wwPDB EM Validation Summary Report (i)

Nov 17, 2022 – 04:21 AM EST

PDB ID	:	8EAQ
EMDB ID	:	EMD-27982
Title	:	Structure of the full-length IP3R1 channel determined at high Ca2+
Authors	:	Fan, G.; Baker, M.R.; Terry, L.E.; Arige, V.; Chen, M.; Seryshev, A.B.; Baker, M.L.; Ludtke, S.J.; Yule, D.I.; Serysheva, I.I.
Deposited on	:	2022-08-29
Resolution	:	3.26 Å(reported)
Based on initial model	:	7LHE

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

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

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

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

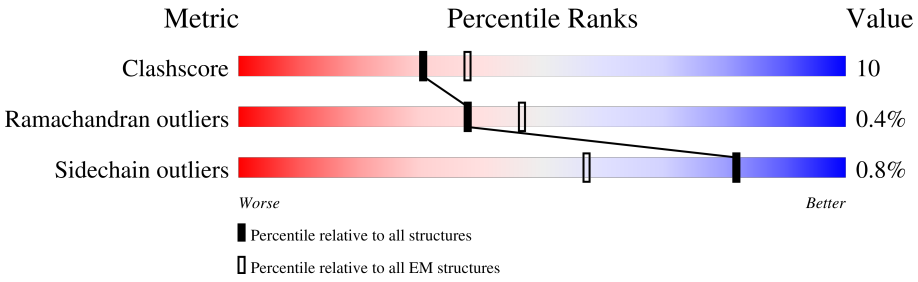
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.26 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	2750	14% 67% 19% · 14%
1	B	2750	14% 67% 18% · 14%
1	C	2750	14% 67% 19% · 14%
1	D	2750	14% 67% 19% · 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 77928 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2374	Total 19195	C 12189	N 3321	O 3567	S 118	1	0
1	B	2374	Total 19195	C 12189	N 3321	O 3567	S 118	1	0
1	C	2374	Total 19195	C 12189	N 3321	O 3567	S 118	1	0
1	D	2374	Total 19195	C 12189	N 3321	O 3567	S 118	1	0

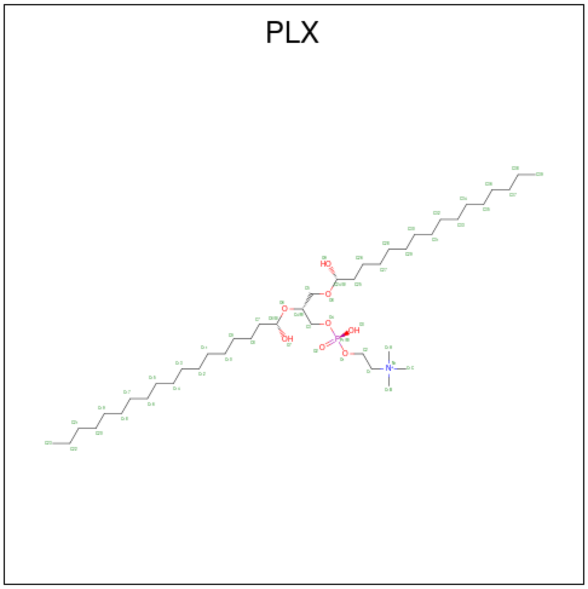
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	6	Total 6	Ca 6	0
3	B	5	Total 5	Ca 5	0
3	C	5	Total 5	Ca 5	0
3	D	4	Total 4	Ca 4	0

- Molecule 4 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
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4	A	1	Total 281	C 211	N 7	O 56	P 7	0
4	A	1	Total 281	C 211	N 7	O 56	P 7	0
4	A	1	Total 281	C 211	N 7	O 56	P 7	0
4	A	1	Total 281	C 211	N 7	O 56	P 7	0
4	A	1	Total 281	C 211	N 7	O 56	P 7	0
4	A	1	Total 281	C 211	N 7	O 56	P 7	0
4	B	1	Total 281	C 211	N 7	O 56	P 7	0
4	B	1	Total 281	C 211	N 7	O 56	P 7	0
4	B	1	Total 281	C 211	N 7	O 56	P 7	0
4	B	1	Total 281	C 211	N 7	O 56	P 7	0
4	B	1	Total 281	C 211	N 7	O 56	P 7	0

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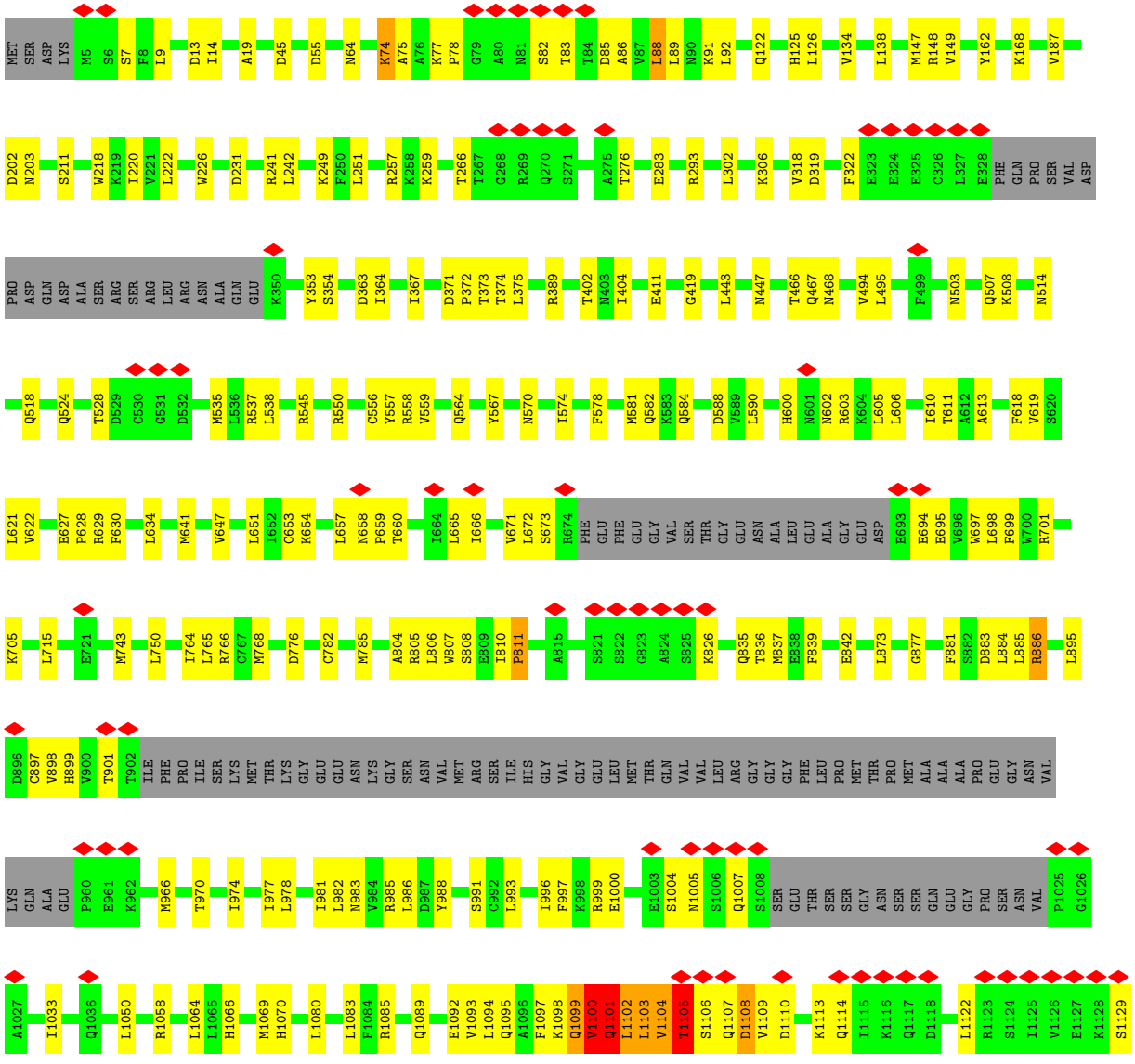
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total 281	C 211	N 7	O 56	P 7	0
4	B	1	Total 281	C 211	N 7	O 56	P 7	0
4	C	1	Total 281	C 211	N 7	O 56	P 7	0
4	C	1	Total 281	C 211	N 7	O 56	P 7	0
4	C	1	Total 281	C 211	N 7	O 56	P 7	0
4	C	1	Total 281	C 211	N 7	O 56	P 7	0
4	C	1	Total 281	C 211	N 7	O 56	P 7	0
4	C	1	Total 281	C 211	N 7	O 56	P 7	0
4	C	1	Total 281	C 211	N 7	O 56	P 7	0
4	D	1	Total 281	C 211	N 7	O 56	P 7	0
4	D	1	Total 281	C 211	N 7	O 56	P 7	0
4	D	1	Total 281	C 211	N 7	O 56	P 7	0
4	D	1	Total 281	C 211	N 7	O 56	P 7	0
4	D	1	Total 281	C 211	N 7	O 56	P 7	0
4	D	1	Total 281	C 211	N 7	O 56	P 7	0
4	D	1	Total 281	C 211	N 7	O 56	P 7	0

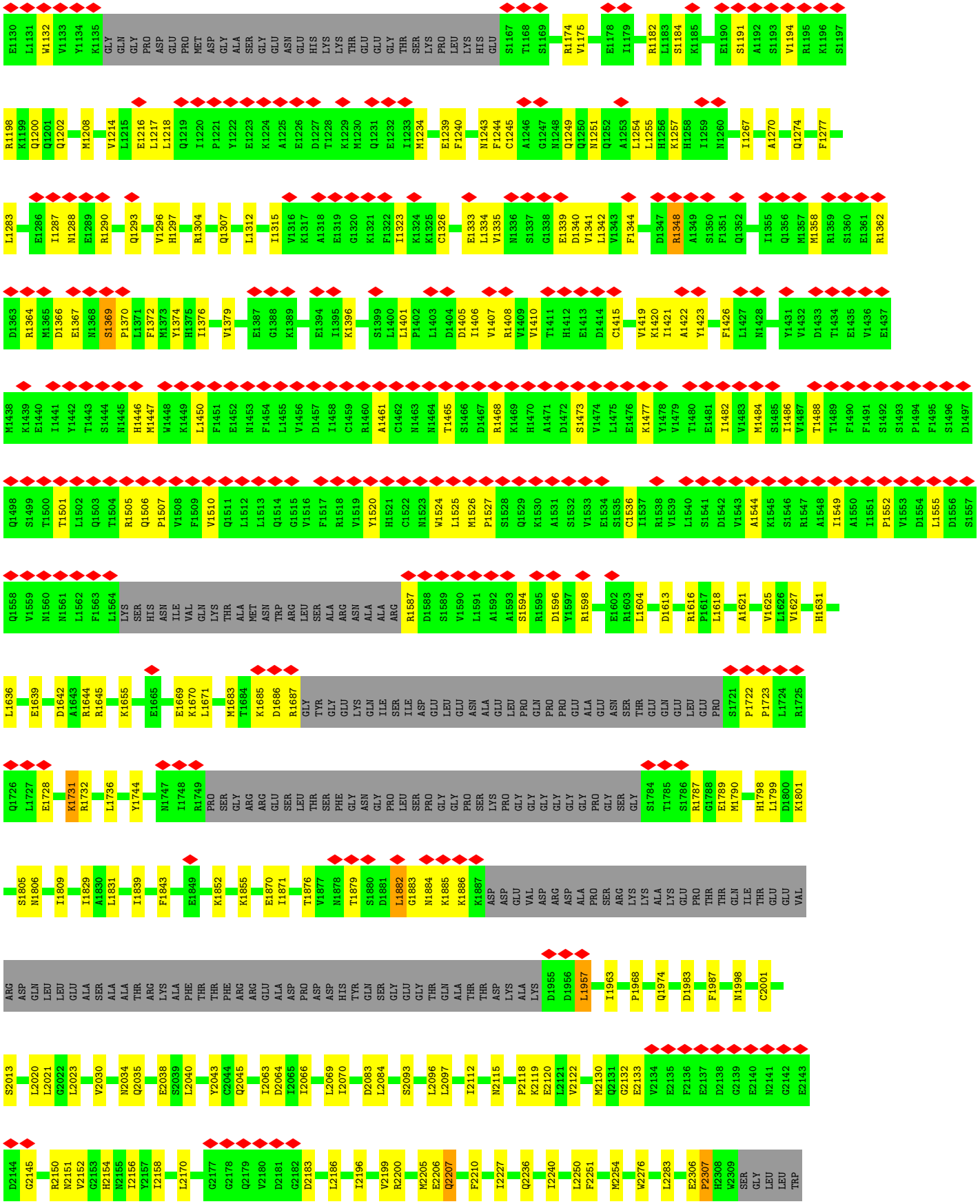
3 Residue-property plots (i)

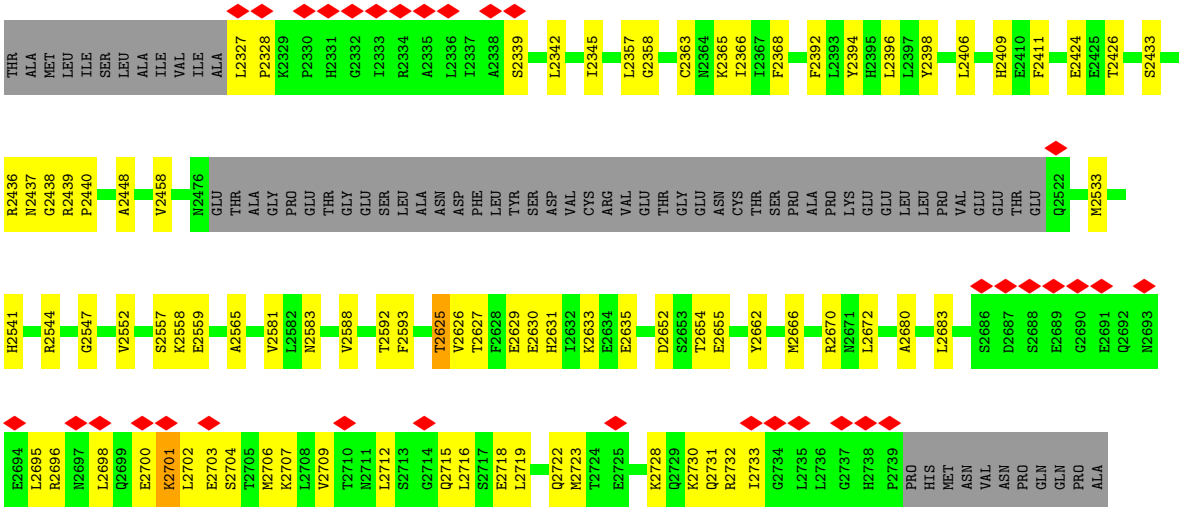
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain A:

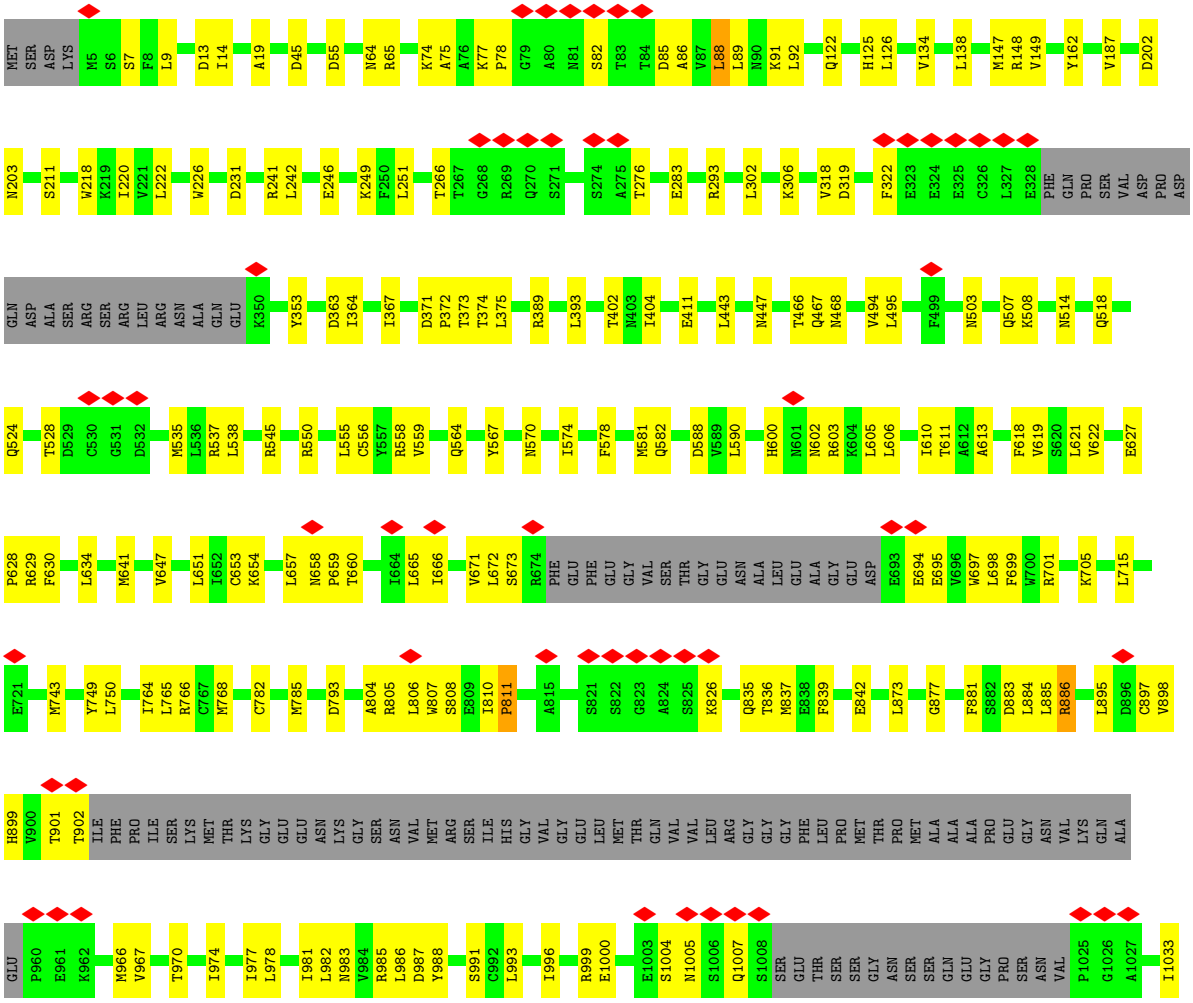


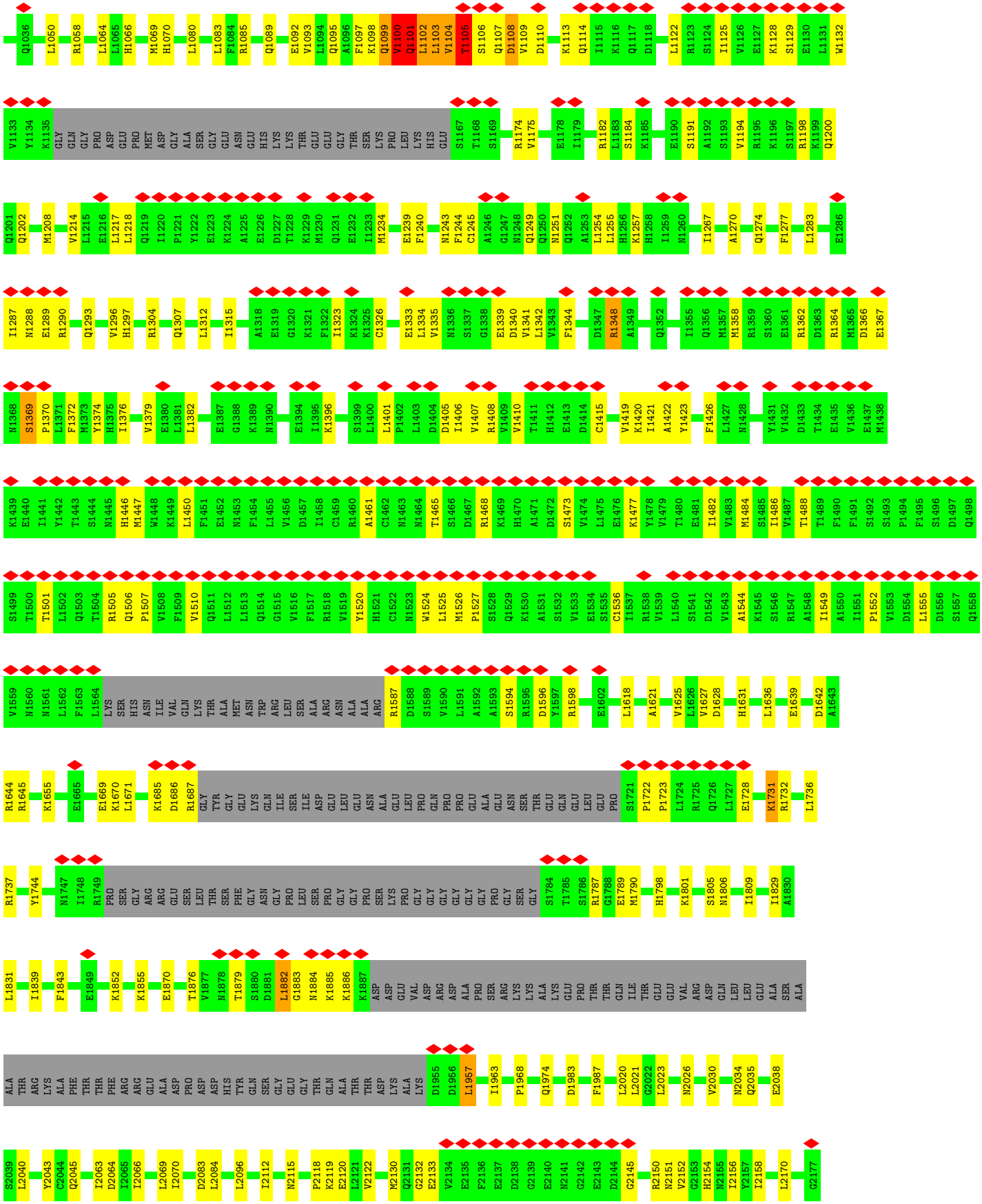




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain B:

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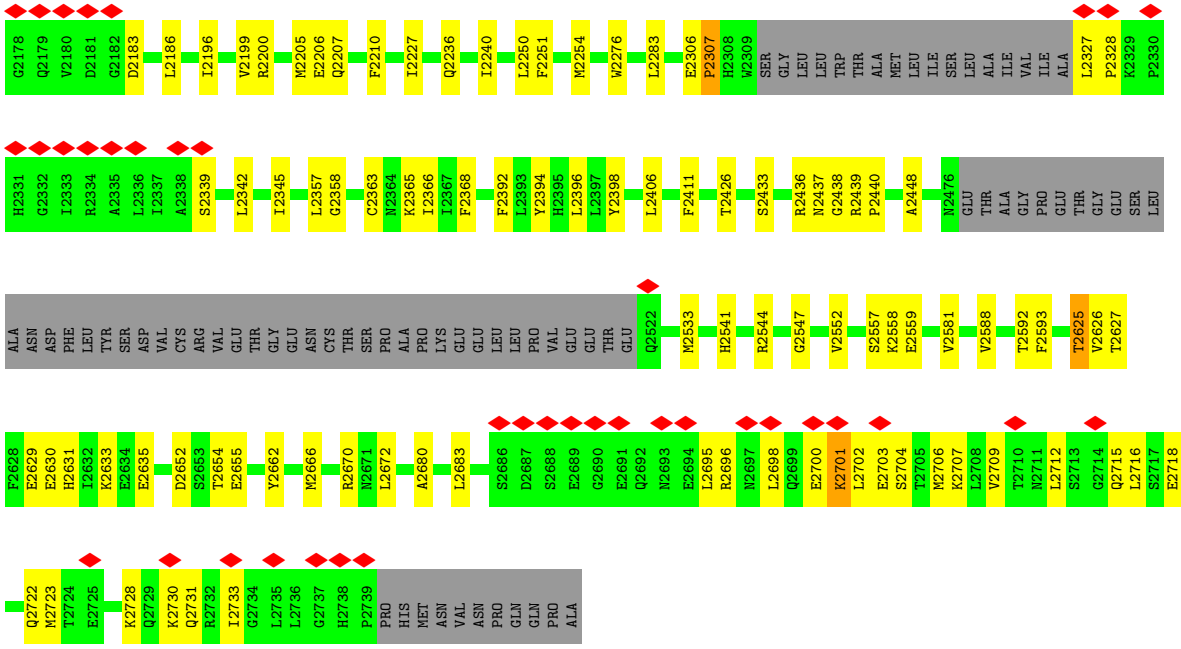
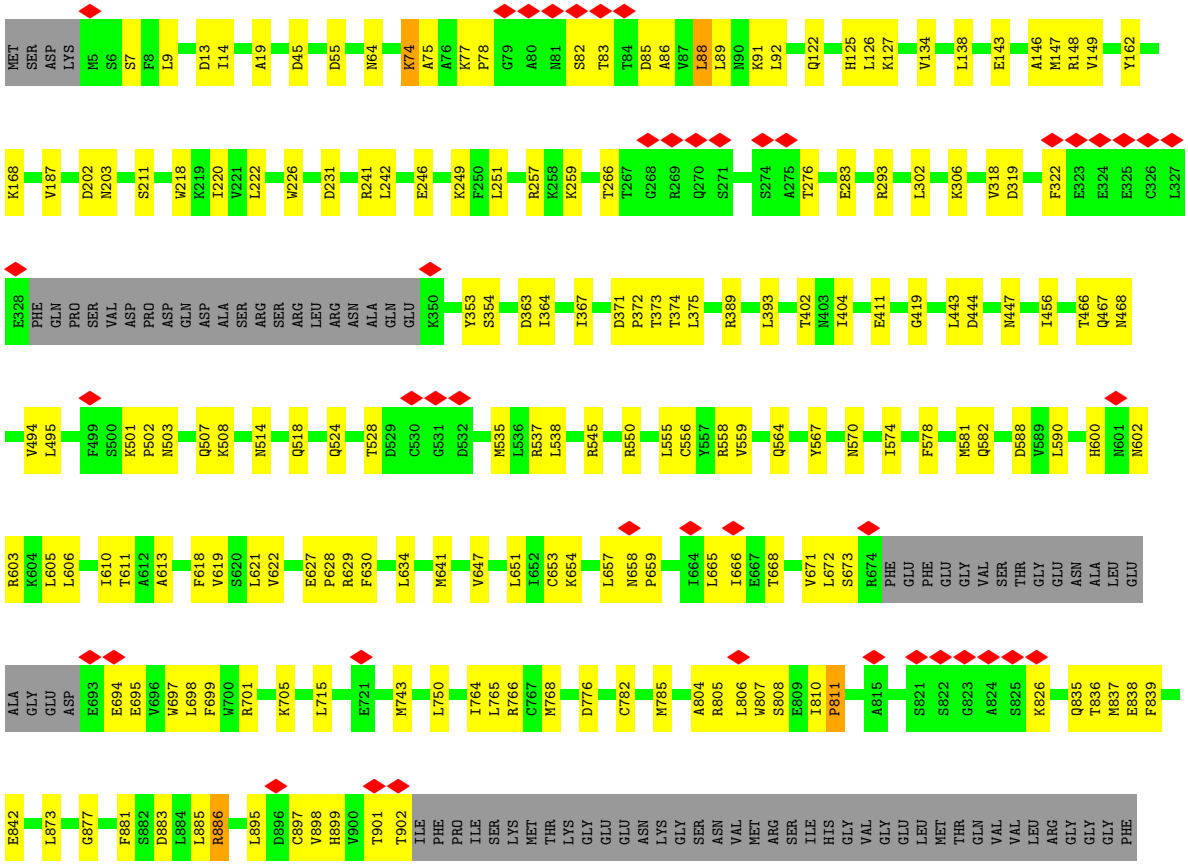
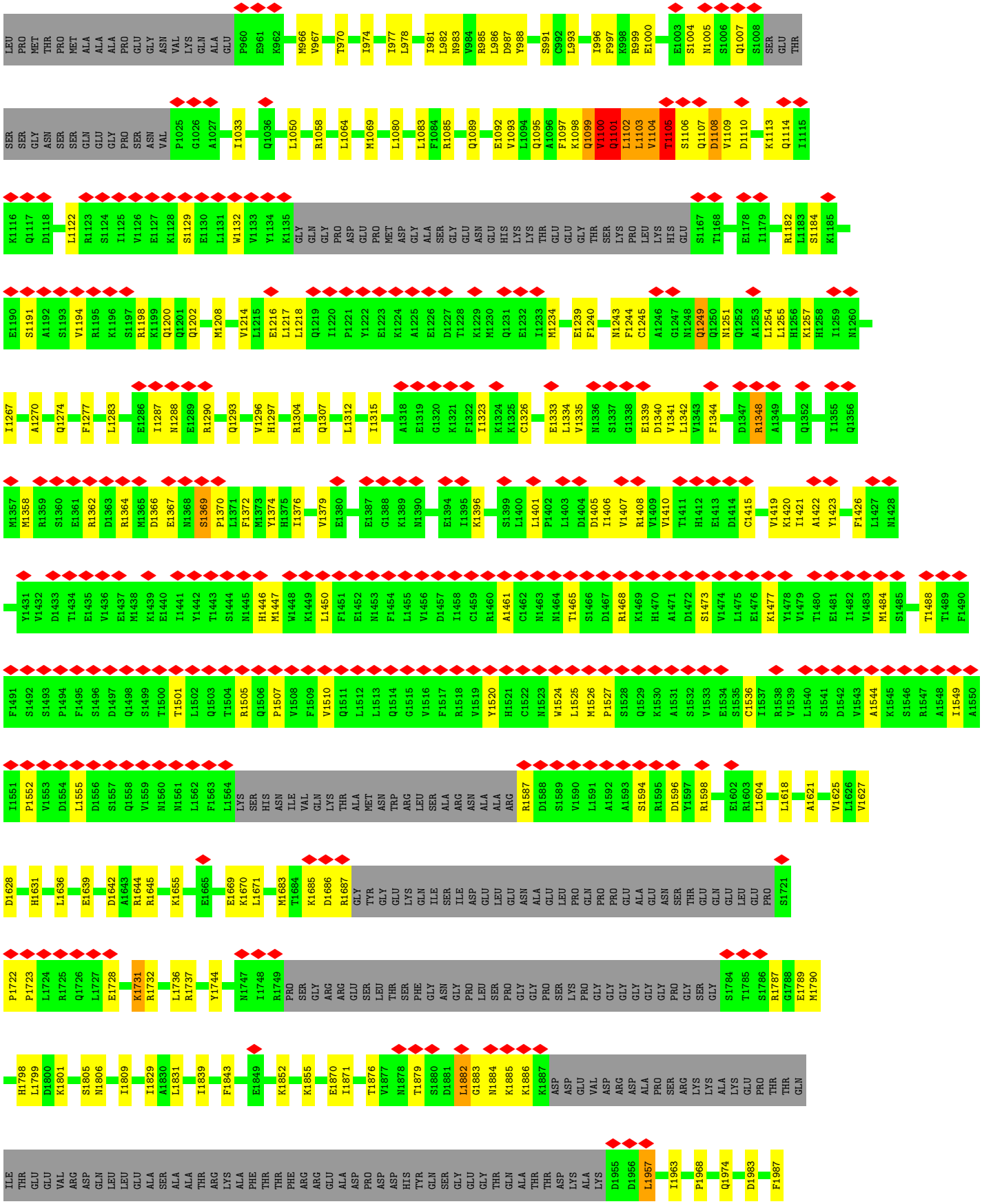
V1133 Y1134 K1135 GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU S1167 T1168 S1169 R1174 V1175 E1178 I1179 R1182 L1183 S1184 K1185 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200
Q1201 Q1202 M1208 V1214 L1215 E1216 L1217 L1218 Q1219 I1220 P1221 Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 E1239 F1240 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 M1251 Q1252 A1253 L1254 L1255 H1256 K1257 H1258 I1259 N1260 I1267 A1270 Q1274 F1277 L1283 E1286
I1287 N1288 E1289 R1290 Q1293 V1296 H1297 R1304 Q1307 L1312 I1315 A1318 E1319 G1320 K1321 F1322 I1323 K1324 K1325 C1326 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 D1347 R1348 A1349 Q1352 I1355 Q1356 M1357 M1358 R1359 S1360 E1361 R1362 D1363 R1364 M1365 D1366 E1367
N1368 S1369 P1370 L1371 F1372 M1373 Y1374 H1375 I1376 V1379 E1380 L1381 L1382 E1387 G1388 K1389 N1390 E1394 I1395 K1396 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 V1419 K1420 I1421 A1422 Y1423 F1426 L1427 N1428 Y1431 V1432 D1433 T1434 E1435 V1436 E1437 M1438
K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 I1458 C1459 R1460 A1461 C1462 N1463 N1464 T1465 S1466 D1467 R1468 K1469 H1470 A1471 D1472 S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 F1491 S1492 S1493 P1494 F1495 S1496 D1497 Q1498
S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 V1539 L1540 S1541 D1542 V1543 A1544 K1545 S1546 R1547 A1548 I1549 A1550 I1551 P1552 V1553 D1554 L1555 D1556 S1557 Q1558
V1559 N1560 N1561 L1562 F1563 L1564 LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG R1587 D1588 S1589 V1590 L1591 A1592 A1593 S1594 R1595 D1596 Y1597 R1598 E1602 L1618 A1621 V1625 L1626 V1627 D1628 H1631 L1636 E1639 D1642 A1643
R1644 R1645 K1655 E1665 E1669 K1670 L1671 K1685 D1686 R1687 GLY TYR GLY GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO S1721 P1722 P1723 L1724 R1725 Q1726 L1727 E1728 K1731 R1732 L1736
R1737 Y1744 N1747 I1748 R1749 PRO SER GLY ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY PRO GLY SER GLY S1784 T1785 S1786 R1787 G1788 E1789 M1790 H1798 K1801 S1805 N1806 I1809 I1829 A1830
L1831 I1839 F1843 E1849 K1852 K1855 E1870 T1876 V1877 N1878 T1879 S1880 D1881 L1882 G1883 N1884 K1885 K1886 K1887 ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA
ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1965 D1966 L1957 I1963 P1968 Q1974 D1983 F1987 L2020 L2021 G2022 L2023 N2026 V2030 N2034 Q2035 E2038
S2039 L2040 Y2043 C2044 Q2045 I2063 D2064 I2065 I2066 L2069 I2070 D2083 L2084 L2096 I2112 N2115 P2118 K2119 E2120 L2121 V2122 N2130 Q2131 G2132 E2133 Y2134 E2135 F2136 E2137 D2138 G2139 E2140 N2141 G2142 E2143 D2144 G2145 R2150 N2151 V2152 G2153 H2154 W2155 I2156 Y2157 I2158 L2170 G2177



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

Chain C:

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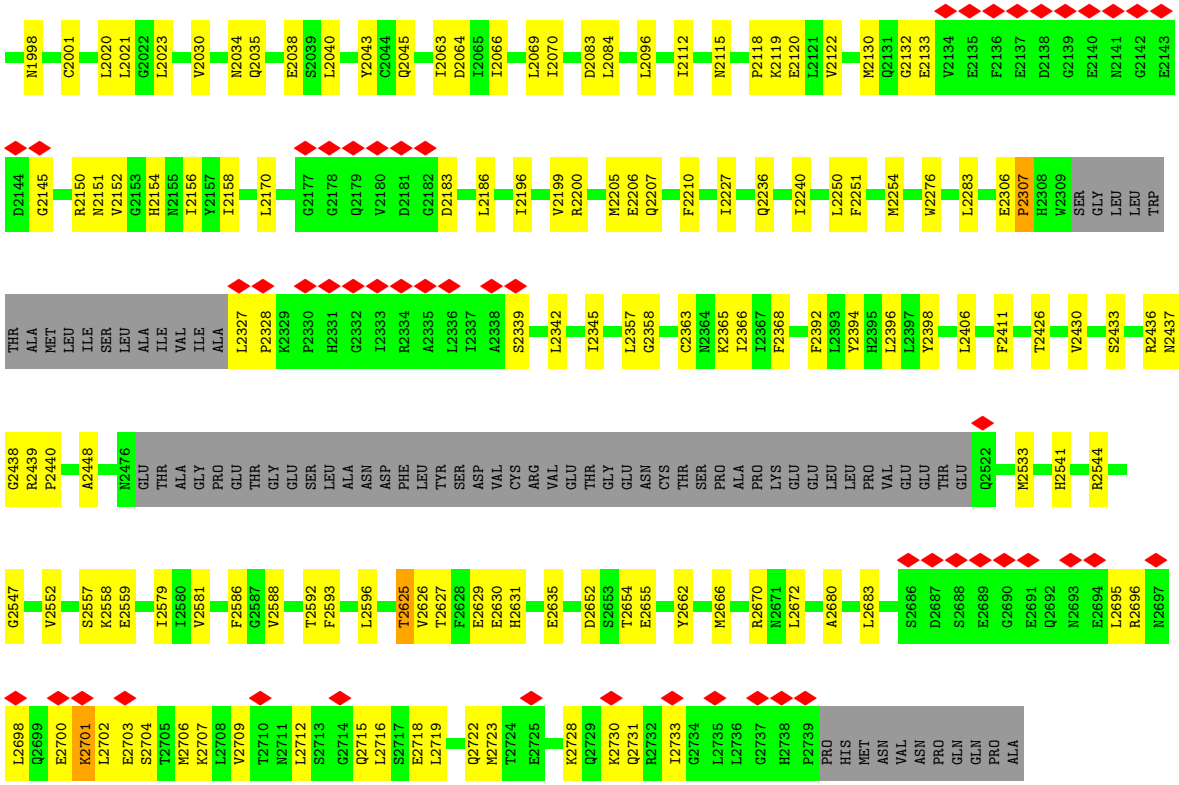
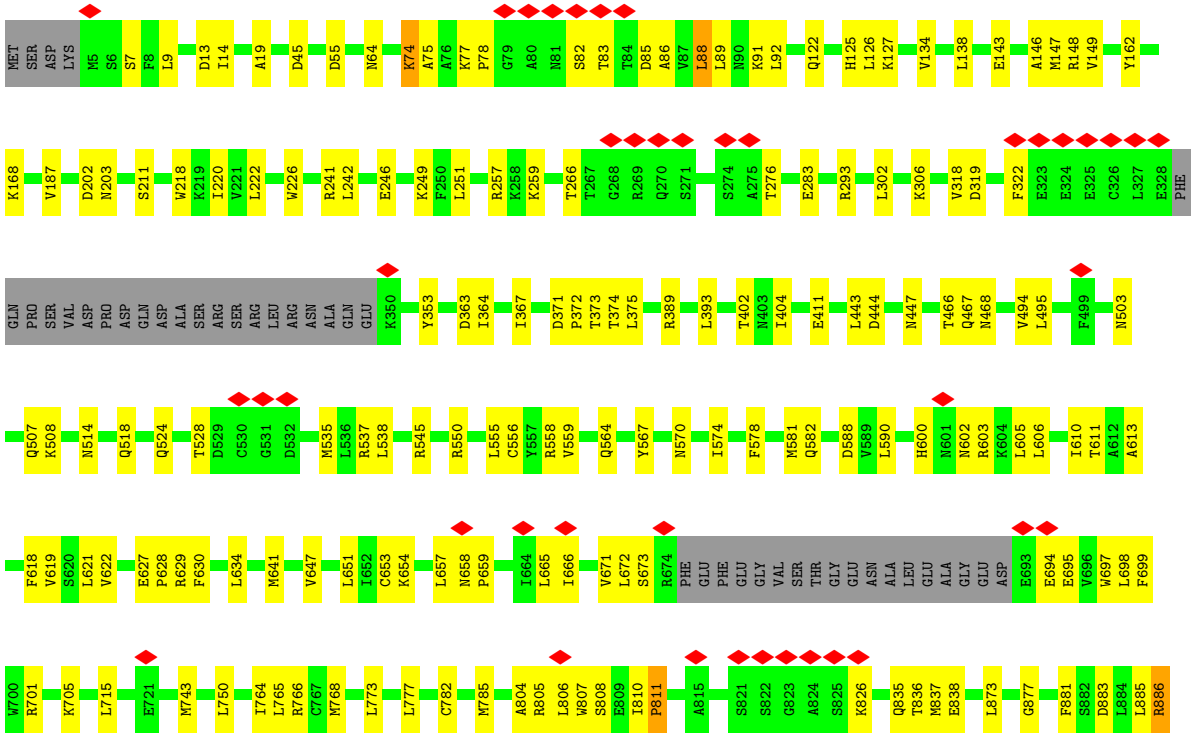
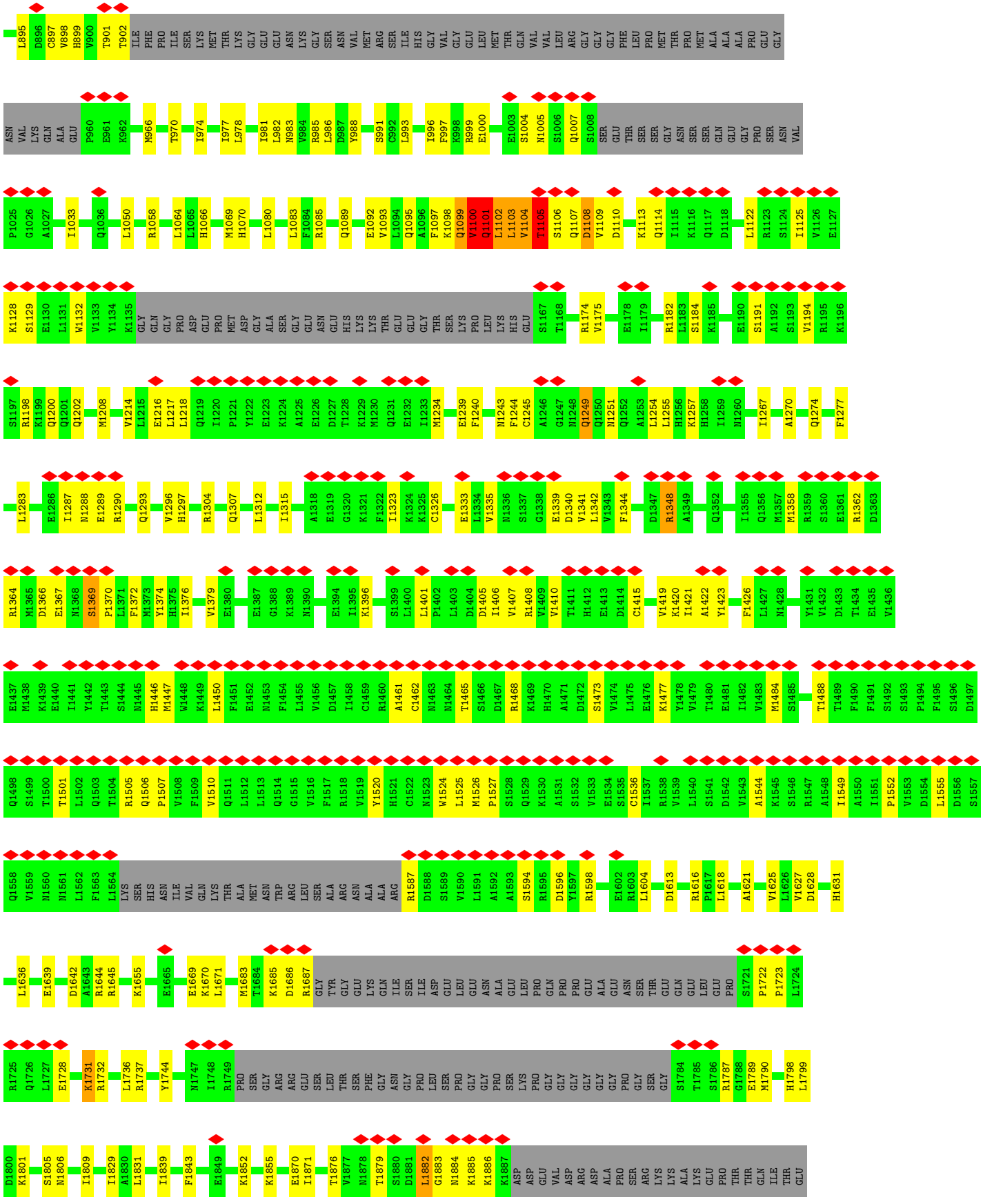
SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL P1025 G1026 A1027 I1033 Q1036 L1050 R1058 L1064 M1069 L1080 L1083 F1084 R1085 Q1089 E1092 V1093 L1094 Q1095 A1096 F1097 K1098 Q1099 V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 V1109 D1110 K1113 Q1114 I1115
K1116 Q1117 D1118 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 E1130 L1131 W1132 V1133 Y1134 K1135 GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU S1167 T1168 E1178 I1179 R1182 L1183 S1184 K1185
E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200 Q1201 Q1202 M1208 V1214 L1215 E1216 L1217 L1218 Q1219 I1220 P1221 Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 E1239 F1240 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 L1254 L1255 H1256 K1257 H1258 I1259 N1260
I1267 A1270 Q1274 F1277 L1283 E1286 I1287 N1288 E1289 R1290 Q1293 V1296 H1297 R1304 Q1307 L1312 I1315 A1318 E1319 G1320 K1321 F1322 I1323 K1324 K1325 C1326 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 D1347 R1348 A1349 Q1352 I1355 Q1356
M1357 M1358 R1359 S1360 E1361 R1362 D1363 R1364 M1365 D1366 E1367 N1368 S1369 P1370 L1371 F1372 M1373 Y1374 H1375 I1376 V1379 E1380 E1387 G1388 K1389 N1390 E1394 I1395 K1396 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 V1419 K1420 I1421 A1422 Y1423 F1426 L1427 N1428
Y1431 V1432 D1433 T1434 E1435 V1436 E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 I1458 C1459 R1460 A1461 C1462 N1463 N1464 T1465 S1466 D1467 R1468 K1469 H1470 A1471 D1472 S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 T1488 T1489 F1490
F1491 S1492 S1493 P1494 F1495 S1496 D1497 Q1498 S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 V1539 L1540 S1541 D1542 V1543 A1544 K1545 S1546 R1547 A1548 I1549 A1550
I1551 P1552 V1553 D1554 L1555 D1556 S1557 Q1558 V1559 N1560 N1561 L1562 F1563 L1564 LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG R1587 D1588 S1589 V1590 L1591 A1592 A1593 S1594 R1595 D1596 Y1597 R1598 E1602 R1603 L1604 L1618 A1621 V1625 L1626 V1627
D1628 H1631 L1636 E1639 D1642 A1643 R1644 R1645 K1655 E1665 E1669 K1670 L1671 M1683 T1684 K1685 D1686 R1687 GLY TYR GLY GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO S1721
P1722 P1723 L1724 R1725 Q1726 L1727 E1728 K1731 R1732 L1736 R1737 Y1744 N1747 I1748 R1749 PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY PRO GLY SER GLY S1784 T1785 S1786 R1787 G1788 E1789 M1790
H1798 L1799 D1800 K1801 S1805 N1806 I1809 I1829 A1830 L1831 I1839 F1843 E1849 K1852 K1855 E1870 I1871 T1876 V1877 N1878 T1879 S1880 D1881 L1882 G1883 N1884 K1885 K1886 K1887 ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN
ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 L1957 I1963 P1968 Q1974 D1983 F1987



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

Chain D:

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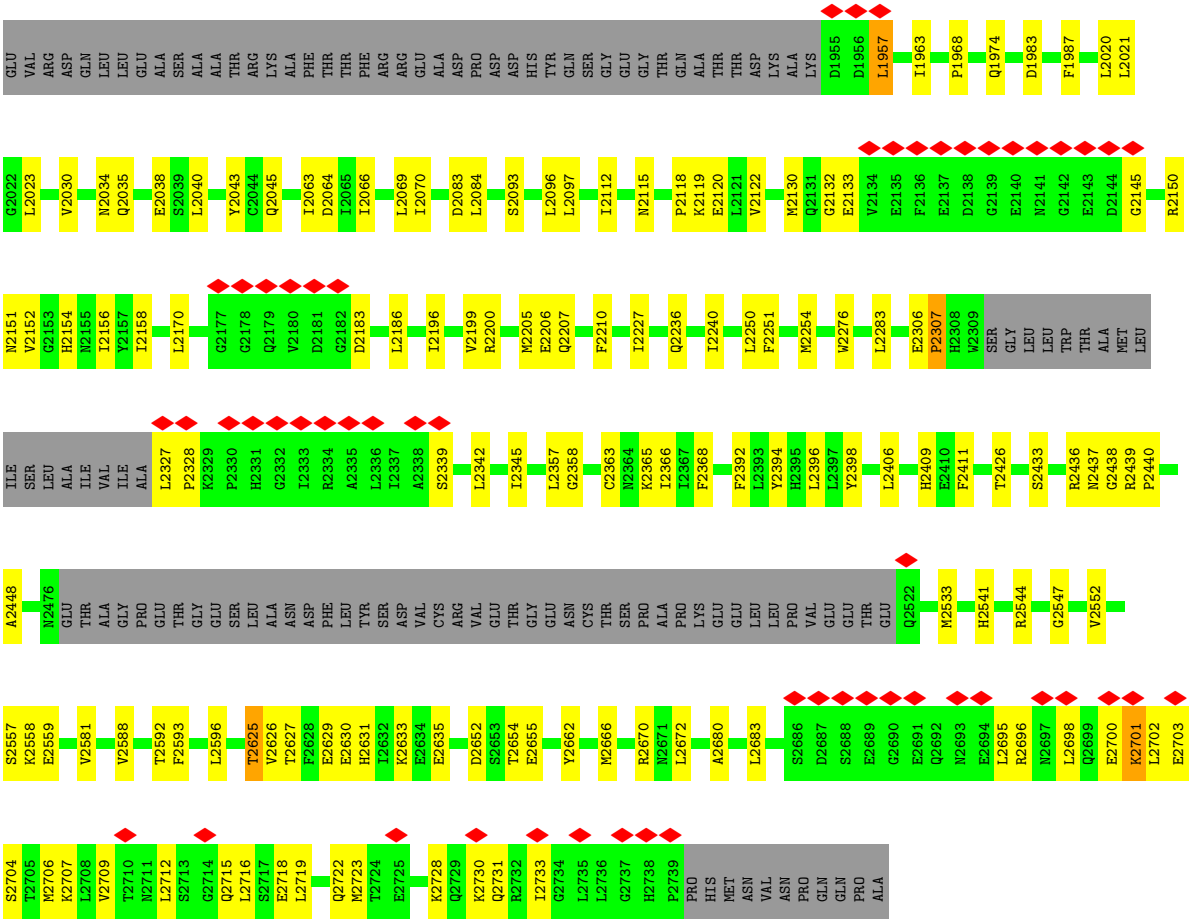
ASN VAL LYS GLN ALA GLU P960 E961 K962 M966 T970 I974 I977 L978 I981 L982 N983 V984 R985 L986 D987 Y988 S991 C992 L993 I996 F997 K998 R999 E1000 E1003 S1004 N1005 S1006 Q1007 S1008 SER GLU THR SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL
P1025 G1026 A1027 I1033 Q1036 L1050 R1058 L1064 L1065 H1066 M1069 H1070 L1080 L1083 F1084 R1085 Q1089 E1092 V1093 L1094 Q1095 A1096 F1097 K1098 Q1099 V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 V1109 D1110 K1113 Q1114 I1115 K1116 Q1117 D1118 L1122 R1123 S1124 I1125 V1126 E1127
K1128 S1129 E1130 L1131 W1132 V1133 Y1134 K1135 GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU S1167 T1168 R1174 V1175 E1178 I1179 R1182 L1183 S1184 K1185 E1190 S1191 A1192 S1193 V1194 R1195 K1196
S1197 R1198 K1199 Q1200 Q1201 Q1202 M1208 V1214 L1215 E1216 L1217 L1218 Q1219 I1220 P1221 Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 E1239 F1240 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 L1254 L1255 H1256 K1257 H1258 I1259 N1260 I1267 A1270 Q1274 F1277
L1283 E1286 I1287 N1288 E1289 R1290 Q1293 V1296 H1297 R1304 Q1307 L1312 I1315 A1318 E1319 G1320 K1321 F1322 I1323 K1324 K1325 C1326 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 D1347 R1348 A1349 Q1352 I1355 Q1356 M1357 M1358 R1359 S1360 E1361 R1362 D1363
R1364 M1365 D1366 E1367 N1368 S1369 P1370 L1371 F1372 M1373 Y1374 H1375 I1376 V1379 E1380 E1387 G1388 K1389 N1390 E1394 I1395 K1396 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 V1419 K1420 I1421 A1422 Y1423 F1426 L1427 N1428 Y1431 V1432 D1433 T1434 E1435 V1436
E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 I1458 C1459 R1460 A1461 C1462 N1463 N1464 T1465 S1466 D1467 R1468 K1469 H1470 A1471 D1472 S1473 V1474 L1475 E1476 K1477 Y1478 Y1479 T1480 E1481 I1482 V1483 M1484 S1485 T1488 T1489 F1490 F1491 S1492 S1493 P1494 F1495 S1496 D1497
Q1498 S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 V1539 L1540 S1541 D1542 V1543 A1544 K1545 S1546 R1547 A1548 I1549 A1550 I1551 P1552 V1553 D1554 L1555 D1556 S1557
Q1558 V1559 N1560 N1561 L1562 F1563 L1564 LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG R1587 D1588 S1589 V1590 L1591 A1592 A1593 S1594 R1595 D1596 Y1597 R1598 E1602 R1603 L1604 D1613 R1616 P1617 L1618 A1621 V1625 L1626 V1627 D1628 H1631
L1636 E1639 D1642 A1643 R1644 R1645 K1655 E1665 E1669 K1670 L1671 M1683 T1684 K1685 D1686 R1687 GLY TYR GLY GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO S1721 P1722 P1723 L1724
R1725 Q1726 L1727 E1728 K1731 R1732 L1736 R1737 Y1744 N1747 I1748 R1749 PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY PRO GLY SER GLY S1784 T1785 S1786 R1787 G1788 E1789 M1790 H1798 L1799
D1800 K1801 S1805 N1806 I1809 I1829 A1830 L1831 I1839 F1843 E1849 K1852 K1855 E1870 I1871 T1876 V1877 N1878 T1879 S1880 D1881 L1882 G1883 N1884 K1885 K1886 K1887 ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU


GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 L1957 I1963 P1968 Q1974 D1983 F1987 L2020 L2021
G2022 L2023 V2030 N2034 Q2035 E2038 S2039 L2040 Y2043 C2044 Q2045 I2063 D2064 I2065 I2066 L2069 I2070 D2083 L2084 S2093 L2096 L2097 I2112 N2115 P2118 K2119 E2120 L2121 V2122 M2130 Q2131 G2132 E2133 V2134 E2135 F2136 E2137 D2138 G2139 E2140 N2141 G2142 E2143 D2144 G2145 R2150
N2151 V2152 G2153 H2154 N2155 I2156 Y2157 I2158 L2170 G2177 G2178 Q2179 V2180 D2181 C2182 D2183 L2186 I2196 V2199 R2200 M2205 E2206 Q2207 F2210 I2227 Q2236 I2240 L2250 F2251 M2254 W2276 L2283 E2306 P2307 H2308 W2309 SER GLY LEU LEU TRP THR ALA MET LEU
ILE SER LEU ALA ILE VAL ILE ALA L2327 P2328 K2329 P2330 H2331 G2332 I2333 R2334 A2335 L2336 I2337 A2338 S2339 L2342 I2345 L2357 G2358 C2363 N2364 K2365 I2366 I2367 F2368 F2392 L2393 Y2394 H2395 L2396 L2397 Y2398 L2406 H2409 E2410 F2411 T2426 S2433 R2436 N2437 G2438 R2439 P2440
A2448 N2476 GLU THR ALA GLY PRO GLU THR GLY GLU SER LEU ALA ASN ASP PHE LEU TYR SER ASP VAL CYS ARG VAL GLU THR GLY GLU ASN CYS THR SER PRO ALA PRO LYS GLU GLU LEU LEU PRO VAL GLU GLU THR GLU Q2522 M2533 H2541 R2544 G2547 V2552
S2557 K2558 E2559 V2581 V2588 T2592 P2593 L2596 T2625 V2626 T2627 P2628 E2629 E2630 H2631 I2632 K2633 E2634 E2635 D2652 S2653 T2654 E2655 Y2662 M2666 R2670 N2671 L2672 A2680 L2683 S2686 D2687 S2688 E2689 G2690 E2691 Q2692 N2693 E2694 L2695 R2696 N2697 L2698 Q2699 E2700 K2701 L2702 E2703
S2704 T2705 M2706 K2707 L2708 V2709 T2710 N2711 L2712 S2713 G2714 Q2715 L2716 S2717 E2718 L2719 Q2722 M2723 T2724 E2725 K2728 Q2729 K2730 Q2731 R2732 I2733 G2734 L2735 L2736 G2737 H2738 P2739 PRO HIS MET ASN VAL ASN PRO GLN GLN PRO ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	346731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/19547	0.50	4/26382 (0.0%)
1	B	0.27	0/19547	0.50	4/26382 (0.0%)
1	C	0.27	0/19547	0.51	4/26382 (0.0%)
1	D	0.27	0/19547	0.50	4/26382 (0.0%)
All	All	0.27	0/78188	0.50	16/105528 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1882	LEU	CA-CB-CG	5.99	129.08	115.30
1	C	1882	LEU	CA-CB-CG	5.99	129.08	115.30
1	D	1882	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	1882	LEU	CA-CB-CG	5.98	129.05	115.30
1	B	1957	LEU	CA-CB-CG	5.47	127.88	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1098	LYS	Mainchain
1	A	665	LEU	Peptide
1	B	1098	LYS	Mainchain
1	B	665	LEU	Peptide
1	C	665	LEU	Peptide

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	19195	0	19276	410	0
1	B	19195	0	19276	400	0
1	C	19195	0	19276	409	0
1	D	19195	0	19276	398	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	6	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
4	A	281	0	412	21	0
4	B	281	0	412	20	0
4	C	281	0	412	19	0
4	D	281	0	412	23	0
All	All	77928	0	78752	1551	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 10.

The worst 5 of 1551 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:D:806:LEU:HD11	1:D:1104:VAL:N	1.84	0.93
1:A:806:LEU:HD11	1:A:1104:VAL:N	1.84	0.92
1:B:806:LEU:HD11	1:B:1104:VAL:N	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:LEU:HD11	1:C:1104:VAL:N	1.84	0.92
1:A:1101:GLN:O	1:A:1102:LEU:HB2	1.75	0.86

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	2351/2750 (86%)	2245 (96%)	97 (4%)	9 (0%)	34	67
1	B	2351/2750 (86%)	2244 (95%)	98 (4%)	9 (0%)	34	67
1	C	2351/2750 (86%)	2245 (96%)	97 (4%)	9 (0%)	34	67
1	D	2351/2750 (86%)	2244 (95%)	98 (4%)	9 (0%)	34	67
All	All	9404/11000 (86%)	8978 (96%)	390 (4%)	36 (0%)	38	67

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	PRO
1	A	1101	GLN
1	A	1102	LEU
1	A	1108	ASP
1	A	2307	PRO

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	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89
1	B	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89
1	C	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89
1	D	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89
All	All	8616/9836 (88%)	8548 (99%)	68 (1%)	82	89

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1101	GLN
1	D	1104	VAL
1	D	2045	GLN
1	B	1103	LEU
1	B	1101	GLN

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

Mol	Chain	Res	Type
1	C	1558	GLN
1	C	2699	GLN
1	C	1998	ASN
1	D	1005	ASN
1	B	1005	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 24 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
4	PLX	A	5108	-	45,45,51	1.14	5 (11%)	49,53,59	0.78	0
4	PLX	D	5112	-	45,45,51	1.14	5 (11%)	49,53,59	0.78	0
4	PLX	D	5109	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	A	5113	-	38,38,51	1.17	3 (7%)	42,46,59	0.80	0
4	PLX	C	5110	-	36,36,51	1.14	4 (11%)	40,44,59	1.22	2 (5%)
4	PLX	A	5110	-	39,39,51	1.18	4 (10%)	43,47,59	0.74	0
4	PLX	C	5111	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	B	5109	-	36,36,51	1.15	4 (11%)	40,44,59	1.22	2 (5%)
4	PLX	A	5114	-	37,37,51	1.20	4 (10%)	41,45,59	0.75	0
4	PLX	B	5113	-	45,45,51	1.13	5 (11%)	49,53,59	0.77	0
4	PLX	D	5110	-	38,38,51	1.16	4 (10%)	42,46,59	0.80	0
4	PLX	C	5113	-	37,37,51	1.19	4 (10%)	41,45,59	0.75	0
4	PLX	B	5108	-	39,39,51	1.18	4 (10%)	43,47,59	0.74	0
4	PLX	D	5108	-	36,36,51	1.14	4 (11%)	40,44,59	1.22	2 (5%)
4	PLX	C	5109	-	39,39,51	1.18	4 (10%)	43,47,59	0.74	0
4	PLX	A	5109	-	44,44,51	1.15	2 (4%)	48,52,59	0.77	0
4	PLX	B	5107	-	44,44,51	1.15	2 (4%)	48,52,59	0.77	0
4	PLX	B	5110	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	D	5106	-	44,44,51	1.16	2 (4%)	48,52,59	0.77	0
4	PLX	B	5112	-	37,37,51	1.20	4 (10%)	41,45,59	0.75	0
4	PLX	A	5111	-	36,36,51	1.15	4 (11%)	40,44,59	1.23	2 (5%)
4	PLX	C	5112	-	38,38,51	1.16	4 (10%)	42,46,59	0.80	0
4	PLX	B	5111	-	38,38,51	1.17	3 (7%)	42,46,59	0.80	0
4	PLX	A	5112	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	D	5107	-	39,39,51	1.19	4 (10%)	43,47,59	0.74	0
4	PLX	C	5107	-	45,45,51	1.14	5 (11%)	49,53,59	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PLX	C	5108	-	44,44,51	1.15	2 (4%)	48,52,59	0.77	0
4	PLX	D	5111	-	37,37,51	1.20	3 (8%)	41,45,59	0.75	0

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
4	PLX	A	5108	-	-	30/49/49/55	-
4	PLX	D	5112	-	-	30/49/49/55	-
4	PLX	D	5109	-	-	26/39/39/55	-
4	PLX	A	5113	-	-	19/42/42/55	-
4	PLX	C	5110	-	-	18/40/40/55	-
4	PLX	A	5110	-	-	20/43/43/55	-
4	PLX	C	5111	-	-	26/39/39/55	-
4	PLX	B	5109	-	-	18/40/40/55	-
4	PLX	A	5114	-	-	14/41/41/55	-
4	PLX	B	5113	-	-	30/49/49/55	-
4	PLX	D	5110	-	-	19/42/42/55	-
4	PLX	C	5113	-	-	14/41/41/55	-
4	PLX	B	5108	-	-	19/43/43/55	-
4	PLX	D	5108	-	-	18/40/40/55	-
4	PLX	C	5109	-	-	20/43/43/55	-
4	PLX	A	5109	-	-	24/48/48/55	-
4	PLX	B	5107	-	-	24/48/48/55	-
4	PLX	B	5110	-	-	26/39/39/55	-
4	PLX	D	5106	-	-	24/48/48/55	-
4	PLX	B	5112	-	-	14/41/41/55	-
4	PLX	A	5111	-	-	18/40/40/55	-
4	PLX	C	5112	-	-	19/42/42/55	-
4	PLX	B	5111	-	-	19/42/42/55	-
4	PLX	A	5112	-	-	26/39/39/55	-
4	PLX	D	5107	-	-	19/43/43/55	-
4	PLX	C	5107	-	-	30/49/49/55	-
4	PLX	C	5108	-	-	24/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLX	D	5111	-	-	14/41/41/55	-

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5106	PLX	O6-C4	-3.59	1.39	1.44
4	D	5111	PLX	O6-C4	-3.52	1.39	1.44
4	A	5109	PLX	O6-C4	-3.52	1.39	1.44
4	B	5107	PLX	O6-C4	-3.52	1.39	1.44
4	C	5108	PLX	O6-C4	-3.52	1.39	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5111	PLX	C6-O6-C4	5.24	125.67	115.20
4	B	5109	PLX	C6-O6-C4	5.24	125.66	115.20
4	D	5108	PLX	C6-O6-C4	5.21	125.59	115.20
4	C	5110	PLX	C6-O6-C4	5.21	125.59	115.20
4	C	5110	PLX	O6-C4-C3	2.53	117.02	109.03

There are no chirality outliers.

5 of 602 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5108	PLX	O7-C6-O6-C4
4	A	5108	PLX	C3-O4-P1-O2
4	A	5108	PLX	C3-O4-P1-O3
4	A	5108	PLX	C2-O1-P1-O2
4	A	5108	PLX	C2-O1-P1-O3

There are no ring outliers.

28 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5108	PLX	4	0
4	D	5112	PLX	2	0
4	D	5109	PLX	3	0
4	A	5113	PLX	2	0
4	C	5110	PLX	4	0
4	A	5110	PLX	3	0
4	C	5111	PLX	3	0

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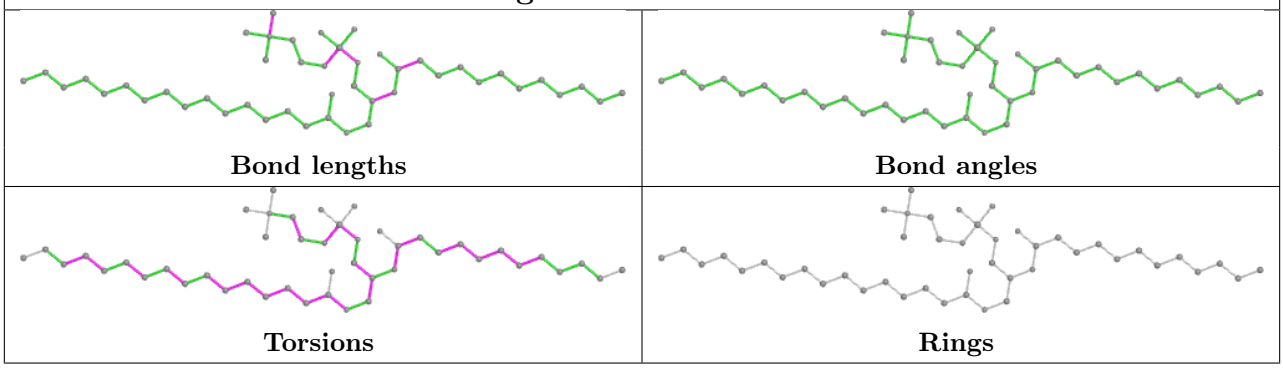
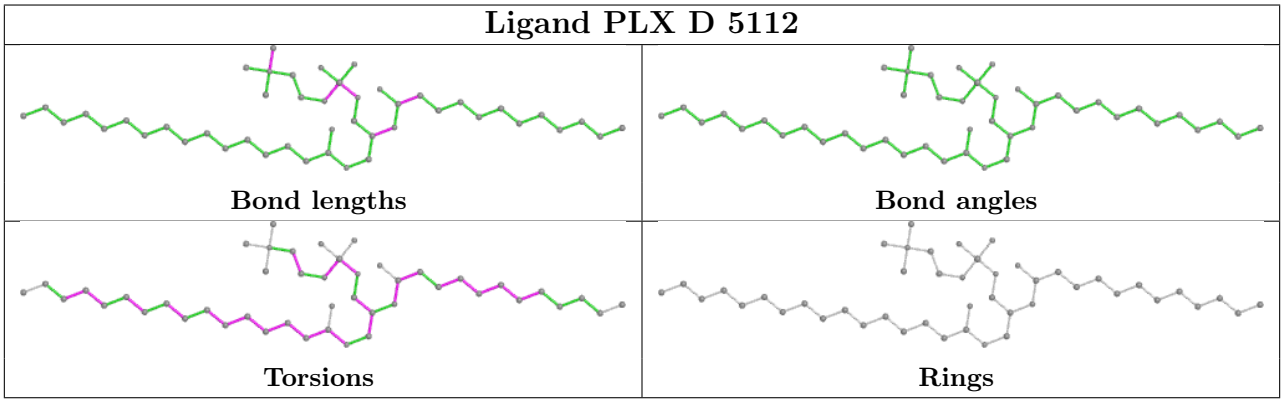
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5109	PLX	3	0
4	A	5114	PLX	3	0
4	B	5113	PLX	2	0
4	D	5110	PLX	3	0
4	C	5113	PLX	3	0
4	B	5108	PLX	3	0
4	D	5108	PLX	5	0
4	C	5109	PLX	3	0
4	A	5109	PLX	4	0
4	B	5107	PLX	4	0
4	B	5110	PLX	2	0
4	D	5106	PLX	3	0
4	B	5112	PLX	3	0
4	A	5111	PLX	4	0
4	C	5112	PLX	2	0
4	B	5111	PLX	3	0
4	A	5112	PLX	1	0
4	D	5107	PLX	3	0
4	C	5107	PLX	1	0
4	C	5108	PLX	3	0
4	D	5111	PLX	4	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.

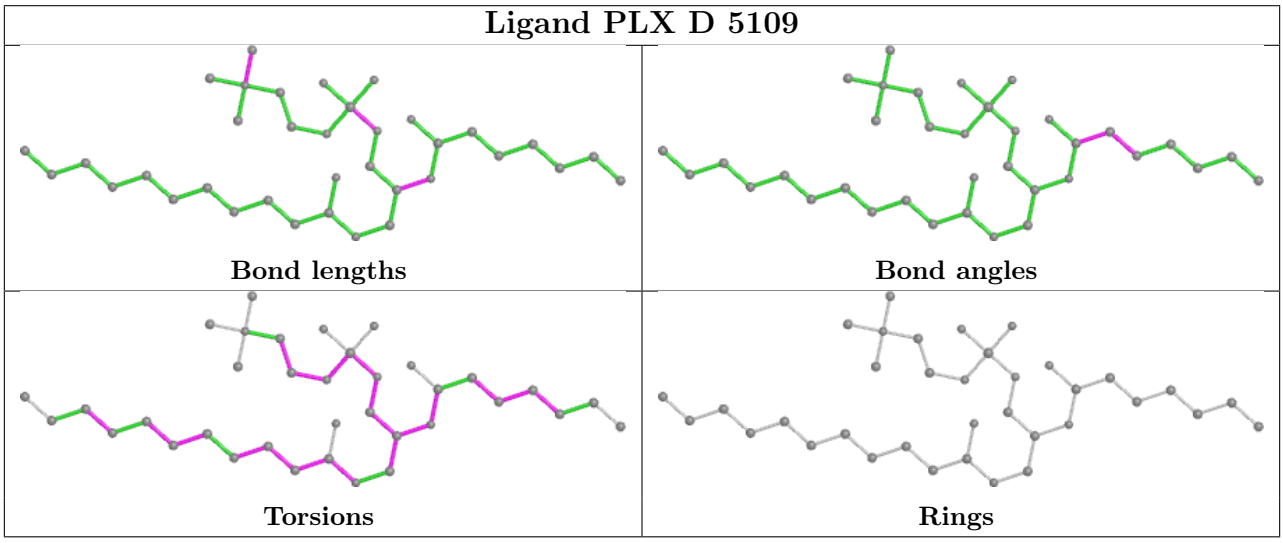
Ligand PLX A 5108



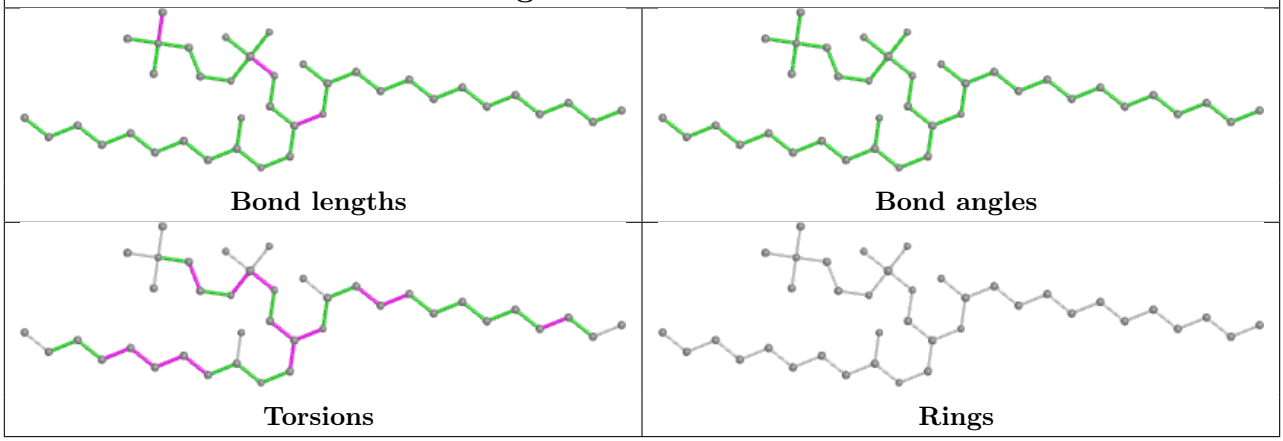
Ligand PLX D 5112



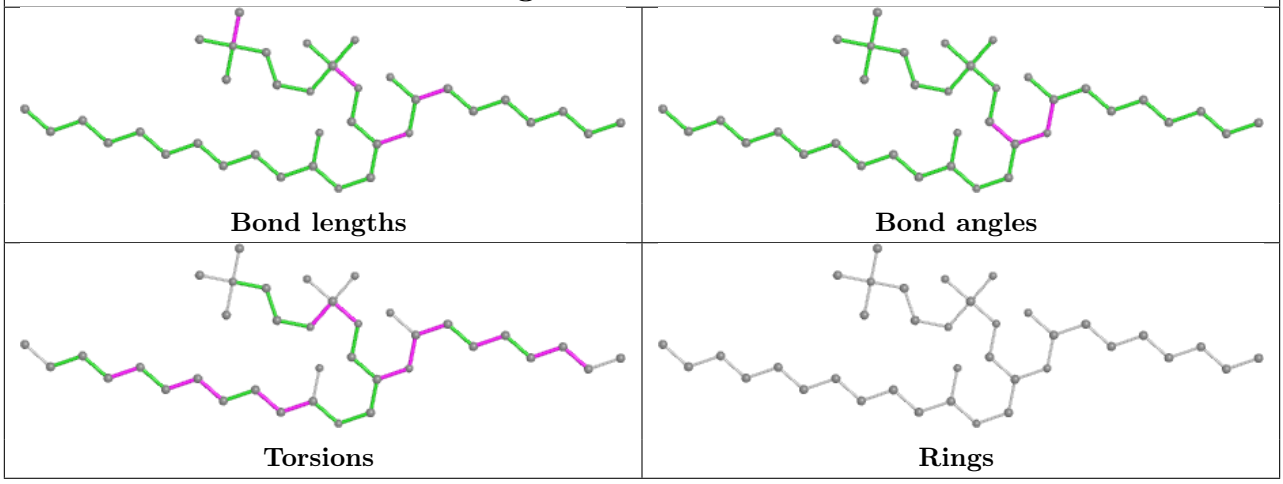
Ligand PLX D 5109



Ligand PLX A 5113



Ligand PLX C 5110



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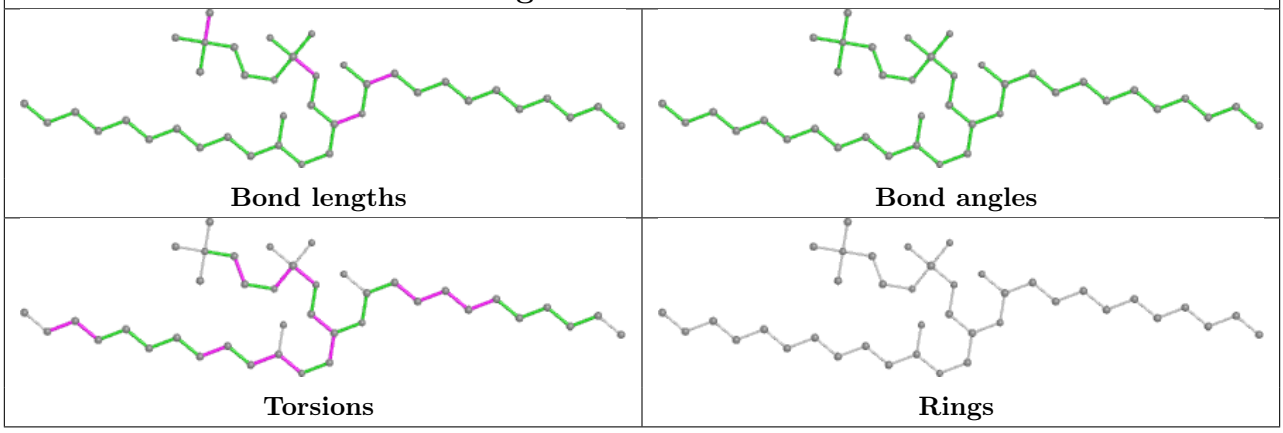
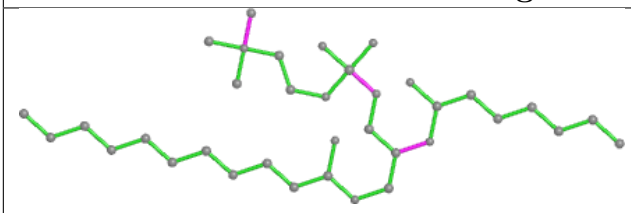
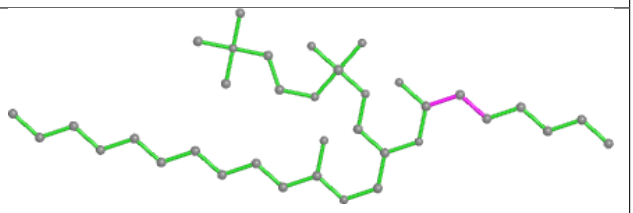
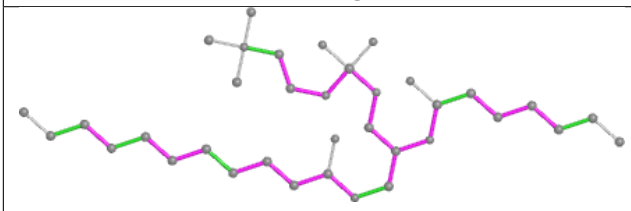
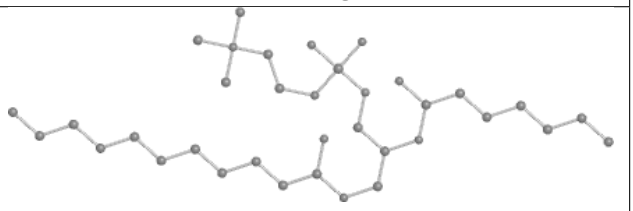


Ligand PLX C 5111

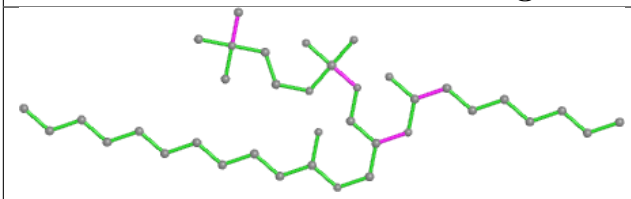

Bond lengths


Bond angles


Torsions


Rings

Ligand PLX B 5109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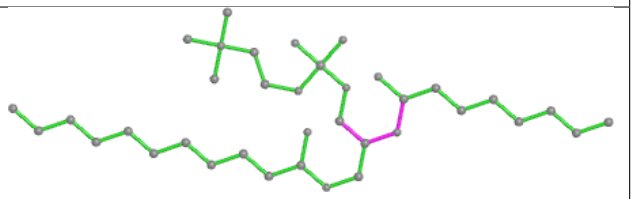
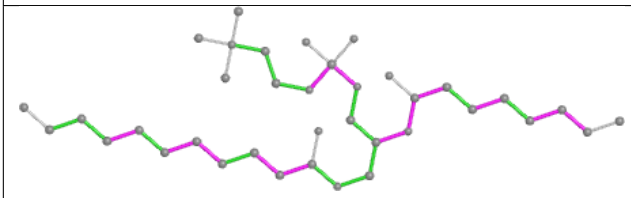

Bond angles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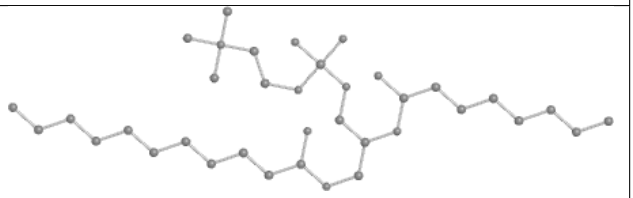
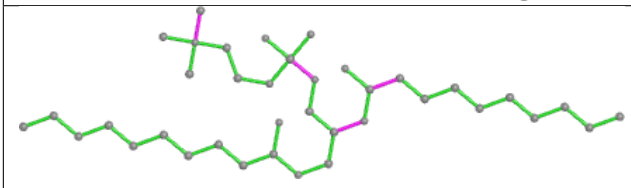

Rings

Ligand PLX A 5114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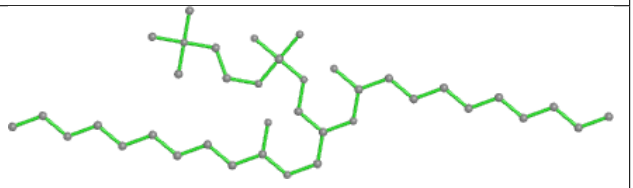
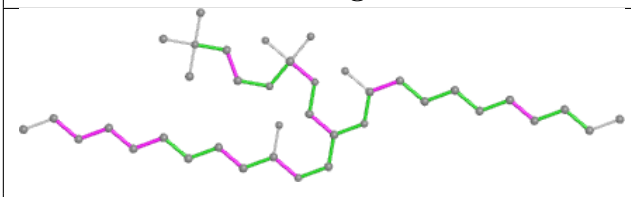
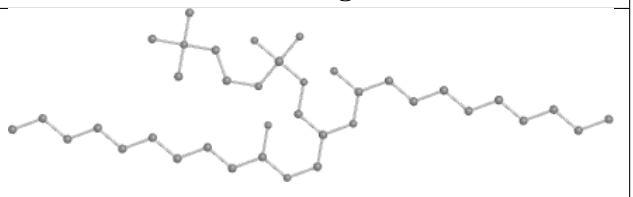
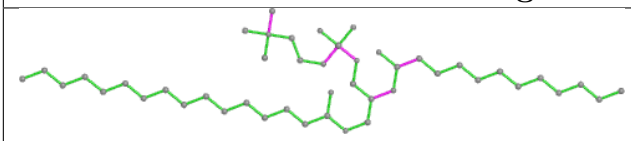
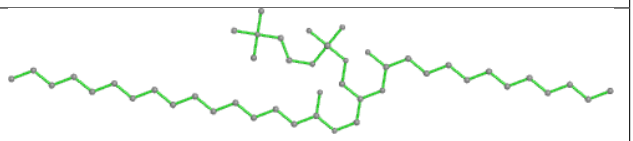
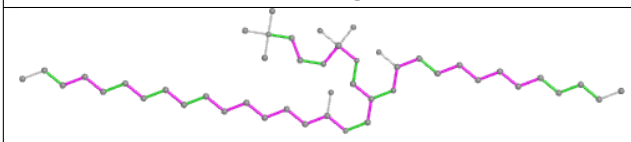
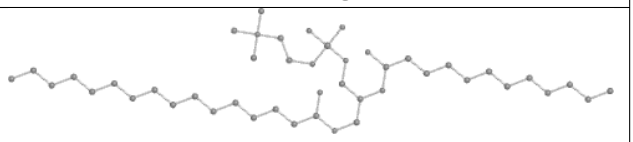
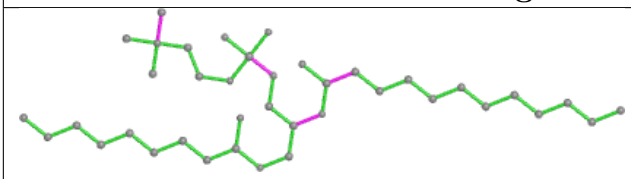
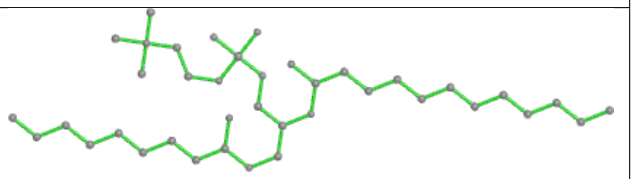
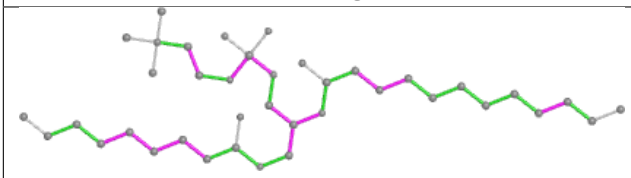
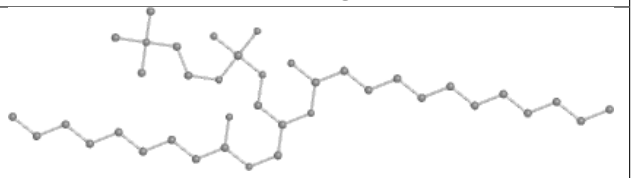
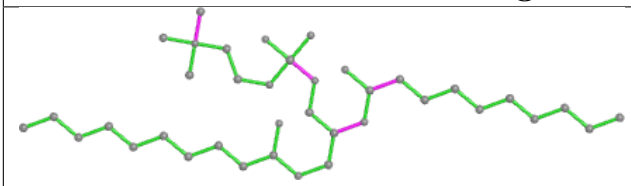
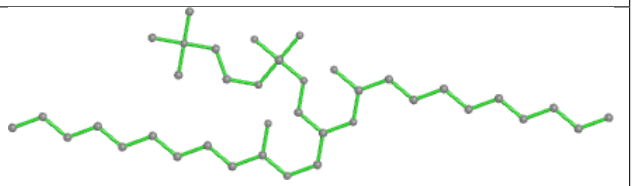
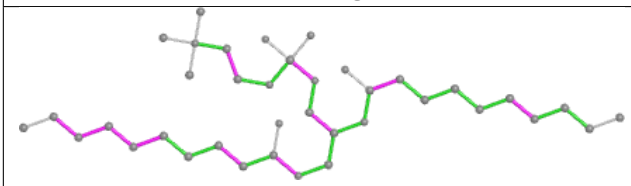
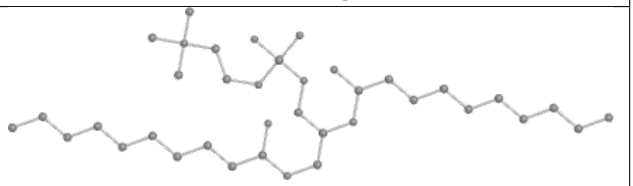

Bond angles


Torsions

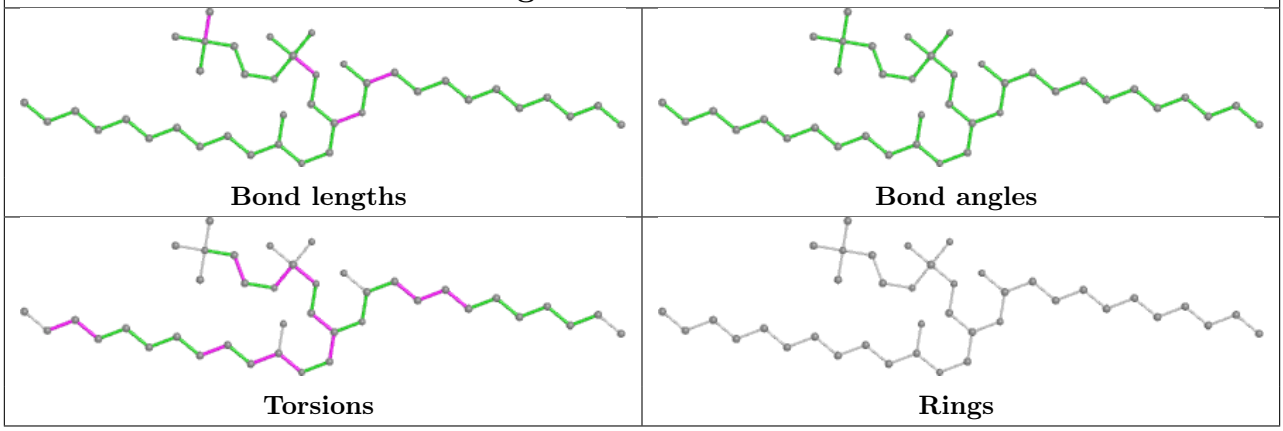

Rings

Ligand PLX B 5113	
 Bond lengths	 Bond angles
 Torsions	 Rings

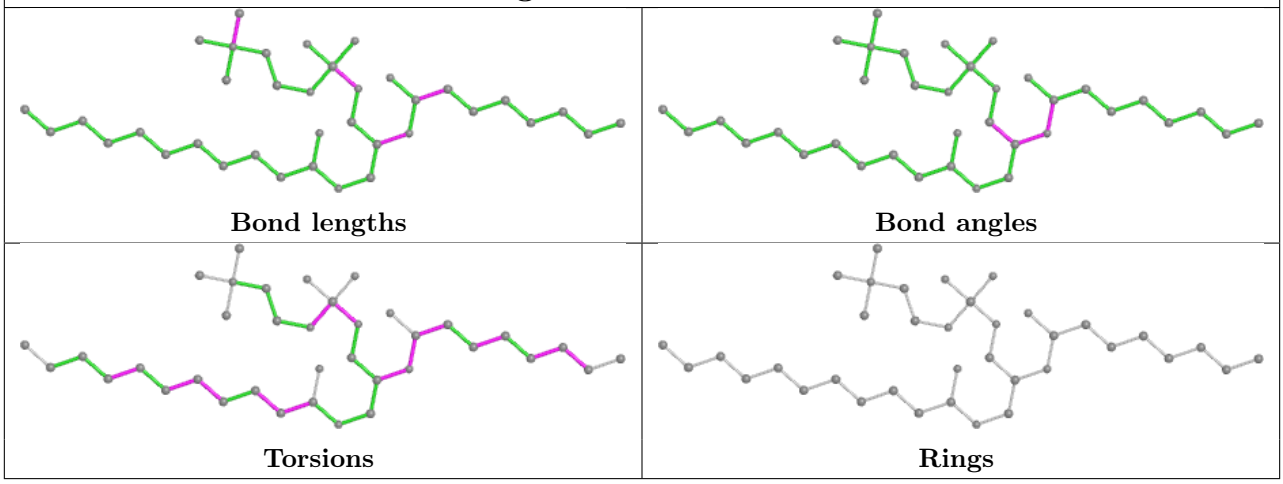
Ligand PLX D 5110	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX C 5113	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX B 5108



Ligand PLX D 5108



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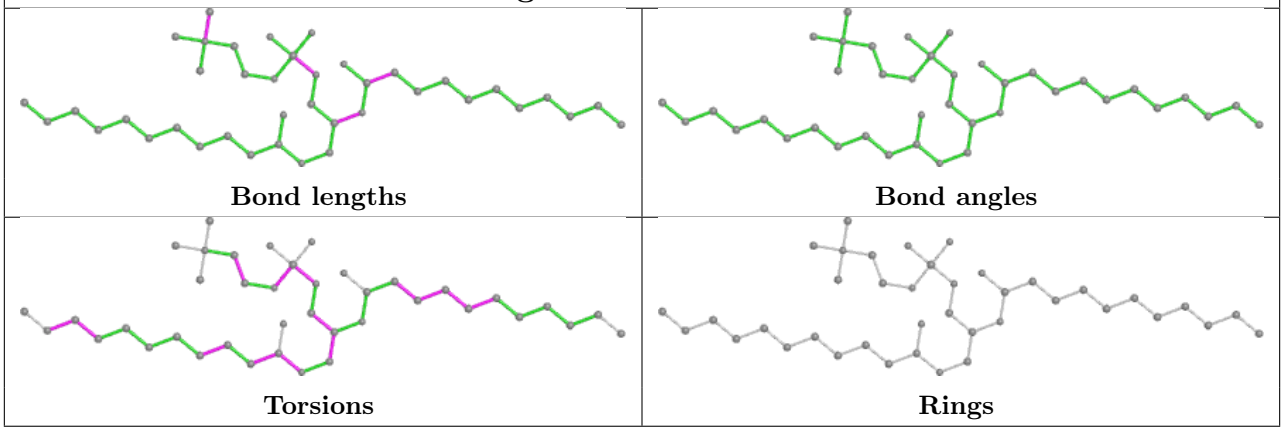
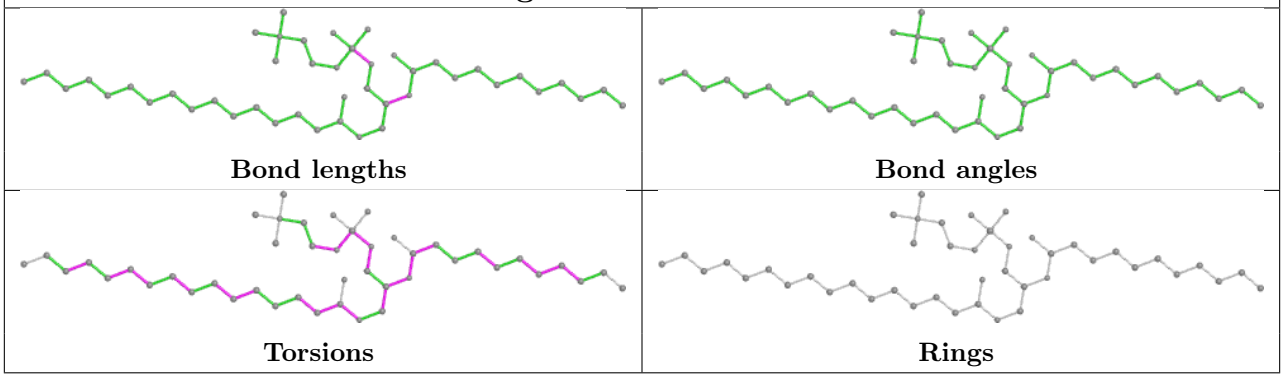
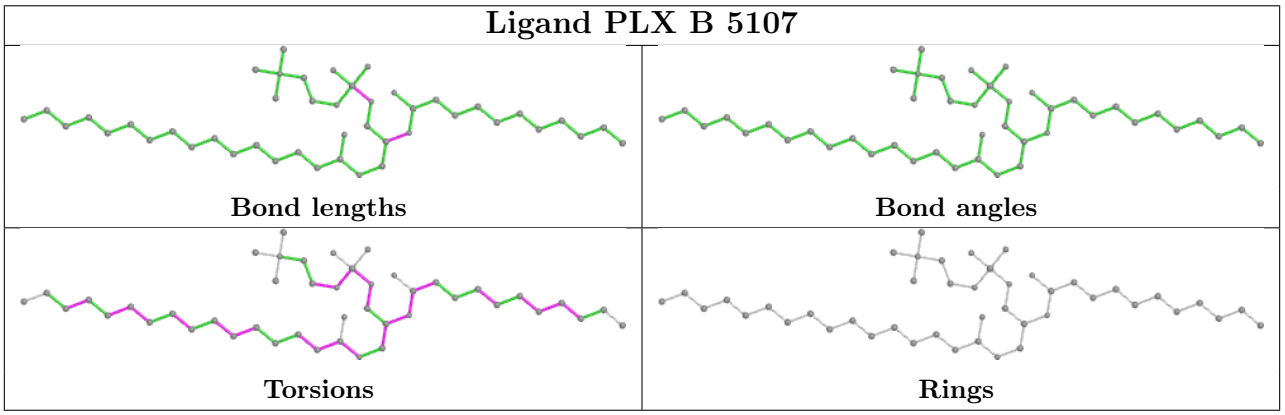


Ligand PLX A 5109



Ligand PLX B 5107



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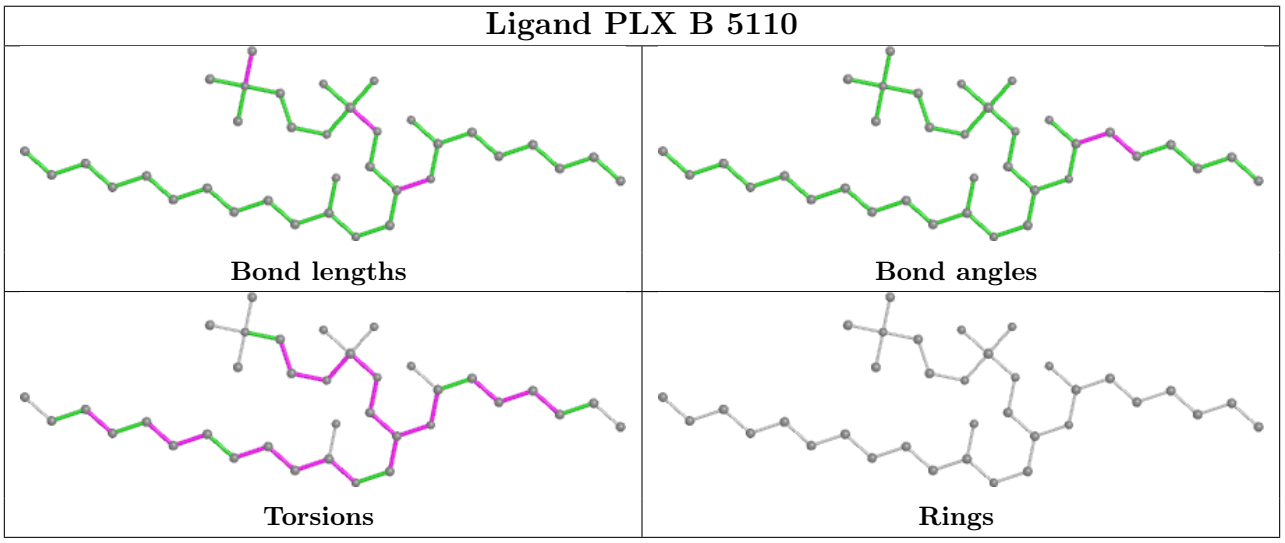
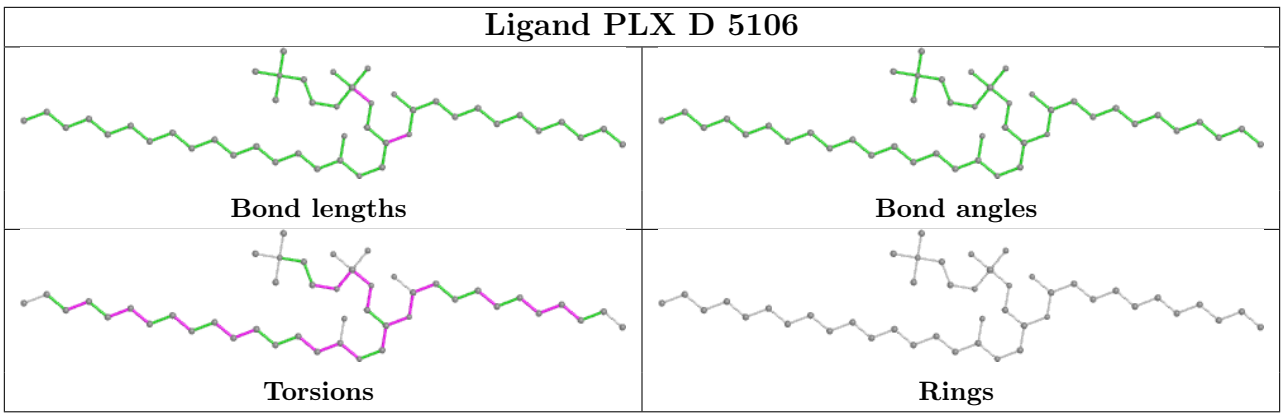
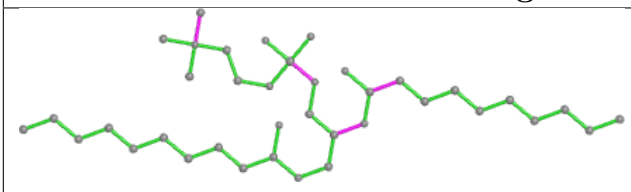
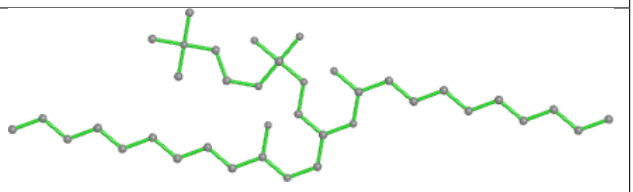
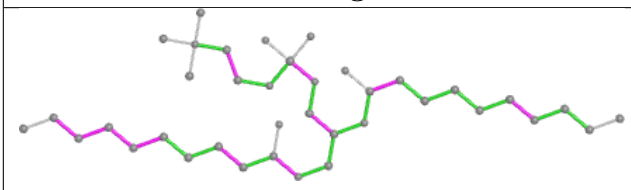
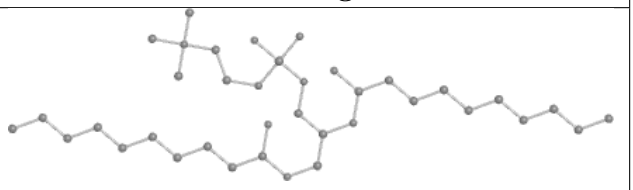


Ligand PLX D 5106



Ligand PLX B 5112	
 Bond lengths	 Bond angles
 Torsions	 Rings

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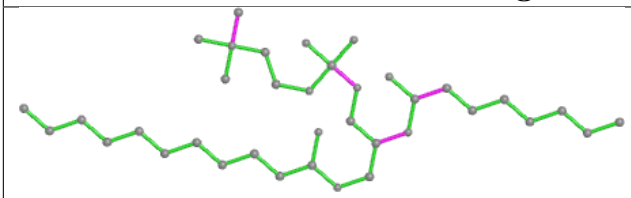
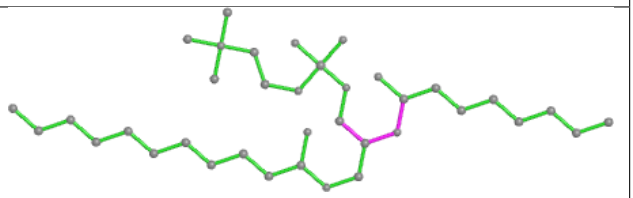
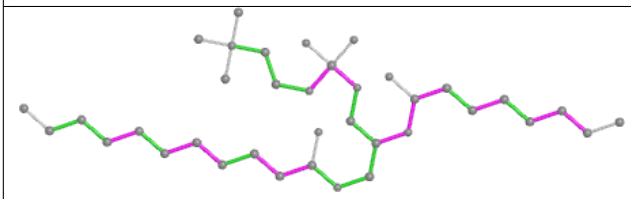
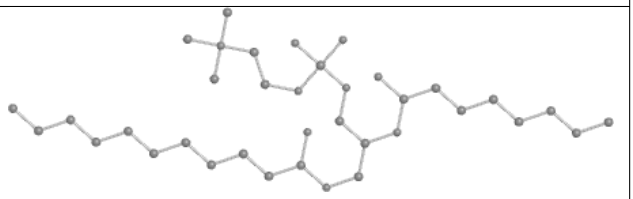
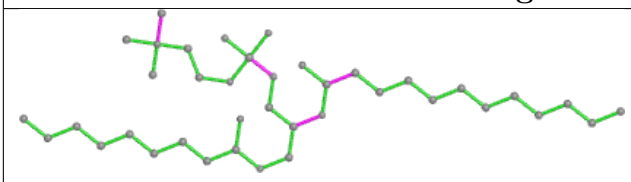
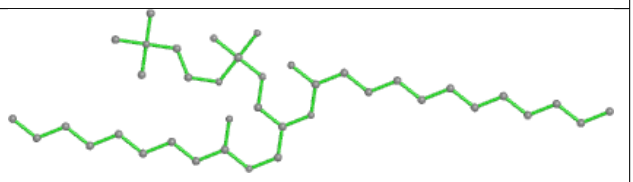
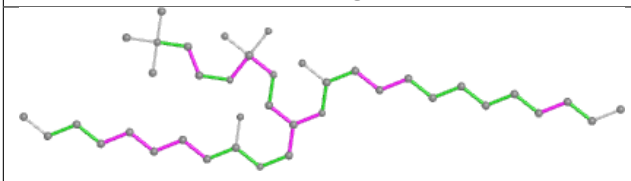
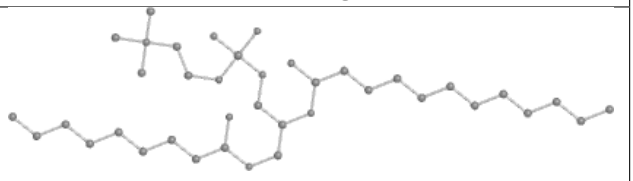
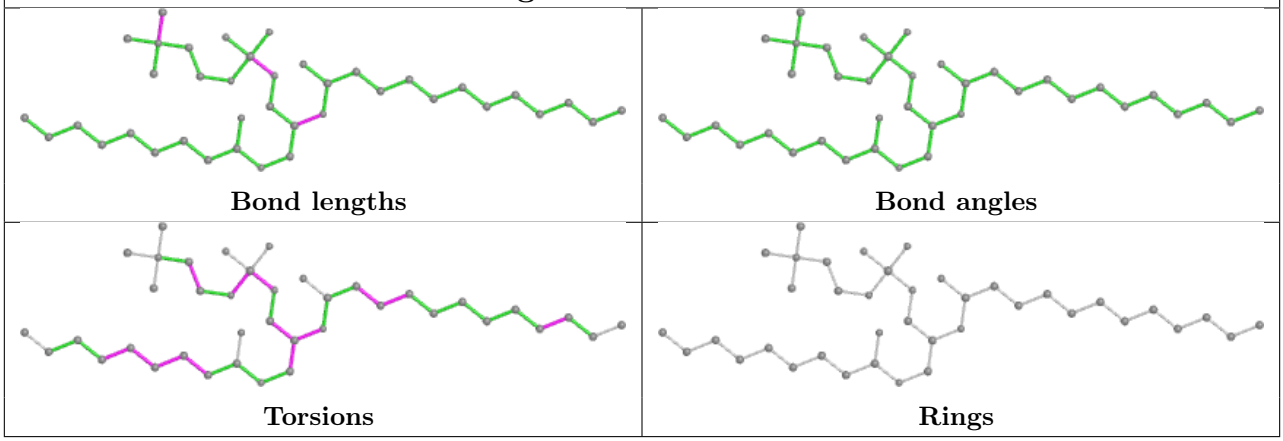
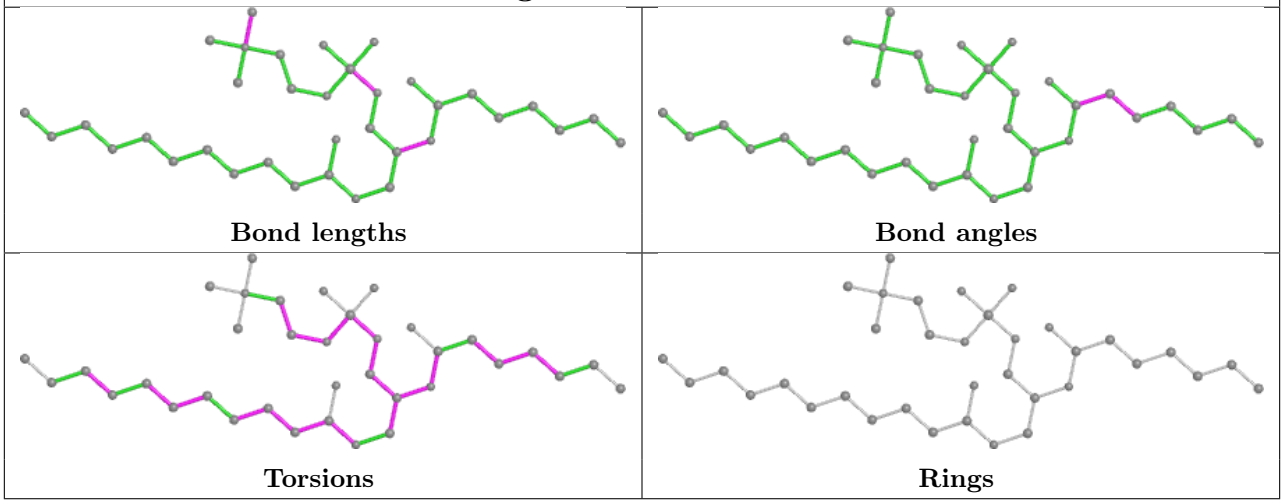
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX C 5112	
 Bond lengths	 Bond angles
 Torsions	 Rings

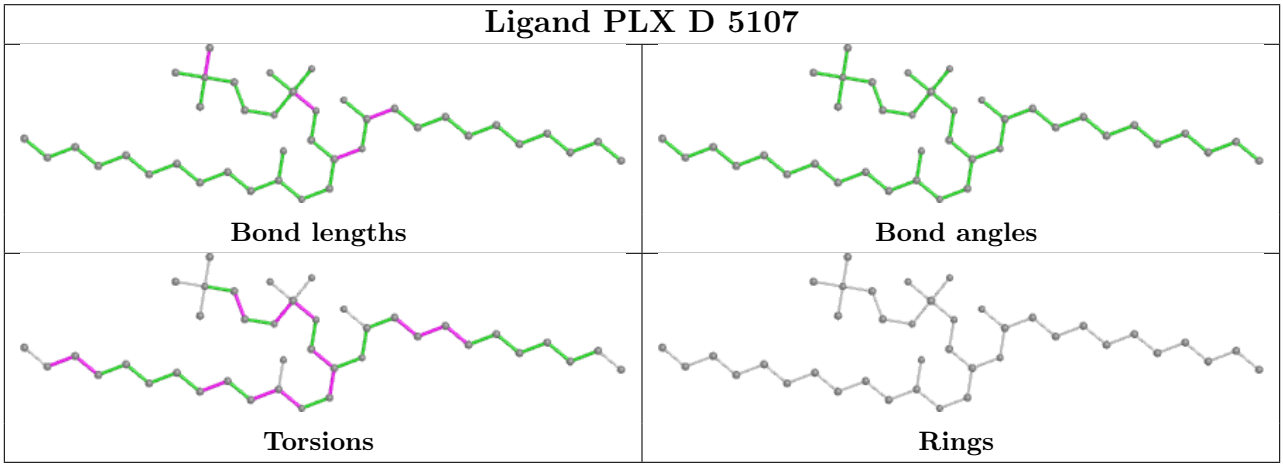
Ligand PLX B 5111



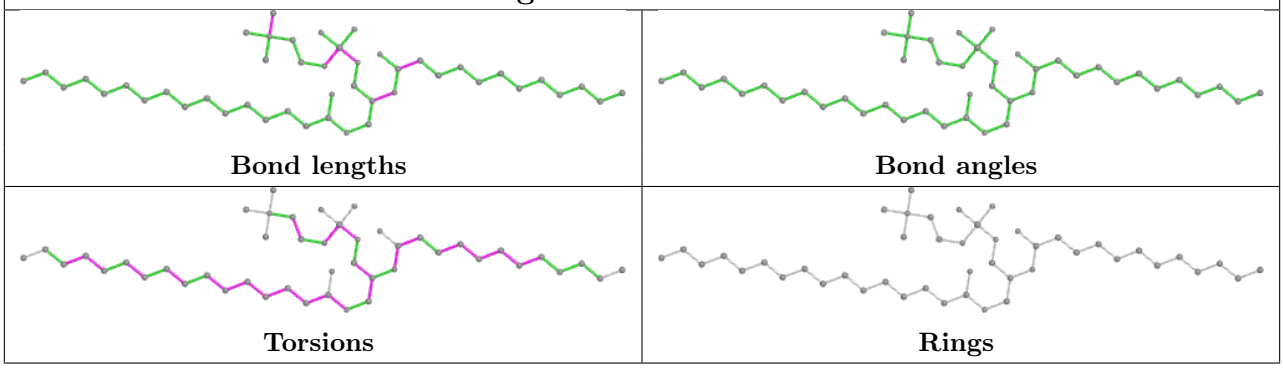
Ligand PLX A 5112



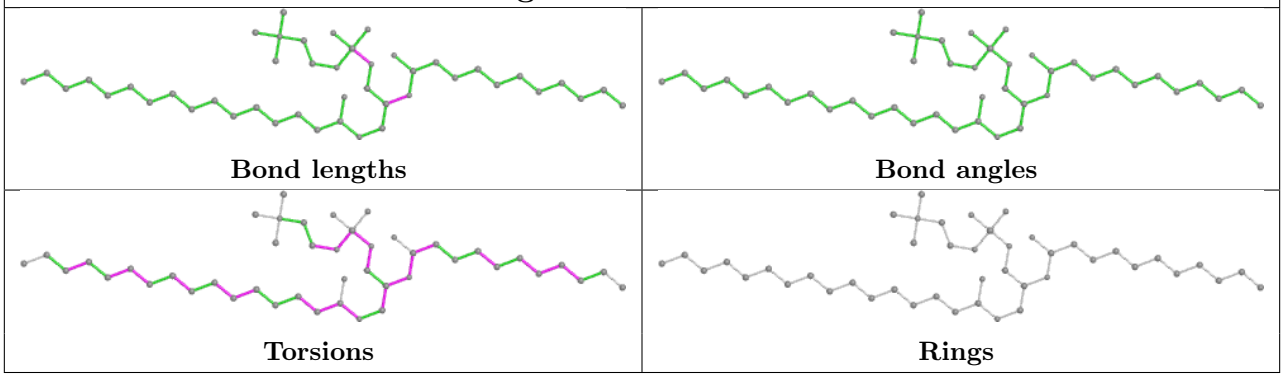
Ligand PLX D 5107



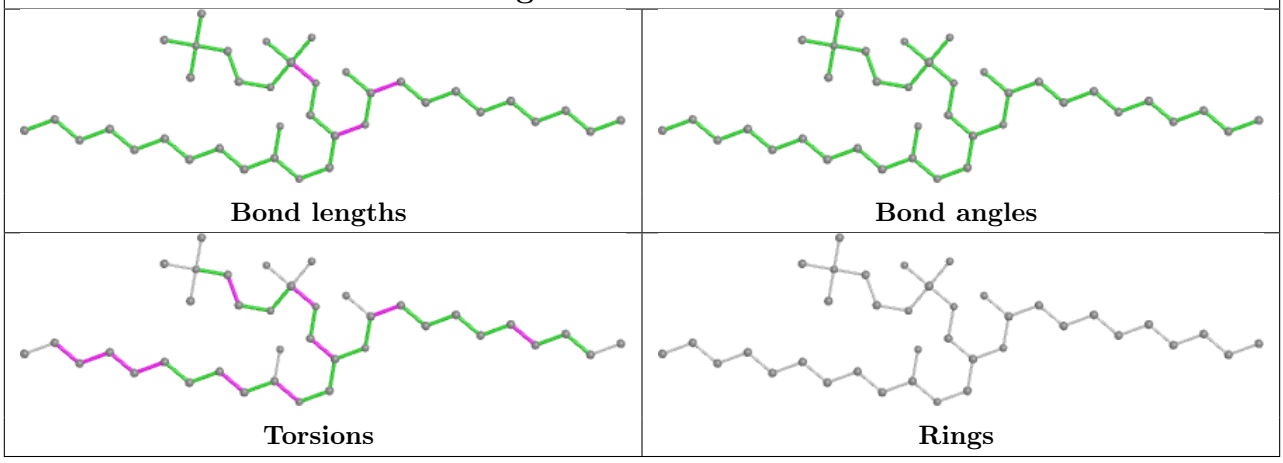
Ligand PLX C 5107



Ligand PLX C 5108



Ligand PLX D 5111



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

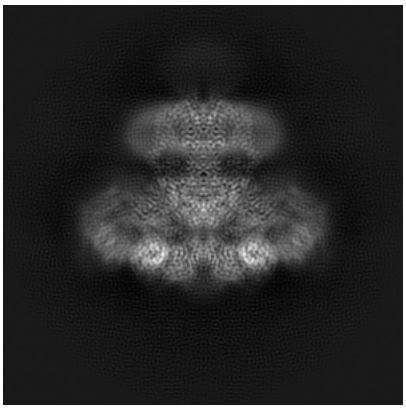
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27982. These allow visual inspection of the internal detail of the map and identification of artifacts.

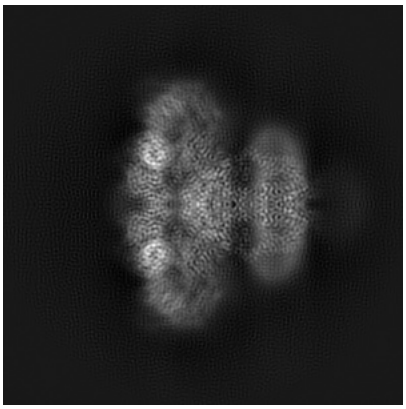
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

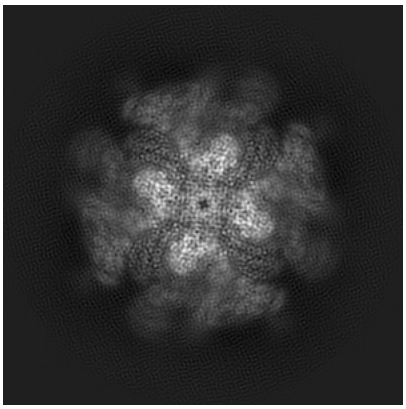
6.1.1 Primary map



X

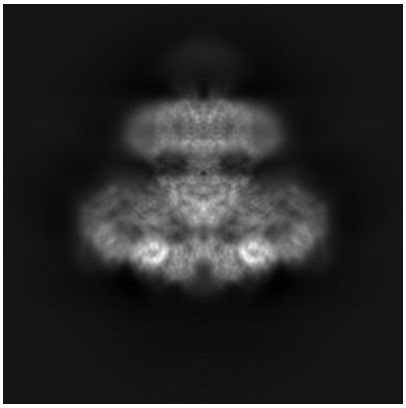


Y

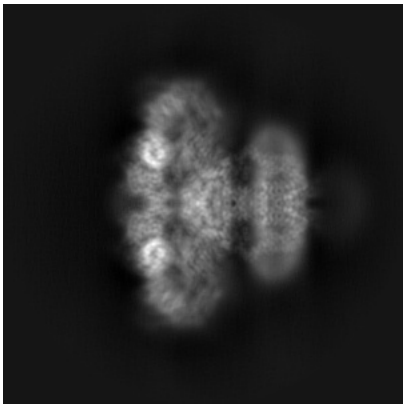


Z

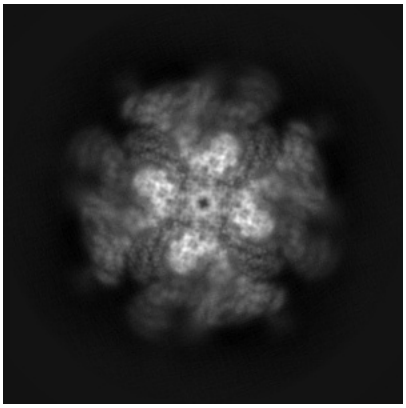
6.1.2 Raw map



X



Y

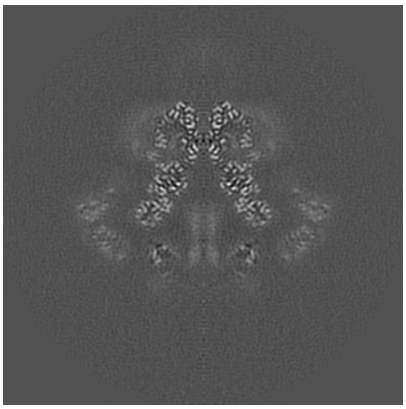


Z

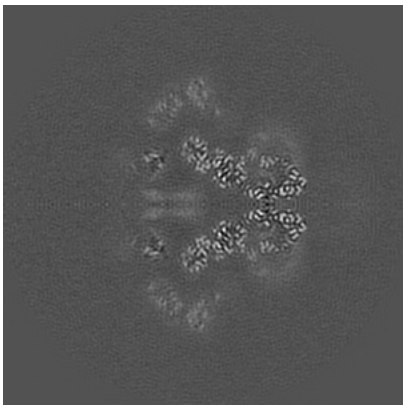
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

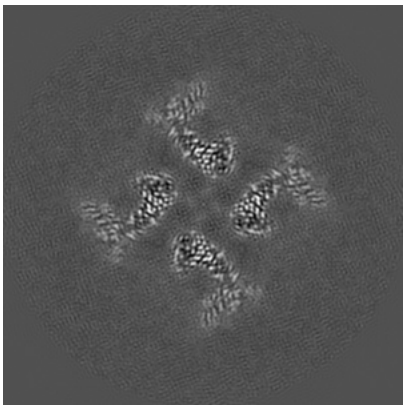
6.2.1 Primary map



X Index: 168

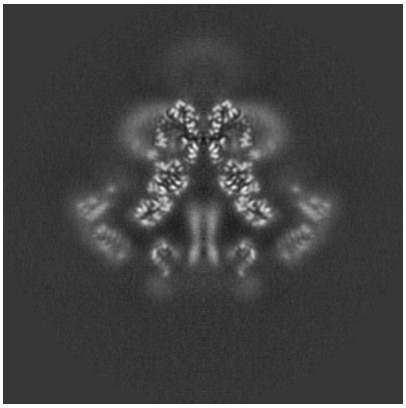


Y Index: 168

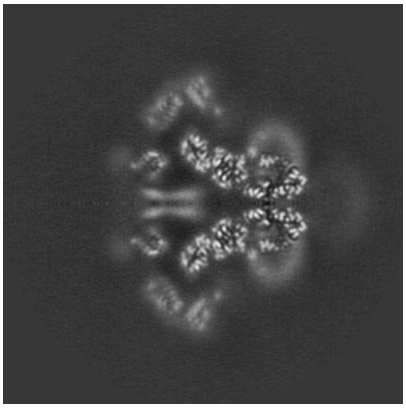


Z Index: 168

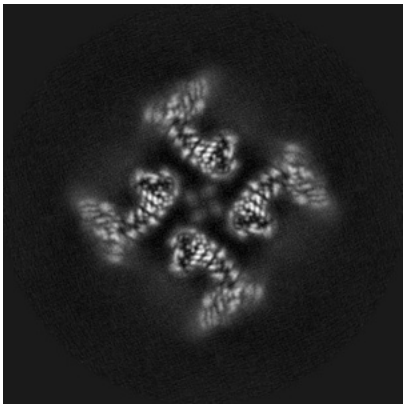
6.2.2 Raw map



X Index: 168



Y Index: 168

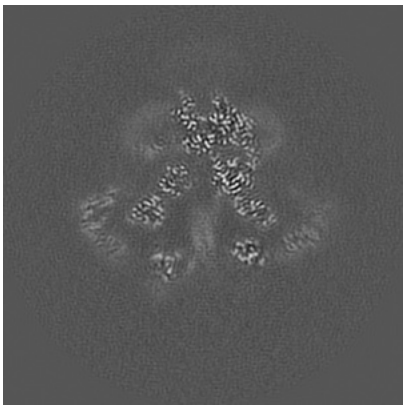


Z Index: 168

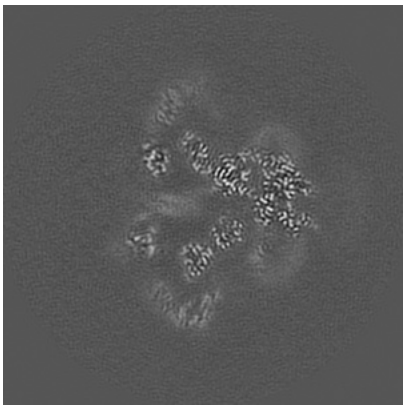
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

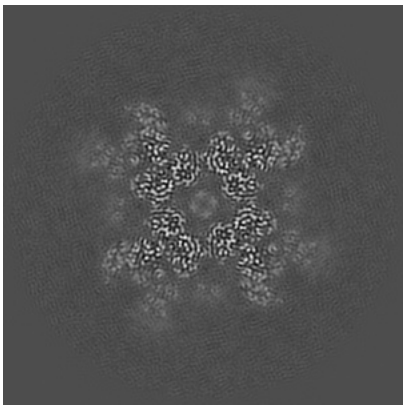
6.3.1 Primary map



X Index: 173

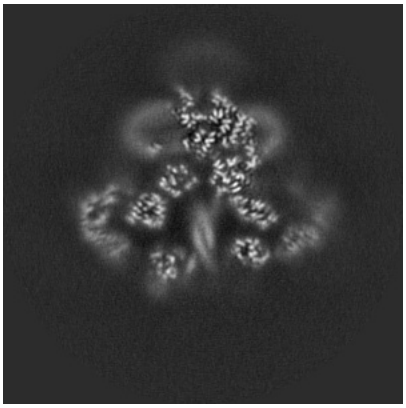


Y Index: 163

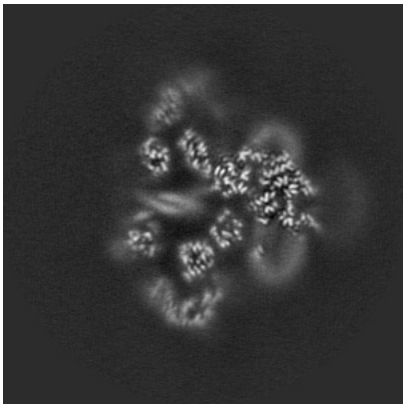


Z Index: 123

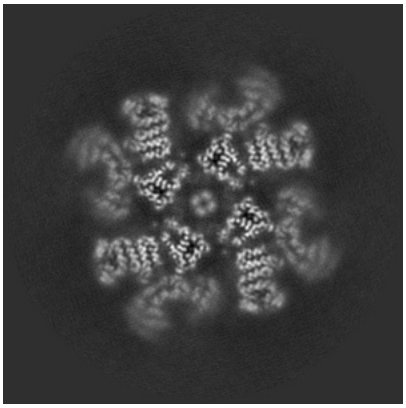
6.3.2 Raw map



X Index: 174



Y Index: 162



Z Index: 131

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 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

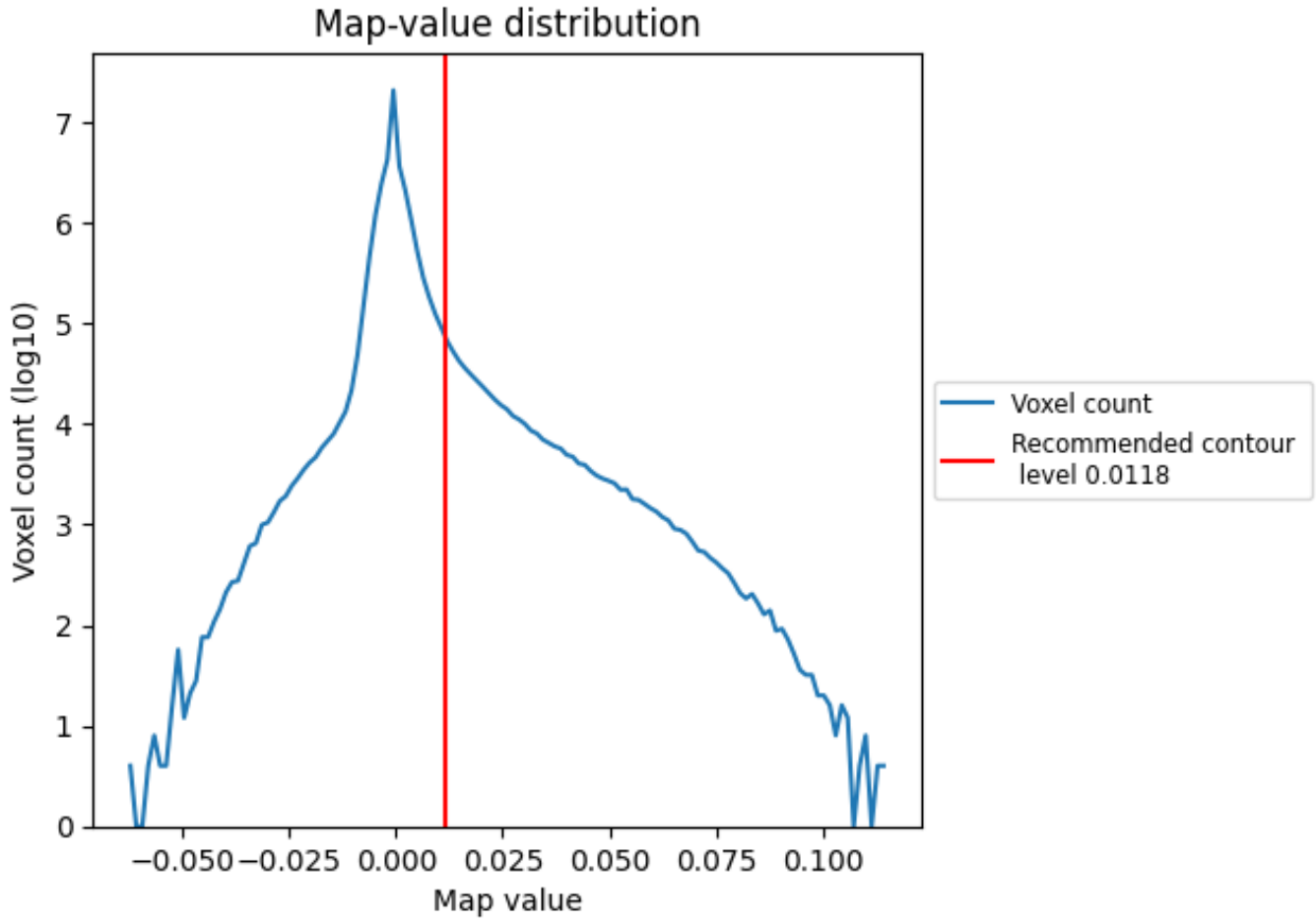
6.5 Mask visualisation (i)

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

7 Map analysis

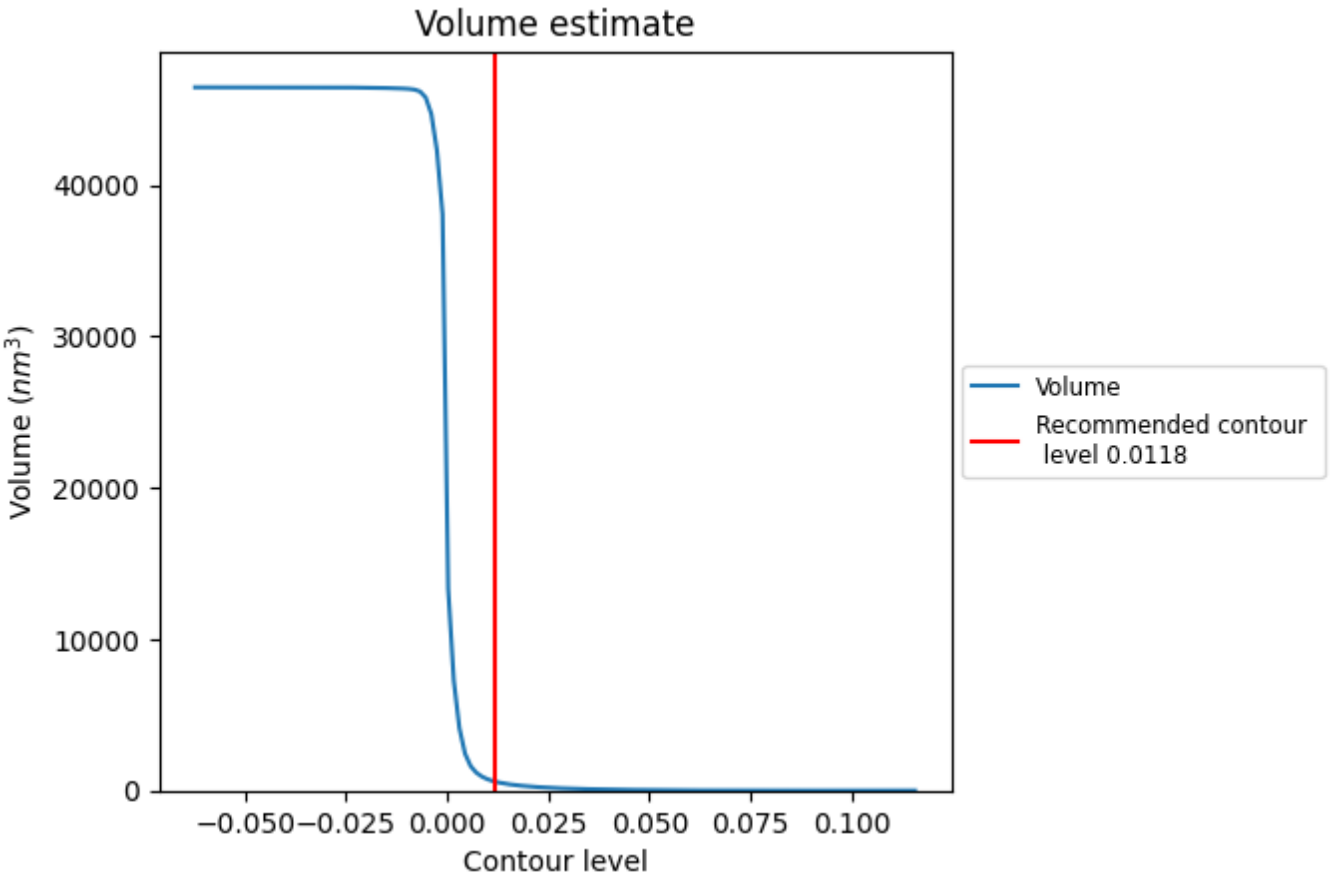
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

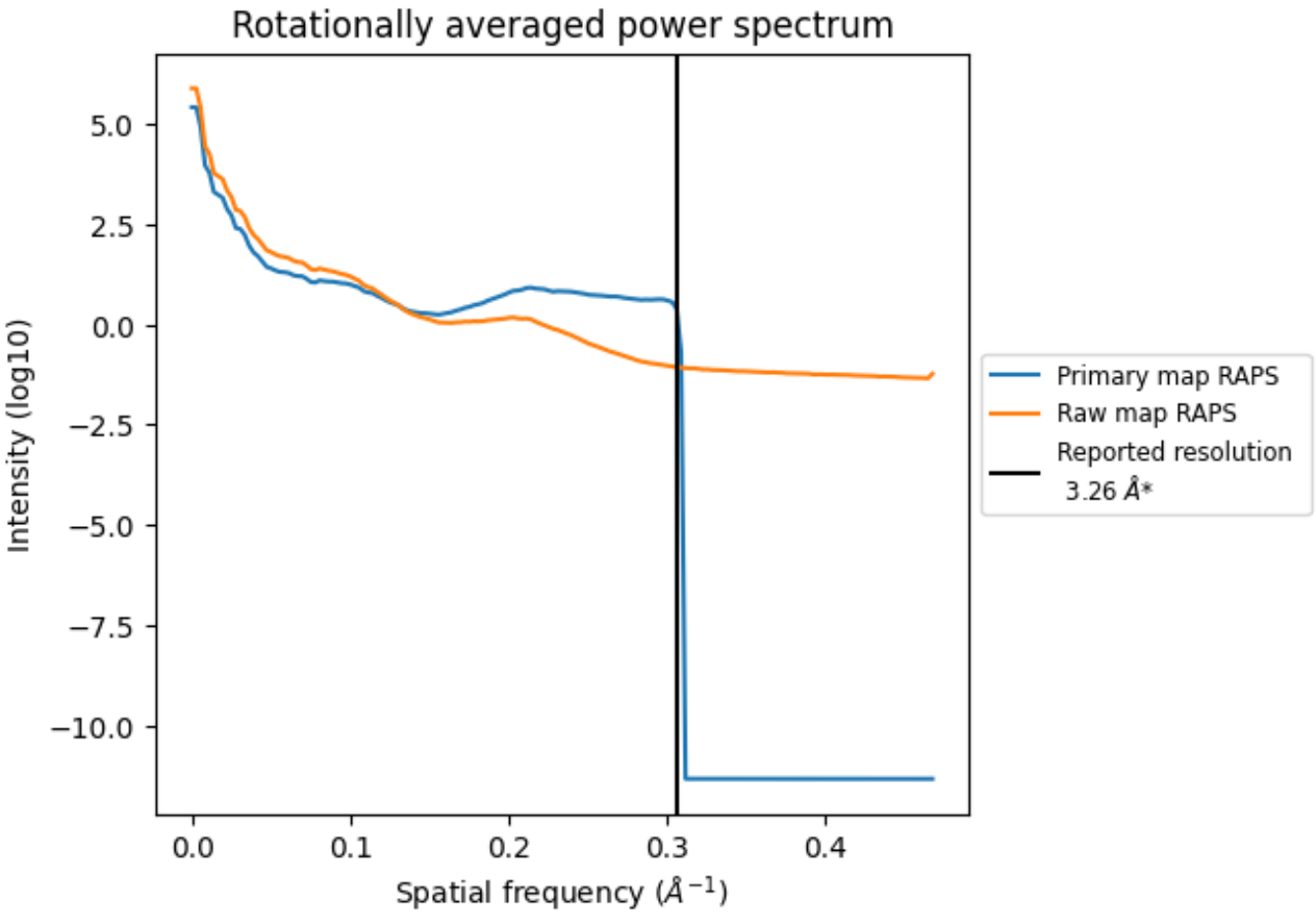
7.2 Volume estimate (i)



The volume at the recommended contour level is 600 nm^3; this corresponds to an approximate mass of 542 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)

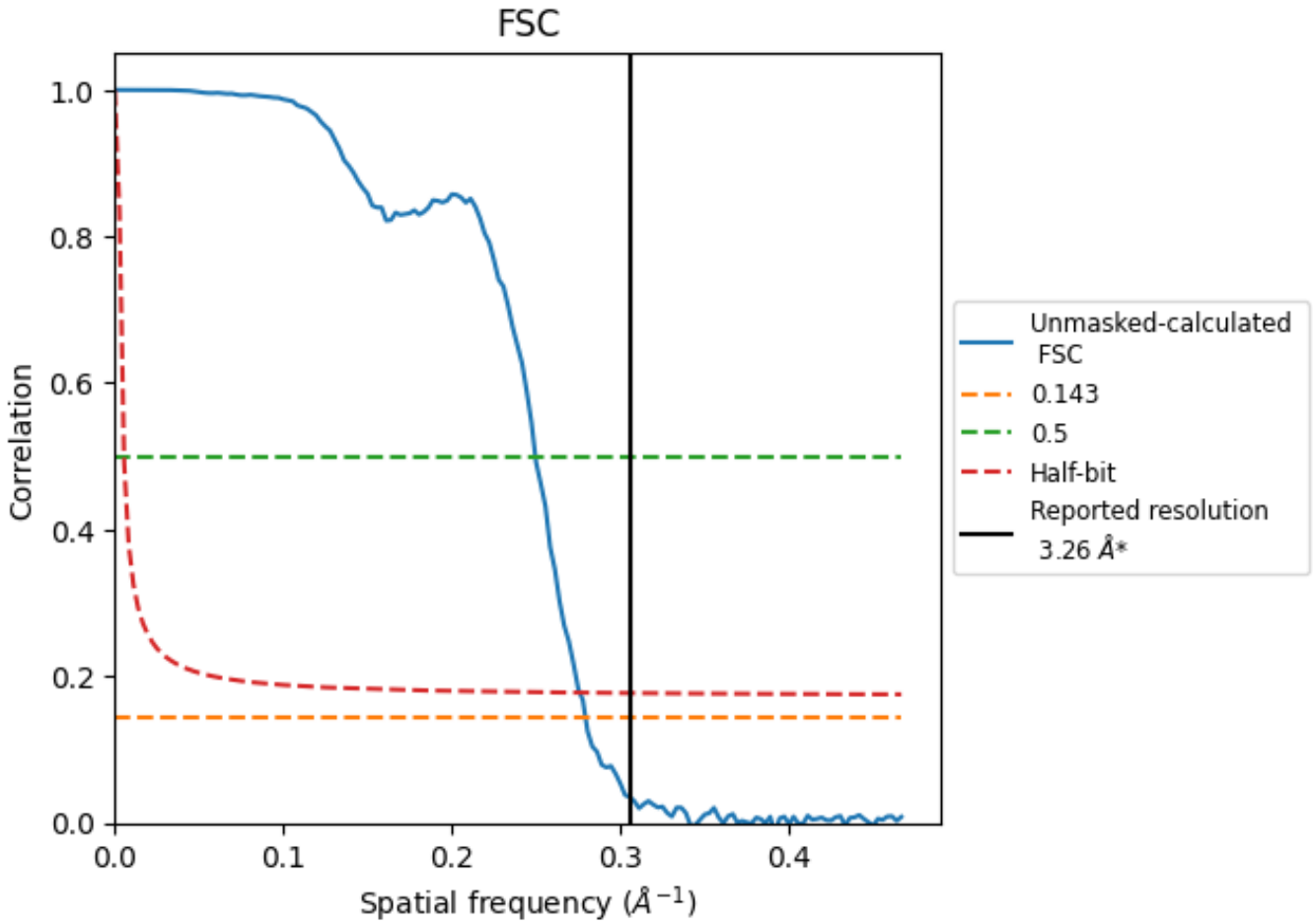


*Reported resolution corresponds to spatial frequency of 0.307 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.307 Å^{-1}

8.2 Resolution estimates (i)

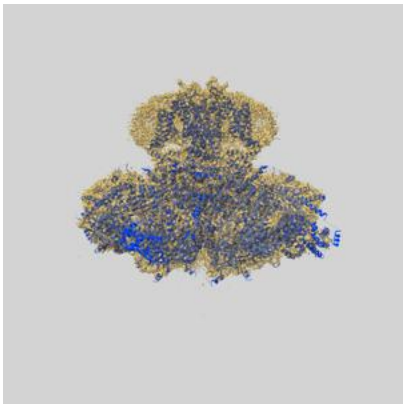
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.00	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

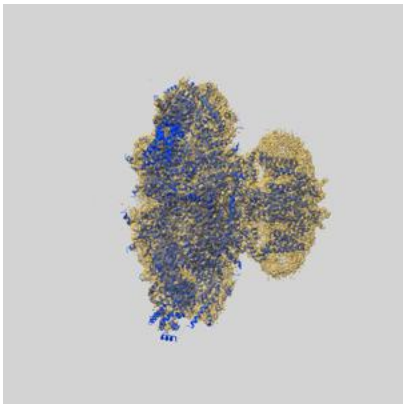
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27982 and PDB model 8EAQ. Per-residue inclusion information can be found in section 3 on page 6.

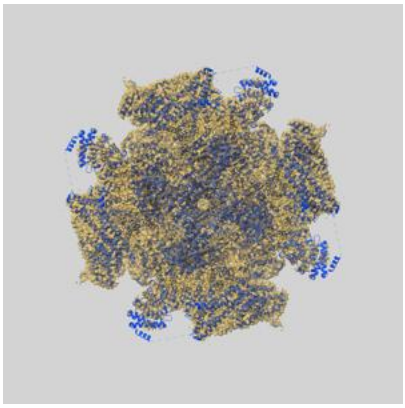
9.1 Map-model overlay



X



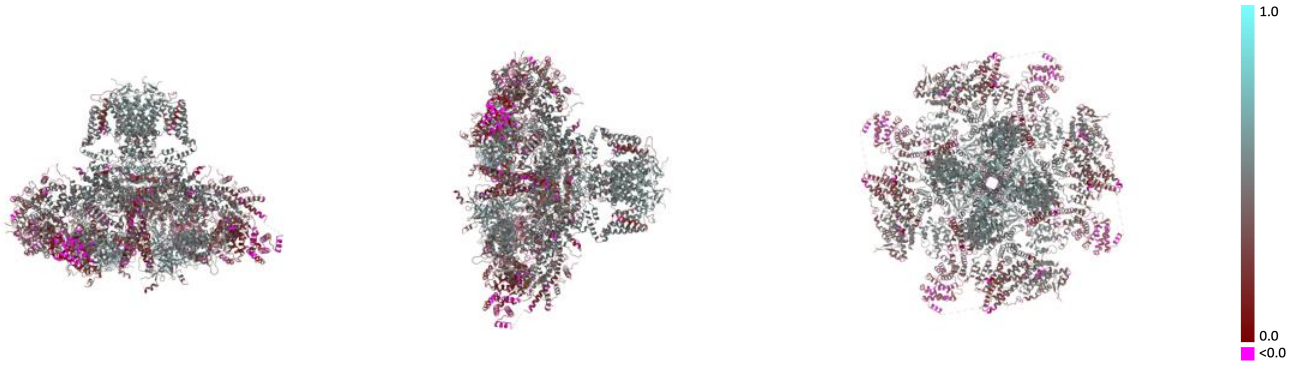
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

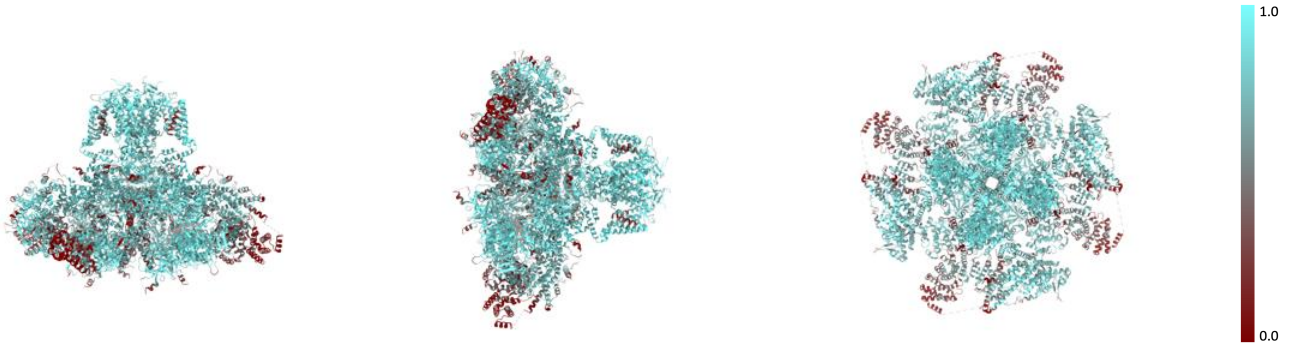
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

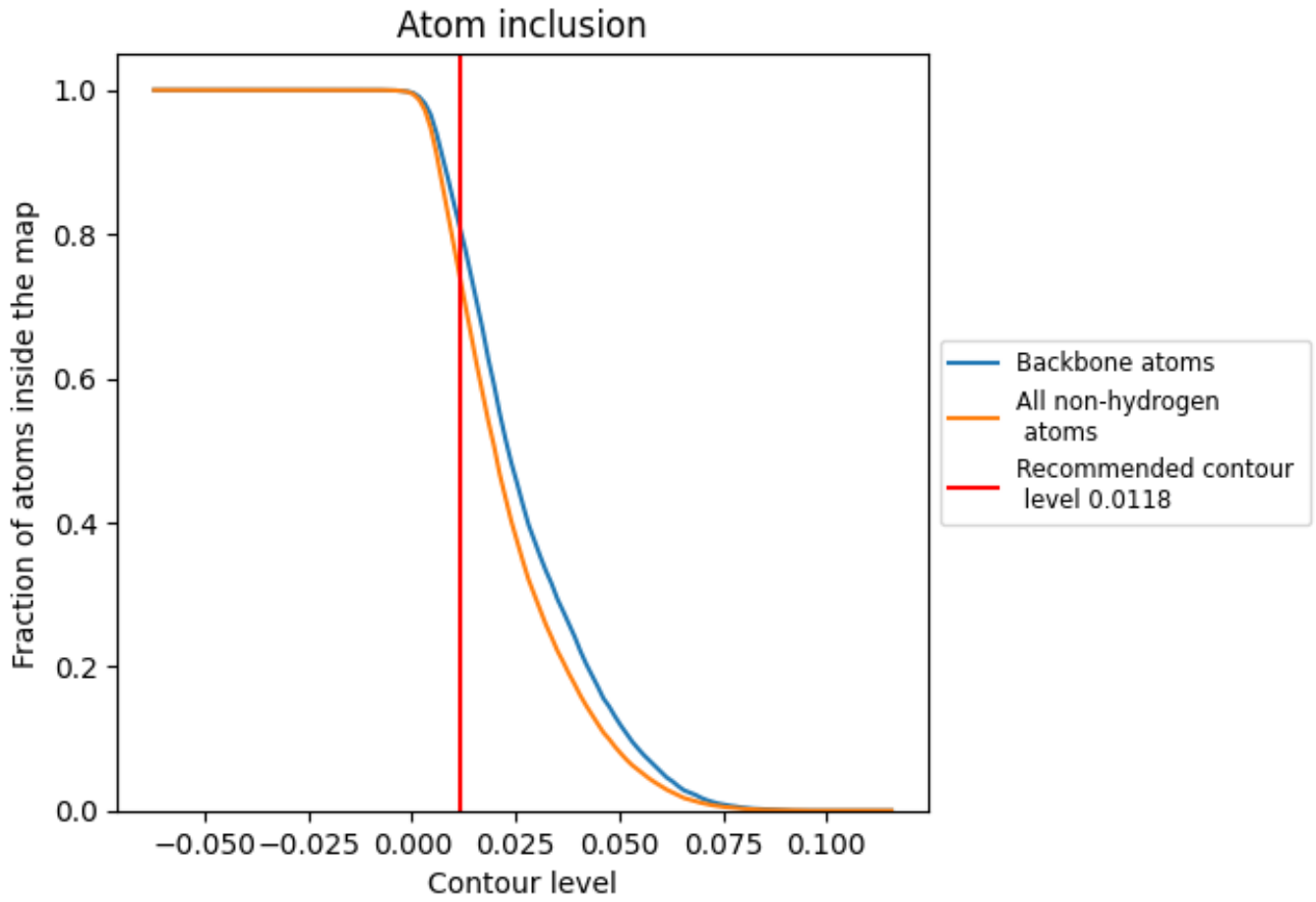
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0118).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7335	0.4030
A	0.7330	0.4030
B	0.7338	0.4030
C	0.7336	0.4030
D	0.7335	0.4030