Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:59 PM EST

PDB ID	:	7T3U
EMDB ID	:	EMD-25671
Title	:	IP3, ATP, and Ca2+ bound type 3 IP3 receptor in the inactive state
Authors	:	Schmitz, E.A.; Takahashi, H.; Karakas, E.
Deposited on	:	2021-12-08
Resolution	:	3.70 Å(reported)
Based on initial model	:	6UQK

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:

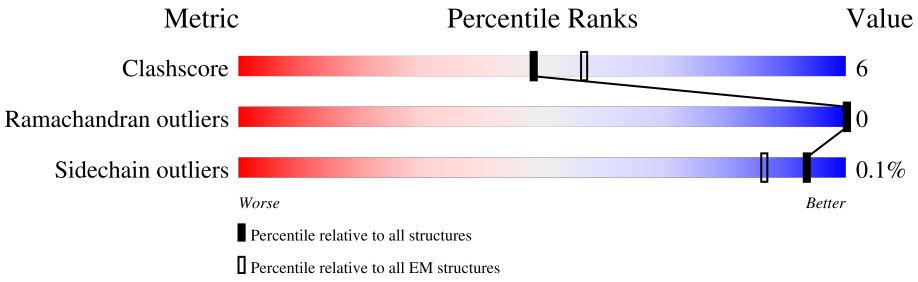
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.70 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	2633	5% 71% 6% 23%
1	B	2633	57% 6% 37%
1	C	2633	35% 53% 7% 40%
1	D	2633	30% 69% 7% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 44501 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

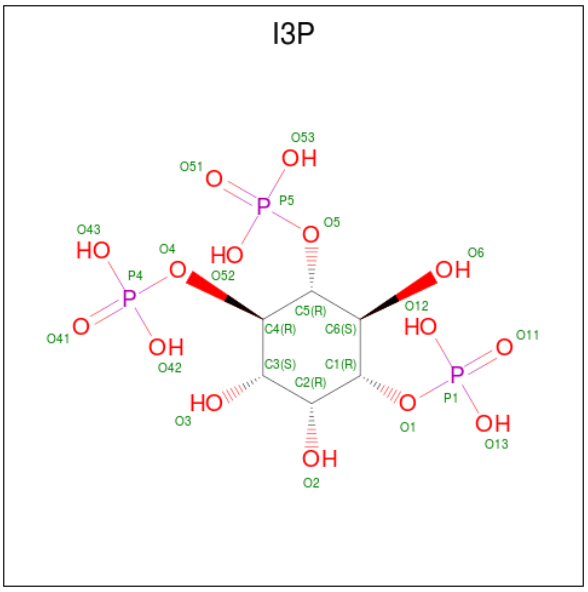
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2020	Total	C	N	O	S	0	0
			12132	7515	2262	2326	29		
1	B	1662	Total	C	N	O	S	0	0
			10375	6470	1906	1968	31		
1	C	1575	Total	C	N	O	S	0	0
			9741	6073	1791	1849	28		
1	D	2012	Total	C	N	O	S	0	0
			12073	7474	2252	2316	31		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

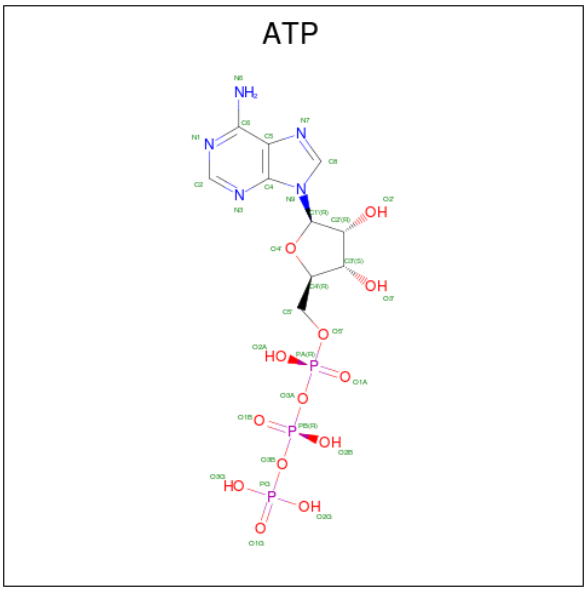
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			24	6	15	3	
3	D	1	Total	C	O	P	0
			24	6	15	3	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

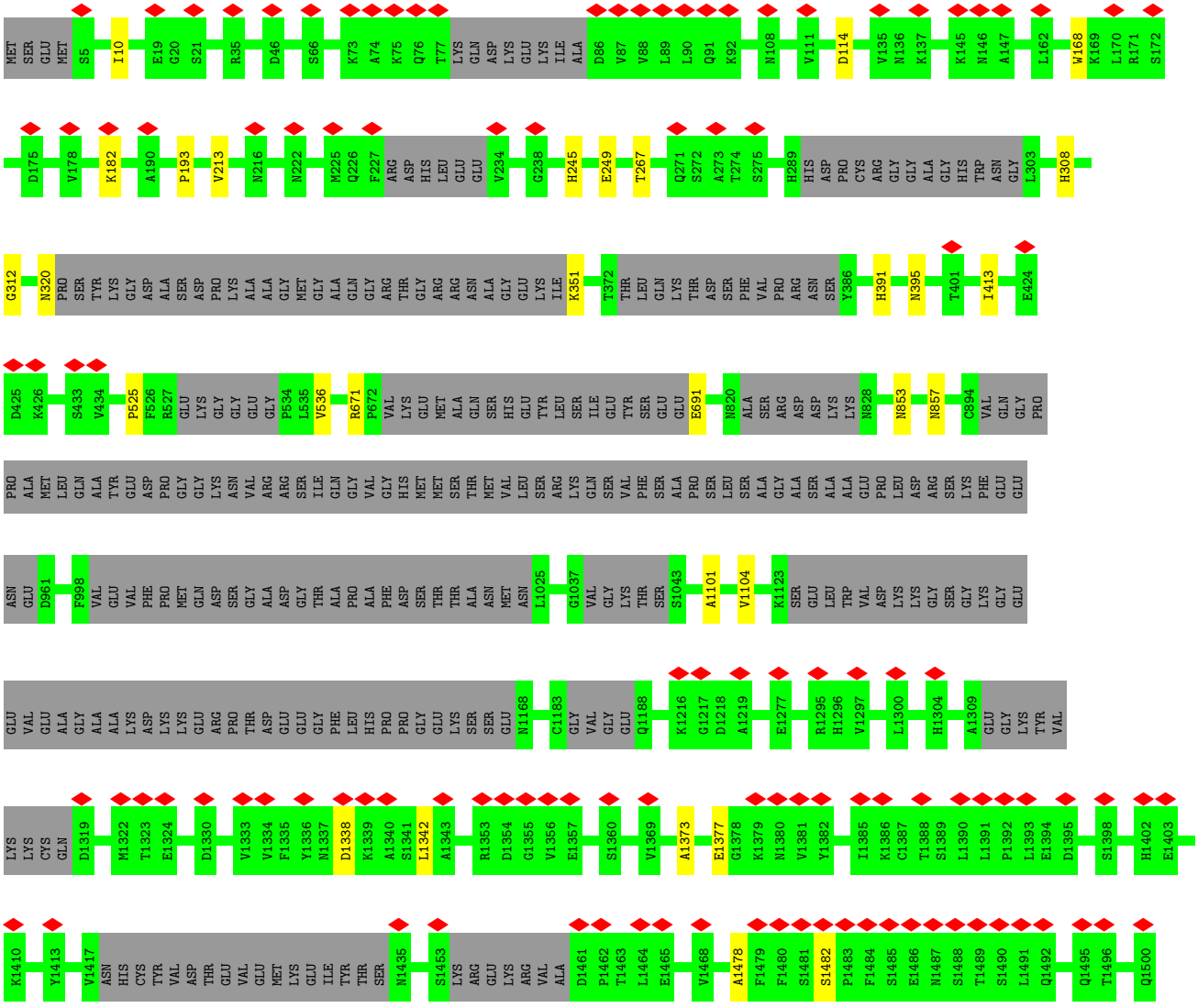
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

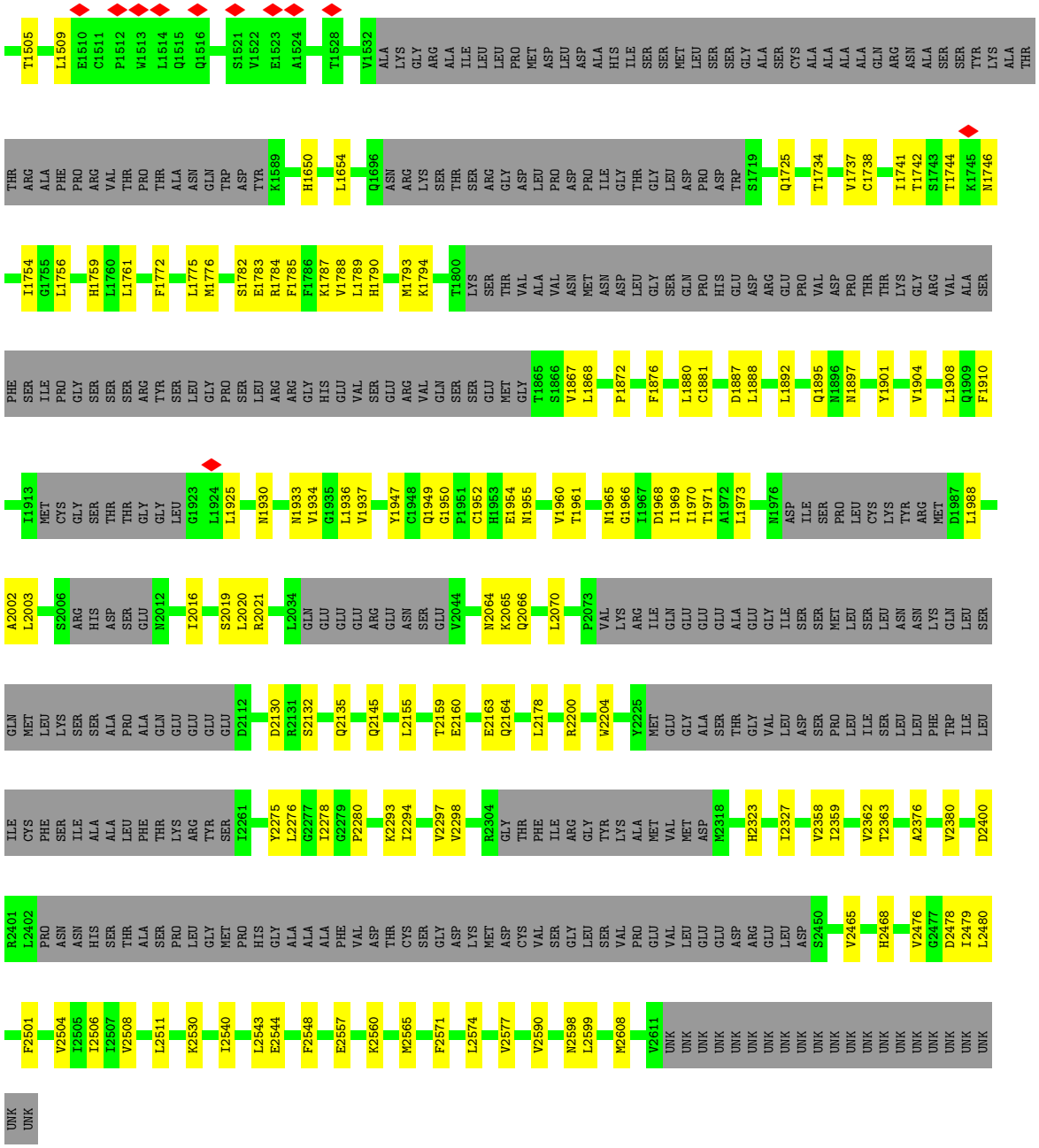
3 Residue-property plots (i)

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

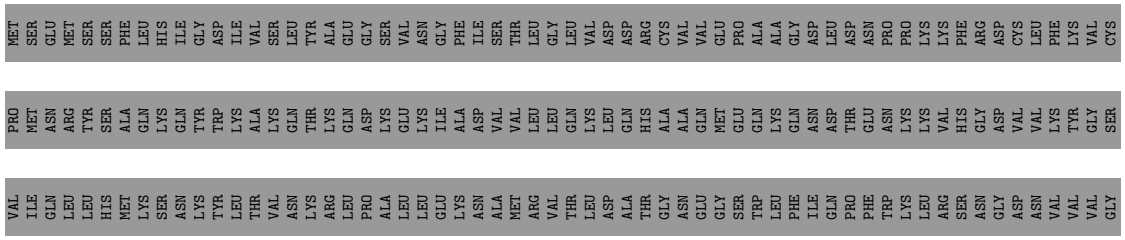
Chain A:

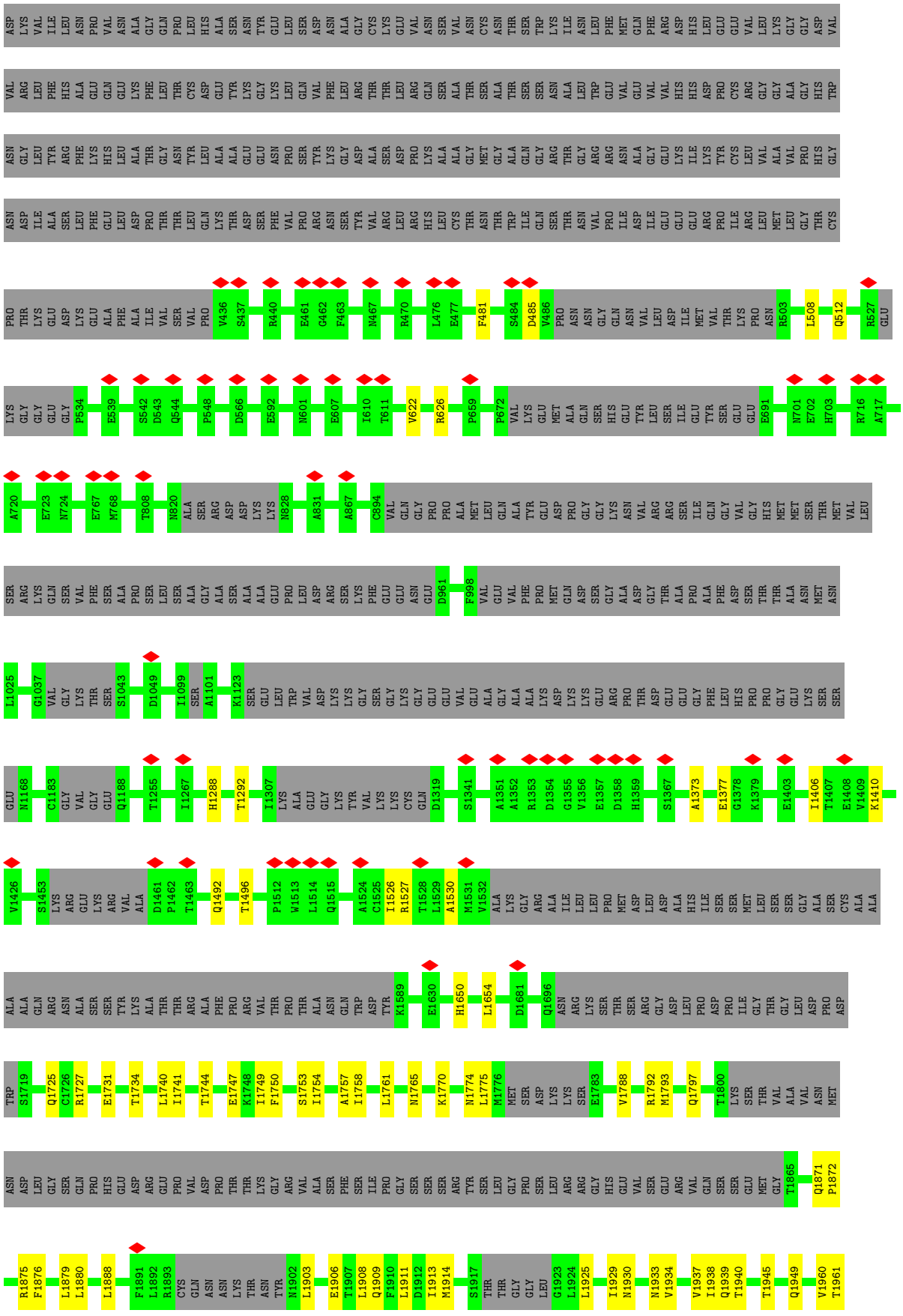


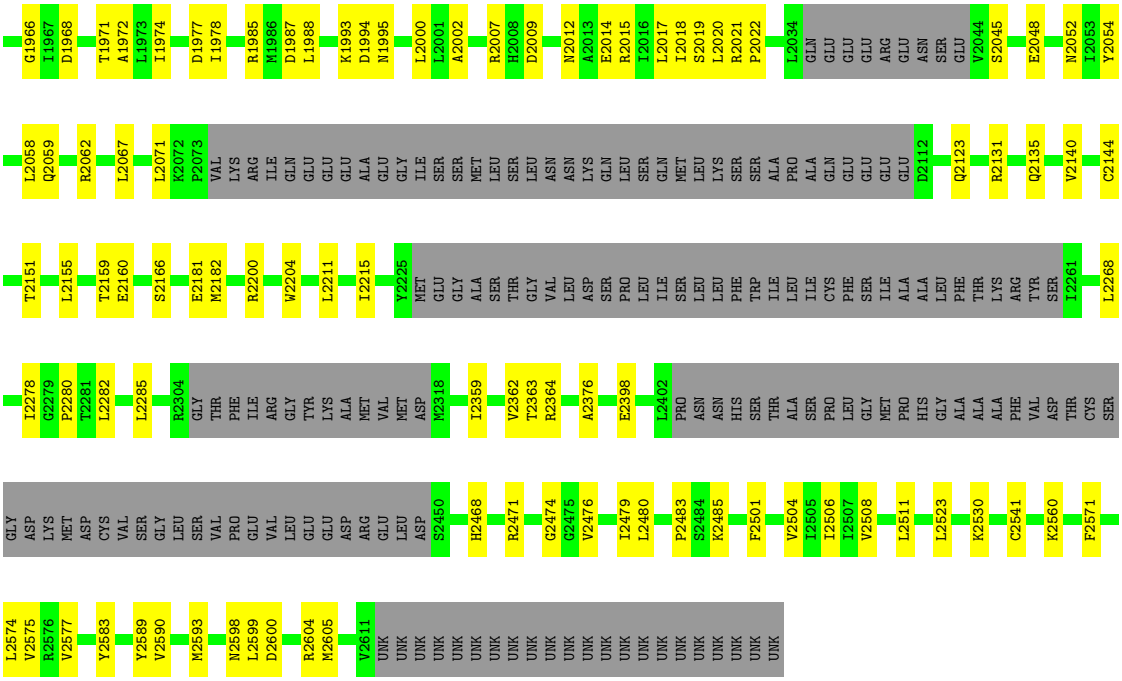


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

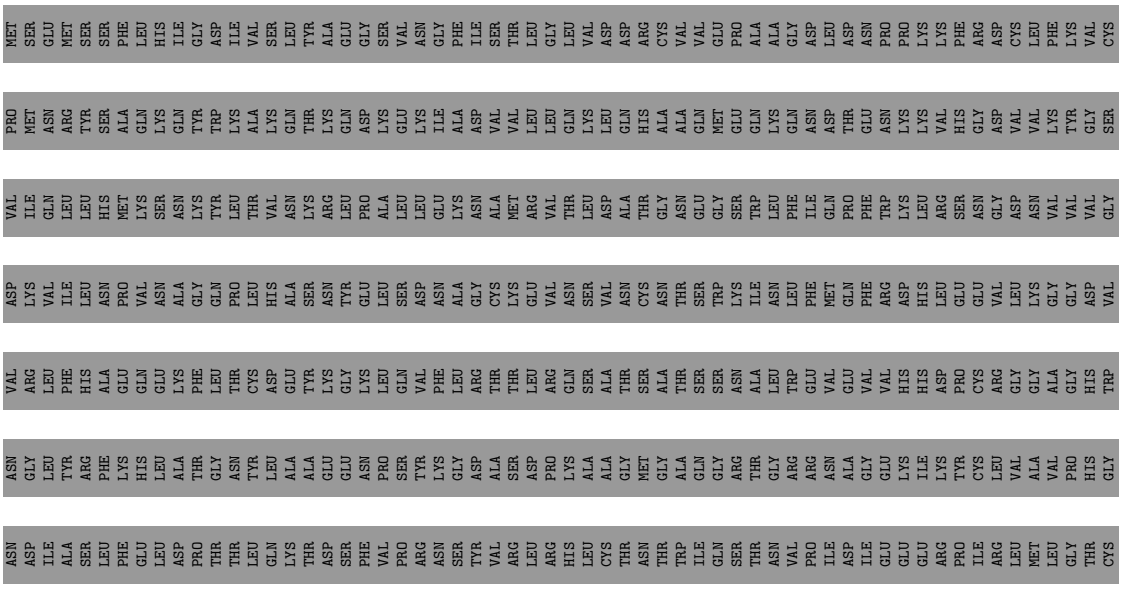
Chain B:

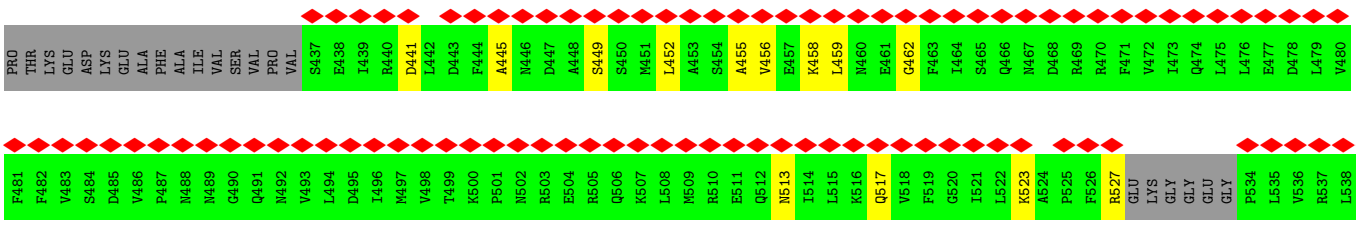


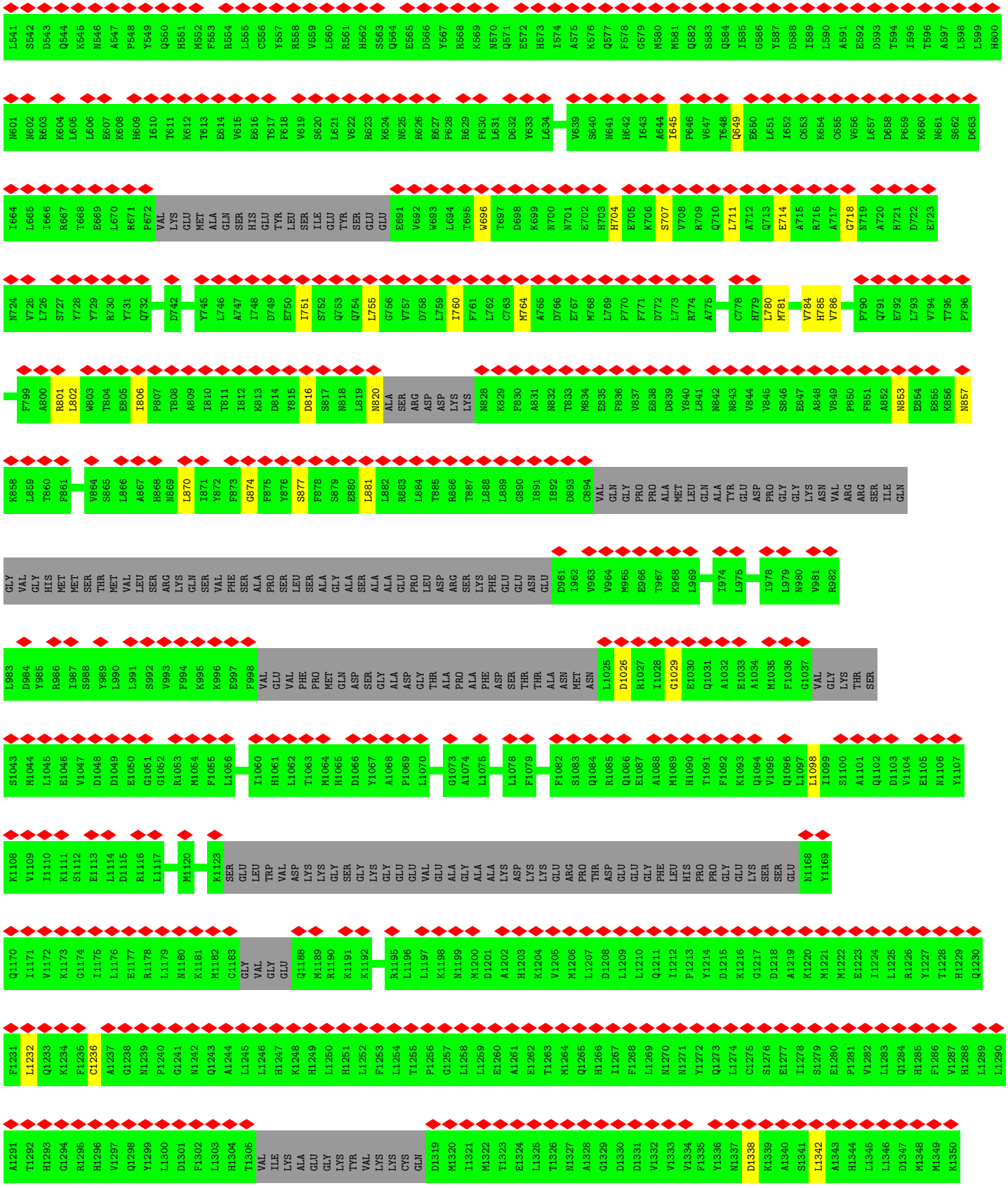




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



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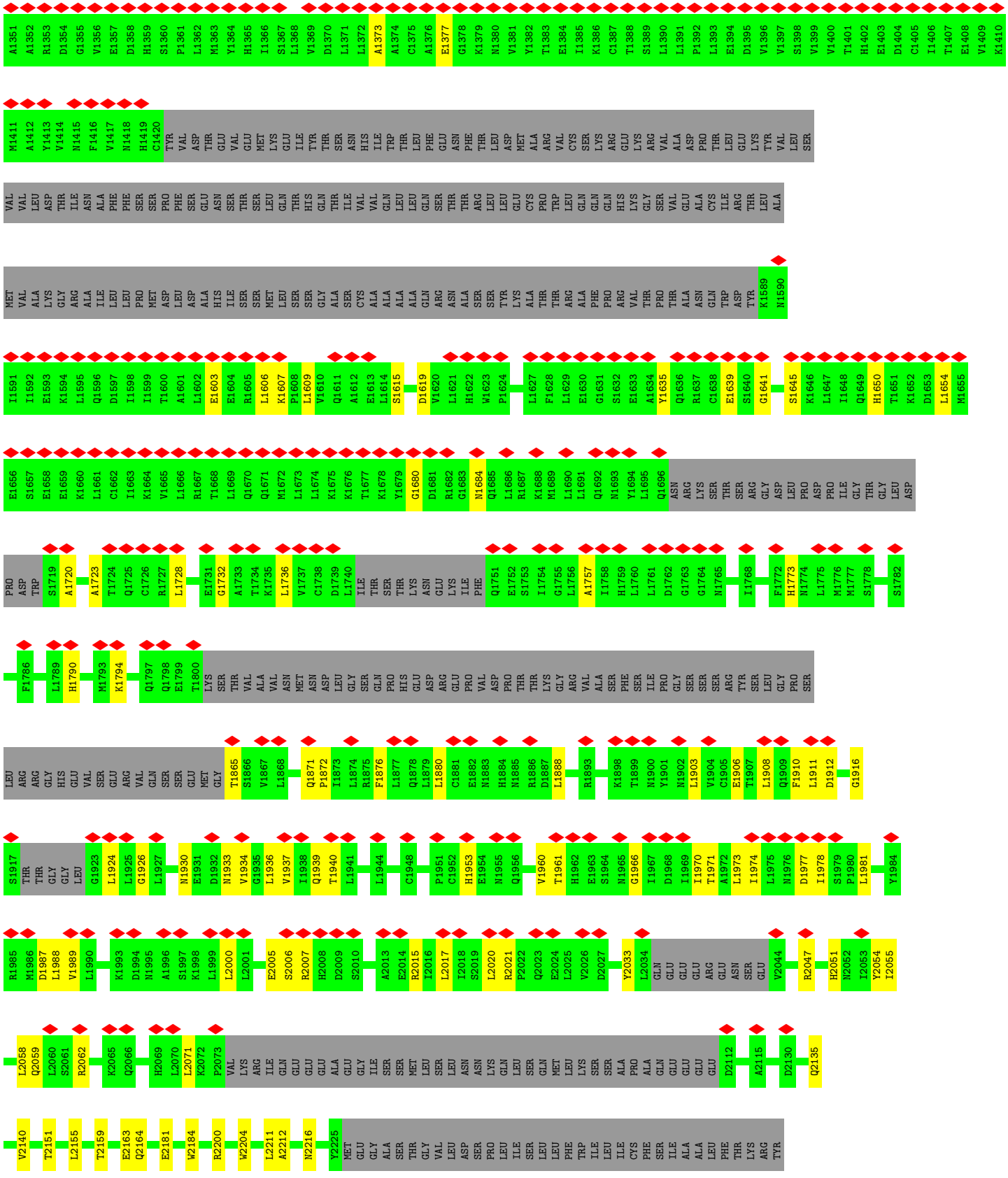
N601 N602 R603 K604 L605 L606 E607 K608 H609 I610 T611 K612 T613 E614 V615 E616 T617 F618 V619 S620 L621 V622 R623 K624 N625 R626 E627 F628 R629 F630 L631 D632 Y633 L634 V639 S640 N641 H642 I643 A644 I645 P646 V647 T648 Q649 E650 L651 I652 C653 K654 C655 V656 L657 D658 P659 K660 N661 S662 D663
I664 L665 I666 R667 T668 E669 L670 R671 P672 VAL LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER GLU GLU E691 V692 W693 L694 T695 W696 T697 D698 K699 N700 N701 E702 H703 H704 E705 K706 S707 V708 R709 Q710 L711 A712 Q713 E714 A715 R716 A717 G718 N719 A720 H721 D722 E723
N724 V725 L726 S727 Y728 Y729 R730 Y731 Q732 D742 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 C778 H779 L780 M781 V784 H785 V786 P790 Q791 E792 L793 V794 T795 P796
F799 A800 R801 L802 W803 T804 E805 I806 P807 T808 A809 I810 T811 I812 K813 D814 Y815 D816 S817 N818 L819 N820 ALA SER ARG ASP ASP LYS LYS N828 K829 F830 A831 N832 T833 M834 E835 F836 V837 E838 D839 Y840 L841 N842 N843 V844 V845 S846 E847 A848 V849 P850 F851 A852 N853 E854 E855 K856 N857
K858 L859 T860 F861 V864 S865 L866 A867 H868 N869 L870 I871 Y872 F873 G874 F875 Y876 S877 F878 S879 E880 L881 L882 R883 L884 T885 R886 T887 L888 L889 G890 I891 I892 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN
GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 I962 V963 V964 M965 E966 T967 K968 L969 I974 L975 I978 L979 N980 V981 R982
L983 D984 Y985 R986 I987 S988 Y989 L990 L991 S992 V993 F994 K995 K996 E997 F998 VAL GLU VAL PHE PRO MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA ASN MET ASN L1025 D1026 R1027 I1028 G1029 E1030 Q1031 A1032 E1033 A1034 M1035 F1036 G1037 VAL GLY LYS THR SER
S1043 M1044 L1045 E1046 V1047 D1048 D1049 E1050 G1051 G1052 R1053 M1054 F1055 L1056 I1060 H1061 L1062 T1063 M1064 H1065 D1066 Y1067 A1068 P1069 L1070 G1073 A1074 L1075 L1078 F1079 F1082 S1083 Q1084 R1085 Q1086 E1087 A1088 M1089 H1090 T1091 F1092 K1093 Q1094 V1095 Q1096 L1097 L1098 I1099 S1100 A1101 Q1102 D1103 V1104 E1105 N1106 Y1107
K1108 V1109 I1110 K1111 S1112 E1113 L1114 D1115 R1116 L1117 M1120 K1123 SER GLU LEU TRP VAL ASP LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER SER GLU N1168 Y1169
Q1170 I1171 V1172 K1173 G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 M1182 C1183 GLY VAL GLY GLU Q1188 M1189 R1190 K1191 K1192 R1195 L1196 L1197 K1198 N1199 M1200 D1201 A1202 H1203 K1204 V1205 M1206 L1207 D1208 L1209 L1210 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222 E1223 I1224 L1225 R1226 Y1227 T1228 H1229 Q1230
F1231 L1232 Q1233 K1234 F1235 C1236 A1237 G1238 N1239 P1240 G1241 N1242 Q1243 A1244 L1245 L1246 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1260 A1261 E1262 T1263 M1264 Q1265 H1266 I1267 F1268 L1269 N1270 N1271 Y1272 Q1273 L1274 C1275 S1276 E1277 I1278 S1279 E1280 P1281 V1282 L1283 Q1284 H1285 F1286 V1287 H1288 L1289 L1290
A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 T1305 VAL ILE LYS ALA GLU GLY LYS TYR VAL LYS LYS CYS GLN 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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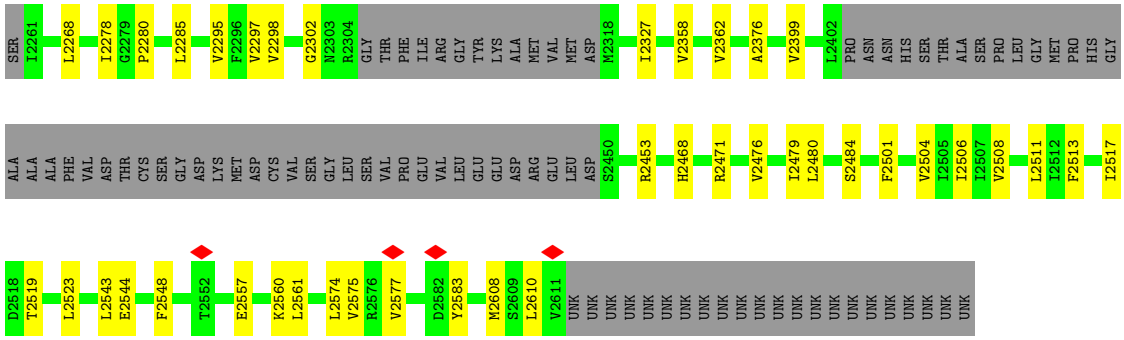
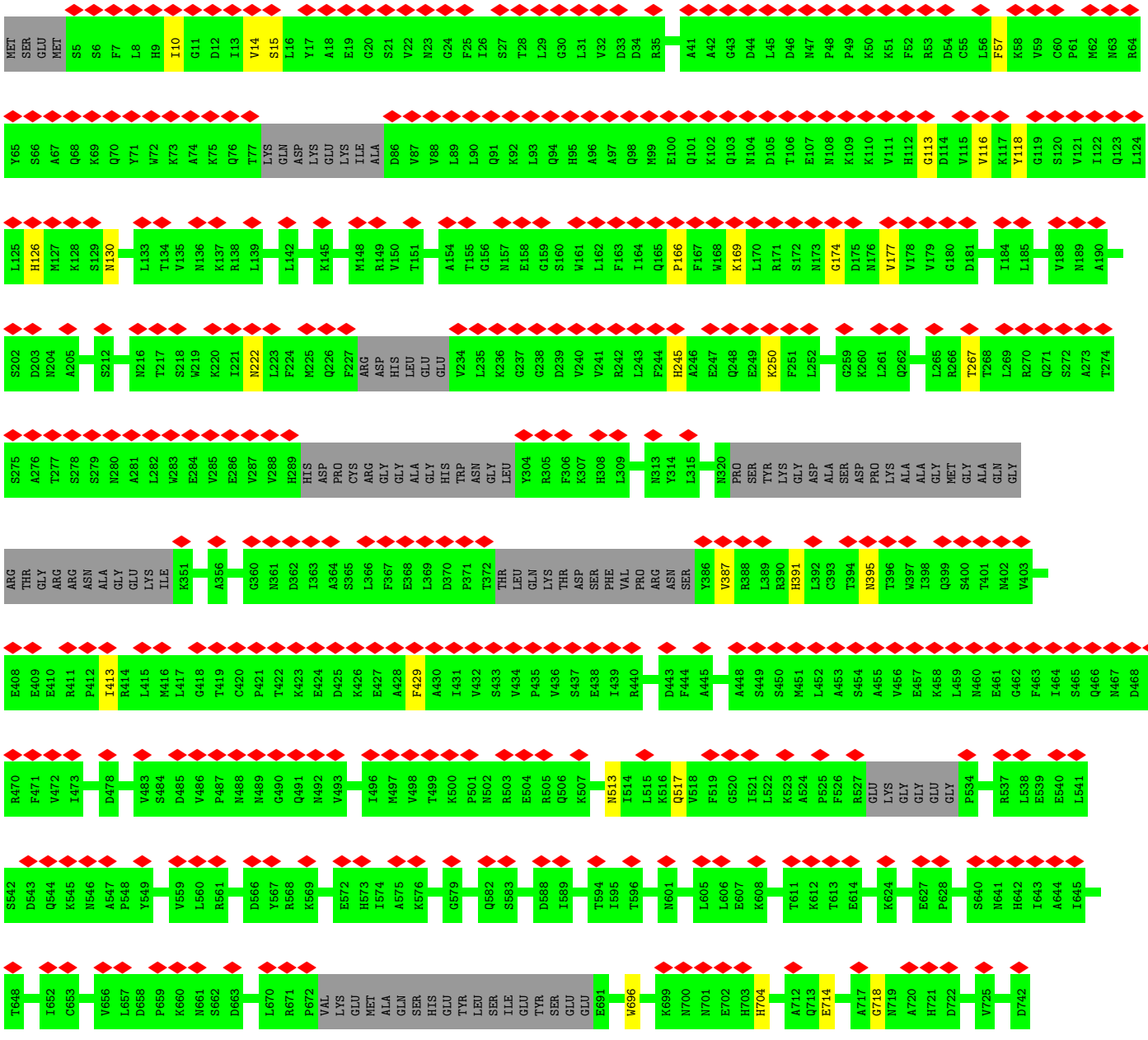
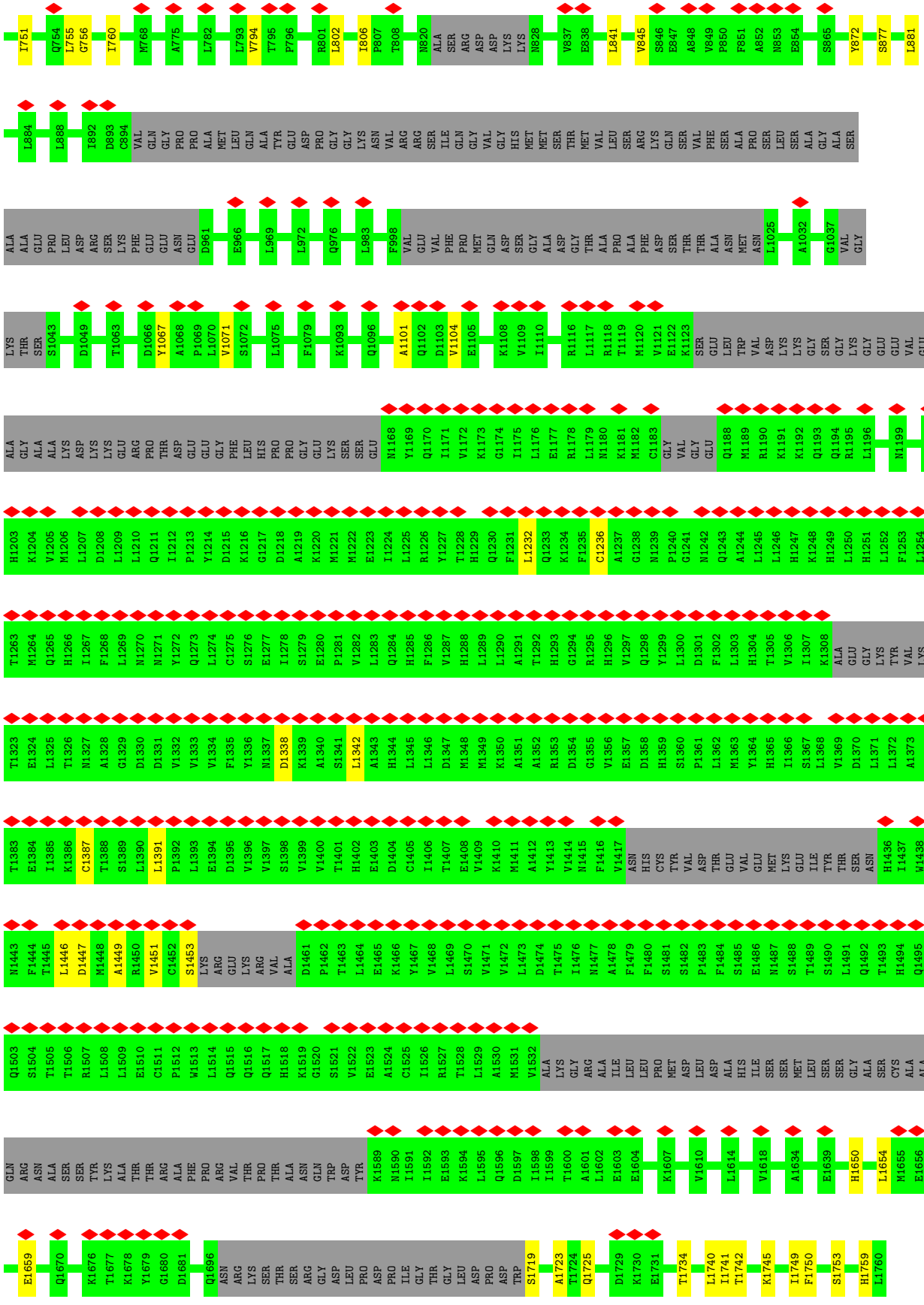
M1411 A1412 Y1413 V1414 N1415 F1416 V1417 N1418 H1419 C1420 TYR VAL ASP THR GLU VAL GLU MET LYS GLU ILE TYR THR SER ASN HIS ILE TRP THR LEU PHE GLU ASN PHE THR LEU ASP MET ALA ARG VAL CYS SER LYS ARG GLU LYS ARG VAL ALA ASP PRO THR LEU GLU LYS TYR VAL LEU SER
VAL VAL LEU ASP THR ILE ASN ALA PHE PHE SER SER PRO PHE SER GLU ASN SER THR SER LEU GLN THR HIS GLN THR ILE VAL VAL GLN LEU LEU GLN SER THR THR ARG LEU LEU GLU CYS PRO TRP LEU GLN GLN GLN HIS LYS GLY SER VAL GLU ALA CYS ILE ARG THR LEU ALA
MET VAL ALA LYS GLY ARG ALA ALA ILE LEU LEU PRO MET ASP LEU ASP ALA HIS ILE SER SER MET LEU SER SER GLY ALA SER CYS ALA ALA ALA ALA GLN ARG ASN ALA SER SER TYR LYS ALA THR THR ARG ALA PHE PRO ARG VAL THR PRO THR ALA ASN GLN TRP ASP TYR K1589 N1590
I1591 I1592 E1593 K1594 L1595 Q1596 D1597 I1598 I1599 T1600 A1601 L1602 E1603 E1604 R1605 L1606 K1607 P1608 L1609 V1610 Q1611 A1612 E1613 L1614 S1615 D1619 V1620 L1621 H1622 W1623 P1624 L1627 F1628 L1629 E1630 G1631 S1632 E1633 A1634 Y1635 Q1636 R1637 C1638 E1639 S1640 G1641 S1645 K1646 L1647 I1648 Q1649 H1650 T1651 K1652 D1653 L1654 M1655
E1656 S1657 E1658 E1659 K1660 L1661 C1662 I1663 K1664 V1665 L1666 R1667 T1668 L1669 Q1670 Q1671 M1672 L1673 L1674 K1675 K1676 T1677 K1678 Y1679 G1680 D1681 R1682 G1683 N1684 Q1685 L1686 R1687 K1688 M1689 L1690 L1691 Q1692 N1693 Y1694 L1695 Q1696 ASN ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP
PRO ASP TRP S1719 A1720 A1723 T1724 Q1725 C1726 R1727 L1728 E1731 G1732 A1733 T1734 K1735 L1736 V1737 C1738 D1739 L1740 ILE THR SER THR LYS ASN GLU LYS ILE PHE Q1751 E1752 S1753 I1754 G1755 L1756 A1757 I1758 H1759 L1760 L1761 D1762 G1763 G1764 N1765 I1768 F1772 H1773 N1774 L1775 M1776 M1777 S1778 S1782
F1786 L1789 H1790 M1793 K1794 Q1797 Q1798 E1799 T1800 LYS SER THR VAL 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 MET GLY T1865 S1866 V1867 L1868 Q1871 P1872 I1873 L1874 R1875 F1876 L1877 Q1878 L1879 L1880 C1881 E1882 N1883 H1884 N1885 R1886 D1887 L1888 R1893 K1898 T1899 N1900 Y1901 N1902 L1903 V1904 C1905 E1906 T1907 L1908 Q1909 F1910 L1911 D1912 G1916
S1917 THR THR GLY GLY LEU G1923 L1924 L1925 G1926 L1927 N1930 E1931 D1932 N1933 V1934 G1935 L1936 V1937 I1938 Q1939 T1940 L1941 L1944 C1948 P1951 C1952 H1953 E1954 N1955 Q1956 V1960 T1961 H1962 E1963 S1964 N1965 G1966 I1967 D1968 I1969 I1970 T1971 A1972 L1973 I1974 L1975 N1976 D1977 I1978 S1979 P1980 L1981 Y1984
R1985 M1986 D1987 L1988 V1989 L1990 K1993 D1994 N1995 A1996 S1997 K1998 L1999 L2000 L2001 E2005 S2006 R2007 H2008 D2009 S2010 A2013 E2014 R2015 I2016 L2017 I2018 S2019 L2020 R2021 P2022 Q2023 E2024 L2025 V2026 D2027 Y2033 L2034 GLN GLU GLU GLU ARG GLU ASN SER GLU V2044 R2047 H2051 W2052 I2053 Y2054 I2055
L2058 Q2059 L2060 S2061 R2062 K2065 Q2066 H2069 L2070 L2071 K2072 P2073 VAL LYS ARG ILE GLN GLU GLU GLU ALA GLU GLY ILE SER SER MET LEU LEU SER LEU ASN ASN LYS GLN LEU SER GLN MET LEU LEU LYS SER SER ALA PRO ALA GLN GLU GLU GLU GLU D2112 A2115 D2130 Q2135
V2140 T2151 L2155 T2159 E2163 Q2164 E2181 W2184 R2200 W2204 L2211 A2212 N2216 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO LEU ILE SER LEU LEU PHE TRP ILE LEU ILE CYS PHE SER ILE ALA ALA LEU PHE THR LYS ARG TYR



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

Chain D:

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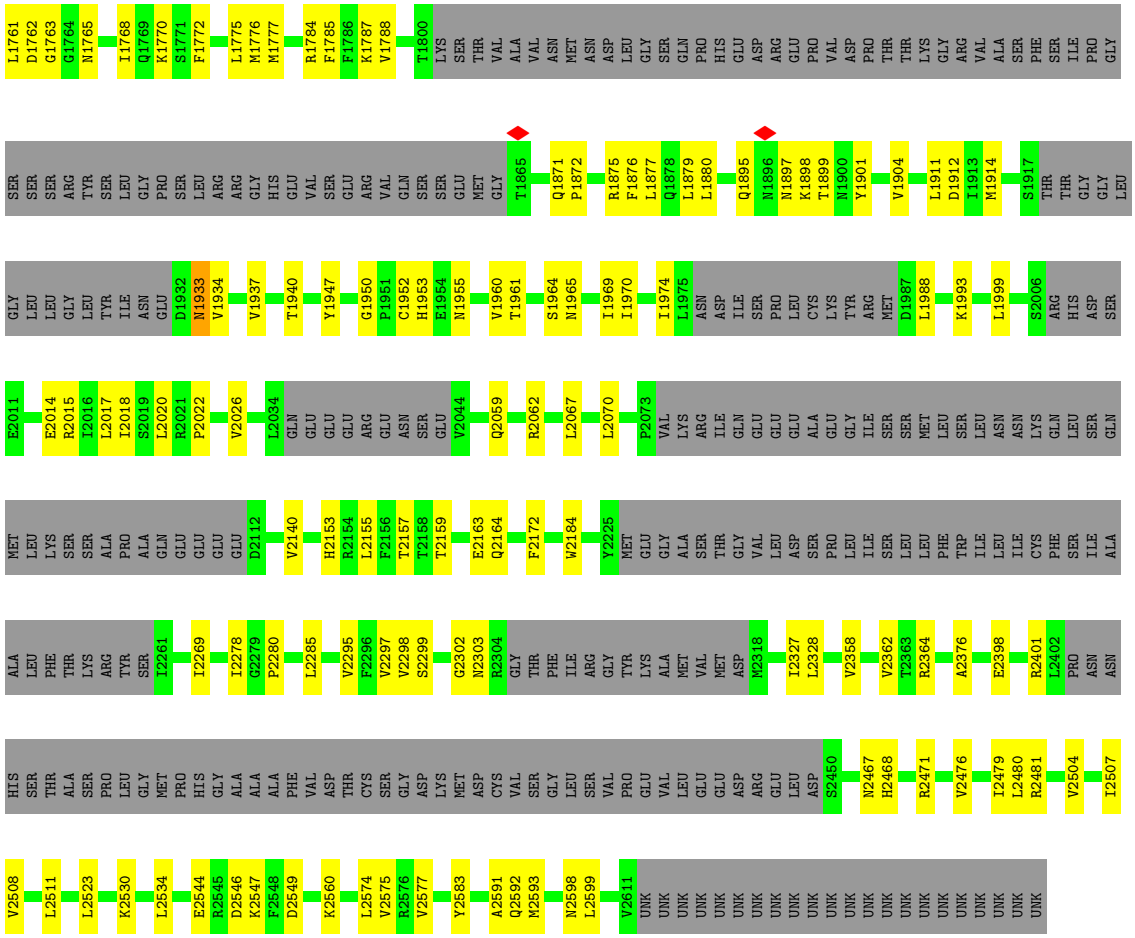
L884 L888 I892 D893 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER
ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 E966 L969 L972 Q976 L983 F998 VAL GLU VAL PHE PRO MET GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA ASN MET ASN L1025 A1032 G1037 VAL GLY
LYS THR SER S1043 D1049 T1063 D1066 Y1067 A1068 P1069 L1070 V1071 S1072 L1075 F1079 K1093 Q1096 A1101 Q1102 D1103 V1104 E1105 K1108 V1109 I1110 R1116 L1117 R1118 T1119 M1120 V1121 E1122 K1123 SER GLU LEU TRP VAL ASP LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU
ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER SER GLU N1168 Y1169 Q1170 I1171 V1172 K1173 G1174 I1175 L1176 E1177 R1178 L1179 N1180 K1181 M1182 C1183 GLY VAL GLY GLU Q1188 M1189 R1190 K1191 K1192 Q1193 Q1194 R1195 L1196 N1199 A1202
H1203 K1204 V1205 M1206 L1207 D1208 L1209 L1210 Q1211 I1212 P1213 Y1214 D1215 K1216 G1217 D1218 A1219 K1220 M1221 M1222 E1223 I1224 L1225 R1226 Y1227 T1228 H1229 Q1230 F1231 L1232 Q1233 K1234 F1235 C1236 A1237 G1238 N1239 P1240 G1241 N1242 Q1243 A1244 L1245 L1246 H1247 K1248 H1249 L1250 H1251 L1252 F1253 L1254 T1255 P1256 G1257 L1258 L1259 E1260 A1261 E1262
T1263 M1264 Q1265 H1266 I1267 F1268 L1269 N1270 N1271 Y1272 Q1273 L1274 C1275 S1276 E1277 I1278 S1279 E1280 P1281 V1282 L1283 Q1284 H1285 F1286 V1287 H1288 L1289 L1290 A1291 T1292 H1293 G1294 R1295 H1296 V1297 Q1298 Y1299 L1300 D1301 F1302 L1303 H1304 T1305 V1306 I1307 K1308 ALA GLU GLY LYS TYR VAL LYS LYS CYS GLN D1319 M1320 I1321 M1322
T1323 E1324 L1325 T1326 N1327 A1328 G1329 D1330 D1331 V1332 V1333 V1334 F1335 Y1336 N1337 D1338 K1339 A1340 S1341 L1342 A1343 H1344 L1345 L1346 D1347 M1348 M1349 K1350 A1351 A1352 R1353 D1354 G1355 V1356 E1357 D1358 H1359 S1360 P1361 L1362 M1363 Y1364 H1365 I1366 S1367 L1368 V1369 D1370 L1371 L1372 A1373 A1374 C1375 A1376 E1377 G1378 K1379 N1380 V1381 Y1382
T1383 E1384 I1385 K1386 C1387 T1388 S1389 L1390 L1391 P1392 L1393 E1394 D1395 V1396 V1397 S1398 V1399 V1400 T1401 H1402 E1403 D1404 C1405 I1406 T1407 E1408 V1409 K1410 M1411 A1412 Y1413 V1414 N1415 F1416 V1417 ASN HIS CYS TYR VAL ASP THR GLU VAL GLU MET LYS GLU ILE TYR THR SER ASN H1436 I1437 W1438 T1439 L1440 F1441 E1442
N1443 F1444 T1445 L1446 D1447 M1448 A1449 R1450 V1451 C1452 S1453 LYS ARG GLU LYS ARG VAL ALA D1461 P1462 T1463 L1464 E1465 K1466 Y1467 V1468 L1469 S1470 V1471 V1472 L1473 D1474 T1475 I1476 N1477 A1478 F1479 F1480 S1481 S1482 P1483 F1484 S1485 E1486 N1487 S1488 T1489 S1490 L1491 Q1492 T1493 H1494 Q1495 T1496 I1497 V1498 V1499 Q1500 L1501 L1502
Q1503 S1504 T1505 T1506 R1507 L1508 L1509 E1510 C1511 P1512 W1513 L1514 Q1515 Q1516 Q1517 H1518 K1519 G1520 S1521 V1522 E1523 A1524 C1525 I1526 R1527 T1528 L1529 A1530 M1531 V1532 ALA LYS GLY ARG ALA ILE LEU LEU PRO MET ASP LEU ASP ALA HIS ILE SER SER MET LEU SER SER GLY ALA SER CYS ALA ALA ALA ALA ALA
GLN ARG ASN ALA SER SER TYR LYS ALA THR THR ARG ALA PHE PRO PRO ARG VAL THR PRO THR ALA ASN GLN TRP ASP TYR K1589 N1590 I1591 I1592 E1593 K1594 L1595 Q1596 D1597 I1598 I1599 T1600 A1601 L1602 E1603 E1604 K1607 V1610 L1614 V1618 A1634 E1639 H1650 L1654 M1655 E1656
E1659 Q1670 K1676 T1677 K1678 Y1679 G1680 D1681 Q1696 ASN ARG LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP TRP S1719 A1723 T1724 Q1725 D1729 K1730 E1731 T1734 L1740 I1741 T1742 K1745 I1749 F1750 S1753 H1759 L1760


L1761 D1762 G1763 G1764 N1765 I1768 Q1769 K1770 S1771 F1772 L1775 M1776 M1777 R1784 F1785 F1786 K1787 V1788 T1800 LYS SER THR VAL 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 MET GLY T1865 Q1871 P1872 R1875 F1876 L1877 Q1878 L1879 L1880 Q1895 N1896 N1897 K1898 T1899 N1900 Y1901 V1904 L1911 D1912 T1913 M1914 S1917 THR THR GLY GLY LEU
GLY LEU LEU GLY LEU TYR ILE ASN GLU D1932 N1933 V1934 V1937 T1940 Y1947 G1950 P1951 C1952 H1953 E1954 N1955 V1960 T1961 S1964 N1965 I1969 I1970 I1974 L1975 ASN ASP ILE SER PRO LEU CYS LYS TYR ARG MET D1987 L1988 K1993 L1999 S2006 ARG HIS ASP SER
E2011 E2014 R2015 I2016 L2017 I2018 S2019 L2020 R2021 P2022 V2026 L2034 GLN GLU GLU GLU ARG GLU ASN SER GLU V2044 Q2059 R2062 L2067 L2070 P2073 VAL 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 GLU D2112 V2140 H2153 R2154 L2155 F2156 T2157 T2158 T2159 E2163 Q2164 F2172 W2184 Y2225 MET GLU GLY ALA SER THR GLY VAL LEU ASP SER PRO LEU ILE SER LEU LEU PHE TRP ILE LEU ILE CYS PHE SER ILE ALA
ALA LEU PHE THR LYS ARG TYR SER I2261 I2269 I2278 G2279 P2280 L2285 V2295 F2296 V2297 V2298 S2299 G2302 N2303 R2304 GLY THR PHE ILE ARG GLY TYR LYS ALA MET VAL MET ASP M2318 I2327 L2328 V2358 V2362 T2363 R2364 A2376 E2398 R2401 L2402 PRO 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 ASP S2450 N2467 H2468 R2471 V2476 I2479 L2480 R2481 V2504 I2507
V2508 L2511 L2523 K2530 L2534 E2544 R2545 D2546 K2547 F2548 D2549 K2560 L2574 V2575 R2576 V2577 Y2583 A2591 Q2592 M2593 N2598 L2599 V2611 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	198441	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.911	Depositor
Minimum map value	-1.171	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I3P, CA, ZN, ATP

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	0.24	0/12209	0.43	0/16761
1	B	0.24	0/10458	0.43	0/14326
1	C	0.24	0/9822	0.42	0/13474
1	D	0.24	0/12149	0.43	0/16677
All	All	0.24	0/44638	0.43	0/61238

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	12132	0	8448	112	0
1	B	10375	0	7682	134	0
1	C	9741	0	7105	120	0
1	D	12073	0	8390	129	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	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	24	0	9	0	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
4	C	31	0	12	1	0
4	D	31	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	44501	0	31691	474	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 6.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2297:VAL:HG21	1:D:2327:ILE:HD11	1.33	1.06
1:C:2297:VAL:HG21	1:C:2327:ILE:HD11	1.40	1.00
1:D:1740:LEU:HD21	1:D:1749:ILE:HG22	1.47	0.95
1:A:2297:VAL:HG21	1:A:2327:ILE:HD11	1.51	0.92
1:B:1934:VAL:HG21	1:B:1988:LEU:HD13	1.55	0.89
1:A:2066:GLN:NE2	1:A:2070:LEU:HD11	1.90	0.86
1:B:1968:ASP:OD1	1:B:2019:SER:OG	1.97	0.82
1:C:1373:ALA:O	1:C:1377:GLU:N	2.14	0.81
1:C:2575:VAL:O	1:C:2583:TYR:OH	1.99	0.80
1:B:2166:SER:OG	1:B:2604:ARG:NH1	2.15	0.80
1:C:2155:LEU:O	1:C:2159:THR:OG1	1.99	0.79
1:D:1725:GLN:NE2	1:D:1759:HIS:O	2.17	0.78
1:B:1747:GLU:OE2	1:B:1792:ARG:NH1	2.17	0.78
1:C:1728:LEU:O	1:C:1732:GLY:N	2.16	0.78
1:C:1650:HIS:O	1:C:1654:LEU:CB	2.33	0.75
1:D:2155:LEU:O	1:D:2159:THR:OG1	2.04	0.74
1:B:2155:LEU:O	1:B:2159:THR:OG1	2.06	0.73
1:B:1933:ASN:O	1:B:1937:VAL:HG23	1.89	0.72
1:A:2066:GLN:O	1:A:2070:LEU:HD12	1.88	0.72
1:B:1492:GLN:O	1:B:1496:THR:N	2.23	0.72
1:D:1650:HIS:O	1:D:1654:LEU:CB	2.37	0.72
1:A:2362:VAL:HG21	1:D:2511:LEU:HD11	1.72	0.71
1:C:1603:GLU:O	1:C:1607:LYS:N	2.23	0.71
1:D:877:SER:O	1:D:881:LEU:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:LEU:O	1:C:806:ILE:N	2.23	0.71
1:B:1526:ILE:O	1:B:1530:ALA:N	2.24	0.70
1:B:2468:HIS:HB3	1:B:2479:ILE:HG21	1.74	0.70
1:B:1945:THR:O	1:B:1949:GLN:N	2.25	0.69
1:A:2468:HIS:HB3	1:A:2479:ILE:HG21	1.74	0.69
1:C:2511:LEU:HD11	1:D:2362:VAL:HG21	1.72	0.69
1:A:2155:LEU:HD22	1:A:2178:LEU:HD11	1.75	0.69
1:B:1909:GLN:HE22	1:B:1913:ILE:HD11	1.58	0.69
1:D:1449:ALA:O	1:D:1453:SER:N	2.25	0.69
1:B:1740:LEU:HD21	1:B:1749:ILE:HG22	1.73	0.69
1:A:1478:ALA:O	1:A:1482:SER:N	2.26	0.69
1:B:1914:MET:CE	1:B:1937:VAL:HG22	2.23	0.69
1:A:2362:VAL:CG2	1:D:2511:LEU:HD11	2.23	0.68
1:D:1974:ILE:O	1:D:1993:LYS:NZ	2.26	0.68
1:C:1680:GLY:O	1:C:1684:ASN:N	2.27	0.68
1:D:2575:VAL:O	1:D:2583:TYR:OH	2.06	0.68
1:C:2511:LEU:HD11	1:D:2362:VAL:CG2	2.24	0.68
1:B:2123:GLN:OE1	1:B:2135:GLN:NE2	2.28	0.67
1:A:2511:LEU:HD21	1:B:2362:VAL:HG23	1.77	0.67
1:B:2511:LEU:HD11	1:C:2362:VAL:HG21	1.75	0.67
1:C:870:LEU:O	1:C:874:GLY:N	2.28	0.67
1:A:1101:ALA:O	1:A:1104:VAL:N	2.28	0.66
1:B:1740:LEU:HD22	1:B:1753:SER:HB3	1.77	0.66
1:B:1740:LEU:HD22	1:B:1753:SER:CB	2.25	0.66
1:A:1650:HIS:O	1:A:1654:LEU:CB	2.43	0.66
1:A:1738:CYS:O	1:A:1742:THR:HG22	1.94	0.66
1:B:2015:ARG:NH1	1:B:2015:ARG:O	2.28	0.66
1:B:2511:LEU:HD11	1:C:2362:VAL:CG2	2.25	0.66
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	1.77	0.66
1:B:1960:VAL:HG23	1:B:1961:THR:HG23	1.76	0.66
1:D:1960:VAL:HG23	1:D:1961:THR:HG23	1.78	0.66
1:C:2511:LEU:HD13	1:D:2358:VAL:CG1	2.26	0.66
1:C:801:ARG:O	1:C:1098:LEU:N	2.29	0.66
1:D:1897:ASN:OD1	1:D:1898:LYS:N	2.29	0.66
1:A:2163:GLU:OE1	1:A:2163:GLU:N	2.29	0.65
1:D:2468:HIS:HB3	1:D:2479:ILE:HG21	1.79	0.65
1:C:2557:GLU:OE2	1:C:2561:LEU:HD12	1.97	0.65
1:B:1987:ASP:OD1	1:B:1988:LEU:N	2.30	0.65
1:B:2501:PHE:CE2	1:B:2506:ILE:HD11	2.32	0.65
1:A:1338:ASP:O	1:A:1342:LEU:N	2.29	0.64
1:C:2015:ARG:O	1:C:2015:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2160:GLU:OE2	1:B:2530:LYS:NZ	2.29	0.64
1:A:2064:ASN:OD1	1:A:2065:LYS:N	2.31	0.64
1:D:751:ILE:O	1:D:755:LEU:N	2.29	0.64
1:D:1933:ASN:O	1:D:1937:VAL:HG23	1.98	0.64
1:A:320:ASN:N	1:A:351:LYS:O	2.31	0.64
1:A:2155:LEU:O	1:A:2159:THR:OG1	2.15	0.64
1:C:2005:GLU:O	1:C:2007:ARG:N	2.31	0.63
1:B:2211:LEU:HD22	1:B:2285:LEU:HD22	1.80	0.63
1:B:2511:LEU:HD13	1:C:2358:VAL:CG1	2.29	0.63
1:D:387:VAL:N	1:D:429:PHE:O	2.31	0.63
1:C:707:SER:O	1:C:711:LEU:N	2.31	0.62
1:D:802:LEU:O	1:D:806:ILE:N	2.30	0.62
1:D:391:HIS:O	1:D:395:ASN:N	2.33	0.62
1:A:1887:ASP:OD1	1:A:1888:LEU:N	2.32	0.61
1:B:2476:VAL:HG22	1:B:2480:LEU:HD13	1.81	0.61
1:C:2544:GLU:N	1:C:2544:GLU:OE1	2.33	0.61
1:A:2557:GLU:OE1	1:A:2557:GLU:N	2.33	0.61
1:A:2544:GLU:OE1	1:A:2544:GLU:N	2.33	0.61
1:C:2059:GLN:OE1	1:C:2062:ARG:NH2	2.34	0.61
1:D:756:GLY:O	1:D:760:ILE:N	2.33	0.61
1:B:1875:ARG:O	1:B:1879:LEU:HD23	2.01	0.61
1:C:645:ILE:O	1:C:649:GLN:N	2.29	0.61
1:A:2478:ASP:OD1	1:B:2471:ARG:NH2	2.35	0.60
1:A:1867:VAL:HG23	1:A:1868:LEU:HD22	1.81	0.60
1:B:1741:ILE:HG22	1:B:1788:VAL:HG11	1.82	0.60
1:B:1911:LEU:HB2	1:B:1940:THR:HG21	1.82	0.60
1:A:1960:VAL:HG23	1:A:1961:THR:HG23	1.83	0.60
1:B:1914:MET:HE1	1:B:1937:VAL:HG22	1.83	0.60
1:D:2467:ASN:OD1	1:D:2471:ARG:NH1	2.33	0.60
1:D:1741:ILE:HG21	1:D:1785:PHE:HE1	1.67	0.59
1:D:1912:ASP:OD2	1:D:1964:SER:OG	2.19	0.59
1:C:1930:ASN:O	1:C:1934:VAL:HG13	2.00	0.59
1:D:245:HIS:N	1:D:250:LYS:O	2.34	0.59
1:D:1761:LEU:HD13	1:D:1880:LEU:HD12	1.83	0.59
1:A:1734:THR:HG23	1:A:1772:PHE:CD1	2.37	0.59
1:C:751:ILE:O	1:C:755:LEU:N	2.34	0.59
1:C:2020:LEU:HD12	1:C:2020:LEU:O	2.01	0.59
1:C:2484:SER:OG	1:D:2401:ARG:NH1	2.35	0.59
1:A:2358:VAL:CG1	1:D:2511:LEU:HD13	2.32	0.59
1:C:1978:ILE:CD1	1:C:1989:VAL:HG23	2.32	0.59
1:D:2364:ARG:HD2	1:D:2523:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1789:LEU:O	1:A:1793:MET:N	2.36	0.59
1:D:2269:ILE:HD12	1:D:2285:LEU:HD11	1.85	0.59
1:D:1387:CYS:O	1:D:1391:LEU:N	2.35	0.58
1:D:2015:ARG:O	1:D:2015:ARG:NH1	2.35	0.58
1:A:245:HIS:O	1:A:249:GLU:N	2.36	0.58
1:B:1757:ALA:HB1	1:B:1876:PHE:CE1	2.37	0.58
1:B:1930:ASN:O	1:B:1934:VAL:HG13	2.03	0.58
1:B:1793:MET:CE	1:B:1903:LEU:HD22	2.34	0.58
1:B:2364:ARG:HD2	1:B:2523:LEU:HD11	1.84	0.58
1:D:14:VAL:N	1:D:57:PHE:O	2.36	0.58
1:D:1734:THR:HG22	1:D:1775:LEU:HD13	1.86	0.58
1:D:2172:PHE:CD2	1:D:2599:LEU:HD21	2.38	0.58
1:B:2059:GLN:OE1	1:B:2062:ARG:NH2	2.37	0.58
1:C:445:ALA:O	1:C:449:SER:N	2.30	0.58
1:D:1965:ASN:O	1:D:1969:ILE:HD12	2.03	0.58
1:D:2530:LYS:O	1:D:2534:LEU:HD23	2.04	0.58
1:B:1288:HIS:O	1:B:1292:THR:N	2.32	0.58
1:A:193:PRO:O	1:A:213:VAL:N	2.37	0.57
1:B:2598:ASN:OD1	1:B:2599:LEU:N	2.38	0.57
1:C:1977:ASP:OD1	1:C:1978:ILE:N	2.38	0.57
1:C:1978:ILE:HD12	1:C:1989:VAL:HG23	1.84	0.57
1:D:1785:PHE:O	1:D:1788:VAL:HG12	2.03	0.57
1:A:10:ILE:N	1:A:114:ASP:O	2.35	0.57
1:A:1783:GLU:OE1	1:A:1897:ASN:ND2	2.38	0.57
1:D:1933:ASN:O	1:D:1933:ASN:ND2	2.37	0.57
1:D:2026:VAL:HG21	1:D:2070:LEU:HD22	1.85	0.57
1:C:781:MET:O	1:C:786:VAL:N	2.33	0.57
1:D:1934:VAL:HG21	1:D:1988:LEU:HD13	1.86	0.57
1:B:1974:ILE:O	1:B:1993:LYS:NZ	2.34	0.57
1:B:1974:ILE:CD1	1:B:2000:LEU:HD12	2.35	0.57
1:D:696:TRP:O	1:D:704:HIS:CB	2.53	0.57
1:D:1447:ASP:O	1:D:1451:VAL:N	2.35	0.57
1:D:1741:ILE:HG23	1:D:1750:PHE:CE1	2.39	0.57
1:B:2007:ARG:NE	1:B:2012:ASN:OD1	2.36	0.57
1:C:2560:LYS:NZ	4:C:2702:ATP:O3A	2.37	0.57
1:B:1909:GLN:NE2	1:B:1913:ILE:HD11	2.20	0.56
1:A:1741:ILE:HG21	1:A:1785:PHE:CE1	2.40	0.56
1:D:794:VAL:N	1:D:872:TYR:O	2.37	0.56
1:A:1968:ASP:OD1	1:A:2019:SER:OG	2.20	0.56
1:D:1101:ALA:O	1:D:1104:VAL:N	2.34	0.56
1:D:2476:VAL:HG22	1:D:2480:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1741:ILE:HG23	1:B:1750:PHE:CE1	2.41	0.56
1:C:1933:ASN:O	1:C:1937:VAL:HG23	2.05	0.56
1:C:513:ASN:O	1:C:517:GLN:N	2.35	0.56
1:A:2543:LEU:HD23	1:A:2548:PHE:CE1	2.40	0.56
1:C:877:SER:O	1:C:881:LEU:N	2.35	0.56
1:D:2017:LEU:HD23	1:D:2020:LEU:HD11	1.88	0.56
1:A:2358:VAL:HG12	1:D:2511:LEU:HD13	1.88	0.56
1:D:1659:GLU:HA	1:D:1749:ILE:HD11	1.88	0.55
1:D:2598:ASN:OD1	1:D:2599:LEU:N	2.40	0.55
1:B:1744:THR:HG21	1:B:1749:ILE:HG21	1.88	0.55
1:B:2474:GLY:O	1:C:2471:ARG:NH1	2.40	0.55
1:C:853:ASN:O	1:C:857:ASN:N	2.36	0.55
1:C:2211:LEU:HD22	1:C:2285:LEU:HD22	1.88	0.55
1:A:1505:THR:O	1:A:1509:LEU:N	2.35	0.55
1:C:2543:LEU:HD23	1:C:2548:PHE:CZ	2.41	0.55
1:D:2468:HIS:HB3	1:D:2479:ILE:HD13	1.89	0.55
1:D:1895:GLN:OE1	1:D:1901:TYR:N	2.40	0.54
1:B:1740:LEU:HD21	1:B:1749:ILE:CG2	2.38	0.54
1:C:781:MET:O	1:C:785:HIS:N	2.41	0.54
1:C:2200:ARG:O	1:C:2204:TRP:NE1	2.40	0.54
1:C:2543:LEU:HD23	1:C:2548:PHE:CE1	2.43	0.54
1:C:1732:GLY:O	1:C:1736:LEU:N	2.38	0.54
1:D:2059:GLN:OE1	1:D:2062:ARG:NH1	2.40	0.54
1:A:2376:ALA:HB2	1:A:2508:VAL:HG11	1.90	0.54
1:A:1971:THR:HG23	1:A:2020:LEU:HB3	1.89	0.54
1:C:458:LYS:O	1:C:462:GLY:N	2.41	0.54
1:C:1908:LEU:HD11	1:C:1966:GLY:HA3	1.91	0.53
1:C:523:LYS:O	1:C:527:ARG:N	2.39	0.53
1:C:2163:GLU:OE2	1:C:2164:GLN:NE2	2.42	0.53
1:D:267:THR:N	1:D:413:ILE:O	2.40	0.53
1:D:1777:MET:HE2	1:D:1777:MET:HA	1.90	0.53
1:A:1910:PHE:CE2	1:A:1936:LEU:HD21	2.43	0.53
1:A:1965:ASN:O	1:A:1968:ASP:N	2.40	0.53
1:B:1977:ASP:OD1	1:B:1978:ILE:N	2.42	0.53
1:B:2574:LEU:HA	1:B:2577:VAL:HG12	1.91	0.53
1:C:2376:ALA:HB2	1:C:2508:VAL:HG11	1.90	0.53
1:B:2359:ILE:O	1:B:2363:THR:HG22	2.08	0.53
1:C:696:TRP:O	1:C:704:HIS:N	2.42	0.53
1:A:1933:ASN:O	1:A:1937:VAL:HG23	2.08	0.53
1:A:1970:ILE:HA	1:A:1973:LEU:HD12	1.90	0.53
1:C:2184:TRP:NE1	1:C:2302:GLY:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1871:GLN:HB3	1:B:1872:PRO:HD3	1.91	0.53
1:B:1908:LEU:HD11	1:B:1966:GLY:HA3	1.91	0.53
1:A:525:PRO:O	1:A:536:VAL:N	2.39	0.53
1:B:1527:ARG:O	1:B:1530:ALA:HB3	2.09	0.53
1:C:2501:PHE:CE2	1:C:2506:ILE:HD11	2.44	0.53
1:A:2066:GLN:CD	1:A:2070:LEU:HD11	2.28	0.53
1:B:1876:PHE:CZ	1:B:1880:LEU:HD11	2.44	0.53
1:C:1790:HIS:O	1:C:1794:LYS:N	2.41	0.53
1:D:513:ASN:O	1:D:517:GLN:N	2.34	0.52
1:A:391:HIS:O	1:A:395:ASN:N	2.38	0.52
1:C:1641:GLY:O	1:C:1645:SER:N	2.39	0.52
1:B:1974:ILE:HD12	1:B:2000:LEU:HD12	1.90	0.52
1:D:714:GLU:O	1:D:718:GLY:N	2.40	0.52
1:B:2511:LEU:HD13	1:C:2358:VAL:HG12	1.92	0.52
1:A:1954:GLU:N	1:A:1954:GLU:OE1	2.42	0.52
1:B:2476:VAL:HG22	1:B:2480:LEU:CD1	2.40	0.52
1:A:1904:VAL:HG23	1:A:1947:TYR:HD2	1.75	0.52
1:A:2160:GLU:OE2	1:A:2530:LYS:NZ	2.40	0.52
1:C:1615:SER:O	1:C:1619:ASP:N	2.40	0.52
1:B:1740:LEU:HD23	1:B:1740:LEU:C	2.30	0.52
1:B:2501:PHE:CZ	1:B:2506:ILE:HD11	2.45	0.52
1:B:2560:LYS:NZ	4:B:2702:ATP:O3A	2.43	0.51
1:C:816:ASP:O	1:C:820:ASN:N	2.42	0.51
1:C:1934:VAL:HG11	1:C:1981:LEU:HD21	1.91	0.51
1:A:1876:PHE:CE1	1:A:1880:LEU:HD11	2.44	0.51
1:B:2511:LEU:HD22	1:C:2358:VAL:HG13	1.92	0.51
1:C:760:ILE:O	1:C:764:MET:N	2.44	0.51
1:C:2511:LEU:HD13	1:D:2358:VAL:HG12	1.92	0.51
1:A:2155:LEU:CD2	1:A:2178:LEU:HD11	2.39	0.51
1:B:2504:VAL:HG12	1:B:2504:VAL:O	2.11	0.51
1:C:2543:LEU:HD21	1:C:2610:LEU:HD22	1.92	0.51
1:D:1770:LYS:HA	1:D:1770:LYS:HE2	1.91	0.51
1:A:1785:PHE:O	1:A:1788:VAL:HG12	2.11	0.51
1:B:1793:MET:HE2	1:B:1903:LEU:HD22	1.92	0.51
1:D:1741:ILE:HG23	1:D:1750:PHE:HE1	1.76	0.51
1:A:2376:ALA:O	1:A:2380:VAL:HG23	2.11	0.50
1:B:1373:ALA:O	1:B:1377:GLU:N	2.44	0.50
1:A:1734:THR:HG22	1:A:1775:LEU:HD13	1.93	0.50
1:B:1985:ARG:HE	1:B:1988:LEU:HD12	1.76	0.50
1:D:1876:PHE:CE1	1:D:1880:LEU:HD11	2.46	0.50
1:D:2376:ALA:HB2	1:D:2508:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1960:VAL:HG13	1:A:2003:LEU:HD22	1.92	0.50
1:D:166:PRO:O	1:D:169:LYS:N	2.43	0.50
1:A:1734:THR:HG23	1:A:1772:PHE:HD1	1.77	0.50
1:C:1635:TYR:O	1:C:1639:GLU:N	2.45	0.50
1:A:2504:VAL:HG12	1:A:2504:VAL:O	2.11	0.49
1:B:2021:ARG:HA	1:B:2021:ARG:NE	2.27	0.49
1:C:2504:VAL:HG12	1:C:2504:VAL:O	2.12	0.49
1:A:1934:VAL:HG21	1:A:1988:LEU:HD22	1.95	0.49
1:B:1930:ASN:OD1	1:B:1933:ASN:N	2.45	0.49
1:A:671:ARG:O	1:A:691:GLU:N	2.45	0.49
1:B:481:PHE:O	1:B:485:ASP:N	2.46	0.49
1:C:2033:TYR:O	1:C:2047:ARG:NH1	2.45	0.49
1:A:1741:ILE:HG21	1:A:1785:PHE:HE1	1.78	0.49
1:D:2153:HIS:CE1	1:D:2157:THR:HG21	2.47	0.49
1:C:2278:ILE:O	1:C:2280:PRO:HD2	2.13	0.49
1:A:2511:LEU:HD21	1:B:2362:VAL:CG2	2.42	0.49
1:B:1740:LEU:HD22	1:B:1753:SER:OG	2.11	0.49
1:A:267:THR:N	1:A:413:ILE:O	2.37	0.49
1:C:714:GLU:O	1:C:718:GLY:N	2.40	0.49
1:C:1930:ASN:OD1	1:C:1933:ASN:N	2.45	0.49
1:A:853:ASN:O	1:A:857:ASN:N	2.43	0.49
1:A:1930:ASN:O	1:A:1934:VAL:HG13	2.13	0.49
1:B:1734:THR:HG22	1:B:1775:LEU:HD13	1.95	0.49
1:A:1904:VAL:HG23	1:A:1947:TYR:CD2	2.48	0.48
1:A:1910:PHE:HE2	1:A:1936:LEU:HD21	1.78	0.48
1:A:2501:PHE:CE2	1:A:2506:ILE:HD11	2.47	0.48
1:A:2275:TYR:HD2	1:A:2276:LEU:HD12	1.78	0.48
1:C:455:ALA:O	1:C:459:LEU:N	2.38	0.48
1:D:1911:LEU:HB2	1:D:1940:THR:HG21	1.94	0.48
1:D:2504:VAL:HG12	1:D:2504:VAL:O	2.13	0.48
1:A:1761:LEU:HD11	1:A:1772:PHE:CE2	2.48	0.48
1:C:1232:LEU:O	1:C:1236:CYS:N	2.47	0.48
1:B:2007:ARG:NH2	1:B:2009:ASP:OD2	2.46	0.48
1:B:2571:PHE:HE2	1:B:2590:VAL:HG21	1.79	0.48
1:C:1903:LEU:HA	1:C:1906:GLU:HG3	1.96	0.48
1:B:622:VAL:O	1:B:626:ARG:N	2.38	0.48
1:B:1757:ALA:HB1	1:B:1876:PHE:HE1	1.77	0.48
1:C:1871:GLN:HB3	1:C:1872:PRO:HD3	1.96	0.48
1:B:2575:VAL:O	1:B:2583:TYR:OH	2.15	0.48
1:C:1924:LEU:HD23	1:C:1924:LEU:H	1.79	0.48
1:B:2022:PRO:HB3	1:B:2067:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:TYR:O	1:D:174:GLY:N	2.46	0.48
1:A:2468:HIS:CB	1:A:2479:ILE:HD13	2.44	0.47
1:A:2571:PHE:HE2	1:A:2590:VAL:HG21	1.78	0.47
1:B:1741:ILE:HG22	1:B:1788:VAL:CG1	2.43	0.47
1:B:2014:GLU:O	1:B:2018:ILE:HG12	2.14	0.47
1:D:1904:VAL:HG21	1:D:1955:ASN:OD1	2.15	0.47
1:D:2022:PRO:HB3	1:D:2067:LEU:HD13	1.95	0.47
1:A:2200:ARG:O	1:A:2204:TRP:NE1	2.47	0.47
1:B:1761:LEU:HD13	1:B:1880:LEU:HD12	1.96	0.47
1:B:1770:LYS:O	1:B:1774:ASN:ND2	2.47	0.47
1:D:2020:LEU:HD12	1:D:2020:LEU:O	2.14	0.47
1:B:1949:GLN:HA	1:B:2002:ALA:HB1	1.95	0.47
1:B:2018:ILE:O	1:B:2021:ARG:NH1	2.47	0.47
1:C:1912:ASP:O	1:C:1916:GLY:N	2.48	0.47
1:D:1897:ASN:ND2	1:D:1899:THR:O	2.48	0.47
1:A:1881:CYS:SG	1:A:1892:LEU:HD12	2.55	0.47
1:B:1971:THR:HG23	1:B:2020:LEU:HB3	1.96	0.47
1:B:2045:SER:N	1:B:2048:GLU:OE2	2.48	0.47
1:A:1949:GLN:HA	1:A:2002:ALA:HB1	1.97	0.47
1:B:1797:GLN:NE2	1:B:1906:GLU:O	2.48	0.47
1:D:1784:ARG:O	1:D:1787:LYS:HB3	2.15	0.47
1:B:1725:GLN:OE1	1:B:1765:ASN:ND2	2.43	0.47
1:C:2017:LEU:O	1:C:2021:ARG:NH2	2.48	0.47
1:D:2070:LEU:O	1:D:2070:LEU:HD23	2.15	0.47
1:A:1790:HIS:O	1:A:1794:LYS:N	2.47	0.46
1:B:508:LEU:O	1:B:512:GLN:N	2.48	0.46
1:D:1442:GLU:O	1:D:1446:LEU:N	2.48	0.46
1:D:1740:LEU:HD23	1:D:1740:LEU:O	2.15	0.46
1:A:2476:VAL:HG22	1:A:2480:LEU:CD1	2.45	0.46
1:D:1914:MET:CE	1:D:1937:VAL:HG22	2.46	0.46
1:A:1373:ALA:O	1:A:1377:GLU:N	2.48	0.46
1:A:1904:VAL:HG21	1:A:1955:ASN:OD1	2.16	0.46
1:C:1910:PHE:CE2	1:C:1936:LEU:HD21	2.50	0.46
1:D:1725:GLN:HB3	1:D:1768:ILE:HD11	1.98	0.46
1:A:2016:ILE:HG22	1:A:2020:LEU:CD2	2.45	0.46
1:B:2017:LEU:HD23	1:B:2020:LEU:HD11	1.98	0.46
1:C:1757:ALA:HB1	1:C:1876:PHE:CE1	2.50	0.46
1:C:2151:THR:OG1	1:C:2181:GLU:OE2	2.33	0.46
1:A:2540:ILE:HD11	1:A:2565:MET:CB	2.45	0.46
1:A:2543:LEU:HD23	1:A:2548:PHE:CZ	2.51	0.46
1:B:2017:LEU:O	1:B:2021:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1934:VAL:CG2	1:C:1988:LEU:HD22	2.46	0.46
1:A:2278:ILE:O	1:A:2280:PRO:HD2	2.16	0.46
1:C:1876:PHE:CZ	1:C:1880:LEU:HD11	2.51	0.46
1:C:1953:HIS:NE2	1:C:2006:SER:O	2.45	0.46
1:D:1950:GLY:O	1:D:1952:CYS:N	2.49	0.46
1:A:2163:GLU:OE2	1:A:2164:GLN:NE2	2.49	0.46
1:C:2513:PHE:CZ	1:C:2517:ILE:HD11	2.51	0.46
1:A:2598:ASN:OD1	1:A:2599:LEU:N	2.49	0.46
1:B:1741:ILE:HG23	1:B:1750:PHE:CD1	2.51	0.46
1:A:1725:GLN:NE2	1:A:1759:HIS:O	2.48	0.45
1:A:2135:GLN:HB2	1:A:2608:MET:HE1	1.98	0.45
1:B:2485:LYS:NZ	1:C:2453:ARG:O	2.29	0.45
1:B:2278:ILE:O	1:B:2280:PRO:HD2	2.16	0.45
1:D:1338:ASP:O	1:D:1342:LEU:N	2.40	0.45
1:A:1761:LEU:HD11	1:A:1772:PHE:HE2	1.81	0.45
1:B:1876:PHE:O	1:B:1880:LEU:HD13	2.16	0.45
1:C:1971:THR:HG23	1:C:2020:LEU:HB3	1.99	0.45
1:D:2549:ASP:OD1	1:D:2549:ASP:O	2.35	0.45
1:C:441:ASP:O	1:C:445:ALA:N	2.42	0.45
1:C:2058:LEU:HD23	1:C:2071:LEU:CD2	2.47	0.45
1:A:2560:LYS:NZ	4:A:2703:ATP:O2G	2.27	0.45
1:C:1934:VAL:HG11	1:C:1981:LEU:CD2	2.47	0.45
1:D:2163:GLU:OE2	1:D:2164:GLN:NE2	2.49	0.45
1:D:2468:HIS:CB	1:D:2479:ILE:HD13	2.47	0.45
1:D:2507:ILE:O	1:D:2511:LEU:N	2.48	0.45
1:D:1762:ASP:OD1	1:D:1763:GLY:N	2.49	0.45
1:D:1875:ARG:CZ	1:D:1879:LEU:HD21	2.46	0.45
1:D:2398:GLU:N	1:D:2398:GLU:OE1	2.50	0.45
1:B:2589:TYR:CZ	1:B:2593:MET:HE3	2.52	0.45
1:D:1877:LEU:HD13	1:D:1947:TYR:OH	2.16	0.45
1:D:2560:LYS:NZ	4:D:2703:ATP:O2G	2.26	0.45
1:B:2054:TYR:CE2	1:B:2058:LEU:HD11	2.52	0.44
1:C:2476:VAL:HG22	1:C:2480:LEU:CD1	2.48	0.44
1:D:1232:LEU:O	1:D:1236:CYS:N	2.50	0.44
1:D:2278:ILE:O	1:D:2280:PRO:HD2	2.18	0.44
1:B:1994:ASP:OD1	1:B:2052:ASN:ND2	2.49	0.44
1:B:2144:CYS:HA	1:B:2182:MET:CE	2.47	0.44
1:D:1871:GLN:HB2	1:D:1872:PRO:HD3	1.99	0.44
1:D:2328:LEU:C	1:D:2328:LEU:HD23	2.38	0.44
1:B:1793:MET:HE1	1:B:1903:LEU:HD22	1.99	0.44
1:C:780:LEU:O	1:C:784:VAL:N	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2054:TYR:HE1	1:C:2058:LEU:HD11	1.83	0.44
1:D:1772:PHE:O	1:D:1776:MET:SD	2.76	0.44
1:B:1754:ILE:O	1:B:1758:ILE:HG12	2.18	0.44
1:B:1925:LEU:HD11	1:B:1972:ALA:CB	2.47	0.44
1:B:1788:VAL:HG22	1:B:1788:VAL:O	2.17	0.44
1:D:2299:SER:O	1:D:2303:ASN:N	2.51	0.44
1:A:168:TRP:N	1:A:182:LYS:O	2.51	0.44
1:D:2269:ILE:HD11	1:D:2285:LEU:HD21	2.00	0.44
1:C:2268:LEU:C	1:C:2268:LEU:HD23	2.38	0.44
1:A:2400:ASP:O	1:D:2481:ARG:NH1	2.48	0.44
1:B:2268:LEU:HD23	1:B:2268:LEU:C	2.39	0.44
1:C:1026:ASP:O	1:C:1029:GLY:N	2.51	0.43
1:D:2467:ASN:O	1:D:2471:ARG:NH1	2.51	0.43
1:C:1338:ASP:O	1:C:1342:LEU:N	2.38	0.43
1:C:1926:GLY:HA2	1:C:1978:ILE:HG23	2.00	0.43
1:C:1974:ILE:CD1	1:C:2000:LEU:HD12	2.48	0.43
1:A:1784:ARG:O	1:A:1787:LYS:HB3	2.19	0.43
1:A:1965:ASN:O	1:A:1969:ILE:HD12	2.18	0.43
1:A:2359:ILE:O	1:A:2363:THR:HG22	2.19	0.43
1:A:2574:LEU:HA	1:A:2577:VAL:HG12	2.00	0.43
1:B:2144:CYS:HA	1:B:2182:MET:HE3	1.99	0.43
1:A:2465:VAL:HG22	1:A:2476:VAL:HG21	2.01	0.43
1:B:1741:ILE:HG23	1:B:1750:PHE:HE1	1.83	0.43
1:D:10:ILE:O	1:D:113:GLY:N	2.41	0.43
1:A:308:HIS:O	1:A:312:GLY:N	2.48	0.43
1:C:1987:ASP:OD1	1:C:1988:LEU:N	2.52	0.43
1:D:1719:SER:O	1:D:1723:ALA:N	2.42	0.43
1:B:1871:GLN:OE1	1:B:1939:GLN:HG3	2.19	0.43
1:B:2364:ARG:CD	1:B:2523:LEU:HD11	2.49	0.43
1:D:1067:TYR:O	1:D:1071:VAL:N	2.47	0.43
1:A:1876:PHE:O	1:A:1880:LEU:HD13	2.19	0.43
1:B:1727:ARG:O	1:B:1731:GLU:HG2	2.19	0.43
1:B:1750:PHE:O	1:B:1753:SER:OG	2.30	0.43
1:C:1773:HIS:CB	1:C:1888:LEU:HD21	2.49	0.43
1:D:1742:THR:O	1:D:1784:ARG:NH1	2.52	0.43
1:D:1876:PHE:CE1	1:D:1880:LEU:CD1	3.02	0.43
1:C:1720:ALA:O	1:C:1723:ALA:N	2.52	0.42
1:A:1908:LEU:HD11	1:A:1966:GLY:HA3	2.01	0.42
1:B:1650:HIS:O	1:B:1654:LEU:CB	2.67	0.42
1:C:452:LEU:O	1:C:456:VAL:N	2.37	0.42
1:A:1744:THR:HG22	1:A:1746:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1880:LEU:HD23	1:B:1888:LEU:HD22	2.01	0.42
1:D:2140:VAL:HG23	1:D:2140:VAL:O	2.19	0.42
1:D:2546:ASP:OD1	1:D:2547:LYS:N	2.52	0.42
1:D:2575:VAL:HG13	1:D:2591:ALA:HB2	2.01	0.42
1:A:1737:VAL:HG12	1:A:1756:LEU:HD23	2.01	0.42
1:A:1950:GLY:O	1:A:1952:CYS:N	2.46	0.42
1:C:1606:LEU:O	1:C:1609:LEU:N	2.53	0.42
1:C:2054:TYR:CE2	1:C:2071:LEU:HD11	2.54	0.42
1:D:126:HIS:O	1:D:130:ASN:N	2.48	0.42
1:A:2130:ASP:OD1	1:A:2132:SER:OG	2.26	0.42
1:A:2145:GLN:HA	1:A:2145:GLN:OE1	2.20	0.42
1:A:2468:HIS:HB3	1:A:2479:ILE:HD13	2.01	0.42
1:B:2215:ILE:HG23	1:B:2282:LEU:CD1	2.49	0.42
1:D:2574:LEU:HA	1:D:2577:VAL:HG12	2.01	0.42
1:A:2021:ARG:CZ	1:A:2021:ARG:HA	2.49	0.42
1:B:1938:ILE:HG23	1:B:1995:ASN:OD1	2.19	0.42
1:B:2278:ILE:C	1:B:2280:PRO:HD2	2.40	0.42
1:D:2560:LYS:NZ	4:D:2703:ATP:O3A	2.53	0.42
1:B:1758:ILE:HD11	1:B:1876:PHE:HB2	2.02	0.42
1:B:1925:LEU:HD11	1:B:1972:ALA:HB1	2.01	0.42
1:B:2376:ALA:HB2	1:B:2508:VAL:CG1	2.50	0.42
1:C:2135:GLN:HB2	1:C:2608:MET:HE1	2.02	0.42
1:C:2501:PHE:CZ	1:C:2506:ILE:HD11	2.54	0.42
1:C:2577:VAL:HG22	1:C:2577:VAL:O	2.20	0.42
1:D:841:LEU:O	1:D:845:VAL:N	2.53	0.42
1:D:1952:CYS:O	1:D:1953:HIS:HB2	2.20	0.42
1:B:1929:ILE:CG2	1:B:1934:VAL:HG12	2.50	0.41
1:B:2058:LEU:HD12	1:B:2071:LEU:HD21	2.01	0.41
1:C:1970:ILE:HA	1:C:1973:LEU:HD12	2.02	0.41
1:D:1970:ILE:HD12	1:D:1999:LEU:HD23	2.02	0.41
1:B:2020:LEU:HD12	1:B:2020:LEU:O	2.20	0.41
1:C:2519:THR:O	1:C:2523:LEU:HD13	2.19	0.41
1:A:1895:GLN:NE2	1:A:1901:TYR:O	2.53	0.41
1:A:1734:THR:HG23	1:A:1772:PHE:CE1	2.54	0.41
1:A:1925:LEU:HD23	1:A:1925:LEU:H	1.85	0.41
1:A:2501:PHE:CZ	1:A:2506:ILE:HD11	2.55	0.41
1:B:1914:MET:HE3	1:B:1937:VAL:HG22	2.00	0.41
1:B:2604:ARG:HE	1:B:2605:MET:HG2	1.85	0.41
1:B:1406:ILE:O	1:B:1410:LYS:N	2.41	0.41
1:B:1934:VAL:CG2	1:B:1988:LEU:HD13	2.38	0.41
1:B:1945:THR:HG22	1:B:1949:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1745:LYS:HE3	1:D:1745:LYS:HA	2.02	0.41
1:D:2184:TRP:NE1	1:D:2302:GLY:O	2.49	0.41
1:D:2544:GLU:OE1	1:D:2544:GLU:N	2.47	0.41
1:B:2200:ARG:O	1:B:2204:TRP:NE1	2.53	0.41
1:D:2163:GLU:CD	1:D:2164:GLN:HE21	2.24	0.41
1:A:2294:ILE:O	1:A:2298:VAL:HG23	2.21	0.41
1:B:2483:PRO:O	1:C:2399:VAL:HG12	2.20	0.41
1:B:2541:CYS:O	1:B:2604:ARG:NH2	2.53	0.41
1:C:1910:PHE:CZ	1:C:1936:LEU:HD21	2.56	0.41
1:C:2058:LEU:HD23	1:C:2071:LEU:HD23	2.03	0.41
1:A:1776:MET:HE2	1:A:1782:SER:HA	2.03	0.41
1:A:2293:LYS:O	1:A:2297:VAL:HG23	2.20	0.41
1:B:1871:GLN:CB	1:B:1872:PRO:HD3	2.50	0.41
1:B:1974:ILE:HD12	1:B:2000:LEU:CD1	2.51	0.41
1:D:1740:LEU:HD22	1:D:1753:SER:HB3	2.01	0.41
1:D:2593:MET:SD	1:D:2598:ASN:ND2	2.93	0.41
1:B:2151:THR:OG1	1:B:2181:GLU:OE2	2.39	0.41
1:C:2140:VAL:O	1:C:2140:VAL:HG23	2.20	0.41
1:C:2574:LEU:HA	1:C:2577:VAL:HG12	2.03	0.41
1:D:1788:VAL:O	1:D:1788:VAL:HG22	2.20	0.41
1:D:2295:VAL:O	1:D:2298:VAL:HG12	2.20	0.41
1:D:116:VAL:O	1:D:177:VAL:N	2.41	0.41
1:A:1754:ILE:HG21	1:A:1872:PRO:HB2	2.03	0.40
1:A:2323:HIS:O	1:A:2327:ILE:HG13	2.21	0.40
1:B:2140:VAL:O	1:B:2140:VAL:HG23	2.21	0.40
1:C:1960:VAL:HG23	1:C:1961:THR:HG23	2.03	0.40
1:D:1741:ILE:HG22	1:D:1788:VAL:HG11	2.03	0.40
1:D:1914:MET:HE3	1:D:1937:VAL:HG22	2.02	0.40
1:D:2014:GLU:O	1:D:2018:ILE:HG13	2.21	0.40
1:C:2295:VAL:O	1:C:2298:VAL:HG12	2.21	0.40
1:C:1865:THR:O	1:C:1865:THR:HG22	2.20	0.40
1:C:1911:LEU:HB2	1:C:1940:THR:HG21	2.03	0.40
1:D:2476:VAL:HG22	1:D:2480:LEU:HD11	2.02	0.40
1:C:1871:GLN:OE1	1:C:1939:GLN:HG3	2.21	0.40
1:D:15:SER:O	1:D:222:ASN:N	2.54	0.40
1:B:2131:ARG:NH2	1:B:2600:ASP:OD2	2.55	0.40
1:B:2398:GLU:OE1	1:B:2398:GLU:N	2.55	0.40
1:C:2051:HIS:O	1:C:2055:ILE:HG12	2.22	0.40
1:C:2212:ALA:O	1:C:2216:ASN:ND2	2.54	0.40
1:D:1725:GLN:OE1	1:D:1765:ASN:ND2	2.49	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	1964/2633 (75%)	1875 (96%)	89 (4%)	0	100	100
1	B	1614/2633 (61%)	1560 (97%)	54 (3%)	0	100	100
1	C	1535/2633 (58%)	1469 (96%)	66 (4%)	0	100	100
1	D	1956/2633 (74%)	1866 (95%)	90 (5%)	0	100	100
All	All	7069/10532 (67%)	6770 (96%)	299 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/2329 (26%)	609 (100%)	0	100	100
1	B	613/2329 (26%)	613 (100%)	0	100	100
1	C	555/2329 (24%)	555 (100%)	0	100	100
1	D	605/2329 (26%)	603 (100%)	2 (0%)	92	96
All	All	2382/9316 (26%)	2380 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1933	ASN
1	D	2592	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1797	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	D	2703	-	26,33,33	0.61	0	31,52,52	1.06	2 (6%)
4	ATP	B	2702	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
3	I3P	D	2702	-	24,24,24	1.30	3 (12%)	36,39,39	0.65	0
4	ATP	C	2702	-	26,33,33	0.60	0	31,52,52	1.06	2 (6%)
4	ATP	A	2703	-	26,33,33	0.62	0	31,52,52	1.06	2 (6%)
3	I3P	A	2702	-	24,24,24	1.30	3 (12%)	36,39,39	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	2703	-	-	8/18/38/38	0/3/3/3
4	ATP	B	2702	-	-	10/18/38/38	0/3/3/3
3	I3P	D	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	C	2702	-	-	5/18/38/38	0/3/3/3
4	ATP	A	2703	-	-	9/18/38/38	0/3/3/3
3	I3P	A	2702	-	-	2/15/39/39	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2702	I3P	P4-O4	3.17	1.65	1.59
3	D	2702	I3P	P5-O5	3.17	1.65	1.59
3	A	2702	I3P	P5-O5	3.14	1.65	1.59
3	D	2702	I3P	P4-O4	3.14	1.65	1.59
3	A	2702	I3P	P1-O1	3.11	1.65	1.59
3	D	2702	I3P	P1-O1	3.09	1.65	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2702	ATP	C5-C6-N6	2.32	123.89	120.35
4	A	2703	ATP	C5-C6-N6	2.32	123.88	120.35
4	D	2703	ATP	C5-C6-N6	2.30	123.85	120.35
4	C	2702	ATP	C5-C6-N6	2.30	123.84	120.35
4	C	2702	ATP	PB-O3B-PG	2.06	139.89	132.83
4	A	2703	ATP	PB-O3B-PG	2.04	139.84	132.83
4	D	2703	ATP	PB-O3B-PG	2.03	139.80	132.83
4	B	2702	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2702	I3P	C5-O5-P5-O51
4	A	2703	ATP	PB-O3B-PG-O2G
4	A	2703	ATP	C5'-O5'-PA-O1A
4	B	2702	ATP	PB-O3B-PG-O2G
4	B	2702	ATP	C5'-O5'-PA-O3A
4	C	2702	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	C	2702	ATP	O4'-C4'-C5'-O5'
4	D	2703	ATP	PB-O3B-PG-O2G
4	D	2703	ATP	C5'-O5'-PA-O1A
4	A	2703	ATP	O4'-C4'-C5'-O5'
4	B	2702	ATP	O4'-C4'-C5'-O5'
4	D	2703	ATP	O4'-C4'-C5'-O5'
4	C	2702	ATP	PB-O3B-PG-O1G
4	A	2703	ATP	PB-O3A-PA-O1A
4	B	2702	ATP	C3'-C4'-C5'-O5'
3	A	2702	I3P	C3-C4-O4-P4
3	D	2702	I3P	C1-O1-P1-O13
3	D	2702	I3P	C5-O5-P5-O53
4	A	2703	ATP	C5'-O5'-PA-O3A
4	A	2703	ATP	PA-O3A-PB-O2B
4	D	2703	ATP	PA-O3A-PB-O2B
4	B	2702	ATP	C5'-O5'-PA-O1A
4	B	2702	ATP	PA-O3A-PB-O2B
4	C	2702	ATP	PA-O3A-PB-O1B
4	D	2703	ATP	PB-O3A-PA-O2A
4	B	2702	ATP	PB-O3B-PG-O1G
4	D	2703	ATP	PB-O3B-PG-O1G
4	A	2703	ATP	PB-O3B-PG-O3G
4	B	2702	ATP	PB-O3B-PG-O3G
3	A	2702	I3P	C5-C4-O4-P4
4	D	2703	ATP	C5'-O5'-PA-O3A
4	A	2703	ATP	PA-O3A-PB-O1B
4	A	2703	ATP	PB-O3A-PA-O2A
4	B	2702	ATP	PB-O3A-PA-O1A
4	B	2702	ATP	PB-O3A-PA-O2A
4	C	2702	ATP	PA-O3A-PB-O2B
4	D	2703	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

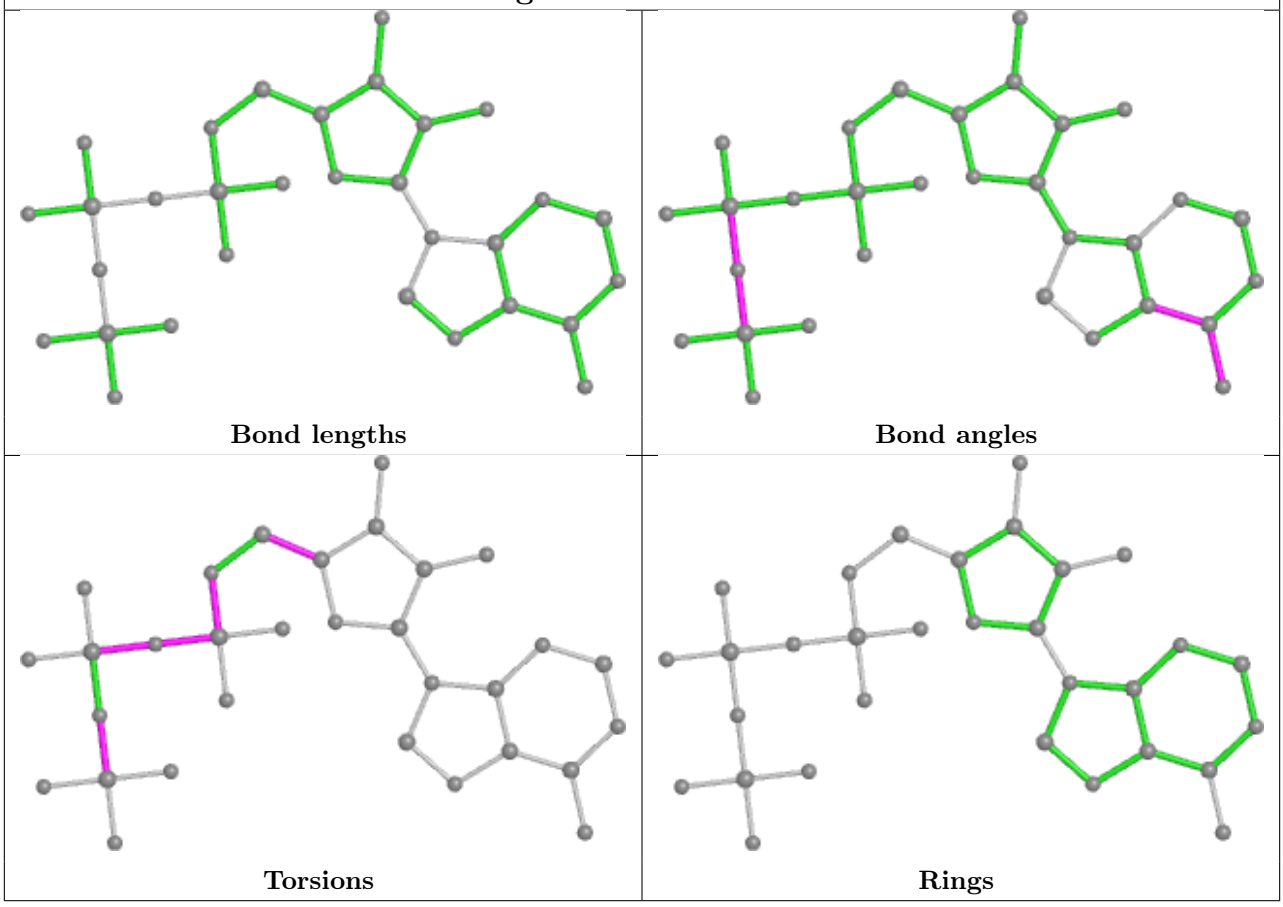
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2703	ATP	2	0
4	B	2702	ATP	1	0
4	C	2702	ATP	1	0
4	A	2703	ATP	1	0

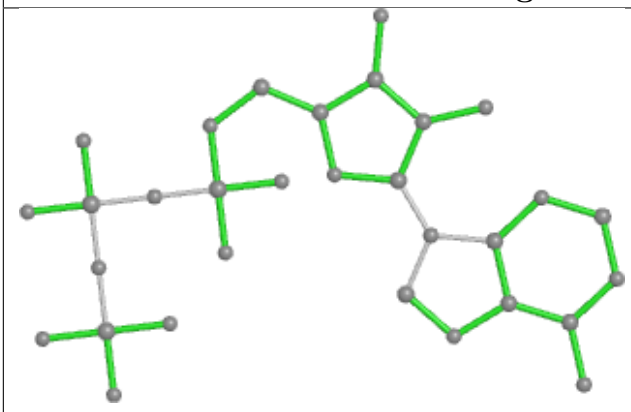
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

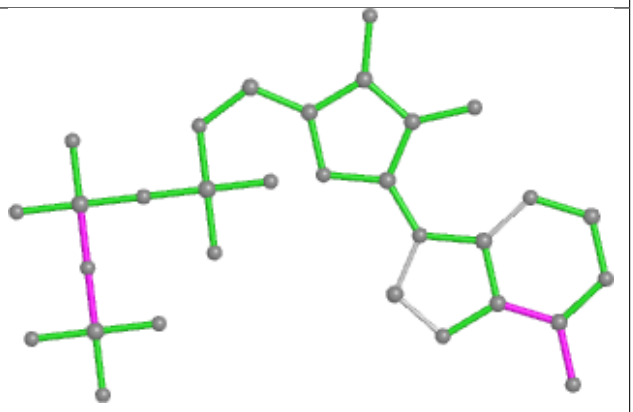
Ligand ATP D 2703



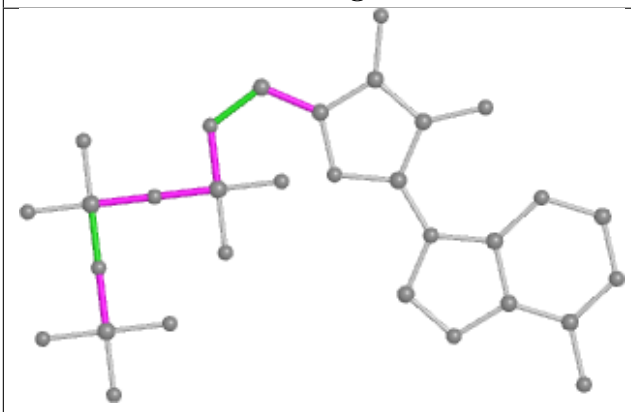
Ligand ATP B 2702



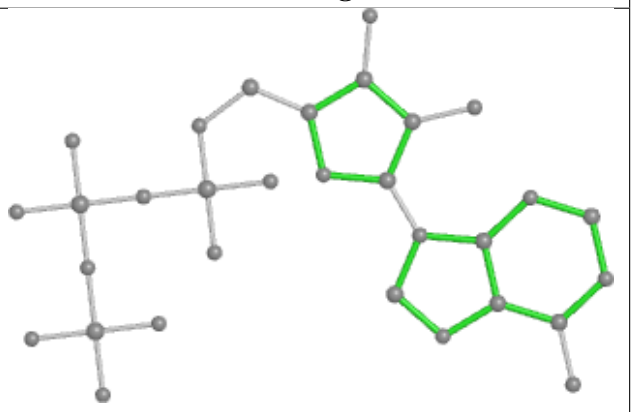
Bond lengths



Bond angles

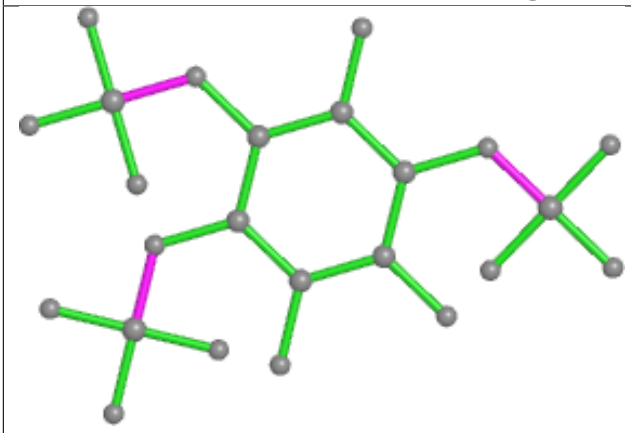


Torsions

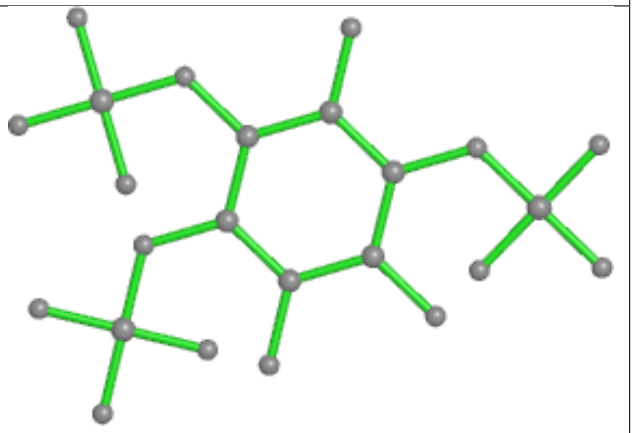


Rings

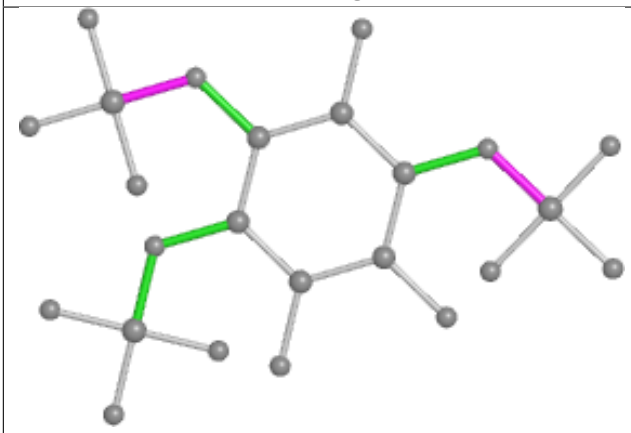
Ligand I3P D 2702



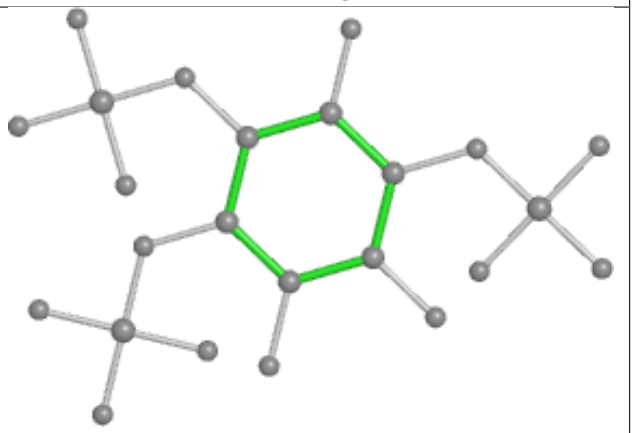
Bond lengths



Bond angles

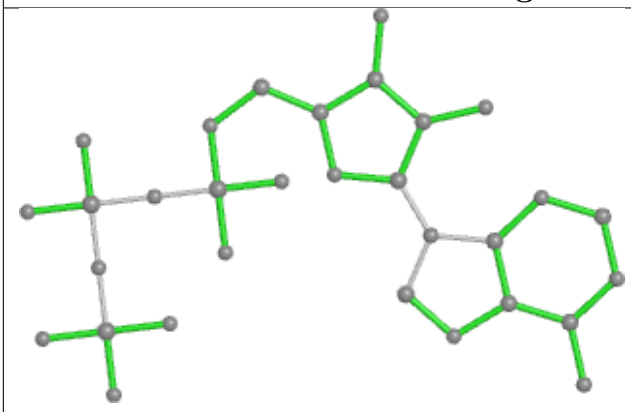


Torsions

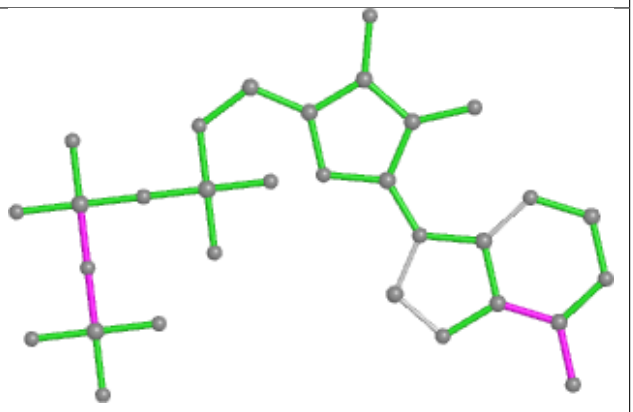


Rings

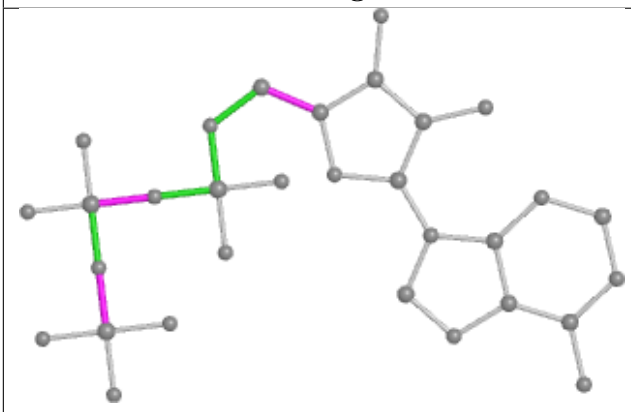
Ligand ATP C 2702



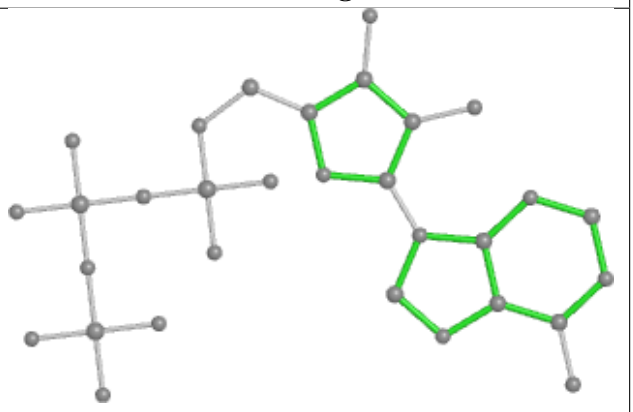
Bond lengths



Bond angles

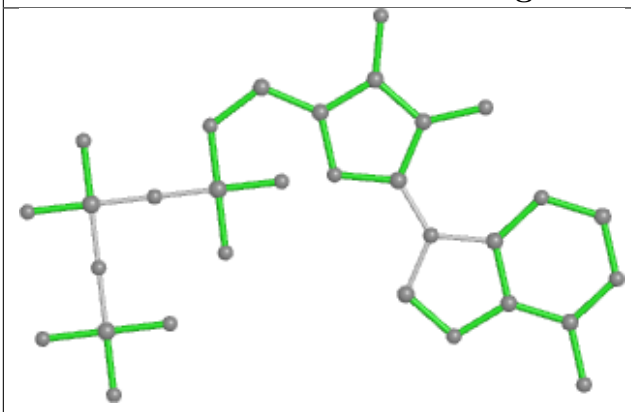


Torsions

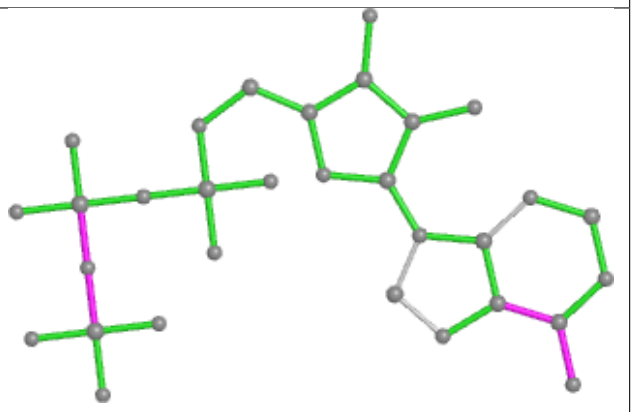


Rings

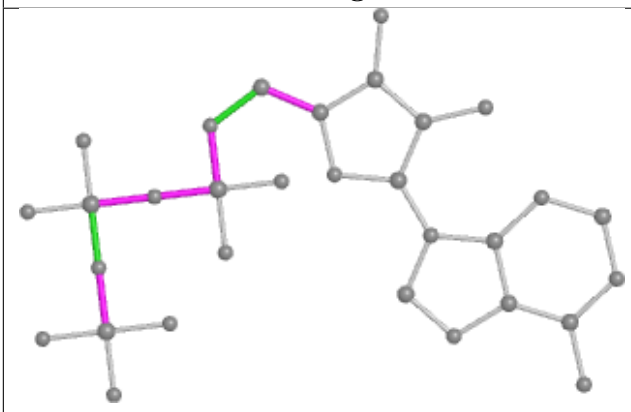
Ligand ATP A 2703



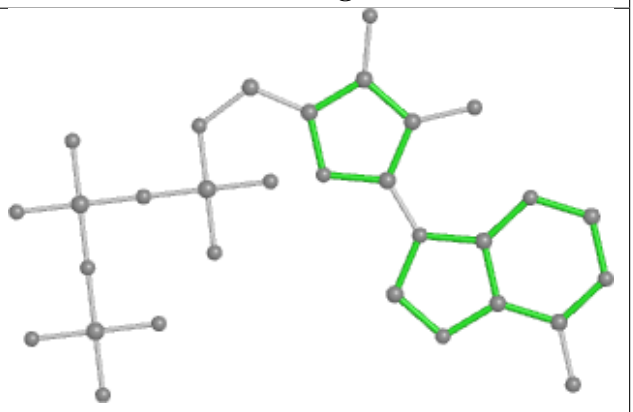
Bond lengths



Bond angles

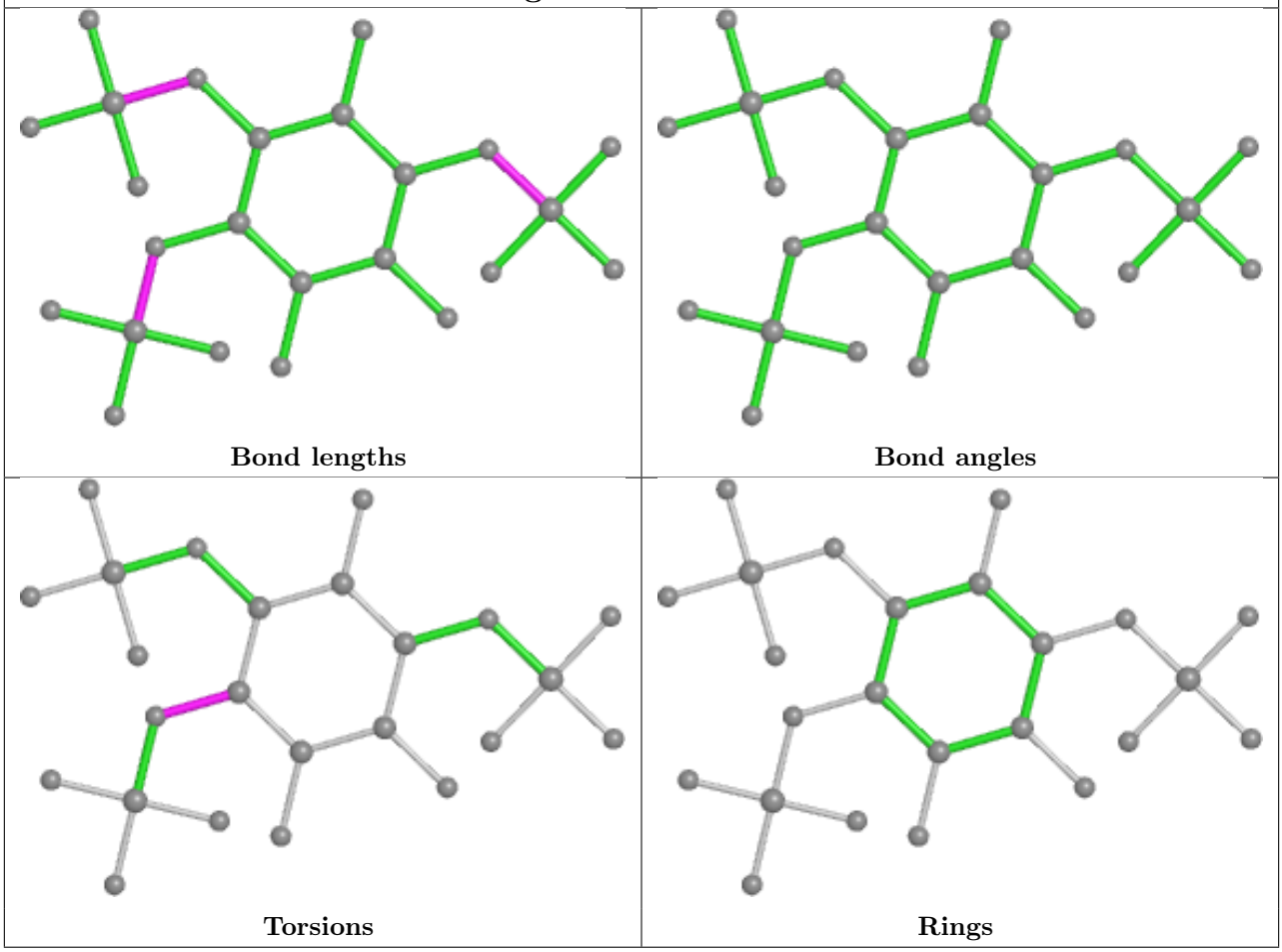


Torsions



Rings

Ligand I3P A 2702



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

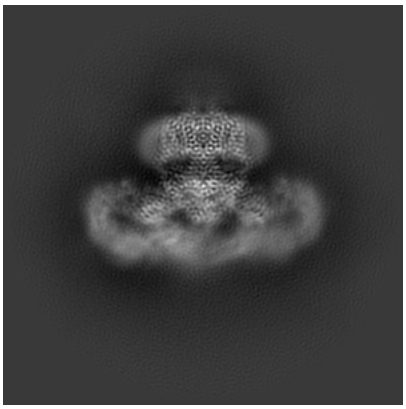
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25671. These allow visual inspection of the internal detail of the map and identification of artifacts.

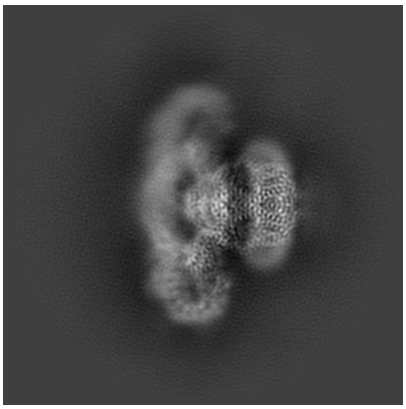
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

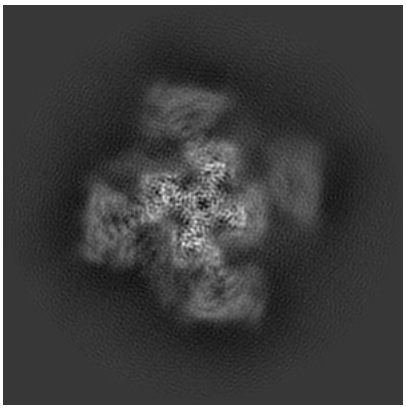
6.1.1 Primary map



X

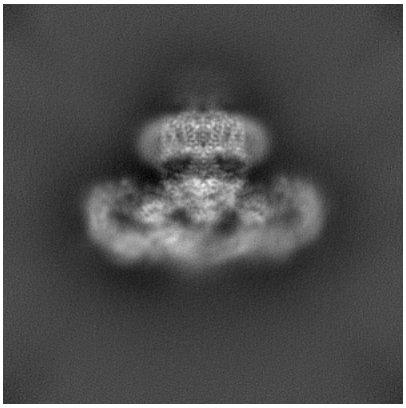


Y

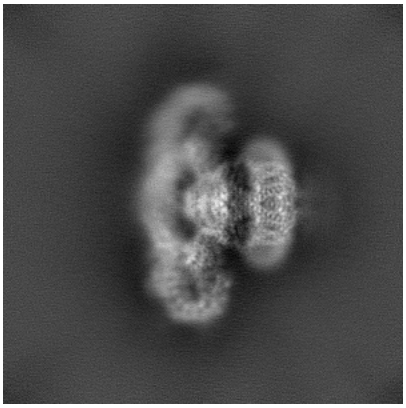


Z

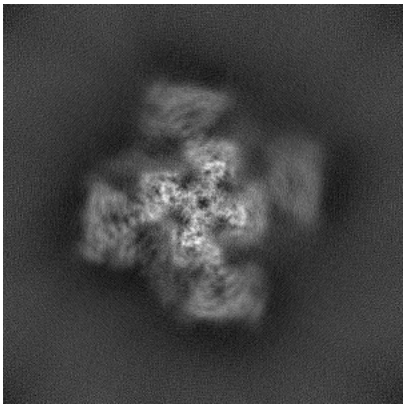
6.1.2 Raw map



X



Y

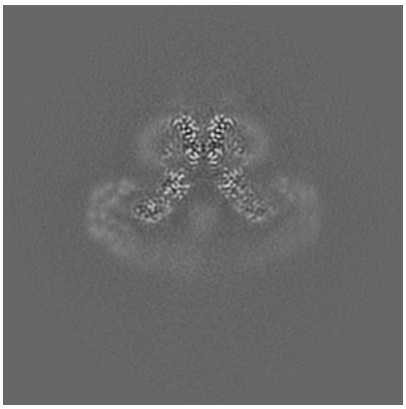


Z

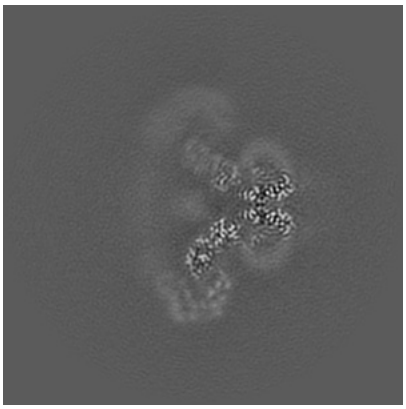
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

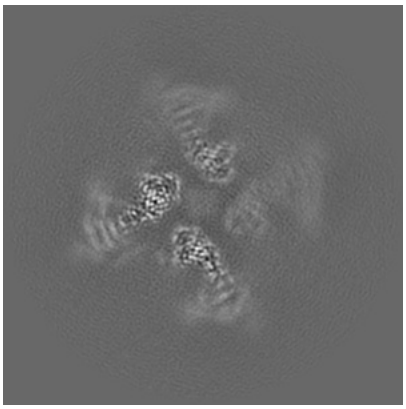
6.2.1 Primary map



X Index: 240

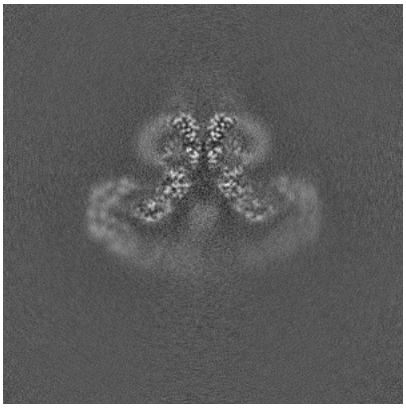


Y Index: 240

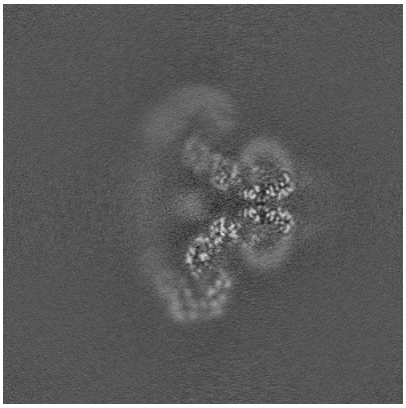


Z Index: 240

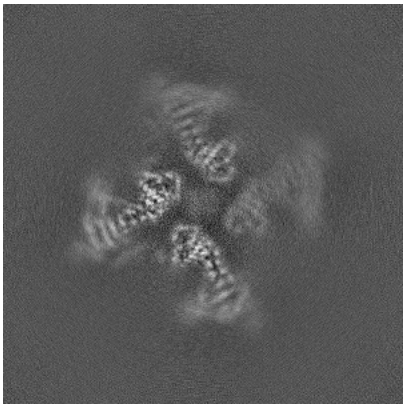
6.2.2 Raw map



X Index: 240



Y Index: 240

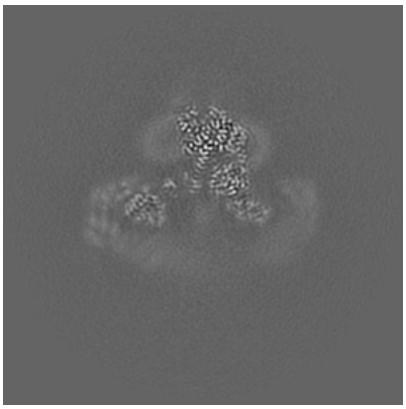


Z Index: 240

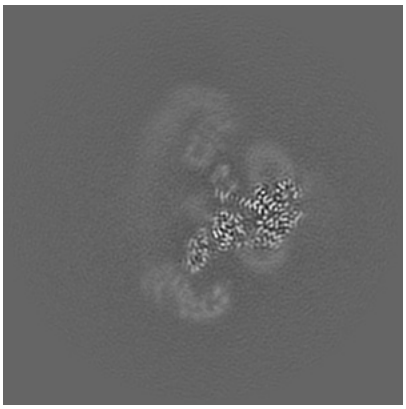
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

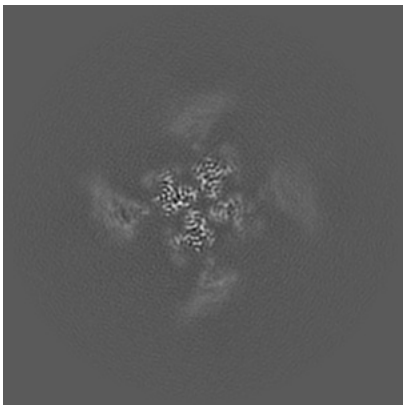
6.3.1 Primary map



X Index: 250

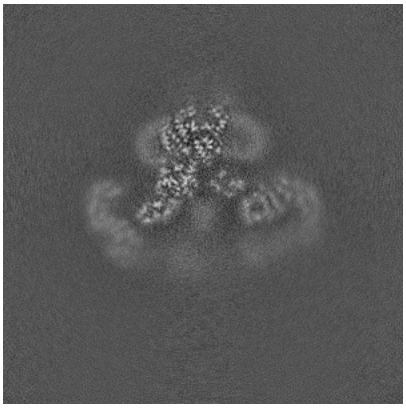


Y Index: 250

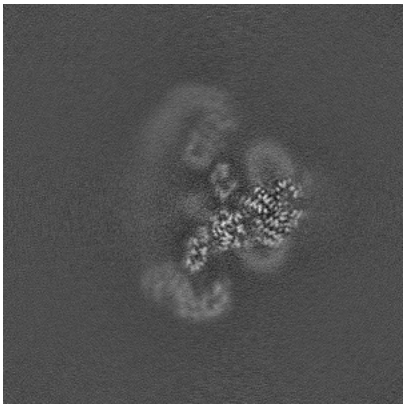


Z Index: 262

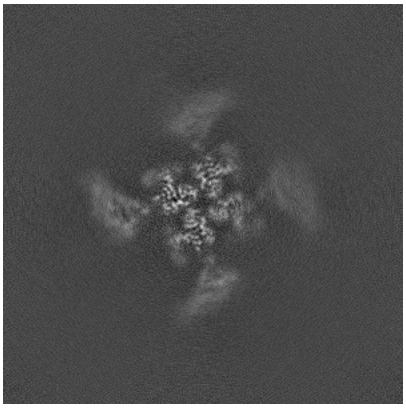
6.3.2 Raw map



X Index: 232



Y Index: 249



Z Index: 262

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

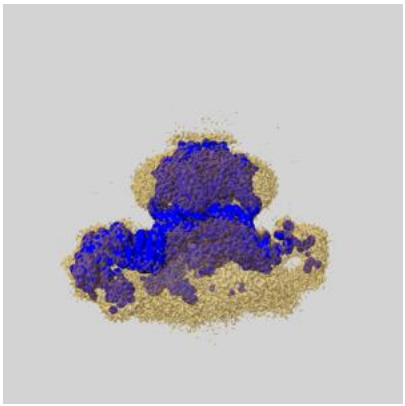
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

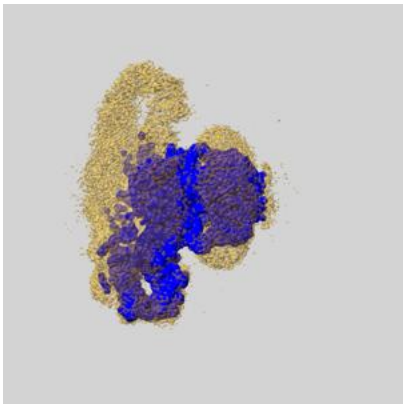
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

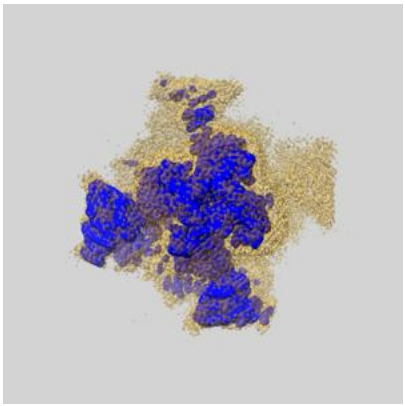
6.5.1 emd_25671_msk_1.map (i)



X



Y

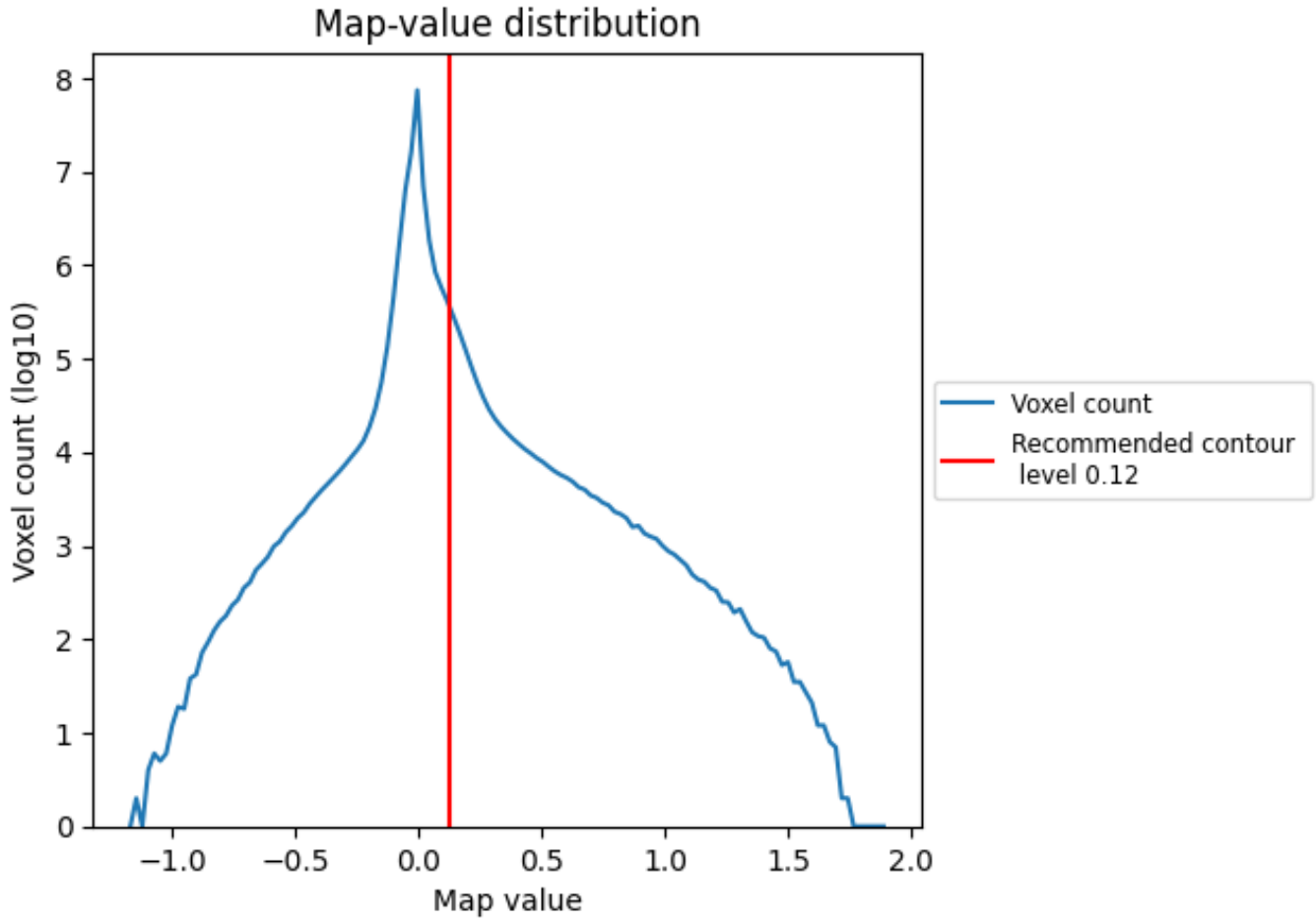


Z

7 Map analysis

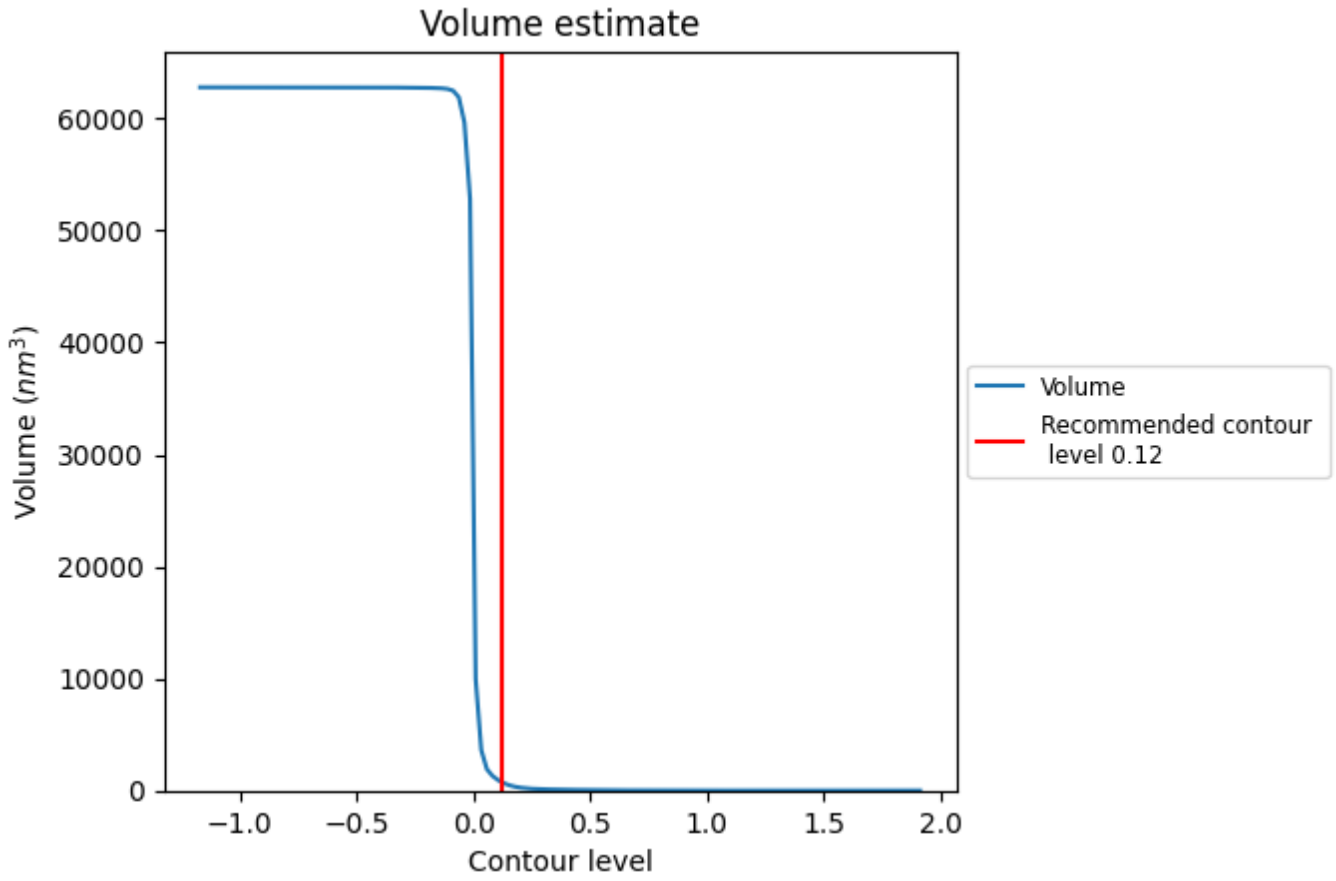
This section contains the results of statistical analysis of the map.

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.

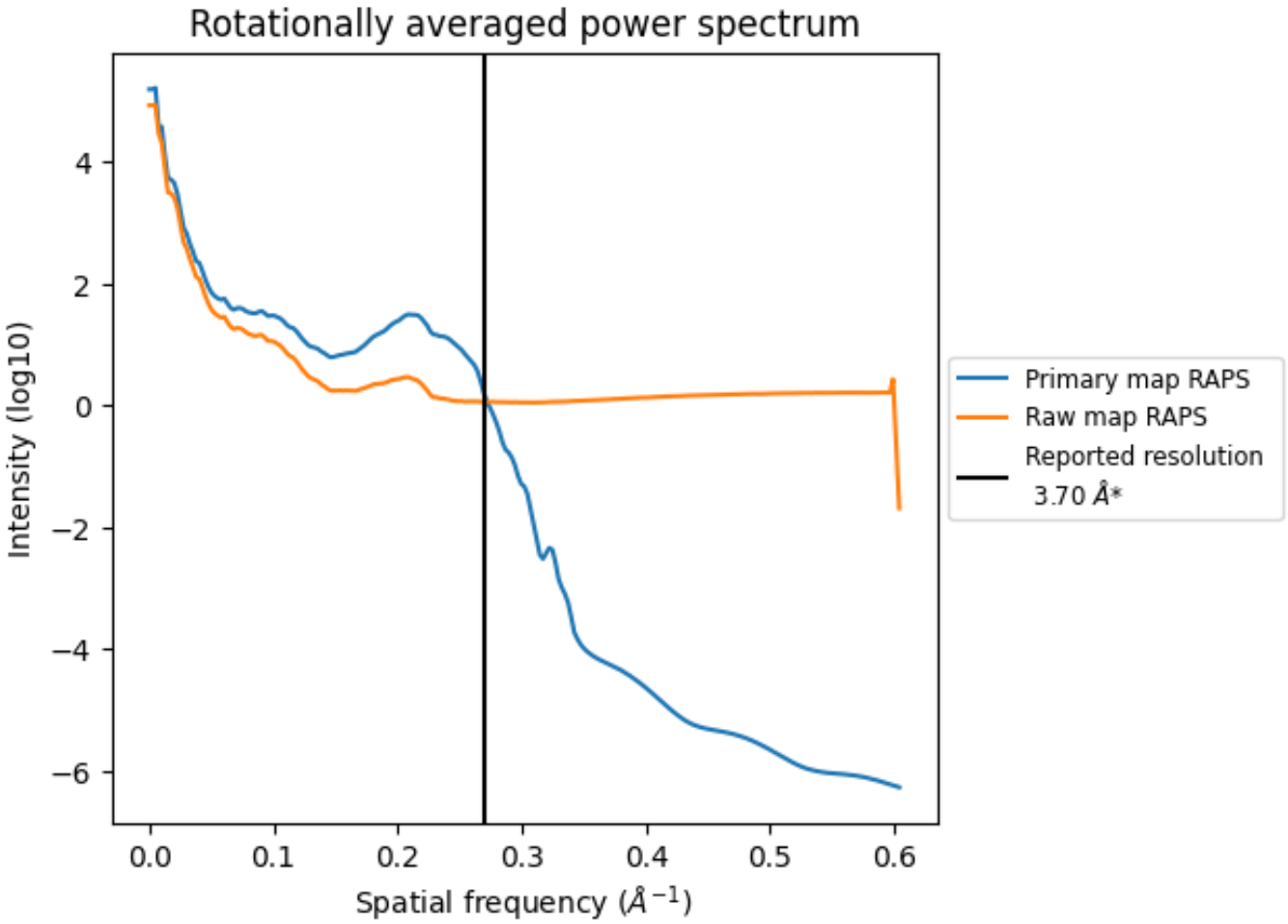
7.2 Volume estimate



The volume at the recommended contour level is 762 nm^3; this corresponds to an approximate mass of 689 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)

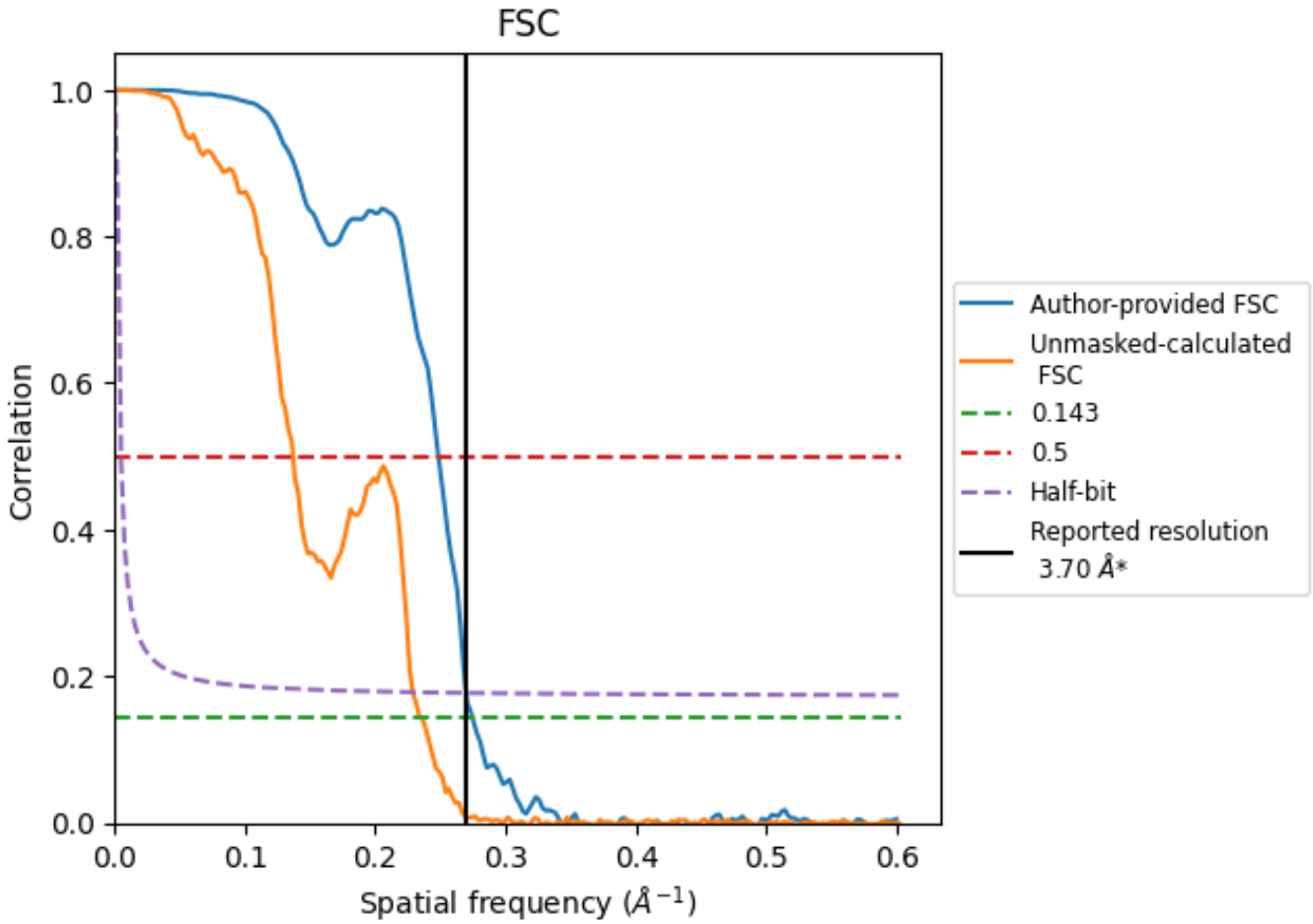


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

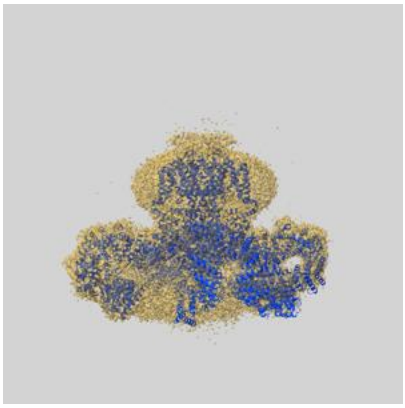
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.64	4.02	3.71
Unmasked-calculated*	4.26	7.30	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.7 by more than 10 %

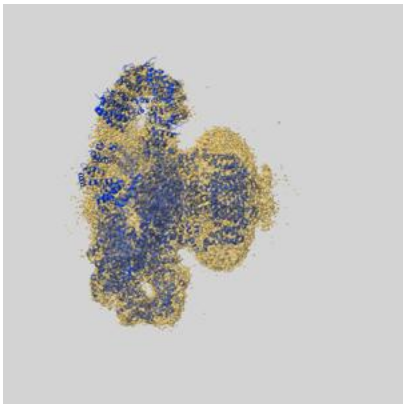
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25671 and PDB model 7T3U. Per-residue inclusion information can be found in section 3 on page 6.

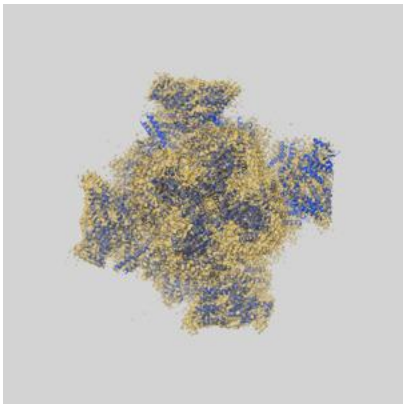
9.1 Map-model overlay



X



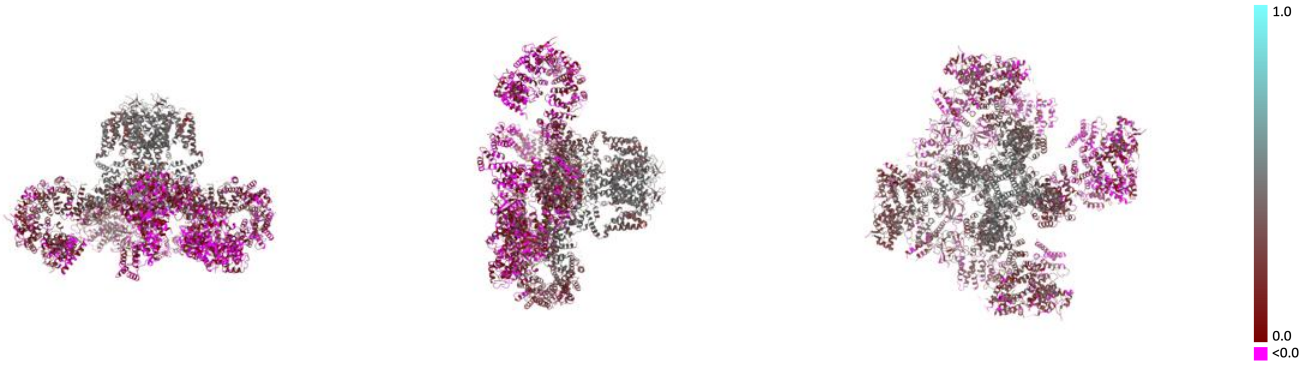
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

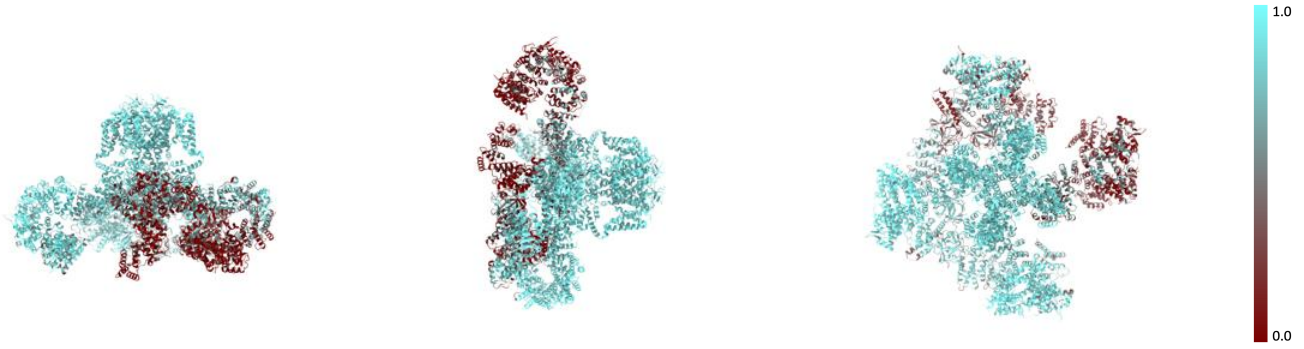
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

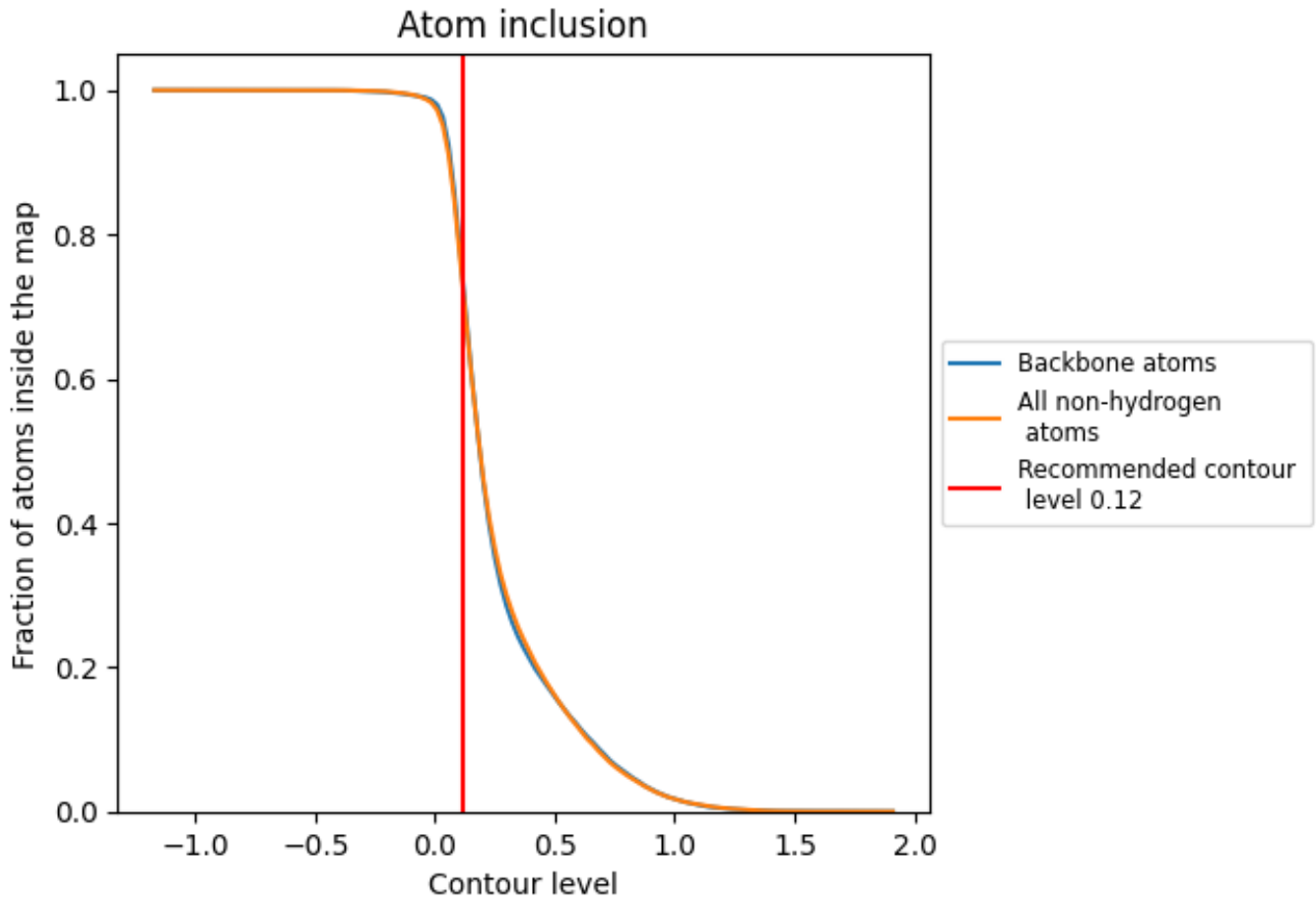
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7153	0.2550
A	0.8737	0.3140
B	0.8743	0.2900
C	0.4706	0.1810
D	0.6169	0.2230