Full wwPDB EM Validation Report

Nov 7, 2022 – 11:53 PM EST

PDB ID	:	6DR2
EMDB ID	:	EMD-7988
Title	:	Ca2+-bound human type 3 1,4,5-inositol trisphosphate receptor
Authors	:	Hite, R.K.; Paknejad, N.
Deposited on	:	2018-06-11
Resolution	:	4.33 Å(reported)

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

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

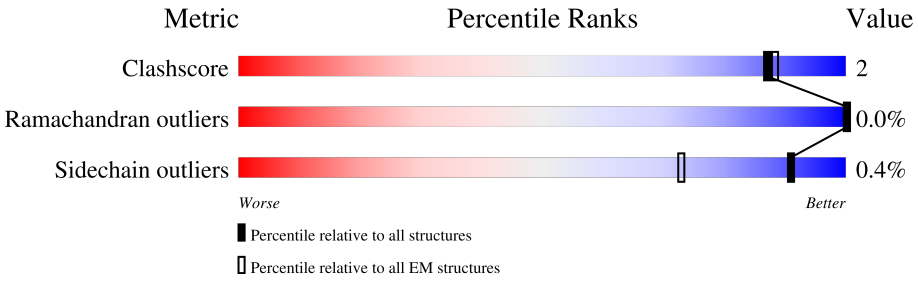
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2671	38% 77% 5% 18%
1	B	2671	39% 77% 5% 18%
1	C	2671	39% 76% 5% 18%
1	D	2671	39% 77% 5% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 139084 atoms, of which 69544 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2191	Total 34768	C 11084	H 17386	N 2990	O 3202	S 106	0	0
1	B	2191	Total 34768	C 11084	H 17386	N 2990	O 3202	S 106	0	0
1	C	2191	Total 34768	C 11084	H 17386	N 2990	O 3202	S 106	0	0
1	D	2191	Total 34768	C 11084	H 17386	N 2990	O 3202	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

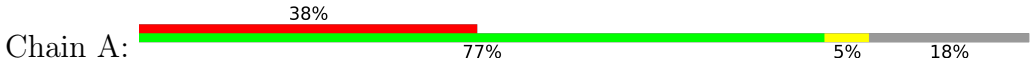
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Ca 2	0
3	B	2	Total 2	Ca 2	0
3	C	2	Total 2	Ca 2	0
3	D	2	Total 2	Ca 2	0

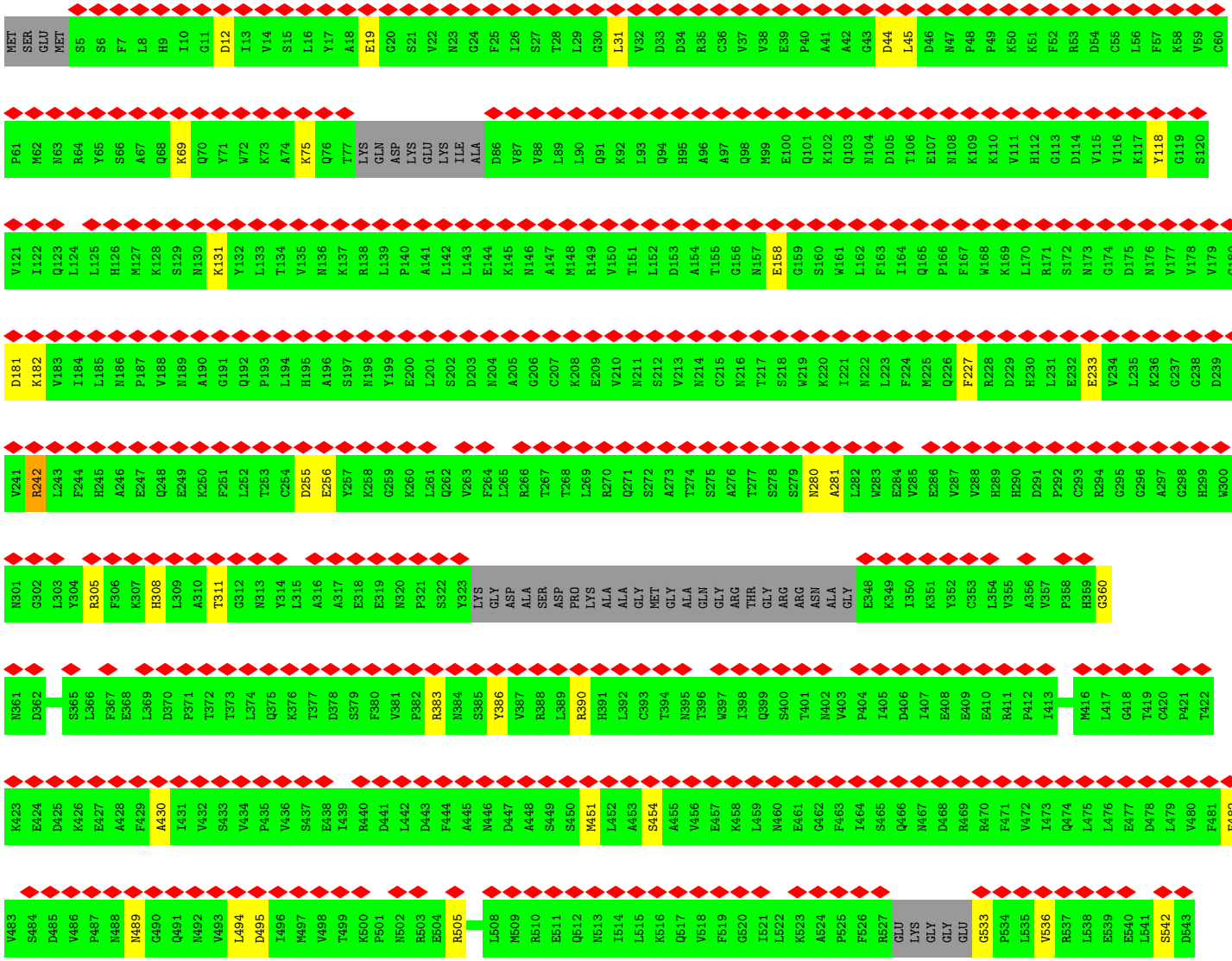
3 Residue-property plots (i)

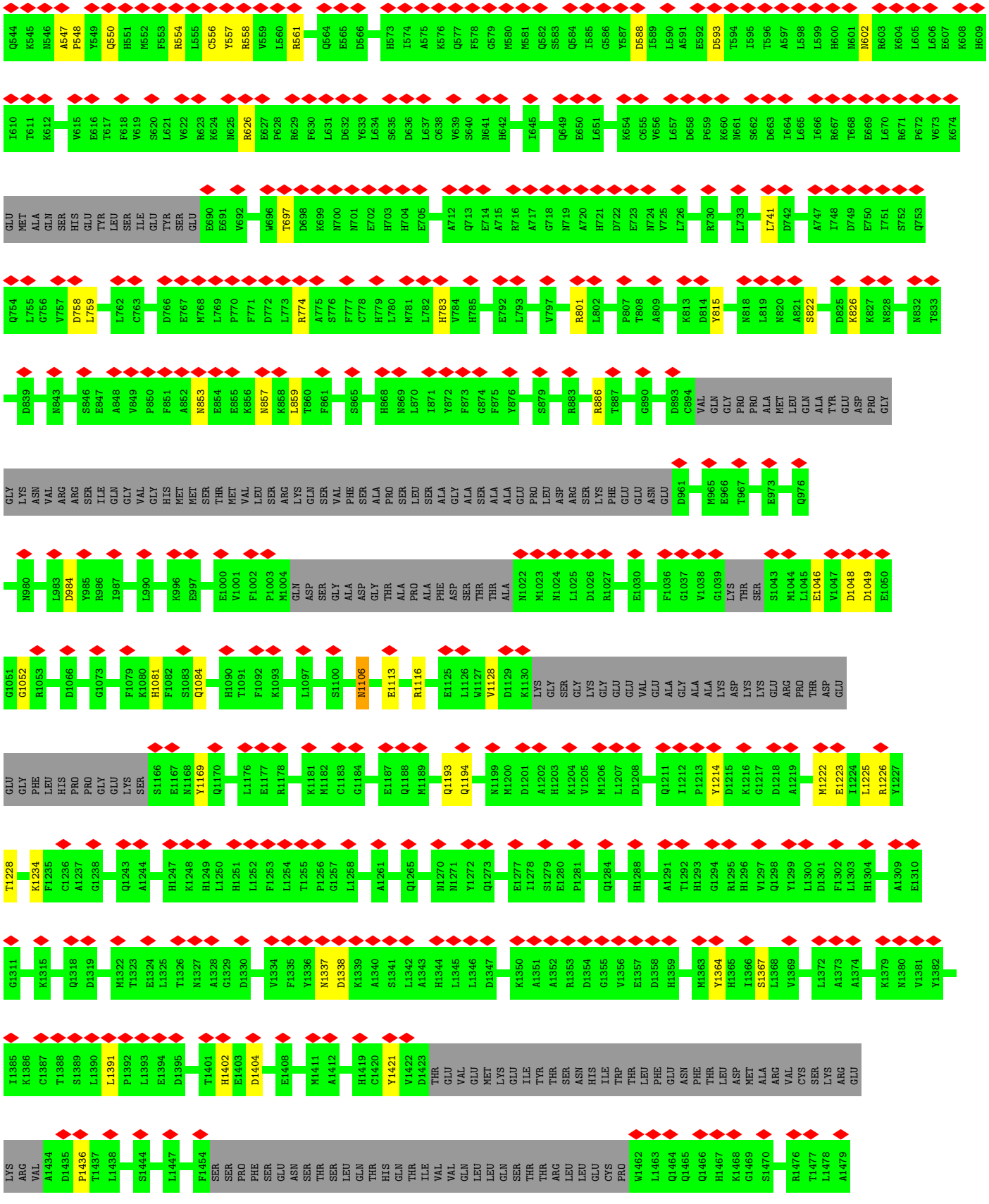
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

Chain A:



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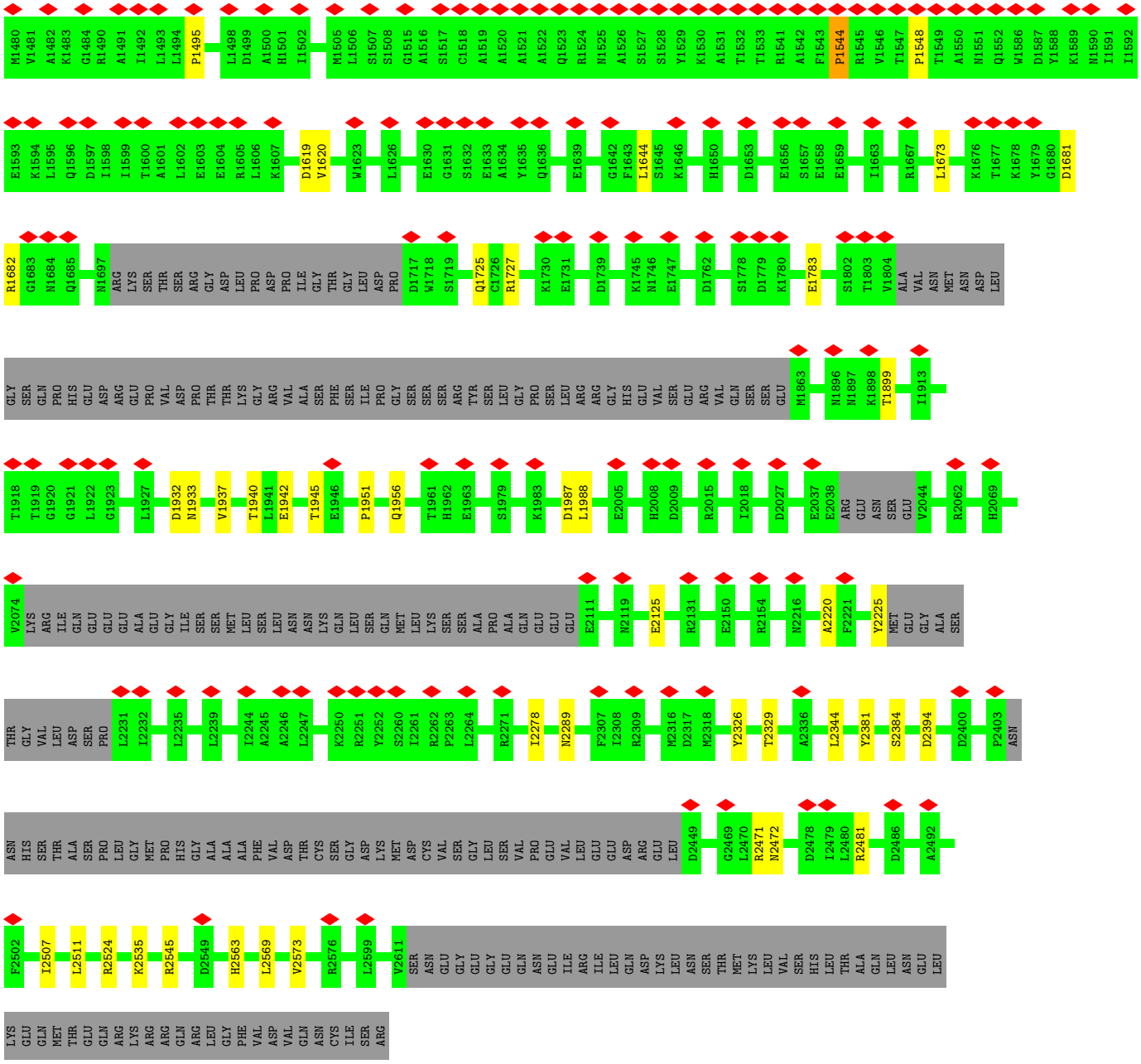
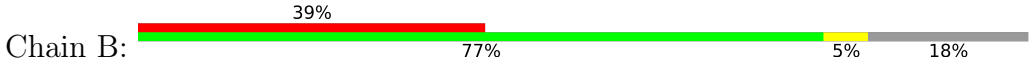
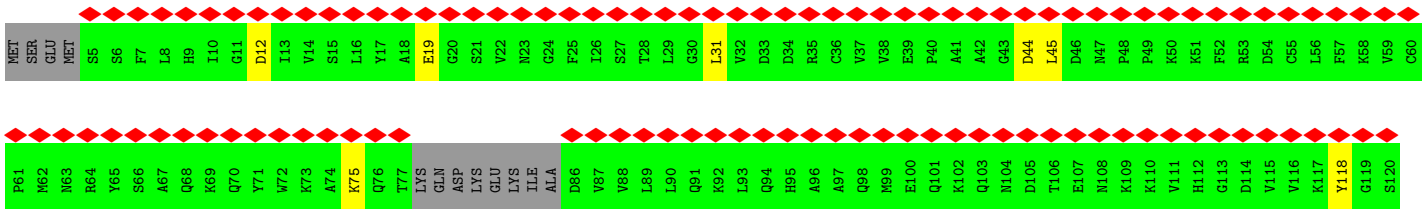
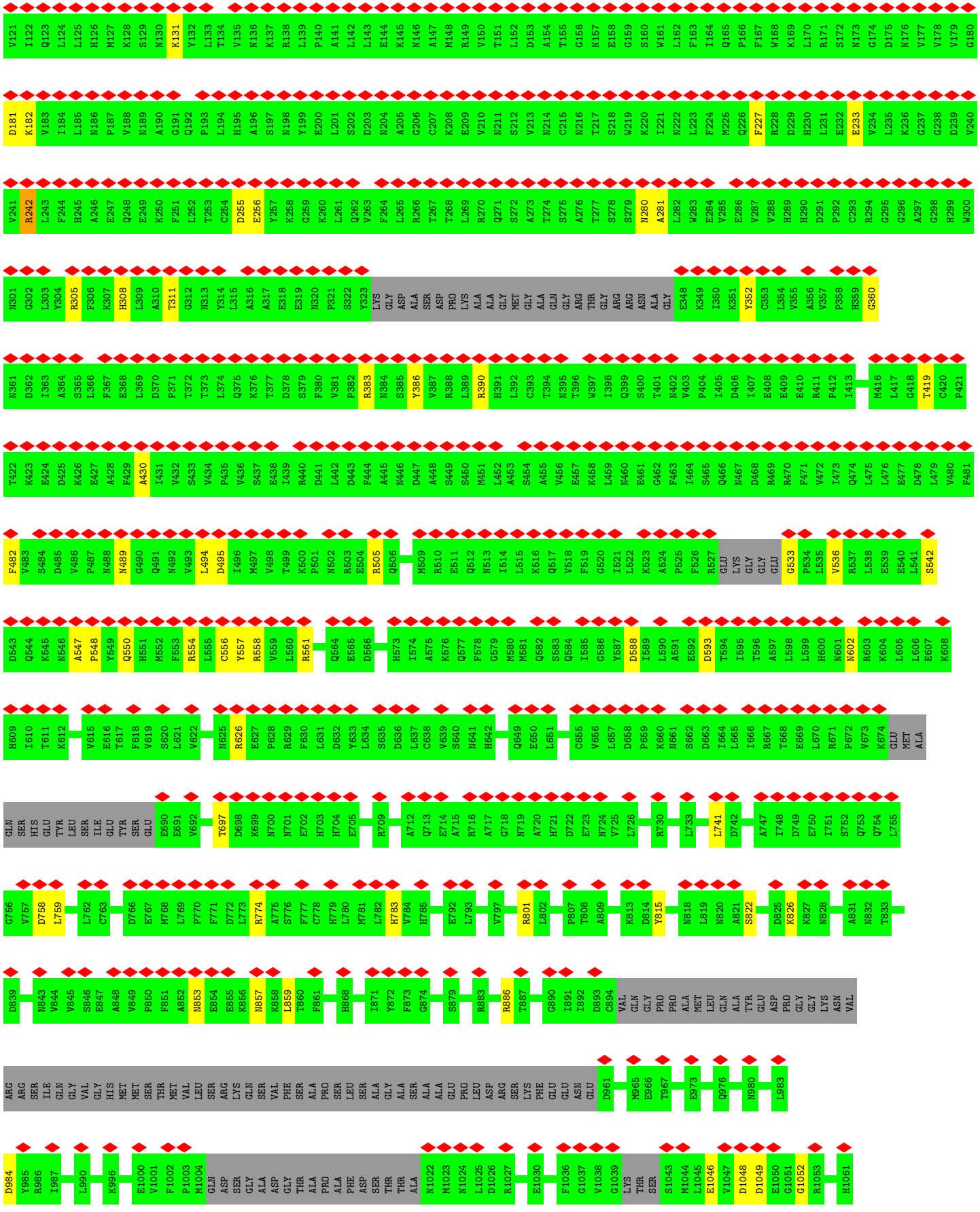
I610 T611 K612 V615 E616 T617 F618 V619 S620 L621 V622 R623 K624 N625 R626 E627 P628 R629 F630 L631 D632 Y633 L634 S635 D636 L637 C638 V639 S640 N641 H642 I645 Q649 E650 L651 K654 C655 V656 L657 D658 P659 K660 W661 S662 D663 I664 L665 I666 R667 T668 E669 L670 R671 P672 V673 K674
GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER GLU E690 E691 V692 W696 T697 D698 K699 N700 N701 E702 H703 H704 E705 A712 Q713 E714 A715 R716 A717 G718 N719 A720 H721 D722 E723 N724 V725 L726 R730 L733 L741 D742 A747 I748 D749 E750 I751 S752 Q753
Q754 L755 G756 V757 D758 L759 L762 C763 D766 E767 M768 L769 P770 F771 D772 L773 R774 A775 S776 F777 C778 H779 L780 M781 L782 H783 V784 H785 E792 L793 V797 R801 L802 P807 T808 A809 K813 D814 Y815 N818 L819 N820 A821 S822 D825 K826 K827 N828 N832 T833
D839 N843 S846 E847 A848 V849 P850 F851 A852 N853 E854 E855 K856 N857 K858 L859 T860 F861 S865 H868 N869 L870 I871 Y872 F873 G874 F875 Y876 S879 R883 R886 T887 G890 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY
GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 M965 E966 T967 E973 Q976
N980 L983 D984 Y985 R986 I987 L990 K996 E997 E1000 V1001 F1002 P1003 M1004 GLN ASP SER GLY GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 M1023 N1024 L1025 D1026 R1027 E1030 F1036 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050
G1051 G1052 R1053 D1066 G1073 F1079 K1080 H1081 F1082 S1083 Q1084 H1090 T1091 F1092 K1093 L1097 S1100 N1106 E1113 R1116 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 L1176 E1177 R1178 K1181 M1182 C1183 G1184 E1187 Q1188 M1189 Q1193 Q1194 N1199 M1200 D1201 A1202 H1203 K1204 V1205 M1206 L1207 D1208 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 M1222 E1223 I1224 L1225 R1226 Y1227
T1228 K1234 F1235 C1236 A1237 G1238 Q1243 A1244 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 A1261 Q1265 N1270 N1271 Y1272 Q1273 E1277 I1278 S1279 E1280 P1281 Q1284 H1288 A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 A1309 E1310
G1311 K1315 Q1318 D1319 M1322 T1323 E1324 L1325 T1326 N1327 A1328 G1329 D1330 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 M1363 Y1364 H1365 I1366 S1367 L1368 V1369 L1372 A1373 A1374 K1379 N1380 V1381 Y1382
I1385 K1386 C1387 T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 T1401 H1402 E1403 D1404 E1408 M1411 A1412 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 S1444 L1447 F1454 SER SER PRO PHE SER GLU ASN SER THR SER LEU GLN THR HIS GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO W1462 L1463 Q1464 Q1465 Q1466 H1467 K1468 G1469 S1470 R1476 T1477 L1478 A1479



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



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D181 K182 V183 I184 L185 N186 P187 V188 N189 A190 G191 Q192 P193 L194 H195 A196 S197 N198 Y199 E200 L201 S202 D203 N204 A205 G206 C207 K208 E209 V210 N211 S212 V213 N214 C215 N216 T217 S218 W219 K220 I221 N222 L223 F224 M225 Q226 F227 R228 D229 H230 L231 E232 E233 V234 L235 K236 G237 G238 D239 V240
V241 R242 L243 F244 H245 A246 E247 Q248 E249 K250 F251 L252 T253 C254 D255 E256 Y257 K258 G259 K260 L261 Q262 V263 F264 L265 R266 T267 T268 L269 R270 Q271 S272 A273 T274 S275 A276 T277 S278 S279 N280 A281 L282 W283 E284 V285 E286 V287 V288 H289 H290 D291 P292 C293 R294 G295 G296 A297 G298 H299 W300
N301 G302 L303 Y304 R305 F306 K307 H308 L309 A310 T311 G312 N313 Y314 L315 A316 A317 E318 E319 N320 P321 S322 Y323 LYS GLY ASP ALA SER ASP PRO LYS ALA ALA GLY MET GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA GLY E348 K349 I350 K351 Y352 C353 L354 V355 A356 V357 P358 H359 G360
N361 D362 I363 A364 S365 L366 F367 E368 L369 D370 P371 T372 T373 L374 Q375 K376 T377 D378 S379 F380 V381 P382 R383 N384 S385 Y386 V387 R388 L389 R390 H391 L392 C393 T394 N395 T396 W397 I398 Q399 S400 T401 N402 V403 P404 I405 D406 I407 E408 E409 E410 R411 P412 I413 M416 L417 G418 T419 C420 P421
T422 K423 E424 D425 K426 E427 A428 F429 A430 I431 V432 S433 V434 P435 V436 S437 E438 I439 R440 D441 L442 D443 F444 A445 N446 D447 A448 S449 S450 M451 L452 A453 S454 A455 V456 E457 K458 L459 N460 E461 G462 F463 I464 S465 Q466 N467 D468 R469 R470 F471 V472 I473 Q474 L475 L476 E477 D478 L479 V480 F481
F482 V483 S484 D485 V486 P487 N488 N489 G490 Q491 N492 V493 L494 D495 I496 M497 V498 T499 K500 P501 N502 R503 E504 R505 Q506 M509 R510 E511 Q512 N513 I514 L515 K516 Q517 V518 F519 G520 I521 L522 K523 A524 P525 F526 R527 GLU LYS GLY GLU G533 P534 L535 V536 R537 L538 E539 E540 L541 S542
D543 Q544 K545 N546 A547 P548 Y549 Q550 H551 M552 F553 R554 L555 C556 Y557 R558 V559 L560 R561 Q564 E565 D566 H573 I574 A575 K576 Q577 F578 G579 M580 M581 Q582 S583 Q584 I585 G586 Y587 D588 I589 L590 A591 E592 D593 T594 L595 T596 A597 L598 L599 H600 N601 N602 R603 K604 L605 L606 E607 K608
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GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER GLU E690 E691 V692 T697 D698 K699 N700 N701 E702 H703 H704 E705 R709 A712 Q713 E714 A715 R716 A717 G718 N719 A720 H721 D722 E723 N724 V725 L726 R730 L733 L741 D742 A747 I748 D749 E750 I751 S752 Q753 Q754 L755
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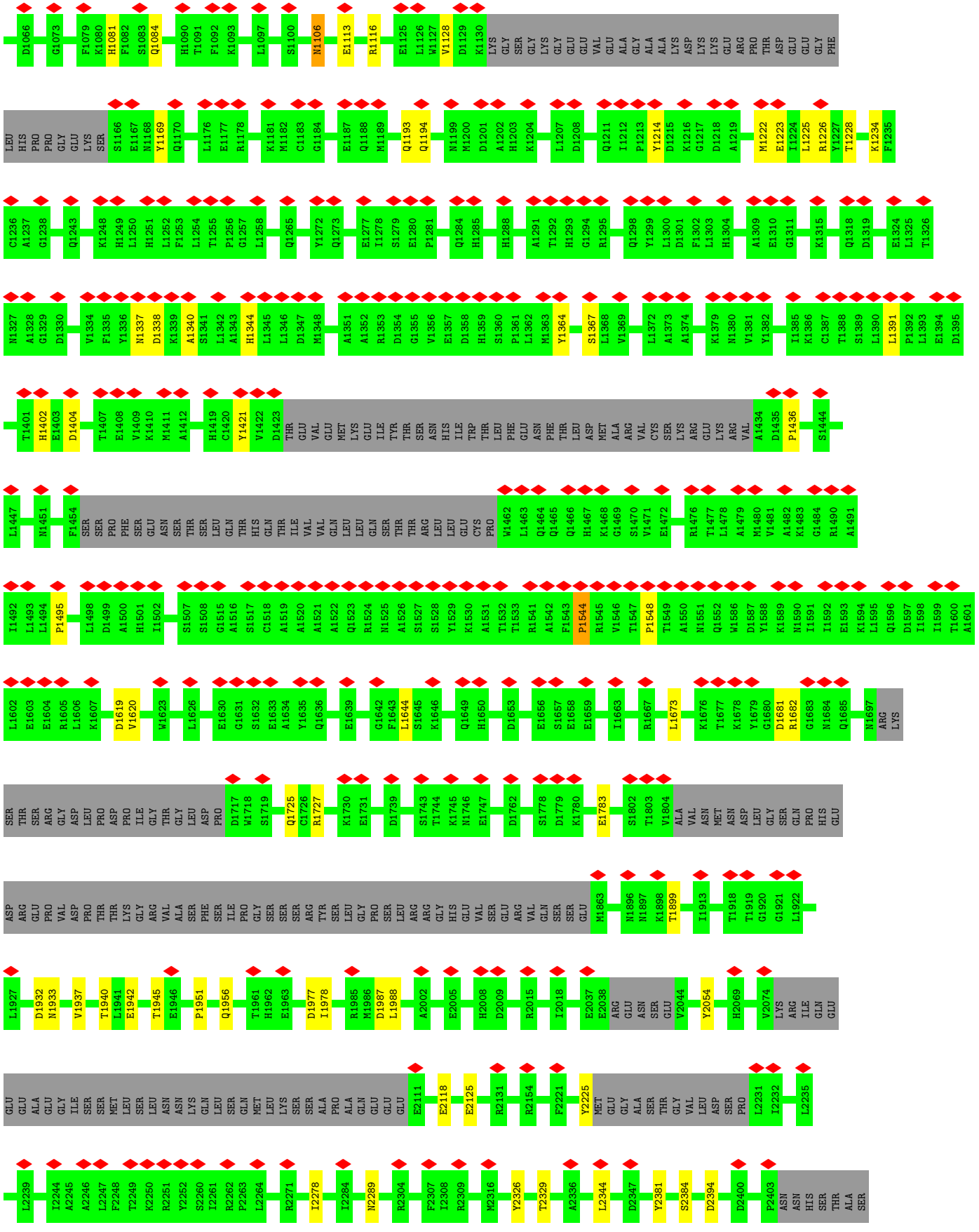
D839 N843 V844 V845 S846 E847 A848 V849 P850 F851 A852 N853 E854 E855 K856 N857 K858 L859 T860 F861 H868 I871 Y872 F873 G874 S879 R883 R886 T887 G890 I891 I892 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL
ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 M965 E966 T967 E973 Q976 N980 L983
D984 Y985 R986 I987 L990 K996 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 F1036 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052 R1053 H1061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LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 N1168 Y1169 Q1170 L1176 E1177 R1178 K1181 M1182 C1183 G1184 E1187 Q1188 M1189 Q1193 Q1194 N1199 M1200 D1201 A1202 H1203 K1204 L1207 D1208 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 M1222 E1223 I1224 L1225 R1226 Y1227 T1228 K1234 F1235
G1236 A1237 G1238 Q1243 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 Q1265 Y1272 Q1273 E1277 I1278 S1279 E1280 P1281 Q1284 H1285 H1288 A1291 T1292 H1293 G1294 R1295 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 A1309 E1310 G1311 K1315 Q1318 D1319 E1324 L1325 T1326
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T1401 H1402 E1403 D1404 T1407 E1408 V1409 K1410 M1411 A1412 H1419 C1420 Y1421 V1422 D1423 THR GLU VAL GLU MET LYS GLU ILE TYR THR 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 S1444
L1447 N1451 F1454 SER SER PRO PHE SER GLU ASN SER THR SER LEU GLN THR HIS GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO W1462 L1463 Q1464 Q1465 Q1466 H1467 K1468 G1469 S1470 V1471 E1472 R1476 T1477 L1478 A1479 M1480 V1481 A1482 K1483 G1484 R1490 A1491
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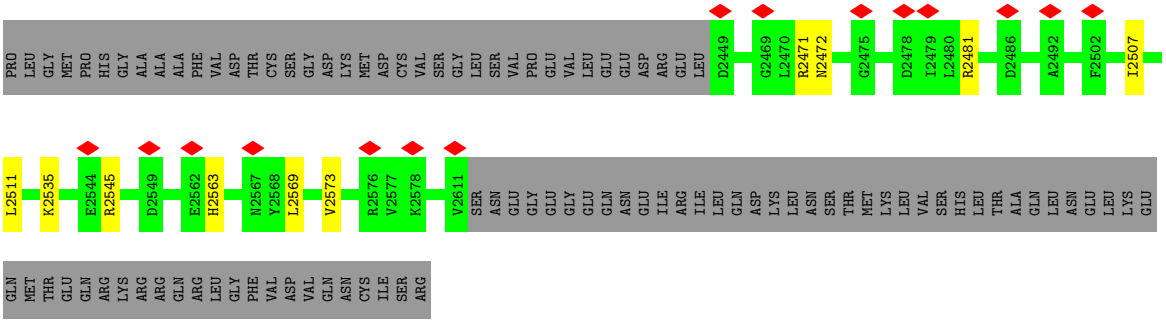
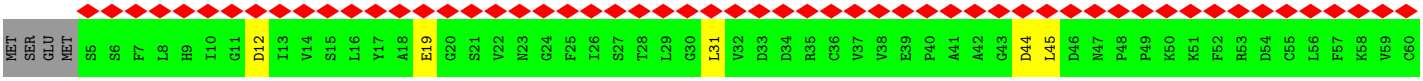
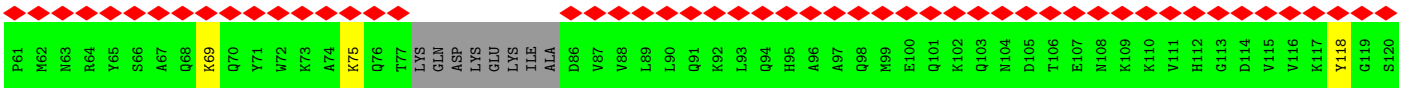
SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO D1717 W1718 S1719 Q1725 C1726 R1727 K1730 E1731 D1739 S1743 T1744 K1745 N1746 E1747 D1762 S1778 D1779 K1780 E1783 S1802 T1803 V1804 ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU
ASP ARG GLU PRO VAL ASP PRO THR THR LYS GLY ARG VAL 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 N1896 N1897 K1898 T1899 I1913 T1918 T1919 G1920 G1921 L1922
L1927 D1932 N1933 V1937 T1940 L1941 E1942 T1945 E1946 P1951 Q1956 T1961 H1962 E1963 D1977 I1978 R1985 M1986 D1987 L1988 A2002 E2005 H2008 D2009 R2015 I2018 E2037 E2038 ARG GLU ASN SER GLU V2044 Y2054 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 E2118 E2125 R2131 R2154 F2221 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO L2231 I2232 L2235
L2239 T2244 A2245 A2246 L2247 F2248 T2249 K2250 R2251 Y2252 S2260 I2261 R2262 P2263 L2264 R2271 I2278 I2284 N2289 R2304 F2307 I2308 R2309 M2316 Y2326 T2329 A2336 L2344 D2347 Y2381 S2384 D2394 D2400 P2403 ASN ASN HIS SER THR ALA SER

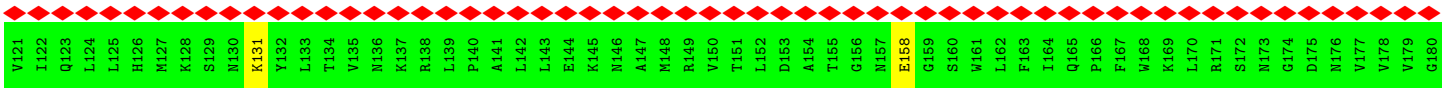


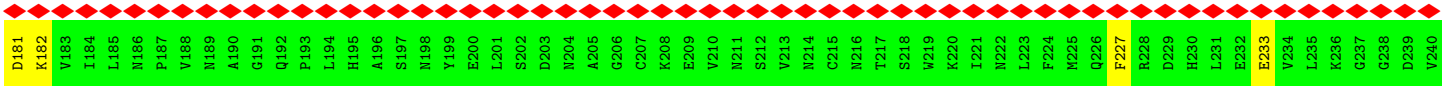
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

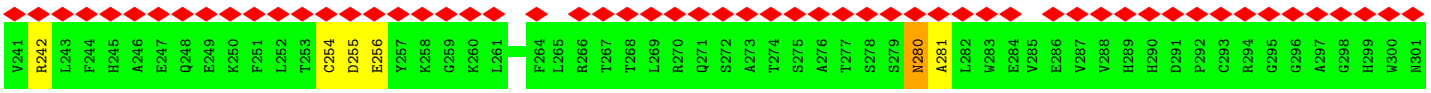
Chain C:

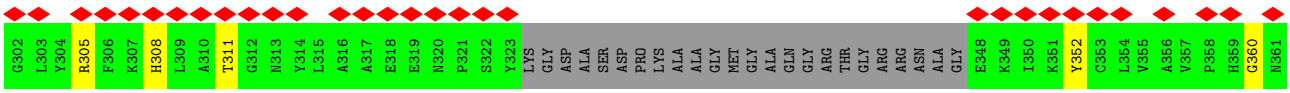


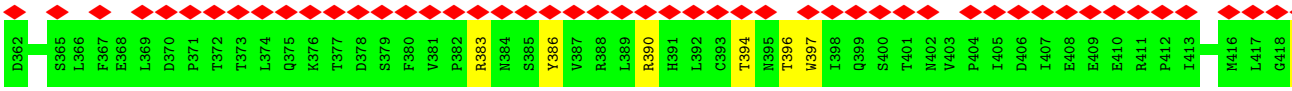


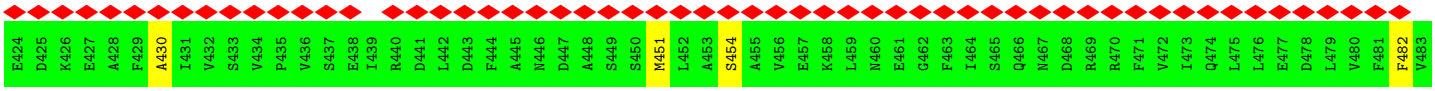


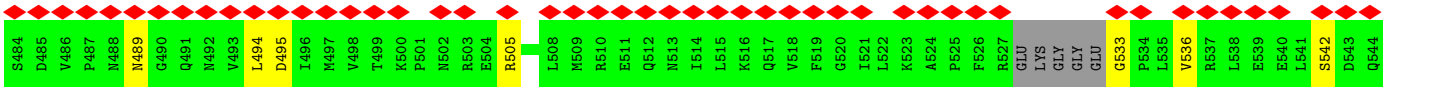


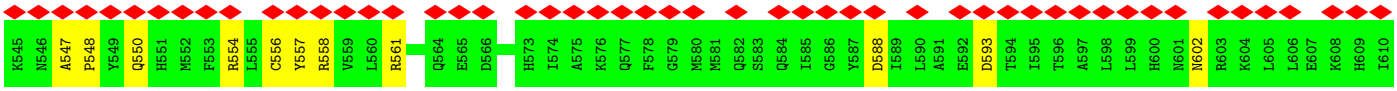


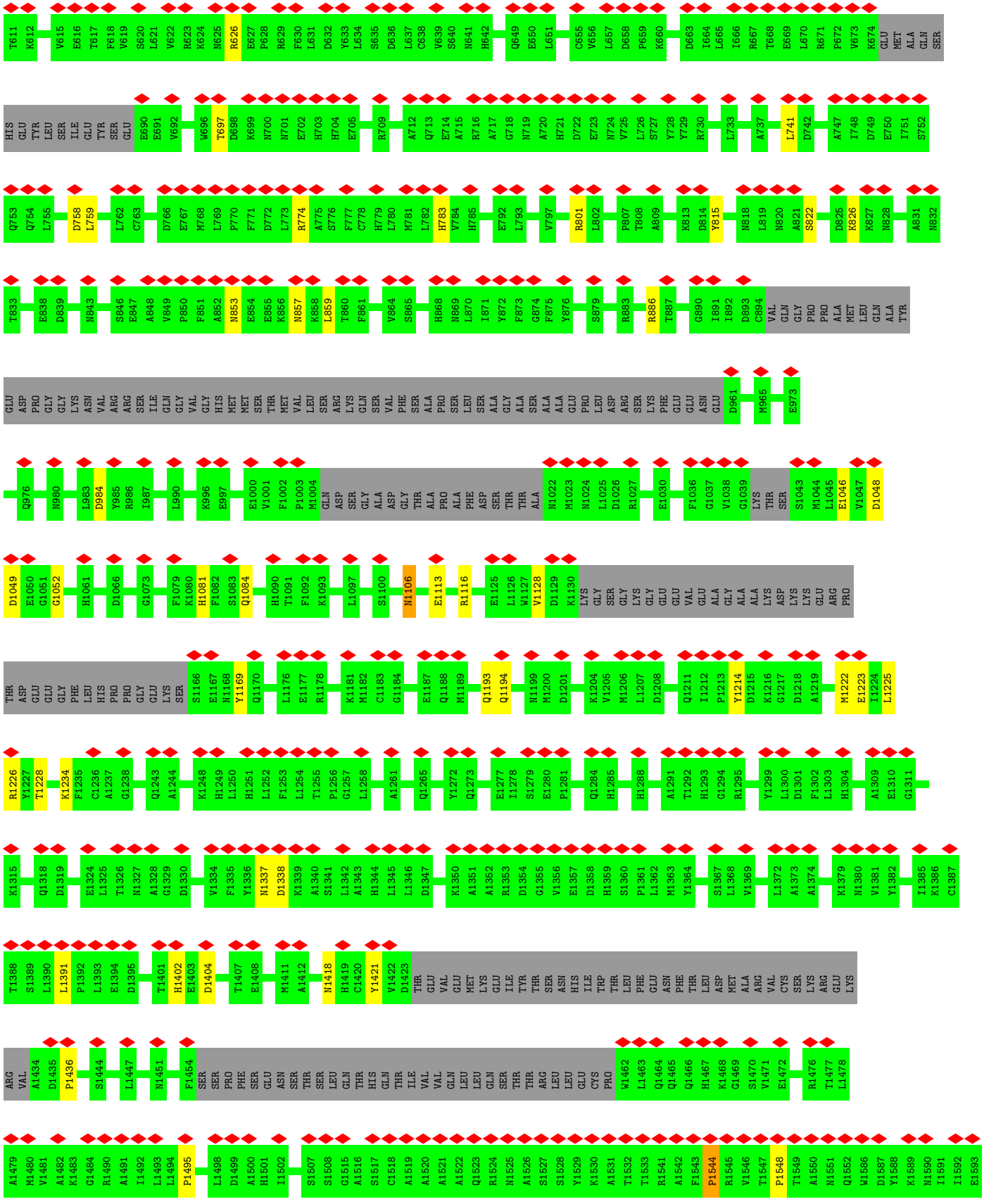








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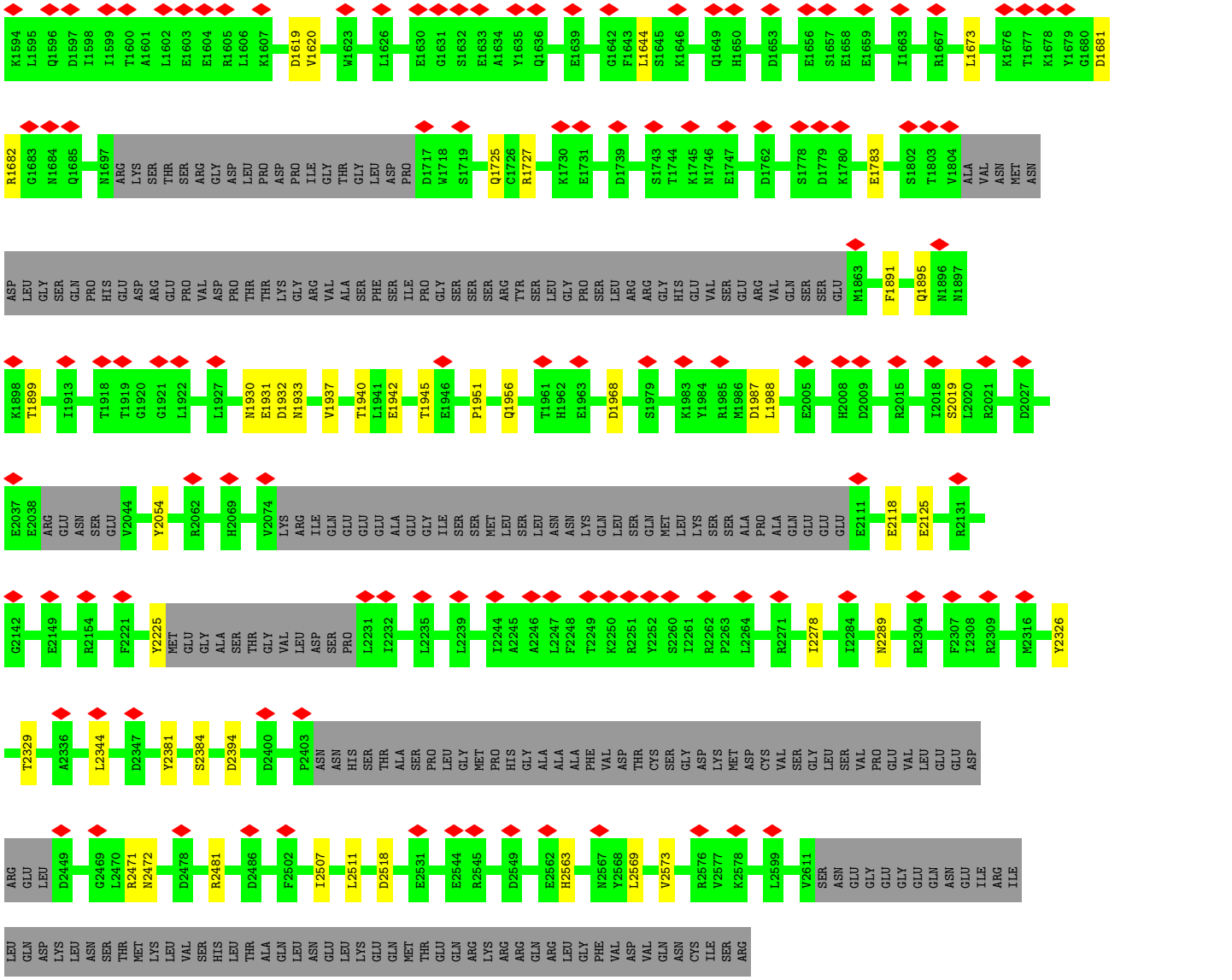
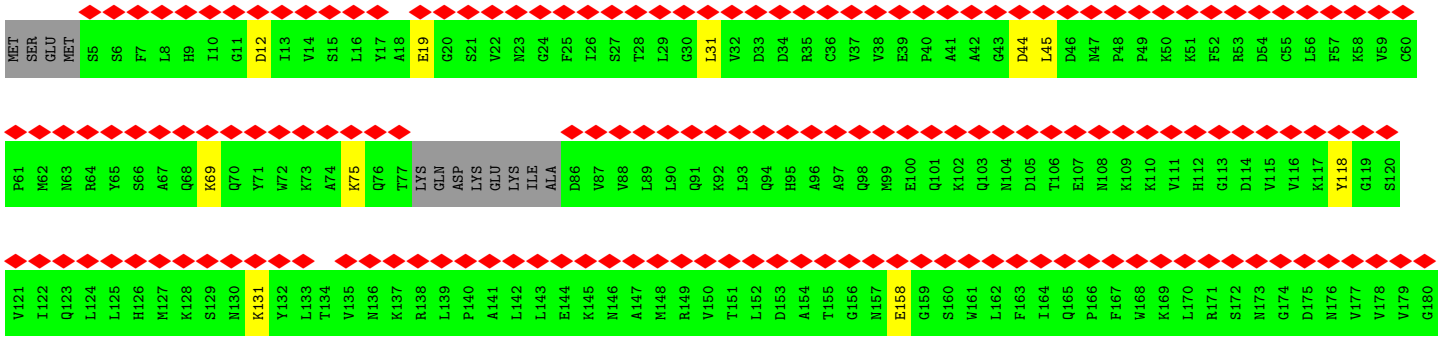
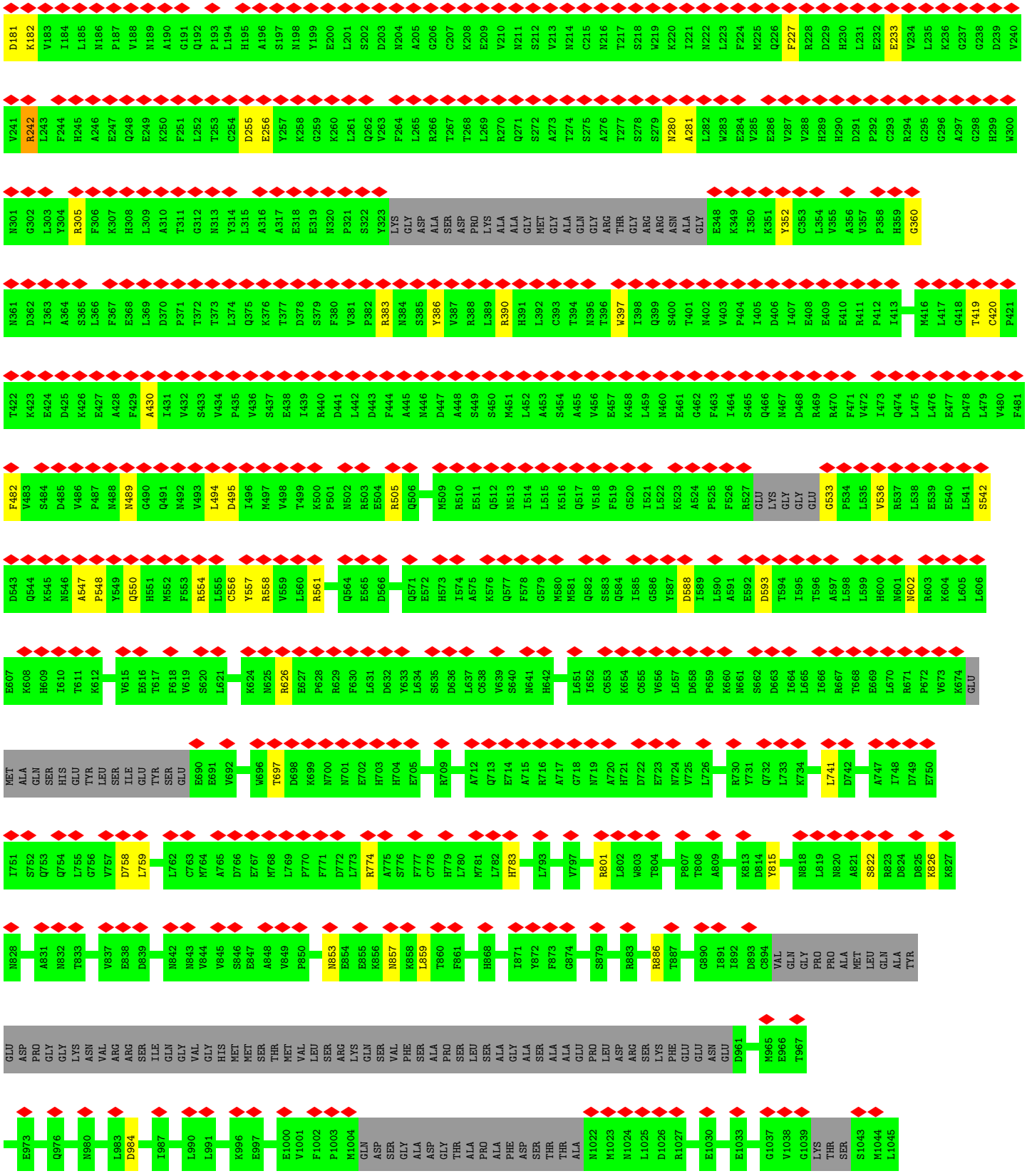
HIS GLU TYR LEU SER ILE GLU TYR SER GLU E690 E691 V692 W696 T697 D698 K699 N700 N701 E702 H703 H704 E705 R709 A712 Q713 E714 A715 R716 A717 G718 N719 A720 H721 D722 E723 N724 V725 L726 S727 Y728 Y729 R730 L733 A737 L741 D742 A747 T748 D749 E750 I751 S752
Q753 Q754 L755 D758 L759 L762 C763 D766 E767 M768 L769 P770 F771 D772 L773 R774 A775 S776 F777 C778 H779 L780 M781 L782 H783 V784 H785 E792 L793 V797 R801 L802 P807 T808 A809 K813 D814 Y815 N818 L819 N820 A821 S822 D825 K826 K827 N828 A831 N832
T833 E838 D839 N843 S846 E847 A848 V849 P850 F851 A852 N853 E854 E855 K856 N857 K858 L859 T860 F861 V864 S865 H868 N869 L870 I871 Y872 F873 G874 F875 Y876 S879 R883 R886 T887 G890 I891 I892 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR
GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 M965 E973
Q976 N980 L983 D984 Y985 R986 I987 L990 K996 E997 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 F1036 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045 E1046 V1047 D1048
D1049 E1050 G1051 G1052 H1061 D1066 G1073 F1079 K1080 H1081 F1082 S1083 Q1084 H1090 T1091 F1092 K1093 L1097 S1100 N1106 E1113 R1116 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 L1176 E1177 R1178 K1181 M1182 C1183 G1184 E1187 Q1188 M1189 Q1193 Q1194 N1199 M1200 D1201 K1204 V1205 M1206 L1207 D1208 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 M1222 E1223 I1224 L1225
R1226 Y1227 T1228 K1234 F1235 C1236 A1237 G1238 Q1243 A1244 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 A1261 Q1265 Y1272 Q1273 E1277 I1278 S1279 E1280 P1281 Q1284 H1285 H1288 A1291 T1292 H1293 G1294 R1295 Y1299 L1300 D1301 F1302 L1303 H1304 A1309 E1310 G1311
K1315 Q1318 D1319 E1324 L1325 T1326 N1327 A1328 G1329 D1330 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 S1360 P1361 L1362 M1363 Y1364 S1367 L1368 V1369 L1372 A1373 A1374 K1379 N1380 V1381 Y1382 I1385 K1386 C1387
T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 T1401 H1402 E1403 D1404 T1407 E1408 M1411 A1412 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 GLU ASN PHE THR LEU ASP MET ALA ARG VAL CYS SER LYS ARG GLU LYS
ARG VAL A1434 D1435 P1436 S1444 L1447 N1451 F1454 SER SER PRO PHE SER GLU ASN SER THR SER LEU GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO W1462 L1463 Q1464 Q1465 Q1466 H1467 K1468 G1469 S1470 V1471 E1472 R1476 T1477 L1478
A1479 M1480 V1481 A1482 K1483 G1484 R1490 A1491 I1492 L1493 L1494 P1495 L1498 D1499 A1500 H1501 I1502 S1507 S1508 G1515 A1516 S1517 C1518 A1519 A1520 A1521 A1522 Q1523 R1524 N1525 A1526 S1527 S1528 Y1529 K1530 A1531 T1532 T1533 R1541 A1542 F1543 P1544 R1545 V1546 T1547 P1548 T1549 A1550 N1551 Q1552 W1586 D1587 Y1588 K1589 N1590 I1591 I1592 E1593



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

Chain D:

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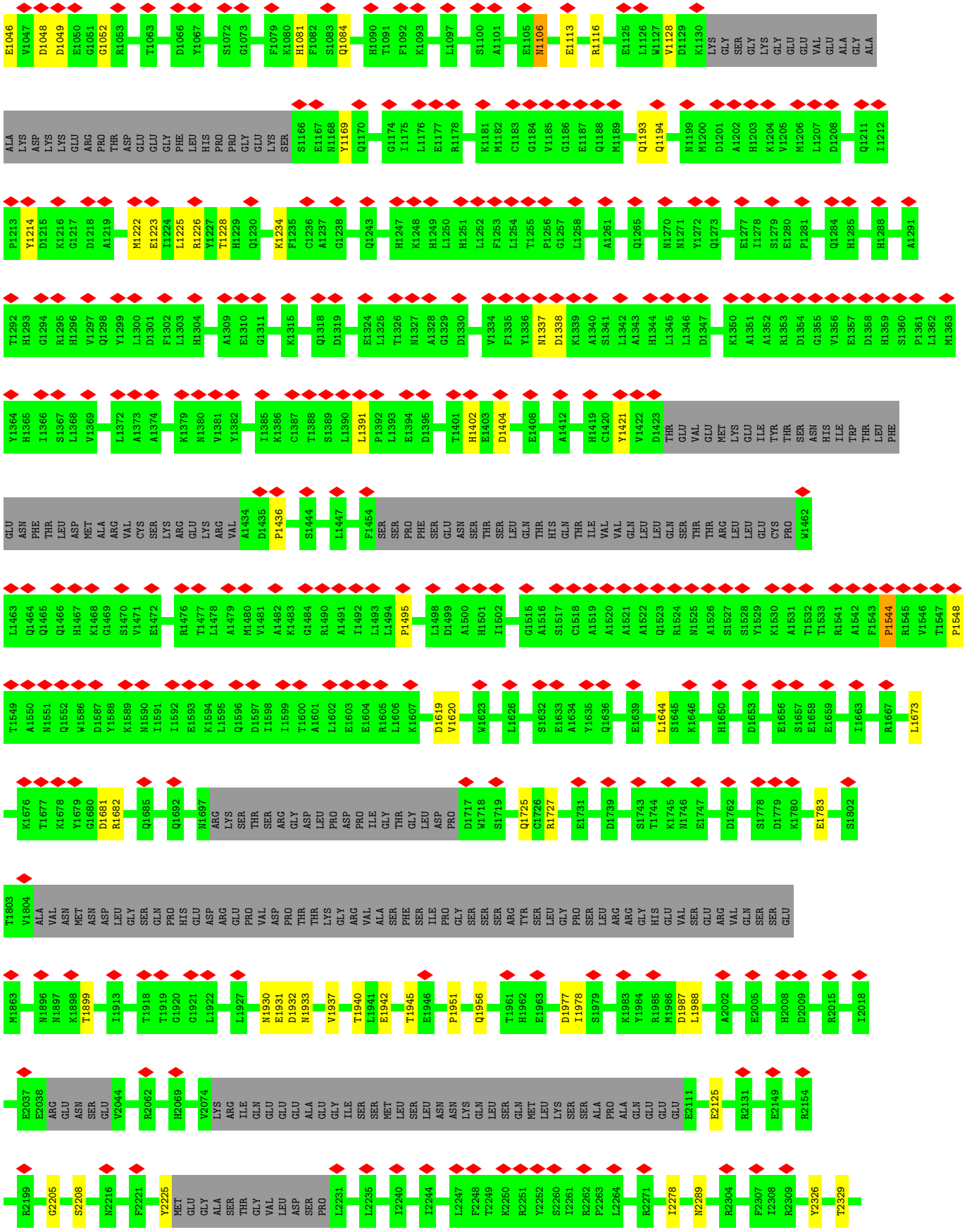
V241 R242 L243 F244 H245 A246 E247 Q248 E249 K250 F251 L252 T253 C254 D255 E256 Y257 K258 G259 K260 L261 Q262 V263 F264 L265 R266 T267 T268 L269 R270 Q271 S272 A273 T274 S275 A276 T277 S278 S279 N280 A281 L282 W283 E284 V285 E286 V287 V288 H289 H290 D291 P292 C293 R294 G295 G296 A297 G298 H299 W300
N301 G302 L303 Y304 R305 F306 K307 H308 L309 A310 T311 G312 N313 Y314 L315 A316 A317 E318 E319 N320 P321 S322 Y323 LYS GLY ASP ALA SER ASP PRO LYS ALA ALA GLY MET GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA GLY E348 K349 I350 K351 Y352 C353 L354 V355 A356 V357 P358 H359 G360
N361 D362 I363 A364 S365 L366 F367 E368 L369 D370 P371 T372 T373 L374 Q375 K376 T377 D378 S379 F380 V381 P382 R383 N384 S385 Y386 V387 R388 L389 R390 H391 L392 C393 T394 N395 T396 W397 I398 Q399 S400 T401 N402 V403 P404 I405 D406 I407 E408 E409 E410 R411 P412 I413 M416 L417 G418 T419 C420 P421
T422 K423 E424 D425 K426 E427 A428 F429 A430 I431 V432 S433 V434 P435 V436 S437 E438 I439 R440 D441 L442 D443 F444 A445 N446 D447 A448 S449 S450 M451 L452 A453 S454 A455 V456 E457 K458 L459 N460 E461 G462 F463 I464 S465 Q466 N467 D468 R469 R470 F471 V472 I473 Q474 L475 L476 E477 D478 L479 V480 F481
F482 V483 S484 D485 V486 P487 N488 N489 G490 Q491 N492 V493 L494 D495 I496 M497 V498 T499 K500 P501 N502 R503 E504 R505 Q506 M509 R510 E511 Q512 N513 I514 L515 K516 Q517 V518 F519 G520 I521 L522 K523 A524 P525 F526 R527 GLU LYS GLY GLU G533 P534 L535 V536 R537 L538 E539 E540 L541 S542
D543 Q544 K545 N546 A547 P548 Y549 Q550 H551 M552 F553 R554 L555 C556 Y557 R558 V559 L560 R561 Q564 E565 D566 Q571 E572 H573 I574 A575 K576 Q577 F578 G579 M580 M581 Q582 S583 Q584 I585 G586 Y587 D588 I589 L590 A591 E592 D593 T594 I595 T596 A597 L598 L599 H600 N601 N602 R603 K604 L605 L606
E607 K608 H609 I610 T611 K612 V615 E616 T617 F618 V619 S620 L621 K624 N625 R626 E627 P628 R629 F630 L631 D632 Y633 L634 S635 D636 L637 C638 V639 S640 M641 H642 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 W696 T697 D698 K699 N700 N701 E702 H703 H704 E705 R709 A712 Q713 E714 A715 R716 A717 G718 N719 A720 H721 D722 E723 N724 V725 L726 R730 Y731 Q732 L733 K734 L741 D742 A747 I748 D749 E750
I751 S752 Q753 Q754 L755 G756 V757 D758 L759 L762 C763 M764 A765 D766 E767 M768 L769 P770 F771 D772 L773 R774 A775 S776 F777 C778 H779 L780 M781 L782 H783 L793 V797 R801 L802 W803 T804 P807 T808 A809 K813 D814 Y815 N818 L819 N820 A821 S822 R823 D824 D825 K826 K827
N828 A831 N832 T833 V837 E838 D839 N842 N843 V844 V845 S846 E847 A848 V849 P850 N853 E854 E855 K856 N857 K858 L859 T860 F861 H868 I871 Y872 F873 G874 S879 R883 R886 T887 G890 I891 I892 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR
GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 M965 E966 T967
E973 Q976 N980 L983 D984 I987 L990 L991 K996 E997 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 E1033 G1037 V1038 G1039 LYS THR SER S1043 M1044 L1045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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 G1174 I1175 L1176 E1177 R1178 K1181 M1182 C1183 G1184 V1185 G1186 E1187 Q1188 M1189 Q1193 Q1194 N1199 M1200 D1201 A1202 H1203 K1204 V1205 M1206 L1207 D1208 Q1211 I1212
P1213 Y1214 D1215 K1216 G1217 D1218 A1219 M1222 E1223 I1224 L1225 R1226 Y1227 T1228 H1229 Q1230 K1234 F1235 C1236 A1237 G1238 Q1243 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 A1261 Q1265 N1270 N1271 Y1272 Q1273 E1277 I1278 S1279 E1280 P1281 Q1284 H1285 H1288 A1291
T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 A1309 E1310 G1311 K1315 Q1318 D1319 E1324 L1325 T1326 N1327 A1328 G1329 D1330 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 S1360 P1361 L1362 M1363
Y1364 H1365 I1366 S1367 L1368 V1369 L1372 A1373 A1374 K1379 N1380 V1381 Y1382 I1385 K1386 C1387 T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 T1401 H1402 E1403 D1404 E1408 A1412 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 S1444 L1447 F1454 SER SER PRO PHE SER GLU ASN SER THR SER LEU GLN THR HIS GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO W1462
L1463 Q1464 Q1465 Q1466 H1467 K1468 G1469 S1470 V1471 E1472 R1476 T1477 L1478 A1479 M1480 V1481 A1482 K1483 G1484 R1490 A1491 I1492 L1493 L1494 P1495 L1498 D1499 A1500 H1501 I1502 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
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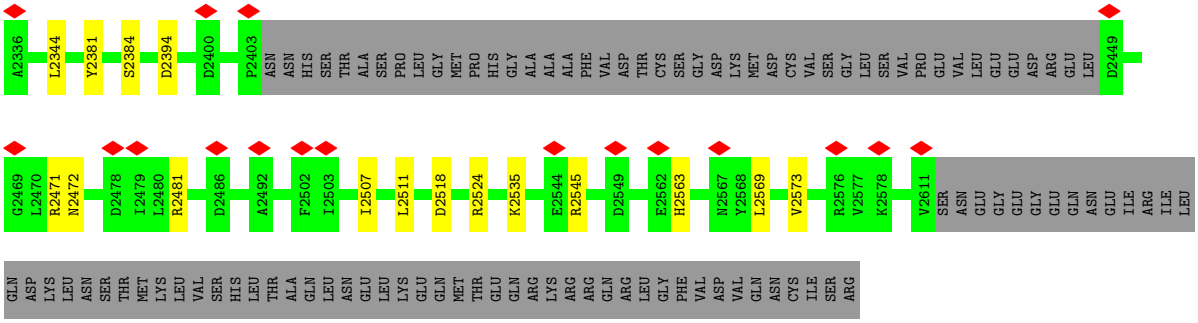
K1676 T1677 K1678 Y1679 G1680 D1681 R1682 Q1685 Q1692 N1697 ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO D1717 W1718 S1719 Q1725 C1726 R1727 E1731 D1739 S1743 T1744 K1745 N1746 E1747 D1762 S1778 D1779 K1780 E1783 S1802
T1803 V1804 ALA VAL ASN MET ASN ASP LEU GLY SER GLN PRO HIS GLU 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 N1896 N1897 K1898 T1899 I1913 T1918 T1919 G1920 G1921 L1922 L1927 N1930 E1931 D1932 N1933 V1937 T1940 L1941 E1942 T1945 E1946 P1951 Q1956 T1961 H1962 E1963 D1977 I1978 S1979 K1983 Y1984 R1985 M1986 D1987 L1988 A2002 E2005 H2008 D2009 R2015 I2018
E2037 E2038 ARG GLU ASN SER GLU V2044 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 E2125 R2131 E2149 R2154
R2199 G2205 S2208 N2216 F2221 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO L2231 L2235 I2240 I2244 L2247 F2248 T2249 K2250 R2251 Y2252 S2260 I2261 R2262 P2263 L2264 R2271 I2278 N2289 R2304 F2307 I2308 R2309 Y2326 T2329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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	33807	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	8.663	Depositor
Minimum map value	-5.040	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.407	Depositor
Recommended contour level	1.91	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: CA, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/17689	0.52	5/23903 (0.0%)
1	B	0.28	0/17689	0.52	5/23903 (0.0%)
1	C	0.28	0/17689	0.52	4/23903 (0.0%)
1	D	0.28	0/17689	0.52	5/23903 (0.0%)
All	All	0.28	0/70756	0.52	19/95612 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1544	PRO	N-CA-CB	5.67	110.10	103.30
1	A	1544	PRO	N-CA-CB	5.65	110.08	103.30
1	D	1544	PRO	N-CA-CB	5.65	110.08	103.30
1	C	1544	PRO	N-CA-CB	5.64	110.07	103.30
1	B	1495	PRO	N-CA-CB	5.61	110.03	103.30
1	A	1495	PRO	N-CA-CB	5.59	110.00	103.30
1	D	1548	PRO	N-CA-CB	5.57	109.99	103.30
1	C	1495	PRO	N-CA-CB	5.57	109.99	103.30
1	C	1548	PRO	N-CA-CB	5.57	109.98	103.30
1	D	1495	PRO	N-CA-CB	5.56	109.97	103.30
1	A	1548	PRO	N-CA-CB	5.54	109.95	103.30
1	B	1548	PRO	N-CA-CB	5.54	109.94	103.30
1	B	1436	PRO	N-CA-CB	5.45	109.84	103.30
1	D	1436	PRO	N-CA-CB	5.44	109.83	103.30
1	A	1436	PRO	N-CA-CB	5.43	109.82	103.30
1	C	1436	PRO	N-CA-CB	5.41	109.79	103.30
1	B	242	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	242	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	242	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17382	17386	17215	68	0
1	B	17382	17386	17215	68	0
1	C	17382	17386	17215	72	0
1	D	17382	17386	17215	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	69540	69544	68860	275	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.

All (275) 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:2524:ARG:NE	1:D:2518:ASP:OD2	2.13	0.82
1:A:561:ARG:NH1	1:A:593:ASP:O	2.21	0.74
1:C:561:ARG:NH1	1:C:593:ASP:O	2.21	0.73
1:B:561:ARG:NH1	1:B:593:ASP:O	2.21	0.73
1:D:561:ARG:NH1	1:D:593:ASP:O	2.21	0.73
1:A:1783:GLU:OE2	1:A:1899:THR:OG1	2.09	0.71
1:D:1783:GLU:OE2	1:D:1899:THR:OG1	2.09	0.70
1:B:1783:GLU:OE2	1:B:1899:THR:OG1	2.09	0.70
1:C:1783:GLU:OE2	1:C:1899:THR:OG1	2.09	0.69
1:A:1942:GLU:O	1:A:1945:THR:OG1	2.12	0.68
1:D:1942:GLU:O	1:D:1945:THR:OG1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1942:GLU:O	1:C:1945:THR:OG1	2.12	0.67
1:A:1391:LEU:O	1:A:1421:TYR:OH	2.13	0.67
1:C:1391:LEU:O	1:C:1421:TYR:OH	2.13	0.66
1:D:1391:LEU:O	1:D:1421:TYR:OH	2.13	0.66
1:A:550:GLN:OE1	1:A:554:ARG:NE	2.29	0.66
1:C:550:GLN:OE1	1:C:554:ARG:NE	2.29	0.66
1:D:550:GLN:OE1	1:D:554:ARG:NE	2.29	0.65
1:B:550:GLN:OE1	1:B:554:ARG:NE	2.29	0.65
1:B:1391:LEU:O	1:B:1421:TYR:OH	2.13	0.65
1:A:815:TYR:OH	1:A:984:ASP:OD2	2.15	0.65
1:D:815:TYR:OH	1:D:984:ASP:OD2	2.15	0.65
1:C:352:TYR:O	1:C:419:THR:OG1	2.13	0.64
1:A:31:LEU:O	1:A:131:LYS:NZ	2.25	0.64
1:B:1942:GLU:O	1:B:1945:THR:OG1	2.12	0.64
1:D:886:ARG:NE	1:D:1049:ASP:OD1	2.31	0.64
1:B:815:TYR:OH	1:B:984:ASP:OD2	2.15	0.64
1:A:886:ARG:NE	1:A:1049:ASP:OD1	2.31	0.63
1:C:815:TYR:OH	1:C:984:ASP:OD2	2.15	0.63
1:A:305:ARG:NH1	1:A:360:GLY:O	2.32	0.63
1:B:886:ARG:NE	1:B:1049:ASP:OD1	2.31	0.63
1:C:886:ARG:NE	1:C:1049:ASP:OD1	2.31	0.62
1:D:305:ARG:NH1	1:D:360:GLY:O	2.32	0.62
1:C:305:ARG:NH1	1:C:360:GLY:O	2.32	0.62
1:A:1951:PRO:O	1:A:1956:GLN:NE2	2.33	0.62
1:C:1951:PRO:O	1:C:1956:GLN:NE2	2.33	0.61
1:D:1951:PRO:O	1:D:1956:GLN:NE2	2.33	0.61
1:B:12:ASP:OD1	1:B:227:PHE:N	2.34	0.61
1:B:305:ARG:NH1	1:B:360:GLY:O	2.32	0.61
1:C:12:ASP:OD1	1:C:227:PHE:N	2.34	0.61
1:B:31:LEU:O	1:B:131:LYS:NZ	2.25	0.61
1:D:12:ASP:OD1	1:D:227:PHE:N	2.34	0.61
1:B:1951:PRO:O	1:B:1956:GLN:NE2	2.33	0.61
1:C:31:LEU:O	1:C:131:LYS:NZ	2.25	0.61
1:A:12:ASP:OD1	1:A:227:PHE:N	2.34	0.60
1:D:1194:GLN:NE2	1:D:1234:LYS:O	2.34	0.60
1:D:233:GLU:OE1	1:D:383:ARG:NH2	2.36	0.59
1:B:1194:GLN:NE2	1:B:1234:LYS:O	2.34	0.59
1:A:1194:GLN:NE2	1:A:1234:LYS:O	2.34	0.59
1:C:1194:GLN:NE2	1:C:1234:LYS:O	2.34	0.59
1:C:233:GLU:OE1	1:C:383:ARG:NH2	2.36	0.58
1:B:1106:ASN:OD1	1:B:1193:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:O	1:D:131:LYS:NZ	2.25	0.58
1:D:1106:ASN:OD1	1:D:1193:GLN:NE2	2.37	0.58
1:A:1106:ASN:OD1	1:A:1193:GLN:NE2	2.37	0.58
1:B:1113:GLU:OE1	1:B:1116:ARG:NH2	2.37	0.58
1:A:233:GLU:OE1	1:A:383:ARG:NH2	2.36	0.58
1:D:1113:GLU:OE1	1:D:1116:ARG:NH2	2.37	0.57
1:C:1113:GLU:OE1	1:C:1116:ARG:NH2	2.37	0.57
1:B:233:GLU:OE1	1:B:383:ARG:NH2	2.36	0.57
1:D:2381:TYR:O	1:D:2384:SER:OG	2.21	0.57
1:C:1106:ASN:OD1	1:C:1193:GLN:NE2	2.37	0.57
1:A:482:PHE:O	1:A:505:ARG:NH1	2.38	0.57
1:A:1113:GLU:OE1	1:A:1116:ARG:NH2	2.37	0.57
1:B:482:PHE:O	1:B:505:ARG:NH1	2.38	0.56
1:C:482:PHE:O	1:C:505:ARG:NH1	2.38	0.56
1:D:482:PHE:O	1:D:505:ARG:NH1	2.38	0.56
1:A:2381:TYR:O	1:A:2384:SER:OG	2.21	0.56
1:B:2225:TYR:OH	1:B:2278:ILE:HG21	2.06	0.55
1:C:2381:TYR:O	1:C:2384:SER:OG	2.21	0.55
1:B:2381:TYR:O	1:B:2384:SER:OG	2.21	0.55
1:C:2394:ASP:OD1	1:C:2481:ARG:NH2	2.40	0.55
1:A:2394:ASP:OD1	1:A:2481:ARG:NH2	2.40	0.55
1:A:2225:TYR:OH	1:A:2278:ILE:HG21	2.06	0.55
1:D:2394:ASP:OD1	1:D:2481:ARG:NH2	2.40	0.55
1:C:2225:TYR:OH	1:C:2278:ILE:HG21	2.07	0.55
1:D:2225:TYR:OH	1:D:2278:ILE:HG21	2.06	0.55
1:B:494:LEU:O	1:B:558:ARG:NE	2.40	0.54
1:C:494:LEU:O	1:C:558:ARG:NE	2.40	0.54
1:B:2394:ASP:OD1	1:B:2481:ARG:NH2	2.40	0.54
1:A:774:ARG:HE	1:A:859:LEU:HD13	1.73	0.54
1:A:494:LEU:O	1:A:558:ARG:NE	2.40	0.54
1:D:774:ARG:HE	1:D:859:LEU:HD13	1.73	0.54
1:B:1937:VAL:O	1:B:1940:THR:OG1	2.23	0.54
1:D:494:LEU:O	1:D:558:ARG:NE	2.40	0.54
1:C:774:ARG:HE	1:C:859:LEU:HD13	1.73	0.53
1:B:352:TYR:O	1:B:419:THR:OG1	2.13	0.53
1:D:19:GLU:OE1	1:D:182:LYS:NZ	2.37	0.53
1:D:352:TYR:O	1:D:419:THR:OG1	2.13	0.53
1:A:1046:GLU:OE2	1:A:1052:GLY:N	2.42	0.53
1:B:774:ARG:HE	1:B:859:LEU:HD13	1.73	0.53
1:D:1046:GLU:OE2	1:D:1052:GLY:N	2.42	0.53
1:A:1937:VAL:O	1:A:1940:THR:OG1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ARG:NH2	1:B:697:THR:O	2.42	0.53
1:B:1214:TYR:OH	1:B:1222:MET:SD	2.66	0.53
1:C:626:ARG:NH2	1:C:697:THR:O	2.42	0.53
1:C:1046:GLU:OE2	1:C:1052:GLY:N	2.42	0.53
1:A:1214:TYR:OH	1:A:1222:MET:SD	2.66	0.52
1:B:1046:GLU:OE2	1:B:1052:GLY:N	2.42	0.52
1:A:118:TYR:OH	1:A:181:ASP:OD2	2.28	0.52
1:C:822:SER:O	1:C:826:LYS:NZ	2.43	0.52
1:D:822:SER:O	1:D:826:LYS:NZ	2.43	0.52
1:C:118:TYR:OH	1:C:181:ASP:OD2	2.28	0.52
1:D:2125:GLU:OE1	1:D:2563:HIS:NE2	2.43	0.52
1:A:626:ARG:NH2	1:A:697:THR:O	2.42	0.52
1:B:822:SER:O	1:B:826:LYS:NZ	2.43	0.52
1:D:495:ASP:OD1	1:D:558:ARG:NH2	2.43	0.52
1:A:822:SER:O	1:A:826:LYS:NZ	2.43	0.52
1:B:118:TYR:OH	1:B:181:ASP:OD2	2.28	0.52
1:A:19:GLU:OE1	1:A:182:LYS:NZ	2.37	0.52
1:D:626:ARG:NH2	1:D:697:THR:O	2.42	0.52
1:C:495:ASP:OD1	1:C:558:ARG:NH2	2.43	0.51
1:C:2125:GLU:OE1	1:C:2563:HIS:NE2	2.43	0.51
1:D:118:TYR:OH	1:D:181:ASP:OD2	2.28	0.51
1:A:495:ASP:OD1	1:A:558:ARG:NH2	2.43	0.51
1:C:1214:TYR:OH	1:C:1222:MET:SD	2.66	0.51
1:B:495:ASP:OD1	1:B:558:ARG:NH2	2.43	0.51
1:C:1937:VAL:O	1:C:1940:THR:OG1	2.23	0.50
1:B:19:GLU:OE1	1:B:182:LYS:NZ	2.37	0.50
1:D:1214:TYR:OH	1:D:1222:MET:SD	2.66	0.50
1:D:547:ALA:HB3	1:D:548:PRO:HD3	1.94	0.50
1:B:2125:GLU:OE1	1:B:2563:HIS:NE2	2.43	0.50
1:A:547:ALA:HB3	1:A:548:PRO:HD3	1.94	0.49
1:A:1619:ASP:OD1	1:A:1620:VAL:N	2.46	0.49
1:B:1225:LEU:O	1:B:1228:THR:OG1	2.27	0.49
1:B:547:ALA:HB3	1:B:548:PRO:HD3	1.94	0.49
1:B:1619:ASP:OD1	1:B:1620:VAL:N	2.46	0.49
1:D:242:ARG:NE	1:D:281:ALA:O	2.45	0.49
1:A:2125:GLU:OE1	1:A:2563:HIS:NE2	2.43	0.49
1:B:386:TYR:CE1	1:B:430:ALA:HB2	2.48	0.49
1:D:1937:VAL:O	1:D:1940:THR:OG1	2.23	0.49
1:A:242:ARG:NE	1:A:281:ALA:O	2.45	0.49
1:B:2507:ILE:O	1:B:2511:LEU:N	2.43	0.49
1:A:451:MET:O	1:A:454:SER:OG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ARG:NE	1:B:281:ALA:O	2.45	0.49
1:C:1619:ASP:OD1	1:C:1620:VAL:N	2.46	0.49
1:C:19:GLU:OE1	1:C:182:LYS:NZ	2.37	0.49
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.46	0.48
1:C:242:ARG:NE	1:C:281:ALA:O	2.45	0.48
1:D:1619:ASP:OD1	1:D:1620:VAL:N	2.46	0.48
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.46	0.48
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.46	0.48
1:A:386:TYR:CE1	1:A:430:ALA:HB2	2.48	0.48
1:C:386:TYR:CE1	1:C:430:ALA:HB2	2.48	0.48
1:C:542:SER:OG	1:C:588:ASP:OD2	2.32	0.48
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.46	0.48
1:A:542:SER:OG	1:A:588:ASP:OD2	2.32	0.48
1:B:542:SER:OG	1:B:588:ASP:OD2	2.32	0.48
1:C:547:ALA:HB3	1:C:548:PRO:HD3	1.94	0.48
1:D:75:LYS:NZ	1:D:489:ASN:O	2.47	0.47
1:D:386:TYR:CE1	1:D:430:ALA:HB2	2.48	0.47
1:C:75:LYS:NZ	1:C:489:ASN:O	2.47	0.47
1:C:1225:LEU:O	1:C:1228:THR:OG1	2.27	0.47
1:A:75:LYS:NZ	1:A:489:ASN:O	2.47	0.47
1:A:1644:LEU:HD22	1:A:1727:ARG:NH2	2.30	0.47
1:D:1644:LEU:HD22	1:D:1727:ARG:NH2	2.30	0.47
1:B:2326:TYR:O	1:B:2329:THR:OG1	2.30	0.47
1:C:1644:LEU:HD22	1:C:1727:ARG:NH2	2.30	0.47
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.48	0.47
1:D:542:SER:OG	1:D:588:ASP:OD2	2.32	0.47
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.48	0.46
1:B:1644:LEU:HD22	1:B:1727:ARG:NH2	2.30	0.46
1:A:1225:LEU:O	1:A:1228:THR:OG1	2.27	0.46
1:B:75:LYS:NZ	1:B:489:ASN:O	2.47	0.46
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.48	0.46
1:D:1081:HIS:O	1:D:1084:GLN:NE2	2.49	0.46
1:B:1081:HIS:O	1:B:1084:GLN:NE2	2.49	0.46
1:A:1081:HIS:O	1:A:1084:GLN:NE2	2.49	0.46
1:C:533:GLY:N	1:C:536:VAL:O	2.49	0.46
1:D:533:GLY:N	1:D:536:VAL:O	2.49	0.46
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.48	0.46
1:A:533:GLY:N	1:A:536:VAL:O	2.49	0.45
1:B:533:GLY:N	1:B:536:VAL:O	2.49	0.45
1:D:1225:LEU:O	1:D:1228:THR:OG1	2.27	0.45
1:C:1081:HIS:O	1:C:1084:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2507:ILE:O	1:D:2511:LEU:N	2.43	0.45
1:A:2507:ILE:O	1:A:2511:LEU:N	2.43	0.45
1:A:2535:LYS:O	1:A:2545:ARG:NH2	2.48	0.45
1:A:758:ASP:OD1	1:A:759:LEU:N	2.50	0.45
1:D:758:ASP:OD1	1:D:759:LEU:N	2.50	0.45
1:B:758:ASP:OD1	1:B:759:LEU:N	2.50	0.45
1:D:44:ASP:OD1	1:D:45:LEU:N	2.50	0.45
1:A:741:LEU:O	1:A:783:HIS:ND1	2.48	0.44
1:C:2326:TYR:O	1:C:2329:THR:OG1	2.30	0.44
1:D:2326:TYR:O	1:D:2329:THR:OG1	2.30	0.44
1:B:255:ASP:OD1	1:B:256:GLU:N	2.51	0.44
1:C:44:ASP:OD1	1:C:45:LEU:N	2.50	0.44
1:A:1337:ASN:OD1	1:A:1338:ASP:N	2.51	0.44
1:C:255:ASP:OD1	1:C:256:GLU:N	2.51	0.44
1:D:255:ASP:OD1	1:D:256:GLU:N	2.51	0.44
1:A:2220:ALA:HB2	1:D:2381:TYR:HE1	1.81	0.44
1:C:758:ASP:OD1	1:C:759:LEU:N	2.50	0.44
1:C:2518:ASP:OD2	1:D:2524:ARG:NE	2.40	0.44
1:A:255:ASP:OD1	1:A:256:GLU:N	2.51	0.43
1:B:1337:ASN:OD1	1:B:1338:ASP:N	2.51	0.43
1:C:1337:ASN:OD1	1:C:1338:ASP:N	2.51	0.43
1:D:1337:ASN:OD1	1:D:1338:ASP:N	2.51	0.43
1:B:44:ASP:OD1	1:B:45:LEU:N	2.50	0.43
1:C:741:LEU:O	1:C:783:HIS:ND1	2.48	0.43
1:B:308:HIS:HD1	1:B:311:THR:HG1	1.64	0.43
1:D:2205:GLY:O	1:D:2208:SER:OG	2.30	0.43
1:A:2220:ALA:HB2	1:D:2381:TYR:CE1	2.54	0.43
1:C:2507:ILE:O	1:C:2511:LEU:N	2.43	0.43
1:B:308:HIS:ND1	1:B:311:THR:OG1	2.47	0.43
1:B:2569:LEU:O	1:B:2573:VAL:HG23	2.19	0.43
1:A:44:ASP:OD1	1:A:45:LEU:N	2.50	0.43
1:A:2569:LEU:O	1:A:2573:VAL:HG23	2.19	0.43
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.52	0.43
1:C:2569:LEU:O	1:C:2573:VAL:HG23	2.19	0.43
1:A:308:HIS:ND1	1:A:311:THR:OG1	2.47	0.42
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.52	0.42
1:D:69:LYS:NZ	1:D:158:GLU:OE1	2.51	0.42
1:D:1930:ASN:OD1	1:D:1931:GLU:N	2.51	0.42
1:C:1968:ASP:OD1	1:C:2019:SER:OG	2.25	0.42
1:A:69:LYS:NZ	1:A:158:GLU:OE1	2.51	0.42
1:B:1681:ASP:OD1	1:B:1682:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1681:ASP:OD1	1:D:1682:ARG:N	2.53	0.42
1:A:1681:ASP:OD1	1:A:1682:ARG:N	2.53	0.42
1:C:1681:ASP:OD1	1:C:1682:ARG:N	2.53	0.42
1:D:2569:LEU:O	1:D:2573:VAL:HG23	2.19	0.42
1:D:853:ASN:O	1:D:857:ASN:ND2	2.52	0.42
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.52	0.42
1:B:741:LEU:O	1:B:783:HIS:ND1	2.48	0.42
1:B:1364:TYR:O	1:B:1367:SER:OG	2.31	0.42
1:A:1048:ASP:OD1	1:A:1049:ASP:N	2.52	0.42
1:A:2326:TYR:O	1:A:2329:THR:OG1	2.30	0.42
1:C:308:HIS:ND1	1:C:311:THR:OG1	2.47	0.42
1:C:1930:ASN:OD1	1:C:1931:GLU:N	2.51	0.42
1:C:2054:TYR:OH	1:C:2118:GLU:OE1	2.38	0.42
1:D:741:LEU:O	1:D:783:HIS:ND1	2.48	0.42
1:B:853:ASN:O	1:B:857:ASN:ND2	2.52	0.42
1:B:2326:TYR:CZ	1:B:2344:LEU:HD22	2.55	0.42
1:C:853:ASN:O	1:C:857:ASN:ND2	2.52	0.42
1:C:2326:TYR:CZ	1:C:2344:LEU:HD22	2.55	0.42
1:D:2326:TYR:CZ	1:D:2344:LEU:HD22	2.55	0.42
1:B:2535:LYS:O	1:B:2545:ARG:NH2	2.48	0.41
1:C:1223:GLU:OE1	1:C:1226:ARG:NH2	2.54	0.41
1:C:1402:HIS:NE2	1:C:1404:ASP:OD2	2.53	0.41
1:C:1128:VAL:O	1:C:1169:TYR:OH	2.38	0.41
1:D:556:CYS:SG	1:D:557:TYR:N	2.94	0.41
1:D:1128:VAL:O	1:D:1169:TYR:OH	2.38	0.41
1:A:1673:LEU:HD22	1:A:1725:GLN:HG3	2.03	0.41
1:B:1340:ALA:O	1:B:1344:HIS:ND1	2.53	0.41
1:C:69:LYS:NZ	1:C:158:GLU:OE1	2.51	0.41
1:D:1402:HIS:NE2	1:D:1404:ASP:OD2	2.53	0.41
1:D:1987:ASP:OD1	1:D:1988:LEU:N	2.54	0.41
1:D:2535:LYS:O	1:D:2545:ARG:NH2	2.48	0.41
1:A:853:ASN:O	1:A:857:ASN:ND2	2.52	0.41
1:A:1128:VAL:O	1:A:1169:TYR:OH	2.38	0.41
1:A:2326:TYR:CZ	1:A:2344:LEU:HD22	2.55	0.41
1:B:1128:VAL:O	1:B:1169:TYR:OH	2.38	0.41
1:B:1223:GLU:OE1	1:B:1226:ARG:NH2	2.54	0.41
1:B:1673:LEU:HD22	1:B:1725:GLN:HG3	2.02	0.41
1:B:2054:TYR:OH	1:B:2118:GLU:OE1	2.38	0.41
1:C:394:THR:OG1	1:C:396:THR:OG1	2.18	0.41
1:B:1987:ASP:OD1	1:B:1988:LEU:N	2.54	0.41
1:C:451:MET:O	1:C:454:SER:OG	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1977:ASP:OD1	1:D:1978:ILE:N	2.54	0.41
1:A:1987:ASP:OD1	1:A:1988:LEU:N	2.54	0.41
1:A:556:CYS:SG	1:A:557:TYR:N	2.94	0.41
1:A:1223:GLU:OE1	1:A:1226:ARG:NH2	2.54	0.41
1:D:1673:LEU:HD22	1:D:1725:GLN:HG3	2.03	0.41
1:A:1402:HIS:NE2	1:A:1404:ASP:OD2	2.53	0.41
1:B:1402:HIS:NE2	1:B:1404:ASP:OD2	2.53	0.41
1:B:1977:ASP:OD1	1:B:1978:ILE:N	2.54	0.41
1:C:1673:LEU:HD22	1:C:1725:GLN:HG3	2.03	0.41
1:B:556:CYS:SG	1:B:557:TYR:N	2.94	0.41
1:C:556:CYS:SG	1:C:557:TYR:N	2.94	0.41
1:C:1987:ASP:OD1	1:C:1988:LEU:N	2.54	0.40
1:D:1223:GLU:OE1	1:D:1226:ARG:NH2	2.53	0.40
1:A:1364:TYR:O	1:A:1367:SER:OG	2.31	0.40
1:C:397:TRP:O	1:C:420:CYS:N	2.54	0.40
1:C:254:CYS:O	1:C:280:ASN:ND2	2.46	0.40
1:C:1891:PHE:O	1:C:1895:GLN:NE2	2.55	0.40
1:D:397:TRP:O	1:D:420:CYS:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2147/2671 (80%)	2055 (96%)	91 (4%)	1 (0%)	100	100
1	B	2147/2671 (80%)	2054 (96%)	92 (4%)	1 (0%)	100	100
1	C	2147/2671 (80%)	2055 (96%)	91 (4%)	1 (0%)	100	100
1	D	2147/2671 (80%)	2053 (96%)	93 (4%)	1 (0%)	100	100
All	All	8588/10684 (80%)	8217 (96%)	367 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1544	PRO
1	B	1544	PRO
1	C	1544	PRO
1	D	1544	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1883/2385 (79%)	1876 (100%)	7 (0%)	91	94
1	B	1883/2385 (79%)	1876 (100%)	7 (0%)	91	94
1	C	1883/2385 (79%)	1875 (100%)	8 (0%)	91	94
1	D	1883/2385 (79%)	1876 (100%)	7 (0%)	91	94
All	All	7532/9540 (79%)	7503 (100%)	29 (0%)	91	94

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
1	A	390	ARG
1	A	602	ASN
1	A	1106	ASN
1	A	2289	ASN
1	A	2471	ARG
1	A	2472	ASN
1	B	280	ASN
1	B	390	ARG
1	B	602	ASN
1	B	1106	ASN
1	B	2289	ASN
1	B	2471	ARG
1	B	2472	ASN
1	C	280	ASN
1	C	390	ARG
1	C	602	ASN
1	C	1106	ASN

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Mol	Chain	Res	Type
1	C	1418	ASN
1	C	2289	ASN
1	C	2471	ARG
1	C	2472	ASN
1	D	280	ASN
1	D	390	ARG
1	D	602	ASN
1	D	1106	ASN
1	D	2289	ASN
1	D	2471	ARG
1	D	2472	ASN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
1	B	5
1	C	5
1	D	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1552:GLN	C	1586:TRP	N	55.70
1	B	1552:GLN	C	1586:TRP	N	55.70
1	C	1552:GLN	C	1586:TRP	N	55.70
1	D	1552:GLN	C	1586:TRP	N	55.70
1	A	1533:THR	C	1541:ARG	N	15.48
1	B	1533:THR	C	1541:ARG	N	15.48
1	C	1533:THR	C	1541:ARG	N	15.48
1	D	1533:THR	C	1541:ARG	N	15.48
1	A	1484:GLY	C	1490:ARG	N	11.29
1	B	1484:GLY	C	1490:ARG	N	11.29
1	C	1484:GLY	C	1490:ARG	N	11.29
1	D	1484:GLY	C	1490:ARG	N	11.29
1	A	1508:SER	C	1515:GLY	N	10.86
1	B	1508:SER	C	1515:GLY	N	10.86
1	C	1508:SER	C	1515:GLY	N	10.86
1	D	1508:SER	C	1515:GLY	N	10.86
1	A	2252:TYR	C	2260:SER	N	6.44
1	B	2252:TYR	C	2260:SER	N	6.44
1	C	2252:TYR	C	2260:SER	N	6.44
1	D	2252:TYR	C	2260:SER	N	6.44

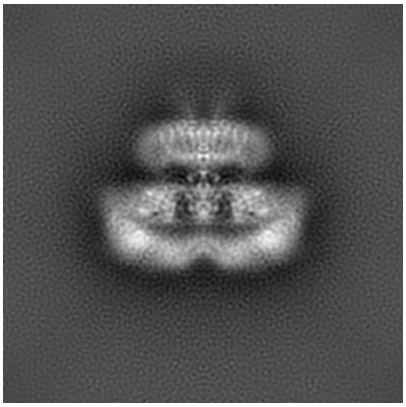
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7988. These allow visual inspection of the internal detail of the map and identification of artifacts.

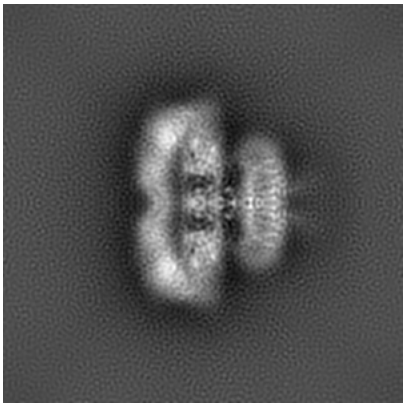
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

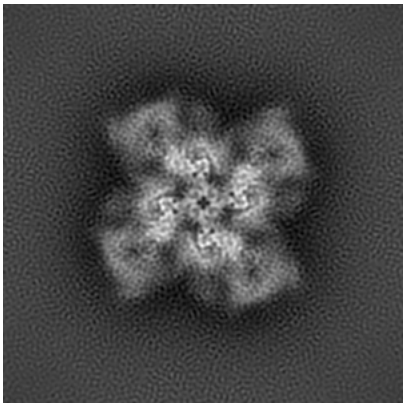
6.1.1 Primary map



X



Y

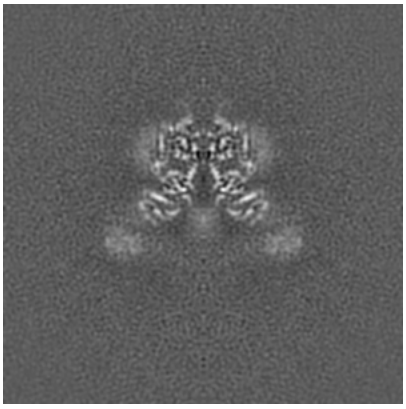


Z

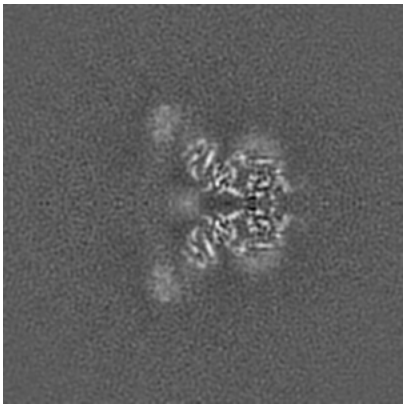
The images above show the map projected in three orthogonal directions.

6.2 Central slices

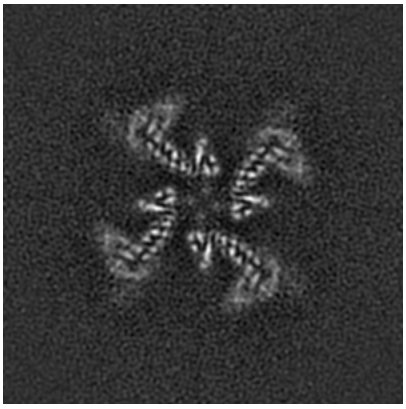
6.2.1 Primary map



X Index: 192



Y Index: 192

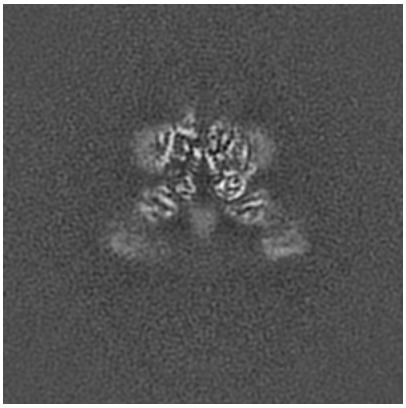


Z Index: 192

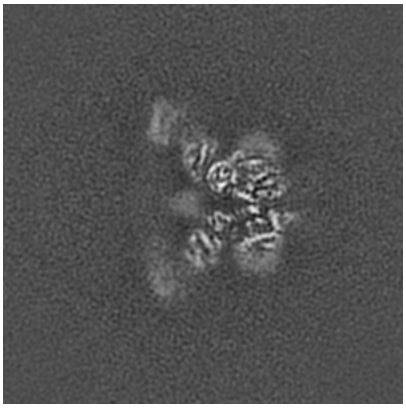
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

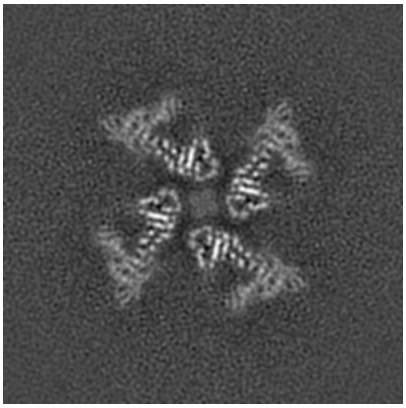
6.3.1 Primary map



X Index: 189



Y Index: 195



Z Index: 187

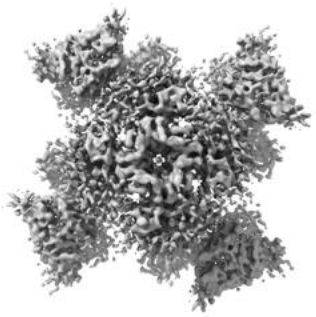
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.91. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

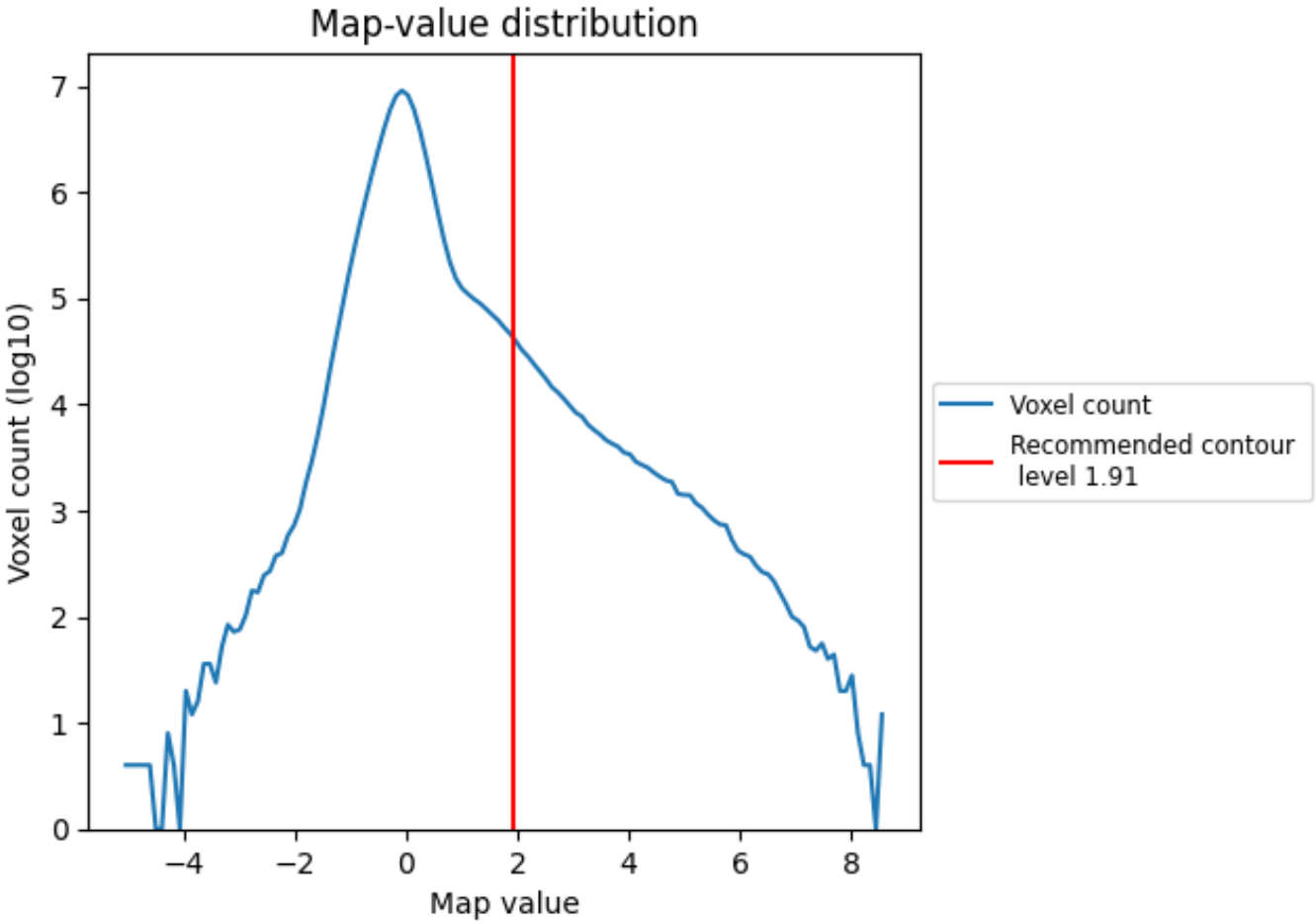
6.5 Mask visualisation (i)

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

7 Map analysis

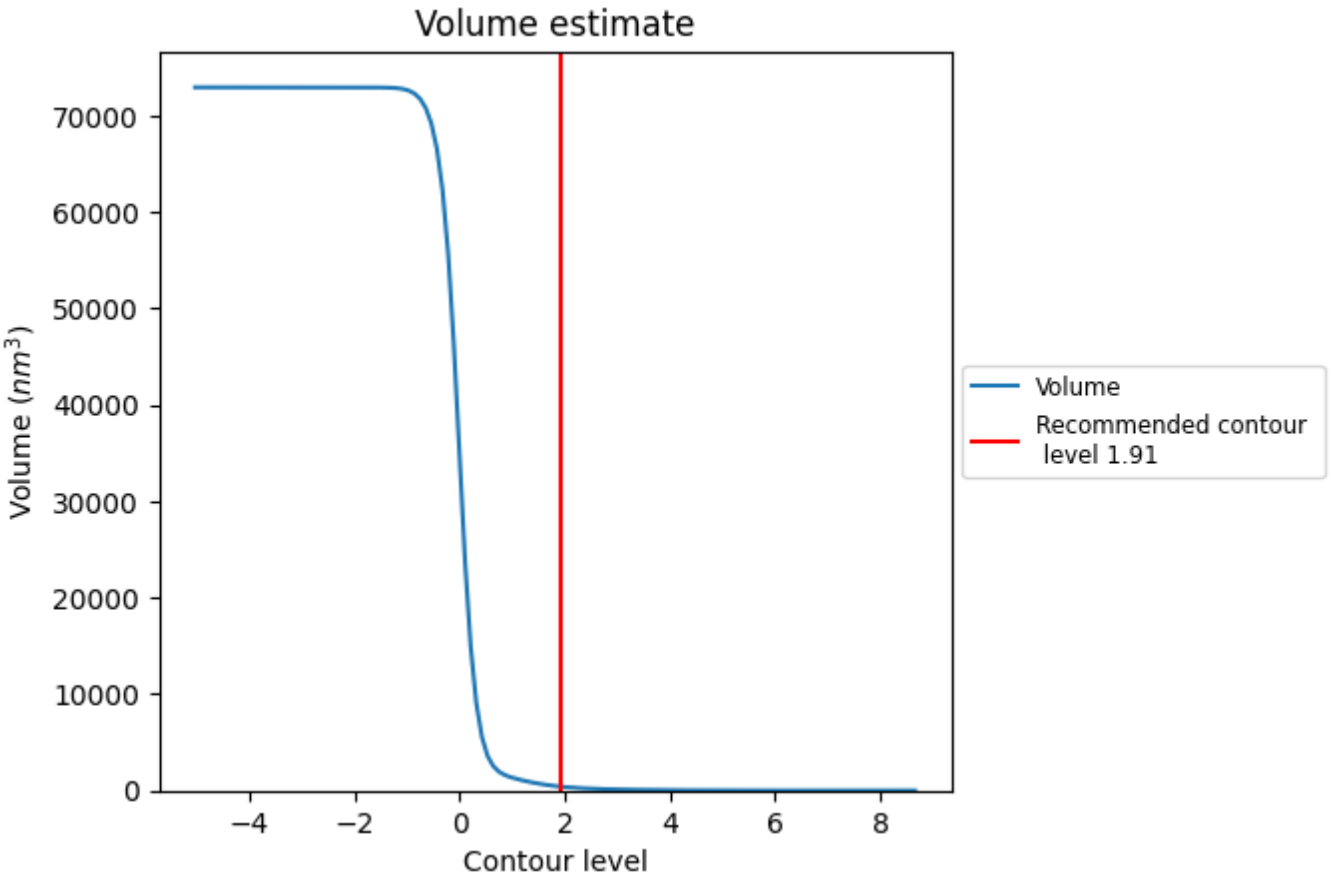
This section contains the results of statistical analysis of the map.

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.

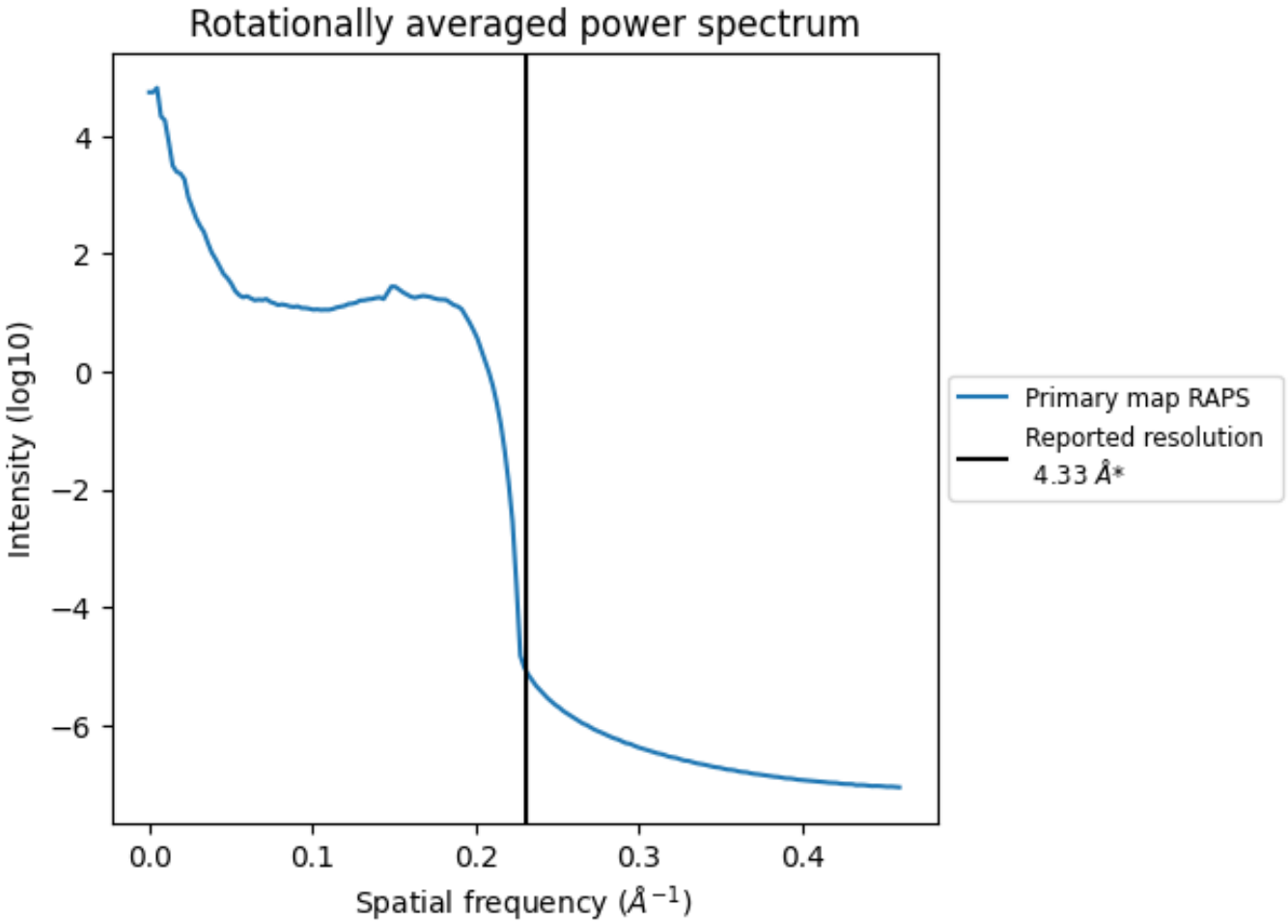
7.2 Volume estimate



The volume at the recommended contour level is 413 nm^3; this corresponds to an approximate mass of 373 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 0.231 Å^{-1}

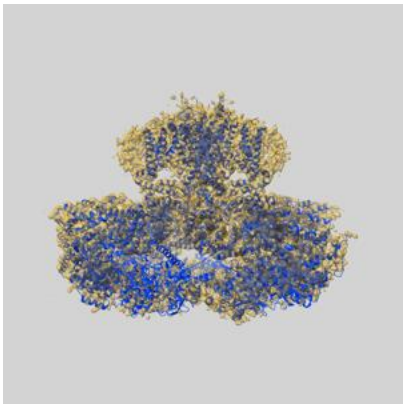
8 Fourier-Shell correlation (i)

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

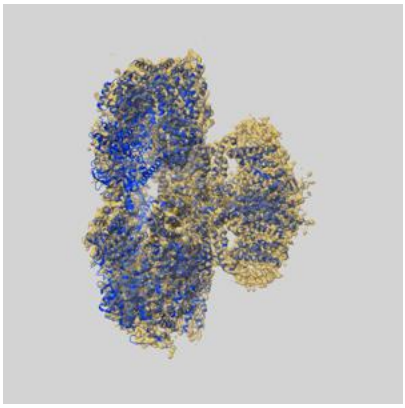
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7988 and PDB model 6DR2. Per-residue inclusion information can be found in section 3 on page 4.

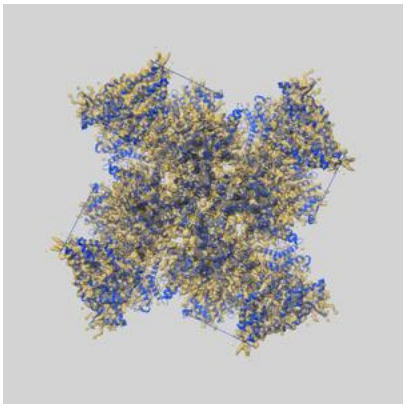
9.1 Map-model overlay



X



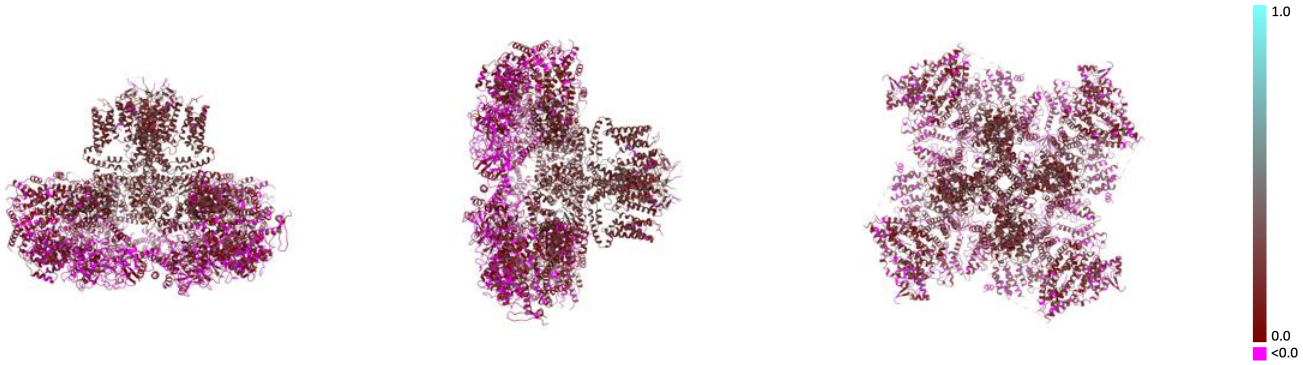
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.91 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.

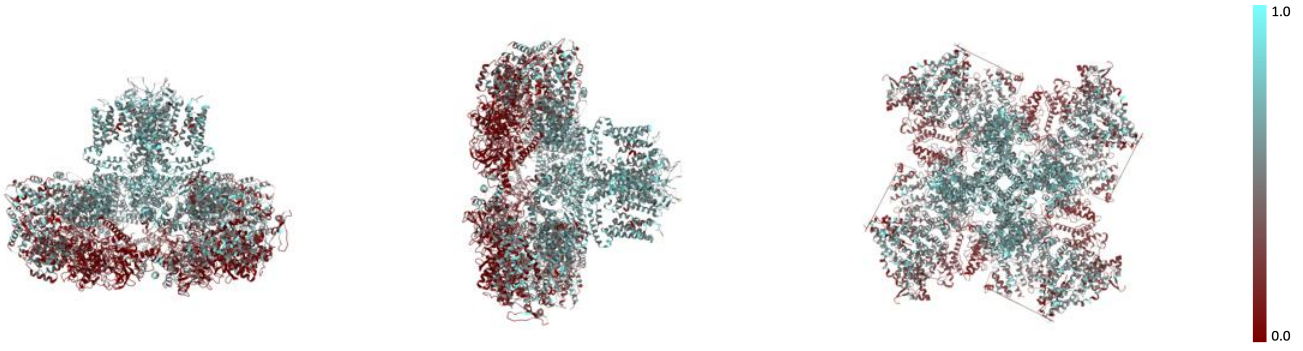
9.2 Q-score mapped to coordinate model (i)



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.

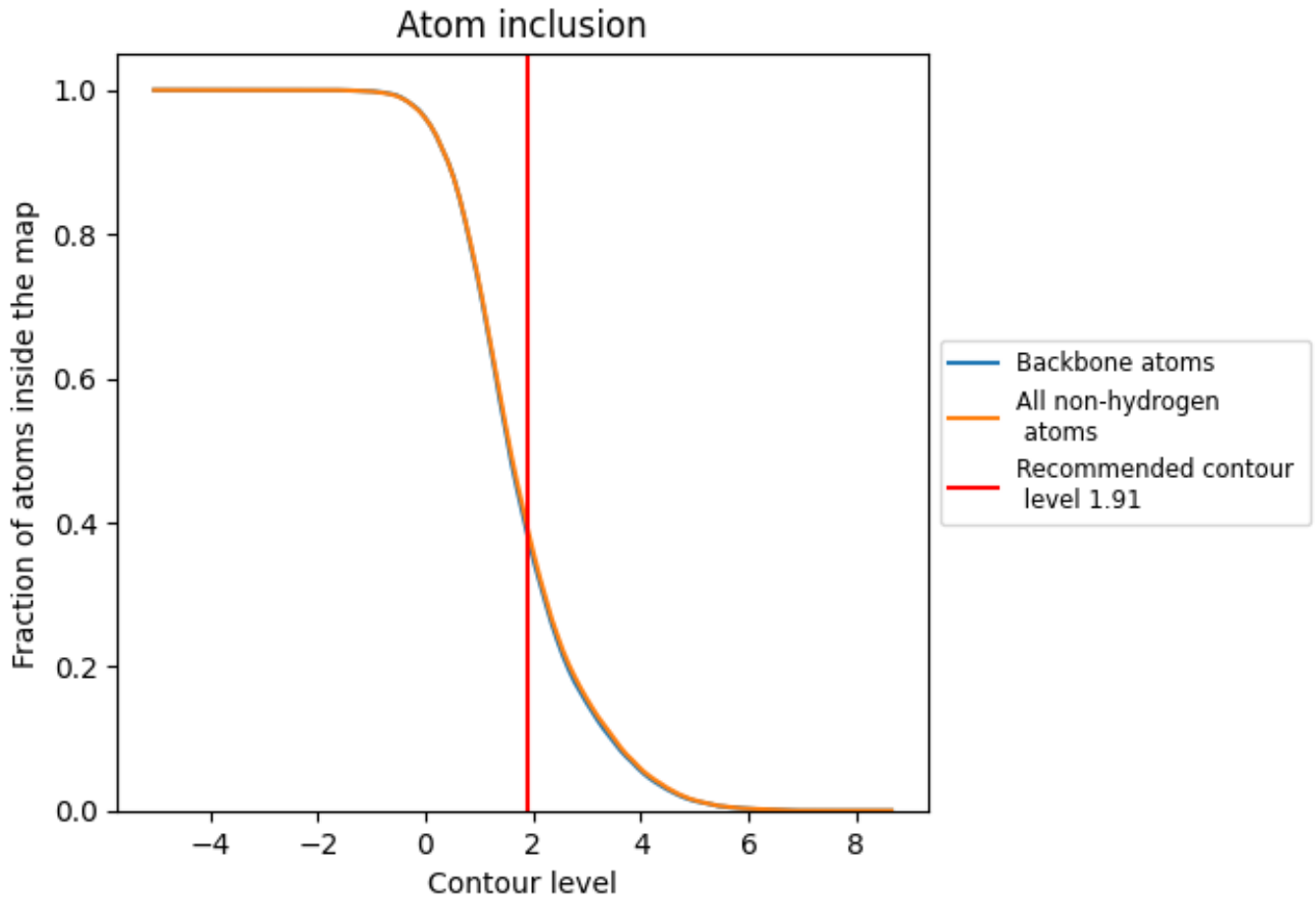
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.91).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 39% 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 (1.91) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3887	0.1290
A	0.3980	0.1300
B	0.3982	0.1290
C	0.3973	0.1300
D	0.3956	0.1270