wwPDB EM Validation Summary Report

Oct 5, 2024 – 10:53 PM EDT

PDB ID	:	6DRC
EMDB ID	:	EMD-7994
Title	:	High IP3 Ca2+ human type 3 1,4,5-inositol trisphosphate receptor
Authors	:	Hite, R.K.; Paknejad, N.
Deposited on	:	2018-06-11
Resolution	:	3.92 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

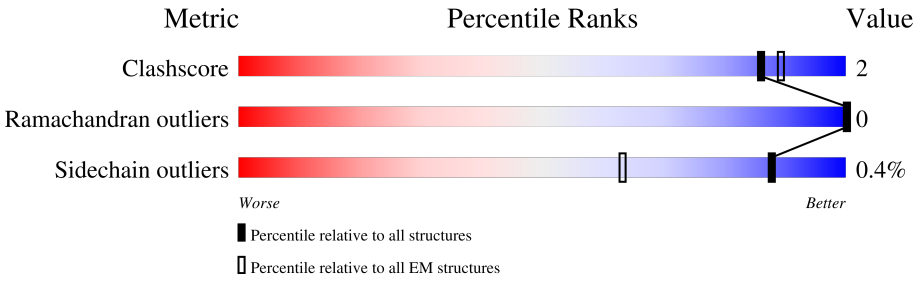
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.92 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	44% 76% 5% 18%
1	B	2671	45% 77% 5% 18%
1	C	2671	44% 77% 5% 18%
1	D	2671	45% 77% 5% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 138896 atoms, of which 69420 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.

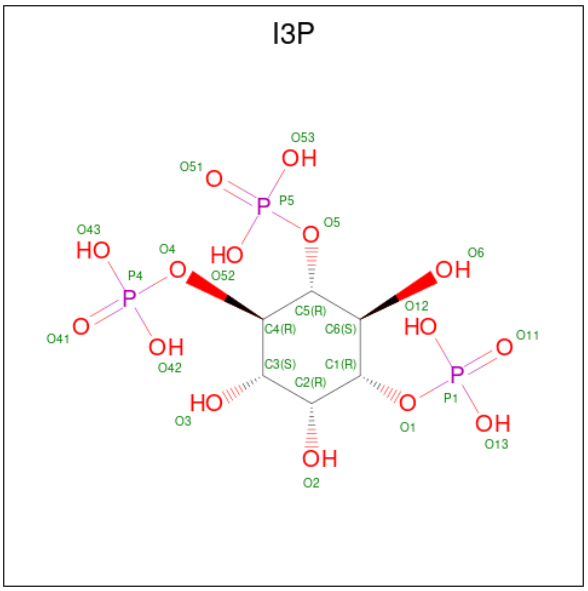
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2186	Total 34688	C 11057	H 17346	N 2984	O 3195	S 106	0	0
1	B	2186	Total 34688	C 11057	H 17346	N 2984	O 3195	S 106	0	0
1	C	2186	Total 34688	C 11057	H 17346	N 2984	O 3195	S 106	0	0
1	D	2186	Total 34688	C 11057	H 17346	N 2984	O 3195	S 106	0	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 D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

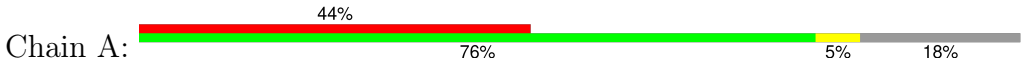
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	D	2	Total	Ca	0
			2	2	

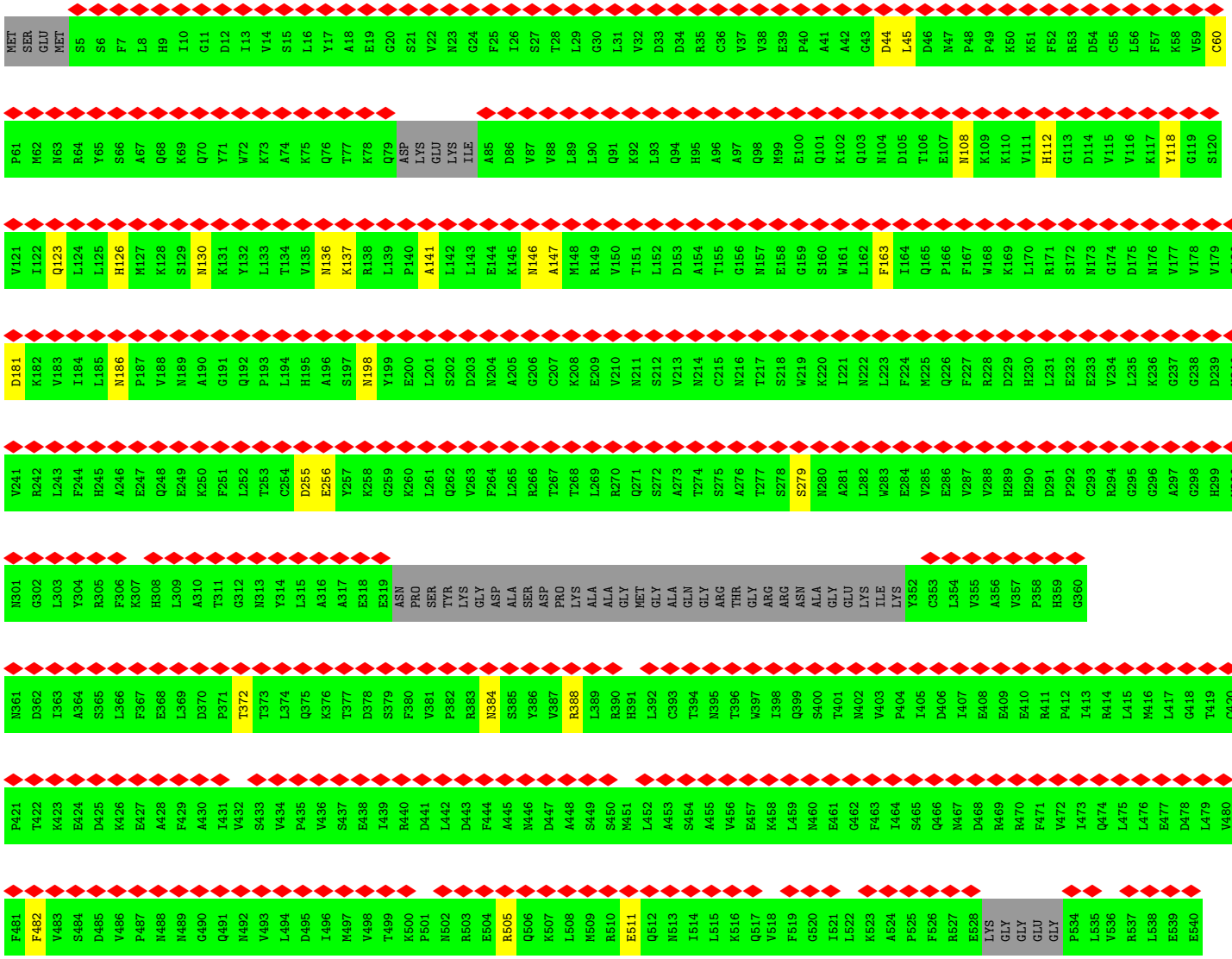
3 Residue-property plots (i)

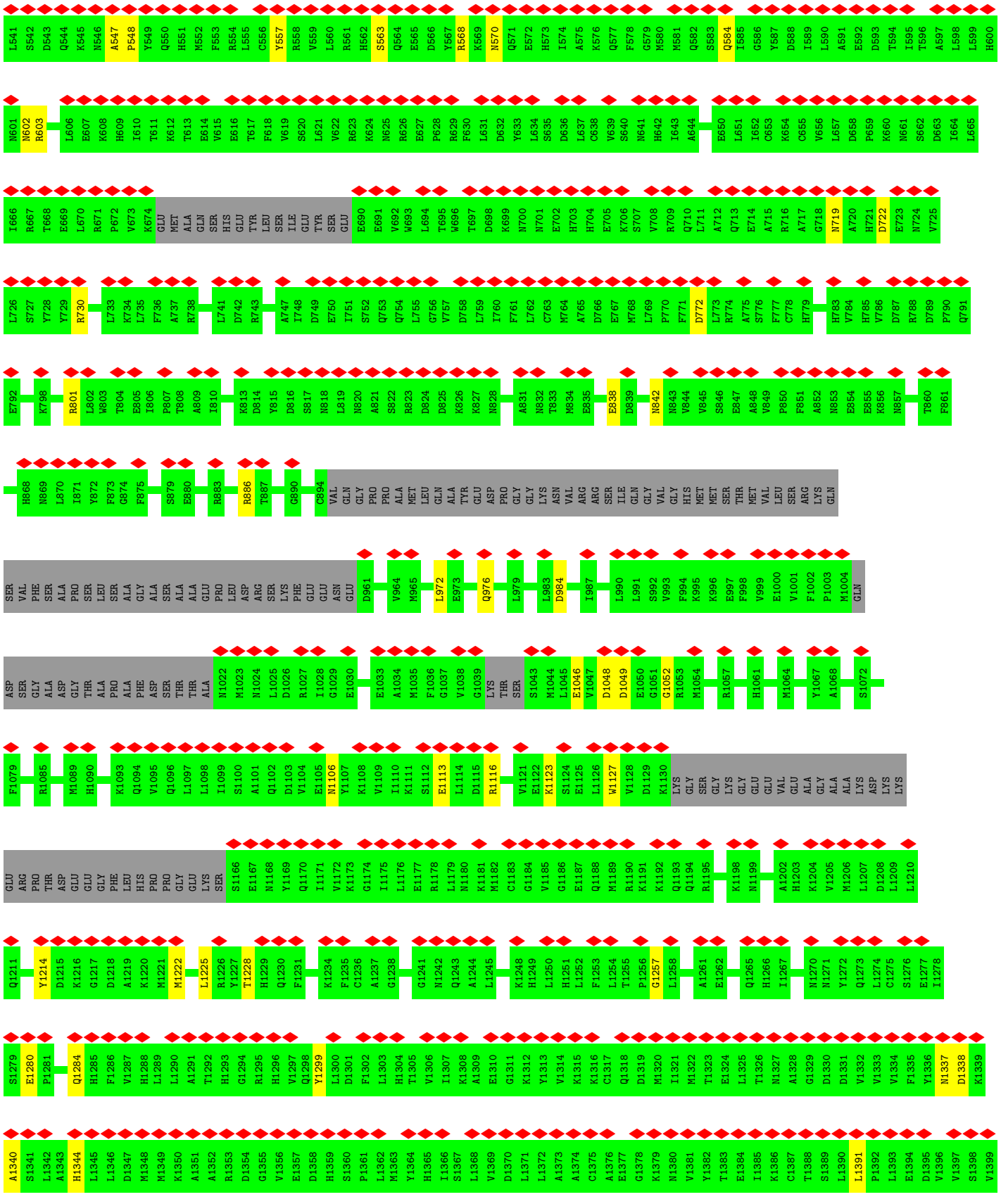
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



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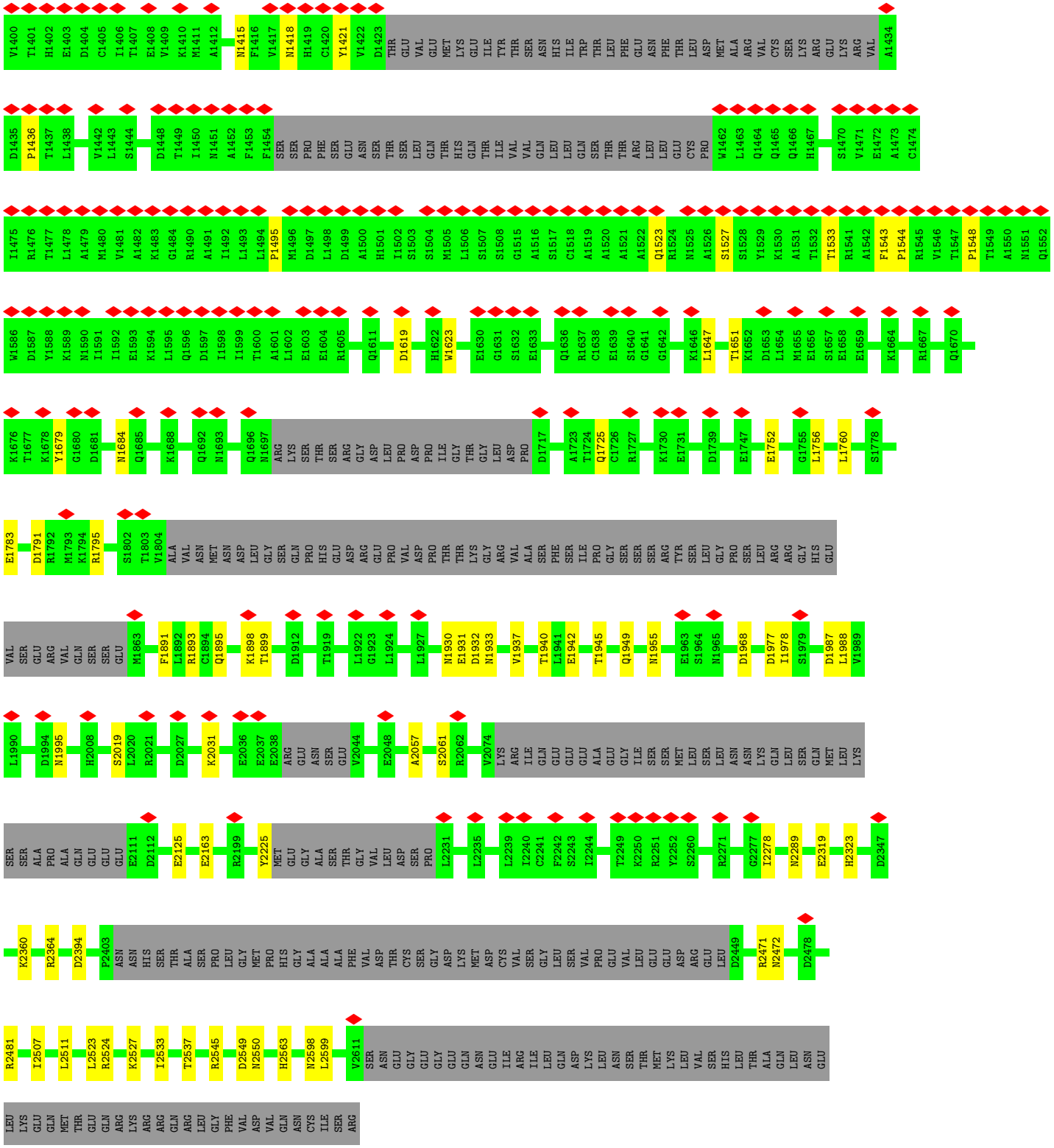
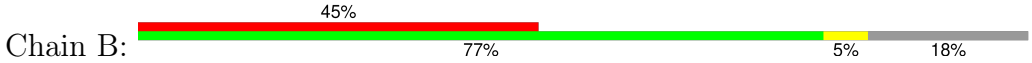
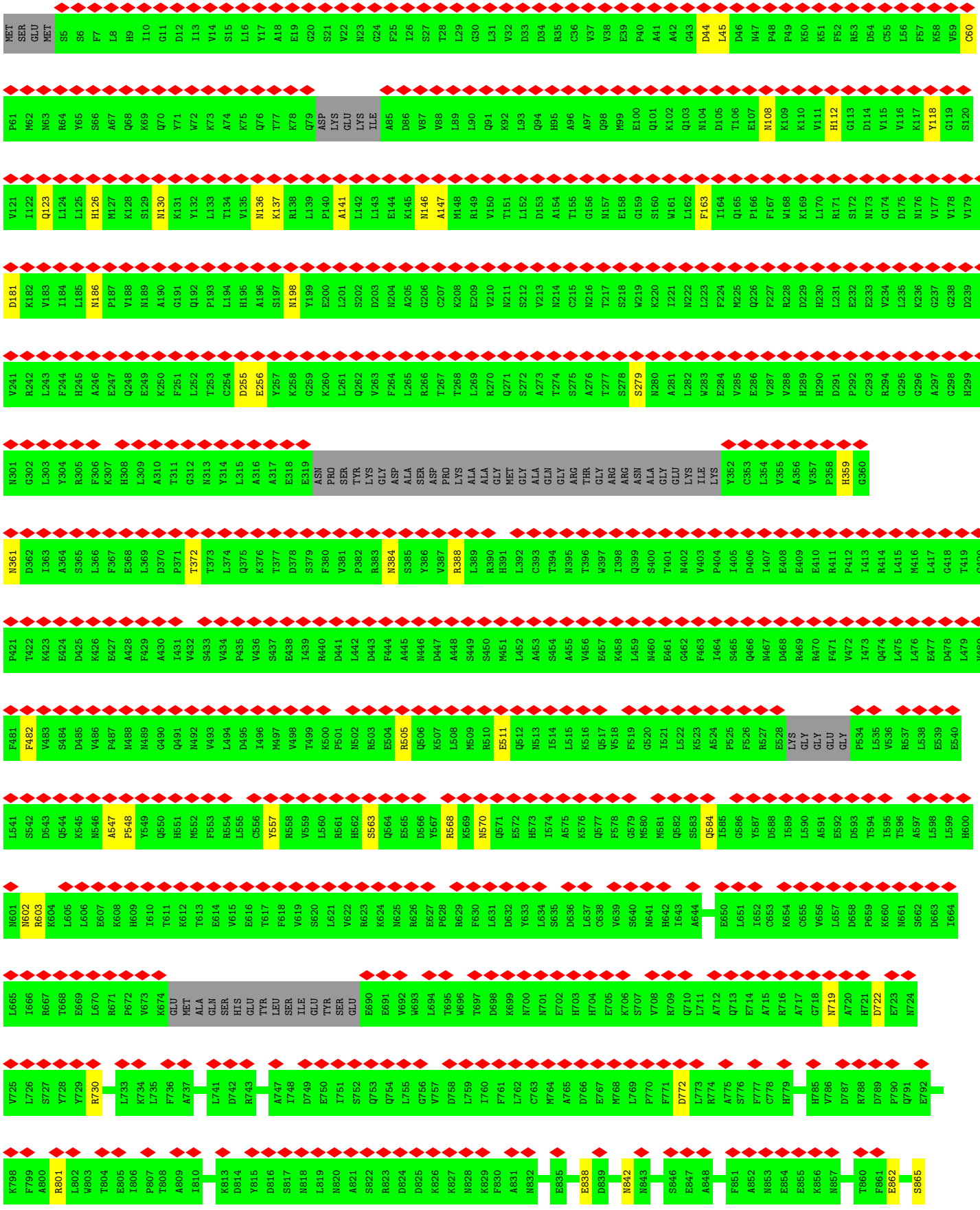
N601 N602 R603 L606 E607 K608 H609 I610 T611 K612 T613 E614 V615 E616 T617 F618 V619 S620 L621 V622 R623 K624 N625 R626 E627 P628 R629 F630 L631 D632 Y633 L634 S635 D636 L637 C638 V639 S640 N641 H642 I643 A644 E650 L651 I652 C653 K654 C655 V656 L657 D658 P659 K660 N661 S662 D663 I664 L665
I666 R667 T668 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 L733 K734 L735 F736 A737 R738 L741 D742 R743 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 H783 V784 H785 V786 D787 R788 D789 P790 Q791
E792 K798 R801 L802 W803 T804 E805 I806 P807 T808 A809 I810 K813 D814 Y815 D816 S817 N818 L819 N820 A821 S822 R823 D824 D825 K826 K827 N828 A831 N832 T833 M834 E835 E838 D839 N842 N843 V844 V845 S846 E847 A848 V849 P850 F851 A852 N853 E854 E855 K856 N857 T860 F861
H868 N869 L870 I871 Y872 F873 G874 F875 S879 E880 R883 R886 T887 G890 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 ASP PRO SER LEU SER ALA GLY GLY ALA SER ALA ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 V964 M965 L972 E973 Q976 L979 L983 D984 I987 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 E1033 A1034 M1035 F1036 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 R1057 H1061 M1064 Y1067 A1068 S1072
F1079 R1085 M1089 H1090 K1093 Q1094 V1095 Q1096 L1097 L1098 I1099 S1100 A1101 Q1102 D1103 V1104 E1105 N1106 Y1107 K1108 V1109 I1110 K1111 S1112 E1113 L1114 D1115 R1116 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 K1198 N1199 A1202 H1203 K1204 V1205 M1206 L1207 D1208 L1209 L1210
Q1211 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222 L1225 R1226 Y1227 T1228 H1229 Q1230 F1231 K1234 F1235 C1236 A1237 G1238 G1241 N1242 Q1243 A1244 L1245 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 A1261 E1262 Q1265 H1266 I1267 N1270 N1271 Y1272 Q1273 L1274 C1275 S1276 E1277 I1278
S1279 E1280 P1281 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



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

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P61 M62 N63 R64 Y65 S66 A67 Q68 K69 Q70 Y71 W72 K73 A74 K75 Q76 T77 K78 Q79 ASP LYS GLU LYS ILE A85 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
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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
N301 G302 L303 Y304 R305 F306 K307 H308 L309 A310 T311 G312 N313 Y314 L315 A316 A317 E318 E319 ASN PRO SER TYR LYS GLY ASP ALA SER ASP PRO LYS ALA ALA GLY MET GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA GLY GLU LYS ILE LYS Y352 C353 L354 V355 A356 V357 P358 H359 G360
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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
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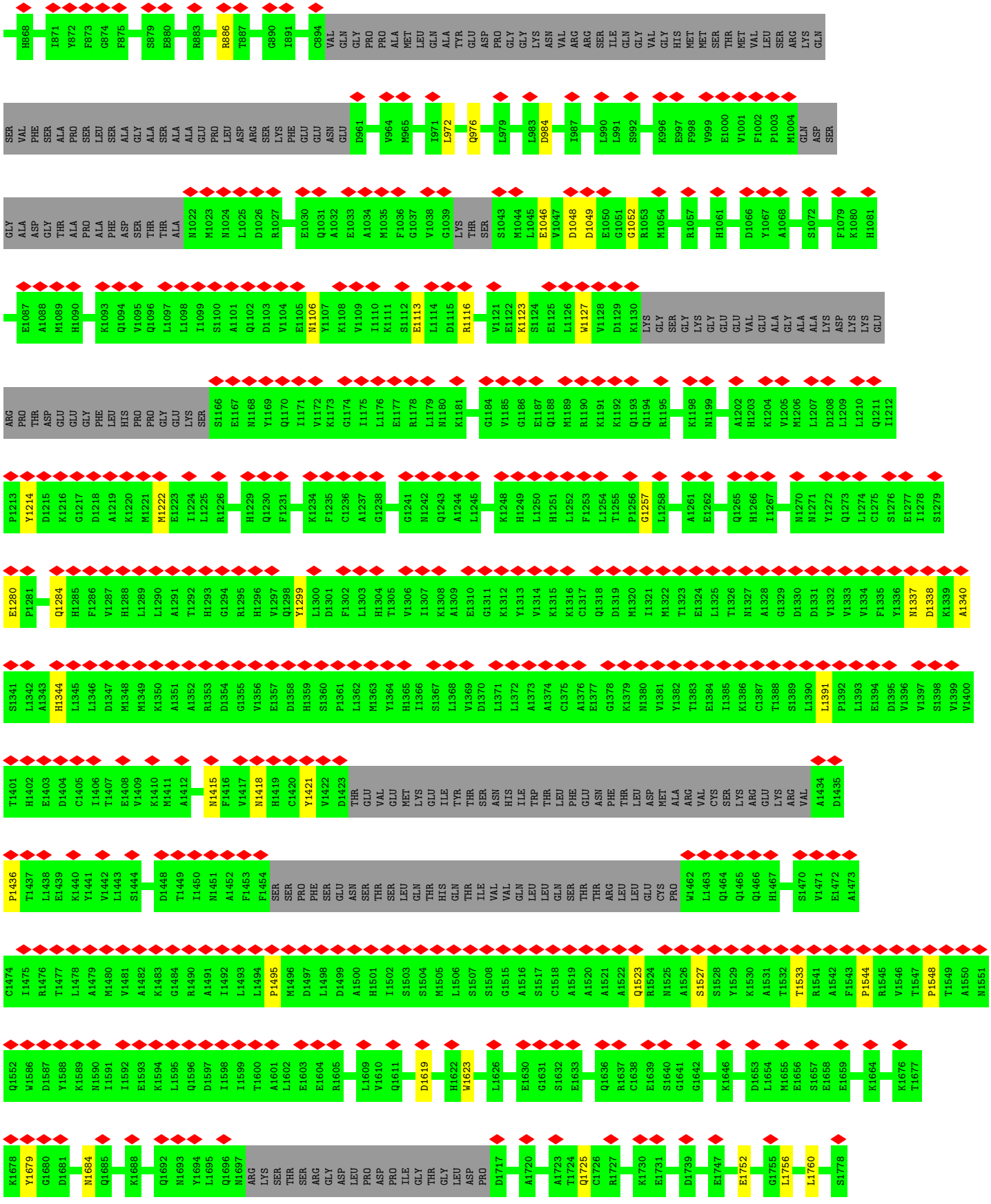
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SER VAL PHE SER ALA PRO SER LEU SER ALA GLY GLY ALA SER ALA ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 V964 M965 I971 L972 Q976 L979 L983 D984 I987 L990 L991 S992 K996 E997 F998 V999 E1000 V1001 F1002 P1003 M1004 GLN ASP SER
GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 M1023 N1024 L1025 D1026 R1027 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 R1057 H1061 D1066 Y1067 A1068 S1072 F1079 K1080 H1081
E1087 A1088 M1089 H1090 K1093 Q1094 V1095 Q1096 L1097 L1098 I1099 S1100 A1101 Q1102 D1103 V1104 E1105 N1106 Y1107 K1108 V1109 I1110 K1111 S1112 E1113 L1114 D1115 R1116 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 G1184 V1185 G1186 E1187 Q1188 M1189 R1190 K1191 K1192 Q1193 Q1194 R1195 K1198 N1199 A1202 H1203 K1204 V1205 M1206 L1207 D1208 L1209 L1210 Q1211 I1212
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T1401 H1402 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412 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 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 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
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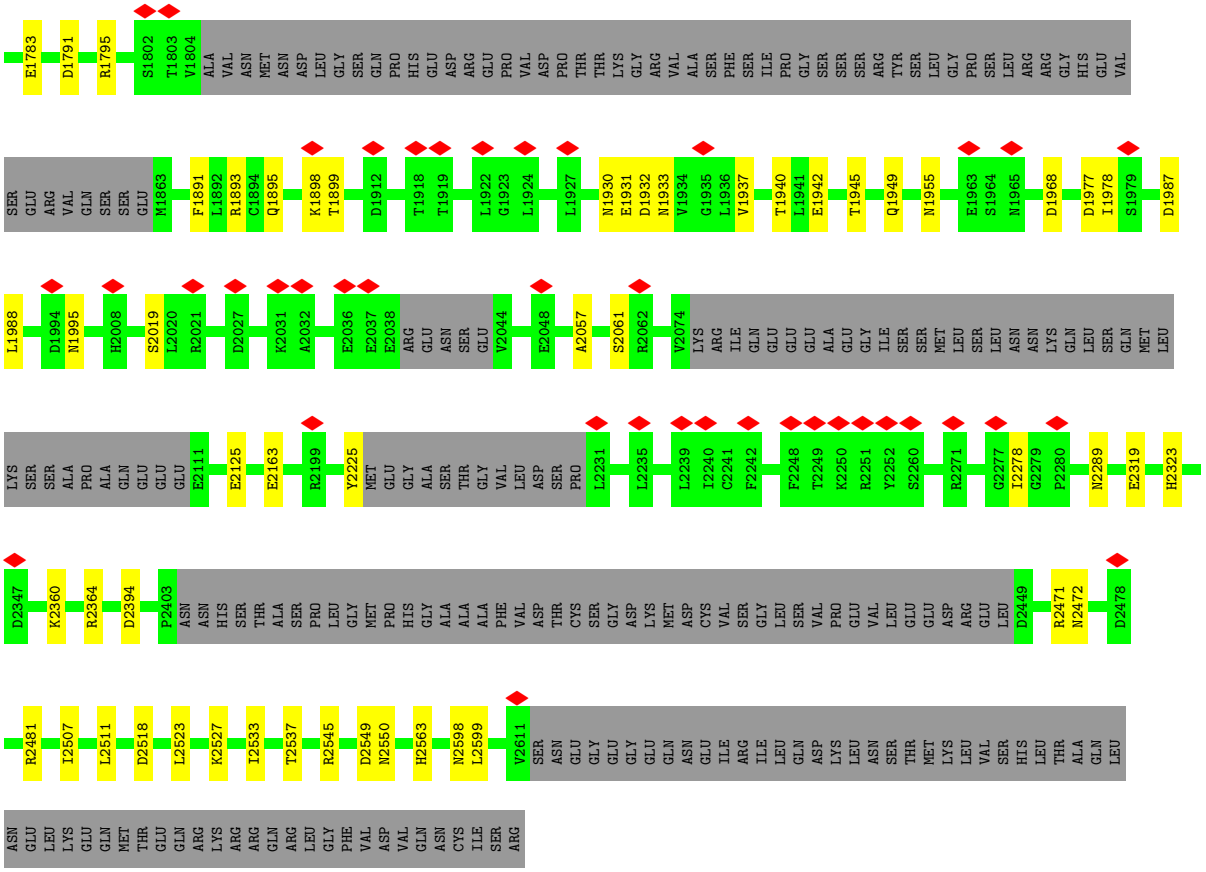
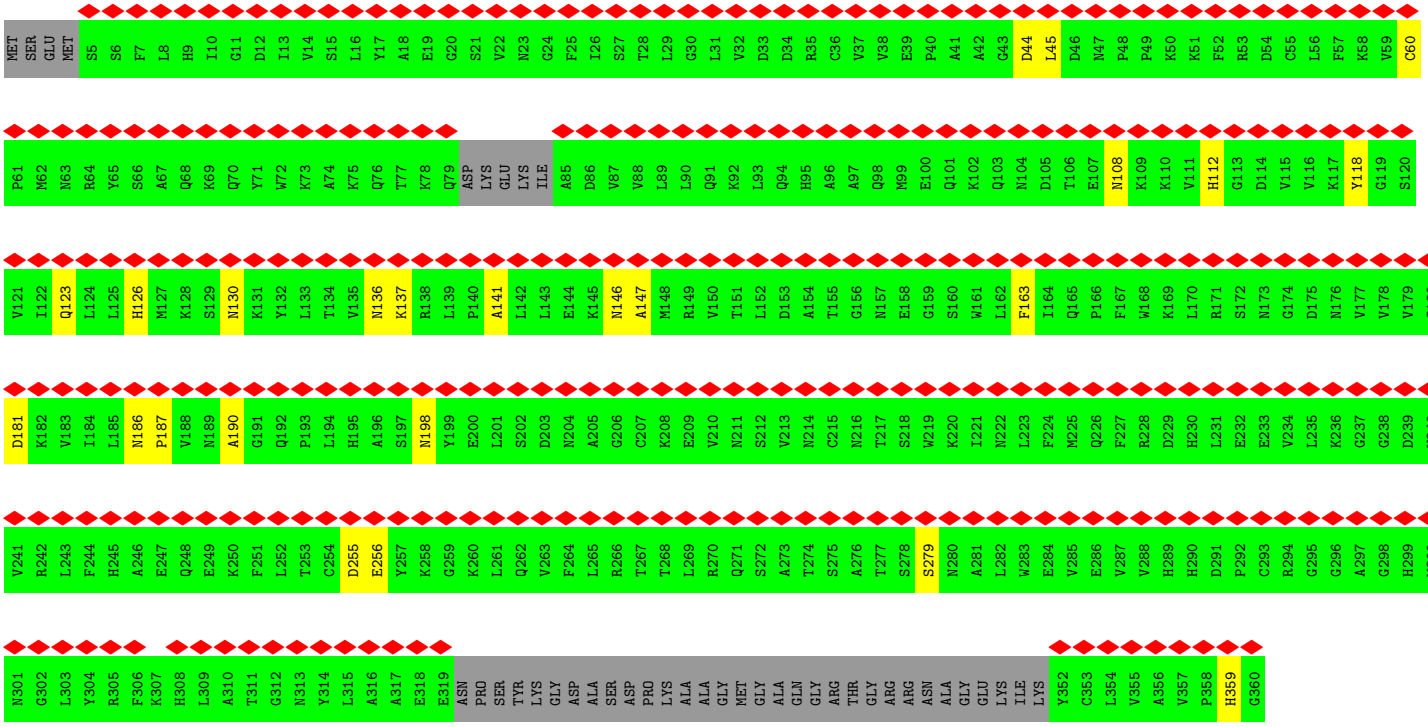
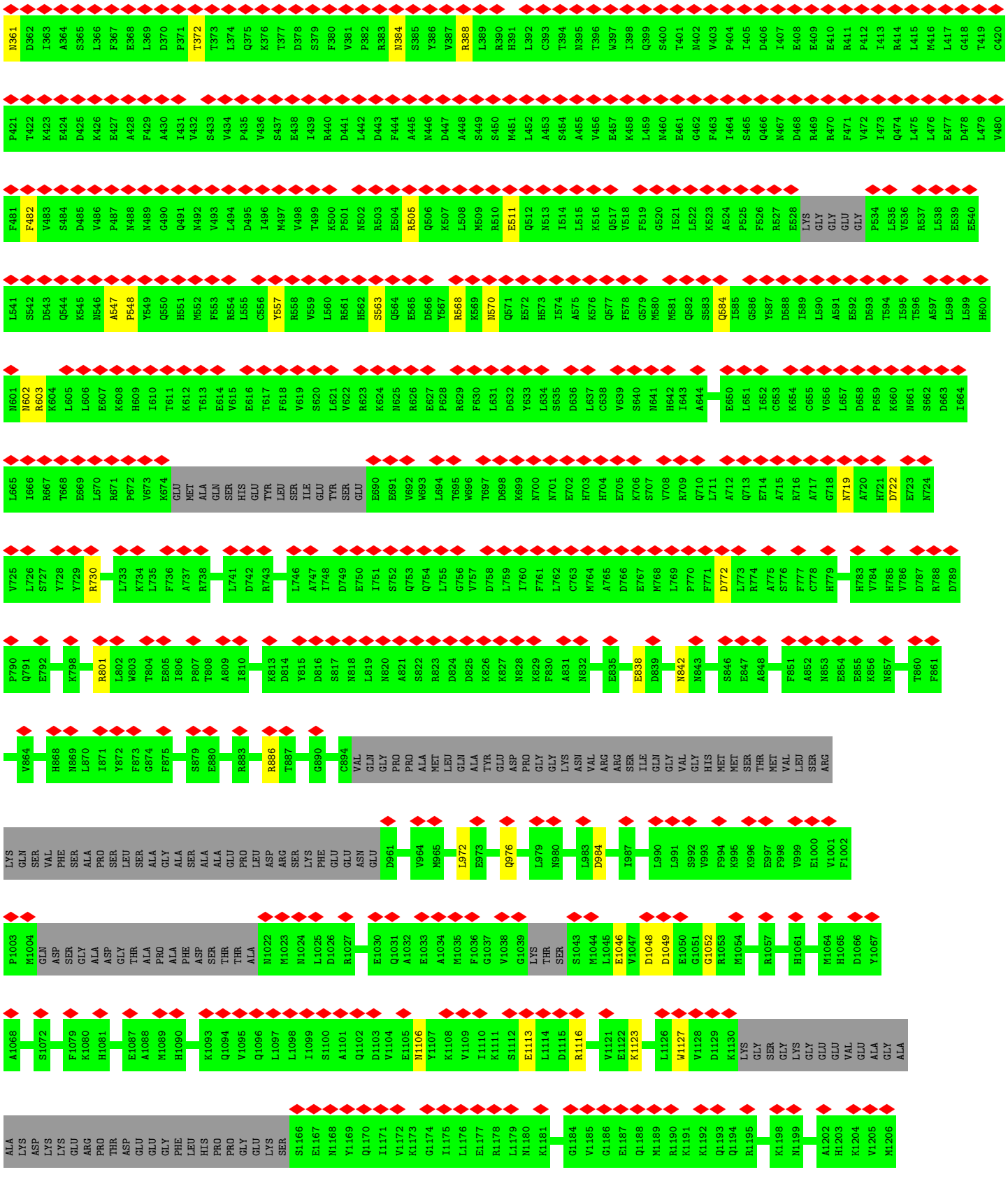
K1678 Y1679 G1680 D1681 N1684 Q1685 K1688 Q1692 N1693 Y1694 L1695 Q1696 N1697 ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO D1717 A1720 A1723 T1724 Q1725 C1726 R1727 K1730 E1731 D1739 E1747 E1752 G1755 L1756 L1760 S1778



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

Chain C:

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LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 V964 M965 L972 E973 Q976 L979 M980 L983 D984 I987 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 E1030 Q1031 A1032 E1033 A1034 M1035 F1036 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045 E1046 Y1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 R1057 H1061 M1064 H1065 D1066 Y1067
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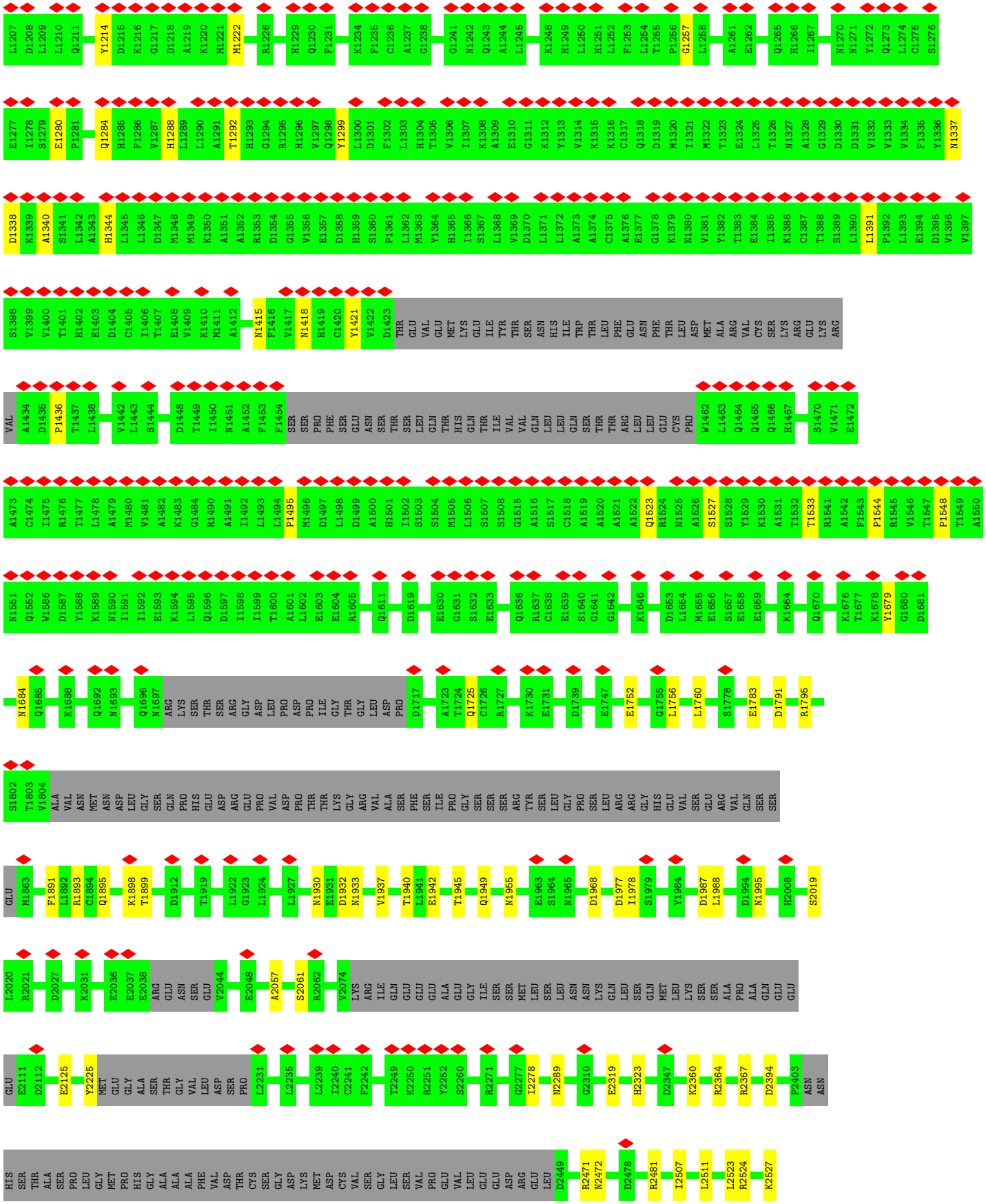
ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 I1171 V1172 K1173 G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 G1184 V1185 G1186 E1187 Q1188 M1189 R1190 K1191 K1192 Q1193 Q1194 R1195 K1198 N1199 A1202 H1203 K1204 V1205 M1206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G1241 N1242 Q1243 A1244 L1245
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Q1265 H1266 I1267
N1270 N1271 Y1272 Q1273 L1274 C1275 S1276
E1277 I1278 S1279 E1280 P1281
Q1284 H1285 F1286 V1287 H1288 L1289 L1290 A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299
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S1398 V1399 V1400 T1401 H1402 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412
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THR GLU VAL GLU MET LYS GLU 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 V1442 L1443 S1444 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 S1470 V1471 E1472
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N1694 Q1695 K1688 Q1692 N1693 Q1696 N1697
ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO
D1717 A1723 T1724 Q1725 C1726 R1727 K1730 E1731 D1739 E1747 E1752 G1755 L1756 L1760 S1778 E1783 D1791 R1795
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 F1891 L1892 R1893 C1894 Q1895 K1898 T1899 D1912 T1919 L1922 G1923 L1924 L1927 N1930 E1931 D1932 N1933 V1937 T1940 L1941 E1942 T1945 Q1949 N1955 E1963 S1964 N1965 D1968 D1977 I1978 S1979 Y1984 D1987 L1988 D1994 N1995 H2008 S2019
L2020 R2021 D2027 K2031 E2036 E2037 E2038
ARG GLU ASN SER GLU
V2044 E2048 A2057 S2061 R2062 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 E2125 Y2225
MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO
L2231 L2235 L2239 I2240 C2241 F2242 T2249 K2250 R2251 Y2252 S2260 R2271 G2277 I2278 N2289 G2310 E2319 H2323 D2347 K2360 R2364 R2367 D2394 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
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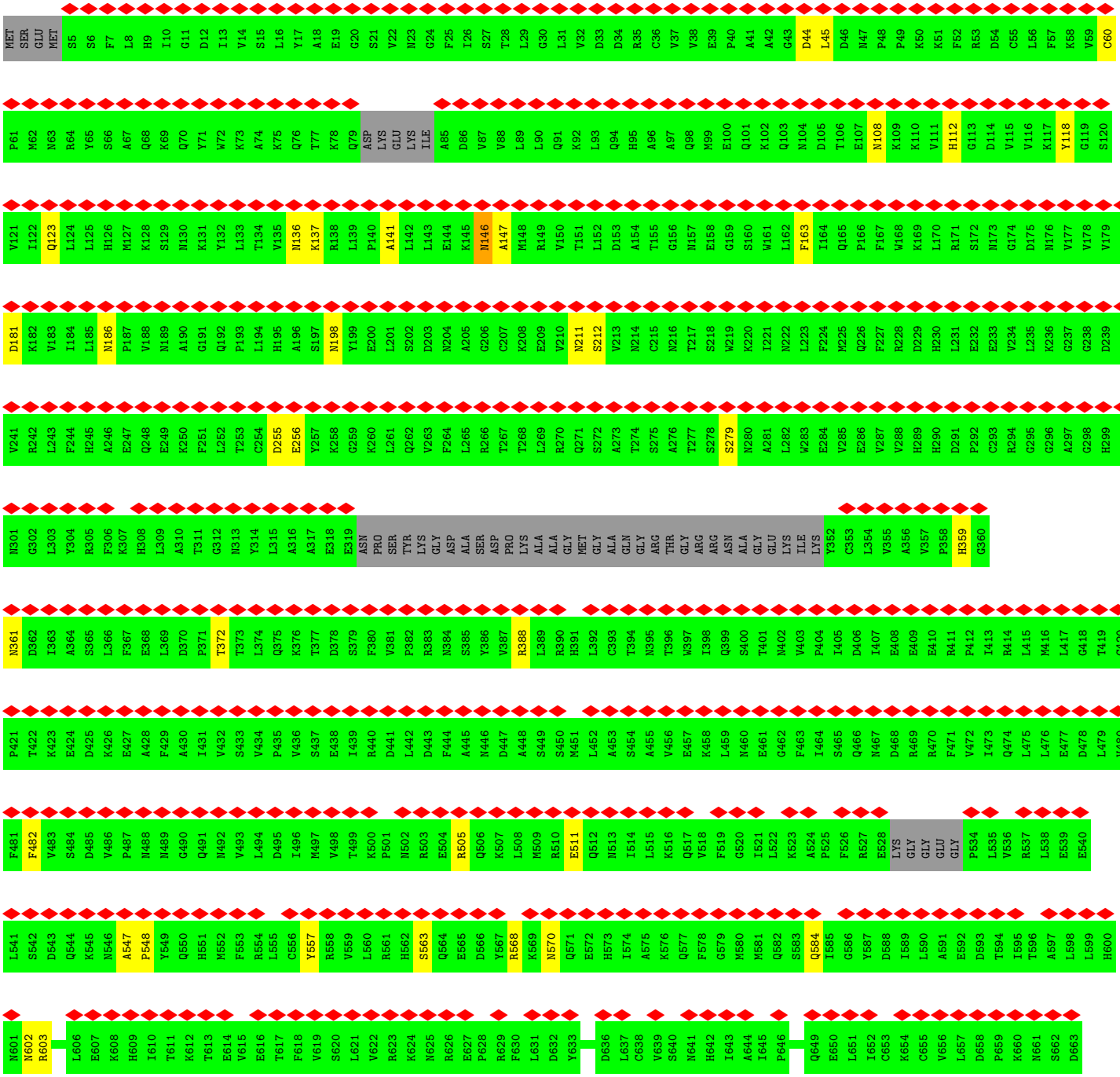
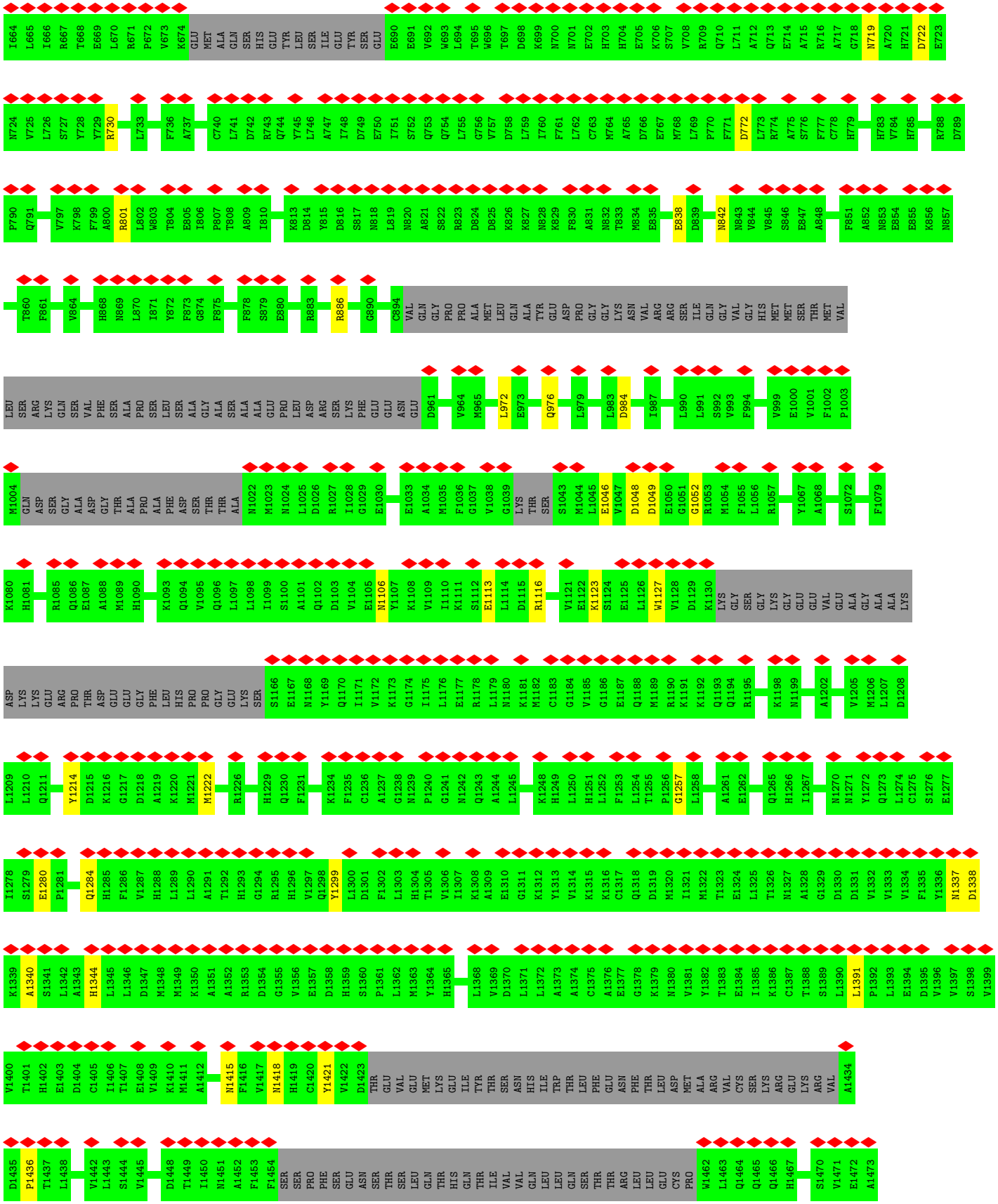
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D:

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N724 V725 L726 S727 Y728 Y729 R730 L733 F736 A737 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 H783 V784 H785 R788 D789
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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 K1198 N1199 A1202 V1205 M1206 L1207 D1208
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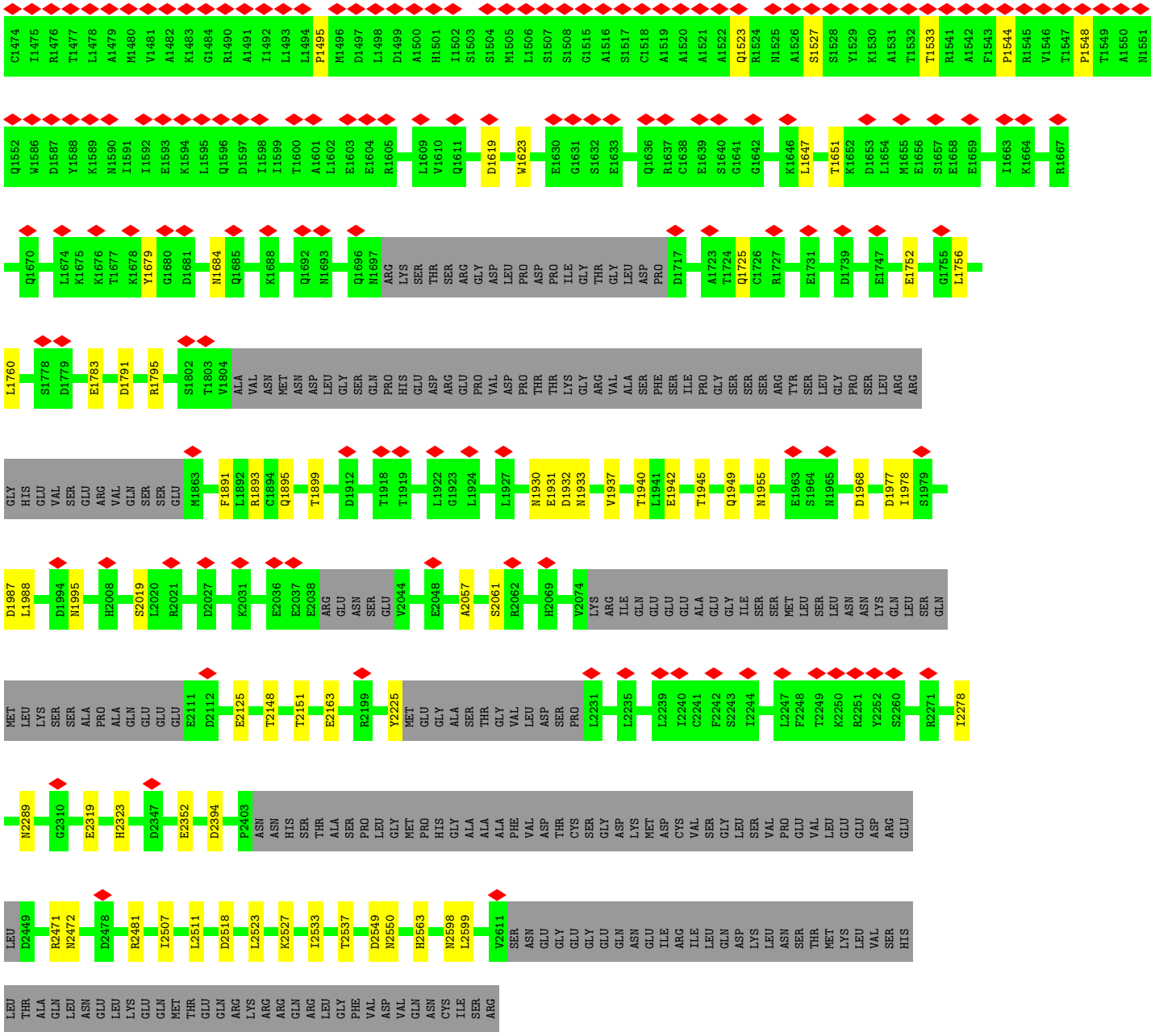
V1400 T1401 H1402 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412 N1415 F1416 V1417 N1418 H1419 C1420 Y1421 V1422 D1423 THR GLU VAL GLU MET LYS GLU ILE TYR THR SER ASN HIS ILE TRP THR LEU PHE GLU ASN PHE THR LEU ASP MET ALA ARG VAL CYS SER LYS ARG GLU LYS ARG VAL A1434
D1435 P1436 T1437 L1438 V1442 L1443 S1444 V1445 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 S1470 V1471 E1472 A1473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Q1670 L1674 K1675 K1676 T1677 K1678 Y1679 G1680 D1681 N1684 Q1685 K1688 Q1692 N1693 Q1696 N1697 ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO D1717 A1723 T1724 Q1725 C1726 R1727 E1731 D1739 E1747 E1752 G1755 L1756
L1760 S1778 D1779 E1783 D1791 R1795 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 F1891 L1892 R1893 C1894 Q1895 T1899 D1912 T1918 T1919 L1922 G1923 L1924 L1927 N1930 E1931 D1932 N1933 V1937 T1940 L1941 E1942 T1945 Q1949 N1955 E1963 S1964 N1965 D1968 D1977 I1978 S1979
D1987 L1988 D1994 N1995 H2008 S2019 L2020 R2021 D2027 K2031 E2036 E2037 E2038 ARG GLU ASN SER GLU V2044 E2048 A2057 S2061 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 E2125 T2148 T2151 E2163 R2199 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO L2231 L2235 L2239 I2240 C2241 F2242 S2243 I2244 L2247 F2248 T2249 K2250 R2251 Y2252 S2260 R2271 I2278
N2289 G2310 E2319 H2323 D2347 E2352 D2394 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 GLU ASP ARG GLU
LEU D2449 R2471 N2472 D2478 R2481 I2507 L2511 D2518 L2523 K2527 I2533 T2537 D2549 N2550 H2563 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	131437	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	30.948	Depositor
Minimum map value	-23.778	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.817	Depositor
Recommended contour level	3	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, I3P, 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	0/17647	0.50	4/23845 (0.0%)
1	B	0.27	0/17647	0.50	4/23845 (0.0%)
1	C	0.27	0/17647	0.50	4/23845 (0.0%)
1	D	0.27	0/17647	0.50	4/23845 (0.0%)
All	All	0.27	0/70588	0.50	16/95380 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

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	A	1548	PRO	N-CA-CB	5.73	110.17	103.30
1	D	1548	PRO	N-CA-CB	5.67	110.10	103.30
1	C	1548	PRO	N-CA-CB	5.67	110.10	103.30
1	D	1495	PRO	N-CA-CB	5.67	110.10	103.30
1	B	1548	PRO	N-CA-CB	5.65	110.08	103.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASN	Peptide
1	B	146	ASN	Peptide
1	C	146	ASN	Peptide
1	D	146	ASN	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	17342	17346	17176	75	0
1	B	17342	17346	17176	72	0
1	C	17342	17346	17176	71	0
1	D	17342	17346	17176	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	1	0
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	69476	69420	68740	278	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 278 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:147:ALA:HB1	1:B:1533:THR:CB	2.13	0.78
1:A:1725:GLN:NE2	1:A:1760:LEU:O	2.18	0.76
1:D:1725:GLN:NE2	1:D:1760:LEU:O	2.18	0.76
1:C:1725:GLN:NE2	1:C:1760:LEU:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1725:GLN:NE2	1:B:1760:LEU:O	2.18	0.75

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	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
1	B	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
1	C	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
1	D	2142/2671 (80%)	2036 (95%)	106 (5%)	0	100	100
All	All	8568/10684 (80%)	8144 (95%)	424 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91
1	B	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91
1	C	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91
1	D	1878/2385 (79%)	1871 (100%)	7 (0%)	89	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7512/9540 (79%)	7484 (100%)	28 (0%)	88 91

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	198	ASN
1	D	2472	ASN
1	C	1418	ASN
1	D	1418	ASN
1	C	1415	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1725	GLN
1	C	1897	ASN
1	D	1725	GLN
1	D	146	ASN
1	B	1725	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	I3P	A	3002	-	24,24,24	1.35	3 (12%)	39,39,39	0.84	0
3	I3P	D	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.83	0
3	I3P	C	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.83	0
3	I3P	B	3002	-	24,24,24	1.34	3 (12%)	39,39,39	0.83	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
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	C	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	2/15/39/39	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3002	I3P	P1-O1	3.31	1.65	1.59
3	A	3002	I3P	P1-O1	3.29	1.65	1.59
3	A	3002	I3P	P4-O4	3.29	1.65	1.59
3	C	3002	I3P	P4-O4	3.28	1.65	1.59
3	B	3002	I3P	P5-O5	3.26	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3002	I3P	C5-O5-P5-O51
3	B	3002	I3P	C5-O5-P5-O51
3	C	3002	I3P	C5-O5-P5-O51
3	D	3002	I3P	C5-O5-P5-O51
3	A	3002	I3P	C5-O5-P5-O53

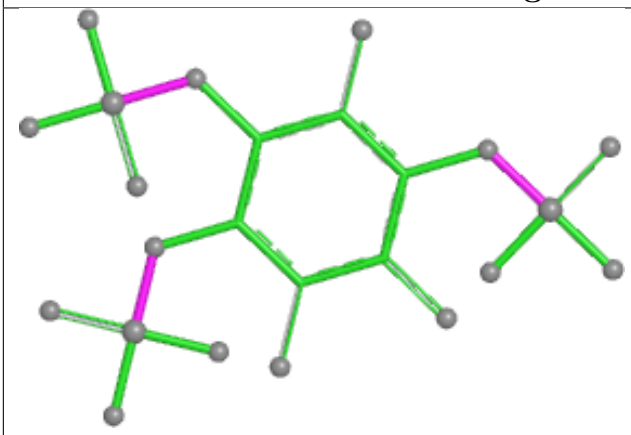
There are no ring outliers.

4 monomers are involved in 4 short contacts:

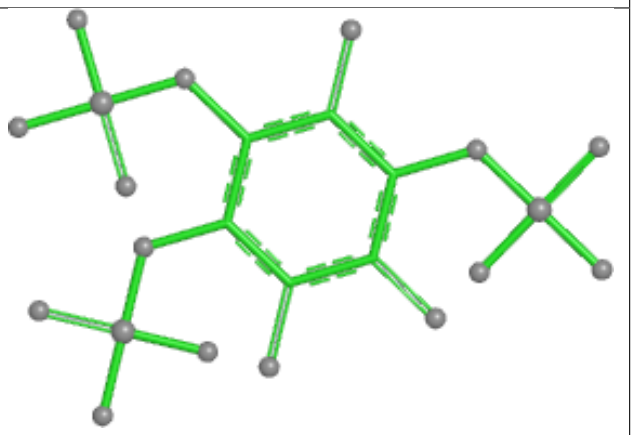
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	I3P	1	0
3	D	3002	I3P	1	0
3	C	3002	I3P	1	0
3	B	3002	I3P	1	0

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

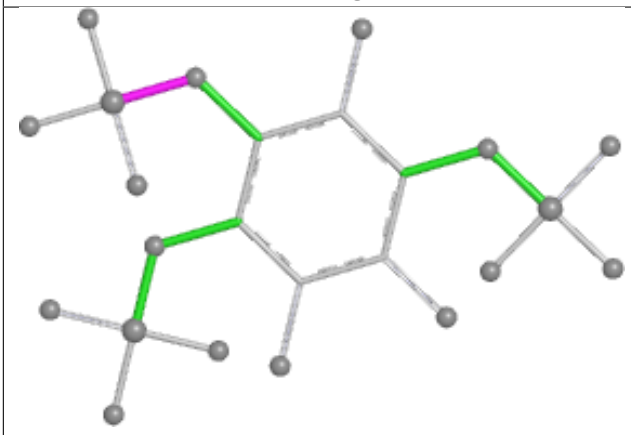
Ligand I3P A 3002



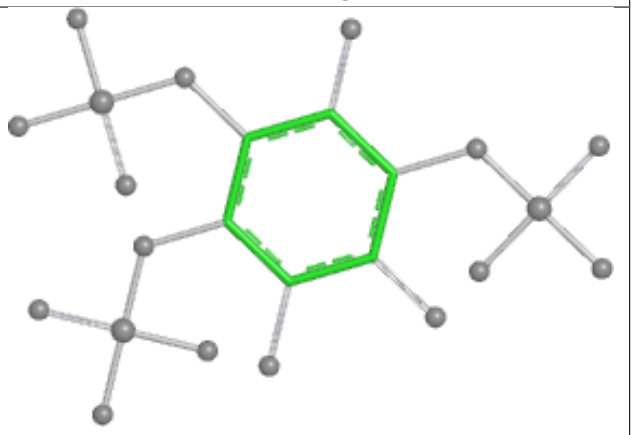
Bond lengths



Bond angles

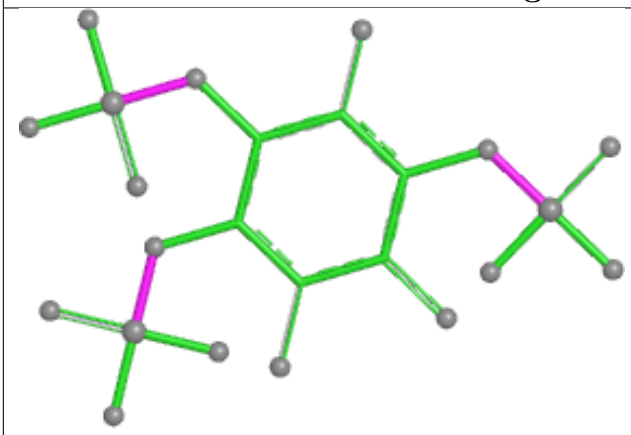


Torsions

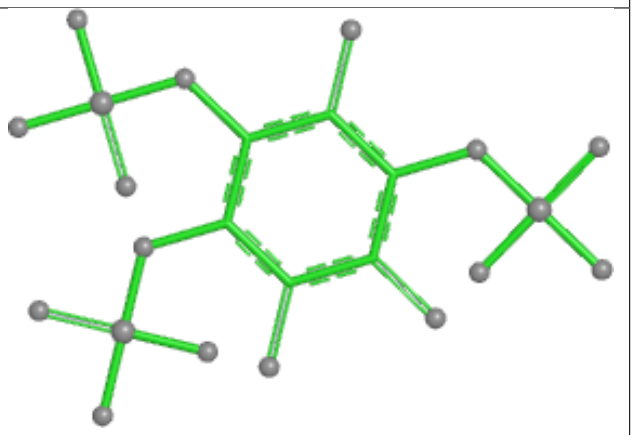


Rings

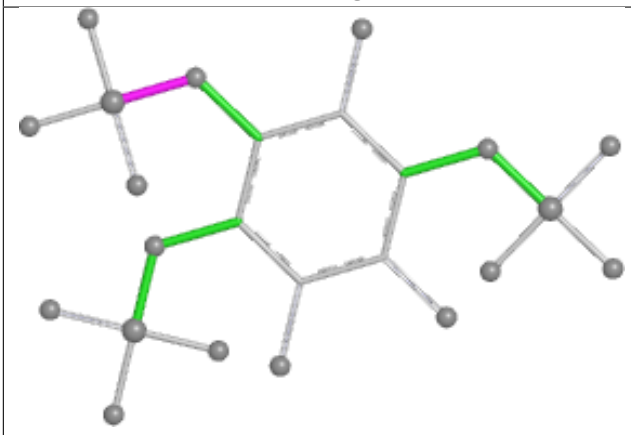
Ligand I3P D 3002



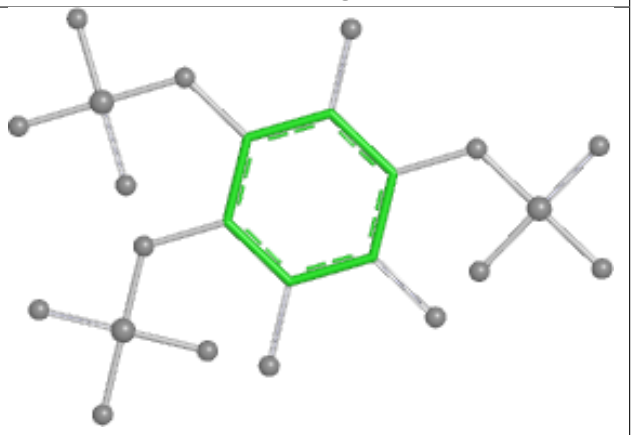
Bond lengths



Bond angles

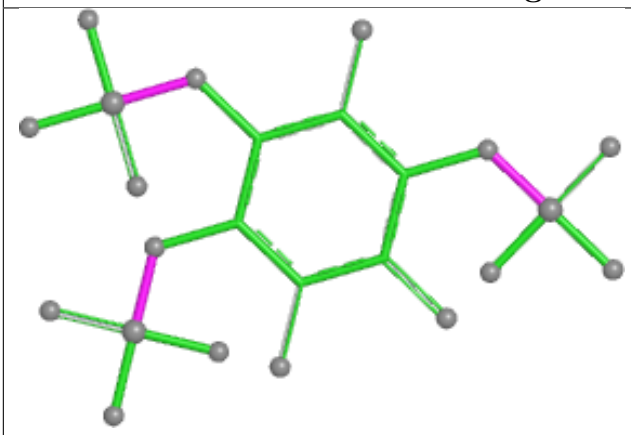


Torsions

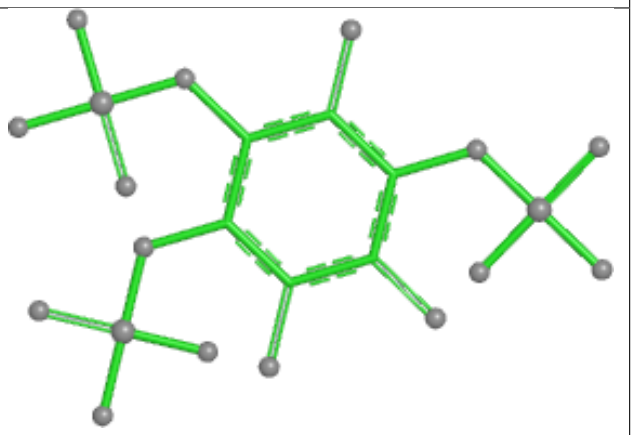


Rings

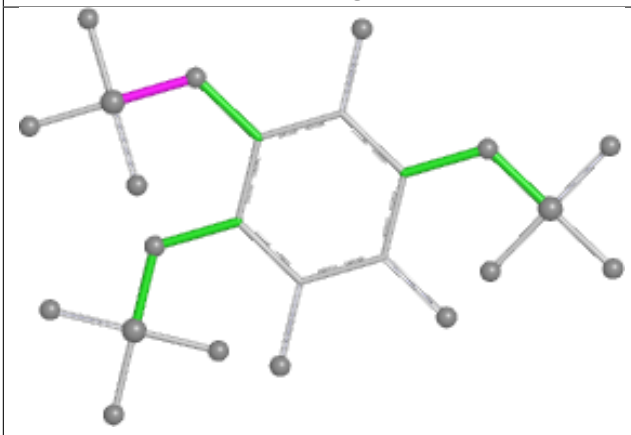
Ligand I3P C 3002



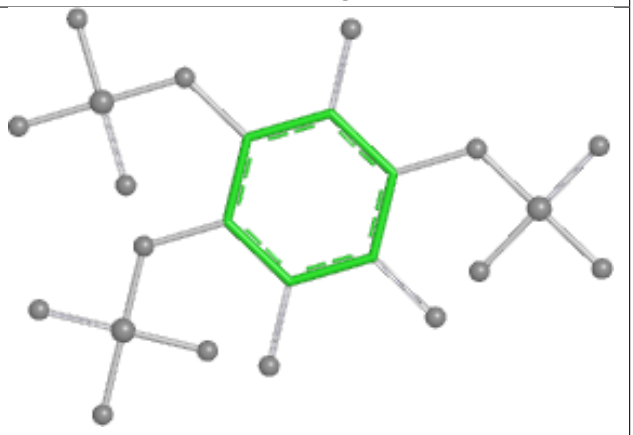
Bond lengths



Bond angles

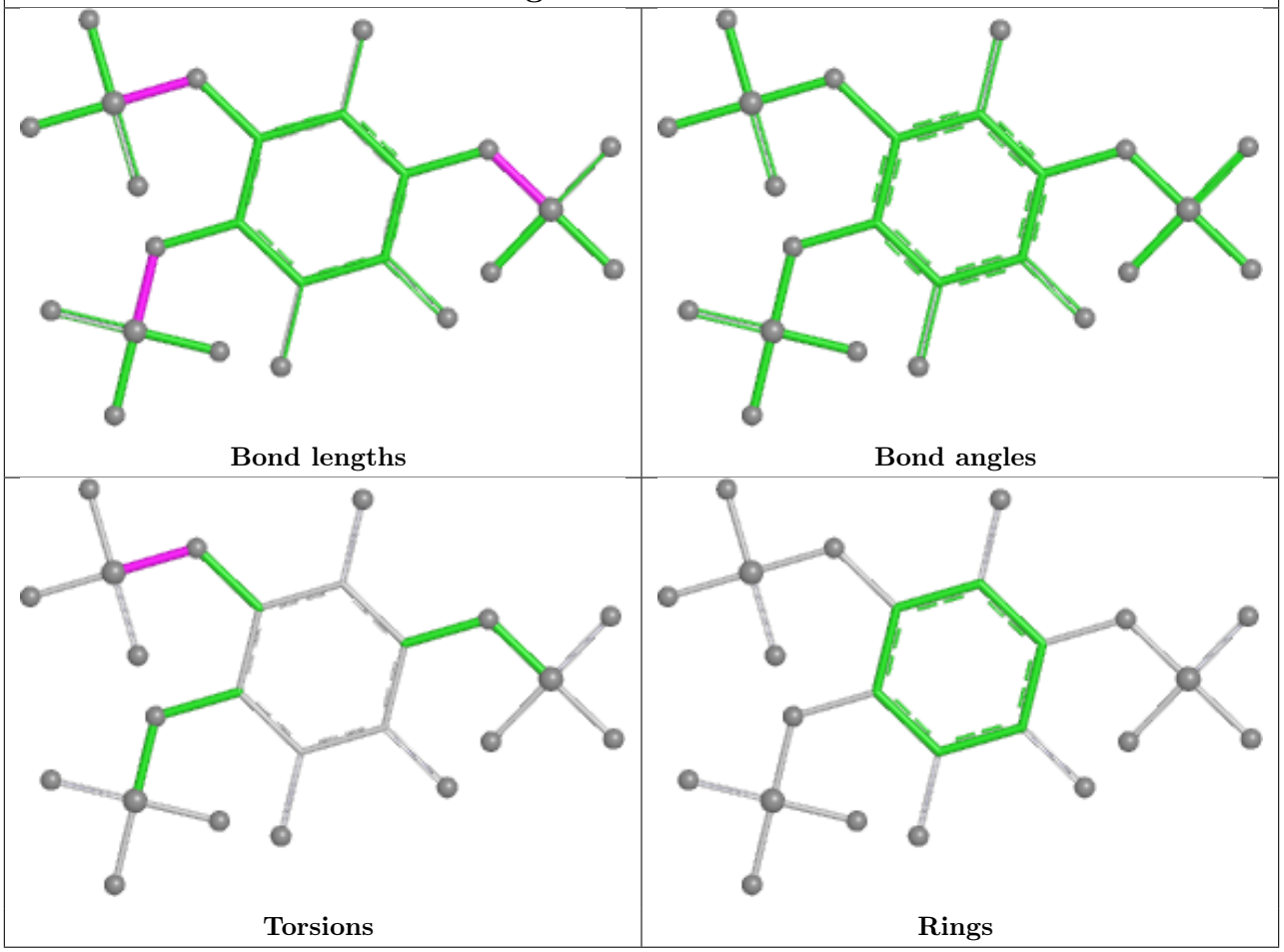


Torsions



Rings

Ligand I3P B 3002



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

The worst 5 of 20 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	56.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1552:GLN	C	1586:TRP	N	56.29
1	C	1552:GLN	C	1586:TRP	N	56.29
1	D	1552:GLN	C	1586:TRP	N	56.29
1	A	1533:THR	C	1541:ARG	N	17.36

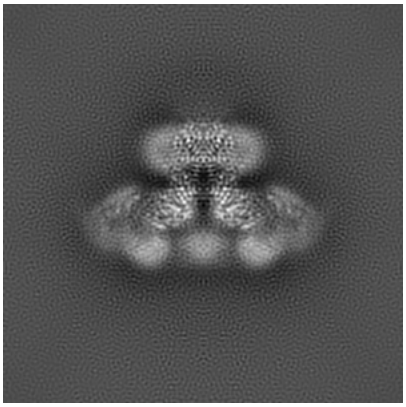
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7994. These allow visual inspection of the internal detail of the map and identification of artifacts.

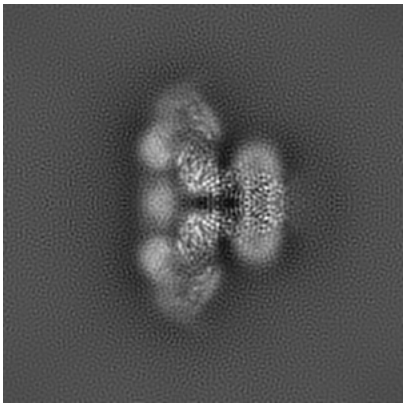
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

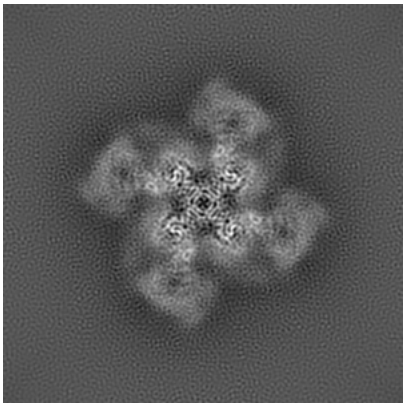
6.1.1 Primary map



X



Y

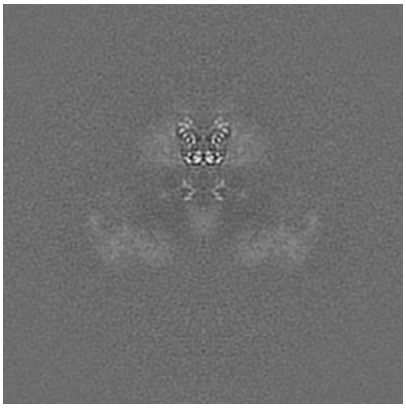


Z

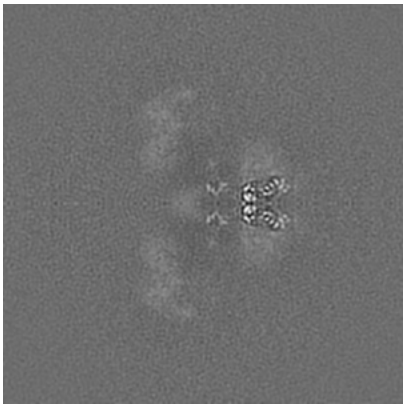
The images above show the map projected in three orthogonal directions.

6.2 Central slices

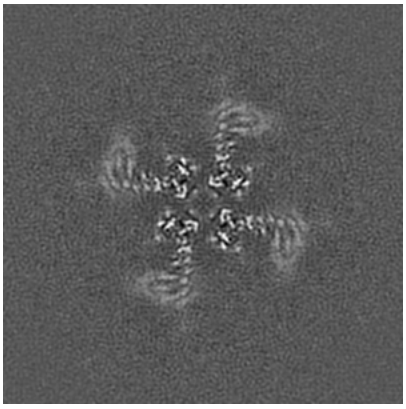
6.2.1 Primary map



X Index: 192



Y Index: 192

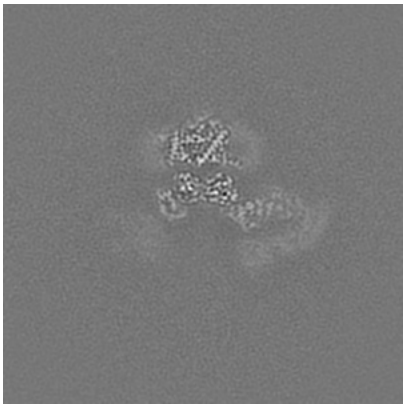


Z Index: 192

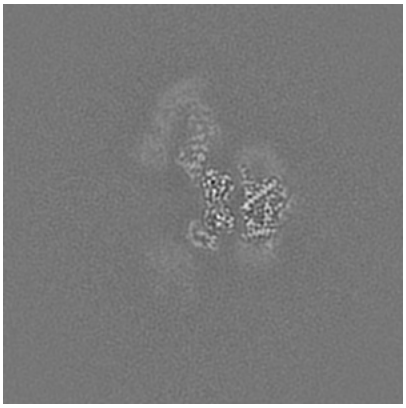
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

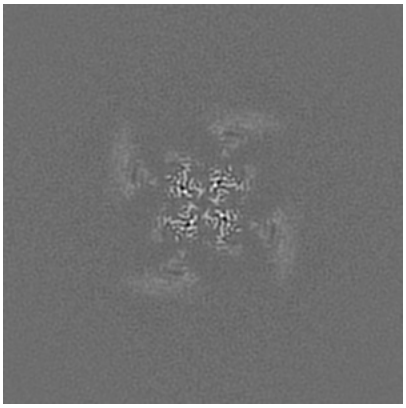
6.3.1 Primary map



X Index: 207



Y Index: 177

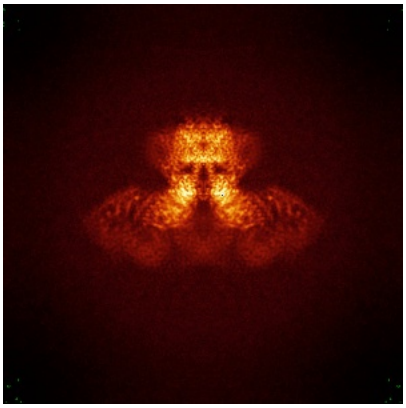


Z Index: 201

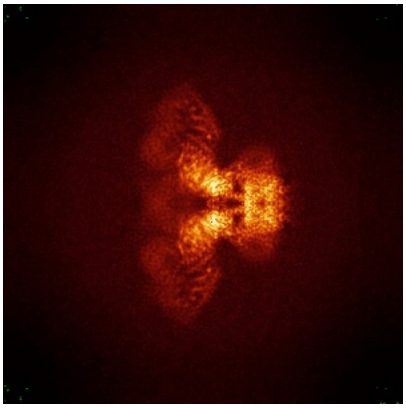
The images above show the largest variance slices of the map in three orthogonal directions.

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

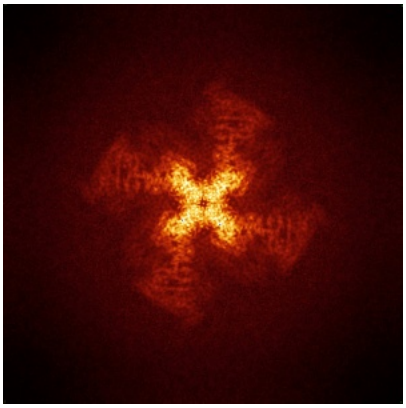
6.4.1 Primary map



X



Y

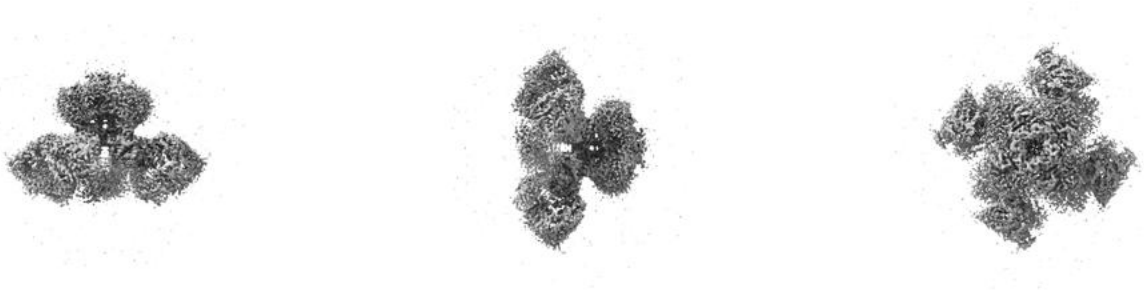


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

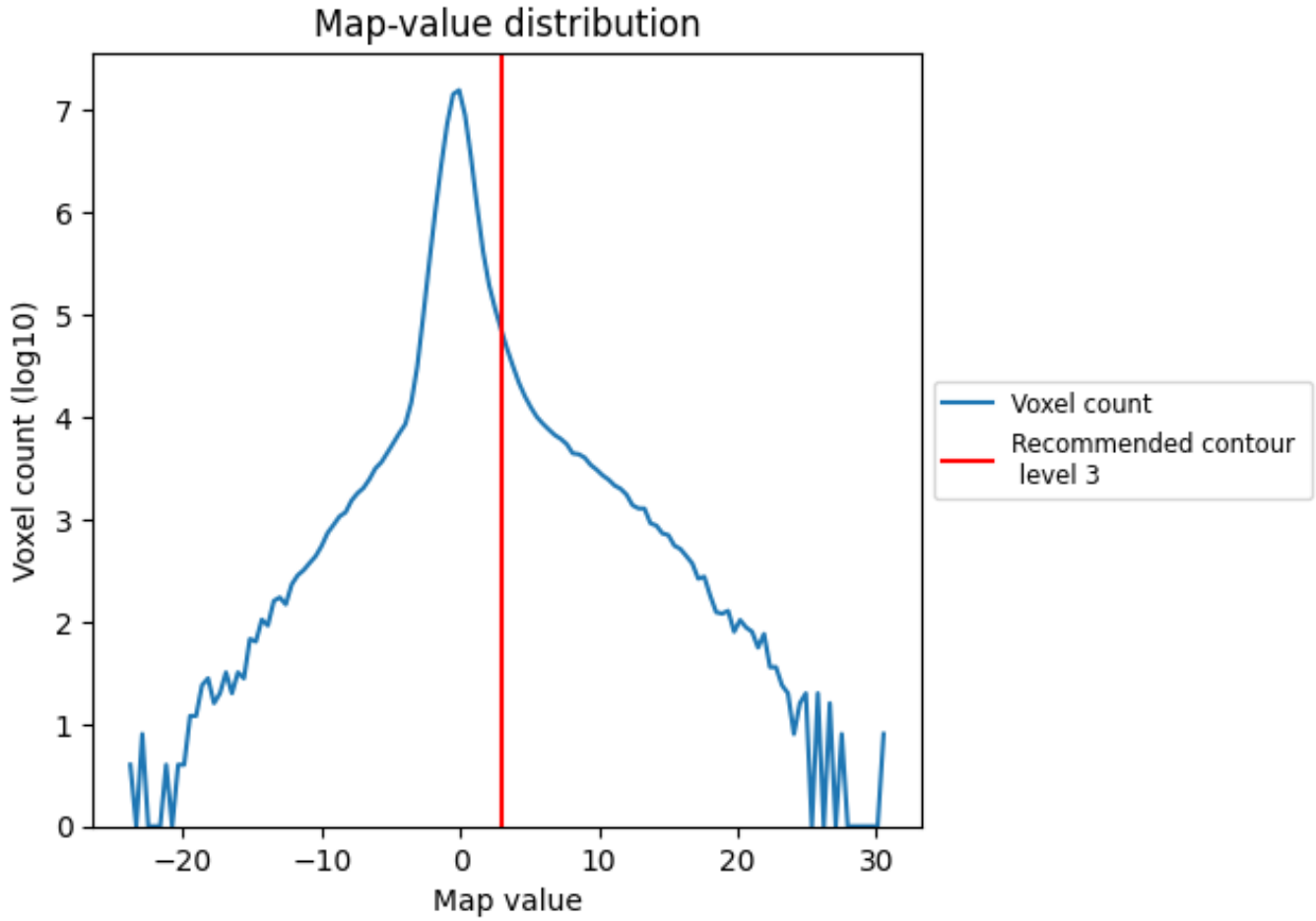
6.6 Mask visualisation (i)

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

7 Map analysis

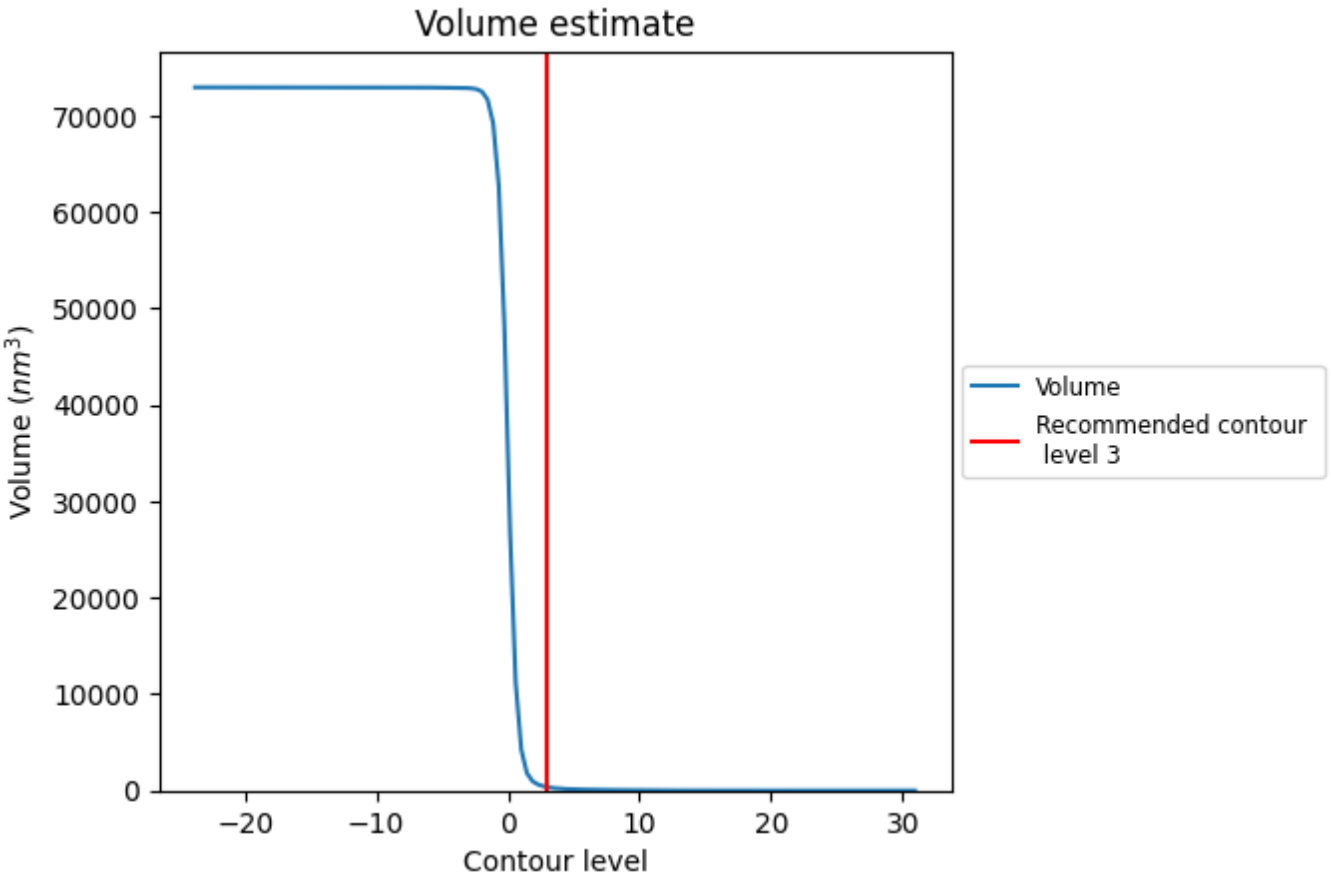
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

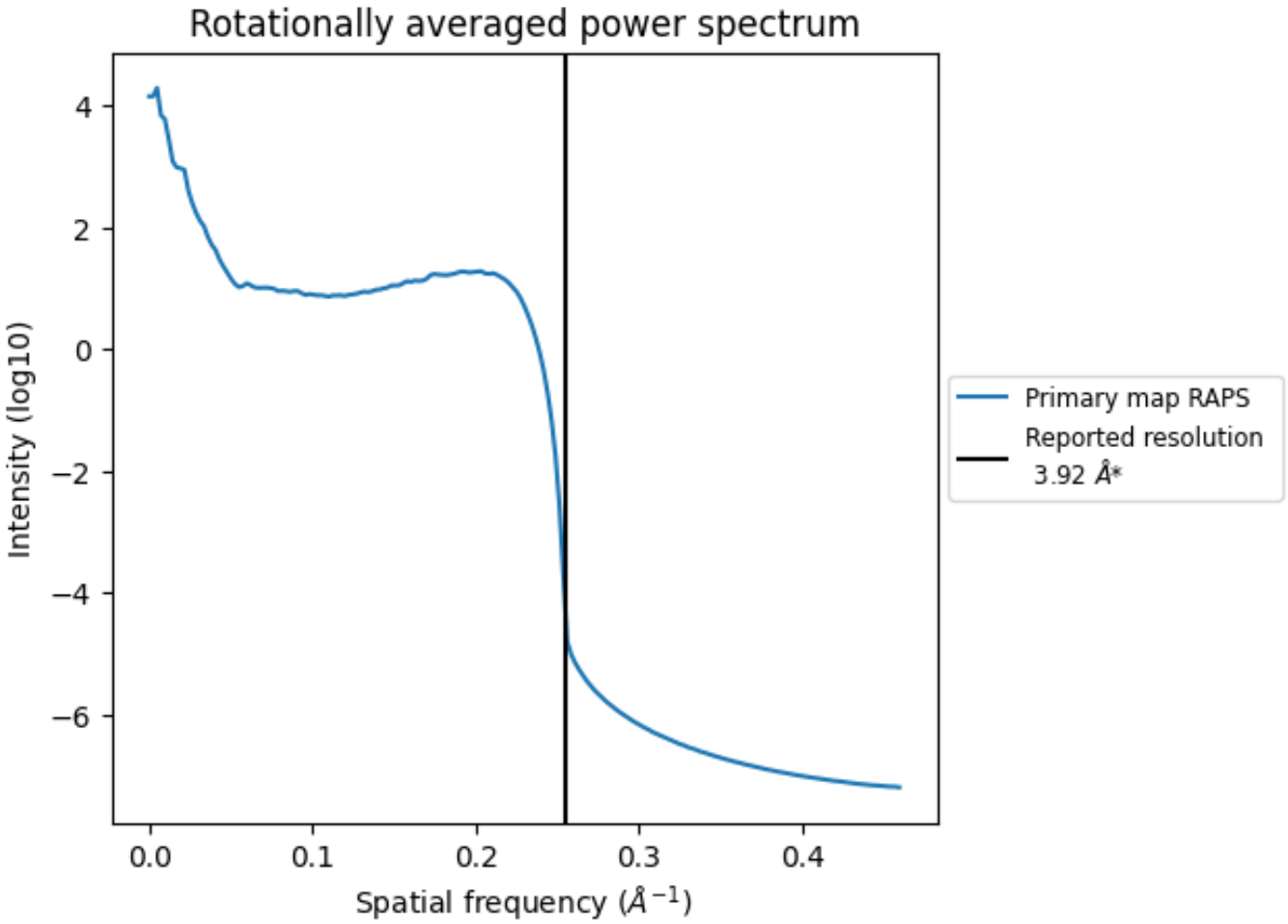
7.2 Volume estimate (i)



The volume at the recommended contour level is 362 nm^3; this corresponds to an approximate mass of 327 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 0.255 Å^{-1}

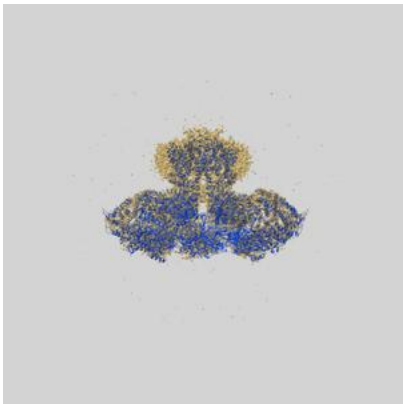
8 Fourier-Shell correlation

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

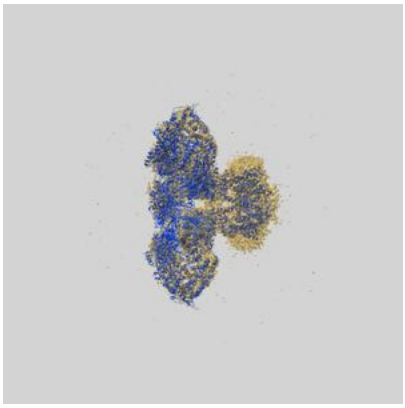
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7994 and PDB model 6DRC. Per-residue inclusion information can be found in section 3 on page 5.

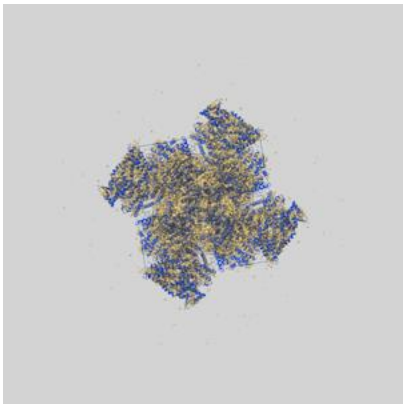
9.1 Map-model overlay



X



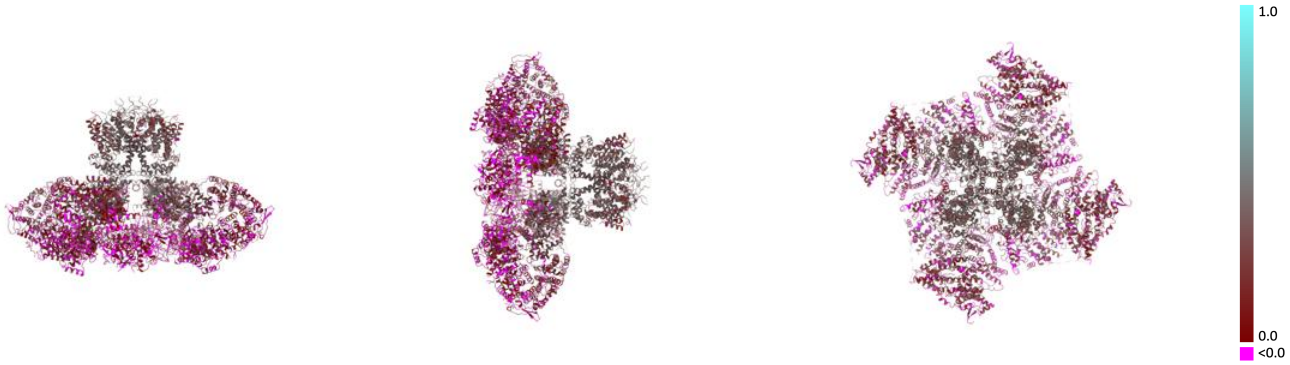
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

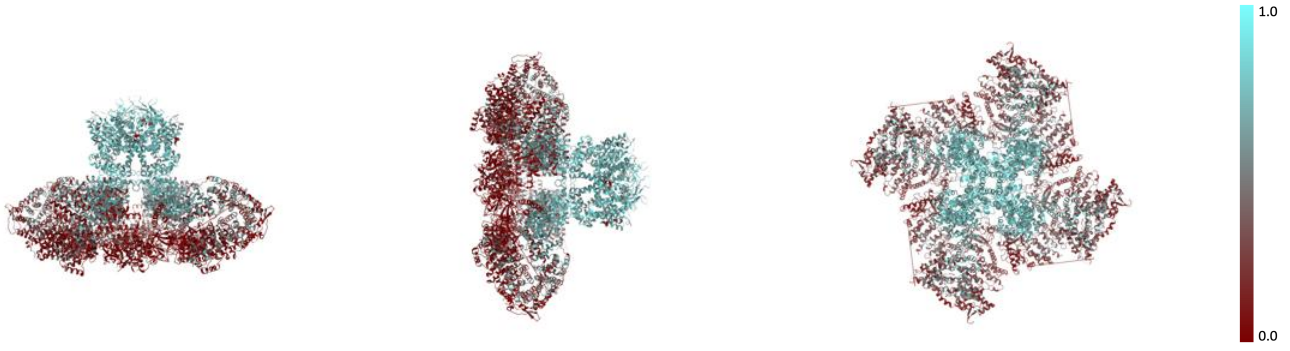
9.2 Q-score mapped to coordinate model



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.

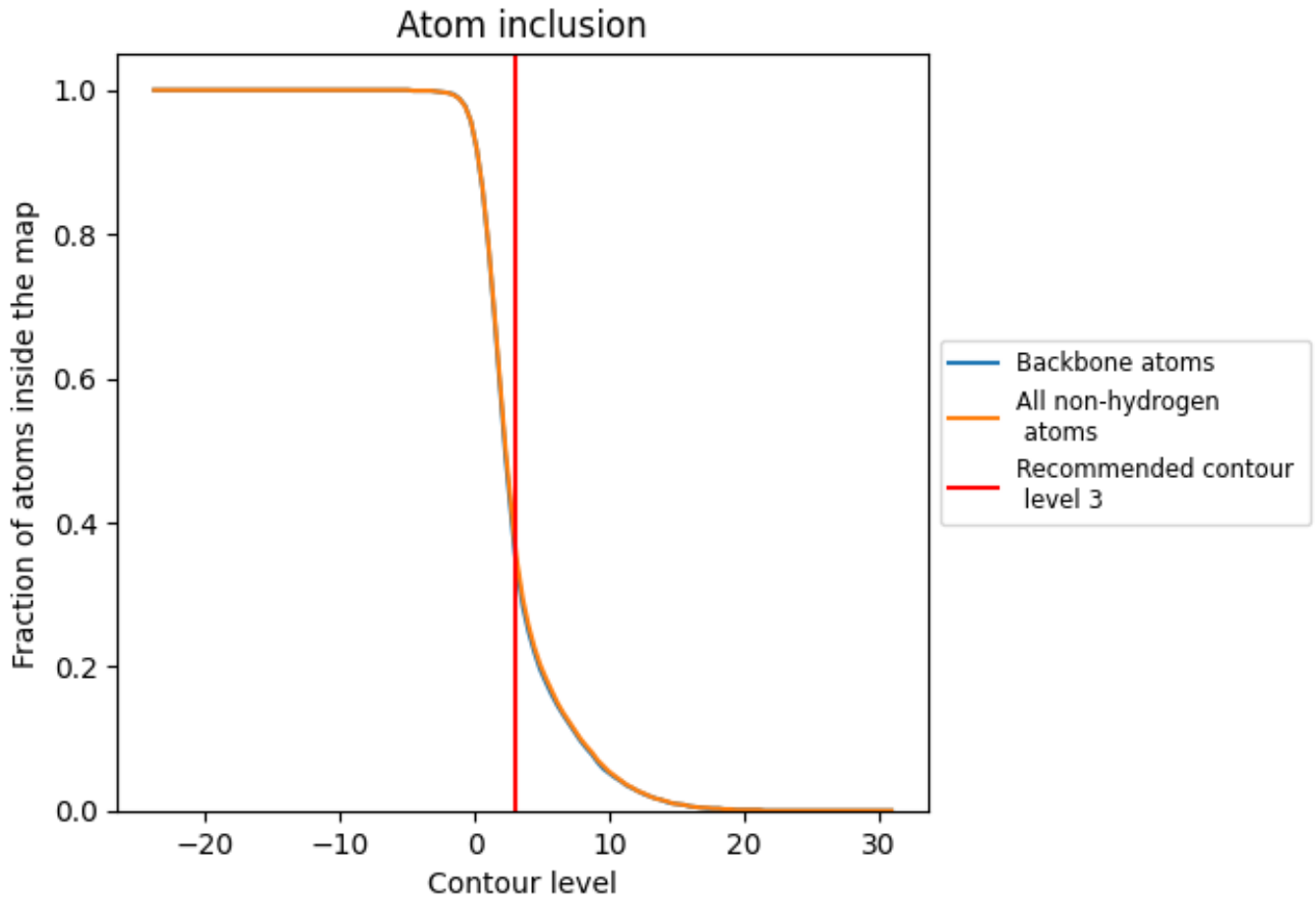
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 36% of all backbone atoms, 37% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3700	0.1790
A	0.3770	0.1790
B	0.3770	0.1790
C	0.3760	0.1790
D	0.3770	0.1790