41 A42 G43 D44 L45 D46 N47 P48 P49 K50 K51 F52 R53 D54 C55 L56 F57 K58 V59 C60

P61 M62 N63 R64 Y65 S66 A67 Q68 K69 Q70 Y71 W72 K73 A74 K75 Q76 T77 LYS GLN ASP LYS GLU LYS ILE ALA D86 V87 V88 L89 L90 Q91 K92 L93 Q94 H95 A96 A97 Q98 M99 E100 Q101 K102 Q103 N104 D105 T106 E107 N108 K109 K110 V111 H112 G113 D114 V115 V116 K117 Y118 G119 S120

V121 I122 Q123 L124 L125 H126 M127 K128 S129 N130 K131 Y132 L133 T134 V135 N136 K137 R138 L139 Y140 A141 L142 L143 E144 K145 N146 A147 M148 R149 V150 T151 L152 D153 A154 T155 G156 N157 E158 G159 S160 W161 L162 F163 I164 Q165 P166 F167 W168 K169 L170 R171 S172 N173 G174 D175 N176 V177 V178 V179 G180

D181 K182 V183 I184 L185 N186 P187 V188 N189 A190 G191 Q192 P193 L194 H195 A196 S197 N198 Y199 E200 L201 S202 D203 N204 A205 G206 C207 K208 E209 V210 N211 S212 V213 N214 C215 N216 T217 S218 W219 K220 I221 N222 L223 F224 M225 Q226 F227 R228 D229 H230 L231 E232 E233 V234 L235 K236 G237 G238 D239 V240

V241 R242 L243 F244 H245 A246 E247 Q248 E249 K250 F251 L252 T253 C254 D255 E256 Y257 K258 G259 K260 L261 Q262 V263 F264 L265 R266 T267 T268 L269 R270 Q271 S272 A273 T274 S275 A276 T277 S278 S279 N280 A281 L282 W283 E284 V285 E286 V287 V288 H289 H290 D291 P292 C293 R294 G295 G296 A297 G298 H299 W300

N301 G302 L303 Y304 R305 F306 K307 H308 L309 A310 T311 G312 N313 Y314 L315 A316 A317 E318 E319 N320 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 E348 K349 I350 K351 Y352 C353 L354 V355 A356 V357 P358 H359 G360

N361 D362 I363 A364 S365 L366 F367 E368 L369 D370 P371 T372 T373 L374 Q375 K376 T377 D378 S379 F380 V381 P382 R383 N384 S385 Y386 V387 R388 L389 R390 H391 L392 C393 T394 N395 T396 W397 I398 Q399 S400 T401 N402 V403 P404 I405 D406 I407 E408 E409 E410 R411 P412 I413 R414 L415 M416 L417 G418 T419 C420

P421 T422 K423 E424 D425 K426 E427 A428 F429 A430 I431 V432 S433 V434 P435 V436 S437 E438 I439 R440 D441 L442 D443 F444 A445 N446 D447 A448 S449 S450 M451 L452 A453 S454 A455 V456 E457 K458 L459 N460 E461 G462 F463 I464 S465 Q466 N467 D468 R469 R470 F471 V472 I473 Q474 L475 L476 E477 D478 L479 V480

F481 F482 V483 S484 D485 V486 P487 N488 N489 G490 Q491 N492 V493 L494 D495 I496 M497 N498 T499 K500 P501 N502 R503 E504 R505 Q506 K507 L508 M509 R510 E511 Q512 N513 I514 L515 K516 Q517 V518 F519 G520 I521 L522 K523 A524 P525 F526 R527 GLU LYS GLY GLY GLU G533 P534 L535 V536 R537 L538 E539 E540

L541 S542 D543 Q544 K545 N546 A547 P548 Y549 Q550 H551 N552 F553 R554 L555 C556 Y557 R558 V559 L560 R561 H562 S563 Q564 E565 D566 Y567 R568 K569 N570 Q571 E572 H573 I574 A575 K576 Q577 F578 G579 M580 M581 Q582 S583 Q584 I585 G586 Y587 D588 I589 L590 A591 E592 D593 T594 I595 T596 A597 L598 L599 H600

N601 M602 R603 K604 L605 L606 E607 K608 H609 I610 T611 K612 T613 E614 V615 E616 T617 F618 V619 S620 L621 V622 R623 K624 M625 R626 E627 P628 R629 F630 L631 D632 Y633 L634 S635 D636 L637 C638 V639 S640 N641 H642 I643 A644 I645 P646 V647 T648 Q649 E650 L651 I652 C653 K654 C655 V656 L657 D658 P659 K660

N661 S662 D663 I664 L665 I666 R667 T668 E669 L670 R671 P672 V673 K674 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 L711 A712 Q713 E714 A715 R716 A717 G718 N719 A720

H721 D722 E723 N724 V725 L726 S727 Y728 Y729 R730 Y731 Q732 L733 K734 L735 F736 A737 R738 M739 C740 L741 D742 R743 Q744 Y745 L746 A747 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 L780

M781 L782 H783 V784 H785 V786 D787 R788 D789 P790 Q791 E792 L793 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 F861 V864 H868 N869 L870 I871 Y872 F873 G874 F875 Y876 S877 F878 S879 E880 R883 R886 T887 L888 L889 G890 I891 I892 D893 C894 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 I971

L972 E973 I974 L975 Q976 L979 L983 D984 Y985 R986 I987 S988 Y989 L990 L991 S992 V993 F994 K995 K996 E997 F998 V999 E1000 V1001 F1002 P1003 M1004 GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 M1023 N1024 L1025 D1026 R1027 I1028 G1029 E1030 Q1031 A1032 E1033 A1034

M1035 F1036 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 F1055 L1056 R1057 H1061 M1064 H1065 D1066 Y1067 A1068 P1069 L1070 V1071 S1072 Q1076 F1079 K1080 H1081 F1082 S1083 Q1084 R1085 Q1086 H1090 T1091 F1092 K1093 Q1094 V1095 Q1096 L1097 L1098 I1099 S1100 A1101 Q1102

D1103 V1104 E1105 N1106 Y1107 I1110 K1111 S1112 E1113 L1114 D1115 R1116 T1119 M1120 V1121 E1122 K1123 S1124 E1125 L1126 W1127 V1128 D1129 K1130 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

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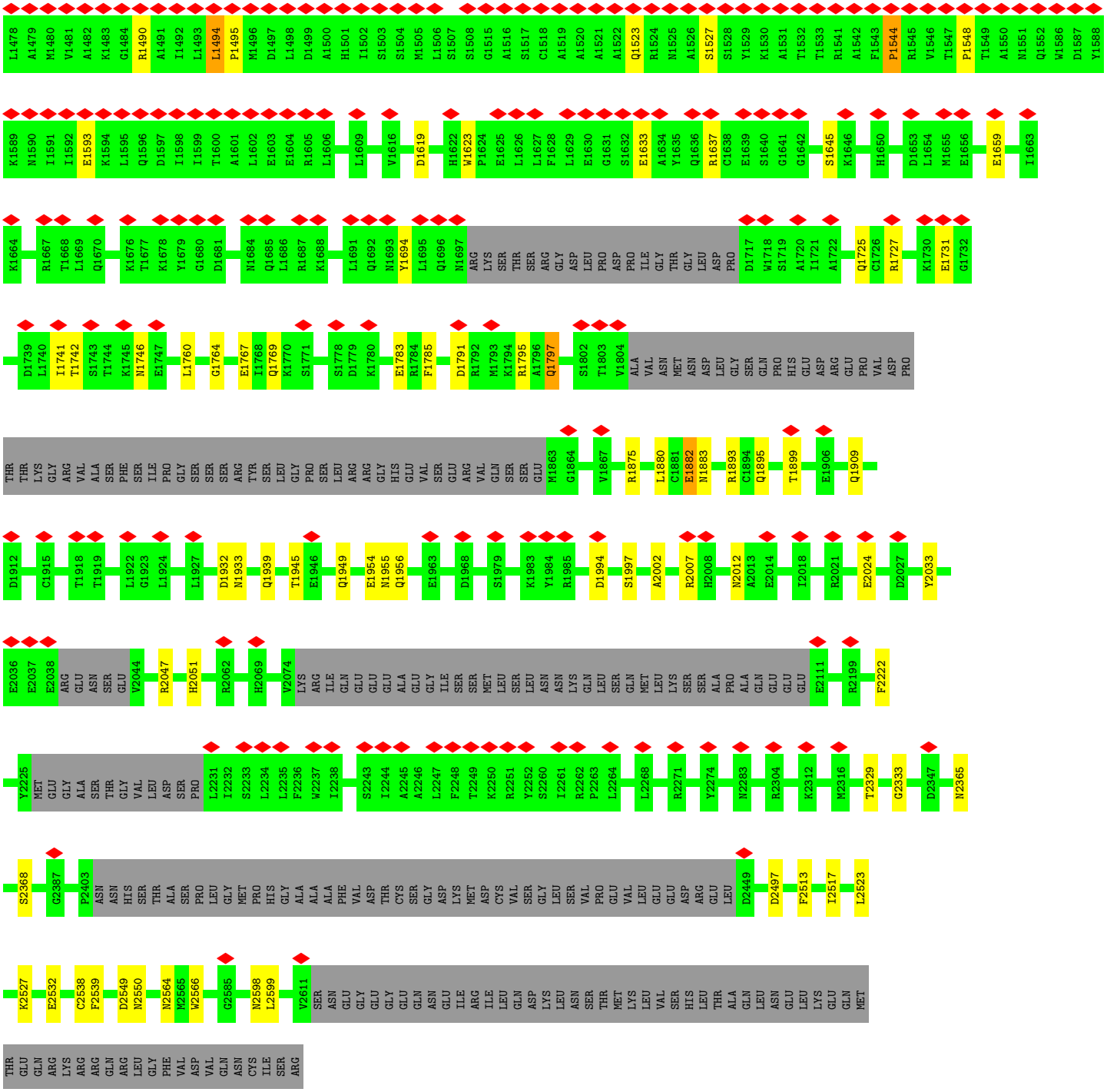
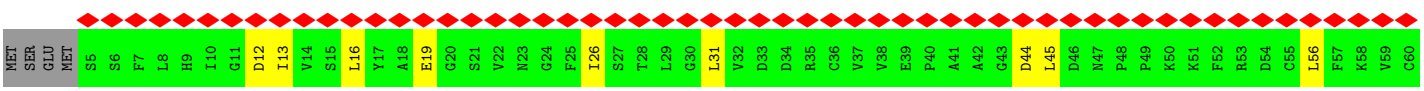


- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain C:



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V121 I122 Q123 L124 L125 H126 M127 K128 S129 N130 K131 Y132 L133 T134 V135 N136 K137 R138 L139 P140 A141 L142 L143 E144 K145 N146 A147 M148 R149 V150 T151 L152 D153 A154 T155 G156 N157 E158 G159 S160 W161 L162 F163 I164 Q165 P166 F167 W168 K169 L170 R171 S172 N173 G174 D175 N176 V177 V178 V179 G180

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V241 R242 L243 F244 H245 A246 E247 Q248 E249 K250 F251 L252 T253 C254 D255 E256 Y257 K258 G259 K260 L261 Q262 V263 F264 L265 R266 T267 T268 L269 R270 Q271 S272 A273 T274 S275 A276 T277 S278 S279 N280 A281 L282 W283 E284 V285 E286 V287 V288 H289 H290 D291 P292 C293 R294 G295 G296 A297 G298 H299 W300

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F481 F482 V483 S484 D485 V486 P487 N488 N489 G490 Q491 N492 V493 L494 D495 I496 M497 V498 T499 K500 P501 N502 R503 E504 R505 Q506 K507 L508 M509 R510 E511 Q512 N513 I514 L515 K516 Q517 V518 F519 G520 I521 L522 K523 A524 P525 F526 R527 GLU LYS GLY GLY GLU G533 P534 L535 V536 R537 L538 E539 E540

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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 I971

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D1103 V1104 E1105 N1106 Y1107 I1110 K1111 S1112 E1113 L1114 D1115 R1116 T1119 M1120 V1121 E1122 K1123 S1124 E1125 L1126 W1127 V1128 D1129 K1130 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

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V1409 K1410 M1411 A1412 Y1413 V1414 N1415 F1416 V1417 N1418 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 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 W1462 L1463 Q1464 Q1465 Q1466 H1467 K1468 G1469 S1470 V1471 E1472 A1473 C1474 I1475 R1476 T1477

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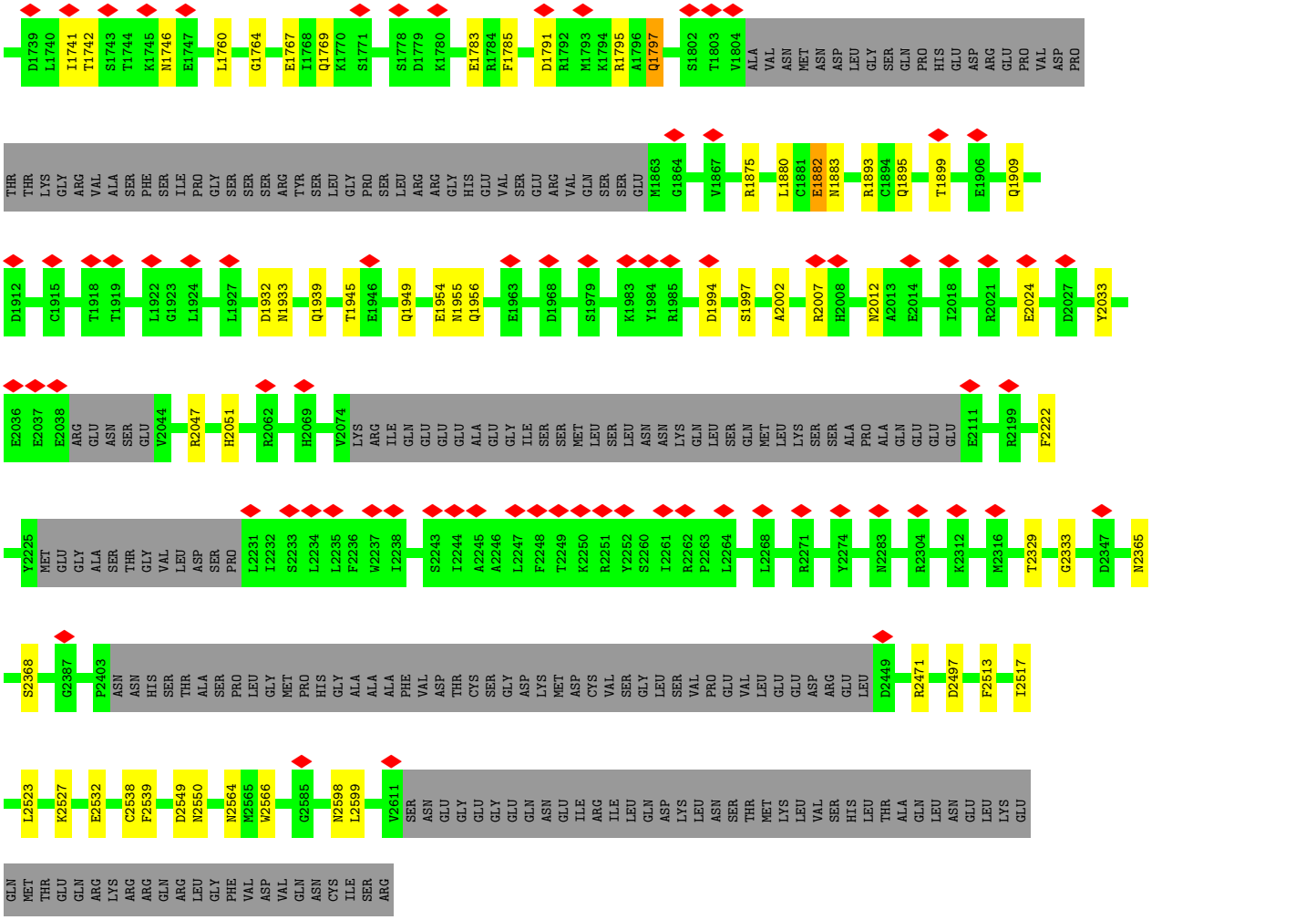
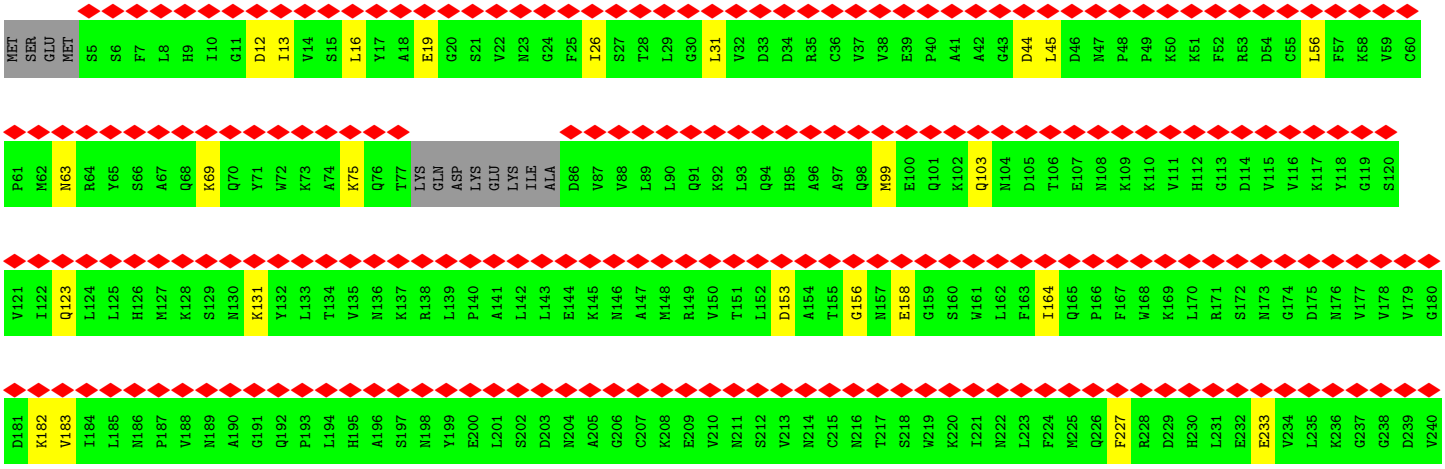
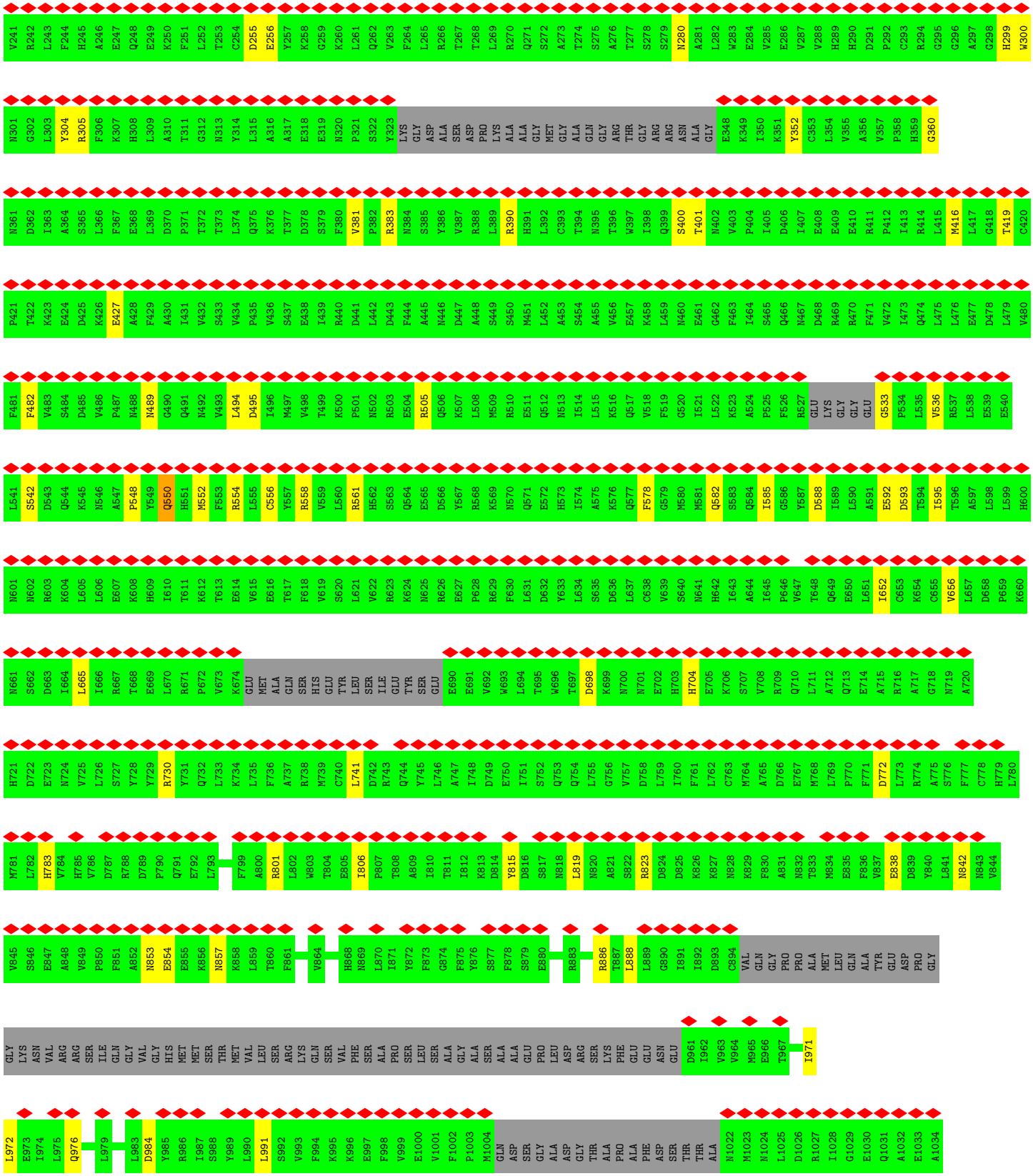



- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D:

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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 I971
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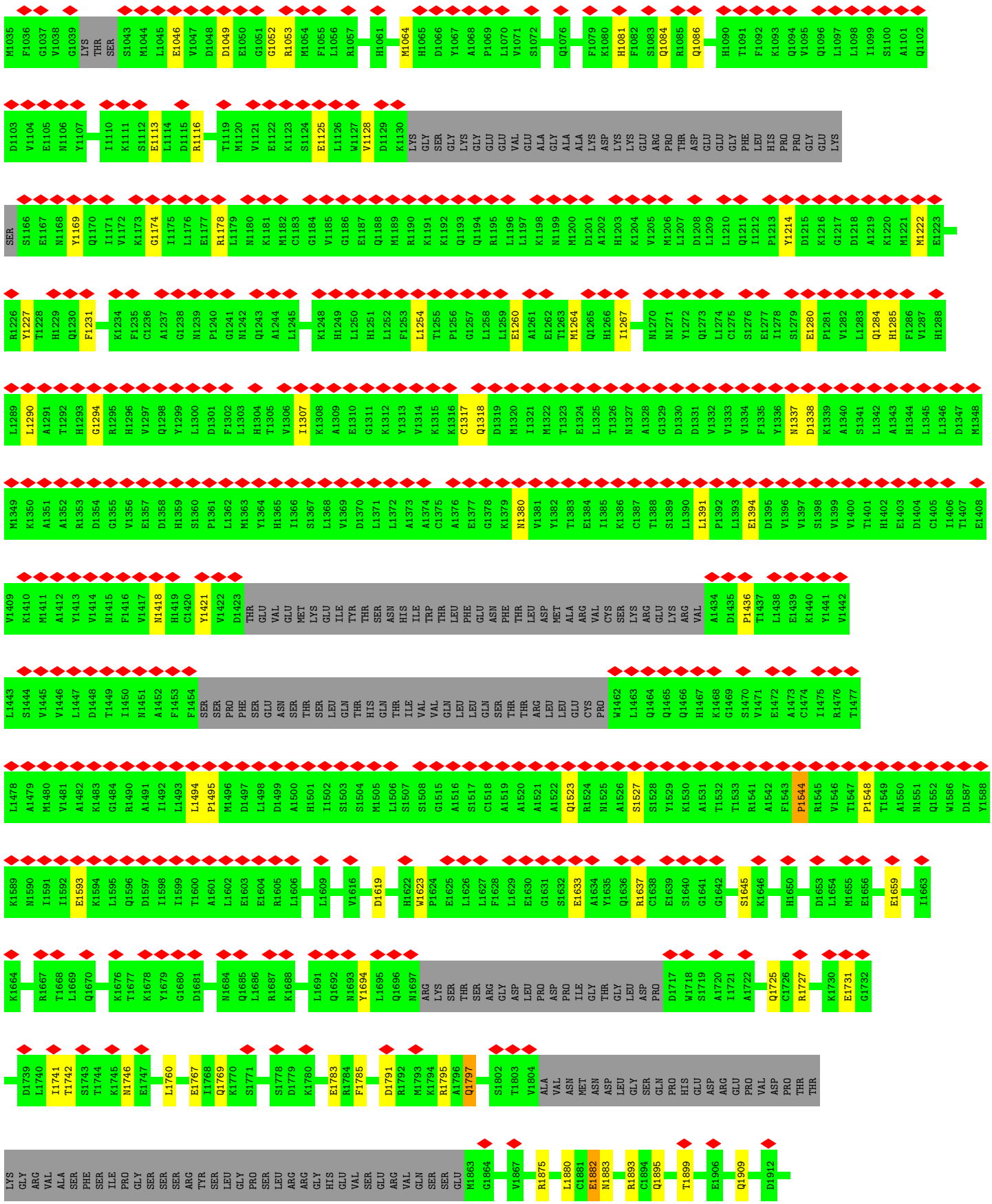
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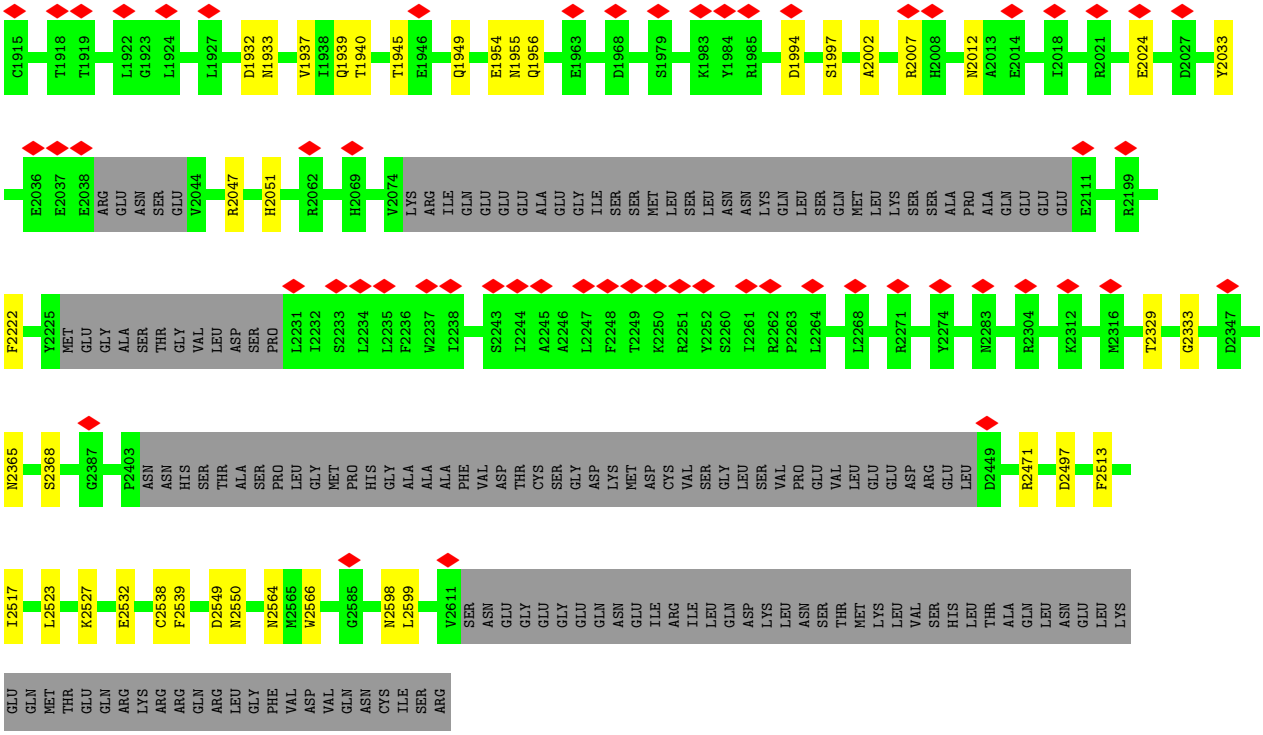
D1103 V1104 E1105 N1106 Y1107 I1110 K1111 S1112 E1113 L1114 D1115 R1116 T1119 M1120 V1121 E1122 K1123 S1124 E1125 L1126 V1127 V1128 D1129 K1130 LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS
SER S1166 E1167 N1168 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
R1226 Y1227 T1228 H1229 Q1230 F1231 K1234 F1235 C1236 A1237 G1238 N1239 P1240 G1241 N1242 Q1243 A1244 L1245 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1260 A1261 E1262 T1263 M1264 Q1265 H1266 I1267 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 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 GLU GLN SER THR THR ARG LEU LEU GLU CYS PRO W1462 L1463 Q1464 Q1465 Q1466 H1467 K1468 G1469 S1470 V1471 E1472 A1473 C1474 I1475 R1476 T1477
L1478 A1479 M1480 V1481 A1482 K1483 G1484 R1490 A1491 I1492 I1493 L1494 P1495 M1496 D1497 L1498 D1499 A1500 H1501 I1502 S1503 S1504 M1505 L1506 S1507 S1508 G1515 A1516 S1517 C1518 A1519 A1520 A1521 A1522 Q1523 R1524 N1525 A1526 S1527 S1528 Y1529 K1530 A1531 T1532 T1533 R1541 A1542 E1543 P1544 R1545 V1546 V1547 P1548 T1549 A1550 N1551 Q1552 W1586 D1587 Y1588
K1589 N1590 I1591 I1592 E1593 K1594 L1595 Q1596 D1597 I1598 I1599 T1600 A1601 L1602 E1603 E1604 R1605 L1606 L1609 V1616 D1619 H1622 W1623 P1624 E1625 L1626 L1627 F1628 L1629 E1630 G1631 S1632 E1633 A1634 Y1635 Q1636 R1637 C1638 E1639 S1640 G1641 G1642 S1645 K1646 H1650 D1653 L1654 M1655 E1656 E1659 I1663
K1664 R1667 T1668 L1669 Q1670 K1676 T1677 K1678 Y1679 G1680 D1681 N1684 Q1685 L1686 R1687 K1688 L1691 Q1692 N1693 Y1694 L1695 Q1696 N1697 ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO D1717 W1718 S1719 A1720 I1721 A1722 Q1725 C1726 R1727 K1730 E1731 G1732
D1739 L1740 I1741 T1742 S1743 T1744 K1745 N1746 E1747 L1760 E1767 I1768 Q1769 K1770 S1771 S1778 D1779 K1780 E1783 R1784 F1785 D1791 R1792 M1793 K1794 R1795 A1796 Q1797 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 V1867 R1875 L1880 C1881 E1882 N1883 R1893 C1894 Q1895 T1899 E1906 Q1909 D1912


C1915
T1918
T1919
L1922
G1923
L1924
L1927
D1932
N1933
V1937
I1938
Q1939
T1940
T1945
E1946
Q1949
E1954
N1955
Q1956
E1963
D1968
S1979
K1983
Y1984
R1985
D1994
S1997
A2002
R2007
H2008
N2012
A2013
E2014
I2018
R2021
E2024
D2027
Y2033
E2036
E2037
E2038
ARG GLU ASN SER GLU
V2044
R2047
H2051
R2062
H2069
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
R2199
F2222
Y2225
MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO
L2231
I2232
S2233
L2234
L2235
F2236
W2237
I2238
S2243
I2244
A2245
A2246
L2247
F2248
T2249
K2250
R2251
Y2252
S2260
I2261
R2262
P2263
L2264
L2268
R2271
Y2274
N2283
R2304
K2312
M2316
T2329
G2333
D2347
N2365
S2368
G2387
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
R2471
D2497
F2513
I2517
L2523
K2527
E2532
C2538
F2539
D2549
N2550
N2564
M2565
W2566
G2585
N2598
L2599
V2611
SER ASN GLU GLY 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 | 49087 | 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 | 22.614 | Depositor |
| Minimum map value | -17.513 | Depositor |
| Average map value | -0.008 | Depositor |
| Map value standard deviation | 0.623 | Depositor |
| Recommended contour level | 2.8 | 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: CA, 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 | 0.25 | 0/17689 | 0.45 | 4/23903 (0.0%) |
| 1 | B | 0.25 | 0/17689 | 0.45 | 4/23903 (0.0%) |
| 1 | C | 0.25 | 0/17689 | 0.45 | 4/23903 (0.0%) |
| 1 | D | 0.25 | 0/17689 | 0.45 | 4/23903 (0.0%) |
| All | All | 0.25 | 0/70756 | 0.45 | 16/95612 (0.0%) |

There are no bond length outliers.

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1544 | PRO | N-CA-CB | 5.80 | 110.26 | 103.30 |
| 1 | B | 1544 | PRO | N-CA-CB | 5.80 | 110.26 | 103.30 |
| 1 | D | 1544 | PRO | N-CA-CB | 5.80 | 110.26 | 103.30 |
| 1 | C | 1544 | PRO | N-CA-CB | 5.77 | 110.22 | 103.30 |
| 1 | B | 1495 | PRO | N-CA-CB | 5.70 | 110.14 | 103.30 |
| 1 | C | 1495 | PRO | N-CA-CB | 5.70 | 110.14 | 103.30 |
| 1 | D | 1495 | PRO | N-CA-CB | 5.70 | 110.14 | 103.30 |
| 1 | A | 1495 | PRO | N-CA-CB | 5.69 | 110.12 | 103.30 |
| 1 | A | 1548 | PRO | N-CA-CB | 5.61 | 110.03 | 103.30 |
| 1 | D | 1548 | PRO | N-CA-CB | 5.61 | 110.03 | 103.30 |
| 1 | B | 1548 | PRO | N-CA-CB | 5.58 | 110.00 | 103.30 |
| 1 | C | 1548 | PRO | N-CA-CB | 5.58 | 110.00 | 103.30 |
| 1 | A | 1436 | PRO | N-CA-CB | 5.53 | 109.93 | 103.30 |
| 1 | B | 1436 | PRO | N-CA-CB | 5.52 | 109.93 | 103.30 |
| 1 | C | 1436 | PRO | N-CA-CB | 5.52 | 109.93 | 103.30 |
| 1 | D | 1436 | PRO | N-CA-CB | 5.52 | 109.92 | 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 | 17382 | 17386 | 17215 | 105 | 0 |
| 1 | B | 17382 | 17386 | 17215 | 106 | 0 |
| 1 | C | 17382 | 17386 | 17215 | 109 | 0 |
| 1 | D | 17382 | 17386 | 17215 | 107 | 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 | 2 | 0 | 0 | 0 | 0 |
| 3 | B | 2 | 0 | 0 | 0 | 0 |
| 3 | C | 2 | 0 | 0 | 0 | 0 |
| 3 | D | 2 | 0 | 0 | 0 | 0 |
| All | All | 69540 | 69544 | 68860 | 424 | 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 3.

All (424) 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:1214:TYR:OH | 1:A:1222:MET:SD | 2.46 | 0.74 |
| 1:D:1214:TYR:OH | 1:D:1222:MET:SD | 2.46 | 0.74 |
| 1:A:75:LYS:NZ | 1:A:489:ASN:O | 2.21 | 0.74 |
| 1:B:1893:ARG:NH1 | 1:B:1955:ASN:OD1 | 2.21 | 0.74 |
| 1:A:1893:ARG:NH1 | 1:A:1955:ASN:OD1 | 2.21 | 0.73 |
| 1:C:1893:ARG:NH1 | 1:C:1955:ASN:OD1 | 2.21 | 0.73 |
| 1:D:75:LYS:NZ | 1:D:489:ASN:O | 2.21 | 0.73 |
| 1:C:75:LYS:NZ | 1:C:489:ASN:O | 2.21 | 0.73 |
| 1:D:1893:ARG:NH1 | 1:D:1955:ASN:OD1 | 2.21 | 0.73 |
| 1:B:1214:TYR:OH | 1:B:1222:MET:SD | 2.46 | 0.73 |
| 1:B:75:LYS:NZ | 1:B:489:ASN:O | 2.21 | 0.72 |
| 1:C:1214:TYR:OH | 1:C:1222:MET:SD | 2.46 | 0.72 |
| 1:D:1725:GLN:NE2 | 1:D:1760:LEU:O | 2.24 | 0.71 |
| 1:A:1725:GLN:NE2 | 1:A:1760:LEU:O | 2.23 | 0.71 |
| 1:C:482:PHE:O | 1:C:505:ARG:NH1 | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:482:PHE:O | 1:A:505:ARG:NH1 | 2.24 | 0.70 |
| 1:B:1725:GLN:NE2 | 1:B:1760:LEU:O | 2.24 | 0.70 |
| 1:C:1725:GLN:NE2 | 1:C:1760:LEU:O | 2.24 | 0.70 |
| 1:D:801:ARG:NH2 | 1:D:984:ASP:OD1 | 2.24 | 0.70 |
| 1:B:482:PHE:O | 1:B:505:ARG:NH1 | 2.24 | 0.70 |
| 1:A:1945:THR:O | 1:A:1949:GLN:N | 2.25 | 0.70 |
| 1:B:1945:THR:O | 1:B:1949:GLN:N | 2.25 | 0.70 |
| 1:D:482:PHE:O | 1:D:505:ARG:NH1 | 2.24 | 0.70 |
| 1:A:801:ARG:NH2 | 1:A:984:ASP:OD1 | 2.24 | 0.70 |
| 1:D:352:TYR:O | 1:D:419:THR:OG1 | 2.09 | 0.70 |
| 1:C:561:ARG:NH1 | 1:C:593:ASP:O | 2.25 | 0.70 |
| 1:C:801:ARG:NH2 | 1:C:984:ASP:OD1 | 2.24 | 0.70 |
| 1:A:561:ARG:NH1 | 1:A:593:ASP:O | 2.25 | 0.70 |
| 1:B:1783:GLU:OE2 | 1:B:1899:THR:OG1 | 2.09 | 0.70 |
| 1:D:561:ARG:NH1 | 1:D:593:ASP:O | 2.25 | 0.70 |
| 1:A:1783:GLU:OE2 | 1:A:1899:THR:OG1 | 2.09 | 0.69 |
| 1:C:1945:THR:O | 1:C:1949:GLN:N | 2.25 | 0.69 |
| 1:D:1783:GLU:OE2 | 1:D:1899:THR:OG1 | 2.09 | 0.69 |
| 1:A:305:ARG:NH1 | 1:A:360:GLY:O | 2.26 | 0.69 |
| 1:B:305:ARG:NH1 | 1:B:360:GLY:O | 2.26 | 0.69 |
| 1:D:1945:THR:O | 1:D:1949:GLN:N | 2.25 | 0.69 |
| 1:B:352:TYR:O | 1:B:419:THR:OG1 | 2.09 | 0.69 |
| 1:B:801:ARG:NH2 | 1:B:984:ASP:OD1 | 2.25 | 0.69 |
| 1:D:1391:LEU:O | 1:D:1421:TYR:OH | 2.10 | 0.69 |
| 1:C:1783:GLU:OE2 | 1:C:1899:THR:OG1 | 2.09 | 0.69 |
| 1:B:561:ARG:NH1 | 1:B:593:ASP:O | 2.25 | 0.69 |
| 1:B:1391:LEU:O | 1:B:1421:TYR:OH | 2.10 | 0.69 |
| 1:A:1391:LEU:O | 1:A:1421:TYR:OH | 2.10 | 0.69 |
| 1:C:305:ARG:NH1 | 1:C:360:GLY:O | 2.26 | 0.69 |
| 1:C:1391:LEU:O | 1:C:1421:TYR:OH | 2.10 | 0.68 |
| 1:C:2523:LEU:O | 1:C:2527:LYS:N | 2.26 | 0.68 |
| 1:A:2523:LEU:O | 1:A:2527:LYS:N | 2.26 | 0.68 |
| 1:C:1645:SER:N | 1:C:1731:GLU:OE2 | 2.27 | 0.68 |
| 1:D:1645:SER:N | 1:D:1731:GLU:OE2 | 2.27 | 0.68 |
| 1:D:495:ASP:OD1 | 1:D:558:ARG:NH2 | 2.27 | 0.68 |
| 1:A:495:ASP:OD1 | 1:A:558:ARG:NH2 | 2.27 | 0.68 |
| 1:D:2523:LEU:O | 1:D:2527:LYS:N | 2.26 | 0.68 |
| 1:B:1645:SER:N | 1:B:1731:GLU:OE2 | 2.27 | 0.68 |
| 1:D:305:ARG:NH1 | 1:D:360:GLY:O | 2.26 | 0.68 |
| 1:A:352:TYR:O | 1:A:419:THR:OG1 | 2.09 | 0.68 |
| 1:A:1645:SER:N | 1:A:1731:GLU:OE2 | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2523:LEU:O | 1:B:2527:LYS:N | 2.26 | 0.67 |
| 1:C:401:THR:OG1 | 1:C:416:MET:O | 2.13 | 0.67 |
| 1:A:2033:TYR:O | 1:A:2047:ARG:NH1 | 2.28 | 0.67 |
| 1:B:495:ASP:OD1 | 1:B:558:ARG:NH2 | 2.27 | 0.67 |
| 1:C:2033:TYR:O | 1:C:2047:ARG:NH1 | 2.28 | 0.67 |
| 1:B:2033:TYR:O | 1:B:2047:ARG:NH1 | 2.28 | 0.67 |
| 1:D:401:THR:OG1 | 1:D:416:MET:O | 2.13 | 0.67 |
| 1:C:495:ASP:OD1 | 1:C:558:ARG:NH2 | 2.27 | 0.67 |
| 1:D:2033:TYR:O | 1:D:2047:ARG:NH1 | 2.28 | 0.67 |
| 1:C:352:TYR:O | 1:C:419:THR:OG1 | 2.09 | 0.66 |
| 1:A:401:THR:OG1 | 1:A:416:MET:O | 2.13 | 0.66 |
| 1:B:401:THR:OG1 | 1:B:416:MET:O | 2.13 | 0.66 |
| 1:A:1128:VAL:O | 1:A:1169:TYR:OH | 2.15 | 0.64 |
| 1:C:1128:VAL:O | 1:C:1169:TYR:OH | 2.15 | 0.64 |
| 1:B:1128:VAL:O | 1:B:1169:TYR:OH | 2.15 | 0.64 |
| 1:B:19:GLU:OE1 | 1:B:182:LYS:NZ | 2.27 | 0.63 |
| 1:D:1128:VAL:O | 1:D:1169:TYR:OH | 2.15 | 0.63 |
| 1:B:394:THR:HG1 | 1:B:396:THR:HG1 | 1.38 | 0.63 |
| 1:C:19:GLU:OE1 | 1:C:182:LYS:NZ | 2.27 | 0.62 |
| 1:A:815:TYR:OH | 1:A:984:ASP:OD2 | 2.18 | 0.61 |
| 1:D:164:ILE:HD11 | 1:D:183:VAL:HG21 | 1.83 | 0.61 |
| 1:C:164:ILE:HD11 | 1:C:183:VAL:HG21 | 1.83 | 0.61 |
| 1:D:19:GLU:OE1 | 1:D:182:LYS:NZ | 2.27 | 0.61 |
| 1:D:815:TYR:OH | 1:D:984:ASP:OD2 | 2.18 | 0.61 |
| 1:B:400:SER:OG | 1:B:427:GLU:OE2 | 2.15 | 0.61 |
| 1:B:2365:ASN:O | 1:B:2368:SER:OG | 2.18 | 0.60 |
| 1:A:400:SER:OG | 1:A:427:GLU:OE2 | 2.16 | 0.60 |
| 1:B:815:TYR:OH | 1:B:984:ASP:OD2 | 2.18 | 0.60 |
| 1:A:2365:ASN:O | 1:A:2368:SER:OG | 2.18 | 0.60 |
| 1:B:164:ILE:HD11 | 1:B:183:VAL:HG21 | 1.83 | 0.60 |
| 1:A:164:ILE:HD11 | 1:A:183:VAL:HG21 | 1.83 | 0.60 |
| 1:C:815:TYR:OH | 1:C:984:ASP:OD2 | 2.18 | 0.60 |
| 1:C:2365:ASN:O | 1:C:2368:SER:OG | 2.18 | 0.60 |
| 1:D:819:LEU:O | 1:D:823:ARG:NE | 2.34 | 0.60 |
| 1:C:819:LEU:O | 1:C:823:ARG:NE | 2.34 | 0.59 |
| 1:C:853:ASN:O | 1:C:857:ASN:ND2 | 2.36 | 0.59 |
| 1:B:853:ASN:O | 1:B:857:ASN:ND2 | 2.36 | 0.59 |
| 1:D:1769:GLN:NE2 | 1:D:1880:LEU:O | 2.36 | 0.59 |
| 1:C:1769:GLN:NE2 | 1:C:1880:LEU:O | 2.36 | 0.59 |
| 1:A:1769:GLN:NE2 | 1:A:1880:LEU:O | 2.36 | 0.59 |
| 1:A:853:ASN:O | 1:A:857:ASN:ND2 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1769:GLN:NE2 | 1:B:1880:LEU:O | 2.36 | 0.58 |
| 1:C:12:ASP:OD1 | 1:C:227:PHE:N | 2.36 | 0.58 |
| 1:D:853:ASN:O | 1:D:857:ASN:ND2 | 2.36 | 0.58 |
| 1:A:19:GLU:OE1 | 1:A:182:LYS:NZ | 2.27 | 0.58 |
| 1:A:819:LEU:O | 1:A:823:ARG:NE | 2.34 | 0.58 |
| 1:A:1053:ARG:NH2 | 1:A:1694:TYR:O | 2.37 | 0.58 |
| 1:B:1053:ARG:NH2 | 1:B:1694:TYR:O | 2.37 | 0.58 |
| 1:D:12:ASP:OD1 | 1:D:227:PHE:N | 2.36 | 0.58 |
| 1:B:12:ASP:OD1 | 1:B:227:PHE:N | 2.36 | 0.58 |
| 1:B:2024:GLU:OE1 | 1:B:2024:GLU:N | 2.37 | 0.58 |
| 1:C:1053:ARG:NH2 | 1:C:1694:TYR:O | 2.37 | 0.58 |
| 1:A:2024:GLU:N | 1:A:2024:GLU:OE1 | 2.37 | 0.58 |
| 1:C:400:SER:OG | 1:C:427:GLU:OE2 | 2.15 | 0.58 |
| 1:D:400:SER:OG | 1:D:427:GLU:OE2 | 2.15 | 0.58 |
| 1:D:1053:ARG:NH2 | 1:D:1694:TYR:O | 2.37 | 0.58 |
| 1:D:1882:GLU:OE1 | 1:D:1883:ASN:N | 2.37 | 0.58 |
| 1:A:12:ASP:OD1 | 1:A:227:PHE:N | 2.36 | 0.57 |
| 1:A:1882:GLU:OE1 | 1:A:1883:ASN:N | 2.37 | 0.56 |
| 1:C:2024:GLU:N | 1:C:2024:GLU:OE1 | 2.37 | 0.56 |
| 1:B:1659:GLU:OE1 | 1:B:1746:ASN:ND2 | 2.38 | 0.56 |
| 1:D:2365:ASN:O | 1:D:2368:SER:OG | 2.18 | 0.56 |
| 1:A:1081:HIS:O | 1:A:1084:GLN:NE2 | 2.38 | 0.56 |
| 1:D:2024:GLU:OE1 | 1:D:2024:GLU:N | 2.37 | 0.56 |
| 1:B:1081:HIS:O | 1:B:1084:GLN:NE2 | 2.38 | 0.56 |
| 1:C:1659:GLU:OE1 | 1:C:1746:ASN:ND2 | 2.38 | 0.56 |
| 1:C:1882:GLU:OE1 | 1:C:1883:ASN:N | 2.37 | 0.56 |
| 1:C:1081:HIS:O | 1:C:1084:GLN:NE2 | 2.38 | 0.56 |
| 1:D:31:LEU:O | 1:D:131:LYS:NZ | 2.29 | 0.56 |
| 1:A:1659:GLU:OE1 | 1:A:1746:ASN:ND2 | 2.38 | 0.56 |
| 1:D:1659:GLU:OE1 | 1:D:1746:ASN:ND2 | 2.38 | 0.55 |
| 1:D:1081:HIS:O | 1:D:1084:GLN:NE2 | 2.38 | 0.55 |
| 1:D:1593:GLU:OE1 | 1:D:1593:GLU:N | 2.40 | 0.55 |
| 1:A:1593:GLU:OE1 | 1:A:1593:GLU:N | 2.40 | 0.55 |
| 1:C:854:GLU:OE1 | 1:C:854:GLU:N | 2.40 | 0.55 |
| 1:D:69:LYS:NZ | 1:D:158:GLU:OE1 | 2.39 | 0.55 |
| 1:C:1593:GLU:N | 1:C:1593:GLU:OE1 | 2.40 | 0.55 |
| 1:A:854:GLU:N | 1:A:854:GLU:OE1 | 2.40 | 0.55 |
| 1:B:69:LYS:NZ | 1:B:158:GLU:OE1 | 2.39 | 0.55 |
| 1:B:1882:GLU:OE1 | 1:B:1883:ASN:N | 2.37 | 0.55 |
| 1:A:69:LYS:NZ | 1:A:158:GLU:OE1 | 2.39 | 0.55 |
| 1:B:819:LEU:O | 1:B:823:ARG:NE | 2.34 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:550:GLN:OE1 | 1:B:554:ARG:NE | 2.41 | 0.55 |
| 1:A:1994:ASP:O | 1:A:1997:SER:OG | 2.24 | 0.54 |
| 1:D:1994:ASP:O | 1:D:1997:SER:OG | 2.24 | 0.54 |
| 1:D:854:GLU:N | 1:D:854:GLU:OE1 | 2.40 | 0.54 |
| 1:B:854:GLU:N | 1:B:854:GLU:OE1 | 2.40 | 0.54 |
| 1:C:69:LYS:NZ | 1:C:158:GLU:OE1 | 2.39 | 0.54 |
| 1:A:550:GLN:OE1 | 1:A:554:ARG:NE | 2.41 | 0.54 |
| 1:B:533:GLY:N | 1:B:536:VAL:O | 2.41 | 0.54 |
| 1:B:1994:ASP:O | 1:B:1997:SER:OG | 2.24 | 0.54 |
| 1:D:533:GLY:N | 1:D:536:VAL:O | 2.41 | 0.54 |
| 1:C:1260:GLU:N | 1:C:1260:GLU:OE1 | 2.41 | 0.54 |
| 1:C:550:GLN:OE1 | 1:C:554:ARG:NE | 2.41 | 0.54 |
| 1:D:550:GLN:OE1 | 1:D:554:ARG:NE | 2.41 | 0.54 |
| 1:A:533:GLY:N | 1:A:536:VAL:O | 2.41 | 0.53 |
| 1:C:533:GLY:N | 1:C:536:VAL:O | 2.41 | 0.53 |
| 1:B:1593:GLU:N | 1:B:1593:GLU:OE1 | 2.40 | 0.53 |
| 1:B:1260:GLU:N | 1:B:1260:GLU:OE1 | 2.41 | 0.53 |
| 1:C:1875:ARG:N | 1:C:1939:GLN:OE1 | 2.42 | 0.53 |
| 1:B:1875:ARG:N | 1:B:1939:GLN:OE1 | 2.42 | 0.53 |
| 1:D:1260:GLU:OE1 | 1:D:1260:GLU:N | 2.41 | 0.53 |
| 1:D:1875:ARG:N | 1:D:1939:GLN:OE1 | 2.42 | 0.53 |
| 1:A:1791:ASP:O | 1:A:1795:ARG:N | 2.42 | 0.53 |
| 1:A:1875:ARG:N | 1:A:1939:GLN:OE1 | 2.42 | 0.52 |
| 1:A:99:MET:O | 1:A:103:GLN:N | 2.42 | 0.52 |
| 1:D:1280:GLU:OE2 | 1:D:1284:GLN:NE2 | 2.42 | 0.52 |
| 1:A:1956:GLN:NE2 | 1:A:2002:ALA:O | 2.43 | 0.52 |
| 1:B:1767:GLU:N | 1:B:1767:GLU:OE1 | 2.42 | 0.52 |
| 1:A:1280:GLU:OE2 | 1:A:1284:GLN:NE2 | 2.42 | 0.52 |
| 1:C:1767:GLU:N | 1:C:1767:GLU:OE1 | 2.42 | 0.52 |
| 1:D:2598:ASN:OD1 | 1:D:2599:LEU:N | 2.43 | 0.52 |
| 1:A:1260:GLU:OE1 | 1:A:1260:GLU:N | 2.41 | 0.52 |
| 1:B:99:MET:O | 1:B:103:GLN:N | 2.42 | 0.52 |
| 1:D:1791:ASP:O | 1:D:1795:ARG:N | 2.42 | 0.52 |
| 1:A:1742:THR:HG21 | 1:A:1785:PHE:HA | 1.92 | 0.52 |
| 1:B:1742:THR:HG21 | 1:B:1785:PHE:HA | 1.92 | 0.52 |
| 1:B:1956:GLN:NE2 | 1:B:2002:ALA:O | 2.43 | 0.52 |
| 1:C:1956:GLN:NE2 | 1:C:2002:ALA:O | 2.43 | 0.52 |
| 1:C:1742:THR:HG21 | 1:C:1785:PHE:HA | 1.92 | 0.51 |
| 1:D:838:GLU:O | 1:D:842:ASN:ND2 | 2.43 | 0.51 |
| 1:A:838:GLU:O | 1:A:842:ASN:ND2 | 2.43 | 0.51 |
| 1:A:1767:GLU:N | 1:A:1767:GLU:OE1 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2598:ASN:OD1 | 1:B:2599:LEU:N | 2.43 | 0.51 |
| 1:D:1956:GLN:NE2 | 1:D:2002:ALA:O | 2.43 | 0.51 |
| 1:C:838:GLU:O | 1:C:842:ASN:ND2 | 2.43 | 0.51 |
| 1:C:1791:ASP:O | 1:C:1795:ARG:N | 2.42 | 0.51 |
| 1:B:1280:GLU:OE2 | 1:B:1284:GLN:NE2 | 2.42 | 0.51 |
| 1:B:31:LEU:O | 1:B:131:LYS:NZ | 2.29 | 0.51 |
| 1:B:1791:ASP:O | 1:B:1795:ARG:N | 2.42 | 0.51 |
| 1:B:2497:ASP:OD2 | 1:C:2471:ARG:NH1 | 2.44 | 0.51 |
| 1:C:2497:ASP:OD2 | 1:D:2471:ARG:NH1 | 2.44 | 0.51 |
| 1:D:1742:THR:HG21 | 1:D:1785:PHE:HA | 1.92 | 0.51 |
| 1:B:838:GLU:O | 1:B:842:ASN:ND2 | 2.43 | 0.51 |
| 1:C:99:MET:O | 1:C:103:GLN:N | 2.43 | 0.51 |
| 1:A:2598:ASN:OD1 | 1:A:2599:LEU:N | 2.43 | 0.51 |
| 1:D:1767:GLU:OE1 | 1:D:1767:GLU:N | 2.42 | 0.51 |
| 1:C:1307:ILE:HD12 | 1:C:1317:CYS:SG | 2.52 | 0.50 |
| 1:B:1307:ILE:HD12 | 1:B:1317:CYS:SG | 2.52 | 0.50 |
| 1:C:1994:ASP:O | 1:C:1997:SER:OG | 2.24 | 0.50 |
| 1:C:2598:ASN:OD1 | 1:C:2599:LEU:N | 2.43 | 0.50 |
| 1:C:1280:GLU:OE2 | 1:C:1284:GLN:NE2 | 2.42 | 0.50 |
| 1:D:2564:ASN:OD1 | 1:D:2566:TRP:N | 2.45 | 0.50 |
| 1:A:1307:ILE:HD12 | 1:A:1317:CYS:SG | 2.52 | 0.50 |
| 1:A:2564:ASN:OD1 | 1:A:2566:TRP:N | 2.45 | 0.50 |
| 1:D:1307:ILE:HD12 | 1:D:1317:CYS:SG | 2.52 | 0.50 |
| 1:C:2564:ASN:OD1 | 1:C:2566:TRP:N | 2.45 | 0.49 |
| 1:B:2564:ASN:OD1 | 1:B:2566:TRP:N | 2.45 | 0.49 |
| 1:B:284:GLU:OE1 | 1:B:307:LYS:NZ | 2.36 | 0.49 |
| 1:A:1113:GLU:OE1 | 1:A:1116:ARG:NH2 | 2.46 | 0.49 |
| 1:D:99:MET:O | 1:D:103:GLN:N | 2.43 | 0.49 |
| 1:D:1113:GLU:OE1 | 1:D:1116:ARG:NH2 | 2.46 | 0.49 |
| 1:A:806:ILE:HD13 | 1:A:991:LEU:HD22 | 1.94 | 0.49 |
| 1:B:1113:GLU:OE1 | 1:B:1116:ARG:NH2 | 2.46 | 0.49 |
| 1:A:2471:ARG:NH1 | 1:D:2497:ASP:OD2 | 2.46 | 0.49 |
| 1:C:548:PRO:O | 1:C:552:MET:N | 2.45 | 0.48 |
| 1:B:806:ILE:HD13 | 1:B:991:LEU:HD22 | 1.94 | 0.48 |
| 1:B:1125:GLU:N | 1:B:1125:GLU:OE1 | 2.47 | 0.48 |
| 1:B:548:PRO:O | 1:B:552:MET:N | 2.46 | 0.48 |
| 1:D:1125:GLU:N | 1:D:1125:GLU:OE1 | 2.47 | 0.48 |
| 1:C:494:LEU:O | 1:C:558:ARG:NE | 2.47 | 0.48 |
| 1:B:494:LEU:O | 1:B:558:ARG:NE | 2.47 | 0.48 |
| 1:C:806:ILE:HD13 | 1:C:991:LEU:HD22 | 1.94 | 0.48 |
| 1:C:1741:ILE:HD11 | 1:C:1785:PHE:CE1 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:806:ILE:HD13 | 1:D:991:LEU:HD22 | 1.94 | 0.48 |
| 1:A:1125:GLU:N | 1:A:1125:GLU:OE1 | 2.47 | 0.48 |
| 1:A:494:LEU:O | 1:A:558:ARG:NE | 2.47 | 0.48 |
| 1:C:1125:GLU:OE1 | 1:C:1125:GLU:N | 2.47 | 0.48 |
| 1:B:741:LEU:O | 1:B:783:HIS:ND1 | 2.46 | 0.48 |
| 1:D:741:LEU:O | 1:D:783:HIS:ND1 | 2.46 | 0.48 |
| 1:B:1797:GLN:OE1 | 1:B:1909:GLN:NE2 | 2.47 | 0.48 |
| 1:C:1113:GLU:OE1 | 1:C:1116:ARG:NH2 | 2.46 | 0.48 |
| 1:C:592:GLU:OE1 | 1:C:592:GLU:N | 2.47 | 0.47 |
| 1:D:592:GLU:N | 1:D:592:GLU:OE1 | 2.47 | 0.47 |
| 1:D:1797:GLN:OE1 | 1:D:1909:GLN:NE2 | 2.47 | 0.47 |
| 1:A:592:GLU:N | 1:A:592:GLU:OE1 | 2.47 | 0.47 |
| 1:A:741:LEU:O | 1:A:783:HIS:ND1 | 2.46 | 0.47 |
| 1:D:1741:ILE:HD11 | 1:D:1785:PHE:CE1 | 2.49 | 0.47 |
| 1:B:592:GLU:N | 1:B:592:GLU:OE1 | 2.47 | 0.47 |
| 1:B:1741:ILE:HD11 | 1:B:1785:PHE:CE1 | 2.49 | 0.47 |
| 1:D:63:ASN:OD1 | 1:D:123:GLN:NE2 | 2.47 | 0.47 |
| 1:A:548:PRO:O | 1:A:552:MET:N | 2.46 | 0.47 |
| 1:D:494:LEU:O | 1:D:558:ARG:NE | 2.47 | 0.47 |
| 1:A:972:LEU:O | 1:A:976:GLN:N | 2.48 | 0.47 |
| 1:C:1797:GLN:OE1 | 1:C:1909:GLN:NE2 | 2.47 | 0.47 |
| 1:A:300:TRP:CE2 | 1:A:381:VAL:HG22 | 2.50 | 0.47 |
| 1:A:1797:GLN:OE1 | 1:A:1909:GLN:NE2 | 2.47 | 0.47 |
| 1:B:2513:PHE:CZ | 1:B:2517:ILE:HD11 | 2.50 | 0.47 |
| 1:C:886:ARG:NE | 1:C:1049:ASP:OD1 | 2.47 | 0.47 |
| 1:D:2513:PHE:CZ | 1:D:2517:ILE:HD11 | 2.50 | 0.47 |
| 1:A:886:ARG:NE | 1:A:1049:ASP:OD1 | 2.47 | 0.47 |
| 1:A:1741:ILE:HD11 | 1:A:1785:PHE:CE1 | 2.49 | 0.47 |
| 1:A:1954:GLU:OE1 | 1:A:1954:GLU:N | 2.47 | 0.47 |
| 1:A:2513:PHE:CZ | 1:A:2517:ILE:HD11 | 2.50 | 0.47 |
| 1:D:886:ARG:NE | 1:D:1049:ASP:OD1 | 2.48 | 0.47 |
| 1:D:1954:GLU:OE1 | 1:D:1954:GLU:N | 2.47 | 0.47 |
| 1:B:153:ASP:OD2 | 1:B:156:GLY:N | 2.48 | 0.46 |
| 1:B:886:ARG:NE | 1:B:1049:ASP:OD1 | 2.47 | 0.46 |
| 1:C:153:ASP:OD2 | 1:C:156:GLY:N | 2.48 | 0.46 |
| 1:B:300:TRP:CE2 | 1:B:381:VAL:HG22 | 2.50 | 0.46 |
| 1:C:1290:LEU:O | 1:C:1294:GLY:N | 2.49 | 0.46 |
| 1:C:1307:ILE:HD11 | 1:C:1318:GLN:HG2 | 1.98 | 0.46 |
| 1:D:1307:ILE:HD11 | 1:D:1318:GLN:HG2 | 1.98 | 0.46 |
| 1:A:44:ASP:OD1 | 1:A:45:LEU:N | 2.49 | 0.46 |
| 1:C:2538:CYS:SG | 1:C:2539:PHE:N | 2.89 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:153:ASP:OD2 | 1:A:156:GLY:N | 2.48 | 0.46 |
| 1:A:1290:LEU:O | 1:A:1294:GLY:N | 2.49 | 0.46 |
| 1:B:63:ASN:OD1 | 1:B:123:GLN:NE2 | 2.47 | 0.46 |
| 1:B:2538:CYS:SG | 1:B:2539:PHE:N | 2.89 | 0.46 |
| 1:C:730:ARG:NH2 | 1:C:772:ASP:OD2 | 2.49 | 0.46 |
| 1:A:542:SER:OG | 1:A:588:ASP:OD2 | 2.33 | 0.46 |
| 1:A:1337:ASN:OD1 | 1:A:1338:ASP:N | 2.48 | 0.46 |
| 1:D:300:TRP:CE2 | 1:D:381:VAL:HG22 | 2.50 | 0.46 |
| 1:D:1290:LEU:O | 1:D:1294:GLY:N | 2.49 | 0.46 |
| 1:D:1337:ASN:OD1 | 1:D:1338:ASP:N | 2.48 | 0.46 |
| 1:A:63:ASN:OD1 | 1:A:123:GLN:NE2 | 2.47 | 0.46 |
| 1:D:153:ASP:OD2 | 1:D:156:GLY:N | 2.48 | 0.46 |
| 1:B:1227:TYR:O | 1:B:1231:PHE:N | 2.48 | 0.46 |
| 1:B:1290:LEU:O | 1:B:1294:GLY:N | 2.49 | 0.46 |
| 1:C:542:SER:OG | 1:C:588:ASP:OD2 | 2.33 | 0.46 |
| 1:B:542:SER:OG | 1:B:588:ASP:OD2 | 2.33 | 0.46 |
| 1:B:972:LEU:O | 1:B:976:GLN:N | 2.48 | 0.46 |
| 1:C:13:ILE:HG21 | 1:C:56:LEU:HD22 | 1.98 | 0.46 |
| 1:C:1633:GLU:OE1 | 1:C:1633:GLU:N | 2.49 | 0.46 |
| 1:D:2007:ARG:NE | 1:D:2012:ASN:OD1 | 2.49 | 0.46 |
| 1:A:1741:ILE:HG13 | 1:A:1742:THR:HG23 | 1.98 | 0.46 |
| 1:B:1337:ASN:OD1 | 1:B:1338:ASP:N | 2.48 | 0.46 |
| 1:C:44:ASP:OD1 | 1:C:45:LEU:N | 2.49 | 0.46 |
| 1:C:1064:MET:SD | 1:C:1637:ARG:NE | 2.89 | 0.46 |
| 1:C:2513:PHE:CZ | 1:C:2517:ILE:HD11 | 2.50 | 0.46 |
| 1:A:2538:CYS:SG | 1:A:2539:PHE:N | 2.89 | 0.45 |
| 1:B:44:ASP:OD1 | 1:B:45:LEU:N | 2.49 | 0.45 |
| 1:B:730:ARG:NH2 | 1:B:772:ASP:OD2 | 2.49 | 0.45 |
| 1:B:1307:ILE:HD11 | 1:B:1318:GLN:HG2 | 1.98 | 0.45 |
| 1:D:542:SER:OG | 1:D:588:ASP:OD2 | 2.33 | 0.45 |
| 1:D:2329:THR:O | 1:D:2333:GLY:N | 2.48 | 0.45 |
| 1:C:972:LEU:O | 1:C:976:GLN:N | 2.48 | 0.45 |
| 1:D:972:LEU:O | 1:D:976:GLN:N | 2.48 | 0.45 |
| 1:D:2538:CYS:SG | 1:D:2539:PHE:N | 2.89 | 0.45 |
| 1:B:1064:MET:SD | 1:B:1637:ARG:NE | 2.89 | 0.45 |
| 1:C:656:VAL:O | 1:C:665:LEU:HD11 | 2.17 | 0.45 |
| 1:C:1227:TYR:O | 1:C:1231:PHE:N | 2.48 | 0.45 |
| 1:C:1337:ASN:OD1 | 1:C:1338:ASP:N | 2.48 | 0.45 |
| 1:C:2549:ASP:OD1 | 1:C:2550:ASN:N | 2.49 | 0.45 |
| 1:A:1307:ILE:HD11 | 1:A:1318:GLN:HG2 | 1.98 | 0.45 |
| 1:B:2007:ARG:NE | 1:B:2012:ASN:OD1 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2329:THR:O | 1:B:2333:GLY:N | 2.48 | 0.45 |
| 1:D:730:ARG:NH2 | 1:D:772:ASP:OD2 | 2.49 | 0.45 |
| 1:A:578:PHE:CE1 | 1:A:595:ILE:HD13 | 2.52 | 0.45 |
| 1:A:656:VAL:O | 1:A:665:LEU:HD11 | 2.17 | 0.45 |
| 1:C:31:LEU:O | 1:C:131:LYS:NZ | 2.29 | 0.45 |
| 1:C:300:TRP:CE2 | 1:C:381:VAL:HG22 | 2.50 | 0.45 |
| 1:D:44:ASP:OD1 | 1:D:45:LEU:N | 2.49 | 0.45 |
| 1:A:730:ARG:NH2 | 1:A:772:ASP:OD2 | 2.49 | 0.45 |
| 1:B:13:ILE:HG21 | 1:B:56:LEU:HD22 | 1.98 | 0.45 |
| 1:B:578:PHE:CE1 | 1:B:595:ILE:HD13 | 2.52 | 0.45 |
| 1:D:13:ILE:HG21 | 1:D:56:LEU:HD22 | 1.98 | 0.45 |
| 1:B:1633:GLU:OE1 | 1:B:1633:GLU:N | 2.49 | 0.45 |
| 1:B:1741:ILE:HG13 | 1:B:1742:THR:HG23 | 1.98 | 0.45 |
| 1:C:1741:ILE:HG13 | 1:C:1742:THR:HG23 | 1.98 | 0.45 |
| 1:D:1633:GLU:OE1 | 1:D:1633:GLU:N | 2.49 | 0.45 |
| 1:B:299:HIS:N | 1:B:304:TYR:OH | 2.50 | 0.44 |
| 1:B:1954:GLU:OE1 | 1:B:1954:GLU:N | 2.47 | 0.44 |
| 1:C:164:ILE:HG23 | 1:C:164:ILE:O | 2.18 | 0.44 |
| 1:C:578:PHE:CE1 | 1:C:595:ILE:HD13 | 2.52 | 0.44 |
| 1:D:299:HIS:N | 1:D:304:TYR:OH | 2.50 | 0.44 |
| 1:B:2549:ASP:OD1 | 1:B:2550:ASN:N | 2.49 | 0.44 |
| 1:C:741:LEU:O | 1:C:783:HIS:ND1 | 2.46 | 0.44 |
| 1:C:2007:ARG:NE | 1:C:2012:ASN:OD1 | 2.49 | 0.44 |
| 1:D:164:ILE:HG23 | 1:D:164:ILE:O | 2.18 | 0.44 |
| 1:D:578:PHE:CE1 | 1:D:595:ILE:HD13 | 2.52 | 0.44 |
| 1:A:2549:ASP:OD1 | 1:A:2550:ASN:N | 2.49 | 0.44 |
| 1:B:164:ILE:HG23 | 1:B:164:ILE:O | 2.18 | 0.44 |
| 1:D:656:VAL:O | 1:D:665:LEU:HD11 | 2.17 | 0.44 |
| 1:D:1227:TYR:O | 1:D:1231:PHE:N | 2.48 | 0.44 |
| 1:A:13:ILE:HG21 | 1:A:56:LEU:HD22 | 1.98 | 0.44 |
| 1:A:1064:MET:SD | 1:A:1637:ARG:NE | 2.89 | 0.44 |
| 1:B:1046:GLU:OE2 | 1:B:1052:GLY:N | 2.51 | 0.44 |
| 1:C:299:HIS:N | 1:C:304:TYR:OH | 2.51 | 0.44 |
| 1:B:656:VAL:O | 1:B:665:LEU:HD11 | 2.17 | 0.44 |
| 1:D:1741:ILE:HG13 | 1:D:1742:THR:HG23 | 1.98 | 0.44 |
| 1:C:1046:GLU:OE2 | 1:C:1052:GLY:N | 2.51 | 0.44 |
| 1:A:299:HIS:N | 1:A:304:TYR:OH | 2.50 | 0.44 |
| 1:A:16:LEU:HD12 | 1:A:26:ILE:HD12 | 2.00 | 0.44 |
| 1:C:1954:GLU:OE1 | 1:C:1954:GLU:N | 2.47 | 0.44 |
| 1:C:2329:THR:O | 1:C:2333:GLY:N | 2.48 | 0.44 |
| 1:D:1064:MET:SD | 1:D:1637:ARG:NE | 2.89 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1619:ASP:O | 1:D:1623:TRP:N | 2.51 | 0.44 |
| 1:A:1046:GLU:OE2 | 1:A:1052:GLY:N | 2.51 | 0.43 |
| 1:A:1227:TYR:O | 1:A:1231:PHE:N | 2.48 | 0.43 |
| 1:B:16:LEU:HD12 | 1:B:26:ILE:HD12 | 2.00 | 0.43 |
| 1:A:164:ILE:O | 1:A:164:ILE:HG23 | 2.18 | 0.43 |
| 1:A:2329:THR:O | 1:A:2333:GLY:N | 2.48 | 0.43 |
| 1:D:548:PRO:O | 1:D:552:MET:N | 2.46 | 0.43 |
| 1:A:31:LEU:O | 1:A:131:LYS:NZ | 2.29 | 0.43 |
| 1:A:1619:ASP:O | 1:A:1623:TRP:N | 2.51 | 0.43 |
| 1:C:1174:GLY:O | 1:C:1178:ARG:NH1 | 2.52 | 0.43 |
| 1:D:255:ASP:OD1 | 1:D:256:GLU:N | 2.52 | 0.43 |
| 1:A:1633:GLU:OE1 | 1:A:1633:GLU:N | 2.49 | 0.43 |
| 1:A:2007:ARG:NE | 1:A:2012:ASN:OD1 | 2.49 | 0.43 |
| 1:C:255:ASP:OD1 | 1:C:256:GLU:N | 2.52 | 0.43 |
| 1:D:2549:ASP:OD1 | 1:D:2550:ASN:N | 2.49 | 0.43 |
| 1:B:1490:ARG:O | 1:B:1494:LEU:N | 2.48 | 0.43 |
| 1:B:1619:ASP:O | 1:B:1623:TRP:N | 2.51 | 0.43 |
| 1:C:16:LEU:HD12 | 1:C:26:ILE:HD12 | 2.00 | 0.43 |
| 1:D:16:LEU:HD12 | 1:D:26:ILE:HD12 | 2.00 | 0.43 |
| 1:B:888:LEU:HD21 | 1:B:971:ILE:HG23 | 2.01 | 0.43 |
| 1:D:1046:GLU:OE2 | 1:D:1052:GLY:N | 2.51 | 0.43 |
| 1:A:888:LEU:HD21 | 1:A:971:ILE:HG23 | 2.01 | 0.43 |
| 1:B:1895:GLN:N | 1:B:1895:GLN:OE1 | 2.52 | 0.42 |
| 1:C:1895:GLN:N | 1:C:1895:GLN:OE1 | 2.52 | 0.42 |
| 1:B:1174:GLY:O | 1:B:1178:ARG:NH1 | 2.52 | 0.42 |
| 1:C:1307:ILE:HD11 | 1:C:1318:GLN:CG | 2.50 | 0.42 |
| 1:D:1307:ILE:HD11 | 1:D:1318:GLN:CG | 2.50 | 0.42 |
| 1:A:1307:ILE:HD11 | 1:A:1318:GLN:CG | 2.50 | 0.42 |
| 1:B:652:ILE:O | 1:B:656:VAL:HG12 | 2.20 | 0.42 |
| 1:C:63:ASN:OD1 | 1:C:123:GLN:NE2 | 2.47 | 0.42 |
| 1:D:652:ILE:O | 1:D:656:VAL:HG12 | 2.20 | 0.42 |
| 1:D:888:LEU:HD21 | 1:D:971:ILE:HG23 | 2.01 | 0.42 |
| 1:D:1174:GLY:O | 1:D:1178:ARG:NH1 | 2.52 | 0.42 |
| 1:A:1174:GLY:O | 1:A:1178:ARG:NH1 | 2.52 | 0.42 |
| 1:B:1307:ILE:HD11 | 1:B:1318:GLN:CG | 2.50 | 0.42 |
| 1:C:888:LEU:HD21 | 1:C:971:ILE:HG23 | 2.01 | 0.42 |
| 1:D:1254:LEU:O | 1:D:1285:HIS:NE2 | 2.53 | 0.42 |
| 1:D:1264:MET:HA | 1:D:1267:ILE:HD12 | 2.02 | 0.42 |
| 1:D:1523:GLN:O | 1:D:1527:SER:N | 2.53 | 0.42 |
| 1:D:1932:ASP:OD1 | 1:D:1933:ASN:N | 2.53 | 0.42 |
| 1:A:652:ILE:O | 1:A:656:VAL:HG12 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1619:ASP:O | 1:C:1623:TRP:N | 2.51 | 0.42 |
| 1:A:1264:MET:HA | 1:A:1267:ILE:HD12 | 2.01 | 0.41 |
| 1:A:1932:ASP:OD1 | 1:A:1933:ASN:N | 2.53 | 0.41 |
| 1:C:1490:ARG:O | 1:C:1494:LEU:N | 2.48 | 0.41 |
| 1:C:1523:GLN:O | 1:C:1527:SER:N | 2.53 | 0.41 |
| 1:D:698:ASP:OD2 | 1:D:704:HIS:NE2 | 2.52 | 0.41 |
| 1:A:255:ASP:OD1 | 1:A:256:GLU:N | 2.52 | 0.41 |
| 1:A:1523:GLN:O | 1:A:1527:SER:N | 2.53 | 0.41 |
| 1:B:255:ASP:OD1 | 1:B:256:GLU:N | 2.52 | 0.41 |
| 1:C:1254:LEU:O | 1:C:1285:HIS:NE2 | 2.53 | 0.41 |
| 1:D:1895:GLN:OE1 | 1:D:1895:GLN:N | 2.52 | 0.41 |
| 1:D:1937:VAL:O | 1:D:1940:THR:OG1 | 2.36 | 0.41 |
| 1:A:1937:VAL:O | 1:A:1940:THR:OG1 | 2.36 | 0.41 |
| 1:B:1523:GLN:O | 1:B:1527:SER:N | 2.53 | 0.41 |
| 1:A:1254:LEU:O | 1:A:1285:HIS:NE2 | 2.53 | 0.41 |
| 1:B:1254:LEU:O | 1:B:1285:HIS:NE2 | 2.53 | 0.41 |
| 1:C:1691:LEU:O | 1:C:1695:LEU:N | 2.50 | 0.41 |
| 1:C:1932:ASP:OD1 | 1:C:1933:ASN:N | 2.53 | 0.41 |
| 1:A:1194:GLN:NE2 | 1:A:1234:LYS:O | 2.51 | 0.41 |
| 1:B:1932:ASP:OD1 | 1:B:1933:ASN:N | 2.53 | 0.41 |
| 1:C:652:ILE:O | 1:C:656:VAL:HG12 | 2.20 | 0.41 |
| 1:D:2513:PHE:CE2 | 1:D:2517:ILE:HD11 | 2.56 | 0.41 |
| 1:C:698:ASP:OD2 | 1:C:704:HIS:NE2 | 2.52 | 0.41 |
| 1:B:698:ASP:OD2 | 1:B:704:HIS:NE2 | 2.52 | 0.41 |
| 1:B:1764:GLY:O | 1:B:1883:ASN:ND2 | 2.54 | 0.41 |
| 1:B:2513:PHE:CE2 | 1:B:2517:ILE:HD11 | 2.56 | 0.41 |
| 1:C:2513:PHE:CE2 | 1:C:2517:ILE:HD11 | 2.56 | 0.41 |
| 1:A:1895:GLN:OE1 | 1:A:1895:GLN:N | 2.52 | 0.40 |
| 1:C:536:VAL:HG21 | 1:C:546:ASN:CG | 2.42 | 0.40 |
| 1:D:1394:GLU:OE1 | 1:D:1394:GLU:N | 2.52 | 0.40 |
| 1:B:1264:MET:HA | 1:B:1267:ILE:HD12 | 2.01 | 0.40 |
| 1:C:233:GLU:OE1 | 1:C:383:ARG:NH2 | 2.52 | 0.40 |
| 1:C:1264:MET:HA | 1:C:1267:ILE:HD12 | 2.01 | 0.40 |
| 1:D:233:GLU:OE1 | 1:D:383:ARG:NH2 | 2.52 | 0.40 |
| 1:A:698:ASP:OD2 | 1:A:704:HIS:NE2 | 2.52 | 0.40 |
| 1:C:1340:ALA:O | 1:C:1344:HIS:ND1 | 2.54 | 0.40 |
| 1:A:1968:ASP:OD1 | 1:A:2019:SER:OG | 2.35 | 0.40 |
| 1:A:2513:PHE:CE2 | 1:A:2517:ILE:HD11 | 2.56 | 0.40 |
| 1:C:1764:GLY:O | 1:C:1883:ASN:ND2 | 2.54 | 0.40 |
| 1:D:582:GLN:O | 1:D:585:ILE:HG22 | 2.21 | 0.40 |

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 | 2147/2671 (80%) | 2079 (97%) | 66 (3%) | 2 (0%) | 51 | 83 |
| 1 | B | 2147/2671 (80%) | 2078 (97%) | 67 (3%) | 2 (0%) | 51 | 83 |
| 1 | C | 2147/2671 (80%) | 2080 (97%) | 65 (3%) | 2 (0%) | 51 | 83 |
| 1 | D | 2147/2671 (80%) | 2080 (97%) | 65 (3%) | 2 (0%) | 51 | 83 |
| All | All | 8588/10684 (80%) | 8317 (97%) | 263 (3%) | 8 (0%) | 54 | 83 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1544 | PRO |
| 1 | B | 1544 | PRO |
| 1 | C | 1544 | PRO |
| 1 | D | 1544 | PRO |
| 1 | A | 1494 | LEU |
| 1 | B | 1494 | LEU |
| 1 | C | 1494 | LEU |
| 1 | D | 1494 | LEU |

### 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 | 1883/2385 (79%) | 1870 (99%) | 13 (1%) | 84 | 90 |
| 1 | B | 1883/2385 (79%) | 1870 (99%) | 13 (1%) | 84 | 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | C | 1883/2385 (79%) | 1870 (99%) | 13 (1%) | 84 | 90 |
| 1 | D | 1883/2385 (79%) | 1870 (99%) | 13 (1%) | 84 | 90 |
| All | All | 7532/9540 (79%) | 7480 (99%) | 52 (1%) | 84 | 90 |

All (52) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 280 | ASN |
| 1 | A | 390 | ARG |
| 1 | A | 550 | GLN |
| 1 | A | 556 | CYS |
| 1 | A | 1086 | GLN |
| 1 | A | 1380 | ASN |
| 1 | A | 1418 | ASN |
| 1 | A | 1727 | ARG |
| 1 | A | 1797 | GLN |
| 1 | A | 1882 | GLU |
| 1 | A | 2051 | HIS |
| 1 | A | 2222 | PHE |
| 1 | A | 2532 | GLU |
| 1 | B | 280 | ASN |
| 1 | B | 390 | ARG |
| 1 | B | 550 | GLN |
| 1 | B | 556 | CYS |
| 1 | B | 1086 | GLN |
| 1 | B | 1380 | ASN |
| 1 | B | 1418 | ASN |
| 1 | B | 1727 | ARG |
| 1 | B | 1797 | GLN |
| 1 | B | 1882 | GLU |
| 1 | B | 2051 | HIS |
| 1 | B | 2222 | PHE |
| 1 | B | 2532 | GLU |
| 1 | C | 280 | ASN |
| 1 | C | 390 | ARG |
| 1 | C | 550 | GLN |
| 1 | C | 556 | CYS |
| 1 | C | 1086 | GLN |
| 1 | C | 1380 | ASN |
| 1 | C | 1418 | ASN |
| 1 | C | 1727 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 1797 | GLN |
| 1 | C | 1882 | GLU |
| 1 | C | 2051 | HIS |
| 1 | C | 2222 | PHE |
| 1 | C | 2532 | GLU |
| 1 | D | 280 | ASN |
| 1 | D | 390 | ARG |
| 1 | D | 550 | GLN |
| 1 | D | 556 | CYS |
| 1 | D | 1086 | GLN |
| 1 | D | 1380 | ASN |
| 1 | D | 1418 | ASN |
| 1 | D | 1727 | ARG |
| 1 | D | 1797 | GLN |
| 1 | D | 1882 | GLU |
| 1 | D | 2051 | HIS |
| 1 | D | 2222 | PHE |
| 1 | D | 2532 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 94 | GLN |
| 1 | B | 94 | GLN |

### 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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (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 | A | 5 |
| 1 | B | 5 |
| 1 | C | 5 |
| 1 | D | 5 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 1552:GLN | C | 1586:TRP | N | 55.42 |
| 1 | B | 1552:GLN | C | 1586:TRP | N | 55.42 |
| 1 | C | 1552:GLN | C | 1586:TRP | N | 55.42 |
| 1 | D | 1552:GLN | C | 1586:TRP | N | 55.42 |
| 1 | A | 1533:THR | C | 1541:ARG | N | 16.01 |
| 1 | B | 1533:THR | C | 1541:ARG | N | 16.01 |
| 1 | C | 1533:THR | C | 1541:ARG | N | 16.01 |
| 1 | D | 1533:THR | C | 1541:ARG | N | 16.01 |
| 1 | A | 1508:SER | C | 1515:GLY | N | 12.00 |
| 1 | B | 1508:SER | C | 1515:GLY | N | 12.00 |
| 1 | C | 1508:SER | C | 1515:GLY | N | 12.00 |
| 1 | D | 1508:SER | C | 1515:GLY | N | 12.00 |
| 1 | A | 1484:GLY | C | 1490:ARG | N | 11.59 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | B | 1484:GLY | C | 1490:ARG | N | 11.59 |
| 1 | C | 1484:GLY | C | 1490:ARG | N | 11.59 |
| 1 | D | 1484:GLY | C | 1490:ARG | N | 11.59 |
| 1 | A | 2252:TYR | C | 2260:SER | N | 7.49 |
| 1 | B | 2252:TYR | C | 2260:SER | N | 7.49 |
| 1 | C | 2252:TYR | C | 2260:SER | N | 7.49 |
| 1 | D | 2252:TYR | C | 2260:SER | N | 7.49 |

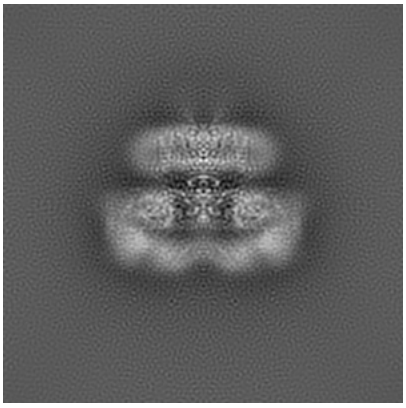
# 6 Map visualisation (i)

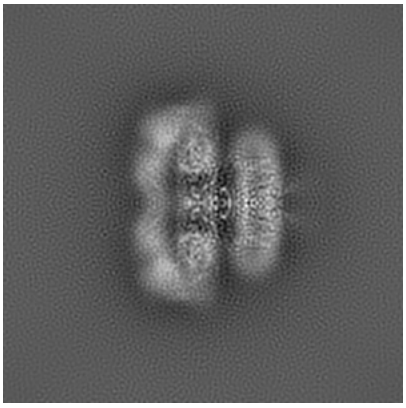
This section contains visualisations of the EMDB entry EMD-7991. These allow visual inspection of the internal detail of the map and identification of artifacts.

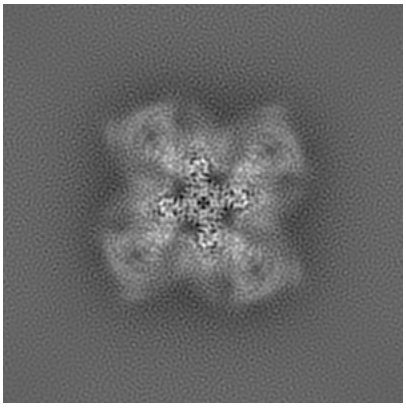
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

### 6.1.1 Primary map


X


Y

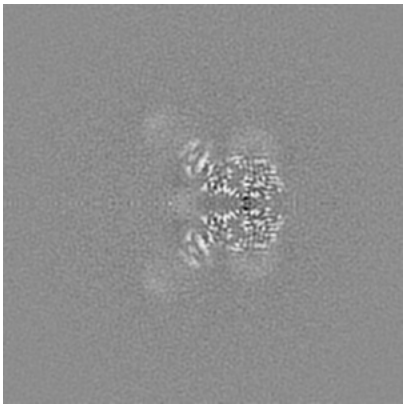

Z

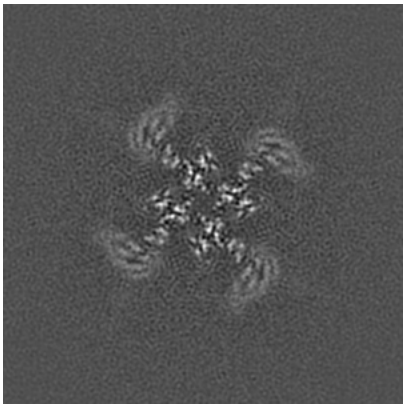
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

### 6.2.1 Primary map

X Index: 192

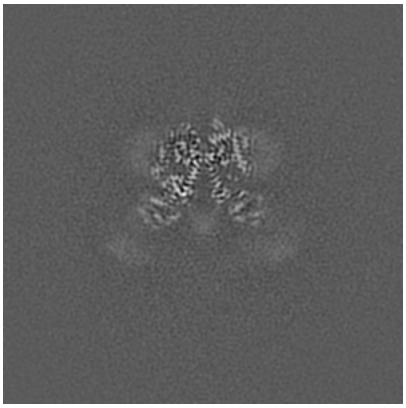

Y Index: 192


Z Index: 192

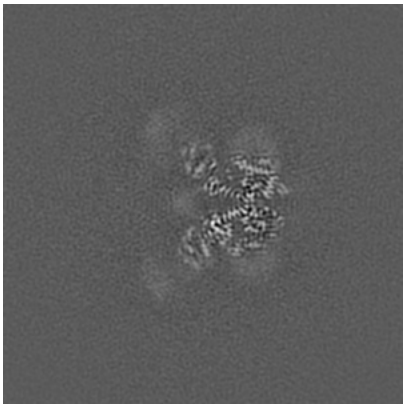
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

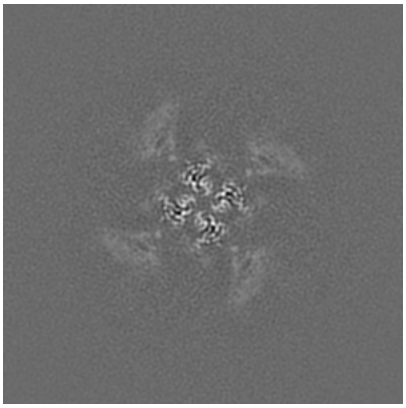
### 6.3.1 Primary map



X Index: 194



Y Index: 190



Z Index: 200

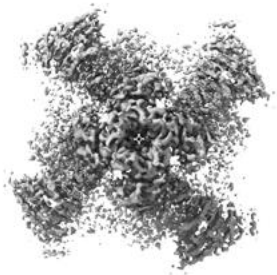
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

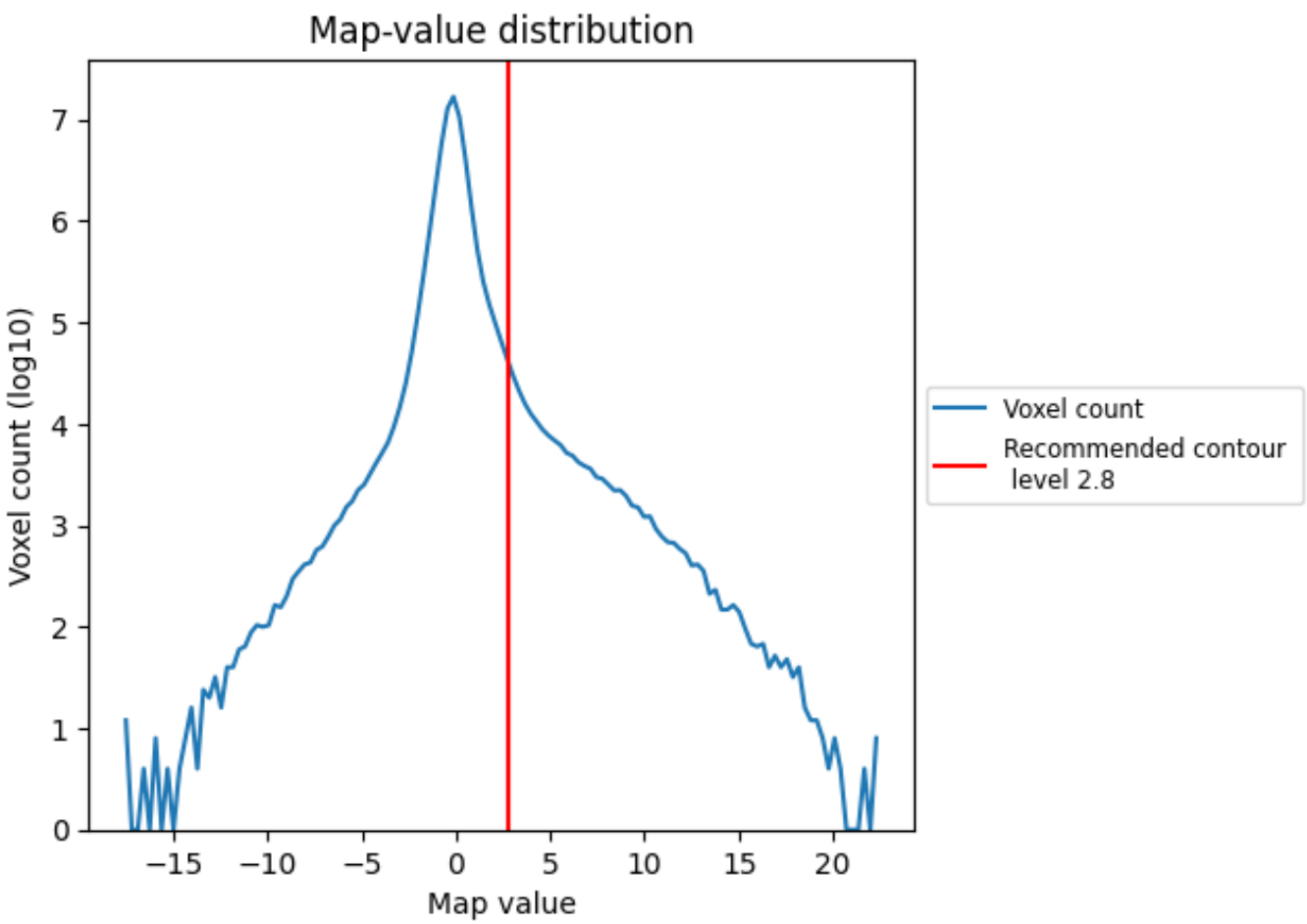
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

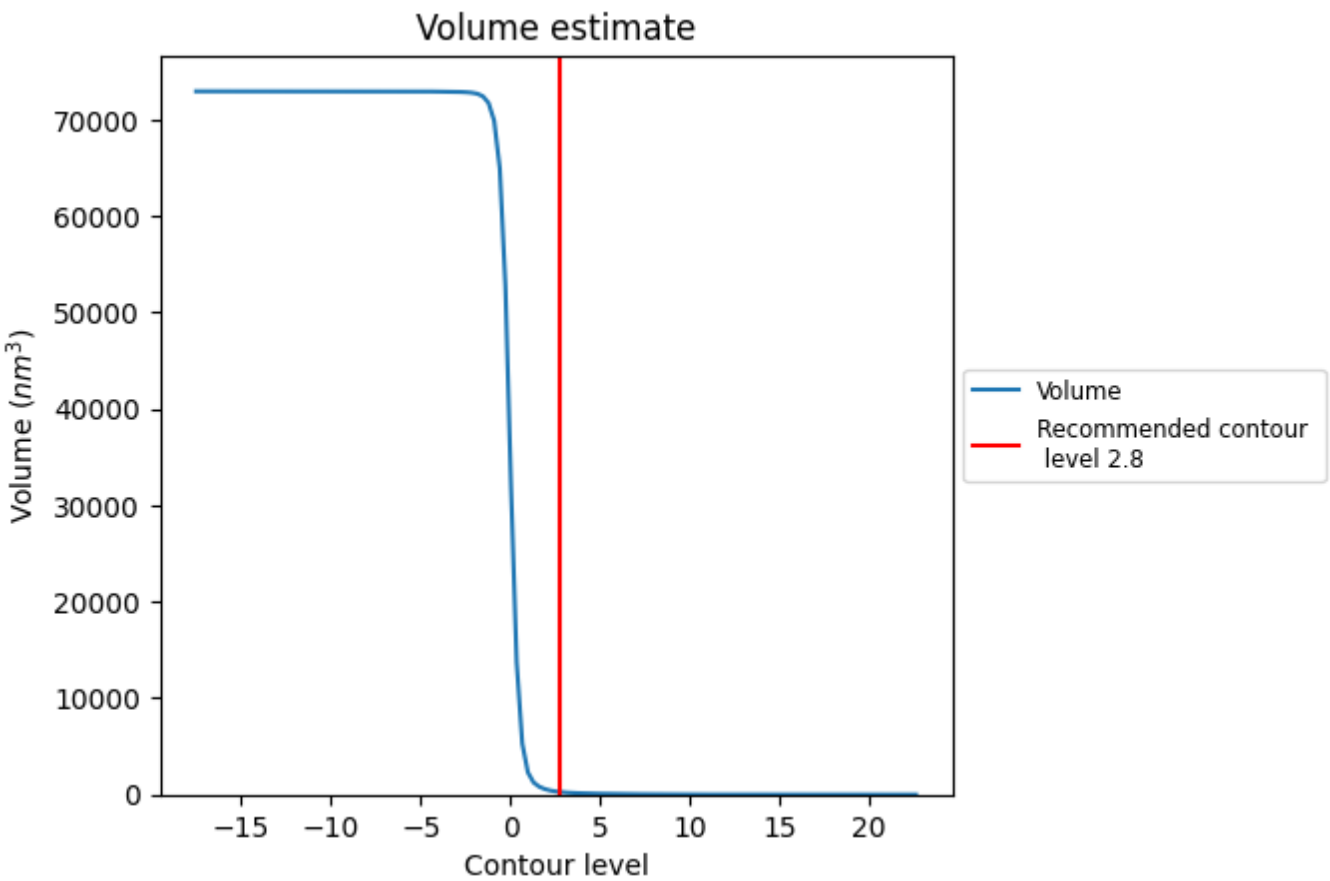
This section contains the results of statistical analysis of the map.

## 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.

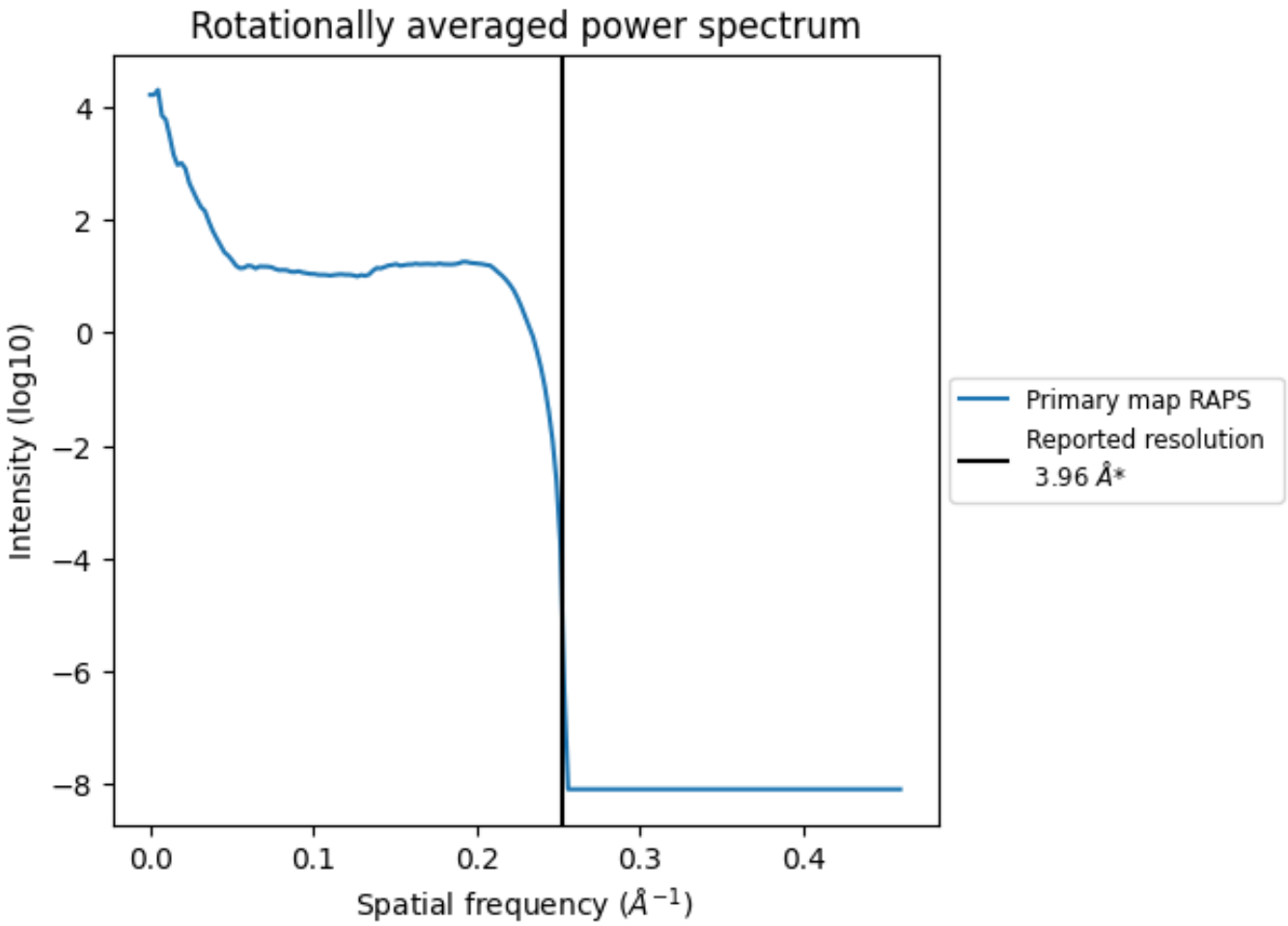
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 258 $nm^3$; this corresponds to an approximate mass of 233 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 0.253 Å$^{-1}$

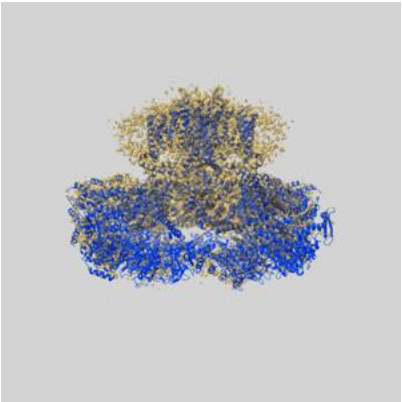
# 8 Fourier-Shell correlation (i)

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

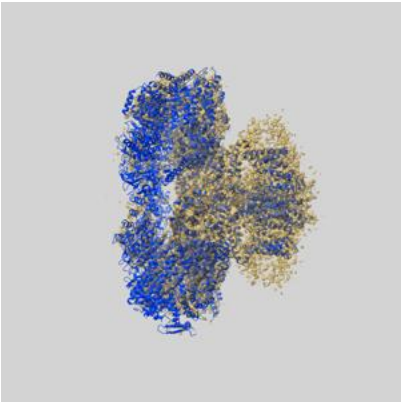
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7991 and PDB model 6DRA. Per-residue inclusion information can be found in section 3 on page 4.

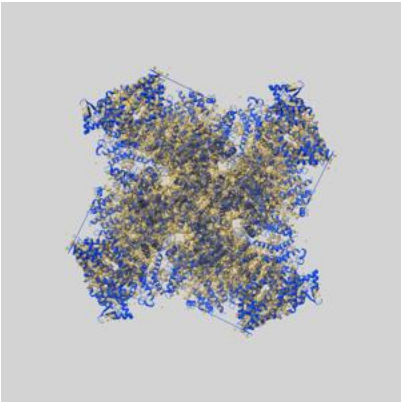
## 9.1 Map-model overlay (i)



X



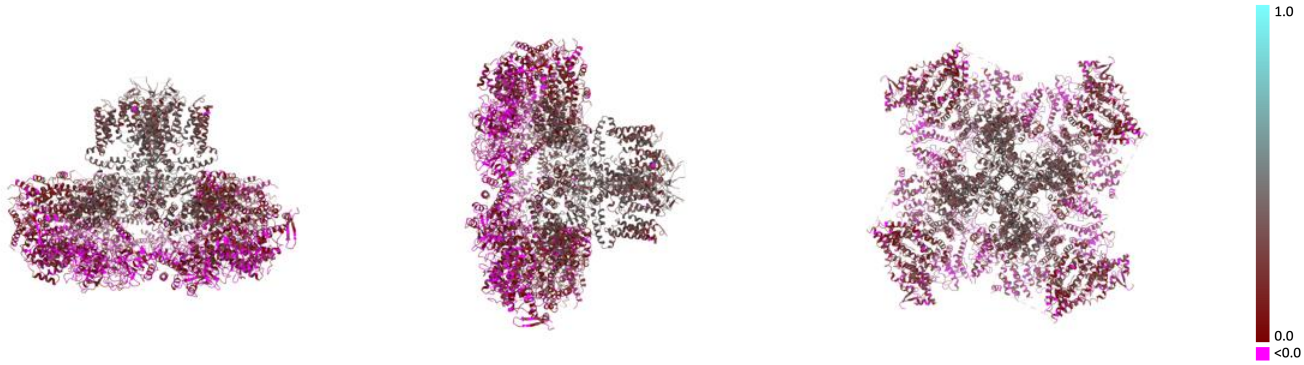
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8 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.

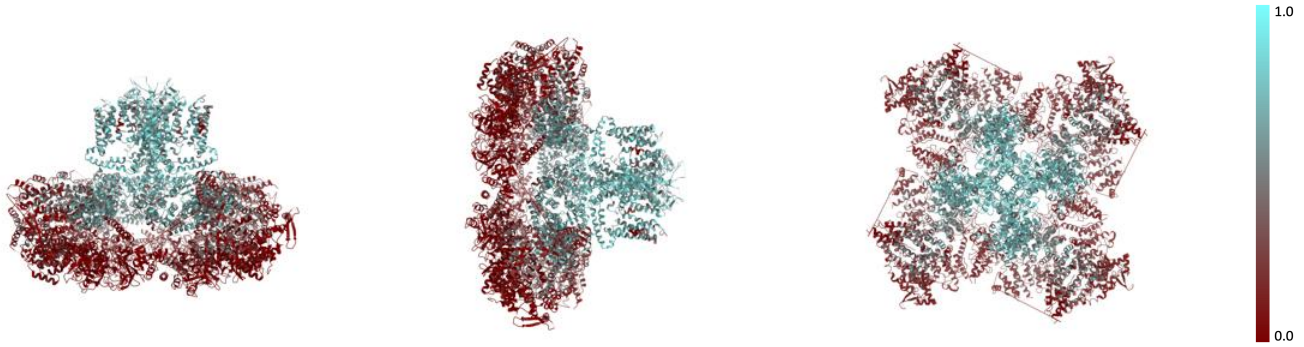
## 9.2 Q-score mapped to coordinate model (i)




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.

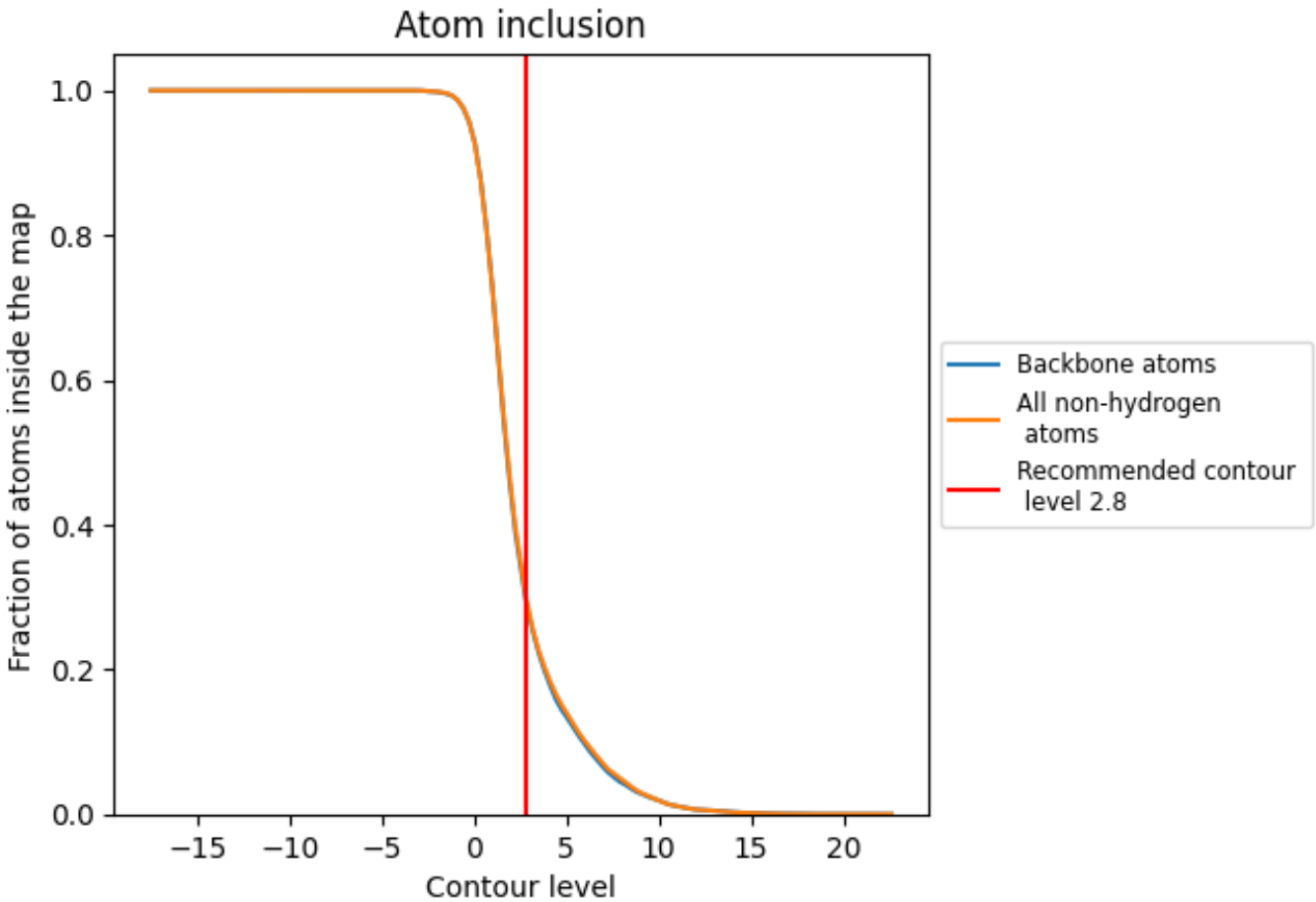
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (2.8).

## 9.4 Atom inclusion (i)




At the recommended contour level, 29% of all backbone atoms, 30% 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 (2.8) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.3011 | 0.1690 |
| A | 0.3099 | 0.1680 |
| B | 0.3101 | 0.1690 |
| C | 0.3101 | 0.1690 |
| D | 0.3100 | 0.1680 |