Full wwPDB EM Validation Report ⓘ

Nov 17, 2022 – 04:24 AM EST

PDB ID	:	8EAR
EMDB ID	:	EMD-27983
Title	:	Structure of the full-length IP3R1 channel determined in the presence of Calcium/IP3/ATP
Authors	:	Fan, G.; Baker, M.R.; Terry, L.E.; Arige, V.; Chen, M.; Seryshev, A.B.; Baker, M.L.; Ludtke, S.J.; Yule, D.I.; Serysheva, I.I.
Deposited on	:	2022-08-29
Resolution	:	3.50 Å(reported)
Based on initial model	:	7LHE

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:

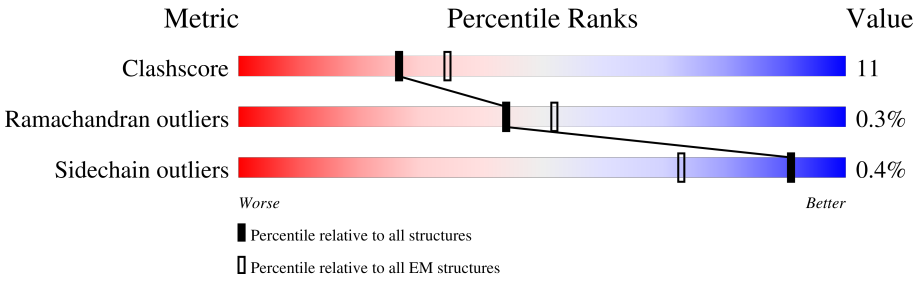
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2750	20% 64% 22% 13%
1	B	2750	20% 64% 22% 13%
1	C	2750	20% 64% 22% 13%
1	D	2750	20% 64% 22% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 78512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

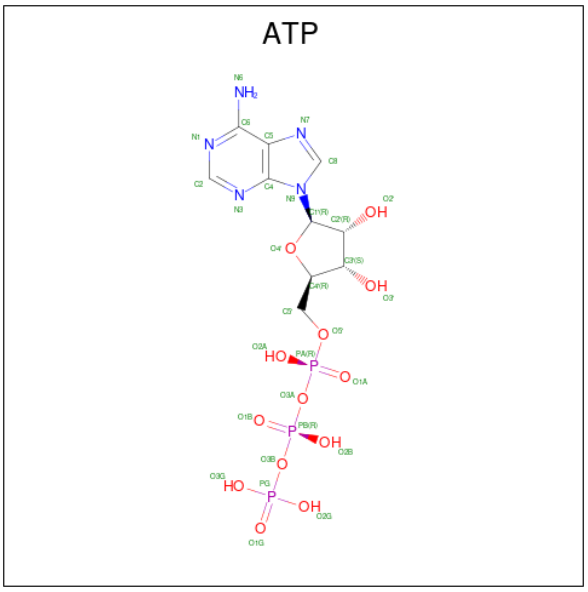
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0
1	B	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0
1	C	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0
1	D	2389	Total 19296	C 12263	N 3334	O 3582	S 117	2	0

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

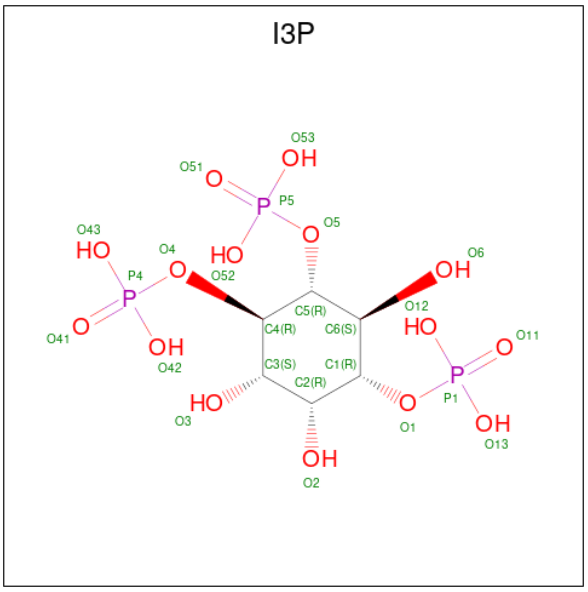
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is 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
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 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).

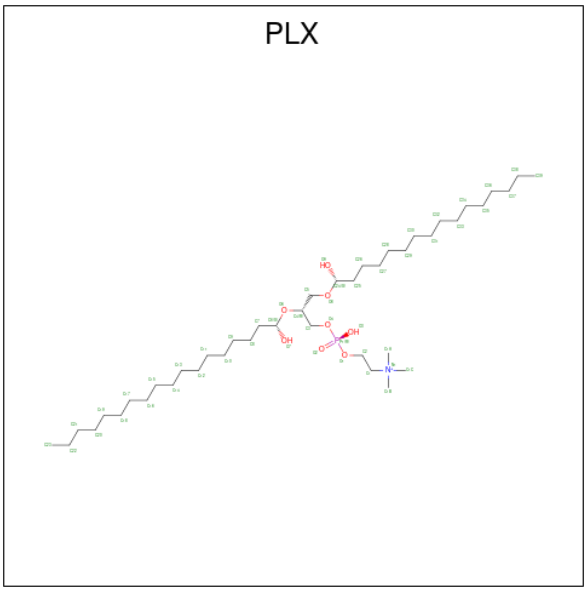


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			24	6	15	3	
4	B	1	Total	C	O	P	0
			24	6	15	3	
4	C	1	Total	C	O	P	0
			24	6	15	3	
4	D	1	Total	C	O	P	0
			24	6	15	3	

- 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	4	Total	Ca	0
			4	4	
5	B	4	Total	Ca	0
			4	4	
5	C	4	Total	Ca	0
			4	4	
5	D	4	Total	Ca	0
			4	4	

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



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total 272	C 202	N 7	O 56	P 7	0
6	A	1	Total 272	C 202	N 7	O 56	P 7	0
6	A	1	Total 272	C 202	N 7	O 56	P 7	0
6	A	1	Total 272	C 202	N 7	O 56	P 7	0
6	A	1	Total 272	C 202	N 7	O 56	P 7	0
6	A	1	Total 272	C 202	N 7	O 56	P 7	0
6	A	1	Total 272	C 202	N 7	O 56	P 7	0
6	B	1	Total 272	C 202	N 7	O 56	P 7	0
6	B	1	Total 272	C 202	N 7	O 56	P 7	0
6	B	1	Total 272	C 202	N 7	O 56	P 7	0
6	B	1	Total 272	C 202	N 7	O 56	P 7	0
6	B	1	Total 272	C 202	N 7	O 56	P 7	0
6	B	1	Total 272	C 202	N 7	O 56	P 7	0
6	B	1	Total 272	C 202	N 7	O 56	P 7	0
6	C	1	Total 272	C 202	N 7	O 56	P 7	0
6	C	1	Total 272	C 202	N 7	O 56	P 7	0
6	C	1	Total 272	C 202	N 7	O 56	P 7	0
6	C	1	Total 272	C 202	N 7	O 56	P 7	0
6	C	1	Total 272	C 202	N 7	O 56	P 7	0
6	C	1	Total 272	C 202	N 7	O 56	P 7	0
6	C	1	Total 272	C 202	N 7	O 56	P 7	0
6	D	1	Total 272	C 202	N 7	O 56	P 7	0

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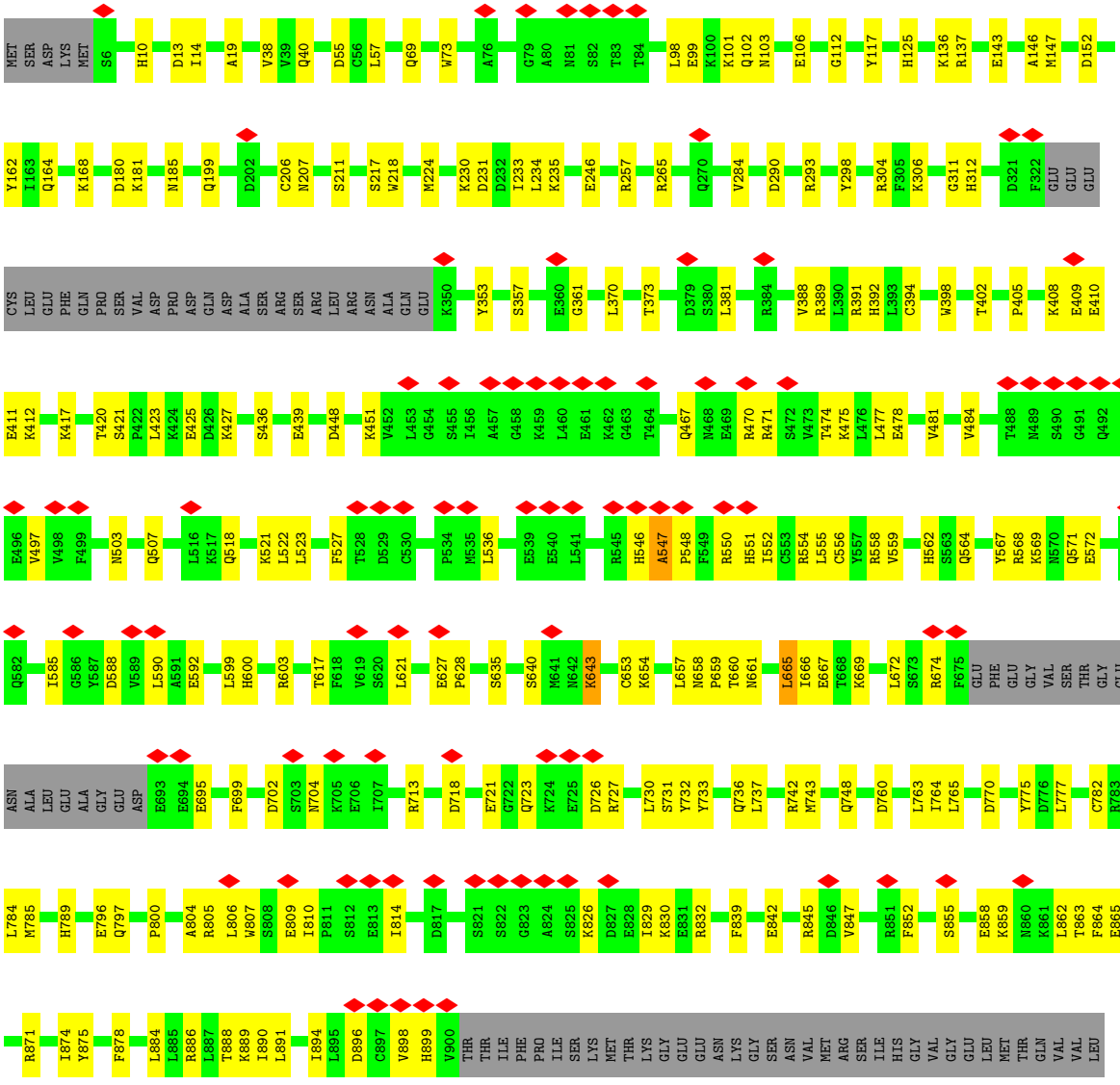
Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total 272	C 202	N 7	O 56	P 7	0
6	D	1	Total 272	C 202	N 7	O 56	P 7	0
6	D	1	Total 272	C 202	N 7	O 56	P 7	0
6	D	1	Total 272	C 202	N 7	O 56	P 7	0
6	D	1	Total 272	C 202	N 7	O 56	P 7	0
6	D	1	Total 272	C 202	N 7	O 56	P 7	0

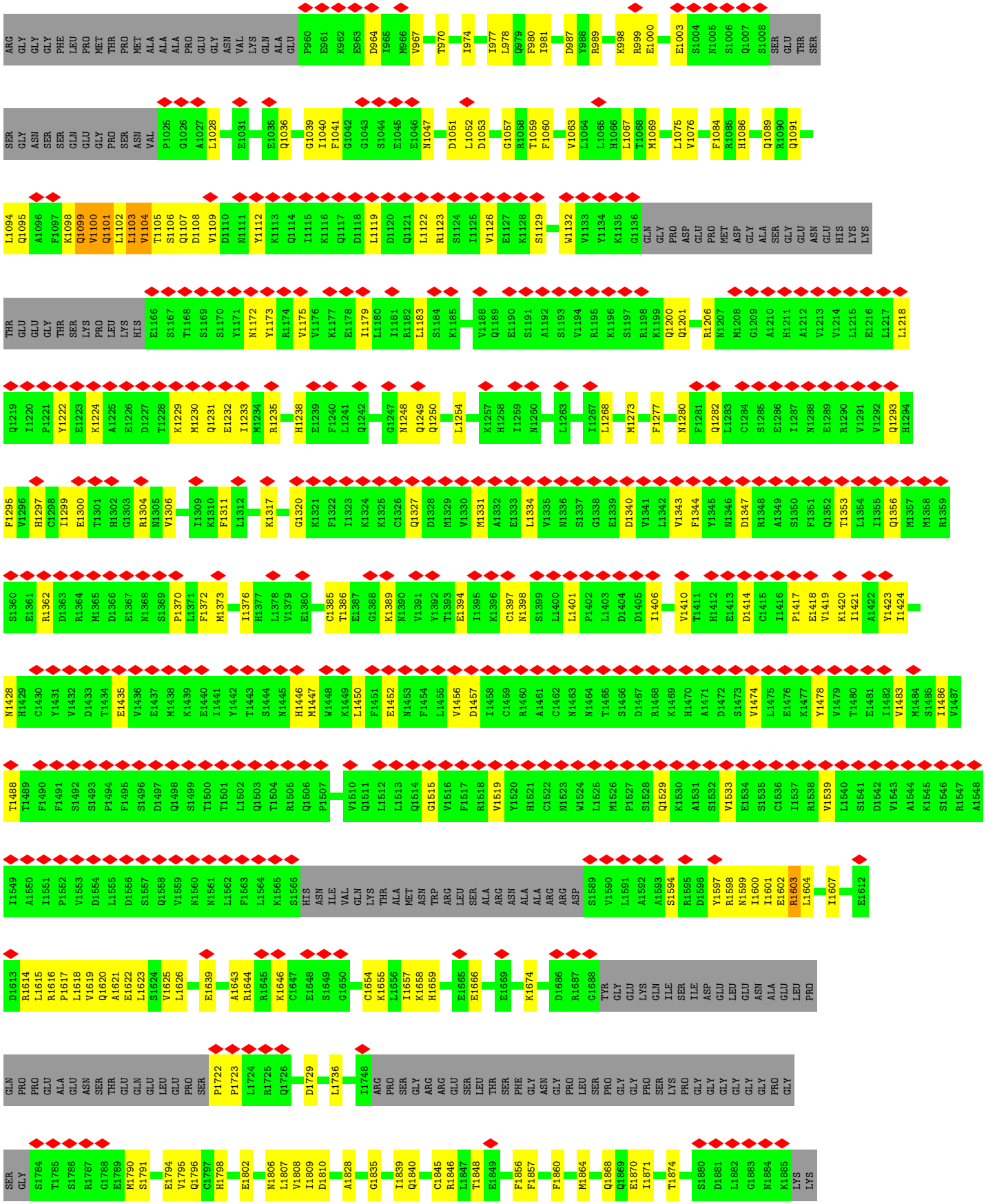
3 Residue-property plots (i)

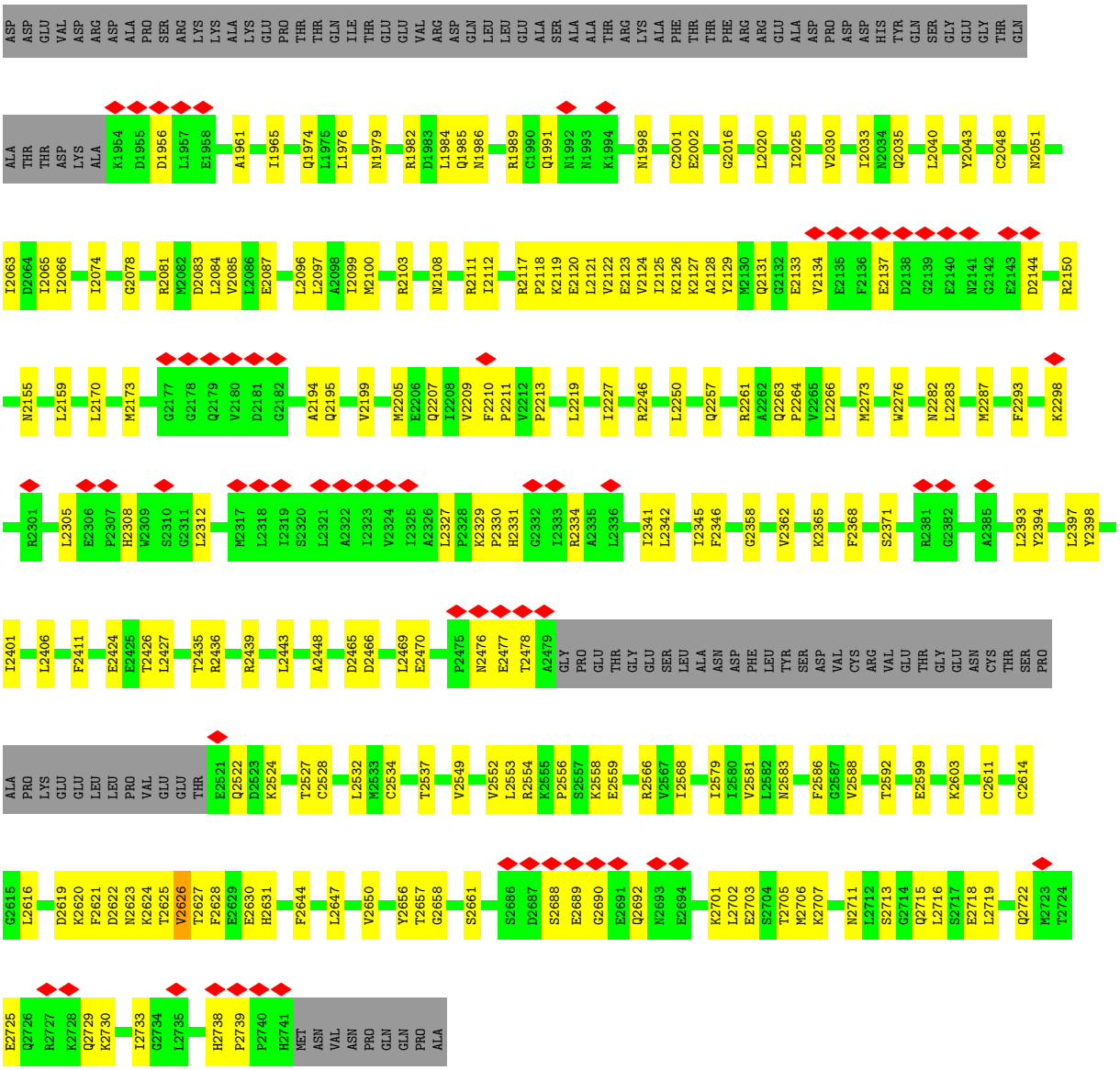
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

Chain A:

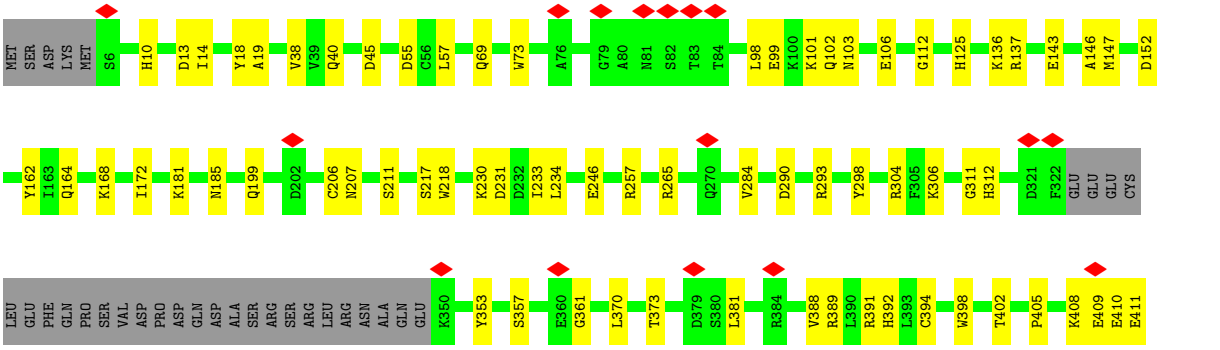


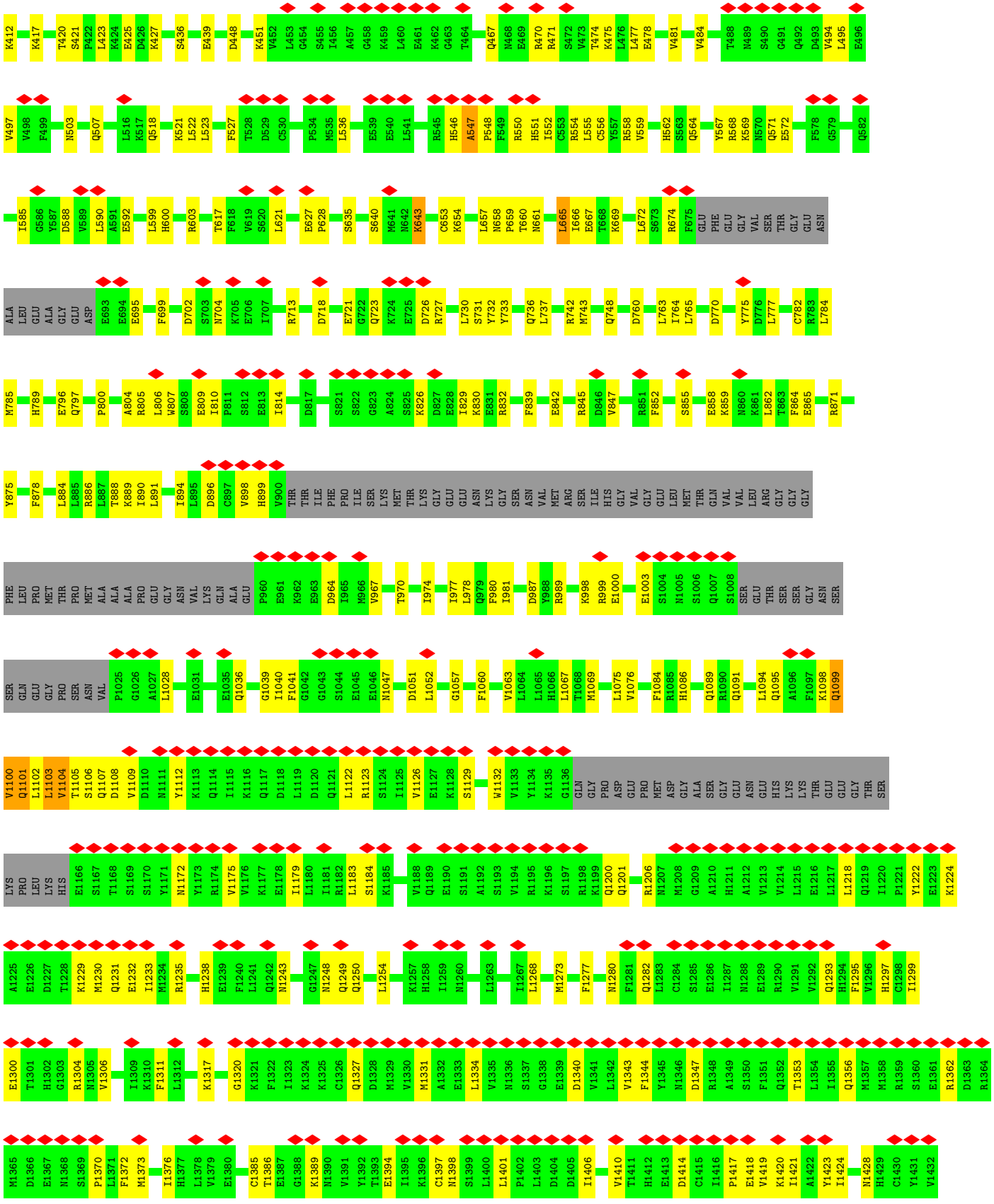




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain B:

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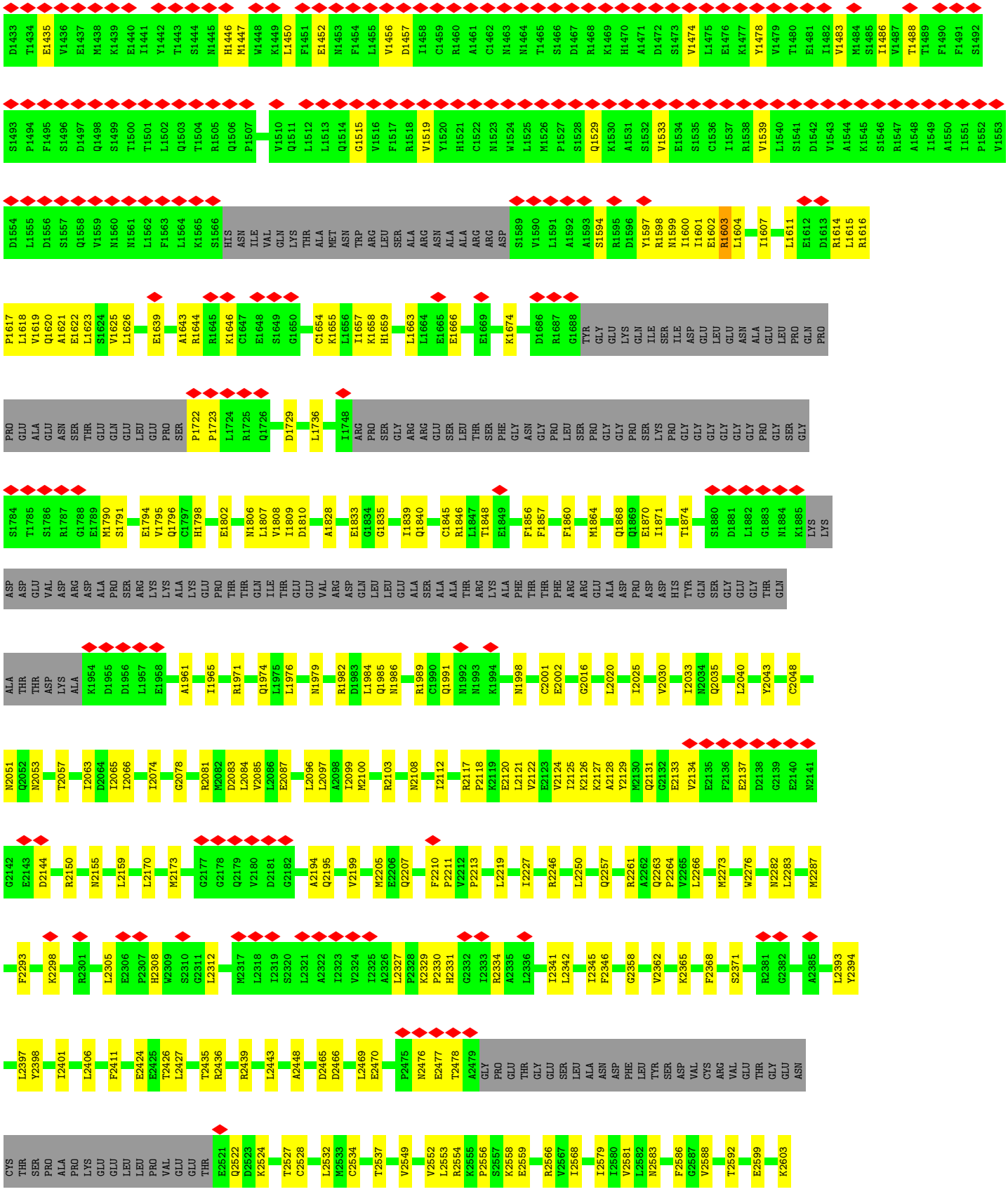
V497 V498 F499 N503 Q507 L516 K517 Q518 K521 L522 L523 F527 T528 D529 C530 P534 M535 L536 E539 E540 L541 R545 H546 A547 P548 F549 R550 H551 I552 C553 R554 L555 C556 Y557 R558 V559 H562 S563 Q564 Y567 R568 K569 N570 Q571 E572 F578 G579 Q582
I585 G586 Y587 D588 V589 L590 A591 E592 L599 H600 R603 T617 F618 V619 S620 L621 E627 P628 S635 S640 M641 N642 K643 C653 K654 L657 N658 P659 T660 N661 L665 I666 E667 T668 K669 L672 S673 R674 F675 GLU PHE GLU GLY VAL SER THR GLY GLU ASN
ALA LEU GLU ALA GLY GLU ASP E693 E694 E695 F699 D702 S703 N704 K705 E706 I707 R713 D718 E721 G722 Q723 K724 E725 D726 R727 L730 S731 Y732 Y733 Q736 L737 R742 M743 Q748 D760 L763 I764 L765 D770 Y775 D776 L777 C782 R783 L784
M785 H789 E796 Q797 P800 A804 R805 L806 W807 S808 E809 I810 P811 S812 E813 I814 D817 S821 S822 G823 A824 S825 K826 D827 E828 I829 K830 E831 R832 F839 E842 R845 D846 V847 R851 F852 S855 E858 K859 N860 K861 L862 T863 F864 E865 R871
Y875 F878 L884 L885 R886 L887 T888 K889 I890 L891 I894 L895 D896 C897 V898 H899 V900 THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL VAL LEU ARG GLY GLY GLY
PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E961 K962 E963 D964 I965 M966 V967 T970 I974 I977 L978 Q979 F980 I981 D987 Y988 R989 K998 R999 E1000 E1003 S1004 N1005 S1006 Q1007 S1008 SER GLU THR SER SER GLY ASN SER
SER GLN GLU GLY PRO SER ASN VAL P1025 G1026 A1027 L1028 E1031 E1035 Q1036 G1039 I1040 F1041 G1042 G1043 S1044 E1045 E1046 N1047 D1051 L1052 G1057 F1060 V1063 L1064 L1065 H1066 L1067 T1068 M1069 L1075 V1076 F1084 R1085 H1086 Q1089 R1090 Q1091 L1094 Q1095 A1096 F1097 K1098 Q1099
V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 V1109 D1110 N1111 Y1112 K1113 Q1114 I1115 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 W1132 V1133 Y1134 K1135 G1136 GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER
LYS PRO LEU LYS HIS E1166 S1167 T1168 S1169 S1170 Y1171 N1172 Y1173 R1174 V1175 V1176 K1177 E1178 I1179 L1180 I1181 R1182 L1183 S1184 K1185 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200 Q1201 R1206 N1207 M1208 G1209 A1210 H1211 A1212 V1213 V1214 L1215 E1216 L1217 L1218 Q1219 I1220 P1221 Y1222 E1223 K1224
A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 R1235 H1238 E1239 F1240 L1241 Q1242 N1243 G1247 N1248 Q1249 Q1250 L1254 K1257 H1258 I1259 N1260 L1263 I1267 L1268 M1273 F1277 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291 V1292 Q1293 H1294 F1295 V1296 H1297 C1298 I1299
E1300 T1301 H1302 G1303 R1304 N1305 V1306 I1309 K1310 F1311 L1312 K1317 G1320 K1321 F1322 I1323 K1324 K1325 C1326 Q1327 D1328 M1329 V1330 M1331 A1332 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 Y1345 N1346 D1347 R1348 A1349 S1350 F1351 Q1352 T1353 L1354 I1355 Q1356 M1357 M1358 R1359 S1360 E1361 R1362 D1363 R1364
M1365 D1366 E1367 N1368 S1369 P1370 L1371 F1372 M1373 I1376 H1377 L1378 V1379 E1380 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 Y1423 I1424 N1428 H1429 C1430 Y1431 V1432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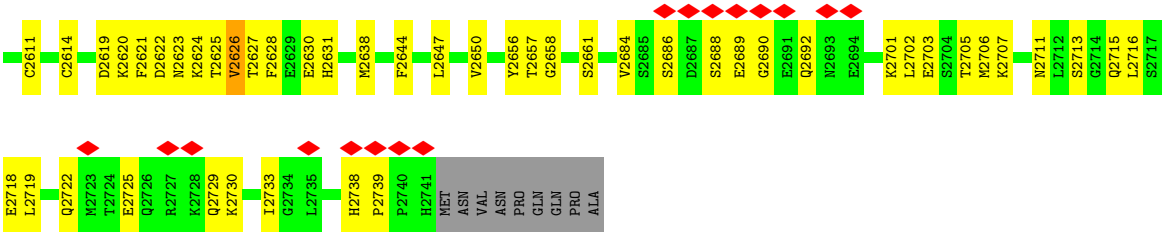
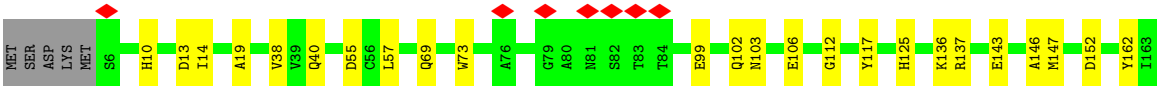
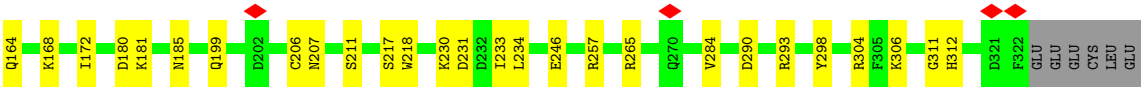
S1493 P1494 F1495 S1496 D1497 Q1498 S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 V1539 L1540 S1541 D1542 V1543 A1544 K1545 S1546 R1547 A1548 I1549 A1550 I1551 P1552 V1553
D1554 L1555 D1556 S1557 Q1558 V1559 N1560 N1561 L1562 F1563 L1564 K1565 S1566 HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP S1589 V1590 L1591 A1592 A1593 S1594 R1595 D1596 Y1597 R1598 N1599 I1600 I1601 E1602 R1603 L1604 I1607 L1611 E1612 D1613 R1614 L1615 R1616
P1617 L1618 V1619 Q1620 A1621 E1622 L1623 S1624 V1625 L1626 E1639 A1643 R1644 R1645 K1646 C1647 E1648 S1649 G1650 C1654 K1655 L1656 I1657 K1658 H1659 L1663 L1664 E1665 E1666 E1669 K1674 D1686 R1687 G1688 TYR GLY GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO
PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER P1722 P1723 L1724 R1725 Q1726 D1729 L1736 I1748 ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY GLY PRO GLY SER GLY
S1784 T1785 S1786 R1787 G1788 E1789 M1790 S1791 E1794 V1795 Q1796 C1797 H1798 E1802 N1806 L1807 V1808 I1809 D1810 A1828 E1833 G1834 G1835 I1839 Q1840 C1845 R1846 L1847 T1848 E1849 F1856 F1857 F1860 M1864 Q1868 Q1869 E1870 I1871 T1874 S1880 D1881 L1882 G1883 N1884 K1885 LYS LYS
ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN
ALA THR THR ASP LYS ALA K1954 D1955 D1956 L1957 E1958 A1961 I1965 R1971 Q1974 L1975 L1976 N1979 R1982 D1983 L1984 Q1985 N1986 R1989 C1990 Q1991 N1992 N1993 K1994 N1998 C2001 E2002 G2016 L2020 I2025 V2030 I2033 N2034 Q2035 L2040 Y2043 C2048
N2051 Q2052 N2053 T2057 I2063 D2064 I2065 I2066 I2074 G2078 R2081 M2082 D2083 L2084 V2085 K2086 E2087 L2096 L2097 A2098 I2099 M2100 R2103 N2108 I2112 R2117 P2118 K2119 E2120 L2121 V2122 E2123 V2124 I2125 K2126 K2127 A2128 Y2129 M2130 Q2131 G2132 E2133 V2134 E2135 F2136 E2137 D2138 G2139 E2140 N2141
G2142 E2143 D2144 R2150 N2155 L2159 L2170 M2173 G2177 G2178 Q2179 V2180 D2181 G2182 A2194 Q2195 V2199 M2205 E2206 Q2207 F2210 P2211 V2212 P2213 L2219 I2227 R2246 L2250 Q2257 R2261 A2262 Q2263 P2264 V2265 L2266 M2273 W2276 N2282 L2283 M2287
F2293 K2298 R2301 L2305 E2306 P2307 H2308 W2309 S2310 G2311 L2312 M2317 L2318 I2319 S2320 L2321 A2322 I2323 V2324 I2325 A2326 L2327 P2328 K2329 P2330 H2331 G2332 I2333 R2334 A2335 L2336 I2341 L2342 I2345 F2346 G2358 V2362 K2365 F2368 S2371 R2381 G2382 A2385 L2393 Y2394
L2397 Y2398 I2401 L2406 F2411 E2424 E2425 T2426 L2427 T2435 R2436 R2439 L2443 A2448 D2465 D2466 L2469 E2470 P2475 N2476 E2477 T2478 A2479 GLY PRO GLU THR GLY GLU SER LEU ALA ASN ASP PHE LEU TYR SER ASP VAL CYS ARG VAL GLU THR GLY GLU ASN
CYS THR SER PRO ALA PRO LYS GLU GLU LEU LEU PRO VAL GLU GLU THR E2521 Q2522 D2523 K2524 T2527 C2528 L2532 M2533 C2534 T2537 V2549 V2552 L2553 R2554 K2555 P2556 S2557 K2558 E2559 R2566 V2567 I2568 I2579 I2580 V2581 L2582 N2583 F2586 G2587 V2588 T2592 E2599 K2603

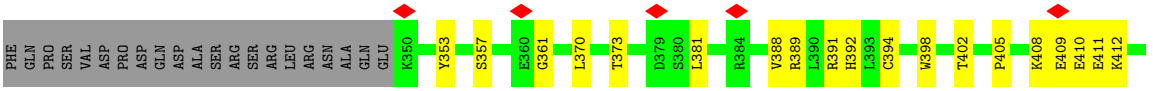


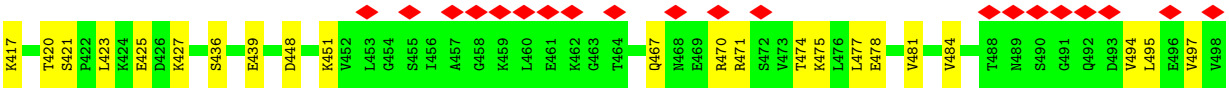
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

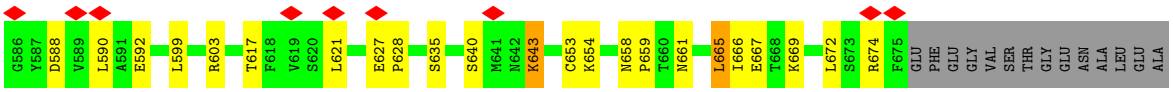
Chain C:

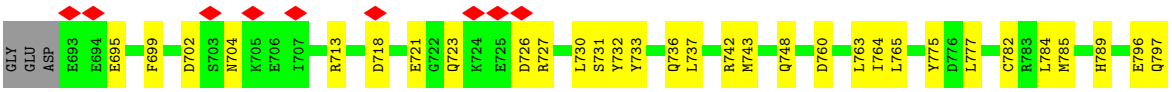


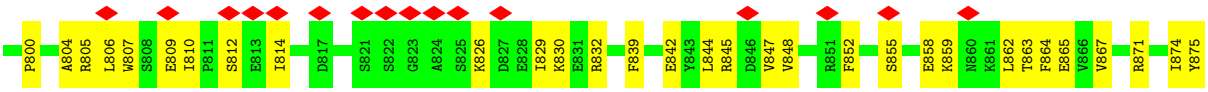


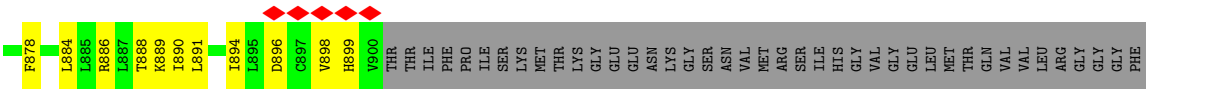


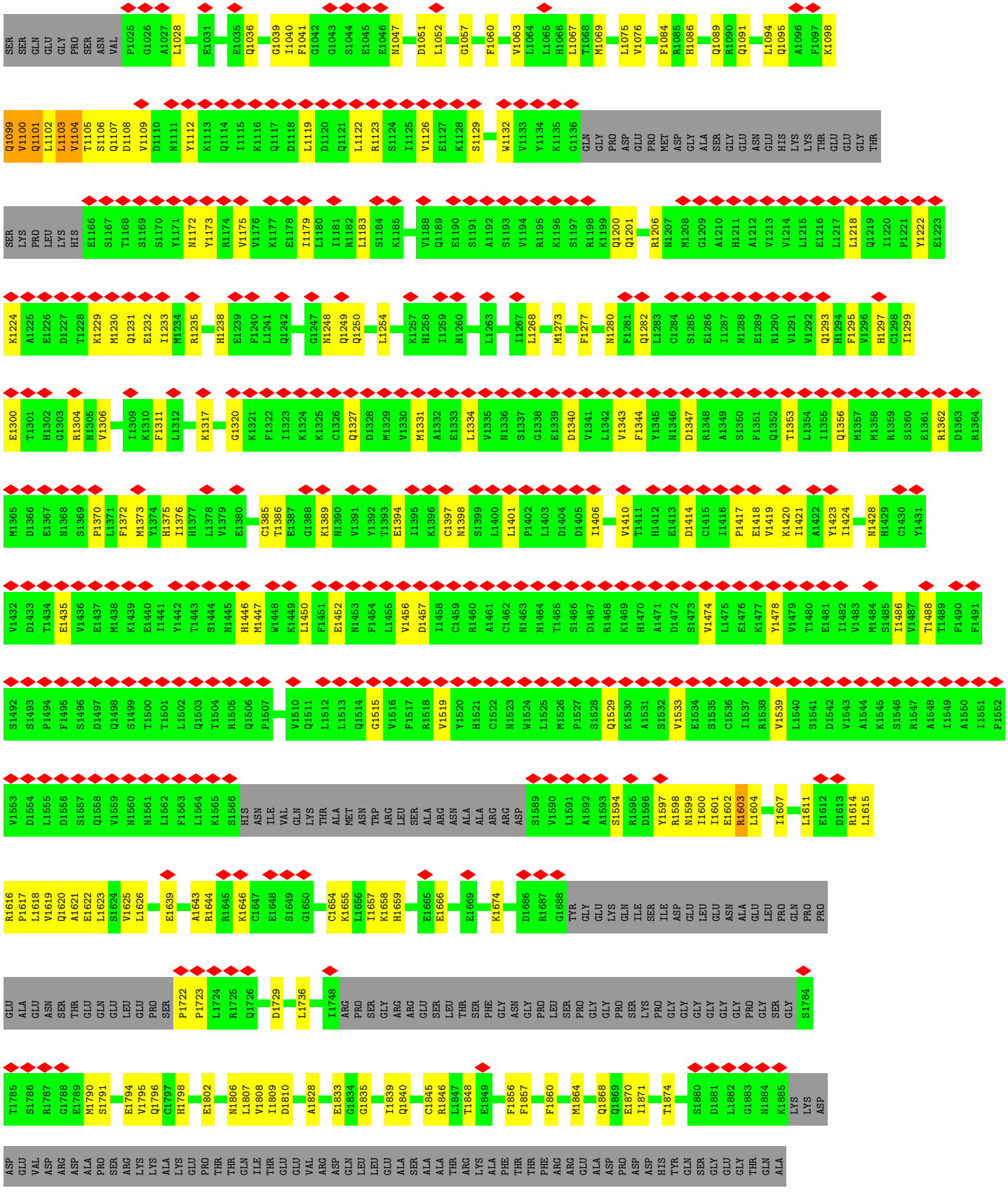


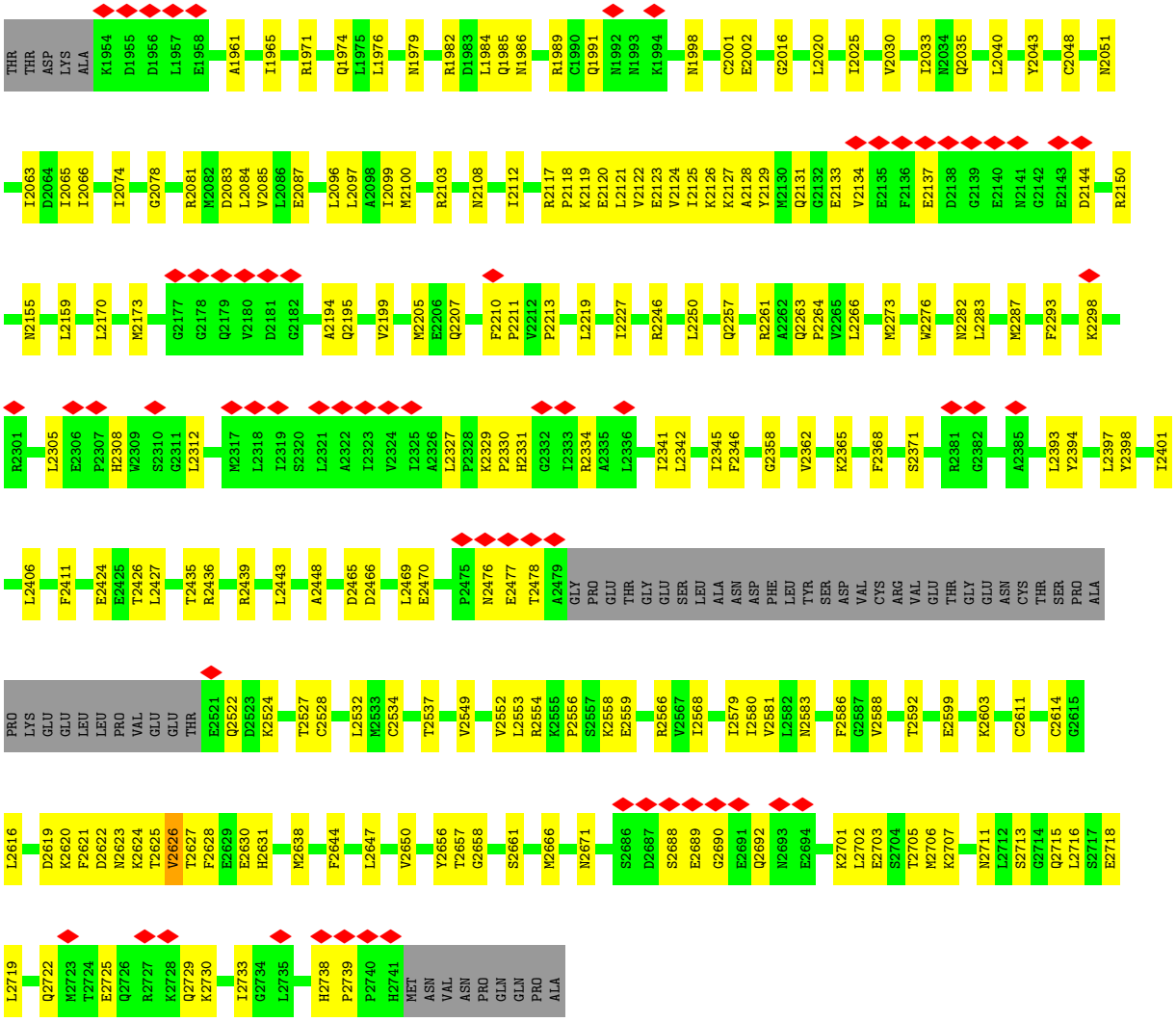






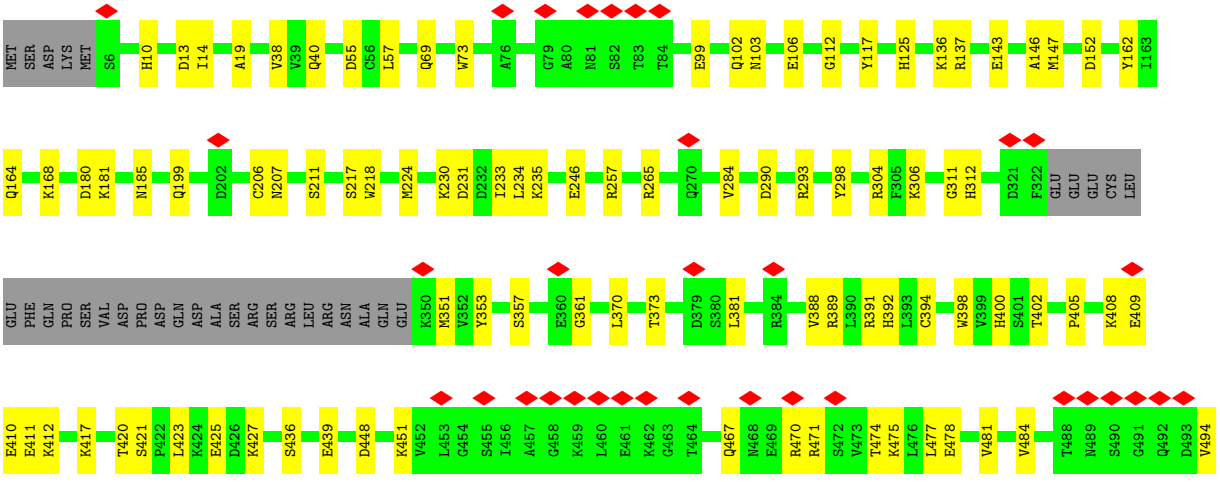


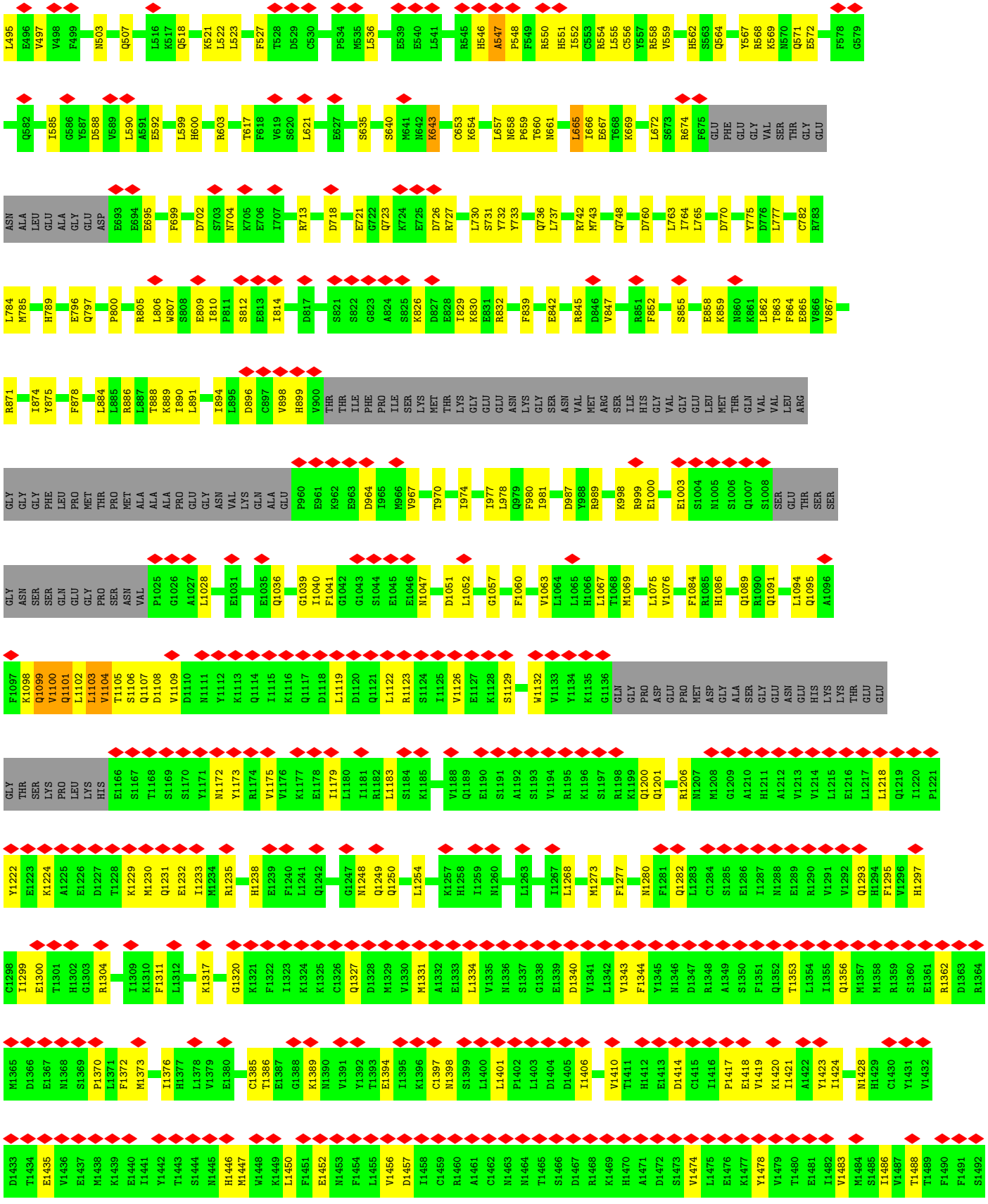




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain D:

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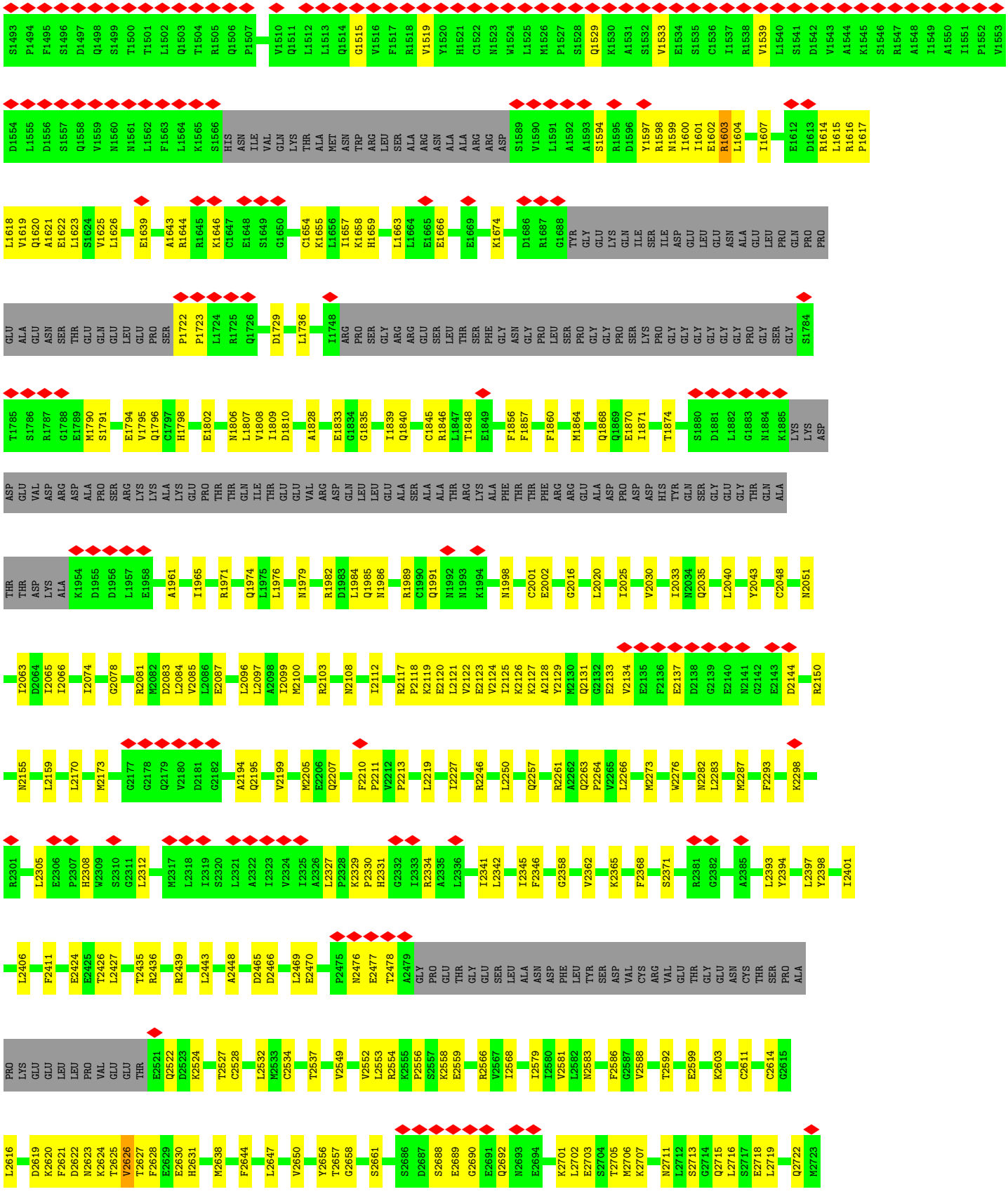
Q582 I585 G586 Y587 D588 V589 L590 A591 E592 L599 H600 R603 T617 F618 V619 S620 L621 E627 S635 S640 M641 N642 K643 C653 K654 L657 N658 P659 T660 N661 L665 I666 E667 T668 K669 L672 S673 R674 F675 GLU PHE GLU GLY VAL SER THR GLY GLU
ASN ALA LEU GLU ALA GLY GLU ASP E693 E694 E695 F699 D702 S703 N704 K705 E706 I707 R713 D718 E721 G722 Q723 K724 E725 D726 R727 L730 S731 Y732 Y733 Q736 L737 R742 M743 Q748 D760 L763 I764 L765 D770 Y775 D776 L777 C782 R783
L784 M785 H789 E796 Q797 P800 R805 L806 W807 S808 E809 I810 P811 S812 E813 I814 D817 S821 S822 G823 A824 S825 K826 D827 E828 I829 K830 E831 R832 F839 E842 R845 D846 V847 R851 F852 S855 E858 K859 N860 K861 L862 T863 F864 E865 V866 V867
R871 I874 Y875 F878 L884 L885 R886 L887 T888 K889 I890 L891 I894 L895 D896 C897 V898 H899 V900 THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL VAL LEU ARG
GLY GLY GLY PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E961 K962 E963 D964 I965 M966 V967 T970 I974 I977 L978 Q979 F980 I981 D987 Y988 R989 K998 R999 E1000 E1003 S1004 N1005 S1006 Q1007 S1008 SER GLU THR SER SER
GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL P1025 G1026 A1027 L1028 E1031 E1035 Q1036 G1039 I1040 F1041 G1042 G1043 S1044 E1045 E1046 N1047 D1051 L1052 G1057 F1060 V1063 L1064 L1065 H1066 L1067 T1068 M1069 L1075 V1076 F1084 R1085 H1086 Q1089 R1090 Q1091 L1094 Q1095 A1096
F1097 K1098 Q1099 V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 V1109 D1110 N1111 Y1112 K1113 Q1114 I1115 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 W1132 V1133 Y1134 K1135 G1136 GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU
GLY THR SER LYS PRO LEU LYS HIS E1166 S1167 T1168 S1169 S1170 Y1171 N1172 Y1173 R1174 V1175 V1176 K1177 E1178 I1179 L1180 I1181 R1182 L1183 S1184 K1185 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 K1199 Q1200 Q1201 R1206 N1207 M1208 G1209 A1210 H1211 A1212 V1213 V1214 L1215 E1216 L1217 L1218 Q1219 I1220 P1221
Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 R1235 H1238 E1239 F1240 L1241 Q1242 G1247 N1248 Q1249 Q1250 L1254 K1257 H1258 I1259 N1260 L1263 I1267 L1268 M1273 F1277 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291 V1292 Q1293 H1294 F1295 V1296 H1297
C1298 I1299 E1300 T1301 H1302 G1303 R1304 I1309 K1310 F1311 L1312 K1317 G1320 K1321 F1322 I1323 K1324 K1325 C1326 Q1327 D1328 M1329 V1330 M1331 A1332 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 L1342 V1343 F1344 Y1345 N1346 D1347 R1348 A1349 S1350 F1351 Q1352 T1353 L1354 I1355 Q1356 M1357 M1358 R1359 S1360 E1361 R1362 D1363 R1364
M1365 D1366 E1367 N1368 S1369 P1370 L1371 F1372 M1373 I1376 H1377 L1378 V1379 E1380 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 Y1423 I1424 N1428 H1429 C1430 Y1431 V1432
D1433 T1434 E1435 V1436 E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 I1458 C1459 R1460 A1461 C1462 N1463 N1464 T1465 S1466 D1467 R1468 K1469 H1470 A1471 D1472 S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 F1491 S1492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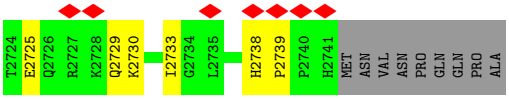
D1554 L1555 D1556 S1557 Q1558 V1559 N1560 N1561 L1562 F1563 L1564 K1565 S1566
HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP
S1589 V1590 L1591 A1592 A1593 S1594 R1595 D1596 Y1597 R1598 N1599 I1600 I1601 E1602 R1603 L1604 I1607 E1612 D1613 R1614 L1615 R1616 P1617
L1618 V1619 Q1620 A1621 E1622 L1623 S1624 V1625 L1626 E1639 A1643 R1644 R1645 K1646 C1647 E1648 S1649 G1650 C1654 K1655 L1656 I1657 K1658 H1659 L1663 L1664 E1665 E1666 E1669 K1674 D1686 R1687 G1688
TYR GLY GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO
GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER P1722 P1723 L1724 R1725 Q1726 D1729 L1736 I1748
ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY PRO GLY SER GLY S1784
T1785 S1786 R1787 G1788 E1789 M1790 S1791 E1794 V1795 Q1796 C1797 H1798 E1802 N1806 L1807 V1808 I1809 D1810 A1828 E1833 G1834 G1835 I1839 Q1840 C1845 R1846 L1847 T1848 E1849 F1856 F1857 F1860 M1864 Q1868 Q1869 E1870 I1871 T1874 S1880 D1881 L1882 G1883 N1884 K1885
LYS LYS ASP
ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY GLY THR GLN ALA
THR THR ASP LYS ALA K1954 D1955 D1956 L1957 E1958 A1961 I1965 R1971 Q1974 L1975 L1976 N1979 R1982 D1983 L1984 Q1985 N1986 R1989 C1990 Q1991 N1992 N1993 K1994 N1998 C2001 E2002 G2016 L2020 I2025 V2030 I2033 N2034 Q2035 L2040 Y2043 C2048 N2051
I2063 D2064 I2065 I2066 I2074 G2078 R2081 M2082 D2083 L2084 V2085 L2086 E2087 L2096 L2097 A2098 I2099 M2100 R2103 N2108 I2112 R2117 P2118 K2119 E2120 L2121 V2122 E2123 V2124 I2125 K2126 K2127 A2128 Y2129 M2130 Q2131 G2132 E2133 V2134 E2135 F2136 E2137 D2138 G2139 E2140 N2141 G2142 E2143 D2144 R2150
N2155 L2159 L2170 M2173 G2177 G2178 Q2179 V2180 D2181 G2182 A2194 Q2195 V2199 M2205 E2206 Q2207 F2210 P2211 V2212 P2213 L2219 I2227 R2246 L2250 Q2257 R2261 A2262 Q2263 P2264 V2265 L2266 M2273 W2276 N2282 L2283 M2287 F2293 K2298
R2301 L2305 E2306 P2307 H2308 W2309 S2310 G2311 L2312 M2317 L2318 I2319 S2320 L2321 A2322 I2323 V2324 I2325 A2326 L2327 P2328 K2329 P2330 H2331 G2332 I2333 R2334 A2335 L2336 I2341 L2342 I2345 F2346 G2358 V2362 K2365 F2368 S2371 R2381 G2382 A2385 L2393 Y2394 L2397 Y2398 I2401
L2406 F2411 E2424 E2425 T2426 L2427 T2435 R2436 R2439 L2443 A2448 D2465 D2466 L2469 E2470 P2475 N2476 E2477 T2478 A2479
GLY PRO GLU THR GLY GLU SER LEU ALA ASN ASP PHE LEU TYR SER ASP VAL CYS ARG VAL GLU THR GLY GLU ASN CYS THR SER PRO ALA
PRO LYS GLU GLU LEU LEU PRO VAL GLU GLU THR E2521 Q2522 D2523 K2524 T2527 C2528 L2532 M2533 C2534 T2537 V2549 V2552 L2553 R2554 K2555 P2556 S2557 K2558 E2559 R2566 V2567 I2568 I2579 I2580 V2581 L2582 N2583 F2586 G2587 V2588 T2592 E2599 K2603 C2611 C2614 G2615
L2616 D2619 K2620 F2621 D2622 N2623 K2624 T2625 V2626 T2627 F2628 E2629 E2630 H2631 M2638 F2644 L2647 V2650 Y2656 T2657 G2658 S2661 S2686 D2687 S2688 E2689 G2690 E2691 Q2692 N2693 E2694 K2701 L2702 E2703 S2704 T2705 M2706 K2707 N2711 L2712 S2713 G2714 Q2715 L2716 S2717 E2718 L2719 Q2722 M2723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H2738
P2739
P2740
H2741
MET
ASN
VAL
ASN
PRO
GLN
GLN
PRO
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	133740	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/19653	0.50	0/26530
1	B	0.27	0/19653	0.50	0/26530
1	C	0.27	0/19653	0.50	0/26530
1	D	0.27	0/19653	0.50	0/26530
All	All	0.27	0/78612	0.50	0/106120

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1099	GLN	Mainchain
1	B	1099	GLN	Mainchain
1	C	1099	GLN	Mainchain
1	D	1099	GLN	Mainchain

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	19296	0	19387	435	0
1	B	19296	0	19387	437	0
1	C	19296	0	19387	436	0
1	D	19296	0	19387	432	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	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	A	24	0	9	1	0
4	B	24	0	9	1	0
4	C	24	0	9	1	0
4	D	24	0	9	1	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
6	A	272	0	387	18	0
6	B	272	0	387	13	0
6	C	272	0	387	13	0
6	D	272	0	387	16	0
All	All	78512	0	79180	1752	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 11.

All (1752) 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:2213:PRO:HG3	1:D:2647:LEU:HB3	1.54	0.89
1:B:2213:PRO:HG3	1:B:2647:LEU:HB3	1.54	0.88
1:A:2213:PRO:HG3	1:A:2647:LEU:HB3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2213:PRO:HG3	1:C:2647:LEU:HB3	1.54	0.86
1:D:806:LEU:HG	1:D:1103:LEU:HD22	1.58	0.85
1:A:806:LEU:HG	1:A:1103:LEU:HD22	1.58	0.84
1:C:806:LEU:HG	1:C:1103:LEU:HD22	1.58	0.84
1:B:806:LEU:HG	1:B:1103:LEU:HD22	1.58	0.83
1:B:1100:VAL:HG22	1:B:1101:GLN:H	1.42	0.82
1:A:1100:VAL:HG22	1:A:1101:GLN:H	1.42	0.82
1:A:807:TRP:CE3	1:A:1102:LEU:HD11	2.15	0.81
1:C:807:TRP:CE3	1:C:1102:LEU:HD11	2.15	0.81
1:D:807:TRP:HB2	1:D:1102:LEU:HD21	1.63	0.81
1:A:807:TRP:HB2	1:A:1102:LEU:HD21	1.63	0.81
1:B:807:TRP:CE3	1:B:1102:LEU:HD11	2.15	0.81
1:C:1100:VAL:HG22	1:C:1101:GLN:H	1.42	0.81
1:D:807:TRP:CE3	1:D:1102:LEU:HD11	2.15	0.81
1:D:1100:VAL:HG22	1:D:1101:GLN:H	1.42	0.81
1:B:807:TRP:HB2	1:B:1102:LEU:HD21	1.63	0.80
1:C:807:TRP:HB2	1:C:1102:LEU:HD21	1.63	0.80
1:A:1654:CYS:SG	1:A:1658:LYS:NZ	2.57	0.78
1:D:1654:CYS:SG	1:D:1658:LYS:NZ	2.57	0.77
1:B:1654:CYS:SG	1:B:1658:LYS:NZ	2.57	0.76
1:B:807:TRP:HE3	1:B:1102:LEU:HD11	1.50	0.76
1:C:1654:CYS:SG	1:C:1658:LYS:NZ	2.57	0.76
1:C:807:TRP:HE3	1:C:1102:LEU:HD11	1.50	0.76
1:A:978:LEU:HD13	1:A:981:ILE:HD11	1.68	0.76
1:D:978:LEU:HD13	1:D:981:ILE:HD11	1.68	0.76
6:B:2812:PLX:H321	6:B:2814:PLX:H292	1.68	0.75
1:D:2528:CYS:HA	1:D:2534:CYS:HB2	1.68	0.75
1:D:667:GLU:HG3	1:D:732:TYR:HD2	1.51	0.75
1:B:978:LEU:HD13	1:B:981:ILE:HD11	1.68	0.75
1:C:667:GLU:HG3	1:C:732:TYR:HD2	1.51	0.75
1:B:2711:ASN:O	1:B:2715:GLN:NE2	2.20	0.75
1:D:807:TRP:HE3	1:D:1102:LEU:HD11	1.50	0.75
1:A:667:GLU:HG3	1:A:732:TYR:HD2	1.51	0.75
1:A:807:TRP:HE3	1:A:1102:LEU:HD11	1.50	0.74
6:A:2811:PLX:H321	6:A:2813:PLX:H292	1.68	0.74
1:B:667:GLU:HG3	1:B:732:TYR:HD2	1.51	0.74
1:B:2528:CYS:HA	1:B:2534:CYS:HB2	1.68	0.74
6:C:2804:PLX:H321	6:C:2806:PLX:H292	1.68	0.74
1:C:2711:ASN:O	1:C:2715:GLN:NE2	2.20	0.74
1:D:2711:ASN:O	1:D:2715:GLN:NE2	2.20	0.74
1:C:1418:GLU:HG3	1:C:1474:VAL:HG11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:978:LEU:HD13	1:C:981:ILE:HD11	1.68	0.73
6:D:2811:PLX:H321	6:D:2813:PLX:H292	1.68	0.73
1:C:2528:CYS:HA	1:C:2534:CYS:HB2	1.68	0.73
1:A:1418:GLU:HG3	1:A:1474:VAL:HG11	1.70	0.73
1:B:1418:GLU:HG3	1:B:1474:VAL:HG11	1.70	0.73
1:D:1418:GLU:HG3	1:D:1474:VAL:HG11	1.70	0.73
1:A:2528:CYS:HA	1:A:2534:CYS:HB2	1.68	0.73
1:A:2711:ASN:O	1:A:2715:GLN:NE2	2.20	0.73
1:D:2554:ARG:O	1:D:2566:ARG:NH2	2.23	0.71
1:A:1982:ARG:NH1	1:A:2048:CYS:SG	2.63	0.71
1:C:2305:LEU:HB3	1:C:2308:HIS:HB2	1.73	0.71
1:D:1982:ARG:NH1	1:D:2048:CYS:SG	2.63	0.71
1:D:2305:LEU:HB3	1:D:2308:HIS:HB2	1.73	0.71
1:C:2554:ARG:O	1:C:2566:ARG:NH2	2.23	0.71
1:D:2527:THR:OG1	1:D:2537:THR:OG1	2.09	0.71
1:B:2305:LEU:HB3	1:B:2308:HIS:HB2	1.73	0.71
1:B:1982:ARG:NH1	1:B:2048:CYS:SG	2.63	0.71
1:B:807:TRP:H	1:B:1103:LEU:HD23	1.56	0.71
1:A:2305:LEU:HB3	1:A:2308:HIS:HB2	1.73	0.71
1:C:1982:ARG:NH1	1:C:2048:CYS:SG	2.63	0.71
1:A:807:TRP:H	1:A:1103:LEU:HD23	1.56	0.70
1:A:875:TYR:HE1	1:A:980:PHE:HB2	1.56	0.70
1:A:2554:ARG:O	1:A:2566:ARG:NH2	2.23	0.70
1:C:2527:THR:OG1	1:C:2537:THR:OG1	2.09	0.70
1:B:2527:THR:OG1	1:B:2537:THR:OG1	2.09	0.70
1:D:497:VAL:HB	1:D:558:ARG:HH22	1.57	0.70
1:B:2554:ARG:O	1:B:2566:ARG:NH2	2.23	0.70
1:D:1218:LEU:HD22	1:D:1238:HIS:HE1	1.56	0.70
1:A:1218:LEU:HD22	1:A:1238:HIS:HE1	1.56	0.69
1:C:497:VAL:HB	1:C:558:ARG:HH22	1.56	0.69
1:D:875:TYR:HE1	1:D:980:PHE:HB2	1.56	0.69
1:A:99:GLU:OE2	1:A:103:ASN:ND2	2.25	0.69
1:A:1102:LEU:HD23	1:A:1103:LEU:H	1.58	0.69
1:B:304:ARG:NH1	1:B:361:GLY:O	2.26	0.69
1:C:99:GLU:OE2	1:C:103:ASN:ND2	2.25	0.69
1:D:1102:LEU:HD23	1:D:1103:LEU:H	1.58	0.69
1:B:875:TYR:HE1	1:B:980:PHE:HB2	1.56	0.69
1:B:1218:LEU:HD22	1:B:1238:HIS:HE1	1.56	0.69
1:C:807:TRP:H	1:C:1103:LEU:HD23	1.56	0.69
1:D:304:ARG:NH1	1:D:361:GLY:O	2.26	0.69
1:B:495:LEU:HD13	1:B:554:ARG:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:LEU:HD23	1:B:1103:LEU:H	1.58	0.68
1:A:304:ARG:NH1	1:A:361:GLY:O	2.26	0.68
1:C:495:LEU:HD13	1:C:554:ARG:HD3	1.75	0.68
1:C:875:TYR:HE1	1:C:980:PHE:HB2	1.56	0.68
1:A:495:LEU:HD13	1:A:554:ARG:HD3	1.75	0.68
1:B:55:ASP:O	1:B:125:HIS:NE2	2.27	0.68
1:B:99:GLU:OE2	1:B:103:ASN:ND2	2.25	0.68
1:D:495:LEU:HD13	1:D:554:ARG:HD3	1.75	0.68
1:A:497:VAL:HB	1:A:558:ARG:HH22	1.56	0.68
1:D:807:TRP:H	1:D:1103:LEU:HD23	1.56	0.68
1:C:304:ARG:NH1	1:C:361:GLY:O	2.26	0.68
1:C:1102:LEU:HD23	1:C:1103:LEU:H	1.58	0.68
1:C:1104:VAL:HG23	1:C:1105:THR:H	1.59	0.68
1:B:497:VAL:HB	1:B:558:ARG:HH22	1.56	0.68
1:C:1218:LEU:HD22	1:C:1238:HIS:HE1	1.56	0.68
1:D:99:GLU:OE2	1:D:103:ASN:ND2	2.25	0.68
1:C:2199:VAL:HG12	1:C:2205:MET:HG2	1.76	0.67
1:B:2199:VAL:HG12	1:B:2205:MET:HG2	1.76	0.67
1:C:1102:LEU:HD23	1:C:1103:LEU:N	2.09	0.67
1:D:1102:LEU:HD23	1:D:1103:LEU:N	2.09	0.67
1:A:661:ASN:HA	1:A:666:ILE:HD11	1.76	0.67
1:D:550:ARG:NH2	1:D:588:ASP:OD2	2.28	0.67
1:D:1104:VAL:HG23	1:D:1105:THR:H	1.59	0.67
1:D:2199:VAL:HG12	1:D:2205:MET:HG2	1.76	0.67
1:A:1103:LEU:HD12	1:A:1108:ASP:HB3	1.77	0.67
1:A:2199:VAL:HG12	1:A:2205:MET:HG2	1.76	0.67
1:C:550:ARG:NH2	1:C:588:ASP:OD2	2.28	0.67
1:A:550:ARG:NH2	1:A:588:ASP:OD2	2.28	0.67
1:D:661:ASN:HA	1:D:666:ILE:HD11	1.76	0.67
1:A:1331:MET:HA	1:A:1334:LEU:HB2	1.76	0.66
1:B:550:ARG:NH2	1:B:588:ASP:OD2	2.28	0.66
1:B:1102:LEU:HD23	1:B:1103:LEU:N	2.09	0.66
1:B:1331:MET:HA	1:B:1334:LEU:HB2	1.76	0.66
1:C:1331:MET:HA	1:C:1334:LEU:HB2	1.76	0.66
1:B:1104:VAL:HG23	1:B:1105:THR:H	1.59	0.66
1:A:1102:LEU:HD23	1:A:1103:LEU:N	2.09	0.66
1:A:1104:VAL:HG23	1:A:1105:THR:H	1.59	0.66
1:A:2016:GLY:HA2	1:A:2020:LEU:HB2	1.78	0.66
1:B:775:TYR:HB2	1:B:858:GLU:HG2	1.78	0.66
1:B:1293:GLN:O	1:B:1297:HIS:ND1	2.29	0.66
1:C:2657:THR:HG22	1:C:2658:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:733:TYR:HD1	1:D:736:GLN:HE21	1.43	0.66
1:D:1103:LEU:HD12	1:D:1108:ASP:HB3	1.77	0.66
1:D:1331:MET:HA	1:D:1334:LEU:HB2	1.76	0.66
1:A:55:ASP:O	1:A:125:HIS:NE2	2.27	0.66
1:B:1103:LEU:HD12	1:B:1108:ASP:HB3	1.77	0.66
1:D:775:TYR:HB2	1:D:858:GLU:HG2	1.78	0.66
1:A:775:TYR:HB2	1:A:858:GLU:HG2	1.78	0.65
1:C:775:TYR:HB2	1:C:858:GLU:HG2	1.78	0.65
1:A:891:LEU:HD21	1:A:974:ILE:HG23	1.78	0.65
1:B:2016:GLY:HA2	1:B:2020:LEU:HB2	1.78	0.65
1:C:661:ASN:HA	1:C:666:ILE:HD11	1.76	0.65
1:D:2016:GLY:HA2	1:D:2020:LEU:HB2	1.78	0.65
1:A:475:LYS:NZ	1:A:478:GLU:OE1	2.29	0.65
1:B:2657:THR:HG22	1:B:2658:GLY:H	1.60	0.65
1:C:891:LEU:HD21	1:C:974:ILE:HG23	1.78	0.65
1:C:1293:GLN:O	1:C:1297:HIS:ND1	2.29	0.65
1:C:2016:GLY:HA2	1:C:2020:LEU:HB2	1.78	0.65
1:B:661:ASN:HA	1:B:666:ILE:HD11	1.76	0.65
1:D:475:LYS:NZ	1:D:478:GLU:OE1	2.29	0.65
1:C:475:LYS:NZ	1:C:478:GLU:OE1	2.29	0.65
1:C:2627:THR:O	1:C:2628:PHE:C	2.35	0.65
1:D:1293:GLN:O	1:D:1297:HIS:ND1	2.29	0.65
1:D:2657:THR:HG22	1:D:2658:GLY:H	1.60	0.65
1:A:2657:THR:HG22	1:A:2658:GLY:H	1.60	0.65
1:A:2527:THR:OG1	1:A:2537:THR:OG1	2.09	0.65
1:B:475:LYS:NZ	1:B:478:GLU:OE1	2.29	0.65
1:D:2627:THR:O	1:D:2628:PHE:C	2.35	0.65
1:A:2627:THR:O	1:A:2628:PHE:C	2.35	0.65
1:C:1103:LEU:HD12	1:C:1108:ASP:HB3	1.77	0.65
1:D:55:ASP:O	1:D:125:HIS:NE2	2.27	0.65
1:D:1791:SER:OG	1:D:1794:GLU:OE1	2.15	0.65
1:A:1293:GLN:O	1:A:1297:HIS:ND1	2.29	0.65
1:C:733:TYR:HD1	1:C:736:GLN:HE21	1.43	0.65
1:D:891:LEU:HD21	1:D:974:ILE:HG23	1.78	0.65
1:B:1028:LEU:HG	1:B:1607:ILE:HD11	1.79	0.64
1:C:1791:SER:OG	1:C:1794:GLU:OE1	2.15	0.64
1:A:136:LYS:HG3	1:A:137:ARG:HD3	1.80	0.64
1:D:136:LYS:HG3	1:D:137:ARG:HD3	1.79	0.64
1:D:667:GLU:HG3	1:D:732:TYR:CD2	2.32	0.64
1:B:2627:THR:O	1:B:2628:PHE:C	2.35	0.64
1:C:723:GLN:HG3	1:C:726:ASP:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:LEU:HG	1:A:1607:ILE:HD11	1.79	0.64
1:B:136:LYS:HG3	1:B:137:ARG:HD3	1.79	0.64
1:B:723:GLN:HG3	1:B:726:ASP:H	1.63	0.64
1:C:667:GLU:HG3	1:C:732:TYR:CD2	2.32	0.64
1:A:667:GLU:HG3	1:A:732:TYR:CD2	2.32	0.64
1:B:147:MET:HB3	1:B:211:SER:HB3	1.79	0.64
1:A:1976:LEU:HB3	1:A:1984:LEU:HD13	1.79	0.64
1:B:667:GLU:HG3	1:B:732:TYR:CD2	2.32	0.64
1:C:136:LYS:HG3	1:C:137:ARG:HD3	1.80	0.64
1:D:723:GLN:HG3	1:D:726:ASP:H	1.63	0.64
1:A:733:TYR:HD1	1:A:736:GLN:HE21	1.43	0.64
1:B:891:LEU:HD21	1:B:974:ILE:HG23	1.78	0.64
1:C:1976:LEU:HB3	1:C:1984:LEU:HD13	1.79	0.64
1:B:564:GLN:O	1:B:571:GLN:NE2	2.31	0.64
1:D:147:MET:HB3	1:D:211:SER:HB3	1.79	0.64
1:A:564:GLN:O	1:A:571:GLN:NE2	2.31	0.64
1:C:55:ASP:O	1:C:125:HIS:NE2	2.27	0.64
1:C:147:MET:HB3	1:C:211:SER:HB3	1.79	0.64
1:C:164:GLN:OE1	1:C:185:ASN:ND2	2.31	0.64
1:B:1808:VAL:HG11	1:B:1828:ALA:HB2	1.81	0.63
1:C:1028:LEU:HG	1:C:1607:ILE:HD11	1.79	0.63
1:B:1976:LEU:HB3	1:B:1984:LEU:HD13	1.79	0.63
1:C:564:GLN:O	1:C:571:GLN:NE2	2.31	0.63
1:B:2129:TYR:O	1:B:2150:ARG:NH2	2.32	0.63
1:D:564:GLN:O	1:D:571:GLN:NE2	2.31	0.63
1:D:970:THR:O	1:D:974:ILE:HD12	1.99	0.63
1:D:1028:LEU:HG	1:D:1607:ILE:HD11	1.79	0.63
1:B:733:TYR:HD1	1:B:736:GLN:HE21	1.43	0.63
1:C:2128:ALA:HA	1:C:2131:GLN:HE22	1.63	0.63
1:A:147:MET:HB3	1:A:211:SER:HB3	1.79	0.63
1:A:164:GLN:OE1	1:A:185:ASN:ND2	2.31	0.63
1:A:1791:SER:OG	1:A:1794:GLU:OE1	2.15	0.63
1:C:1172:ASN:HA	1:C:1175:VAL:HG12	1.81	0.63
1:D:436:SER:HB3	1:D:439:GLU:HG3	1.80	0.63
1:D:2128:ALA:HA	1:D:2131:GLN:HE22	1.63	0.63
1:D:1976:LEU:HB3	1:D:1984:LEU:HD13	1.79	0.63
1:A:2128:ALA:HA	1:A:2131:GLN:HE22	1.63	0.63
1:B:1791:SER:OG	1:B:1794:GLU:OE1	2.15	0.63
1:A:723:GLN:HG3	1:A:726:ASP:H	1.63	0.63
1:A:2129:TYR:O	1:A:2150:ARG:NH2	2.32	0.63
1:B:970:THR:O	1:B:974:ILE:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2210:PHE:HE2	1:B:2647:LEU:HD11	1.64	0.63
1:D:2210:PHE:HE2	1:D:2647:LEU:HD11	1.64	0.63
1:A:1103:LEU:CD1	1:A:1108:ASP:HB3	2.29	0.62
1:D:1103:LEU:CD1	1:D:1108:ASP:HB3	2.29	0.62
1:D:2628:PHE:O	1:D:2631:HIS:N	2.32	0.62
1:A:1808:VAL:HG11	1:A:1828:ALA:HB2	1.81	0.62
1:B:1618:LEU:HD22	1:B:1736:LEU:HD12	1.81	0.62
1:B:2628:PHE:O	1:B:2631:HIS:N	2.32	0.62
1:C:970:THR:O	1:C:974:ILE:HD12	1.99	0.62
1:D:164:GLN:OE1	1:D:185:ASN:ND2	2.31	0.62
1:D:1808:VAL:HG11	1:D:1828:ALA:HB2	1.81	0.62
1:A:970:THR:O	1:A:974:ILE:HD12	1.99	0.62
1:B:436:SER:HB3	1:B:439:GLU:HG3	1.80	0.62
1:C:1808:VAL:HG11	1:C:1828:ALA:HB2	1.81	0.62
1:C:2210:PHE:HE2	1:C:2647:LEU:HD11	1.64	0.62
1:C:1103:LEU:CD1	1:C:1108:ASP:HB3	2.29	0.62
1:D:1172:ASN:HA	1:D:1175:VAL:HG12	1.81	0.62
1:A:436:SER:HB3	1:A:439:GLU:HG3	1.80	0.62
1:A:2210:PHE:HE2	1:A:2647:LEU:HD11	1.64	0.62
1:B:164:GLN:OE1	1:B:185:ASN:ND2	2.31	0.62
1:C:1618:LEU:HD22	1:C:1736:LEU:HD12	1.81	0.62
1:B:1103:LEU:CD1	1:B:1108:ASP:HB3	2.29	0.62
1:C:2628:PHE:O	1:C:2631:HIS:N	2.32	0.62
1:A:2628:PHE:O	1:A:2631:HIS:N	2.32	0.62
1:B:2128:ALA:HA	1:B:2131:GLN:HE22	1.63	0.62
1:C:2558:LYS:NZ	1:C:2559:GLU:OE2	2.33	0.62
1:D:2129:TYR:O	1:D:2150:ARG:NH2	2.32	0.62
1:A:1172:ASN:HA	1:A:1175:VAL:HG12	1.81	0.62
1:A:2074:ILE:O	1:A:2078:GLY:N	2.30	0.62
1:D:1076:VAL:HG23	1:D:1659:HIS:CE1	2.35	0.61
1:A:1618:LEU:HD22	1:A:1736:LEU:HD12	1.81	0.61
1:C:436:SER:HB3	1:C:439:GLU:HG3	1.80	0.61
1:D:1618:LEU:HD22	1:D:1736:LEU:HD12	1.81	0.61
1:C:665:LEU:HB3	1:C:667:GLU:HG2	1.82	0.61
1:C:2129:TYR:O	1:C:2150:ARG:NH2	2.32	0.61
1:A:1076:VAL:HG23	1:A:1659:HIS:CE1	2.35	0.61
1:B:181:LYS:HB3	1:B:217:SER:HB2	1.83	0.61
1:B:1172:ASN:HA	1:B:1175:VAL:HG12	1.81	0.61
1:C:181:LYS:HB3	1:C:217:SER:HB2	1.83	0.61
1:D:1421:ILE:HG13	1:D:1478:TYR:HD1	1.66	0.61
1:C:1076:VAL:HG23	1:C:1659:HIS:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1857:PHE:CE2	1:D:1991:GLN:HG2	2.36	0.61
1:A:1421:ILE:HG13	1:A:1478:TYR:HD1	1.66	0.61
1:D:669:LYS:HD3	1:D:699:PHE:HB2	1.83	0.61
1:A:181:LYS:HB3	1:A:217:SER:HB2	1.83	0.61
1:D:665:LEU:HB3	1:D:667:GLU:HG2	1.82	0.61
1:D:2219:LEU:HD11	1:D:2250:LEU:HD22	1.83	0.61
1:B:2081:ARG:HB3	1:B:2084:LEU:HD13	1.83	0.60
1:C:669:LYS:HD3	1:C:699:PHE:HB2	1.83	0.60
1:C:2219:LEU:HD11	1:C:2250:LEU:HD22	1.83	0.60
1:D:743:MET:O	1:D:748:GLN:NE2	2.33	0.60
1:A:1857:PHE:CE2	1:A:1991:GLN:HG2	2.36	0.60
1:B:1857:PHE:CE2	1:B:1991:GLN:HG2	2.36	0.60
1:A:2081:ARG:HB3	1:A:2084:LEU:HD13	1.83	0.60
1:B:669:LYS:HD3	1:B:699:PHE:HB2	1.83	0.60
1:D:181:LYS:HB3	1:D:217:SER:HB2	1.83	0.60
1:D:760:ASP:HB2	1:D:763:LEU:HD23	1.83	0.60
1:A:760:ASP:HB2	1:A:763:LEU:HD23	1.84	0.60
1:A:2219:LEU:HD11	1:A:2250:LEU:HD22	1.83	0.60
1:A:523:LEU:HD12	1:A:556:CYS:HB2	1.84	0.60
1:D:2074:ILE:O	1:D:2078:GLY:N	2.30	0.60
1:D:2558:LYS:NZ	1:D:2559:GLU:OE2	2.33	0.60
1:A:669:LYS:HD3	1:A:699:PHE:HB2	1.83	0.60
1:B:1076:VAL:HG23	1:B:1659:HIS:CE1	2.35	0.60
1:A:1428:ASN:HB2	1:A:1486:ILE:HG22	1.84	0.60
1:C:743:MET:O	1:C:748:GLN:NE2	2.33	0.60
1:C:1857:PHE:CE2	1:C:1991:GLN:HG2	2.36	0.60
1:D:523:LEU:HD12	1:D:556:CYS:HB2	1.84	0.60
1:B:1051:ASP:OD2	1:B:1057:GLY:N	2.35	0.60
1:C:2081:ARG:HB3	1:C:2084:LEU:HD13	1.83	0.60
1:A:2327:LEU:HD21	1:A:2331:HIS:CD2	2.37	0.60
1:C:523:LEU:HD12	1:C:556:CYS:HB2	1.84	0.60
1:D:1428:ASN:HB2	1:D:1486:ILE:HG22	1.84	0.60
1:D:2327:LEU:HD21	1:D:2331:HIS:CD2	2.37	0.60
1:C:760:ASP:HB2	1:C:763:LEU:HD23	1.83	0.59
1:C:1421:ILE:HG13	1:C:1478:TYR:HD1	1.66	0.59
1:D:2081:ARG:HB3	1:D:2084:LEU:HD13	1.83	0.59
1:A:2532:LEU:HD12	1:B:2293:PHE:HA	1.85	0.59
1:B:523:LEU:HD12	1:B:556:CYS:HB2	1.84	0.59
1:B:1428:ASN:HB2	1:B:1486:ILE:HG22	1.84	0.59
1:C:1428:ASN:HB2	1:C:1486:ILE:HG22	1.84	0.59
1:D:1051:ASP:OD2	1:D:1057:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:ASP:OD2	1:A:1057:GLY:N	2.35	0.59
1:B:1421:ILE:HG13	1:B:1478:TYR:HD1	1.66	0.59
1:A:665:LEU:HB3	1:A:667:GLU:HG2	1.82	0.59
1:B:10:HIS:ND1	1:B:112:GLY:O	2.32	0.59
1:B:665:LEU:HB3	1:B:667:GLU:HG2	1.82	0.59
1:B:2219:LEU:HD11	1:B:2250:LEU:HD22	1.83	0.59
1:B:2327:LEU:HD21	1:B:2331:HIS:CD2	2.37	0.59
1:C:2327:LEU:HD21	1:C:2331:HIS:CD2	2.37	0.59
1:B:760:ASP:HB2	1:B:763:LEU:HD23	1.84	0.59
1:C:69:GLN:HE22	1:C:73:TRP:HE3	1.51	0.59
1:B:69:GLN:HE22	1:B:73:TRP:HE3	1.51	0.59
1:C:1796:GLN:HB3	1:C:1839:ILE:HD11	1.85	0.59
1:C:1051:ASP:OD2	1:C:1057:GLY:N	2.35	0.59
1:B:2074:ILE:O	1:B:2078:GLY:N	2.30	0.58
1:A:2282:ASN:OD1	1:A:2334:ARG:NH2	2.36	0.58
1:B:2532:LEU:HD12	1:C:2293:PHE:HA	1.85	0.58
1:A:2263:GLN:OE1	1:A:2266:LEU:HB2	2.04	0.58
1:B:1419:VAL:HG13	1:B:1423:TYR:HE2	1.69	0.58
1:B:2558:LYS:NZ	1:B:2559:GLU:OE2	2.33	0.58
1:D:1598:ARG:HH21	1:D:1602:GLU:HB3	1.68	0.58
1:A:1796:GLN:HB3	1:A:1839:ILE:HD11	1.85	0.58
1:C:1419:VAL:HG13	1:C:1423:TYR:CE2	2.38	0.58
1:C:2282:ASN:OD1	1:C:2334:ARG:NH2	2.36	0.58
1:A:1373:MET:HA	1:A:1376:ILE:HD12	1.86	0.58
1:B:1796:GLN:HB3	1:B:1839:ILE:HD11	1.85	0.58
1:C:10:HIS:ND1	1:C:112:GLY:O	2.32	0.58
1:C:2532:LEU:HD12	1:D:2293:PHE:HA	1.85	0.58
1:D:69:GLN:HE22	1:D:73:TRP:HE3	1.51	0.58
1:D:1796:GLN:HB3	1:D:1839:ILE:HD11	1.85	0.58
1:A:69:GLN:HE22	1:A:73:TRP:HE3	1.51	0.58
1:A:1103:LEU:HD13	1:A:1109:VAL:HG23	1.86	0.58
1:A:2586[A]:PHE:HE1	1:D:2579:ILE:HG23	1.68	0.58
1:B:1373:MET:HA	1:B:1376:ILE:HD12	1.86	0.58
1:C:1419:VAL:HG13	1:C:1423:TYR:HE2	1.69	0.58
1:A:1419:VAL:HG13	1:A:1423:TYR:CE2	2.38	0.58
1:A:2558:LYS:NZ	1:A:2559:GLU:OE2	2.33	0.58
1:D:19:ALA:HB2	1:D:218:TRP:CZ3	2.39	0.58
1:D:1419:VAL:HG13	1:D:1423:TYR:CE2	2.38	0.58
1:D:695:GLU:OE2	1:D:713:ARG:NH1	2.32	0.58
1:D:1069:MET:O	1:D:1655:LYS:NZ	2.35	0.58
1:D:1419:VAL:HG13	1:D:1423:TYR:HE2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:HB2	1:A:218:TRP:CZ3	2.39	0.58
1:B:19:ALA:HB2	1:B:218:TRP:CZ3	2.39	0.58
1:C:1373:MET:HA	1:C:1376:ILE:HD12	1.86	0.58
1:A:1419:VAL:HG13	1:A:1423:TYR:HE2	1.69	0.57
1:B:2282:ASN:OD1	1:B:2334:ARG:NH2	2.36	0.57
1:D:2263:GLN:OE1	1:D:2266:LEU:HB2	2.04	0.57
1:C:764:ILE:HG21	1:C:785:MET:HB2	1.87	0.57
1:D:2282:ASN:OD1	1:D:2334:ARG:NH2	2.36	0.57
1:A:527:PHE:HA	1:A:536:LEU:HD13	1.87	0.57
1:A:2293:PHE:HA	1:D:2532:LEU:HD12	1.86	0.57
1:B:1598:ARG:HH21	1:B:1602:GLU:HB3	1.68	0.57
1:C:527:PHE:HA	1:C:536:LEU:HD13	1.87	0.57
1:B:1069:MET:O	1:B:1655:LYS:NZ	2.35	0.57
1:C:1598:ARG:HH21	1:C:1602:GLU:HB3	1.68	0.57
1:D:1103:LEU:HD13	1:D:1109:VAL:HG23	1.86	0.57
1:B:764:ILE:HG21	1:B:785:MET:HB2	1.87	0.57
1:D:1373:MET:HA	1:D:1376:ILE:HD12	1.86	0.57
1:A:1598:ARG:HH21	1:A:1602:GLU:HB3	1.68	0.57
1:C:19:ALA:HB2	1:C:218:TRP:CZ3	2.39	0.57
1:B:695:GLU:OE2	1:B:713:ARG:NH1	2.32	0.57
1:B:2263:GLN:OE1	1:B:2266:LEU:HB2	2.04	0.57
1:B:2443:LEU:HB3	1:C:2427:LEU:HG	1.86	0.57
1:C:1218:LEU:HD22	1:C:1238:HIS:CE1	2.38	0.57
1:A:764:ILE:HG21	1:A:785:MET:HB2	1.87	0.57
1:B:527:PHE:HA	1:B:536:LEU:HD13	1.87	0.57
1:A:1639:GLU:HA	1:A:1644:ARG:HD3	1.87	0.57
1:B:1639:GLU:HA	1:B:1644:ARG:HD3	1.87	0.57
1:C:1639:GLU:HA	1:C:1644:ARG:HD3	1.87	0.57
1:C:2074:ILE:O	1:C:2078:GLY:N	2.30	0.57
1:C:2263:GLN:OE1	1:C:2266:LEU:HB2	2.04	0.57
1:C:1069:MET:O	1:C:1655:LYS:NZ	2.35	0.56
1:C:1103:LEU:HD13	1:C:1109:VAL:HG23	1.86	0.56
1:C:2443:LEU:HB3	1:D:2427:LEU:HG	1.87	0.56
1:D:527:PHE:HA	1:D:536:LEU:HD13	1.87	0.56
1:D:1639:GLU:HA	1:D:1644:ARG:HD3	1.87	0.56
1:B:1103:LEU:HD13	1:B:1109:VAL:HG23	1.86	0.56
1:B:1419:VAL:HG13	1:B:1423:TYR:CE2	2.38	0.56
1:B:2579:ILE:HG23	1:C:2586[A]:PHE:HE1	1.70	0.56
1:D:1961:ALA:O	1:D:1965:ILE:HG12	2.05	0.56
1:A:1277:PHE:HA	1:A:1280:ASN:HD21	1.70	0.56
1:B:1218:LEU:HD22	1:B:1238:HIS:CE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:ARG:NH1	1:D:731:SER:OG	2.39	0.56
1:A:2579:ILE:HG23	1:B:2586[A]:PHE:HE1	1.71	0.56
1:C:1961:ALA:O	1:C:1965:ILE:HG12	2.05	0.56
1:A:2427:LEU:HG	1:D:2443:LEU:HB3	1.88	0.56
1:A:2435:THR:HG21	6:A:2813:PLX:H52	1.88	0.56
1:B:886:ARG:HA	1:B:889:LYS:NZ	2.21	0.56
1:D:764:ILE:HG21	1:D:785:MET:HB2	1.87	0.56
1:C:1389:LYS:HB3	1:C:1435:GLU:HB2	1.88	0.56
1:C:1621:ALA:O	1:C:1625:VAL:HG23	2.06	0.56
1:D:1621:ALA:O	1:D:1625:VAL:HG23	2.06	0.56
1:A:2443:LEU:HB3	1:B:2427:LEU:HG	1.88	0.56
1:B:727:ARG:NH1	1:B:731:SER:OG	2.39	0.56
1:C:1277:PHE:HA	1:C:1280:ASN:HD21	1.70	0.56
1:B:547:ALA:HB3	1:B:548:PRO:HD3	1.88	0.56
1:B:1421:ILE:HD11	1:B:1478:TYR:HB2	1.88	0.56
1:C:886:ARG:HA	1:C:889:LYS:NZ	2.21	0.56
1:A:10:HIS:ND1	1:A:112:GLY:O	2.32	0.55
1:C:2553:LEU:HB3	1:C:2566:ARG:NH2	2.22	0.55
1:D:547:ALA:HB3	1:D:548:PRO:HD3	1.89	0.55
1:D:886:ARG:HA	1:D:889:LYS:NZ	2.21	0.55
1:B:1961:ALA:O	1:B:1965:ILE:HG12	2.05	0.55
1:C:727:ARG:NH1	1:C:731:SER:OG	2.39	0.55
1:C:2579:ILE:HG23	1:D:2586[A]:PHE:HE1	1.70	0.55
1:C:2701:LYS:O	1:C:2705:THR:N	2.39	0.55
1:D:847:VAL:HG13	1:D:894:ILE:HD11	1.88	0.55
1:D:2553:LEU:HB3	1:D:2566:ARG:NH2	2.22	0.55
1:A:1421:ILE:HD11	1:A:1478:TYR:HB2	1.88	0.55
1:A:1961:ALA:O	1:A:1965:ILE:HG12	2.05	0.55
1:D:2628:PHE:O	1:D:2630:GLU:N	2.40	0.55
1:A:743:MET:O	1:A:748:GLN:NE2	2.33	0.55
1:C:2435:THR:HG21	6:C:2806:PLX:H52	1.88	0.55
1:D:1277:PHE:HA	1:D:1280:ASN:HD21	1.70	0.55
1:D:1840:GLN:NE2	1:D:1976:LEU:O	2.40	0.55
1:A:847:VAL:HG13	1:A:894:ILE:HD11	1.88	0.55
1:A:2703:GLU:HA	1:A:2706:MET:HG2	1.88	0.55
1:C:695:GLU:OE2	1:C:713:ARG:NH1	2.32	0.55
1:C:1421:ILE:HD11	1:C:1478:TYR:HB2	1.88	0.55
1:A:1218:LEU:HD22	1:A:1238:HIS:CE1	2.38	0.55
1:A:2628:PHE:O	1:A:2630:GLU:N	2.40	0.55
1:B:743:MET:O	1:B:748:GLN:NE2	2.33	0.55
1:C:2122:VAL:HG12	1:C:2126:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:2813:PLX:H282	6:D:2813:PLX:H112	1.88	0.55
1:B:665:LEU:O	1:B:667:GLU:N	2.40	0.55
1:B:1389:LYS:HB3	1:B:1435:GLU:HB2	1.88	0.55
1:B:1621:ALA:O	1:B:1625:VAL:HG23	2.06	0.55
1:D:425:GLU:OE1	1:D:427:LYS:NZ	2.40	0.55
1:A:547:ALA:HB3	1:A:548:PRO:HD3	1.89	0.55
1:A:1621:ALA:O	1:A:1625:VAL:HG23	2.06	0.55
1:B:306:LYS:NZ	1:B:311:GLY:O	2.38	0.55
1:B:1840:GLN:NE2	1:B:1976:LEU:O	2.40	0.55
1:C:425:GLU:OE1	1:C:427:LYS:NZ	2.40	0.55
1:C:547:ALA:HB3	1:C:548:PRO:HD3	1.89	0.55
1:C:1840:GLN:NE2	1:C:1976:LEU:O	2.40	0.55
1:D:2121:LEU:O	1:D:2125:ILE:HG12	2.07	0.55
1:D:2647:LEU:HA	1:D:2650:VAL:HG12	1.89	0.55
1:A:727:ARG:NH1	1:A:731:SER:OG	2.39	0.55
1:A:886:ARG:HA	1:A:889:LYS:NZ	2.21	0.55
1:B:425:GLU:OE1	1:B:427:LYS:NZ	2.40	0.55
1:B:847:VAL:HG13	1:B:894:ILE:HD11	1.88	0.55
1:B:2628:PHE:O	1:B:2630:GLU:N	2.40	0.55
1:B:1277:PHE:HA	1:B:1280:ASN:HD21	1.70	0.55
1:B:2647:LEU:HA	1:B:2650:VAL:HG12	1.89	0.55
1:D:1389:LYS:HB3	1:D:1435:GLU:HB2	1.88	0.55
1:A:2121:LEU:O	1:A:2125:ILE:HG12	2.07	0.54
1:A:2647:LEU:HA	1:A:2650:VAL:HG12	1.89	0.54
1:B:2553:LEU:HB3	1:B:2566:ARG:NH2	2.21	0.54
1:C:410:GLU:OE1	1:C:412:LYS:N	2.41	0.54
1:D:410:GLU:OE1	1:D:412:LYS:N	2.40	0.54
1:B:1617:PRO:HB3	1:B:1729:ASP:HB3	1.90	0.54
1:C:2703:GLU:HA	1:C:2706:MET:HG2	1.89	0.54
1:D:1421:ILE:HD11	1:D:1478:TYR:HB2	1.88	0.54
1:D:2122:VAL:HG12	1:D:2126:LYS:NZ	2.22	0.54
1:A:1069:MET:O	1:A:1655:LYS:NZ	2.35	0.54
1:A:1389:LYS:HB3	1:A:1435:GLU:HB2	1.88	0.54
1:C:392:HIS:HE1	1:C:394:CYS:HB3	1.72	0.54
1:C:554:ARG:HG3	1:C:590:LEU:HG	1.90	0.54
1:C:2628:PHE:O	1:C:2630:GLU:N	2.40	0.54
1:C:2647:LEU:HA	1:C:2650:VAL:HG12	1.89	0.54
6:C:2806:PLX:H282	6:C:2806:PLX:H112	1.88	0.54
1:D:507:GLN:NE2	1:D:562:HIS:O	2.41	0.54
1:D:554:ARG:HG3	1:D:590:LEU:HG	1.90	0.54
1:D:1218:LEU:HD22	1:D:1238:HIS:CE1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LYS:NZ	1:A:311:GLY:O	2.38	0.54
1:A:425:GLU:OE1	1:A:427:LYS:NZ	2.40	0.54
1:A:507:GLN:NE2	1:A:562:HIS:O	2.41	0.54
1:A:603:ARG:NH1	1:A:640:SER:OG	2.41	0.54
1:C:40:GLN:NE2	1:C:206:CYS:SG	2.81	0.54
1:A:410:GLU:OE1	1:A:412:LYS:N	2.41	0.54
1:A:1840:GLN:NE2	1:A:1976:LEU:O	2.40	0.54
6:A:2813:PLX:H282	6:A:2813:PLX:H112	1.88	0.54
1:B:554:ARG:HG3	1:B:590:LEU:HG	1.90	0.54
1:B:2122:VAL:HG12	1:B:2126:LYS:NZ	2.22	0.54
1:B:2257:GLN:HE22	1:B:2261:ARG:HD3	1.72	0.54
1:B:2527:THR:HG1	1:B:2537:THR:HG1	1.48	0.54
1:C:847:VAL:HG13	1:C:894:ILE:HD11	1.88	0.54
1:D:730:LEU:HD22	1:D:777:LEU:HD21	1.90	0.54
1:D:2703:GLU:HA	1:D:2706:MET:HG2	1.88	0.54
1:B:398:TRP:O	1:B:421:SER:N	2.37	0.54
6:B:2814:PLX:H282	6:B:2814:PLX:H112	1.88	0.54
1:A:2122:VAL:HG12	1:A:2126:LYS:NZ	2.22	0.54
1:A:2257:GLN:HE22	1:A:2261:ARG:HD3	1.72	0.54
1:A:2553:LEU:HB3	1:A:2566:ARG:NH2	2.22	0.54
1:B:1206:ARG:HH21	1:B:1254:LEU:HD11	1.73	0.54
1:C:603:ARG:NH1	1:C:640:SER:OG	2.41	0.54
1:C:859:LYS:NZ	1:C:862:LEU:HD22	2.23	0.54
1:D:392:HIS:HE1	1:D:394:CYS:HB3	1.72	0.54
1:D:1617:PRO:HB3	1:D:1729:ASP:HB3	1.90	0.54
1:A:896:ASP:HA	1:A:899:HIS:CE1	2.43	0.54
1:A:1206:ARG:HH21	1:A:1254:LEU:HD11	1.73	0.54
1:B:40:GLN:NE2	1:B:206:CYS:SG	2.81	0.54
1:B:978:LEU:HA	1:B:981:ILE:HG12	1.90	0.54
1:C:507:GLN:NE2	1:C:562:HIS:O	2.41	0.54
1:C:730:LEU:HD22	1:C:777:LEU:HD21	1.90	0.54
1:D:1835:GLY:O	1:D:1979:ASN:ND2	2.41	0.54
1:D:2025:ILE:HD12	1:D:2033:ILE:HD13	1.90	0.54
1:A:978:LEU:HA	1:A:981:ILE:HG12	1.90	0.54
1:A:1617:PRO:HB3	1:A:1729:ASP:HB3	1.90	0.54
1:A:1835:GLY:O	1:A:1979:ASN:ND2	2.41	0.54
1:D:859:LYS:NZ	1:D:862:LEU:HD22	2.23	0.54
1:D:978:LEU:HA	1:D:981:ILE:HG12	1.90	0.54
1:D:1643:ALA:HA	1:D:1646:LYS:HE3	1.90	0.54
1:D:2435:THR:HG21	6:D:2813:PLX:H52	1.90	0.54
1:A:554:ARG:HG3	1:A:590:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2435:THR:HG21	6:B:2814:PLX:H52	1.90	0.54
1:B:2703:GLU:HA	1:B:2706:MET:HG2	1.88	0.54
1:C:1643:ALA:HA	1:C:1646:LYS:HE3	1.90	0.54
1:D:2466:ASP:OD1	1:D:2554:ARG:NH1	2.41	0.54
1:D:2701:LYS:O	1:D:2705:THR:N	2.39	0.54
1:A:859:LYS:NZ	1:A:862:LEU:HD22	2.23	0.53
1:A:2025:ILE:HD12	1:A:2033:ILE:HD13	1.90	0.53
1:A:2466:ASP:OD1	1:A:2554:ARG:NH1	2.41	0.53
1:C:2144:ASP:OD1	1:C:2144:ASP:N	2.42	0.53
1:D:40:GLN:NE2	1:D:206:CYS:SG	2.81	0.53
1:D:2122:VAL:HG11	1:D:2173:MET:HB3	1.89	0.53
1:A:730:LEU:HD22	1:A:777:LEU:HD21	1.90	0.53
1:A:1809:ILE:HD12	1:A:1846:ARG:HD3	1.91	0.53
1:B:2121:LEU:O	1:B:2125:ILE:HG12	2.07	0.53
1:C:665:LEU:O	1:C:667:GLU:N	2.40	0.53
1:C:896:ASP:HA	1:C:899:HIS:CE1	2.43	0.53
1:C:978:LEU:HA	1:C:981:ILE:HG12	1.90	0.53
1:C:2121:LEU:O	1:C:2125:ILE:HG12	2.07	0.53
6:D:2802:PLX:H6	6:D:2802:PLX:H22	1.90	0.53
1:A:398:TRP:O	1:A:421:SER:N	2.37	0.53
1:A:695:GLU:OE2	1:A:713:ARG:NH1	2.32	0.53
1:B:405:PRO:HG2	1:B:408:LYS:NZ	2.23	0.53
1:B:603:ARG:NH1	1:B:640:SER:OG	2.41	0.53
1:C:1617:PRO:HB3	1:C:1729:ASP:HB3	1.90	0.53
1:C:1835:GLY:O	1:C:1979:ASN:ND2	2.41	0.53
1:D:10:HIS:ND1	1:D:112:GLY:O	2.32	0.53
1:D:896:ASP:HA	1:D:899:HIS:CE1	2.43	0.53
1:B:859:LYS:NZ	1:B:862:LEU:HD22	2.23	0.53
1:B:1105:THR:HG23	1:B:1107:GLN:H	1.74	0.53
1:B:2195:GLN:HG3	1:B:2207:GLN:HE21	1.74	0.53
1:C:2025:ILE:HD12	1:C:2033:ILE:HD13	1.90	0.53
1:D:405:PRO:HG2	1:D:408:LYS:NZ	2.23	0.53
1:A:405:PRO:HG2	1:A:408:LYS:NZ	2.23	0.53
1:A:2195:GLN:HG3	1:A:2207:GLN:HE21	1.74	0.53
1:A:2623:ASN:O	1:A:2624:LYS:C	2.47	0.53
6:A:2808:PLX:H22	6:A:2808:PLX:H6	1.90	0.53
1:B:1809:ILE:HD12	1:B:1846:ARG:HD3	1.91	0.53
1:B:1835:GLY:O	1:B:1979:ASN:ND2	2.41	0.53
1:C:2195:GLN:HG3	1:C:2207:GLN:HE21	1.74	0.53
1:C:2623:ASN:O	1:C:2624:LYS:C	2.47	0.53
1:D:672:LEU:HG	1:D:674:ARG:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:ARG:HH22	1:D:1036:GLN:HG3	1.74	0.53
1:A:2122:VAL:HG11	1:A:2173:MET:HB3	1.89	0.53
1:A:2227:ILE:HD12	1:A:2246:ARG:HD3	1.91	0.53
1:B:2122:VAL:HG11	1:B:2173:MET:HB3	1.89	0.53
1:B:2227:ILE:HD12	1:B:2246:ARG:HD3	1.91	0.53
1:C:1039:GLY:O	1:C:1047:ASN:ND2	2.42	0.53
1:C:1809:ILE:HD12	1:C:1846:ARG:HD3	1.91	0.53
1:C:2257:GLN:HE22	1:C:2261:ARG:HD3	1.72	0.53
1:A:665:LEU:O	1:A:667:GLU:N	2.40	0.53
1:A:2358:GLY:HA3	1:A:2406:LEU:HD13	1.91	0.53
1:B:392:HIS:HE1	1:B:394:CYS:HB3	1.72	0.53
1:B:410:GLU:OE1	1:B:412:LYS:N	2.41	0.53
1:B:999:ARG:HH22	1:B:1036:GLN:HG3	1.74	0.53
1:B:2622:ASP:O	1:B:2624:LYS:HG2	2.09	0.53
1:C:1206:ARG:HH21	1:C:1254:LEU:HD11	1.73	0.53
1:C:2118:PRO:HB3	1:C:2170:LEU:HD13	1.91	0.53
1:D:2257:GLN:HE22	1:D:2261:ARG:HD3	1.72	0.53
1:D:2358:GLY:HA3	1:D:2406:LEU:HD13	1.91	0.53
1:A:40:GLN:NE2	1:A:206:CYS:SG	2.81	0.53
1:A:392:HIS:HE1	1:A:394:CYS:HB3	1.72	0.53
1:A:672:LEU:HG	1:A:674:ARG:H	1.74	0.53
1:A:1039:GLY:O	1:A:1047:ASN:ND2	2.42	0.53
1:A:1105:THR:HG23	1:A:1107:GLN:H	1.74	0.53
1:A:2118:PRO:HB3	1:A:2170:LEU:HD13	1.91	0.53
1:A:2701:LYS:O	1:A:2705:THR:N	2.39	0.53
1:B:730:LEU:HD22	1:B:777:LEU:HD21	1.90	0.53
1:B:1643:ALA:HA	1:B:1646:LYS:HE3	1.90	0.53
1:B:2118:PRO:HB3	1:B:2170:LEU:HD13	1.91	0.53
1:C:1105:THR:HG23	1:C:1107:GLN:H	1.74	0.53
1:D:603:ARG:NH1	1:D:640:SER:OG	2.41	0.53
1:D:1809:ILE:HD12	1:D:1846:ARG:HD3	1.91	0.53
1:D:2195:GLN:HG3	1:D:2207:GLN:HE21	1.74	0.53
1:A:2532:LEU:HD22	6:A:2809:PLX:H4	1.91	0.53
1:B:896:ASP:HA	1:B:899:HIS:CE1	2.43	0.53
1:B:1039:GLY:O	1:B:1047:ASN:ND2	2.42	0.53
1:B:1616:ARG:HA	1:B:1619:VAL:HG12	1.91	0.53
1:B:2025:ILE:HD12	1:B:2033:ILE:HD13	1.90	0.53
1:C:494:VAL:HG22	1:C:555:LEU:HD21	1.91	0.53
1:B:894:ILE:O	1:B:898:VAL:HG23	2.10	0.53
1:B:2623:ASN:O	1:B:2624:LYS:C	2.47	0.53
6:B:2809:PLX:H22	6:B:2809:PLX:H6	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2227:ILE:HD12	1:C:2246:ARG:HD3	1.91	0.53
1:A:2622:ASP:O	1:A:2624:LYS:HG2	2.09	0.52
1:C:989:ARG:HH12	1:C:1089:GLN:HB3	1.74	0.52
1:D:2623:ASN:O	1:D:2624:LYS:C	2.47	0.52
1:A:894:ILE:O	1:A:898:VAL:HG23	2.09	0.52
1:A:1616:ARG:HA	1:A:1619:VAL:HG12	1.91	0.52
1:A:1643:ALA:HA	1:A:1646:LYS:HE3	1.90	0.52
1:B:507:GLN:NE2	1:B:562:HIS:O	2.41	0.52
1:C:405:PRO:HG2	1:C:408:LYS:NZ	2.23	0.52
1:C:672:LEU:HG	1:C:674:ARG:H	1.74	0.52
1:C:999:ARG:HH22	1:C:1036:GLN:HG3	1.74	0.52
1:C:2122:VAL:HG11	1:C:2173:MET:HB3	1.89	0.52
1:A:999:ARG:HH22	1:A:1036:GLN:HG3	1.74	0.52
1:B:2701:LYS:O	1:B:2705:THR:N	2.39	0.52
1:C:411:GLU:HG2	1:C:412:LYS:HG2	1.92	0.52
1:D:306:LYS:NZ	1:D:311:GLY:O	2.38	0.52
1:D:1105:THR:HG23	1:D:1107:GLN:H	1.74	0.52
1:D:2118:PRO:HB3	1:D:2170:LEU:HD13	1.91	0.52
1:D:2144:ASP:N	1:D:2144:ASP:OD1	2.42	0.52
1:A:989:ARG:HH12	1:A:1089:GLN:HB3	1.74	0.52
1:B:1447:MET:HE2	1:B:1447:MET:HA	1.91	0.52
1:C:2622:ASP:O	1:C:2624:LYS:HG2	2.09	0.52
1:D:494:VAL:HG22	1:D:555:LEU:HD21	1.91	0.52
1:D:1039:GLY:O	1:D:1047:ASN:ND2	2.42	0.52
1:D:1206:ARG:HH21	1:D:1254:LEU:HD11	1.73	0.52
1:D:2622:ASP:O	1:D:2624:LYS:HG2	2.09	0.52
1:D:665:LEU:O	1:D:667:GLU:N	2.40	0.52
1:D:2619:ASP:OD2	1:D:2620:LYS:N	2.43	0.52
1:B:2358:GLY:HA3	1:B:2406:LEU:HD13	1.91	0.52
1:B:2619:ASP:OD2	1:B:2620:LYS:N	2.43	0.52
1:B:989:ARG:HH12	1:B:1089:GLN:HB3	1.74	0.52
1:B:1394:GLU:O	1:B:1398:ASN:ND2	2.43	0.52
1:C:1394:GLU:O	1:C:1398:ASN:ND2	2.43	0.52
1:D:894:ILE:O	1:D:898:VAL:HG23	2.10	0.52
1:B:2144:ASP:OD1	1:B:2144:ASP:N	2.42	0.52
1:C:2619:ASP:OD2	1:C:2620:LYS:N	2.43	0.52
6:C:2814:PLX:H22	6:C:2814:PLX:H6	1.90	0.52
1:A:2611:CYS:HB3	1:A:2614:CYS:SG	2.50	0.52
1:A:2619:ASP:OD2	1:A:2620:LYS:N	2.43	0.52
1:B:782:CYS:HB2	1:B:865:GLU:HG3	1.92	0.52
1:B:1104:VAL:HG23	1:B:1105:THR:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1229:LYS:O	1:C:1232:GLU:HG3	2.10	0.52
1:C:2358:GLY:HA3	1:C:2406:LEU:HD13	1.91	0.52
1:A:1091:GLN:O	1:A:1094:LEU:HG	2.10	0.52
1:B:1091:GLN:O	1:B:1094:LEU:HG	2.10	0.52
1:B:2466:ASP:OD1	1:B:2554:ARG:NH1	2.41	0.52
1:D:257:ARG:NH1	1:D:409:GLU:OE2	2.43	0.52
1:D:411:GLU:HG2	1:D:412:LYS:HG2	1.91	0.52
1:A:1229:LYS:O	1:A:1232:GLU:HG3	2.10	0.51
1:B:1229:LYS:O	1:B:1232:GLU:HG3	2.10	0.51
1:B:1273:MET:HG3	1:B:1311:PHE:CE1	2.46	0.51
1:C:2466:ASP:OD1	1:C:2554:ARG:NH1	2.41	0.51
1:C:2532:LEU:HD22	6:C:2802:PLX:H4	1.91	0.51
1:A:1394:GLU:O	1:A:1398:ASN:ND2	2.43	0.51
1:C:298:TYR:HE1	1:C:381:LEU:HD22	1.75	0.51
1:C:1273:MET:HG3	1:C:1311:PHE:CE1	2.46	0.51
1:C:1447:MET:HE2	1:C:1447:MET:HA	1.92	0.51
1:D:1091:GLN:O	1:D:1094:LEU:HG	2.10	0.51
1:D:2227:ILE:HD12	1:D:2246:ARG:HD3	1.91	0.51
1:D:2611:CYS:HB3	1:D:2614:CYS:SG	2.50	0.51
1:A:411:GLU:HG2	1:A:412:LYS:HG2	1.91	0.51
1:A:2273:MET:SD	1:A:2371:SER:OG	2.63	0.51
1:B:672:LEU:HG	1:B:674:ARG:H	1.74	0.51
1:B:1515:GLY:O	1:B:1519:VAL:HG23	2.10	0.51
1:B:2532:LEU:HD22	6:B:2810:PLX:H4	1.92	0.51
1:C:782:CYS:HB2	1:C:865:GLU:HG3	1.92	0.51
1:C:894:ILE:O	1:C:898:VAL:HG23	2.09	0.51
1:C:1616:ARG:HA	1:C:1619:VAL:HG12	1.91	0.51
1:D:1222:TYR:HB2	1:D:1230:MET:CE	2.41	0.51
1:D:1616:ARG:HA	1:D:1619:VAL:HG12	1.91	0.51
1:A:2586[A]:PHE:CE1	1:D:2579:ILE:HG23	2.45	0.51
1:C:1515:GLY:O	1:C:1519:VAL:HG23	2.10	0.51
1:D:989:ARG:HH12	1:D:1089:GLN:HB3	1.74	0.51
1:D:2308:HIS:O	1:D:2312:LEU:N	2.44	0.51
1:A:102:GLN:O	1:A:106:GLU:OE1	2.29	0.51
1:A:1515:GLY:O	1:A:1519:VAL:HG23	2.10	0.51
1:B:411:GLU:HG2	1:B:412:LYS:HG2	1.92	0.51
1:B:2448:ALA:HB2	1:B:2581:VAL:HG11	1.93	0.51
1:C:484:VAL:O	1:C:503:ASN:ND2	2.44	0.51
1:D:1614:ARG:O	1:D:1615:LEU:HD22	2.11	0.51
1:B:298:TYR:HE1	1:B:381:LEU:HD22	1.75	0.51
1:C:1222:TYR:HB2	1:C:1230:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:782:CYS:HB2	1:D:865:GLU:HG3	1.92	0.51
1:A:494:VAL:HG22	1:A:555:LEU:HD21	1.91	0.51
1:A:1619:VAL:HA	1:A:1622:GLU:OE1	2.11	0.51
1:C:1091:GLN:O	1:C:1094:LEU:HG	2.10	0.51
1:D:2448:ALA:HB2	1:D:2581:VAL:HG11	1.93	0.51
1:B:102:GLN:O	1:B:106:GLU:OE1	2.29	0.51
1:B:1235:ARG:HG3	1:B:1268:LEU:HG	1.93	0.51
1:C:2688:SER:C	1:C:2689:GLU:HG3	2.32	0.51
1:D:484:VAL:O	1:D:503:ASN:ND2	2.44	0.51
1:D:1229:LYS:O	1:D:1232:GLU:HG3	2.10	0.51
1:D:1273:MET:HG3	1:D:1311:PHE:CE1	2.46	0.51
1:D:1394:GLU:O	1:D:1398:ASN:ND2	2.43	0.51
1:D:2532:LEU:HD22	6:D:2809:PLX:H4	1.92	0.51
1:A:782:CYS:HB2	1:A:865:GLU:HG3	1.92	0.51
1:A:2308:HIS:O	1:A:2312:LEU:N	2.44	0.51
1:A:2448:ALA:HB2	1:A:2581:VAL:HG11	1.93	0.51
1:B:1488:THR:HG23	1:B:1539:VAL:HG21	1.93	0.51
1:B:2688:SER:C	1:B:2689:GLU:HG3	2.32	0.51
1:D:398:TRP:O	1:D:421:SER:N	2.37	0.51
1:D:2688:SER:C	1:D:2689:GLU:HG3	2.31	0.51
1:A:1104:VAL:HG23	1:A:1105:THR:N	2.25	0.51
1:A:1222:TYR:HB2	1:A:1230:MET:CE	2.41	0.51
1:A:1594:SER:HA	1:A:1597:TYR:CE2	2.47	0.51
1:C:1235:ARG:HG3	1:C:1268:LEU:HG	1.93	0.51
1:A:298:TYR:HE1	1:A:381:LEU:HD22	1.75	0.50
1:A:484:VAL:O	1:A:503:ASN:ND2	2.44	0.50
1:B:1594:SER:HA	1:B:1597:TYR:CE2	2.47	0.50
1:B:1614:ARG:O	1:B:1615:LEU:HD22	2.11	0.50
1:C:830:LYS:HE2	1:C:878:PHE:HA	1.93	0.50
1:C:1614:ARG:O	1:C:1615:LEU:HD22	2.11	0.50
1:C:1619:VAL:HA	1:C:1622:GLU:OE1	2.11	0.50
1:D:1619:VAL:HA	1:D:1622:GLU:OE1	2.11	0.50
1:B:484:VAL:O	1:B:503:ASN:ND2	2.44	0.50
1:C:257:ARG:NH1	1:C:409:GLU:OE2	2.43	0.50
1:D:102:GLN:O	1:D:106:GLU:OE1	2.29	0.50
1:B:1222:TYR:HB2	1:B:1230:MET:CE	2.41	0.50
1:B:2611:CYS:HB3	1:B:2614:CYS:SG	2.50	0.50
1:C:1104:VAL:HG23	1:C:1105:THR:N	2.25	0.50
1:C:2448:ALA:HB2	1:C:2581:VAL:HG11	1.93	0.50
1:D:298:TYR:HE1	1:D:381:LEU:HD22	1.75	0.50
1:A:402:THR:OG1	1:A:417:LYS:O	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1224:LYS:HE2	1:B:1231:GLN:HG3	1.94	0.50
1:D:830:LYS:HE2	1:D:878:PHE:HA	1.93	0.50
1:A:246:GLU:HA	1:D:168:LYS:HD2	1.94	0.50
1:A:1224:LYS:HE2	1:A:1231:GLN:HG3	1.94	0.50
1:B:494:VAL:HG22	1:B:555:LEU:HD21	1.91	0.50
1:C:2611:CYS:HB3	1:C:2614:CYS:SG	2.50	0.50
1:D:1447:MET:HA	1:D:1447:MET:HE2	1.92	0.50
1:A:1488:THR:HG23	1:A:1539:VAL:HG21	1.93	0.50
1:A:1614:ARG:O	1:A:1615:LEU:HD22	2.11	0.50
1:C:102:GLN:O	1:C:106:GLU:OE1	2.29	0.50
1:C:891:LEU:HD11	1:C:974:ILE:HG12	1.93	0.50
1:D:859:LYS:HZ3	1:D:862:LEU:HD22	1.75	0.50
1:D:2688:SER:O	1:D:2689:GLU:HG3	2.12	0.50
1:A:1273:MET:HG3	1:A:1311:PHE:CE1	2.46	0.50
1:A:2688:SER:O	1:A:2689:GLU:HG3	2.12	0.50
1:B:2124:VAL:HA	1:B:2127:LYS:HB2	1.94	0.50
1:D:1515:GLY:O	1:D:1519:VAL:HG23	2.10	0.50
1:D:1594:SER:HA	1:D:1597:TYR:CE2	2.47	0.50
1:A:2124:VAL:HA	1:A:2127:LYS:HB2	1.94	0.50
1:A:845:ARG:NH1	1:A:890:ILE:HD13	2.27	0.50
1:A:891:LEU:HD11	1:A:974:ILE:HG12	1.93	0.50
1:C:1488:THR:HG23	1:C:1539:VAL:HG21	1.93	0.50
1:C:2719:LEU:O	1:C:2722:GLN:HG3	2.12	0.50
1:A:830:LYS:HE2	1:A:878:PHE:HA	1.93	0.49
1:B:845:ARG:NH1	1:B:890:ILE:HD13	2.27	0.49
1:B:1619:VAL:HA	1:B:1622:GLU:OE1	2.11	0.49
1:B:2043:TYR:O	1:B:2051:ASN:ND2	2.33	0.49
1:C:1224:LYS:HE2	1:C:1231:GLN:HG3	1.94	0.49
1:C:1372:PHE:CE2	1:C:1376:ILE:HD11	2.47	0.49
1:D:1224:LYS:HE2	1:D:1231:GLN:HG3	1.94	0.49
1:D:1235:ARG:HG3	1:D:1268:LEU:HG	1.93	0.49
1:A:2043:TYR:O	1:A:2051:ASN:ND2	2.33	0.49
1:A:2144:ASP:N	1:A:2144:ASP:OD1	2.42	0.49
1:B:830:LYS:HE2	1:B:878:PHE:HA	1.93	0.49
1:B:2273:MET:SD	1:B:2371:SER:OG	2.63	0.49
1:D:842:GLU:HA	1:D:845:ARG:HD3	1.94	0.49
1:D:1249:GLN:NE2	1:D:1282:GLN:OE1	2.45	0.49
1:A:1372:PHE:CE2	1:A:1376:ILE:HD11	2.47	0.49
1:C:845:ARG:NH1	1:C:890:ILE:HD13	2.27	0.49
1:C:1594:SER:HA	1:C:1597:TYR:CE2	2.47	0.49
1:D:845:ARG:NH1	1:D:890:ILE:HD13	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:GLN:NE2	1:A:1282:GLN:OE1	2.46	0.49
1:B:168:LYS:HD2	1:C:246:GLU:HA	1.94	0.49
1:B:2210:PHE:CE2	1:B:2647:LEU:HD21	2.47	0.49
1:D:2719:LEU:O	1:D:2722:GLN:HG3	2.12	0.49
1:A:1235:ARG:HG3	1:A:1268:LEU:HG	1.93	0.49
1:A:2210:PHE:CE2	1:A:2647:LEU:HD21	2.47	0.49
1:B:257:ARG:NH1	1:B:409:GLU:OE2	2.43	0.49
1:B:2439:ARG:NH2	1:C:2424:GLU:OE1	2.46	0.49
1:C:398:TRP:O	1:C:421:SER:N	2.37	0.49
1:D:2096:LEU:HB3	1:D:2159:LEU:HD22	1.94	0.49
1:D:2711:ASN:HB3	1:D:2715:GLN:HE22	1.77	0.49
1:A:2688:SER:C	1:A:2689:GLU:HG3	2.31	0.49
1:B:891:LEU:HD11	1:B:974:ILE:HG12	1.93	0.49
1:B:1372:PHE:CE2	1:B:1376:ILE:HD11	2.47	0.49
1:B:2688:SER:O	1:B:2689:GLU:HG3	2.12	0.49
1:C:306:LYS:NZ	1:C:311:GLY:O	2.38	0.49
1:C:1864:MET:HE1	1:C:2002:GLU:HB2	1.95	0.49
1:C:2688:SER:O	1:C:2689:GLU:HG3	2.12	0.49
1:D:891:LEU:HD11	1:D:974:ILE:HG12	1.93	0.49
1:B:842:GLU:HA	1:B:845:ARG:HD3	1.94	0.49
1:B:353:TYR:HB2	1:B:420:THR:OG1	2.13	0.49
1:C:2133:GLU:O	1:C:2137:GLU:HG3	2.13	0.49
1:D:1998:ASN:HB3	1:D:2001:CYS:HB2	1.95	0.49
1:D:2210:PHE:CE2	1:D:2647:LEU:HD21	2.47	0.49
1:B:807:TRP:CH2	1:B:998:LYS:HG2	2.48	0.49
1:C:2579:ILE:HG23	1:D:2586[A]:PHE:CE1	2.47	0.49
1:D:800:PRO:HB3	1:D:980:PHE:HE1	1.78	0.49
1:A:2030:VAL:HG21	1:A:2084:LEU:HD23	1.95	0.49
1:A:2108:ASN:O	1:A:2112:ILE:HG12	2.13	0.49
1:B:2711:ASN:HB3	1:B:2715:GLN:HE22	1.77	0.49
1:C:99:GLU:O	1:C:102:GLN:HG3	2.13	0.49
1:C:796:GLU:OE1	1:C:1123:ARG:NH1	2.46	0.49
1:C:1998:ASN:HB3	1:C:2001:CYS:HB2	1.95	0.49
1:D:807:TRP:CH2	1:D:998:LYS:HG2	2.48	0.49
1:D:1488:THR:HG23	1:D:1539:VAL:HG21	1.93	0.49
1:D:1864:MET:HE1	1:D:2002:GLU:HB2	1.95	0.49
1:A:842:GLU:HA	1:A:845:ARG:HD3	1.94	0.48
1:B:1249:GLN:NE2	1:B:1282:GLN:OE1	2.46	0.48
1:B:2133:GLU:O	1:B:2137:GLU:HG3	2.13	0.48
1:B:2719:LEU:O	1:B:2722:GLN:HG3	2.12	0.48
1:C:2124:VAL:HA	1:C:2127:LYS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2210:PHE:CE2	1:C:2647:LEU:HD21	2.47	0.48
1:D:2133:GLU:O	1:D:2137:GLU:HG3	2.13	0.48
1:A:99:GLU:O	1:A:102:GLN:HG3	2.13	0.48
1:A:1446:HIS:O	1:A:1450:LEU:HG	2.13	0.48
1:C:800:PRO:HB3	1:C:980:PHE:HE1	1.78	0.48
1:C:842:GLU:HA	1:C:845:ARG:HD3	1.94	0.48
1:C:1249:GLN:NE2	1:C:1282:GLN:OE1	2.45	0.48
1:D:162:TYR:N	1:D:185:ASN:O	2.40	0.48
1:D:1104:VAL:HG23	1:D:1105:THR:N	2.25	0.48
1:D:1372:PHE:CE2	1:D:1376:ILE:HD11	2.47	0.48
1:D:1798:HIS:O	1:D:1802:GLU:HG2	2.13	0.48
1:D:2030:VAL:HG21	1:D:2084:LEU:HD23	1.95	0.48
1:D:2124:VAL:HA	1:D:2127:LYS:HB2	1.94	0.48
1:A:2439:ARG:NH2	1:B:2424:GLU:OE1	2.46	0.48
1:B:99:GLU:O	1:B:102:GLN:HG3	2.13	0.48
1:B:796:GLU:OE1	1:B:1123:ARG:NH1	2.46	0.48
1:B:2096:LEU:O	1:B:2099:ILE:HG22	2.14	0.48
1:B:2096:LEU:HB3	1:B:2159:LEU:HD22	1.94	0.48
1:C:807:TRP:CH2	1:C:998:LYS:HG2	2.48	0.48
1:C:1870:GLU:OE2	1:C:1874:THR:OG1	2.32	0.48
1:C:2096:LEU:O	1:C:2099:ILE:HG22	2.14	0.48
1:C:2308:HIS:O	1:C:2312:LEU:N	2.44	0.48
1:A:257:ARG:NH1	1:A:409:GLU:OE2	2.43	0.48
1:A:353:TYR:HB2	1:A:420:THR:OG1	2.13	0.48
1:A:796:GLU:OE1	1:A:1123:ARG:NH1	2.46	0.48
1:A:1998:ASN:HB3	1:A:2001:CYS:HB2	1.95	0.48
1:A:800:PRO:HB3	1:A:980:PHE:HE1	1.78	0.48
1:B:1104:VAL:CG2	1:B:1108:ASP:HB2	2.44	0.48
1:B:1798:HIS:O	1:B:1802:GLU:HG2	2.14	0.48
1:B:2108:ASN:O	1:B:2112:ILE:HG12	2.13	0.48
1:C:2096:LEU:HB3	1:C:2159:LEU:HD22	1.94	0.48
1:D:1722:PRO:HG2	1:D:1723:PRO:HD3	1.96	0.48
1:A:1870:GLU:OE2	1:A:1874:THR:OG1	2.32	0.48
1:A:2341:ILE:O	1:A:2345:ILE:HG23	2.13	0.48
1:A:2719:LEU:O	1:A:2722:GLN:HG3	2.12	0.48
1:B:2341:ILE:O	1:B:2345:ILE:HG23	2.13	0.48
1:C:1798:HIS:O	1:C:1802:GLU:HG2	2.13	0.48
1:D:796:GLU:OE1	1:D:1123:ARG:NH1	2.46	0.48
1:A:1104:VAL:CG2	1:A:1108:ASP:HB2	2.44	0.48
1:A:2711:ASN:HB3	1:A:2715:GLN:HE22	1.77	0.48
1:C:1722:PRO:HG2	1:C:1723:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TYR:N	1:A:185:ASN:O	2.40	0.48
1:A:2096:LEU:HB3	1:A:2159:LEU:HD22	1.94	0.48
1:A:2096:LEU:O	1:A:2099:ILE:HG22	2.14	0.48
1:B:477:LEU:HD12	1:B:552:ILE:HG22	1.96	0.48
1:B:800:PRO:HB3	1:B:980:PHE:HE1	1.78	0.48
1:B:964:ASP:HB3	1:B:967:VAL:HG12	1.96	0.48
1:B:2579:ILE:HG23	1:C:2586[A]:PHE:CE1	2.47	0.48
1:C:168:LYS:HD2	1:D:246:GLU:HA	1.95	0.48
1:C:1104:VAL:CG2	1:C:1108:ASP:HB2	2.43	0.48
1:D:1446:HIS:O	1:D:1450:LEU:HG	2.13	0.48
1:D:2096:LEU:O	1:D:2099:ILE:HG22	2.14	0.48
1:B:1446:HIS:O	1:B:1450:LEU:HG	2.13	0.48
1:B:2308:HIS:O	1:B:2312:LEU:N	2.44	0.48
1:C:353:TYR:HB2	1:C:420:THR:OG1	2.13	0.48
1:C:2341:ILE:O	1:C:2345:ILE:HG23	2.13	0.48
1:C:2030:VAL:HG21	1:C:2084:LEU:HD23	1.95	0.48
1:D:964:ASP:HB3	1:D:967:VAL:HG12	1.96	0.48
1:D:1986:ASN:HA	1:D:1989:ARG:HH12	1.78	0.48
1:D:2108:ASN:O	1:D:2112:ILE:HG12	2.13	0.48
1:D:2273:MET:SD	1:D:2371:SER:OG	2.63	0.48
1:D:2341:ILE:O	1:D:2345:ILE:HG23	2.13	0.48
1:A:168:LYS:HD2	1:B:246:GLU:HA	1.96	0.47
1:A:807:TRP:CH2	1:A:998:LYS:HG2	2.48	0.47
1:A:964:ASP:HB3	1:A:967:VAL:HG12	1.96	0.47
1:A:1722:PRO:HG2	1:A:1723:PRO:HD3	1.96	0.47
1:B:14:ILE:HG22	1:B:57:LEU:HD12	1.96	0.47
1:B:1998:ASN:HB3	1:B:2001:CYS:HB2	1.95	0.47
1:B:2469:LEU:HD22	1:B:2552:VAL:HG22	1.96	0.47
1:C:14:ILE:HG22	1:C:57:LEU:HD12	1.96	0.47
1:C:1446:HIS:O	1:C:1450:LEU:HG	2.13	0.47
1:C:2108:ASN:O	1:C:2112:ILE:HG12	2.13	0.47
1:C:2711:ASN:HB3	1:C:2715:GLN:HE22	1.77	0.47
1:B:1986:ASN:HA	1:B:1989:ARG:HH12	1.78	0.47
1:C:477:LEU:HD12	1:C:552:ILE:HG22	1.96	0.47
1:C:2439:ARG:NH2	1:D:2424:GLU:OE1	2.46	0.47
1:C:2469:LEU:HD22	1:C:2552:VAL:HG22	1.96	0.47
1:D:1104:VAL:CG2	1:D:1108:ASP:HB2	2.44	0.47
1:A:14:ILE:HG22	1:A:57:LEU:HD12	1.96	0.47
1:A:1798:HIS:O	1:A:1802:GLU:HG2	2.13	0.47
1:A:2133:GLU:O	1:A:2137:GLU:HG3	2.13	0.47
1:D:353:TYR:HB2	1:D:420:THR:OG1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2327:LEU:HD21	1:D:2331:HIS:HD2	1.78	0.47
1:A:1353:THR:O	1:A:1356:GLN:HG2	2.15	0.47
1:B:599:LEU:O	1:B:603:ARG:NH2	2.47	0.47
1:B:1353:THR:O	1:B:1356:GLN:HG2	2.15	0.47
1:B:2030:VAL:HG21	1:B:2084:LEU:HD23	1.95	0.47
1:D:14:ILE:HG22	1:D:57:LEU:HD12	1.96	0.47
1:A:448:ASP:HA	1:A:451:LYS:HG2	1.96	0.47
1:A:2074:ILE:HD12	1:A:2085:VAL:HG13	1.96	0.47
1:A:2327:LEU:HD21	1:A:2331:HIS:HD2	1.78	0.47
1:B:1370:PRO:HA	1:B:1373:MET:SD	2.55	0.47
1:C:859:LYS:HZ3	1:C:862:LEU:HD22	1.80	0.47
1:C:1986:ASN:HA	1:C:1989:ARG:HH12	1.78	0.47
1:D:567:TYR:CE2	1:D:569:LYS:HB2	2.50	0.47
1:A:886:ARG:HA	1:A:889:LYS:HZ3	1.78	0.47
1:B:38:VAL:HG11	1:B:206:CYS:HB3	1.97	0.47
1:C:1857:PHE:HE2	1:C:1991:GLN:HG2	1.79	0.47
1:D:1857:PHE:HE2	1:D:1991:GLN:HG2	1.79	0.47
1:A:1370:PRO:HA	1:A:1373:MET:SD	2.55	0.47
1:A:1806:ASN:OD1	1:A:1846:ARG:NE	2.44	0.47
1:C:448:ASP:HA	1:C:451:LYS:HG2	1.96	0.47
1:C:567:TYR:CE2	1:C:569:LYS:HB2	2.50	0.47
1:C:806:LEU:HD11	1:C:1109:VAL:HG13	1.97	0.47
1:C:964:ASP:HB3	1:C:967:VAL:HG12	1.96	0.47
1:C:2128:ALA:HA	1:C:2131:GLN:NE2	2.29	0.47
1:C:2690:GLY:C	1:C:2692:GLN:H	2.18	0.47
1:D:99:GLU:O	1:D:102:GLN:HG3	2.13	0.47
1:D:1974:GLN:OE1	1:D:2035:GLN:NE2	2.48	0.47
1:D:2074:ILE:HD12	1:D:2085:VAL:HG13	1.96	0.47
1:D:2128:ALA:HA	1:D:2131:GLN:NE2	2.29	0.47
1:D:2276:TRP:HB2	1:D:2368:PHE:HD2	1.80	0.47
1:A:2579:ILE:HG23	1:B:2586[A]:PHE:CE1	2.48	0.47
1:B:392:HIS:CE1	1:B:394:CYS:HB3	2.50	0.47
1:B:804:ALA:O	1:B:1112:TYR:OH	2.29	0.47
1:B:2476:ASN:O	1:B:2478:THR:N	2.48	0.47
1:C:2083:ASP:O	1:C:2087:GLU:OE1	2.33	0.47
1:D:599:LEU:O	1:D:603:ARG:NH2	2.47	0.47
1:D:1370:PRO:HA	1:D:1373:MET:SD	2.55	0.47
1:D:1870:GLU:OE2	1:D:1874:THR:OG1	2.32	0.47
1:A:765:LEU:HD21	1:A:839:PHE:CE2	2.50	0.47
1:A:2276:TRP:HB2	1:A:2368:PHE:HD2	1.80	0.47
1:B:13:ASP:OD1	1:B:14:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:TYR:CE2	1:B:569:LYS:HB2	2.50	0.47
1:B:1722:PRO:HG2	1:B:1723:PRO:HD3	1.96	0.47
1:B:2730:LYS:HA	1:B:2733:ILE:HG22	1.97	0.47
1:C:392:HIS:CE1	1:C:394:CYS:HB3	2.50	0.47
1:C:2273:MET:SD	1:C:2371:SER:OG	2.63	0.47
1:D:152:ASP:N	1:D:152:ASP:OD1	2.48	0.47
1:D:477:LEU:HD12	1:D:552:ILE:HG22	1.96	0.47
1:D:806:LEU:HD11	1:D:1109:VAL:HG13	1.97	0.47
1:D:1060:PHE:O	1:D:1063:VAL:HG22	2.15	0.47
1:D:1353:THR:O	1:D:1356:GLN:HG2	2.15	0.47
1:D:2588:VAL:O	1:D:2592:THR:HG23	2.15	0.47
1:A:477:LEU:HD12	1:A:552:ILE:HG22	1.96	0.47
1:A:599:LEU:O	1:A:603:ARG:NH2	2.47	0.47
1:A:1974:GLN:OE1	1:A:2035:GLN:NE2	2.48	0.47
1:A:2083:ASP:O	1:A:2087:GLU:OE1	2.33	0.47
1:A:2553:LEU:HB3	1:A:2566:ARG:HH22	1.80	0.47
1:B:2083:ASP:O	1:B:2087:GLU:OE1	2.33	0.47
1:B:2365:LYS:HA	1:B:2365:LYS:HD3	1.70	0.47
1:B:2656:TYR:HB3	1:B:2661:SER:HB2	1.96	0.47
1:C:402:THR:OG1	1:C:417:LYS:O	2.25	0.47
1:C:1353:THR:O	1:C:1356:GLN:HG2	2.15	0.47
1:D:810:ILE:HG23	1:D:814:ILE:HD11	1.97	0.47
1:A:1060:PHE:O	1:A:1063:VAL:HG22	2.15	0.46
1:A:1986:ASN:HA	1:A:1989:ARG:HH12	1.78	0.46
1:A:2424:GLU:OE1	1:D:2439:ARG:NH2	2.47	0.46
1:B:448:ASP:HA	1:B:451:LYS:HG2	1.96	0.46
1:B:2690:GLY:C	1:B:2692:GLN:H	2.18	0.46
1:C:2476:ASN:O	1:C:2478:THR:N	2.48	0.46
1:D:2690:GLY:C	1:D:2692:GLN:H	2.18	0.46
1:A:2476:ASN:O	1:A:2478:THR:N	2.48	0.46
1:B:1060:PHE:O	1:B:1063:VAL:HG22	2.15	0.46
1:B:1974:GLN:OE1	1:B:2035:GLN:NE2	2.48	0.46
1:C:599:LEU:O	1:C:603:ARG:NH2	2.47	0.46
1:C:1452:GLU:O	1:C:1456:VAL:HG23	2.16	0.46
1:C:2588:VAL:O	1:C:2592:THR:HG23	2.15	0.46
1:A:13:ASP:OD1	1:A:14:ILE:N	2.48	0.46
1:A:884:LEU:HD23	1:A:981:ILE:HG22	1.98	0.46
1:A:2588:VAL:O	1:A:2592:THR:HG23	2.15	0.46
1:B:152:ASP:OD1	1:B:152:ASP:N	2.48	0.46
1:B:1100:VAL:HG22	1:B:1101:GLN:N	2.22	0.46
1:C:1105:THR:OG1	1:C:1106:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1974:GLN:OE1	1:C:2035:GLN:NE2	2.48	0.46
1:C:2074:ILE:HD12	1:C:2085:VAL:HG13	1.96	0.46
1:D:392:HIS:CE1	1:D:394:CYS:HB3	2.50	0.46
1:D:1105:THR:OG1	1:D:1106:SER:N	2.49	0.46
1:A:152:ASP:N	1:A:152:ASP:OD1	2.48	0.46
1:A:392:HIS:CE1	1:A:394:CYS:HB3	2.50	0.46
1:A:1597:TYR:O	1:A:1601:ILE:HG12	2.16	0.46
1:A:2469:LEU:HD22	1:A:2552:VAL:HG22	1.96	0.46
1:A:2549:VAL:HG22	1:A:2553:LEU:HD13	1.97	0.46
1:B:635:SER:HB2	1:B:742:ARG:HD2	1.98	0.46
1:B:1870:GLU:OE2	1:B:1874:THR:OG1	2.32	0.46
1:C:518:GLN:HA	1:C:521:LYS:HB2	1.98	0.46
1:C:635:SER:HB2	1:C:742:ARG:HD2	1.98	0.46
1:C:1370:PRO:HA	1:C:1373:MET:SD	2.55	0.46
1:C:1833:GLU:OE2	1:C:1971:ARG:NH2	2.47	0.46
1:C:2707:LYS:HZ3	1:D:2702:LEU:HD13	1.81	0.46
1:D:448:ASP:HA	1:D:451:LYS:HG2	1.96	0.46
1:A:635:SER:HB2	1:A:742:ARG:HD2	1.98	0.46
1:A:1105:THR:OG1	1:A:1106:SER:N	2.49	0.46
1:B:2715:GLN:HA	1:B:2718:GLU:HG3	1.98	0.46
1:C:810:ILE:HG23	1:C:814:ILE:HD11	1.97	0.46
1:C:1060:PHE:O	1:C:1063:VAL:HG22	2.15	0.46
1:C:1806:ASN:OD1	1:C:1846:ARG:NE	2.44	0.46
1:D:38:VAL:HG11	1:D:206:CYS:HB3	1.97	0.46
1:D:1452:GLU:O	1:D:1456:VAL:HG23	2.16	0.46
1:D:2083:ASP:O	1:D:2087:GLU:OE1	2.33	0.46
1:D:2305:LEU:HD22	1:D:2308:HIS:ND1	2.31	0.46
1:D:2469:LEU:HD22	1:D:2552:VAL:HG22	1.96	0.46
1:D:2553:LEU:HB3	1:D:2566:ARG:HH22	1.80	0.46
1:A:567:TYR:CE2	1:A:569:LYS:HB2	2.50	0.46
1:A:1657:ILE:HG23	1:A:1807:LEU:HD12	1.97	0.46
1:A:2690:GLY:C	1:A:2692:GLN:H	2.18	0.46
1:A:2730:LYS:HA	1:A:2733:ILE:HG22	1.97	0.46
1:B:859:LYS:HZ3	1:B:862:LEU:HD22	1.80	0.46
1:C:864:PHE:CE1	1:C:967:VAL:HA	2.51	0.46
1:C:2276:TRP:HB2	1:C:2368:PHE:HD2	1.80	0.46
1:D:1597:TYR:O	1:D:1601:ILE:HG12	2.16	0.46
1:D:2476:ASN:O	1:D:2478:THR:N	2.48	0.46
6:D:2813:PLX:H102	6:D:2813:PLX:H71	1.68	0.46
1:A:2305:LEU:HD22	1:A:2308:HIS:ND1	2.31	0.46
1:A:2656:TYR:HB3	1:A:2661:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2715:GLN:HA	1:A:2718:GLU:HG3	1.98	0.46
1:B:518:GLN:HA	1:B:521:LYS:HB2	1.98	0.46
1:B:765:LEU:HD21	1:B:839:PHE:CE2	2.50	0.46
1:B:806:LEU:HD11	1:B:1109:VAL:HG13	1.97	0.46
1:C:13:ASP:OD1	1:C:14:ILE:N	2.48	0.46
1:C:2656:TYR:HB3	1:C:2661:SER:HB2	1.96	0.46
1:D:765:LEU:HD21	1:D:839:PHE:CE2	2.50	0.46
1:A:2707:LYS:HZ3	1:B:2702:LEU:HD13	1.81	0.46
1:B:864:PHE:CE1	1:B:967:VAL:HA	2.51	0.46
1:B:884:LEU:HD23	1:B:981:ILE:HG22	1.98	0.46
1:B:1597:TYR:O	1:B:1601:ILE:HG12	2.16	0.46
1:B:1657:ILE:HG23	1:B:1807:LEU:HD12	1.97	0.46
1:B:2657:THR:HG22	1:B:2658:GLY:N	2.29	0.46
1:C:1790:MET:HE2	1:C:1795:VAL:HG22	1.97	0.46
1:D:2549:VAL:HG22	1:D:2553:LEU:HD13	1.97	0.46
1:A:38:VAL:HG11	1:A:206:CYS:HB3	1.97	0.46
1:A:405:PRO:HG2	1:A:408:LYS:HZ3	1.81	0.46
1:A:617:THR:O	1:A:621:LEU:HG	2.16	0.46
1:B:585:ILE:HG23	1:B:592:GLU:HB3	1.98	0.46
1:B:1452:GLU:O	1:B:1456:VAL:HG23	2.16	0.46
1:B:2074:ILE:HD12	1:B:2085:VAL:HG13	1.96	0.46
1:B:2588:VAL:O	1:B:2592:THR:HG23	2.15	0.46
1:C:1327:GLN:HG2	1:C:1385:CYS:HA	1.98	0.46
6:C:2806:PLX:H102	6:C:2806:PLX:H71	1.68	0.46
1:D:1806:ASN:OD1	1:D:1846:ARG:NE	2.44	0.46
1:D:2656:TYR:HB3	1:D:2661:SER:HB2	1.96	0.46
1:A:1452:GLU:O	1:A:1456:VAL:HG23	2.16	0.46
1:A:1864:MET:HE1	1:A:2002:GLU:HB2	1.98	0.46
1:B:617:THR:O	1:B:621:LEU:HG	2.16	0.46
1:B:2305:LEU:HD22	1:B:2308:HIS:ND1	2.31	0.46
1:B:2707:LYS:HZ3	1:C:2702:LEU:HD13	1.80	0.46
1:C:38:VAL:HG11	1:C:206:CYS:HB3	1.97	0.46
1:C:806:LEU:HG	1:C:1103:LEU:CD2	2.40	0.46
1:D:13:ASP:OD1	1:D:14:ILE:N	2.48	0.46
1:D:635:SER:HB2	1:D:742:ARG:HD2	1.98	0.46
1:D:770:ASP:OD1	1:D:770:ASP:N	2.49	0.46
1:D:2715:GLN:HA	1:D:2718:GLU:HG3	1.98	0.46
1:A:864:PHE:CE1	1:A:967:VAL:HA	2.51	0.45
1:A:1084:PHE:HE1	1:A:1674:LYS:HB3	1.81	0.45
1:A:2725:GLU:HG3	1:A:2729:GLN:NE2	2.32	0.45
1:B:1857:PHE:HE2	1:B:1991:GLN:HG2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:THR:HA	1:C:389:ARG:HH12	1.81	0.45
1:C:2725:GLU:HG3	1:C:2729:GLN:NE2	2.32	0.45
1:D:864:PHE:CE1	1:D:967:VAL:HA	2.51	0.45
1:D:1386:THR:HG21	1:D:1397:CYS:SG	2.56	0.45
1:D:2730:LYS:HA	1:D:2733:ILE:HG22	1.97	0.45
1:A:806:LEU:HD11	1:A:1109:VAL:HG13	1.97	0.45
1:B:2128:ALA:HA	1:B:2131:GLN:NE2	2.29	0.45
1:C:2715:GLN:HA	1:C:2718:GLU:HG3	1.98	0.45
1:D:518:GLN:HA	1:D:521:LYS:HB2	1.98	0.45
1:D:546:HIS:HB2	1:D:550:ARG:HD3	1.98	0.45
1:D:826:LYS:O	1:D:830:LYS:HG2	2.17	0.45
1:D:1086:HIS:O	1:D:1089:GLN:HG3	2.17	0.45
1:D:1657:ILE:HG23	1:D:1807:LEU:HD12	1.97	0.45
1:D:1790:MET:HE2	1:D:1795:VAL:HG22	1.98	0.45
1:A:224:MET:HE1	1:A:235:LYS:HD2	1.97	0.45
1:A:600:HIS:O	1:A:603:ARG:NH1	2.42	0.45
1:A:2128:ALA:HA	1:A:2131:GLN:NE2	2.29	0.45
1:B:2725:GLU:HG3	1:B:2729:GLN:NE2	2.32	0.45
1:C:1084:PHE:HE1	1:C:1674:LYS:HB3	1.81	0.45
1:C:2305:LEU:HD22	1:C:2308:HIS:ND1	2.31	0.45
1:C:2549:VAL:HG22	1:C:2553:LEU:HD13	1.97	0.45
1:D:234:LEU:HD21	1:D:284:VAL:HG11	1.98	0.45
1:D:1327:GLN:HG2	1:D:1385:CYS:HA	1.98	0.45
1:A:810:ILE:HG23	1:A:814:ILE:HD11	1.97	0.45
1:A:826:LYS:O	1:A:830:LYS:HG2	2.16	0.45
1:B:826:LYS:O	1:B:830:LYS:HG2	2.16	0.45
1:C:2553:LEU:HB3	1:C:2566:ARG:HH22	1.80	0.45
1:D:481:VAL:HG22	1:D:559:VAL:HB	1.99	0.45
1:D:884:LEU:HD23	1:D:981:ILE:HG22	1.98	0.45
1:D:2725:GLU:HG3	1:D:2729:GLN:NE2	2.32	0.45
1:A:234:LEU:HD21	1:A:284:VAL:HG11	1.98	0.45
1:A:1344:PHE:HD2	1:A:1401:LEU:HD13	1.82	0.45
1:B:1790:MET:HE2	1:B:1795:VAL:HG22	1.97	0.45
1:B:2276:TRP:HB2	1:B:2368:PHE:HD2	1.80	0.45
6:B:2810:PLX:H252	6:B:2810:PLX:H281	1.71	0.45
1:C:1086:HIS:O	1:C:1089:GLN:HG3	2.17	0.45
1:D:1344:PHE:HD2	1:D:1401:LEU:HD13	1.82	0.45
1:A:373:THR:HA	1:A:389:ARG:HH12	1.82	0.45
1:A:518:GLN:HA	1:A:521:LYS:HB2	1.98	0.45
1:B:810:ILE:HG23	1:B:814:ILE:HD11	1.97	0.45
1:B:1040:ILE:HG13	1:B:1041:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2549:VAL:HG22	1:B:2553:LEU:HD13	1.97	0.45
1:B:2553:LEU:HB3	1:B:2566:ARG:HH22	1.80	0.45
6:B:2811:PLX:H1A2	6:B:2811:PLX:H22	1.79	0.45
1:C:585:ILE:HG23	1:C:592:GLU:HB3	1.98	0.45
1:C:1173:TYR:O	1:C:1229:LYS:NZ	2.48	0.45
1:C:1344:PHE:HD2	1:C:1401:LEU:HD13	1.82	0.45
1:C:1657:ILE:HG23	1:C:1807:LEU:HD12	1.97	0.45
1:C:2730:LYS:HA	1:C:2733:ILE:HG22	1.97	0.45
1:B:1344:PHE:HD2	1:B:1401:LEU:HD13	1.82	0.45
1:C:546:HIS:HB2	1:C:550:ARG:HD3	1.98	0.45
1:C:884:LEU:HD23	1:C:981:ILE:HG22	1.98	0.45
1:C:1597:TYR:O	1:C:1601:ILE:HG12	2.16	0.45
6:C:2802:PLX:H21	6:C:2802:PLX:H1C3	1.76	0.45
1:A:585:ILE:HG23	1:A:592:GLU:HB3	1.98	0.45
1:A:804:ALA:O	1:A:1112:TYR:OH	2.29	0.45
1:A:1386:THR:HG21	1:A:1397:CYS:SG	2.57	0.45
1:A:2398:TYR:HA	1:A:2401:ILE:HB	1.99	0.45
1:B:373:THR:HA	1:B:389:ARG:HH12	1.82	0.45
1:B:481:VAL:HG22	1:B:559:VAL:HB	1.99	0.45
1:B:800:PRO:HB3	1:B:980:PHE:CE1	2.52	0.45
1:B:1105:THR:OG1	1:B:1106:SER:N	2.49	0.45
1:B:1386:THR:HG21	1:B:1397:CYS:SG	2.57	0.45
1:C:481:VAL:HG22	1:C:559:VAL:HB	1.99	0.45
1:C:765:LEU:HD21	1:C:839:PHE:CE2	2.50	0.45
1:C:1040:ILE:HG13	1:C:1041:PHE:CD1	2.52	0.45
1:D:1084:PHE:HE1	1:D:1674:LYS:HB3	1.81	0.45
1:A:1362:ARG:NH1	1:A:1414:ASP:OD1	2.50	0.45
6:A:2813:PLX:H71	6:A:2813:PLX:H102	1.68	0.45
1:B:2327:LEU:HD21	1:B:2331:HIS:HD2	1.78	0.45
1:B:2470:GLU:HA	1:B:2524:LYS:HD3	1.99	0.45
1:C:1100:VAL:HG13	1:C:1101:GLN:N	2.32	0.45
1:C:2043:TYR:O	1:C:2051:ASN:ND2	2.33	0.45
1:C:2131:GLN:HA	1:C:2134:VAL:HB	1.99	0.45
1:D:2470:GLU:HA	1:D:2524:LYS:HD3	1.99	0.45
1:A:481:VAL:HG22	1:A:559:VAL:HB	1.99	0.45
1:A:1100:VAL:HG13	1:A:1101:GLN:N	2.32	0.45
1:A:2365:LYS:HD3	1:A:2365:LYS:HA	1.69	0.45
1:C:2465:ASP:OD1	1:C:2465:ASP:N	2.50	0.45
1:D:373:THR:HA	1:D:389:ARG:HH12	1.81	0.45
1:D:585:ILE:HG23	1:D:592:GLU:HB3	1.98	0.45
1:D:1040:ILE:HG13	1:D:1041:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1100:VAL:HG13	1:D:1101:GLN:N	2.32	0.45
1:D:1103:LEU:CD1	1:D:1109:VAL:HG23	2.47	0.45
1:D:2465:ASP:N	1:D:2465:ASP:OD1	2.50	0.45
6:D:2813:PLX:H51	6:D:2813:PLX:H252	1.82	0.45
1:A:1040:ILE:HG13	1:A:1041:PHE:CD1	2.52	0.44
1:A:1086:HIS:O	1:A:1089:GLN:HG3	2.17	0.44
1:A:1327:GLN:HG2	1:A:1385:CYS:HA	1.98	0.44
6:A:2809:PLX:H252	6:A:2809:PLX:H281	1.71	0.44
1:A:806:LEU:HG	1:A:1103:LEU:CD2	2.40	0.44
1:B:974:ILE:HA	1:B:977:ILE:HD12	2.00	0.44
1:C:143:GLU:HB3	1:C:146:ALA:HB3	1.99	0.44
1:C:800:PRO:HB3	1:C:980:PHE:CE1	2.52	0.44
1:C:2063:ILE:HA	1:C:2066:ILE:HD12	1.99	0.44
1:D:1421:ILE:HG13	1:D:1478:TYR:CD1	2.51	0.44
1:A:546:HIS:HB2	1:A:550:ARG:HD3	1.98	0.44
1:A:1248:ASN:OD1	1:A:1249:GLN:N	2.51	0.44
1:B:546:HIS:HB2	1:B:550:ARG:HD3	1.98	0.44
1:C:234:LEU:HD21	1:C:284:VAL:HG11	1.99	0.44
1:C:2657:THR:HG22	1:C:2658:GLY:N	2.29	0.44
1:D:617:THR:O	1:D:621:LEU:HG	2.16	0.44
1:D:974:ILE:HA	1:D:977:ILE:HD12	2.00	0.44
1:D:1620:GLN:HA	1:D:1623:LEU:HB2	2.00	0.44
1:A:497:VAL:H	1:A:558:ARG:HH12	1.65	0.44
1:A:800:PRO:HB3	1:A:980:PHE:CE1	2.52	0.44
1:A:2713:SER:HA	1:A:2716:LEU:HG	2.00	0.44
1:B:1248:ASN:OD1	1:B:1249:GLN:N	2.51	0.44
1:B:1806:ASN:OD1	1:B:1846:ARG:NE	2.44	0.44
1:B:2393:LEU:O	1:B:2397:LEU:HG	2.18	0.44
1:C:1103:LEU:CD1	1:C:1109:VAL:HG23	2.47	0.44
1:C:2470:GLU:HA	1:C:2524:LYS:HD3	1.99	0.44
6:C:2802:PLX:H362	6:C:2802:PLX:H331	1.83	0.44
1:D:2398:TYR:HA	1:D:2401:ILE:HB	1.99	0.44
1:A:1200:GLN:HG2	1:A:1201:GLN:N	2.33	0.44
1:A:1599:ASN:C	1:A:1603:ARG:HE	2.21	0.44
1:A:1736:LEU:HD23	1:A:1736:LEU:HA	1.82	0.44
1:A:1986:ASN:HA	1:A:1989:ARG:NH1	2.33	0.44
1:B:1086:HIS:O	1:B:1089:GLN:HG3	2.17	0.44
1:C:152:ASP:N	1:C:152:ASP:OD1	2.48	0.44
1:C:804:ALA:O	1:C:1112:TYR:OH	2.29	0.44
1:C:1620:GLN:HA	1:C:1623:LEU:HB2	2.00	0.44
1:D:497:VAL:H	1:D:558:ARG:HH12	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1300:GLU:HG3	1:D:1340:ASP:HB3	2.00	0.44
1:D:1833:GLU:OE2	1:D:1971:ARG:NH2	2.47	0.44
1:A:974:ILE:HA	1:A:977:ILE:HD12	2.00	0.44
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.48	0.44
1:A:2411:PHE:HB2	6:A:2810:PLX:H81	1.99	0.44
1:A:2702:LEU:HD13	1:D:2707:LYS:HZ3	1.83	0.44
1:B:852:PHE:HB3	1:B:855:SER:OG	2.18	0.44
1:B:1327:GLN:HG2	1:B:1385:CYS:HA	1.98	0.44
1:B:1986:ASN:HA	1:B:1989:ARG:NH1	2.33	0.44
1:B:2063:ILE:HA	1:B:2066:ILE:HD12	1.99	0.44
1:B:2443:LEU:HD12	1:C:2426:THR:OG1	2.18	0.44
1:C:617:THR:O	1:C:621:LEU:HG	2.16	0.44
1:C:974:ILE:HA	1:C:977:ILE:HD12	2.00	0.44
1:C:1248:ASN:OD1	1:C:1249:GLN:N	2.51	0.44
1:C:1986:ASN:HA	1:C:1989:ARG:NH1	2.33	0.44
1:A:1410:VAL:HG21	1:A:1424:ILE:HD11	2.00	0.44
1:B:477:LEU:HD21	1:B:522:LEU:HD13	2.00	0.44
1:B:1100:VAL:HG13	1:B:1101:GLN:N	2.32	0.44
1:B:1103:LEU:CD1	1:B:1109:VAL:HG23	2.47	0.44
1:B:1420:LYS:HZ3	1:B:1457:ASP:HB2	1.82	0.44
1:C:826:LYS:O	1:C:830:LYS:HG2	2.16	0.44
1:D:2210:PHE:HB2	1:D:2211:PRO:HD2	2.00	0.44
1:D:2611:CYS:CB	1:D:2614:CYS:SG	3.06	0.44
1:C:1386:THR:HG21	1:C:1397:CYS:SG	2.56	0.44
1:C:1421:ILE:HG13	1:C:1478:TYR:CD1	2.51	0.44
1:C:2628:PHE:C	1:C:2630:GLU:N	2.71	0.44
1:D:1986:ASN:HA	1:D:1989:ARG:NH1	2.33	0.44
1:D:2283:LEU:HD23	1:D:2283:LEU:HA	1.87	0.44
1:A:852:PHE:HB3	1:A:855:SER:OG	2.18	0.44
1:A:2627:THR:O	1:A:2630:GLU:N	2.30	0.44
1:B:143:GLU:HB3	1:B:146:ALA:HB3	1.99	0.44
1:B:1084:PHE:HE1	1:B:1674:LYS:HB3	1.81	0.44
1:B:1810:ASP:OD1	1:B:1846:ARG:NH2	2.51	0.44
1:C:2210:PHE:HB2	1:C:2211:PRO:HD2	2.00	0.44
1:C:2398:TYR:HA	1:C:2401:ILE:HB	1.99	0.44
1:D:806:LEU:HG	1:D:1103:LEU:CD2	2.40	0.44
1:D:1200:GLN:HG2	1:D:1201:GLN:N	2.33	0.44
1:D:1417:PRO:O	1:D:1421:ILE:HD12	2.18	0.44
1:A:117:TYR:OH	1:A:180:ASP:OD2	2.35	0.43
6:A:2813:PLX:H51	6:A:2813:PLX:H252	1.82	0.43
1:B:234:LEU:HD21	1:B:284:VAL:HG11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ARG:HG2	1:B:572:GLU:OE1	2.18	0.43
1:B:1300:GLU:HG3	1:B:1340:ASP:HB3	2.00	0.43
1:C:477:LEU:HD21	1:C:522:LEU:HD13	2.00	0.43
1:C:568:ARG:HG2	1:C:572:GLU:OE1	2.18	0.43
1:C:875:TYR:CE1	1:C:980:PHE:HB2	2.45	0.43
1:C:2327:LEU:HD21	1:C:2331:HIS:HD2	1.78	0.43
1:C:2394:TYR:CZ	1:C:2398:TYR:HE2	2.36	0.43
1:D:999:ARG:NH2	1:D:1036:GLN:HG3	2.34	0.43
1:A:1620:GLN:HA	1:A:1623:LEU:HB2	2.00	0.43
1:A:2131:GLN:HA	1:A:2134:VAL:HB	1.99	0.43
1:A:2611:CYS:CB	1:A:2614:CYS:SG	3.06	0.43
6:A:2811:PLX:H281	6:A:2811:PLX:H311	1.75	0.43
1:B:1417:PRO:O	1:B:1421:ILE:HD12	2.18	0.43
1:B:2394:TYR:CZ	1:B:2398:TYR:HE2	2.36	0.43
1:B:2628:PHE:C	1:B:2630:GLU:N	2.71	0.43
1:C:852:PHE:HB3	1:C:855:SER:OG	2.18	0.43
1:C:1300:GLU:HG3	1:C:1340:ASP:HB3	2.00	0.43
1:C:2527:THR:HG1	1:C:2537:THR:HG1	1.51	0.43
1:D:2043:TYR:O	1:D:2051:ASN:ND2	2.33	0.43
1:D:2628:PHE:C	1:D:2630:GLU:N	2.71	0.43
1:A:474:THR:HG23	1:A:552:ILE:HG21	2.01	0.43
1:A:805:ARG:NH2	1:A:987:ASP:OD1	2.51	0.43
1:A:859:LYS:HZ3	1:A:862:LEU:HD22	1.82	0.43
1:A:2470:GLU:HA	1:A:2524:LYS:HD3	1.99	0.43
1:B:1620:GLN:HA	1:B:1623:LEU:HB2	2.00	0.43
1:B:2131:GLN:HA	1:B:2134:VAL:HB	1.99	0.43
1:C:1103:LEU:O	1:C:1103:LEU:HG	2.18	0.43
1:C:1200:GLN:HG2	1:C:1201:GLN:N	2.33	0.43
1:C:2393:LEU:O	1:C:2397:LEU:HG	2.18	0.43
1:D:199:GLN:NE2	1:D:207:ASN:OD1	2.52	0.43
1:D:805:ARG:NH2	1:D:987:ASP:OD1	2.51	0.43
1:D:852:PHE:HB3	1:D:855:SER:OG	2.18	0.43
1:D:1000:GLU:HB3	1:D:1028:LEU:HD12	2.00	0.43
1:D:1103:LEU:O	1:D:1103:LEU:HG	2.18	0.43
1:D:1248:ASN:OD1	1:D:1250:GLN:HG3	2.18	0.43
1:D:1736:LEU:HA	1:D:1736:LEU:HD23	1.82	0.43
1:A:718:ASP:HA	1:A:721:GLU:CD	2.39	0.43
1:A:2657:THR:HG22	1:A:2658:GLY:N	2.29	0.43
1:B:1248:ASN:OD1	1:B:1250:GLN:HG3	2.18	0.43
1:B:2398:TYR:HA	1:B:2401:ILE:HB	1.99	0.43
1:C:231:ASP:OD1	1:C:231:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:LEU:HD22	1:C:388:VAL:HG21	2.01	0.43
1:C:1206:ARG:HD2	1:C:1250:GLN:HE22	1.84	0.43
1:C:1362:ARG:NH1	1:C:1414:ASP:OD1	2.50	0.43
1:C:1666:GLU:HG2	1:C:1666:GLU:O	2.19	0.43
1:C:2611:CYS:CB	1:C:2614:CYS:SG	3.06	0.43
1:C:2621:PHE:CZ	1:C:2631:HIS:CE1	3.07	0.43
1:D:800:PRO:HB3	1:D:980:PHE:CE1	2.52	0.43
1:D:1410:VAL:HG21	1:D:1424:ILE:HD11	2.00	0.43
1:D:2365:LYS:HD3	1:D:2365:LYS:HA	1.70	0.43
1:A:199:GLN:NE2	1:A:207:ASN:OD1	2.52	0.43
1:A:1000:GLU:HB3	1:A:1028:LEU:HD12	2.00	0.43
1:A:1666:GLU:O	1:A:1666:GLU:HG2	2.19	0.43
1:A:2040:LEU:HA	1:A:2043:TYR:HD2	1.84	0.43
1:A:2063:ILE:HA	1:A:2066:ILE:HD12	1.99	0.43
1:A:2210:PHE:HB2	1:A:2211:PRO:HD2	2.00	0.43
1:A:2393:LEU:O	1:A:2397:LEU:HG	2.18	0.43
1:A:2394:TYR:CZ	1:A:2398:TYR:HE2	2.36	0.43
1:B:199:GLN:NE2	1:B:207:ASN:OD1	2.52	0.43
1:B:497:VAL:H	1:B:558:ARG:HH12	1.65	0.43
1:B:1103:LEU:O	1:B:1103:LEU:HG	2.18	0.43
1:B:1410:VAL:HG21	1:B:1424:ILE:HD11	2.00	0.43
1:B:2040:LEU:HA	1:B:2043:TYR:HD2	1.84	0.43
6:B:2810:PLX:H1C3	6:B:2810:PLX:H21	1.76	0.43
1:C:423:LEU:HD23	1:C:423:LEU:H	1.84	0.43
1:C:1100:VAL:HG22	1:C:1101:GLN:N	2.22	0.43
1:C:2713:SER:HA	1:C:2716:LEU:HG	2.00	0.43
1:D:1598:ARG:NE	1:D:1598:ARG:O	2.52	0.43
1:D:2393:LEU:O	1:D:2397:LEU:HG	2.18	0.43
1:D:2713:SER:HA	1:D:2716:LEU:HG	2.00	0.43
6:D:2809:PLX:H1C3	6:D:2809:PLX:H21	1.76	0.43
1:A:2426:THR:OG1	1:D:2443:LEU:HD12	2.18	0.43
1:A:2624:LYS:O	1:A:2626:VAL:N	2.52	0.43
1:B:1206:ARG:HD2	1:B:1250:GLN:HE22	1.84	0.43
1:B:1362:ARG:NH1	1:B:1414:ASP:OD1	2.50	0.43
1:B:1599:ASN:C	1:B:1603:ARG:HE	2.21	0.43
1:B:2210:PHE:HB2	1:B:2211:PRO:HD2	2.00	0.43
1:C:829:ILE:O	1:C:832:ARG:HG2	2.19	0.43
1:C:999:ARG:NH2	1:C:1036:GLN:HG3	2.33	0.43
1:D:231:ASP:OD1	1:D:231:ASP:N	2.52	0.43
1:D:1229:LYS:O	1:D:1233:ILE:HG12	2.19	0.43
1:A:143:GLU:HB3	1:A:146:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:HG2	1:A:572:GLU:OE1	2.18	0.43
1:A:1122:LEU:HD13	1:A:1179:ILE:HD11	2.01	0.43
1:A:2122:VAL:HG12	1:A:2126:LYS:HZ3	1.82	0.43
1:B:886:ARG:HA	1:B:889:LYS:HZ3	1.81	0.43
1:B:1200:GLN:HG2	1:B:1201:GLN:N	2.33	0.43
1:B:2713:SER:HA	1:B:2716:LEU:HG	2.00	0.43
1:C:805:ARG:NH2	1:C:987:ASP:OD1	2.51	0.43
1:C:1229:LYS:O	1:C:1233:ILE:HG12	2.19	0.43
1:C:1810:ASP:OD1	1:C:1846:ARG:NH2	2.51	0.43
1:D:117:TYR:OH	1:D:180:ASP:OD2	2.35	0.43
1:D:423:LEU:HD23	1:D:423:LEU:H	1.84	0.43
1:D:1362:ARG:NH1	1:D:1414:ASP:OD1	2.50	0.43
1:D:2628:PHE:C	1:D:2630:GLU:H	2.22	0.43
1:A:770:ASP:OD1	1:A:770:ASP:N	2.49	0.43
1:A:999:ARG:NH2	1:A:1036:GLN:HG3	2.33	0.43
1:A:1406:ILE:HG23	1:A:1423:TYR:HB3	2.01	0.43
1:A:2621:PHE:CZ	1:A:2631:HIS:CE1	3.07	0.43
1:A:2628:PHE:C	1:A:2630:GLU:H	2.22	0.43
1:B:474:THR:HG23	1:B:552:ILE:HG21	2.01	0.43
1:B:806:LEU:HG	1:B:1103:LEU:CD2	2.40	0.43
1:B:1598:ARG:NE	1:B:1598:ARG:O	2.52	0.43
1:B:1833:GLU:OE2	1:B:1971:ARG:NH2	2.47	0.43
1:B:2624:LYS:O	1:B:2626:VAL:N	2.52	0.43
1:C:199:GLN:NE2	1:C:207:ASN:OD1	2.52	0.43
1:C:474:THR:HG23	1:C:552:ILE:HG21	2.01	0.43
1:C:1410:VAL:HG21	1:C:1424:ILE:HD11	2.00	0.43
1:C:2628:PHE:C	1:C:2630:GLU:H	2.22	0.43
1:D:143:GLU:HB3	1:D:146:ALA:HB3	1.99	0.43
1:D:764:ILE:HD12	1:D:789:HIS:NE2	2.34	0.43
1:D:1248:ASN:OD1	1:D:1249:GLN:N	2.51	0.43
1:D:2063:ILE:HA	1:D:2066:ILE:HD12	1.99	0.43
1:D:2358:GLY:O	1:D:2362:VAL:HG23	2.19	0.43
1:D:2621:PHE:CZ	1:D:2631:HIS:CE1	3.07	0.43
6:D:2814:PLX:H32	6:D:2814:PLX:H6	1.83	0.43
1:A:477:LEU:HD21	1:A:522:LEU:HD13	2.00	0.43
1:A:1229:LYS:O	1:A:1233:ILE:HG12	2.19	0.43
1:A:1300:GLU:HG3	1:A:1340:ASP:HB3	2.00	0.43
1:A:1810:ASP:OD1	1:A:1846:ARG:NH2	2.51	0.43
1:A:1857:PHE:HE2	1:A:1991:GLN:HG2	1.79	0.43
1:A:2628:PHE:C	1:A:2630:GLU:N	2.71	0.43
1:B:718:ASP:HA	1:B:721:GLU:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ARG:NH2	1:B:987:ASP:OD1	2.51	0.43
1:B:1347:ASP:OD1	1:B:1347:ASP:N	2.52	0.43
1:B:2358:GLY:O	1:B:2362:VAL:HG23	2.19	0.43
1:C:497:VAL:H	1:C:558:ARG:HH12	1.65	0.43
1:C:1248:ASN:OD1	1:C:1250:GLN:HG3	2.18	0.43
1:C:1598:ARG:O	1:C:1598:ARG:NE	2.52	0.43
1:C:2365:LYS:HD3	1:C:2365:LYS:HA	1.69	0.43
1:D:568:ARG:HG2	1:D:572:GLU:OE1	2.18	0.43
1:D:1206:ARG:HD2	1:D:1250:GLN:HE22	1.84	0.43
1:A:829:ILE:O	1:A:832:ARG:HG2	2.19	0.43
1:A:1091:GLN:HG3	1:A:1095:GLN:HE22	1.84	0.43
1:A:1104:VAL:HG23	1:A:1108:ASP:HB2	2.01	0.43
1:A:1420:LYS:HZ3	1:A:1457:ASP:HB2	1.84	0.43
1:B:797:GLN:OE1	1:B:875:TYR:HB3	2.19	0.43
1:B:1104:VAL:HG23	1:B:1108:ASP:HB2	2.01	0.43
1:B:2628:PHE:C	1:B:2630:GLU:H	2.22	0.43
1:C:830:LYS:HD3	1:C:878:PHE:HD1	1.84	0.43
1:C:1095:GLN:O	1:C:1098:LYS:HG2	2.19	0.43
1:C:2358:GLY:O	1:C:2362:VAL:HG23	2.19	0.43
1:C:2411:PHE:HB2	6:C:2803:PLX:H81	1.99	0.43
1:C:2568:ILE:HD11	6:D:2809:PLX:H111	2.01	0.43
1:D:471:ARG:HA	1:D:471:ARG:HD2	1.90	0.43
1:D:797:GLN:OE1	1:D:875:TYR:HB3	2.19	0.43
1:D:1406:ILE:HG23	1:D:1423:TYR:HB3	2.01	0.43
1:D:2040:LEU:HA	1:D:2043:TYR:HD2	1.84	0.43
1:D:2394:TYR:CZ	1:D:2398:TYR:HE2	2.36	0.43
1:D:2738:HIS:N	1:D:2739:PRO:HD2	2.34	0.43
1:A:1173:TYR:O	1:A:1229:LYS:NZ	2.48	0.42
1:A:1790:MET:HE2	1:A:1795:VAL:HG22	2.01	0.42
1:B:806:LEU:HD22	1:B:809:GLU:HG3	2.01	0.42
1:B:2194:ALA:HB3	1:B:2644:PHE:CZ	2.54	0.42
1:B:2621:PHE:CZ	1:B:2631:HIS:CE1	3.07	0.42
1:B:2738:HIS:N	1:B:2739:PRO:HD2	2.34	0.42
6:B:2802:PLX:H1C2	6:B:2802:PLX:H21	1.75	0.42
1:C:764:ILE:HD12	1:C:789:HIS:NE2	2.34	0.42
1:C:797:GLN:OE1	1:C:875:TYR:HB3	2.19	0.42
1:D:477:LEU:HD21	1:D:522:LEU:HD13	2.00	0.42
1:D:658:ASN:HB2	1:D:659:PRO:HD3	2.01	0.42
1:D:737:LEU:HB3	1:D:784:LEU:HD23	2.01	0.42
1:D:1100:VAL:HG22	1:D:1101:GLN:N	2.22	0.42
1:D:1218:LEU:CD2	1:D:1238:HIS:CE1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1810:ASP:OD1	1:D:1846:ARG:NH2	2.51	0.42
1:D:2131:GLN:HA	1:D:2134:VAL:HB	1.99	0.42
1:A:471:ARG:HA	1:A:471:ARG:HD2	1.90	0.42
1:A:1095:GLN:O	1:A:1098:LYS:HG2	2.19	0.42
1:A:1248:ASN:OD1	1:A:1250:GLN:HG3	2.18	0.42
1:A:2342:LEU:O	1:A:2345:ILE:HG12	2.19	0.42
1:A:2715:GLN:HA	1:A:2718:GLU:CG	2.49	0.42
1:B:829:ILE:O	1:B:832:ARG:HG2	2.19	0.42
1:C:658:ASN:HB2	1:C:659:PRO:HD3	2.01	0.42
1:C:1000:GLU:HB3	1:C:1028:LEU:HD12	2.00	0.42
1:C:1067:LEU:HD23	1:C:1075:LEU:HD11	2.01	0.42
1:C:2040:LEU:HA	1:C:2043:TYR:HD2	1.84	0.42
1:C:2122:VAL:HG12	1:C:2126:LYS:HZ3	1.82	0.42
1:D:718:ASP:HA	1:D:721:GLU:CD	2.39	0.42
1:D:1091:GLN:HG3	1:D:1095:GLN:HE22	1.84	0.42
1:D:1119:LEU:HD23	1:D:1119:LEU:HA	1.86	0.42
1:D:1317:LYS:HE2	1:D:1320:GLY:HA2	2.01	0.42
1:D:2342:LEU:O	1:D:2345:ILE:HG12	2.19	0.42
1:D:2624:LYS:O	1:D:2626:VAL:N	2.52	0.42
1:A:1103:LEU:CD1	1:A:1109:VAL:HG23	2.47	0.42
1:A:1317:LYS:HE2	1:A:1320:GLY:HA2	2.01	0.42
1:A:1598:ARG:NE	1:A:1598:ARG:O	2.52	0.42
6:A:2809:PLX:H362	6:A:2809:PLX:H331	1.83	0.42
1:B:875:TYR:CE1	1:B:980:PHE:HB2	2.45	0.42
1:B:1184:SER:O	1:B:1243:ASN:ND2	2.51	0.42
1:B:2100:MET:O	1:B:2103:ARG:HB2	2.20	0.42
1:B:2626:VAL:CG1	1:B:2631:HIS:HB2	2.50	0.42
1:C:162:TYR:N	1:C:185:ASN:O	2.40	0.42
1:C:1091:GLN:HG3	1:C:1095:GLN:HE22	1.84	0.42
1:D:405:PRO:HG2	1:D:408:LYS:HZ3	1.83	0.42
1:D:474:THR:HG23	1:D:552:ILE:HG21	2.01	0.42
1:D:829:ILE:O	1:D:832:ARG:HG2	2.19	0.42
1:D:1095:GLN:O	1:D:1098:LYS:HG2	2.19	0.42
1:D:1122:LEU:O	1:D:1126:VAL:HG23	2.19	0.42
1:D:2411:PHE:HB2	6:D:2810:PLX:H81	2.01	0.42
1:D:2443:LEU:HD23	1:D:2443:LEU:HA	1.89	0.42
1:A:312:HIS:HB3	1:A:357:SER:HB3	2.02	0.42
1:A:797:GLN:OE1	1:A:875:TYR:HB3	2.19	0.42
1:A:830:LYS:HD3	1:A:878:PHE:HD1	1.84	0.42
1:B:312:HIS:HB3	1:B:357:SER:HB3	2.02	0.42
1:B:1091:GLN:HG3	1:B:1095:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1122:LEU:HD13	1:B:1179:ILE:HD11	2.01	0.42
1:B:1229:LYS:O	1:B:1233:ILE:HG12	2.19	0.42
1:B:2715:GLN:HA	1:B:2718:GLU:CG	2.49	0.42
1:C:2738:HIS:N	1:C:2739:PRO:HD2	2.34	0.42
1:D:1856:PHE:CE1	1:D:1860:PHE:HE2	2.38	0.42
1:D:2100:MET:O	1:D:2103:ARG:HB2	2.20	0.42
1:D:2627:THR:O	1:D:2630:GLU:N	2.30	0.42
6:D:2810:PLX:H281	6:D:2810:PLX:H252	1.89	0.42
1:A:1067:LEU:HD23	1:A:1075:LEU:HD11	2.01	0.42
1:A:1122:LEU:O	1:A:1126:VAL:HG23	2.19	0.42
1:A:2100:MET:O	1:A:2103:ARG:HB2	2.20	0.42
1:B:231:ASP:OD1	1:B:231:ASP:N	2.52	0.42
1:B:658:ASN:HB2	1:B:659:PRO:HD3	2.02	0.42
1:B:999:ARG:NH2	1:B:1036:GLN:HG3	2.33	0.42
1:B:1095:GLN:O	1:B:1098:LYS:HG2	2.19	0.42
1:B:1304:ARG:CZ	1:B:1343:VAL:HG21	2.50	0.42
1:C:471:ARG:HA	1:C:471:ARG:HD2	1.90	0.42
1:C:1104:VAL:HG23	1:C:1108:ASP:HB2	2.01	0.42
1:C:1295:PHE:O	1:C:1299:ILE:HG13	2.20	0.42
1:C:1317:LYS:HE2	1:C:1320:GLY:HA2	2.01	0.42
1:C:1417:PRO:O	1:C:1421:ILE:HD12	2.18	0.42
1:C:2556:PRO:HG3	1:C:2566:ARG:HG2	2.01	0.42
1:D:1000:GLU:O	1:D:1003:GLU:HG3	2.20	0.42
1:D:1067:LEU:HD23	1:D:1075:LEU:HD11	2.00	0.42
1:A:658:ASN:HB2	1:A:659:PRO:HD3	2.01	0.42
1:A:1206:ARG:HD2	1:A:1250:GLN:HE22	1.84	0.42
1:A:2556:PRO:HG3	1:A:2566:ARG:HG2	2.01	0.42
1:A:2626:VAL:CG1	1:A:2631:HIS:HB2	2.50	0.42
1:A:2738:HIS:N	1:A:2739:PRO:HD2	2.34	0.42
6:A:2809:PLX:H1C3	6:A:2809:PLX:H21	1.76	0.42
1:B:1000:GLU:HB3	1:B:1028:LEU:HD12	2.00	0.42
1:B:1663:LEU:HD23	1:B:1663:LEU:HA	1.92	0.42
1:B:1868:GLN:HA	1:B:1871:ILE:HG22	2.02	0.42
1:B:2611:CYS:CB	1:B:2614:CYS:SG	3.06	0.42
1:C:290:ASP:OD2	1:C:293:ARG:HG3	2.20	0.42
1:C:627:GLU:HA	1:C:628:PRO:HD3	1.87	0.42
1:C:718:ASP:HA	1:C:721:GLU:CD	2.39	0.42
1:C:737:LEU:HB3	1:C:784:LEU:HD23	2.01	0.42
1:C:806:LEU:HD22	1:C:809:GLU:HG3	2.01	0.42
1:C:1000:GLU:O	1:C:1003:GLU:HG3	2.20	0.42
1:C:1406:ILE:HG23	1:C:1423:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2100:MET:O	1:C:2103:ARG:HB2	2.20	0.42
1:C:2194:ALA:HB3	1:C:2644:PHE:CZ	2.54	0.42
6:C:2805:PLX:H1B2	6:C:2805:PLX:H21	1.79	0.42
1:D:290:ASP:OD2	1:D:293:ARG:HG3	2.20	0.42
1:D:1295:PHE:O	1:D:1299:ILE:HG13	2.20	0.42
1:A:290:ASP:OD2	1:A:293:ARG:HG3	2.20	0.42
1:A:627:GLU:HA	1:A:628:PRO:HD3	1.87	0.42
1:A:1304:ARG:CZ	1:A:1343:VAL:HG21	2.50	0.42
1:A:1417:PRO:O	1:A:1421:ILE:HD12	2.18	0.42
1:A:2194:ALA:HB3	1:A:2644:PHE:CZ	2.54	0.42
1:A:2264:PRO:O	1:A:2266:LEU:N	2.53	0.42
1:A:2358:GLY:O	1:A:2362:VAL:HG23	2.19	0.42
1:B:405:PRO:HG2	1:B:408:LYS:HZ3	1.83	0.42
1:C:1304:ARG:CZ	1:C:1343:VAL:HG21	2.50	0.42
1:C:2117:ARG:HB2	1:C:2120:GLU:OE1	2.20	0.42
1:C:2626:VAL:CG1	1:C:2631:HIS:HB2	2.50	0.42
1:D:402:THR:OG1	1:D:417:LYS:O	2.25	0.42
1:D:1666:GLU:O	1:D:1666:GLU:HG2	2.19	0.42
1:A:265:ARG:HH22	4:A:2803:I3P:P4	2.43	0.42
1:A:1295:PHE:O	1:A:1299:ILE:HG13	2.20	0.42
1:A:2283:LEU:O	1:A:2287:MET:HG3	2.20	0.42
1:A:2599:GLU:O	1:A:2603:LYS:HG2	2.20	0.42
6:A:2809:PLX:H111	1:D:2568:ILE:HD11	2.02	0.42
1:B:402:THR:OG1	1:B:417:LYS:O	2.25	0.42
1:B:423:LEU:HD23	1:B:423:LEU:H	1.84	0.42
1:B:702:ASP:HB3	1:B:704:ASN:OD1	2.20	0.42
1:B:1623:LEU:HA	1:B:1626:LEU:HD23	2.02	0.42
1:B:1666:GLU:HG2	1:B:1666:GLU:O	2.19	0.42
1:B:1864:MET:CE	1:B:2002:GLU:HB2	2.50	0.42
1:C:1529:GLN:O	1:C:1533:VAL:HG23	2.20	0.42
1:C:2443:LEU:HD12	1:D:2426:THR:OG1	2.19	0.42
1:D:230:LYS:HB2	1:D:233:ILE:HG12	2.02	0.42
1:D:370:LEU:HD22	1:D:388:VAL:HG21	2.01	0.42
1:D:1122:LEU:HD13	1:D:1179:ILE:HD11	2.01	0.42
1:D:2626:VAL:CG1	1:D:2631:HIS:HB2	2.50	0.42
1:D:2715:GLN:HA	1:D:2718:GLU:CG	2.49	0.42
1:A:764:ILE:HD12	1:A:789:HIS:NE2	2.34	0.42
1:A:888:THR:HG21	1:A:1052:LEU:HB3	2.02	0.42
1:A:1868:GLN:HA	1:A:1871:ILE:HG22	2.02	0.42
1:B:162:TYR:N	1:B:185:ASN:O	2.40	0.42
1:B:764:ILE:HD12	1:B:789:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1000:GLU:O	1:B:1003:GLU:HG3	2.20	0.42
1:B:2053:ASN:O	1:B:2057:THR:OG1	2.27	0.42
1:B:2465:ASP:N	1:B:2465:ASP:OD1	2.50	0.42
6:B:2813:PLX:H261	6:B:2813:PLX:H291	1.92	0.42
1:C:1420:LYS:O	1:C:1424:ILE:HB	2.20	0.42
1:C:2342:LEU:O	1:C:2345:ILE:HG12	2.19	0.42
1:D:2194:ALA:HB3	1:D:2644:PHE:CZ	2.54	0.42
1:D:2556:PRO:HG3	1:D:2566:ARG:HG2	2.01	0.42
1:A:826:LYS:HA	1:A:829:ILE:HD12	2.02	0.42
1:A:1100:VAL:HG22	1:A:1101:GLN:N	2.22	0.42
1:A:1119:LEU:HD23	1:A:1119:LEU:HA	1.86	0.42
6:A:2812:PLX:H21	6:A:2812:PLX:H1B2	1.79	0.42
1:B:467:GLN:O	1:B:471:ARG:N	2.34	0.42
1:B:600:HIS:O	1:B:603:ARG:NH1	2.42	0.42
1:B:826:LYS:HA	1:B:829:ILE:HD12	2.02	0.42
1:B:1122:LEU:O	1:B:1126:VAL:HG23	2.19	0.42
1:B:1218:LEU:CD2	1:B:1238:HIS:CE1	3.02	0.42
1:B:1401:LEU:HD12	1:B:1401:LEU:HA	1.96	0.42
1:B:1421:ILE:HG13	1:B:1478:TYR:CD1	2.51	0.42
1:B:2117:ARG:HB2	1:B:2120:GLU:OE1	2.20	0.42
1:B:2122:VAL:HG12	1:B:2126:LYS:HZ3	1.82	0.42
1:B:2568:ILE:HD11	6:C:2802:PLX:H111	2.02	0.42
1:B:2638:MET:HG2	3:B:2803:ATP:C8	2.55	0.42
1:C:265:ARG:HH22	4:C:2808:I3P:P4	2.43	0.42
1:C:1347:ASP:OD1	1:C:1347:ASP:N	2.52	0.42
1:C:1353:THR:HG23	1:C:1356:GLN:HE21	1.85	0.42
1:C:2283:LEU:O	1:C:2287:MET:HG3	2.20	0.42
1:D:702:ASP:HB3	1:D:704:ASN:OD1	2.20	0.42
1:D:733:TYR:O	1:D:737:LEU:HG	2.20	0.42
1:D:826:LYS:HA	1:D:829:ILE:HD12	2.02	0.42
1:D:1104:VAL:HG22	1:D:1108:ASP:OD2	2.20	0.42
1:D:1304:ARG:CZ	1:D:1343:VAL:HG21	2.50	0.42
1:D:2065:ILE:H	1:D:2065:ILE:HD12	1.85	0.42
6:D:2814:PLX:H21	6:D:2814:PLX:H1C2	1.75	0.42
1:A:370:LEU:HD22	1:A:388:VAL:HG21	2.01	0.41
1:A:806:LEU:HD22	1:A:809:GLU:HG3	2.01	0.41
1:A:1864:MET:CE	1:A:2002:GLU:HB2	2.50	0.41
1:B:370:LEU:HD22	1:B:388:VAL:HG21	2.01	0.41
1:B:1067:LEU:HD23	1:B:1075:LEU:HD11	2.01	0.41
1:B:1306:VAL:HG11	1:B:1373:MET:HG2	2.02	0.41
1:B:1317:LYS:HE2	1:B:1320:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1406:ILE:HG23	1:B:1423:TYR:HB3	2.01	0.41
1:B:2556:PRO:HG3	1:B:2566:ARG:HG2	2.01	0.41
1:C:2715:GLN:HA	1:C:2718:GLU:CG	2.49	0.41
6:C:2806:PLX:H21	6:C:2806:PLX:H1C2	1.83	0.41
1:D:1104:VAL:HG23	1:D:1108:ASP:HB2	2.01	0.41
1:A:423:LEU:HD23	1:A:423:LEU:H	1.84	0.41
1:A:737:LEU:HB3	1:A:784:LEU:HD23	2.01	0.41
1:A:1000:GLU:O	1:A:1003:GLU:HG3	2.20	0.41
1:B:830:LYS:HD3	1:B:878:PHE:HD1	1.84	0.41
1:B:1611:LEU:O	1:B:1615:LEU:HD23	2.21	0.41
1:C:733:TYR:O	1:C:737:LEU:HG	2.20	0.41
1:C:1122:LEU:O	1:C:1126:VAL:HG23	2.19	0.41
1:C:1856:PHE:CE1	1:C:1860:PHE:HE2	2.38	0.41
1:C:2599:GLU:O	1:C:2603:LYS:HG2	2.20	0.41
1:D:1353:THR:HG23	1:D:1356:GLN:HE21	1.85	0.41
1:D:2097:LEU:HD11	1:D:2155:ASN:HB3	2.02	0.41
1:D:2117:ARG:HB2	1:D:2120:GLU:OE1	2.20	0.41
1:D:2599:GLU:O	1:D:2603:LYS:HG2	2.20	0.41
1:A:875:TYR:CE1	1:A:980:PHE:HB2	2.45	0.41
1:A:1053:ASP:OD2	1:A:1059:THR:OG1	2.26	0.41
1:A:1353:THR:HG23	1:A:1356:GLN:HE21	1.85	0.41
1:A:1529:GLN:O	1:A:1533:VAL:HG23	2.20	0.41
1:A:1856:PHE:CE1	1:A:1860:PHE:HE2	2.38	0.41
1:A:2117:ARG:N	1:A:2120:GLU:OE2	2.53	0.41
1:B:290:ASP:OD2	1:B:293:ARG:HG3	2.20	0.41
1:B:737:LEU:HB3	1:B:784:LEU:HD23	2.01	0.41
1:B:888:THR:HG21	1:B:1052:LEU:HB3	2.02	0.41
1:B:2599:GLU:O	1:B:2603:LYS:HG2	2.20	0.41
1:C:1420:LYS:HZ3	1:C:1457:ASP:HB2	1.85	0.41
1:C:1599:ASN:C	1:C:1603:ARG:HE	2.21	0.41
6:C:2813:PLX:H21	6:C:2813:PLX:H1C2	1.75	0.41
1:D:830:LYS:HD3	1:D:878:PHE:HD1	1.84	0.41
1:D:1173:TYR:O	1:D:1229:LYS:NZ	2.48	0.41
1:D:1420:LYS:O	1:D:1424:ILE:HB	2.20	0.41
1:D:1623:LEU:O	1:D:1626:LEU:HB2	2.21	0.41
1:D:2117:ARG:N	1:D:2120:GLU:OE2	2.53	0.41
1:D:2122:VAL:HG12	1:D:2126:LYS:HZ3	1.84	0.41
1:A:702:ASP:HB3	1:A:704:ASN:OD1	2.20	0.41
1:A:1179:ILE:O	1:A:1183:LEU:HD23	2.20	0.41
1:A:1623:LEU:O	1:A:1626:LEU:HB2	2.21	0.41
1:A:2329:LYS:N	1:A:2330:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HD11	1:B:551:HIS:HA	2.02	0.41
1:B:1295:PHE:O	1:B:1299:ILE:HG13	2.20	0.41
1:B:1845:CYS:HA	1:B:1848:THR:HG22	2.03	0.41
1:B:2117:ARG:N	1:B:2120:GLU:OE2	2.53	0.41
1:B:2264:PRO:O	1:B:2266:LEU:N	2.53	0.41
1:B:2411:PHE:HB2	6:B:2811:PLX:H81	2.01	0.41
1:C:230:LYS:HB2	1:C:233:ILE:HG12	2.02	0.41
1:C:411:GLU:HG2	1:C:412:LYS:N	2.36	0.41
1:C:826:LYS:HA	1:C:829:ILE:HD12	2.02	0.41
1:C:1122:LEU:HD13	1:C:1179:ILE:HD11	2.01	0.41
1:C:1864:MET:CE	1:C:2002:GLU:HB2	2.50	0.41
1:C:2329:LYS:N	1:C:2330:PRO:HD2	2.36	0.41
1:C:2624:LYS:O	1:C:2626:VAL:N	2.52	0.41
1:C:2666:MET:HE3	1:C:2671:ASN:HB3	2.02	0.41
1:D:1600:ILE:O	1:D:1604:LEU:HD23	2.21	0.41
1:D:1623:LEU:HA	1:D:1626:LEU:HD23	2.02	0.41
1:D:1868:GLN:HA	1:D:1871:ILE:HG22	2.02	0.41
1:D:2264:PRO:O	1:D:2266:LEU:N	2.53	0.41
1:A:733:TYR:O	1:A:737:LEU:HG	2.20	0.41
1:A:1306:VAL:HG11	1:A:1373:MET:HG2	2.02	0.41
1:A:1956:ASP:OD1	1:A:1956:ASP:N	2.54	0.41
1:A:2443:LEU:HD12	1:B:2426:THR:OG1	2.20	0.41
6:A:2813:PLX:H1C2	6:A:2813:PLX:H21	1.83	0.41
1:B:69:GLN:NE2	1:B:73:TRP:HE3	2.18	0.41
1:B:653:CYS:SG	1:B:654:LYS:N	2.94	0.41
1:B:1129:SER:HA	1:B:1132:TRP:NE1	2.35	0.41
1:B:2329:LYS:N	1:B:2330:PRO:HD2	2.36	0.41
1:C:702:ASP:HB3	1:C:704:ASN:OD1	2.20	0.41
1:C:1218:LEU:CD2	1:C:1238:HIS:CE1	3.02	0.41
1:C:1845:CYS:HA	1:C:1848:THR:HG22	2.03	0.41
1:C:2580:ILE:HD13	1:C:2580:ILE:HA	1.96	0.41
1:A:1420:LYS:O	1:A:1424:ILE:HB	2.20	0.41
1:B:98:LEU:HA	1:B:101:LYS:HE2	2.03	0.41
1:B:265:ARG:HH22	4:B:2804:I3P:P4	2.43	0.41
1:B:2283:LEU:O	1:B:2287:MET:HG3	2.20	0.41
1:B:2305:LEU:HD23	1:B:2305:LEU:HA	1.98	0.41
1:B:2342:LEU:O	1:B:2345:ILE:HG12	2.19	0.41
1:C:1104:VAL:HG22	1:C:1108:ASP:OD2	2.20	0.41
1:C:1129:SER:HA	1:C:1132:TRP:HE1	1.86	0.41
1:C:1179:ILE:O	1:C:1183:LEU:HD23	2.20	0.41
1:C:1600:ILE:O	1:C:1604:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1623:LEU:O	1:C:1626:LEU:HB2	2.21	0.41
1:C:1868:GLN:HA	1:C:1871:ILE:HG22	2.02	0.41
1:C:2065:ILE:H	1:C:2065:ILE:HD12	1.85	0.41
1:C:2638:MET:HG2	3:C:2807:ATP:C8	2.56	0.41
1:D:265:ARG:HH22	4:D:2804:I3P:P4	2.43	0.41
1:D:653:CYS:SG	1:D:654:LYS:N	2.94	0.41
1:D:806:LEU:HD22	1:D:809:GLU:HG3	2.01	0.41
1:D:1095:GLN:O	1:D:1099:GLN:HG2	2.21	0.41
1:D:1529:GLN:O	1:D:1533:VAL:HG23	2.20	0.41
1:D:2119:LYS:O	1:D:2123:GLU:HG2	2.21	0.41
1:D:2436:ARG:NH2	1:D:2599:GLU:OE2	2.54	0.41
1:A:98:LEU:HA	1:A:101:LYS:HE2	2.03	0.41
1:A:230:LYS:HB2	1:A:233:ILE:HG12	2.02	0.41
1:A:467:GLN:HG2	1:A:470:ARG:HH21	1.86	0.41
1:A:2117:ARG:HB2	1:A:2120:GLU:OE1	2.20	0.41
1:A:2436:ARG:NH2	1:A:2599:GLU:OE2	2.54	0.41
1:A:2568:ILE:HD11	6:B:2810:PLX:H111	2.03	0.41
1:B:18:TYR:OH	1:B:45:ASP:OD1	2.32	0.41
1:B:411:GLU:HG2	1:B:412:LYS:N	2.36	0.41
1:B:1623:LEU:O	1:B:1626:LEU:HB2	2.21	0.41
1:B:1856:PHE:CE1	1:B:1860:PHE:HE2	2.38	0.41
1:B:2283:LEU:HD23	1:B:2283:LEU:HA	1.87	0.41
1:C:117:TYR:OH	1:C:180:ASP:OD2	2.35	0.41
1:C:1623:LEU:HA	1:C:1626:LEU:HD23	2.02	0.41
1:D:1129:SER:HA	1:D:1132:TRP:NE1	2.35	0.41
1:D:2283:LEU:O	1:D:2287:MET:HG3	2.20	0.41
1:D:2329:LYS:N	1:D:2330:PRO:HD2	2.36	0.41
1:D:2657:THR:HG22	1:D:2658:GLY:N	2.29	0.41
1:A:863:THR:O	1:A:867:VAL:HG23	2.21	0.41
1:A:1129:SER:HA	1:A:1132:TRP:NE1	2.35	0.41
1:A:1623:LEU:HA	1:A:1626:LEU:HD23	2.02	0.41
1:A:1985:GLN:HB3	1:A:2051:ASN:ND2	2.36	0.41
1:A:2305:LEU:HD23	1:A:2305:LEU:HA	1.98	0.41
1:B:230:LYS:HB2	1:B:233:ILE:HG12	2.01	0.41
1:C:467:GLN:HG2	1:C:470:ARG:HH21	1.86	0.41
1:C:1306:VAL:HG11	1:C:1373:MET:HG2	2.02	0.41
1:C:1611:LEU:O	1:C:1615:LEU:HD23	2.21	0.41
1:C:2117:ARG:N	1:C:2120:GLU:OE2	2.53	0.41
1:C:2264:PRO:O	1:C:2266:LEU:N	2.53	0.41
1:D:312:HIS:HB3	1:D:357:SER:HB3	2.02	0.41
1:D:812:SER:HA	1:D:998:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1864:MET:CE	1:D:2002:GLU:HB2	2.50	0.41
1:D:2616:LEU:HB2	1:D:2621:PHE:HE1	1.86	0.41
1:A:231:ASP:OD1	1:A:231:ASP:N	2.52	0.41
1:A:653:CYS:SG	1:A:654:LYS:N	2.94	0.41
1:A:1447:MET:HA	1:A:1447:MET:HE2	2.03	0.41
1:A:1845:CYS:HA	1:A:1848:THR:HG22	2.03	0.41
1:A:2195:GLN:HG3	1:A:2207:GLN:NE2	2.36	0.41
1:A:2616:LEU:HB2	1:A:2621:PHE:HE1	1.86	0.41
1:B:733:TYR:O	1:B:737:LEU:HG	2.20	0.41
1:B:1529:GLN:O	1:B:1533:VAL:HG23	2.20	0.41
1:B:1864:MET:HE1	1:B:2002:GLU:HB2	2.02	0.41
1:B:2097:LEU:HD11	1:B:2155:ASN:HB3	2.02	0.41
1:C:69:GLN:NE2	1:C:73:TRP:HE3	2.18	0.41
1:C:312:HIS:HB3	1:C:357:SER:HB3	2.02	0.41
1:C:993:LEU:HD23	1:C:993:LEU:HA	1.96	0.41
1:C:1095:GLN:O	1:C:1099:GLN:HG2	2.21	0.41
1:C:1736:LEU:HD23	1:C:1736:LEU:HA	1.82	0.41
1:C:2083:ASP:OD1	1:C:2083:ASP:N	2.54	0.41
1:C:2097:LEU:HD11	1:C:2155:ASN:HB3	2.02	0.41
1:C:2436:ARG:NH2	1:C:2599:GLU:OE2	2.54	0.41
1:D:467:GLN:HG2	1:D:470:ARG:HH21	1.86	0.41
1:D:888:THR:HG21	1:D:1052:LEU:HB3	2.02	0.41
1:D:1483:VAL:HA	1:D:1486:ILE:HG12	2.03	0.41
1:D:1599:ASN:C	1:D:1603:ARG:HE	2.21	0.41
1:D:1845:CYS:HA	1:D:1848:THR:HG22	2.03	0.41
1:D:2345:ILE:HG13	1:D:2346:PHE:N	2.36	0.41
1:A:640:SER:O	1:A:643:LYS:HG3	2.21	0.41
1:A:1600:ILE:O	1:A:1604:LEU:HD23	2.21	0.41
1:A:2345:ILE:HG13	1:A:2346:PHE:N	2.36	0.41
1:A:2465:ASP:OD1	1:A:2465:ASP:N	2.50	0.41
6:A:2812:PLX:H261	6:A:2812:PLX:H291	1.92	0.41
1:B:640:SER:O	1:B:643:LYS:HG3	2.21	0.41
1:B:1179:ILE:O	1:B:1183:LEU:HD23	2.20	0.41
1:B:1206:ARG:CD	1:B:1250:GLN:HE22	2.34	0.41
1:B:1353:THR:HG23	1:B:1356:GLN:HE21	1.85	0.41
1:B:1985:GLN:HB3	1:B:2051:ASN:ND2	2.36	0.41
1:B:2436:ARG:NH2	1:B:2599:GLU:OE2	2.54	0.41
6:B:2814:PLX:H51	6:B:2814:PLX:H252	1.82	0.41
1:D:69:GLN:NE2	1:D:73:TRP:HE3	2.18	0.41
1:D:351:MET:HE1	1:D:400:HIS:CD2	2.56	0.41
1:D:862:LEU:HA	1:D:865:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1985:GLN:HB3	1:D:2051:ASN:ND2	2.36	0.41
6:D:2802:PLX:H22	6:D:2802:PLX:H1C2	1.83	0.41
6:D:2812:PLX:H291	6:D:2812:PLX:H261	1.92	0.41
1:A:495:LEU:HD11	1:A:551:HIS:HA	2.02	0.40
1:A:2083:ASP:OD1	1:A:2083:ASP:N	2.54	0.40
1:B:627:GLU:HA	1:B:628:PRO:HD3	1.87	0.40
1:B:1420:LYS:O	1:B:1424:ILE:HB	2.20	0.40
1:B:2345:ILE:HG13	1:B:2346:PHE:N	2.36	0.40
1:B:2627:THR:O	1:B:2630:GLU:N	2.30	0.40
1:C:1985:GLN:HB3	1:C:2051:ASN:ND2	2.36	0.40
1:C:2616:LEU:HB2	1:C:2621:PHE:HE1	1.86	0.40
1:D:224:MET:HE1	1:D:235:LYS:HD2	2.02	0.40
1:D:640:SER:O	1:D:643:LYS:HG3	2.21	0.40
1:D:1129:SER:HA	1:D:1132:TRP:HE1	1.86	0.40
1:D:1420:LYS:HZ3	1:D:1457:ASP:HB2	1.85	0.40
1:D:1663:LEU:HD23	1:D:1663:LEU:HA	1.92	0.40
1:A:862:LEU:HA	1:A:865:GLU:OE2	2.21	0.40
1:A:1103:LEU:O	1:A:1103:LEU:HG	2.18	0.40
1:B:172:ILE:H	1:B:172:ILE:HD12	1.87	0.40
1:B:1129:SER:HA	1:B:1132:TRP:HE1	1.86	0.40
1:B:2065:ILE:H	1:B:2065:ILE:HD12	1.85	0.40
1:B:2684:VAL:O	1:B:2686:SER:N	2.54	0.40
1:C:172:ILE:H	1:C:172:ILE:HD12	1.87	0.40
1:C:653:CYS:SG	1:C:654:LYS:N	2.94	0.40
1:C:888:THR:HG21	1:C:1052:LEU:HB3	2.02	0.40
1:C:1129:SER:HA	1:C:1132:TRP:NE1	2.35	0.40
1:C:2119:LYS:O	1:C:2123:GLU:HG2	2.21	0.40
1:C:2627:THR:O	1:C:2630:GLU:N	2.30	0.40
1:D:874:ILE:HG13	1:D:875:TYR:N	2.36	0.40
1:D:1179:ILE:O	1:D:1183:LEU:HD23	2.20	0.40
1:D:1206:ARG:CD	1:D:1250:GLN:HE22	2.34	0.40
1:D:2638:MET:HG2	3:D:2803:ATP:C8	2.56	0.40
1:A:1104:VAL:HG22	1:A:1108:ASP:OD2	2.20	0.40
1:A:1347:ASP:OD1	1:A:1347:ASP:N	2.52	0.40
1:A:1483:VAL:HA	1:A:1486:ILE:HG12	2.03	0.40
1:A:2065:ILE:HD12	1:A:2065:ILE:H	1.85	0.40
1:A:2111:ARG:HA	1:A:2111:ARG:HD2	1.96	0.40
6:A:2810:PLX:H281	6:A:2810:PLX:H252	1.89	0.40
1:B:657:LEU:O	1:B:660:THR:HG22	2.22	0.40
1:B:770:ASP:OD1	1:B:770:ASP:N	2.49	0.40
1:B:862:LEU:HA	1:B:865:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1095:GLN:O	1:B:1099:GLN:HG2	2.21	0.40
1:C:863:THR:O	1:C:867:VAL:HG23	2.21	0.40
1:C:1206:ARG:CD	1:C:1250:GLN:HE22	2.34	0.40
1:D:495:LEU:HD11	1:D:551:HIS:HA	2.02	0.40
1:A:2097:LEU:HD11	1:A:2155:ASN:HB3	2.02	0.40
1:B:467:GLN:HG2	1:B:470:ARG:HH21	1.86	0.40
1:B:1790:MET:HB2	1:B:1794:GLU:OE2	2.22	0.40
1:C:495:LEU:HD11	1:C:551:HIS:HA	2.02	0.40
1:C:640:SER:O	1:C:643:LYS:HG3	2.21	0.40
1:C:844:LEU:O	1:C:848:VAL:HG23	2.22	0.40
1:C:1119:LEU:HD23	1:C:1119:LEU:HA	1.86	0.40
1:C:2345:ILE:HG13	1:C:2346:PHE:N	2.36	0.40
1:D:600:HIS:O	1:D:603:ARG:NH1	2.42	0.40
1:D:657:LEU:O	1:D:660:THR:HG22	2.22	0.40
1:D:863:THR:O	1:D:867:VAL:HG23	2.21	0.40
6:D:2813:PLX:H21	6:D:2813:PLX:H1C2	1.83	0.40
1:A:657:LEU:O	1:A:660:THR:HG22	2.22	0.40
1:A:874:ILE:HG13	1:A:875:TYR:N	2.36	0.40
1:A:1095:GLN:O	1:A:1099:GLN:HG2	2.21	0.40
1:A:2119:LYS:O	1:A:2123:GLU:HG2	2.21	0.40
1:A:2207:GLN:HE22	1:A:2209:VAL:HG23	1.86	0.40
6:A:2814:PLX:H21	6:A:2814:PLX:H1C2	1.75	0.40
1:B:1483:VAL:HA	1:B:1486:ILE:HG12	2.03	0.40
1:B:1600:ILE:O	1:B:1604:LEU:HD23	2.21	0.40
1:C:812:SER:HA	1:C:998:LYS:HD3	2.03	0.40
1:C:874:ILE:HG13	1:C:875:TYR:N	2.36	0.40
1:C:1375:HIS:CD2	1:C:1423:TYR:HH	2.40	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	2369/2750 (86%)	2264 (96%)	98 (4%)	7 (0%)	41	75
1	B	2369/2750 (86%)	2264 (96%)	98 (4%)	7 (0%)	41	75
1	C	2369/2750 (86%)	2265 (96%)	97 (4%)	7 (0%)	41	75
1	D	2369/2750 (86%)	2265 (96%)	97 (4%)	7 (0%)	41	75
All	All	9476/11000 (86%)	9058 (96%)	390 (4%)	28 (0%)	44	75

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	ALA
1	B	547	ALA
1	C	547	ALA
1	D	547	ALA
1	A	665	LEU
1	A	1104	VAL
1	A	2477	GLU
1	B	665	LEU
1	B	1104	VAL
1	B	2477	GLU
1	C	665	LEU
1	C	1104	VAL
1	C	2477	GLU
1	D	665	LEU
1	D	1104	VAL
1	D	2477	GLU
1	A	1100	VAL
1	A	2625	THR
1	B	1100	VAL
1	B	2625	THR
1	C	1100	VAL
1	C	2625	THR
1	D	1100	VAL
1	D	2625	THR
1	A	2522	GLN
1	B	2522	GLN
1	C	2522	GLN
1	D	2522	GLN

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	2163/2459 (88%)	2153 (100%)	10 (0%)	88 94
1	B	2163/2459 (88%)	2153 (100%)	10 (0%)	88 94
1	C	2163/2459 (88%)	2153 (100%)	10 (0%)	88 94
1	D	2163/2459 (88%)	2153 (100%)	10 (0%)	88 94
All	All	8652/9836 (88%)	8612 (100%)	40 (0%)	91 94

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	ARG
1	A	643	LYS
1	A	871	ARG
1	A	1101	GLN
1	A	1103	LEU
1	A	1603	ARG
1	A	2298	LYS
1	A	2583[A]	ASN
1	A	2583[B]	ASN
1	A	2626	VAL
1	B	391	ARG
1	B	643	LYS
1	B	871	ARG
1	B	1101	GLN
1	B	1103	LEU
1	B	1603	ARG
1	B	2298	LYS
1	B	2583[A]	ASN
1	B	2583[B]	ASN
1	B	2626	VAL
1	C	391	ARG
1	C	643	LYS
1	C	871	ARG
1	C	1101	GLN

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Mol	Chain	Res	Type
1	C	1103	LEU
1	C	1603	ARG
1	C	2298	LYS
1	C	2583[A]	ASN
1	C	2583[B]	ASN
1	C	2626	VAL
1	D	391	ARG
1	D	643	LYS
1	D	871	ARG
1	D	1101	GLN
1	D	1103	LEU
1	D	1603	ARG
1	D	2298	LYS
1	D	2583[A]	ASN
1	D	2583[B]	ASN
1	D	2626	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1101	GLN
1	A	1238	HIS
1	A	1280	ASN
1	A	1356	GLN
1	A	1981	ASN
1	A	2207	GLN
1	A	2409	HIS
1	A	2623	ASN
1	A	2715	GLN
1	B	1101	GLN
1	B	1238	HIS
1	B	1280	ASN
1	B	1356	GLN
1	B	1981	ASN
1	B	2207	GLN
1	B	2409	HIS
1	B	2623	ASN
1	B	2715	GLN
1	C	40	GLN
1	C	736	GLN
1	C	1101	GLN
1	C	1238	HIS

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Mol	Chain	Res	Type
1	C	1280	ASN
1	C	1356	GLN
1	C	1981	ASN
1	C	2207	GLN
1	C	2409	HIS
1	C	2623	ASN
1	C	2715	GLN
1	D	40	GLN
1	D	736	GLN
1	D	1101	GLN
1	D	1238	HIS
1	D	1280	ASN
1	D	1981	ASN
1	D	2207	GLN
1	D	2409	HIS
1	D	2623	ASN
1	D	2715	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 20 are monoatomic - leaving 36 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	$\#\|Z\|>2$
6	PLX	B	2802	-	36,36,51	1.19	4 (11%)	40,44,59	0.75	1 (2%)
6	PLX	B	2810	-	44,44,51	1.14	4 (9%)	48,52,59	0.77	0
6	PLX	C	2803	-	36,36,51	1.22	5 (13%)	40,44,59	0.76	1 (2%)
3	ATP	B	2803	-	26,33,33	0.62	0	31,52,52	0.73	2 (6%)
3	ATP	D	2803	-	26,33,33	0.62	0	31,52,52	0.73	2 (6%)
6	PLX	D	2814	-	36,36,51	1.19	4 (11%)	40,44,59	0.75	1 (2%)
4	I3P	A	2803	-	24,24,24	1.28	3 (12%)	36,39,39	0.66	1 (2%)
6	PLX	A	2812	-	38,38,51	1.18	4 (10%)	42,46,59	0.76	0
6	PLX	B	2814	-	37,37,51	1.23	5 (13%)	41,45,59	0.69	0
6	PLX	D	2802	-	39,39,51	1.18	3 (7%)	43,47,59	0.75	0
6	PLX	C	2806	-	37,37,51	1.23	5 (13%)	41,45,59	0.68	0
3	ATP	C	2807	-	26,33,33	0.63	0	31,52,52	0.73	2 (6%)
6	PLX	B	2812	-	35,35,51	1.22	3 (8%)	39,43,59	0.71	0
4	I3P	D	2804	-	24,24,24	1.28	3 (12%)	36,39,39	0.66	1 (2%)
6	PLX	A	2811	-	35,35,51	1.23	4 (11%)	39,43,59	0.72	0
6	PLX	D	2813	-	37,37,51	1.22	5 (13%)	41,45,59	0.68	0
6	PLX	D	2811	-	35,35,51	1.23	4 (11%)	39,43,59	0.72	0
4	I3P	C	2808	-	24,24,24	1.28	3 (12%)	36,39,39	0.65	1 (2%)
6	PLX	A	2808	-	39,39,51	1.19	3 (7%)	43,47,59	0.75	0
3	ATP	A	2802	-	26,33,33	0.61	0	31,52,52	0.74	2 (6%)
6	PLX	D	2809	-	44,44,51	1.15	5 (11%)	48,52,59	0.77	0
6	PLX	A	2813	-	37,37,51	1.23	5 (13%)	41,45,59	0.68	0
6	PLX	A	2814	-	36,36,51	1.19	4 (11%)	40,44,59	0.75	1 (2%)
6	PLX	B	2813	-	38,38,51	1.18	4 (10%)	42,46,59	0.76	0
4	I3P	B	2804	-	24,24,24	1.29	3 (12%)	36,39,39	0.65	1 (2%)
6	PLX	B	2811	-	36,36,51	1.21	4 (11%)	40,44,59	0.76	1 (2%)
6	PLX	C	2805	-	38,38,51	1.18	4 (10%)	42,46,59	0.76	0
6	PLX	A	2809	-	44,44,51	1.15	4 (9%)	48,52,59	0.77	0
6	PLX	C	2802	-	44,44,51	1.15	4 (9%)	48,52,59	0.77	0
6	PLX	B	2809	-	39,39,51	1.19	3 (7%)	43,47,59	0.75	0
6	PLX	D	2810	-	36,36,51	1.21	5 (13%)	40,44,59	0.76	1 (2%)
6	PLX	C	2804	-	35,35,51	1.23	3 (8%)	39,43,59	0.72	0
6	PLX	D	2812	-	38,38,51	1.18	4 (10%)	42,46,59	0.76	0
6	PLX	A	2810	-	36,36,51	1.20	4 (11%)	40,44,59	0.75	1 (2%)
6	PLX	C	2814	-	39,39,51	1.19	3 (7%)	43,47,59	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PLX	C	2813	-	36,36,51	1.18	4 (11%)	40,44,59	0.74	1 (2%)

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
6	PLX	B	2802	-	-	22/40/40/55	-
6	PLX	B	2810	-	-	29/48/48/55	-
6	PLX	C	2803	-	-	14/40/40/55	-
3	ATP	B	2803	-	-	8/18/38/38	0/3/3/3
3	ATP	D	2803	-	-	8/18/38/38	0/3/3/3
6	PLX	D	2814	-	-	22/40/40/55	-
4	I3P	A	2803	-	-	2/15/39/39	0/1/1/1
6	PLX	A	2812	-	-	24/42/42/55	-
6	PLX	B	2814	-	-	21/41/41/55	-
6	PLX	D	2802	-	-	19/43/43/55	-
6	PLX	C	2806	-	-	21/41/41/55	-
3	ATP	C	2807	-	-	8/18/38/38	0/3/3/3
6	PLX	B	2812	-	-	23/39/39/55	-
4	I3P	D	2804	-	-	2/15/39/39	0/1/1/1
6	PLX	A	2811	-	-	23/39/39/55	-
6	PLX	D	2813	-	-	21/41/41/55	-
6	PLX	D	2811	-	-	23/39/39/55	-
4	I3P	C	2808	-	-	2/15/39/39	0/1/1/1
6	PLX	A	2808	-	-	19/43/43/55	-
3	ATP	A	2802	-	-	8/18/38/38	0/3/3/3
6	PLX	D	2809	-	-	29/48/48/55	-
6	PLX	A	2813	-	-	21/41/41/55	-
6	PLX	A	2814	-	-	22/40/40/55	-
6	PLX	B	2813	-	-	25/42/42/55	-
4	I3P	B	2804	-	-	2/15/39/39	0/1/1/1
6	PLX	B	2811	-	-	14/40/40/55	-
6	PLX	C	2805	-	-	25/42/42/55	-
6	PLX	A	2809	-	-	29/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLX	C	2802	-	-	29/48/48/55	-
6	PLX	B	2809	-	-	19/43/43/55	-
6	PLX	D	2810	-	-	14/40/40/55	-
6	PLX	C	2804	-	-	23/39/39/55	-
6	PLX	D	2812	-	-	24/42/42/55	-
6	PLX	A	2810	-	-	14/40/40/55	-
6	PLX	C	2814	-	-	19/43/43/55	-
6	PLX	C	2813	-	-	22/40/40/55	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2804	PLX	O6-C4	-3.61	1.39	1.44
6	B	2809	PLX	O6-C4	-3.55	1.39	1.44
6	C	2814	PLX	O6-C4	-3.55	1.39	1.44
6	B	2812	PLX	O6-C4	-3.54	1.39	1.44
6	D	2809	PLX	O6-C4	-3.53	1.39	1.44
6	A	2809	PLX	O6-C4	-3.53	1.39	1.44
6	A	2811	PLX	O6-C4	-3.53	1.39	1.44
6	D	2811	PLX	O6-C4	-3.53	1.39	1.44
6	A	2808	PLX	O6-C4	-3.52	1.39	1.44
6	C	2802	PLX	O6-C4	-3.52	1.39	1.44
6	C	2803	PLX	O6-C4	-3.49	1.39	1.44
6	D	2810	PLX	O6-C4	-3.49	1.39	1.44
6	D	2802	PLX	O6-C4	-3.48	1.39	1.44
6	B	2814	PLX	O6-C4	-3.46	1.39	1.44
6	C	2806	PLX	O6-C4	-3.46	1.39	1.44
6	B	2810	PLX	O6-C4	-3.45	1.39	1.44
6	B	2811	PLX	O6-C4	-3.45	1.40	1.44
6	A	2812	PLX	O6-C4	-3.42	1.40	1.44
6	B	2813	PLX	O6-C4	-3.42	1.40	1.44
6	C	2805	PLX	O6-C4	-3.42	1.40	1.44
6	D	2812	PLX	O6-C4	-3.42	1.40	1.44
6	A	2810	PLX	O6-C4	-3.40	1.40	1.44
6	A	2813	PLX	O6-C4	-3.39	1.40	1.44
6	D	2813	PLX	O6-C4	-3.39	1.40	1.44
4	B	2804	I3P	P1-O1	3.10	1.65	1.59
4	D	2804	I3P	P1-O1	3.09	1.65	1.59
4	B	2804	I3P	P5-O5	3.08	1.65	1.59
4	C	2808	I3P	P5-O5	3.08	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2804	I3P	P5-O5	3.08	1.65	1.59
4	A	2803	I3P	P1-O1	3.07	1.65	1.59
4	C	2808	I3P	P1-O1	3.07	1.65	1.59
4	A	2803	I3P	P5-O5	3.07	1.65	1.59
4	B	2804	I3P	P4-O4	3.07	1.65	1.59
6	A	2814	PLX	O6-C4	-3.06	1.40	1.44
6	B	2802	PLX	O6-C4	-3.06	1.40	1.44
6	D	2814	PLX	O6-C4	-3.06	1.40	1.44
4	C	2808	I3P	P4-O4	3.06	1.65	1.59
4	A	2803	I3P	P4-O4	3.05	1.65	1.59
4	D	2804	I3P	P4-O4	3.03	1.65	1.59
6	C	2813	PLX	O6-C4	-2.96	1.40	1.44
6	B	2814	PLX	P1-O4	2.45	1.69	1.59
6	C	2806	PLX	P1-O4	2.45	1.69	1.59
6	A	2813	PLX	P1-O4	2.44	1.69	1.59
6	D	2813	PLX	P1-O4	2.44	1.69	1.59
6	C	2814	PLX	P1-O4	2.33	1.68	1.59
6	C	2804	PLX	P1-O4	2.33	1.68	1.59
6	A	2811	PLX	P1-O4	2.33	1.68	1.59
6	D	2811	PLX	P1-O4	2.33	1.68	1.59
6	A	2808	PLX	P1-O4	2.32	1.68	1.59
6	D	2802	PLX	P1-O4	2.32	1.68	1.59
6	A	2809	PLX	P1-O4	2.32	1.68	1.59
6	B	2810	PLX	P1-O4	2.32	1.68	1.59
6	C	2802	PLX	P1-O4	2.32	1.68	1.59
6	B	2812	PLX	P1-O4	2.32	1.68	1.59
6	D	2809	PLX	P1-O4	2.32	1.68	1.59
6	A	2810	PLX	P1-O4	2.31	1.68	1.59
6	B	2811	PLX	P1-O4	2.31	1.68	1.59
6	C	2803	PLX	P1-O4	2.31	1.68	1.59
6	D	2810	PLX	P1-O4	2.31	1.68	1.59
6	B	2809	PLX	P1-O4	2.31	1.68	1.59
6	A	2814	PLX	P1-O4	2.30	1.68	1.59
6	C	2813	PLX	P1-O4	2.30	1.68	1.59
6	D	2814	PLX	P1-O4	2.30	1.68	1.59
6	A	2812	PLX	P1-O4	2.29	1.68	1.59
6	B	2813	PLX	P1-O4	2.29	1.68	1.59
6	D	2812	PLX	P1-O4	2.29	1.68	1.59
6	C	2805	PLX	P1-O4	2.29	1.68	1.59
6	B	2802	PLX	P1-O4	2.27	1.68	1.59
6	A	2814	PLX	C7-C6	2.17	1.55	1.50
6	B	2802	PLX	C7-C6	2.17	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2814	PLX	C7-C6	2.17	1.55	1.50
6	C	2813	PLX	C7-C6	2.13	1.55	1.50
6	B	2809	PLX	C1A-N1	-2.09	1.43	1.50
6	A	2813	PLX	C1A-N1	-2.09	1.43	1.50
6	B	2814	PLX	C1A-N1	-2.09	1.43	1.50
6	C	2806	PLX	C1A-N1	-2.09	1.43	1.50
6	A	2812	PLX	C1A-N1	-2.09	1.43	1.50
6	C	2805	PLX	C1A-N1	-2.08	1.43	1.50
6	D	2812	PLX	C1A-N1	-2.08	1.43	1.50
6	B	2813	PLX	C1A-N1	-2.08	1.43	1.50
6	D	2802	PLX	C1A-N1	-2.08	1.43	1.50
6	C	2803	PLX	C1A-N1	-2.07	1.44	1.50
6	D	2813	PLX	C1A-N1	-2.07	1.44	1.50
6	D	2811	PLX	C1A-N1	-2.07	1.44	1.50
6	D	2812	PLX	C7-C6	2.07	1.55	1.50
6	A	2813	PLX	C7-C6	2.06	1.55	1.50
6	B	2810	PLX	C7-C6	2.06	1.55	1.50
6	D	2809	PLX	C7-C6	2.06	1.55	1.50
6	A	2808	PLX	C1A-N1	-2.05	1.44	1.50
6	C	2814	PLX	C1A-N1	-2.05	1.44	1.50
6	A	2814	PLX	C1A-N1	-2.05	1.44	1.50
6	B	2802	PLX	C1A-N1	-2.05	1.44	1.50
6	C	2813	PLX	C1A-N1	-2.05	1.44	1.50
6	D	2814	PLX	C1A-N1	-2.05	1.44	1.50
6	B	2813	PLX	C7-C6	2.05	1.55	1.50
6	B	2810	PLX	C1A-N1	-2.04	1.44	1.50
6	C	2802	PLX	C1A-N1	-2.04	1.44	1.50
6	D	2809	PLX	C1A-N1	-2.04	1.44	1.50
6	C	2803	PLX	C7-C6	2.03	1.55	1.50
6	A	2811	PLX	C1A-N1	-2.03	1.44	1.50
6	B	2812	PLX	C1A-N1	-2.03	1.44	1.50
6	A	2809	PLX	C1A-N1	-2.03	1.44	1.50
6	C	2804	PLX	C1A-N1	-2.03	1.44	1.50
6	B	2811	PLX	C1A-N1	-2.03	1.44	1.50
6	D	2810	PLX	C7-C6	2.03	1.55	1.50
6	B	2811	PLX	P1-O1	2.03	1.67	1.59
6	A	2813	PLX	P1-O1	2.03	1.67	1.59
6	B	2814	PLX	P1-O1	2.03	1.67	1.59
6	C	2806	PLX	P1-O1	2.03	1.67	1.59
6	A	2811	PLX	C7-C6	2.03	1.55	1.50
6	D	2811	PLX	C7-C6	2.03	1.55	1.50
6	A	2810	PLX	C1A-N1	-2.02	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2814	PLX	C7-C6	2.02	1.55	1.50
6	C	2806	PLX	C7-C6	2.02	1.55	1.50
6	D	2813	PLX	C7-C6	2.02	1.55	1.50
6	D	2813	PLX	P1-O1	2.02	1.67	1.59
6	A	2809	PLX	C7-C6	2.02	1.55	1.50
6	C	2802	PLX	C7-C6	2.02	1.55	1.50
6	D	2809	PLX	P1-O1	2.01	1.67	1.59
6	D	2810	PLX	C1A-N1	-2.01	1.44	1.50
6	A	2810	PLX	P1-O1	2.01	1.67	1.59
6	C	2803	PLX	P1-O1	2.01	1.67	1.59
6	D	2810	PLX	P1-O1	2.01	1.67	1.59
6	A	2812	PLX	C7-C6	2.00	1.55	1.50
6	C	2805	PLX	C7-C6	2.00	1.55	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2802	ATP	C5-C6-N6	2.34	123.91	120.35
3	C	2807	ATP	C5-C6-N6	2.32	123.88	120.35
3	D	2803	ATP	C5-C6-N6	2.29	123.83	120.35
3	B	2803	ATP	C5-C6-N6	2.29	123.83	120.35
6	B	2811	PLX	C8-C7-C6	-2.20	108.30	113.38
6	C	2803	PLX	C8-C7-C6	-2.19	108.31	113.38
6	D	2810	PLX	C8-C7-C6	-2.18	108.35	113.38
6	A	2810	PLX	C8-C7-C6	-2.16	108.38	113.38
4	A	2803	I3P	C5-C6-C1	2.07	113.25	108.96
4	D	2804	I3P	C5-C6-C1	2.07	113.25	108.96
4	B	2804	I3P	C5-C6-C1	2.05	113.22	108.96
4	C	2808	I3P	C5-C6-C1	2.04	113.19	108.96
6	A	2814	PLX	C26-C25-C24	-2.02	108.70	113.38
3	A	2802	ATP	PB-O3B-PG	2.02	139.76	132.83
3	C	2807	ATP	PB-O3B-PG	2.02	139.76	132.83
3	D	2803	ATP	PB-O3B-PG	2.02	139.76	132.83
6	C	2813	PLX	C26-C25-C24	-2.02	108.71	113.38
6	D	2814	PLX	C26-C25-C24	-2.01	108.72	113.38
3	B	2803	ATP	PB-O3B-PG	2.01	139.73	132.83
6	B	2802	PLX	C26-C25-C24	-2.00	108.75	113.38

There are no chirality outliers.

All (650) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2802	ATP	C5'-O5'-PA-O1A
3	A	2802	ATP	C5'-O5'-PA-O2A
3	A	2802	ATP	O4'-C4'-C5'-O5'
3	B	2803	ATP	C5'-O5'-PA-O1A
3	B	2803	ATP	C5'-O5'-PA-O2A
3	B	2803	ATP	O4'-C4'-C5'-O5'
3	C	2807	ATP	C5'-O5'-PA-O1A
3	C	2807	ATP	C5'-O5'-PA-O2A
3	C	2807	ATP	O4'-C4'-C5'-O5'
3	D	2803	ATP	C5'-O5'-PA-O1A
3	D	2803	ATP	C5'-O5'-PA-O2A
3	D	2803	ATP	O4'-C4'-C5'-O5'
6	A	2808	PLX	O7-C6-O6-C4
6	A	2808	PLX	C3-O4-P1-O1
6	A	2808	PLX	C3-O4-P1-O2
6	A	2808	PLX	C3-O4-P1-O3
6	A	2808	PLX	C2-O1-P1-O4
6	A	2808	PLX	C2-O1-P1-O2
6	A	2808	PLX	C2-O1-P1-O3
6	A	2809	PLX	O7-C6-C7-C8
6	A	2809	PLX	O7-C6-O6-C4
6	A	2809	PLX	C2-O1-P1-O2
6	A	2809	PLX	N1-C1-C2-O1
6	A	2809	PLX	O9-C24-O8-C5
6	A	2810	PLX	O7-C6-O6-C4
6	A	2810	PLX	C3-O4-P1-O3
6	A	2810	PLX	N1-C1-C2-O1
6	A	2810	PLX	O9-C24-O8-C5
6	A	2810	PLX	O9-C24-C25-C26
6	A	2811	PLX	O7-C6-C7-C8
6	A	2811	PLX	C3-O4-P1-O2
6	A	2811	PLX	C3-O4-P1-O3
6	A	2811	PLX	C2-O1-P1-O2
6	A	2811	PLX	C2-O1-P1-O3
6	A	2811	PLX	N1-C1-C2-O1
6	A	2812	PLX	O7-C6-C7-C8
6	A	2812	PLX	O7-C6-O6-C4
6	A	2812	PLX	O6-C4-C5-O8
6	A	2812	PLX	C3-O4-P1-O1
6	A	2812	PLX	C3-O4-P1-O2
6	A	2812	PLX	C3-O4-P1-O3
6	A	2812	PLX	O9-C24-C25-C26
6	A	2813	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	A	2813	PLX	O7-C6-O6-C4
6	A	2813	PLX	C4-C3-O4-P1
6	A	2813	PLX	O9-C24-O8-C5
6	A	2814	PLX	O7-C6-C7-C8
6	A	2814	PLX	O6-C6-C7-C8
6	A	2814	PLX	O7-C6-O6-C4
6	A	2814	PLX	C3-C4-O6-C6
6	A	2814	PLX	C3-O4-P1-O2
6	A	2814	PLX	C3-O4-P1-O3
6	A	2814	PLX	C4-C5-O8-C24
6	A	2814	PLX	C25-C24-O8-C5
6	B	2802	PLX	O7-C6-C7-C8
6	B	2802	PLX	O6-C6-C7-C8
6	B	2802	PLX	O7-C6-O6-C4
6	B	2802	PLX	C3-C4-O6-C6
6	B	2802	PLX	C3-O4-P1-O2
6	B	2802	PLX	C3-O4-P1-O3
6	B	2802	PLX	C4-C5-O8-C24
6	B	2802	PLX	C25-C24-O8-C5
6	B	2809	PLX	O7-C6-O6-C4
6	B	2809	PLX	C3-O4-P1-O1
6	B	2809	PLX	C3-O4-P1-O2
6	B	2809	PLX	C3-O4-P1-O3
6	B	2809	PLX	C2-O1-P1-O4
6	B	2809	PLX	C2-O1-P1-O2
6	B	2809	PLX	C2-O1-P1-O3
6	B	2810	PLX	O7-C6-C7-C8
6	B	2810	PLX	O7-C6-O6-C4
6	B	2810	PLX	C2-O1-P1-O2
6	B	2810	PLX	N1-C1-C2-O1
6	B	2810	PLX	O9-C24-O8-C5
6	B	2811	PLX	O7-C6-O6-C4
6	B	2811	PLX	C3-O4-P1-O3
6	B	2811	PLX	N1-C1-C2-O1
6	B	2811	PLX	O9-C24-O8-C5
6	B	2811	PLX	O9-C24-C25-C26
6	B	2812	PLX	O7-C6-C7-C8
6	B	2812	PLX	C3-O4-P1-O2
6	B	2812	PLX	C3-O4-P1-O3
6	B	2812	PLX	C2-O1-P1-O2
6	B	2812	PLX	C2-O1-P1-O3
6	B	2812	PLX	N1-C1-C2-O1

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Mol	Chain	Res	Type	Atoms
6	B	2813	PLX	O7-C6-C7-C8
6	B	2813	PLX	O7-C6-O6-C4
6	B	2813	PLX	O6-C4-C5-O8
6	B	2813	PLX	C3-O4-P1-O1
6	B	2813	PLX	C3-O4-P1-O2
6	B	2813	PLX	C3-O4-P1-O3
6	B	2813	PLX	O9-C24-C25-C26
6	B	2814	PLX	O7-C6-C7-C8
6	B	2814	PLX	O7-C6-O6-C4
6	B	2814	PLX	C4-C3-O4-P1
6	B	2814	PLX	O9-C24-O8-C5
6	C	2802	PLX	O7-C6-C7-C8
6	C	2802	PLX	O7-C6-O6-C4
6	C	2802	PLX	C2-O1-P1-O2
6	C	2802	PLX	N1-C1-C2-O1
6	C	2802	PLX	O9-C24-O8-C5
6	C	2803	PLX	O7-C6-O6-C4
6	C	2803	PLX	C3-O4-P1-O3
6	C	2803	PLX	N1-C1-C2-O1
6	C	2803	PLX	O9-C24-O8-C5
6	C	2803	PLX	O9-C24-C25-C26
6	C	2804	PLX	O7-C6-C7-C8
6	C	2804	PLX	C3-O4-P1-O2
6	C	2804	PLX	C3-O4-P1-O3
6	C	2804	PLX	C2-O1-P1-O2
6	C	2804	PLX	C2-O1-P1-O3
6	C	2804	PLX	N1-C1-C2-O1
6	C	2805	PLX	O7-C6-C7-C8
6	C	2805	PLX	O7-C6-O6-C4
6	C	2805	PLX	O6-C4-C5-O8
6	C	2805	PLX	C3-O4-P1-O1
6	C	2805	PLX	C3-O4-P1-O2
6	C	2805	PLX	C3-O4-P1-O3
6	C	2805	PLX	O9-C24-C25-C26
6	C	2806	PLX	O7-C6-C7-C8
6	C	2806	PLX	O7-C6-O6-C4
6	C	2806	PLX	C4-C3-O4-P1
6	C	2806	PLX	O9-C24-O8-C5
6	C	2813	PLX	O7-C6-C7-C8
6	C	2813	PLX	O6-C6-C7-C8
6	C	2813	PLX	O7-C6-O6-C4
6	C	2813	PLX	C3-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
6	C	2813	PLX	C3-O4-P1-O2
6	C	2813	PLX	C3-O4-P1-O3
6	C	2813	PLX	C4-C5-O8-C24
6	C	2813	PLX	C25-C24-O8-C5
6	C	2814	PLX	O7-C6-O6-C4
6	C	2814	PLX	C3-O4-P1-O1
6	C	2814	PLX	C3-O4-P1-O2
6	C	2814	PLX	C3-O4-P1-O3
6	C	2814	PLX	C2-O1-P1-O4
6	C	2814	PLX	C2-O1-P1-O2
6	C	2814	PLX	C2-O1-P1-O3
6	D	2802	PLX	O7-C6-O6-C4
6	D	2802	PLX	C3-O4-P1-O1
6	D	2802	PLX	C3-O4-P1-O2
6	D	2802	PLX	C3-O4-P1-O3
6	D	2802	PLX	C2-O1-P1-O4
6	D	2802	PLX	C2-O1-P1-O2
6	D	2802	PLX	C2-O1-P1-O3
6	D	2809	PLX	O7-C6-C7-C8
6	D	2809	PLX	O7-C6-O6-C4
6	D	2809	PLX	C2-O1-P1-O2
6	D	2809	PLX	N1-C1-C2-O1
6	D	2809	PLX	O9-C24-O8-C5
6	D	2810	PLX	O7-C6-O6-C4
6	D	2810	PLX	C3-O4-P1-O3
6	D	2810	PLX	N1-C1-C2-O1
6	D	2810	PLX	O9-C24-O8-C5
6	D	2810	PLX	O9-C24-C25-C26
6	D	2811	PLX	O7-C6-C7-C8
6	D	2811	PLX	C3-O4-P1-O2
6	D	2811	PLX	C3-O4-P1-O3
6	D	2811	PLX	C2-O1-P1-O2
6	D	2811	PLX	C2-O1-P1-O3
6	D	2811	PLX	N1-C1-C2-O1
6	D	2812	PLX	O7-C6-C7-C8
6	D	2812	PLX	O7-C6-O6-C4
6	D	2812	PLX	O6-C4-C5-O8
6	D	2812	PLX	C3-O4-P1-O1
6	D	2812	PLX	C3-O4-P1-O2
6	D	2812	PLX	C3-O4-P1-O3
6	D	2812	PLX	O9-C24-C25-C26
6	D	2813	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	D	2813	PLX	O7-C6-O6-C4
6	D	2813	PLX	C4-C3-O4-P1
6	D	2813	PLX	O9-C24-O8-C5
6	D	2814	PLX	O7-C6-C7-C8
6	D	2814	PLX	O6-C6-C7-C8
6	D	2814	PLX	O7-C6-O6-C4
6	D	2814	PLX	C3-C4-O6-C6
6	D	2814	PLX	C3-O4-P1-O2
6	D	2814	PLX	C3-O4-P1-O3
6	D	2814	PLX	C4-C5-O8-C24
6	D	2814	PLX	C25-C24-O8-C5
3	A	2802	ATP	C3'-C4'-C5'-O5'
3	B	2803	ATP	C3'-C4'-C5'-O5'
3	C	2807	ATP	C3'-C4'-C5'-O5'
3	D	2803	ATP	C3'-C4'-C5'-O5'
6	C	2813	PLX	C28-C29-C30-C31
6	A	2814	PLX	C28-C29-C30-C31
6	B	2802	PLX	C28-C29-C30-C31
6	D	2814	PLX	C28-C29-C30-C31
6	A	2809	PLX	C3-O4-P1-O1
6	A	2809	PLX	C2-O1-P1-O4
6	A	2810	PLX	C3-O4-P1-O1
6	A	2811	PLX	C3-O4-P1-O1
6	A	2811	PLX	C2-O1-P1-O4
6	A	2812	PLX	C2-O1-P1-O4
6	A	2813	PLX	C3-O4-P1-O1
6	A	2813	PLX	C2-O1-P1-O4
6	A	2814	PLX	C3-O4-P1-O1
6	B	2802	PLX	C3-O4-P1-O1
6	B	2810	PLX	C3-O4-P1-O1
6	B	2810	PLX	C2-O1-P1-O4
6	B	2811	PLX	C3-O4-P1-O1
6	B	2812	PLX	C3-O4-P1-O1
6	B	2812	PLX	C2-O1-P1-O4
6	B	2813	PLX	C2-O1-P1-O4
6	B	2814	PLX	C3-O4-P1-O1
6	B	2814	PLX	C2-O1-P1-O4
6	C	2802	PLX	C3-O4-P1-O1
6	C	2802	PLX	C2-O1-P1-O4
6	C	2803	PLX	C3-O4-P1-O1
6	C	2804	PLX	C3-O4-P1-O1
6	C	2804	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
6	C	2805	PLX	C2-O1-P1-O4
6	C	2806	PLX	C3-O4-P1-O1
6	C	2806	PLX	C2-O1-P1-O4
6	C	2813	PLX	C3-O4-P1-O1
6	D	2809	PLX	C3-O4-P1-O1
6	D	2809	PLX	C2-O1-P1-O4
6	D	2810	PLX	C3-O4-P1-O1
6	D	2811	PLX	C3-O4-P1-O1
6	D	2811	PLX	C2-O1-P1-O4
6	D	2812	PLX	C2-O1-P1-O4
6	D	2813	PLX	C3-O4-P1-O1
6	D	2813	PLX	C2-O1-P1-O4
6	D	2814	PLX	C3-O4-P1-O1
6	A	2809	PLX	O8-C24-C25-C26
6	A	2812	PLX	O8-C24-C25-C26
6	A	2813	PLX	O8-C24-C25-C26
6	B	2810	PLX	O8-C24-C25-C26
6	B	2813	PLX	O8-C24-C25-C26
6	B	2814	PLX	O8-C24-C25-C26
6	C	2802	PLX	O8-C24-C25-C26
6	C	2805	PLX	O8-C24-C25-C26
6	C	2806	PLX	O8-C24-C25-C26
6	D	2809	PLX	O6-C6-C7-C8
6	D	2809	PLX	O8-C24-C25-C26
6	D	2812	PLX	O8-C24-C25-C26
6	D	2813	PLX	O8-C24-C25-C26
6	A	2810	PLX	C11-C10-C9-C8
6	B	2811	PLX	C11-C10-C9-C8
6	C	2803	PLX	C11-C10-C9-C8
6	D	2810	PLX	C11-C10-C9-C8
6	A	2809	PLX	C12-C13-C14-C15
6	A	2814	PLX	C25-C26-C27-C28
6	B	2802	PLX	C25-C26-C27-C28
6	B	2810	PLX	C12-C13-C14-C15
6	C	2802	PLX	C12-C13-C14-C15
6	C	2813	PLX	C25-C26-C27-C28
6	D	2809	PLX	C12-C13-C14-C15
6	D	2814	PLX	C25-C26-C27-C28
6	A	2808	PLX	C30-C31-C32-C33
6	A	2811	PLX	C27-C28-C29-C30
6	B	2809	PLX	C30-C31-C32-C33
6	B	2812	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
6	C	2804	PLX	C27-C28-C29-C30
6	C	2814	PLX	C30-C31-C32-C33
6	D	2802	PLX	C30-C31-C32-C33
6	D	2811	PLX	C27-C28-C29-C30
6	A	2808	PLX	C28-C29-C30-C31
6	B	2809	PLX	C28-C29-C30-C31
6	C	2814	PLX	C28-C29-C30-C31
6	D	2802	PLX	C28-C29-C30-C31
6	A	2812	PLX	C11-C10-C9-C8
6	B	2813	PLX	C11-C10-C9-C8
6	C	2805	PLX	C11-C10-C9-C8
6	D	2812	PLX	C11-C10-C9-C8
6	A	2810	PLX	C27-C28-C29-C30
6	B	2811	PLX	C27-C28-C29-C30
6	C	2803	PLX	C27-C28-C29-C30
6	D	2810	PLX	C27-C28-C29-C30
6	A	2811	PLX	C28-C29-C30-C31
6	B	2812	PLX	C28-C29-C30-C31
6	D	2811	PLX	C28-C29-C30-C31
6	C	2804	PLX	C28-C29-C30-C31
6	C	2802	PLX	C26-C27-C28-C29
6	A	2811	PLX	O9-C24-C25-C26
6	A	2813	PLX	O9-C24-C25-C26
6	A	2814	PLX	O9-C24-C25-C26
6	B	2802	PLX	O9-C24-C25-C26
6	B	2812	PLX	O9-C24-C25-C26
6	B	2814	PLX	O9-C24-C25-C26
6	C	2804	PLX	O9-C24-C25-C26
6	C	2806	PLX	O9-C24-C25-C26
6	C	2813	PLX	O9-C24-C25-C26
6	D	2811	PLX	O9-C24-C25-C26
6	D	2813	PLX	O9-C24-C25-C26
6	D	2814	PLX	O9-C24-C25-C26
6	A	2809	PLX	C26-C27-C28-C29
6	A	2811	PLX	C29-C30-C31-C32
6	A	2812	PLX	C10-C11-C12-C13
6	B	2810	PLX	C26-C27-C28-C29
6	B	2812	PLX	C29-C30-C31-C32
6	B	2813	PLX	C10-C11-C12-C13
6	C	2804	PLX	C29-C30-C31-C32
6	C	2805	PLX	C10-C11-C12-C13
6	D	2809	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	D	2812	PLX	C10-C11-C12-C13
6	D	2811	PLX	C29-C30-C31-C32
6	D	2809	PLX	C11-C12-C13-C14
6	A	2809	PLX	C11-C12-C13-C14
6	B	2810	PLX	C11-C12-C13-C14
6	C	2802	PLX	C11-C12-C13-C14
6	B	2802	PLX	C11-C10-C9-C8
6	C	2813	PLX	C11-C10-C9-C8
6	A	2814	PLX	C11-C10-C9-C8
6	D	2814	PLX	C11-C10-C9-C8
6	A	2811	PLX	C26-C27-C28-C29
6	B	2812	PLX	C26-C27-C28-C29
6	C	2804	PLX	C26-C27-C28-C29
6	D	2811	PLX	C26-C27-C28-C29
6	A	2814	PLX	C10-C11-C12-C13
6	B	2802	PLX	C10-C11-C12-C13
6	C	2813	PLX	C10-C11-C12-C13
6	D	2814	PLX	C10-C11-C12-C13
6	A	2808	PLX	C11-C10-C9-C8
6	A	2809	PLX	C28-C29-C30-C31
6	B	2809	PLX	C11-C10-C9-C8
6	B	2810	PLX	C28-C29-C30-C31
6	D	2802	PLX	C11-C10-C9-C8
6	D	2809	PLX	C28-C29-C30-C31
6	C	2802	PLX	C28-C29-C30-C31
6	C	2814	PLX	C11-C10-C9-C8
6	A	2813	PLX	C10-C11-C12-C13
6	B	2814	PLX	C10-C11-C12-C13
6	C	2806	PLX	C10-C11-C12-C13
6	D	2813	PLX	C10-C11-C12-C13
6	A	2809	PLX	C30-C31-C32-C33
6	B	2810	PLX	C25-C26-C27-C28
6	B	2810	PLX	C30-C31-C32-C33
6	C	2802	PLX	C25-C26-C27-C28
6	C	2802	PLX	C30-C31-C32-C33
6	D	2809	PLX	C30-C31-C32-C33
6	A	2809	PLX	C25-C26-C27-C28
6	D	2809	PLX	C25-C26-C27-C28
6	C	2806	PLX	C25-C26-C27-C28
6	A	2813	PLX	C25-C26-C27-C28
6	A	2814	PLX	C3-C4-C5-O8
6	B	2802	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
6	B	2814	PLX	C25-C26-C27-C28
6	C	2813	PLX	C3-C4-C5-O8
6	D	2813	PLX	C25-C26-C27-C28
6	D	2814	PLX	C3-C4-C5-O8
6	A	2814	PLX	C30-C31-C32-C33
6	B	2802	PLX	C30-C31-C32-C33
6	C	2806	PLX	C30-C31-C32-C33
6	C	2813	PLX	C30-C31-C32-C33
6	D	2814	PLX	C30-C31-C32-C33
6	A	2808	PLX	C10-C11-C12-C13
6	A	2813	PLX	C30-C31-C32-C33
6	B	2810	PLX	C11-C10-C9-C8
6	B	2814	PLX	C30-C31-C32-C33
6	C	2802	PLX	C11-C10-C9-C8
6	D	2813	PLX	C30-C31-C32-C33
6	A	2809	PLX	C11-C10-C9-C8
6	B	2809	PLX	C10-C11-C12-C13
6	C	2814	PLX	C10-C11-C12-C13
6	D	2802	PLX	C10-C11-C12-C13
6	D	2809	PLX	C11-C10-C9-C8
6	A	2809	PLX	O6-C6-C7-C8
6	A	2814	PLX	O8-C24-C25-C26
6	B	2802	PLX	O8-C24-C25-C26
6	B	2810	PLX	O6-C6-C7-C8
6	C	2802	PLX	O6-C6-C7-C8
6	C	2813	PLX	O8-C24-C25-C26
6	D	2814	PLX	O8-C24-C25-C26
6	A	2808	PLX	C9-C10-C11-C12
6	B	2809	PLX	C9-C10-C11-C12
6	C	2814	PLX	C9-C10-C11-C12
6	D	2802	PLX	C9-C10-C11-C12
6	A	2809	PLX	C10-C11-C12-C13
6	B	2810	PLX	C10-C11-C12-C13
6	C	2802	PLX	C10-C11-C12-C13
6	D	2809	PLX	C10-C11-C12-C13
6	A	2810	PLX	C30-C31-C32-C33
6	B	2811	PLX	C30-C31-C32-C33
6	C	2803	PLX	C30-C31-C32-C33
6	D	2810	PLX	C30-C31-C32-C33
6	A	2812	PLX	C7-C8-C9-C10
6	B	2813	PLX	C7-C8-C9-C10
6	C	2805	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	D	2812	PLX	C7-C8-C9-C10
6	A	2812	PLX	C29-C30-C31-C32
6	C	2805	PLX	C29-C30-C31-C32
6	D	2812	PLX	C29-C30-C31-C32
6	B	2813	PLX	C29-C30-C31-C32
6	A	2808	PLX	O4-C3-C4-C5
6	A	2813	PLX	O4-C3-C4-C5
6	B	2809	PLX	O4-C3-C4-C5
6	B	2814	PLX	O4-C3-C4-C5
6	C	2806	PLX	O4-C3-C4-C5
6	C	2814	PLX	O4-C3-C4-C5
6	D	2802	PLX	O4-C3-C4-C5
6	D	2813	PLX	O4-C3-C4-C5
6	A	2811	PLX	C3-C4-C5-O8
6	B	2812	PLX	C3-C4-C5-O8
6	C	2804	PLX	C3-C4-C5-O8
6	D	2811	PLX	C3-C4-C5-O8
6	A	2811	PLX	C3-C4-O6-C6
6	B	2812	PLX	C3-C4-O6-C6
6	C	2804	PLX	C3-C4-O6-C6
6	D	2811	PLX	C3-C4-O6-C6
6	A	2809	PLX	O9-C24-C25-C26
6	B	2810	PLX	O9-C24-C25-C26
6	C	2802	PLX	O9-C24-C25-C26
6	D	2809	PLX	O9-C24-C25-C26
6	A	2809	PLX	O4-C3-C4-O6
6	A	2812	PLX	O4-C3-C4-O6
6	B	2810	PLX	O4-C3-C4-O6
6	B	2813	PLX	O4-C3-C4-O6
6	C	2802	PLX	O4-C3-C4-O6
6	C	2805	PLX	O4-C3-C4-O6
6	D	2809	PLX	O4-C3-C4-O6
6	D	2812	PLX	O4-C3-C4-O6
6	B	2812	PLX	C25-C26-C27-C28
6	C	2804	PLX	C25-C26-C27-C28
6	D	2811	PLX	C25-C26-C27-C28
6	A	2811	PLX	C25-C26-C27-C28
6	A	2814	PLX	O6-C4-C5-O8
6	B	2802	PLX	O6-C4-C5-O8
6	C	2813	PLX	O6-C4-C5-O8
6	D	2814	PLX	O6-C4-C5-O8
6	A	2809	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
6	B	2810	PLX	C27-C28-C29-C30
6	D	2809	PLX	C27-C28-C29-C30
6	C	2802	PLX	C27-C28-C29-C30
6	A	2809	PLX	C35-C36-C37-C38
6	B	2810	PLX	C35-C36-C37-C38
6	C	2802	PLX	C35-C36-C37-C38
6	A	2811	PLX	C4-C3-O4-P1
6	B	2812	PLX	C4-C3-O4-P1
6	C	2804	PLX	C4-C3-O4-P1
6	D	2811	PLX	C4-C3-O4-P1
6	D	2809	PLX	C33-C34-C35-C36
6	D	2809	PLX	C35-C36-C37-C38
6	A	2809	PLX	C33-C34-C35-C36
6	B	2810	PLX	C33-C34-C35-C36
6	C	2802	PLX	C33-C34-C35-C36
6	A	2808	PLX	C25-C26-C27-C28
6	B	2809	PLX	C25-C26-C27-C28
6	C	2814	PLX	C25-C26-C27-C28
6	D	2802	PLX	C25-C26-C27-C28
6	A	2811	PLX	O6-C6-C7-C8
6	B	2812	PLX	O6-C6-C7-C8
6	C	2804	PLX	O6-C6-C7-C8
6	D	2811	PLX	O6-C6-C7-C8
6	B	2814	PLX	C7-C8-C9-C10
6	D	2813	PLX	C7-C8-C9-C10
6	A	2813	PLX	C7-C8-C9-C10
6	C	2806	PLX	C7-C8-C9-C10
6	A	2812	PLX	C3-C4-C5-O8
6	A	2812	PLX	C4-C3-O4-P1
6	B	2813	PLX	C3-C4-C5-O8
6	B	2813	PLX	C4-C3-O4-P1
6	C	2805	PLX	C3-C4-C5-O8
6	C	2805	PLX	C4-C3-O4-P1
6	D	2812	PLX	C3-C4-C5-O8
6	D	2812	PLX	C4-C3-O4-P1
6	A	2808	PLX	O4-C3-C4-O6
6	B	2809	PLX	O4-C3-C4-O6
6	C	2814	PLX	O4-C3-C4-O6
6	D	2802	PLX	O4-C3-C4-O6
6	A	2811	PLX	O6-C4-C5-O8
6	B	2812	PLX	O6-C4-C5-O8
6	C	2804	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
6	D	2811	PLX	O6-C4-C5-O8
6	A	2809	PLX	C24-C25-C26-C27
6	B	2810	PLX	C24-C25-C26-C27
6	C	2802	PLX	C24-C25-C26-C27
6	D	2809	PLX	C24-C25-C26-C27
3	A	2802	ATP	PG-O3B-PB-O2B
3	B	2803	ATP	PG-O3B-PB-O2B
3	C	2807	ATP	PG-O3B-PB-O2B
3	D	2803	ATP	PG-O3B-PB-O2B
6	A	2809	PLX	C3-O4-P1-O2
6	A	2809	PLX	C3-O4-P1-O3
6	A	2812	PLX	C2-O1-P1-O3
6	A	2813	PLX	C3-O4-P1-O3
6	A	2813	PLX	C2-O1-P1-O2
6	A	2813	PLX	C2-O1-P1-O3
6	B	2810	PLX	C3-O4-P1-O2
6	B	2810	PLX	C3-O4-P1-O3
6	B	2813	PLX	C2-O1-P1-O3
6	B	2814	PLX	C3-O4-P1-O3
6	B	2814	PLX	C2-O1-P1-O2
6	B	2814	PLX	C2-O1-P1-O3
6	C	2802	PLX	C3-O4-P1-O2
6	C	2802	PLX	C3-O4-P1-O3
6	C	2805	PLX	C2-O1-P1-O3
6	C	2806	PLX	C3-O4-P1-O3
6	C	2806	PLX	C2-O1-P1-O2
6	C	2806	PLX	C2-O1-P1-O3
6	D	2809	PLX	C3-O4-P1-O2
6	D	2809	PLX	C3-O4-P1-O3
6	D	2812	PLX	C2-O1-P1-O3
6	D	2813	PLX	C3-O4-P1-O3
6	D	2813	PLX	C2-O1-P1-O2
6	D	2813	PLX	C2-O1-P1-O3
6	A	2809	PLX	O4-C3-C4-C5
6	B	2810	PLX	O4-C3-C4-C5
6	C	2802	PLX	O4-C3-C4-C5
6	D	2809	PLX	O4-C3-C4-C5
6	A	2811	PLX	C25-C24-O8-C5
6	A	2812	PLX	C25-C24-O8-C5
6	B	2812	PLX	C25-C24-O8-C5
6	B	2813	PLX	C25-C24-O8-C5
6	C	2804	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
6	C	2805	PLX	C25-C24-O8-C5
6	D	2811	PLX	C25-C24-O8-C5
6	D	2812	PLX	C25-C24-O8-C5
6	A	2814	PLX	C6-C7-C8-C9
6	B	2802	PLX	C6-C7-C8-C9
6	C	2813	PLX	C6-C7-C8-C9
6	D	2814	PLX	C6-C7-C8-C9
6	A	2813	PLX	O4-C3-C4-O6
6	B	2814	PLX	O4-C3-C4-O6
6	C	2806	PLX	O4-C3-C4-O6
6	D	2813	PLX	O4-C3-C4-O6
6	B	2812	PLX	C30-C31-C32-C33
6	C	2804	PLX	C30-C31-C32-C33
6	D	2811	PLX	C30-C31-C32-C33
6	A	2811	PLX	C30-C31-C32-C33
6	A	2808	PLX	N1-C1-C2-O1
6	A	2812	PLX	N1-C1-C2-O1
6	B	2809	PLX	N1-C1-C2-O1
6	B	2813	PLX	N1-C1-C2-O1
6	C	2805	PLX	N1-C1-C2-O1
6	C	2814	PLX	N1-C1-C2-O1
6	D	2802	PLX	N1-C1-C2-O1
6	D	2812	PLX	N1-C1-C2-O1
6	A	2810	PLX	O8-C24-C25-C26
6	A	2813	PLX	O6-C6-C7-C8
6	B	2811	PLX	O8-C24-C25-C26
6	B	2814	PLX	O6-C6-C7-C8
6	C	2803	PLX	O8-C24-C25-C26
6	C	2806	PLX	O6-C6-C7-C8
6	D	2810	PLX	O8-C24-C25-C26
6	D	2813	PLX	O6-C6-C7-C8
6	A	2808	PLX	O9-C24-C25-C26
6	B	2809	PLX	O9-C24-C25-C26
6	C	2814	PLX	O9-C24-C25-C26
6	D	2802	PLX	O9-C24-C25-C26
6	A	2812	PLX	C27-C28-C29-C30
6	D	2812	PLX	C27-C28-C29-C30
6	B	2813	PLX	C27-C28-C29-C30
6	C	2802	PLX	C13-C14-C15-C16
6	D	2809	PLX	C13-C14-C15-C16
6	A	2809	PLX	C13-C14-C15-C16
6	C	2805	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
6	B	2810	PLX	C13-C14-C15-C16
6	B	2814	PLX	C27-C28-C29-C30
6	C	2806	PLX	C27-C28-C29-C30
6	D	2813	PLX	C27-C28-C29-C30
6	A	2813	PLX	C27-C28-C29-C30
6	C	2805	PLX	C28-C29-C30-C31
6	D	2812	PLX	C28-C29-C30-C31
6	A	2812	PLX	C28-C29-C30-C31
6	B	2813	PLX	C28-C29-C30-C31
6	A	2810	PLX	C29-C30-C31-C32
6	B	2811	PLX	C29-C30-C31-C32
6	C	2803	PLX	C29-C30-C31-C32
6	D	2810	PLX	C29-C30-C31-C32
6	A	2811	PLX	C24-C25-C26-C27
6	B	2812	PLX	C24-C25-C26-C27
6	C	2804	PLX	C24-C25-C26-C27
6	D	2811	PLX	C24-C25-C26-C27
6	D	2810	PLX	C28-C29-C30-C31
6	A	2810	PLX	C28-C29-C30-C31
6	B	2811	PLX	C28-C29-C30-C31
6	C	2803	PLX	C28-C29-C30-C31
6	A	2813	PLX	C6-C7-C8-C9
6	B	2814	PLX	C6-C7-C8-C9
6	C	2806	PLX	C6-C7-C8-C9
6	D	2813	PLX	C6-C7-C8-C9
6	A	2812	PLX	O6-C6-C7-C8
6	B	2813	PLX	O6-C6-C7-C8
6	C	2805	PLX	O6-C6-C7-C8
6	D	2812	PLX	O6-C6-C7-C8
6	A	2808	PLX	C29-C30-C31-C32
6	C	2814	PLX	C29-C30-C31-C32
6	D	2802	PLX	C29-C30-C31-C32
6	B	2809	PLX	C29-C30-C31-C32
6	A	2809	PLX	C5-C4-O6-C6
6	A	2812	PLX	C5-C4-O6-C6
6	A	2814	PLX	C5-C4-O6-C6
6	B	2802	PLX	C5-C4-O6-C6
6	B	2810	PLX	C5-C4-O6-C6
6	B	2813	PLX	C5-C4-O6-C6
6	C	2802	PLX	C5-C4-O6-C6
6	C	2805	PLX	C5-C4-O6-C6
6	C	2813	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
6	D	2809	PLX	C5-C4-O6-C6
6	D	2812	PLX	C5-C4-O6-C6
6	D	2814	PLX	C5-C4-O6-C6
6	A	2813	PLX	C24-C25-C26-C27
6	B	2814	PLX	C24-C25-C26-C27
6	C	2806	PLX	C24-C25-C26-C27
6	D	2813	PLX	C24-C25-C26-C27
6	A	2812	PLX	O4-C3-C4-C5
6	B	2813	PLX	O4-C3-C4-C5
6	C	2805	PLX	O4-C3-C4-C5
6	D	2812	PLX	O4-C3-C4-C5
3	A	2802	ATP	C4'-C5'-O5'-PA
3	B	2803	ATP	C4'-C5'-O5'-PA
3	D	2803	ATP	C4'-C5'-O5'-PA
6	C	2814	PLX	C24-C25-C26-C27
6	D	2802	PLX	C24-C25-C26-C27
4	A	2803	I3P	C1-O1-P1-O11
4	B	2804	I3P	C1-O1-P1-O11
4	C	2808	I3P	C1-O1-P1-O11
4	D	2804	I3P	C1-O1-P1-O11
6	B	2810	PLX	C31-C32-C33-C34
6	C	2802	PLX	C31-C32-C33-C34
6	D	2809	PLX	C31-C32-C33-C34
6	A	2808	PLX	C24-C25-C26-C27
6	B	2809	PLX	C24-C25-C26-C27
6	A	2809	PLX	C31-C32-C33-C34
3	C	2807	ATP	C4'-C5'-O5'-PA
6	C	2813	PLX	C26-C27-C28-C29
6	D	2814	PLX	C26-C27-C28-C29
6	B	2802	PLX	C26-C27-C28-C29
6	A	2814	PLX	C26-C27-C28-C29
3	A	2802	ATP	C5'-O5'-PA-O3A
3	B	2803	ATP	C5'-O5'-PA-O3A
3	C	2807	ATP	C5'-O5'-PA-O3A
3	D	2803	ATP	C5'-O5'-PA-O3A
4	A	2803	I3P	C1-O1-P1-O13
4	B	2804	I3P	C1-O1-P1-O13
4	C	2808	I3P	C1-O1-P1-O13
4	D	2804	I3P	C1-O1-P1-O13
6	A	2814	PLX	C24-C25-C26-C27
6	B	2802	PLX	C24-C25-C26-C27
6	C	2813	PLX	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
6	D	2814	PLX	C24-C25-C26-C27
3	A	2802	ATP	PG-O3B-PB-O1B
3	B	2803	ATP	PG-O3B-PB-O1B
3	C	2807	ATP	PG-O3B-PB-O1B
3	D	2803	ATP	PG-O3B-PB-O1B
6	A	2810	PLX	C25-C24-O8-C5
6	A	2811	PLX	C1-C2-O1-P1
6	B	2811	PLX	C25-C24-O8-C5
6	B	2812	PLX	C1-C2-O1-P1
6	C	2803	PLX	C25-C24-O8-C5
6	C	2804	PLX	C1-C2-O1-P1
6	D	2810	PLX	C25-C24-O8-C5
6	D	2811	PLX	C1-C2-O1-P1
6	B	2811	PLX	C26-C27-C28-C29
6	D	2810	PLX	C26-C27-C28-C29
6	A	2810	PLX	C26-C27-C28-C29
6	C	2803	PLX	C26-C27-C28-C29
6	B	2813	PLX	C9-C10-C11-C12
6	C	2805	PLX	C9-C10-C11-C12

There are no ring outliers.

35 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2802	PLX	1	0
6	B	2810	PLX	4	0
6	C	2803	PLX	1	0
3	B	2803	ATP	1	0
3	D	2803	ATP	1	0
6	D	2814	PLX	2	0
4	A	2803	I3P	1	0
6	A	2812	PLX	2	0
6	B	2814	PLX	4	0
6	D	2802	PLX	2	0
6	C	2806	PLX	5	0
3	C	2807	ATP	1	0
6	B	2812	PLX	1	0
4	D	2804	I3P	1	0
6	A	2811	PLX	2	0
6	D	2813	PLX	6	0
6	D	2811	PLX	1	0
4	C	2808	I3P	1	0

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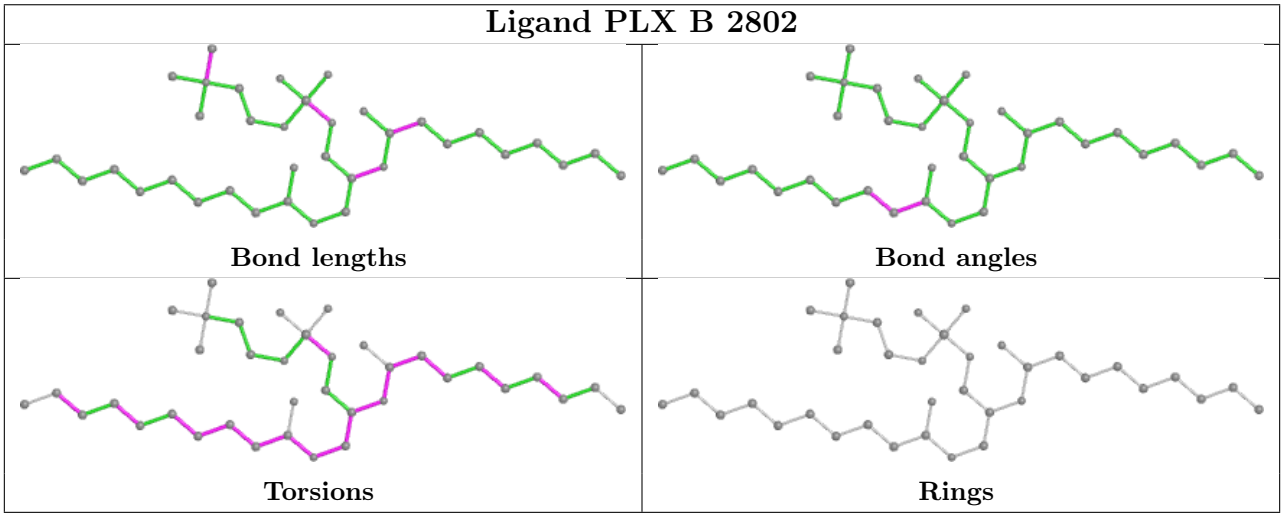
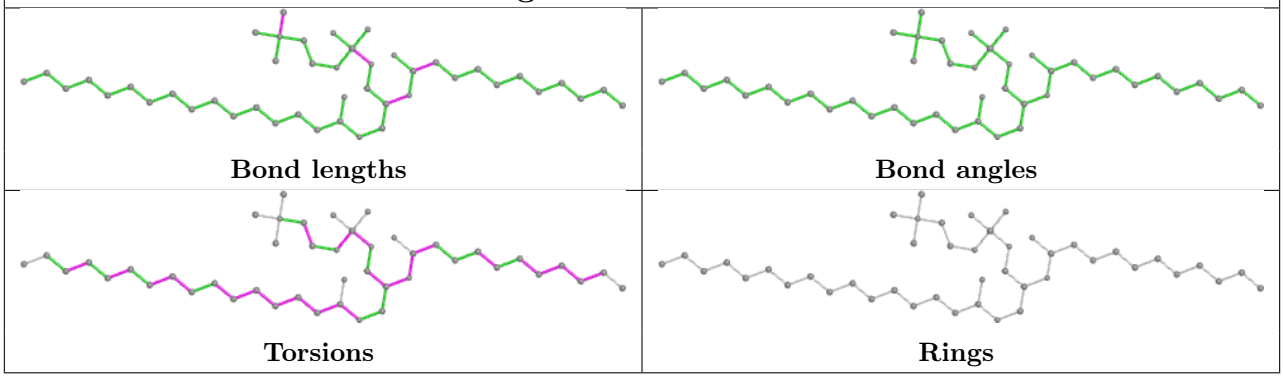
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2808	PLX	1	0
6	D	2809	PLX	3	0
6	A	2813	PLX	6	0
6	A	2814	PLX	1	0
6	B	2813	PLX	1	0
4	B	2804	I3P	1	0
6	B	2811	PLX	2	0
6	C	2805	PLX	1	0
6	A	2809	PLX	5	0
6	C	2802	PLX	4	0
6	B	2809	PLX	1	0
6	D	2810	PLX	2	0
6	C	2804	PLX	1	0
6	D	2812	PLX	1	0
6	A	2810	PLX	2	0
6	C	2814	PLX	1	0
6	C	2813	PLX	1	0

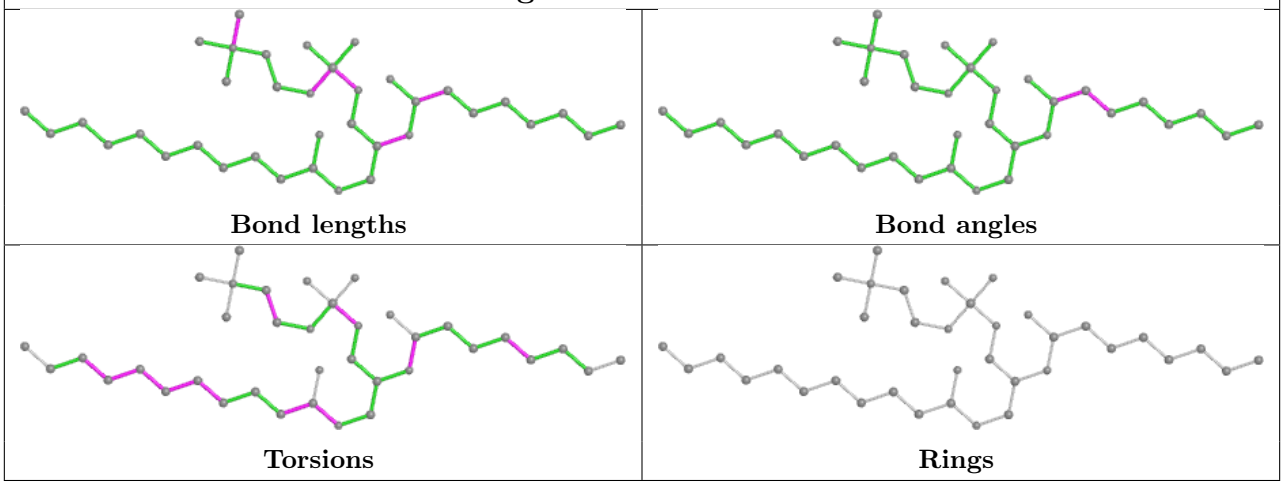
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



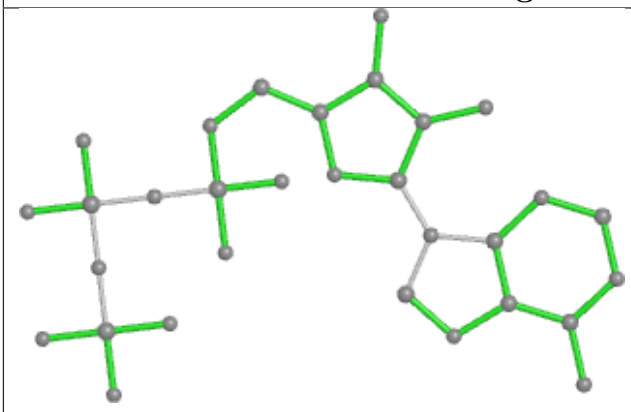
Ligand PLX B 2810



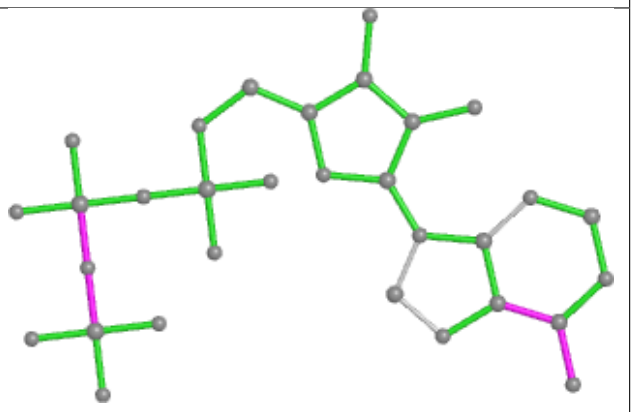
Ligand PLX C 2803



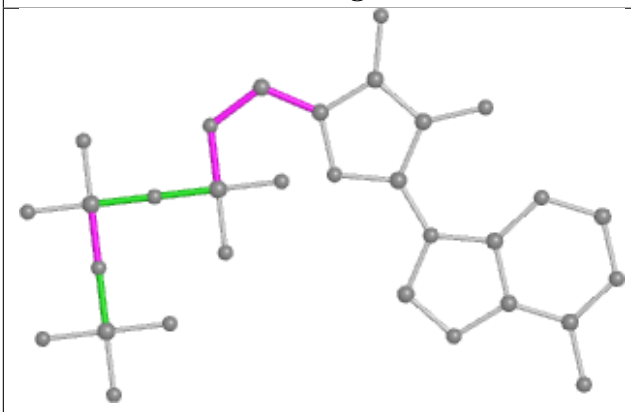
Ligand ATP B 2803



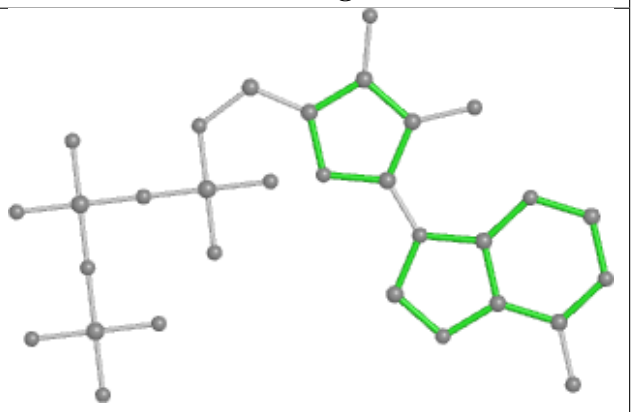
Bond lengths



Bond angles

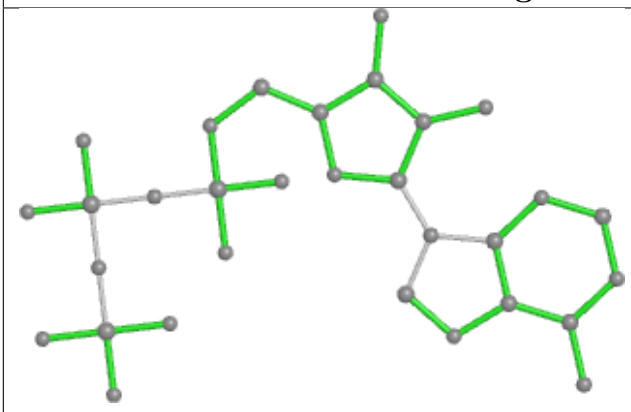


Torsions

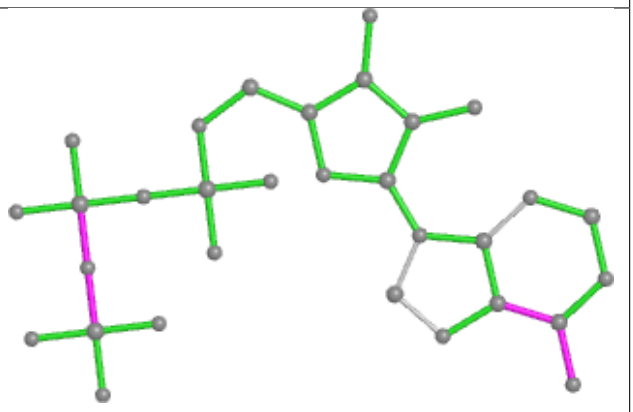


Rings

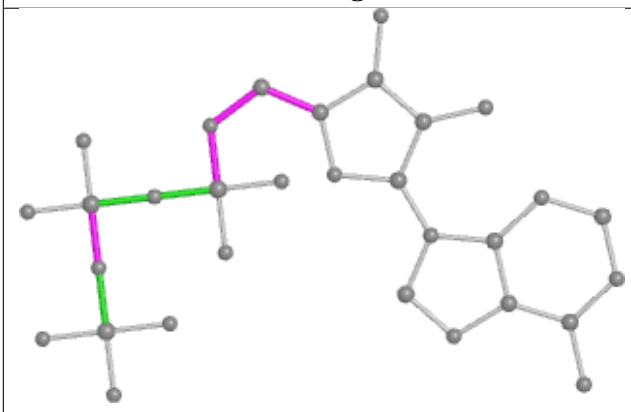
Ligand ATP D 2803



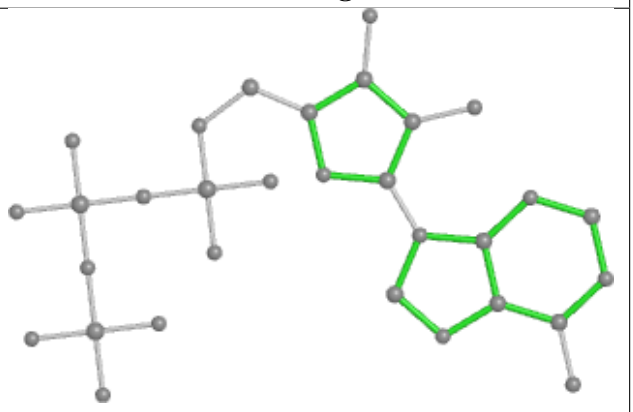
Bond lengths



Bond angles

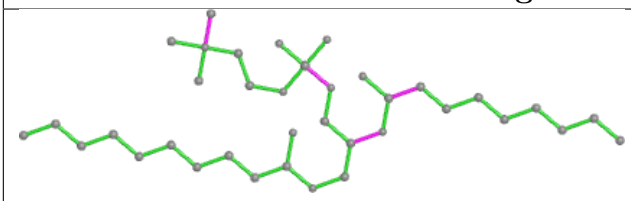


Torsions

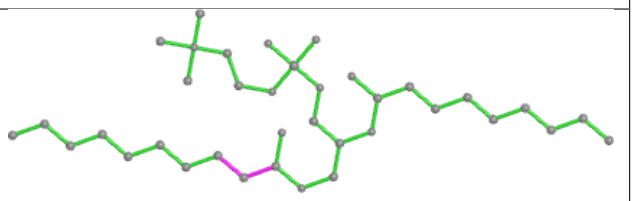


Rings

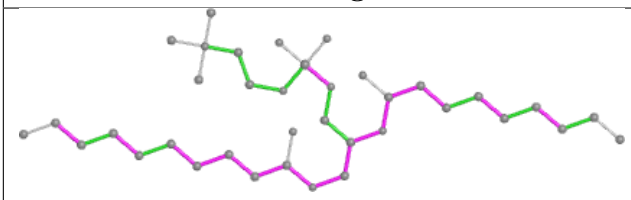
Ligand PLX D 2814



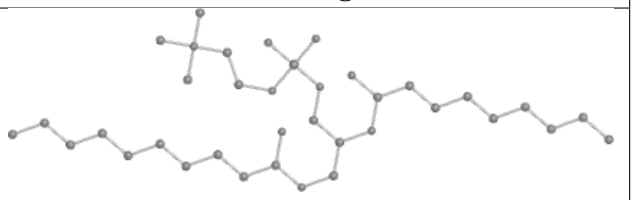
Bond lengths



Bond angles

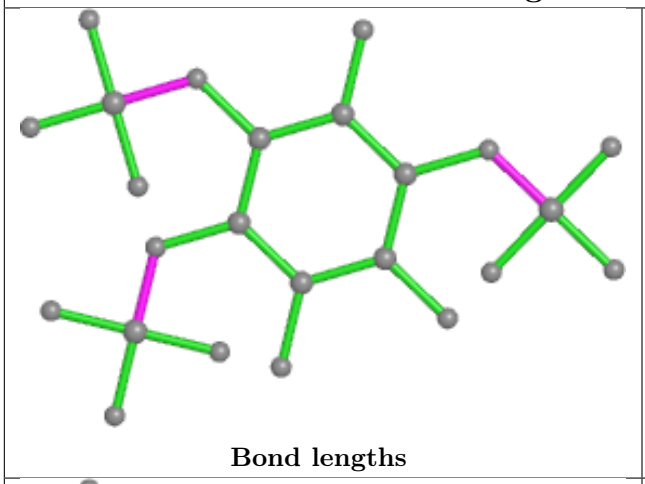


Torsions

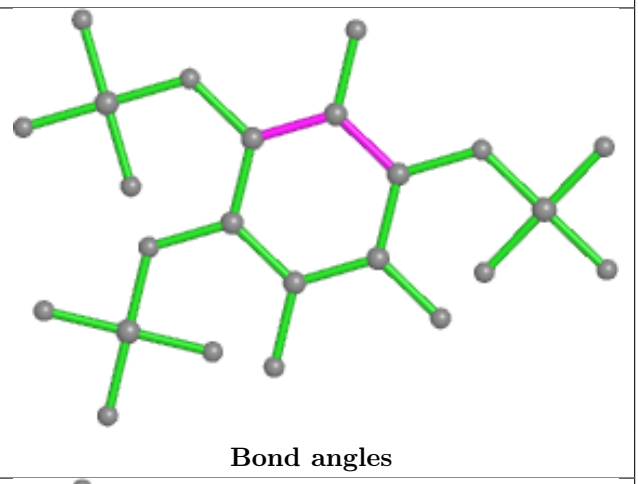


Rings

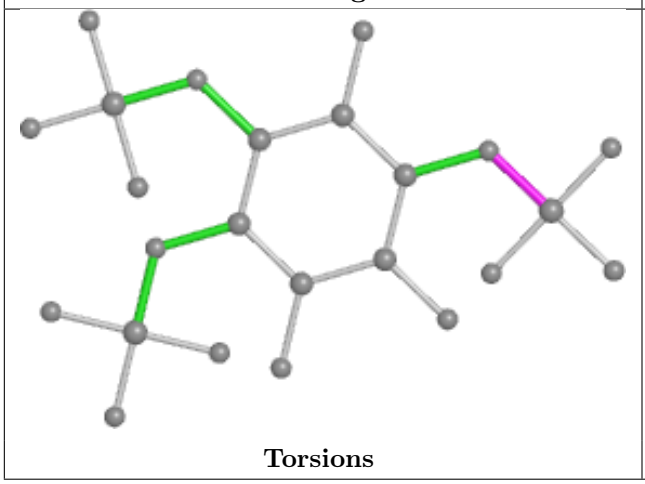
Ligand I3P A 2803



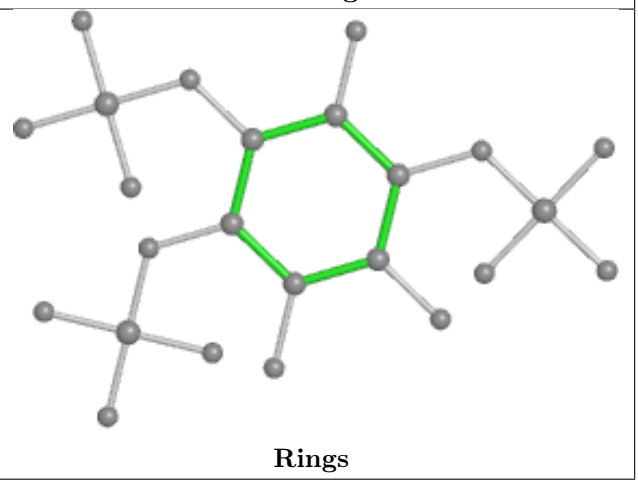
Bond lengths



Bond angles

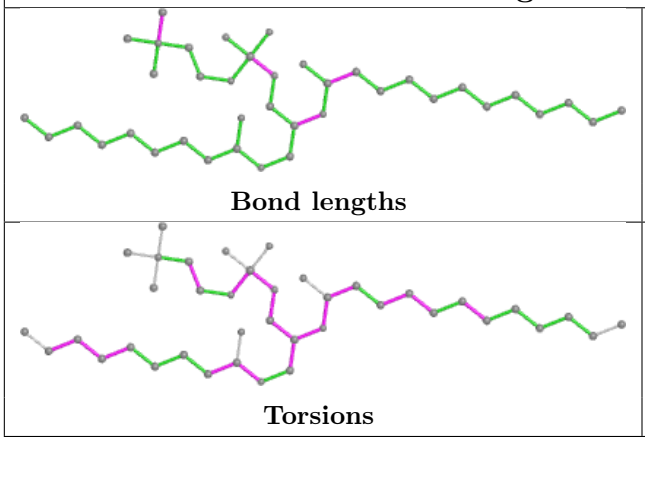


Torsions

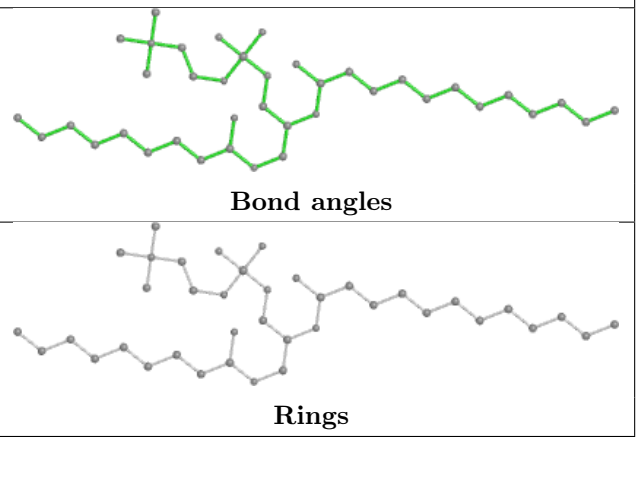


Rings

Ligand PLX A 2812



Bond lengths

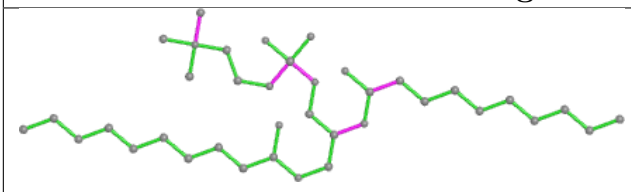


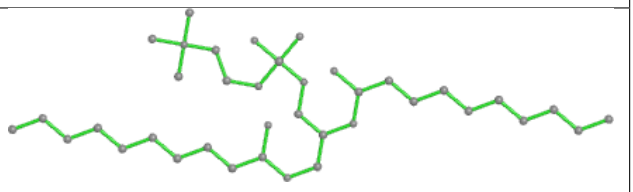
Bond angles

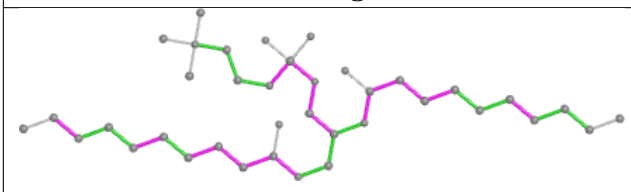
Torsions

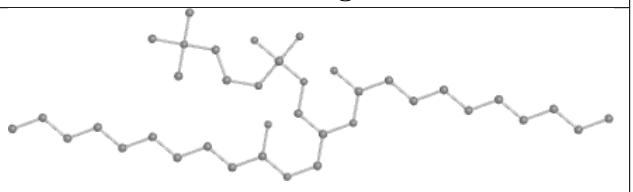
Rings

Ligand PLX B 2814

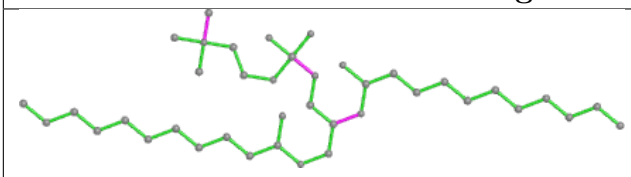

Bond lengths

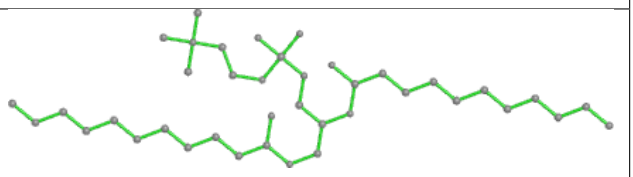

Bond angles

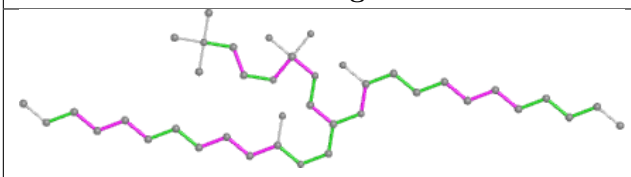

Torsions


Rings

Ligand PLX D 2802


Bond lengths


Bond angles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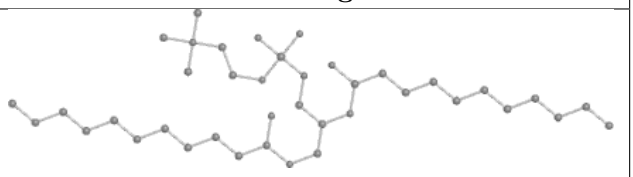
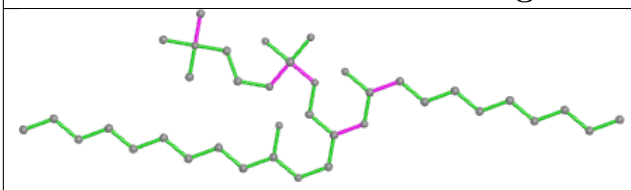
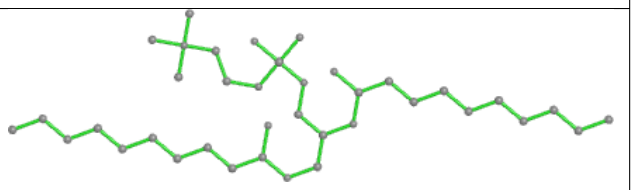
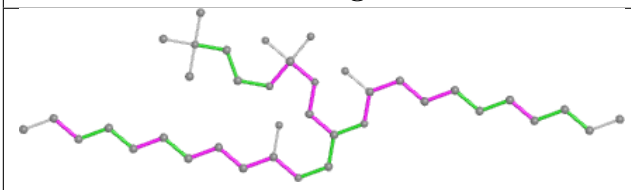
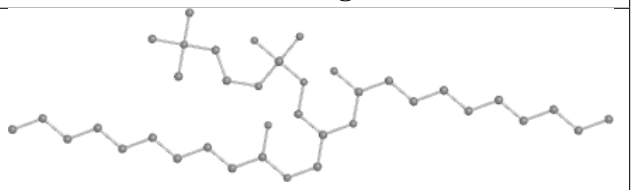

Rings

Ligand PLX C 2806

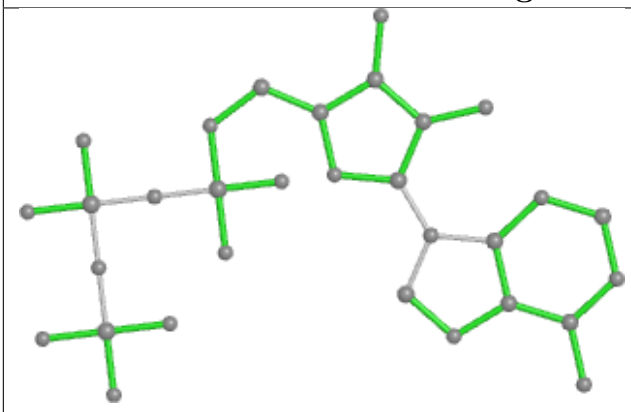

Bond lengths


Bond angles

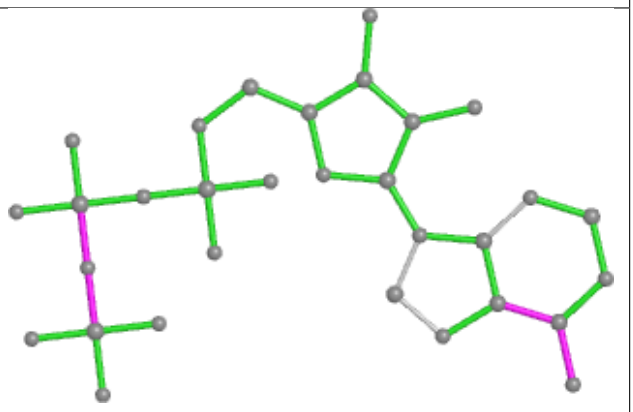

Torsions


Rings

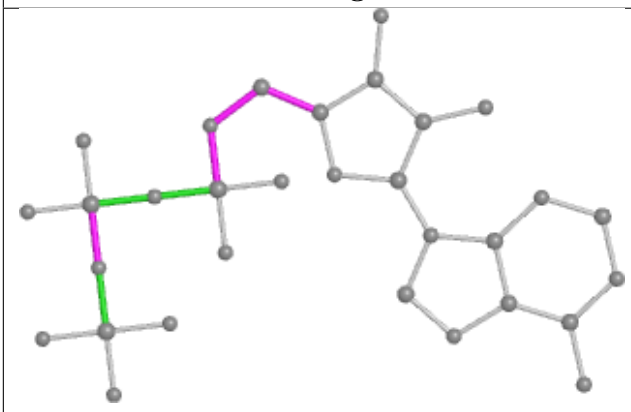
Ligand ATP C 2807



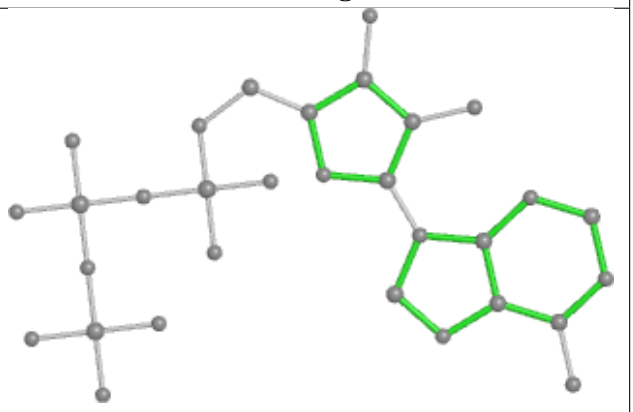
Bond lengths



Bond angles

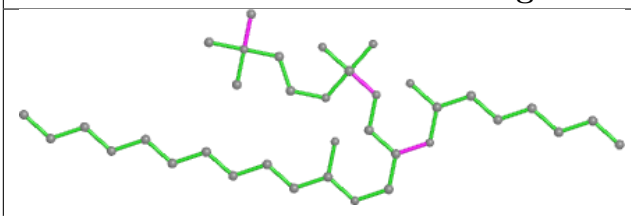


Torsions

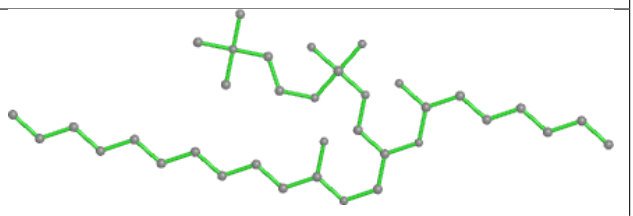


Rings

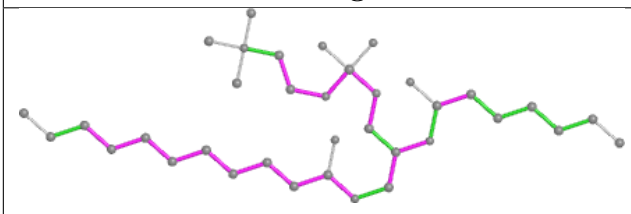
Ligand PLX B 2812



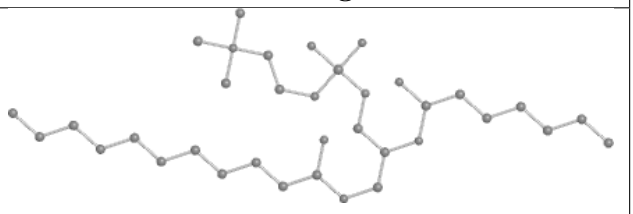
Bond lengths



Bond angles

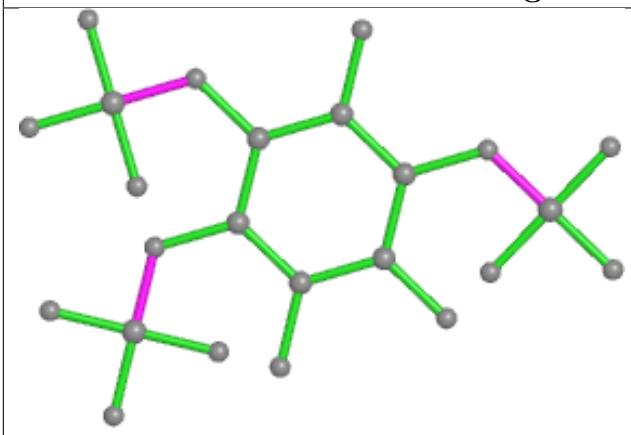


Torsions



Rings

Ligand I3P D 2804



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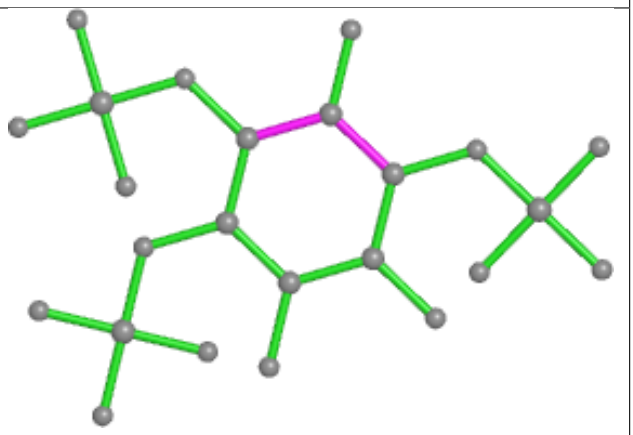
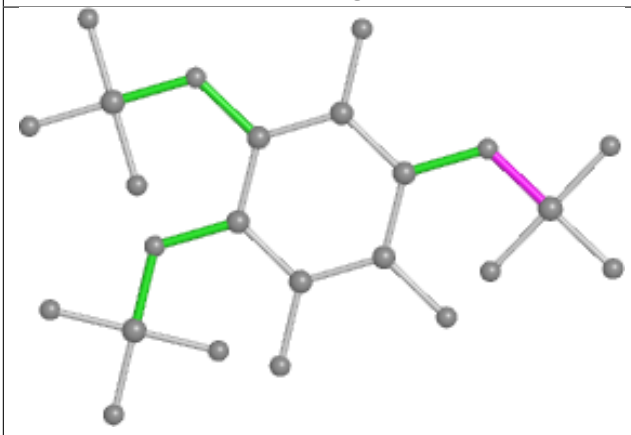
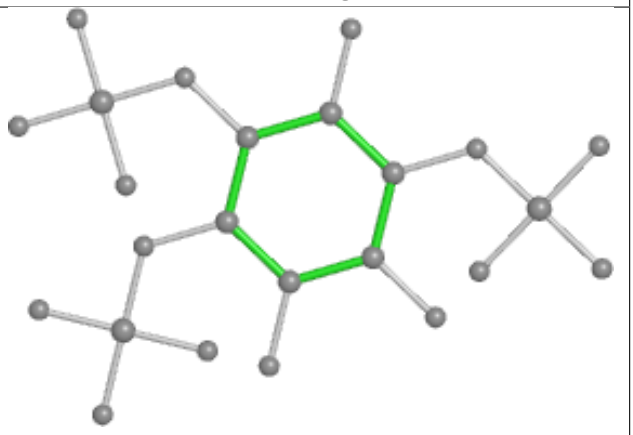


Bond angles

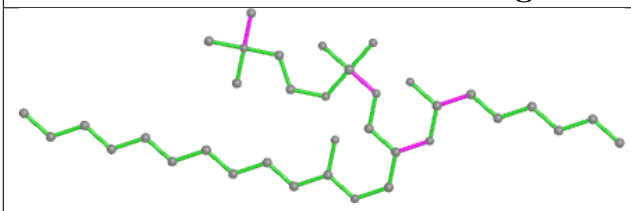


Torsions



Rings

Ligand PLX A 2811



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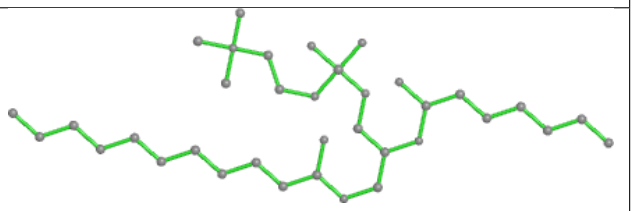
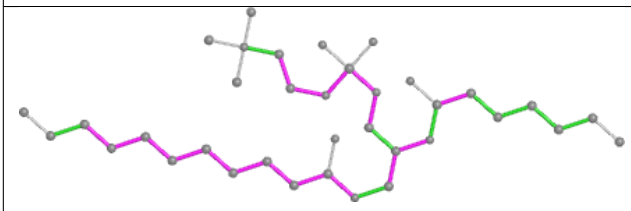


Bond angles



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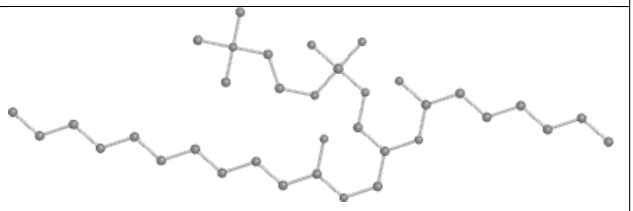
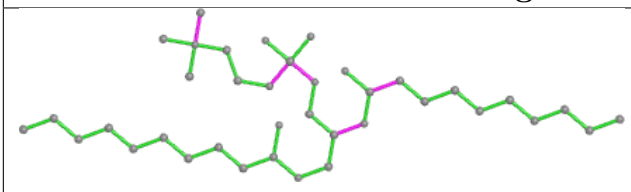


Rings

Ligand PLX D 2813



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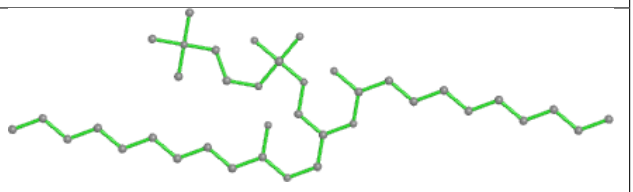
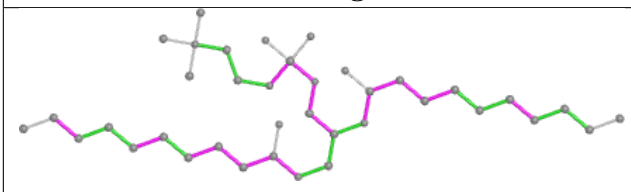


Bond angles



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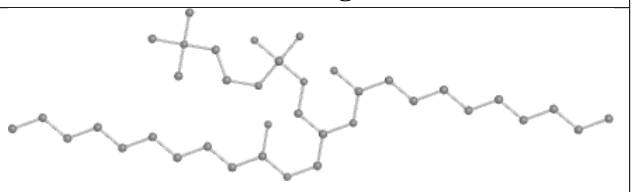
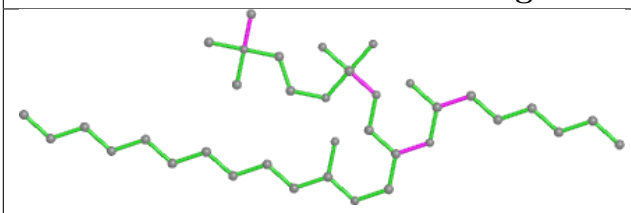


Rings

Ligand PLX D 2811



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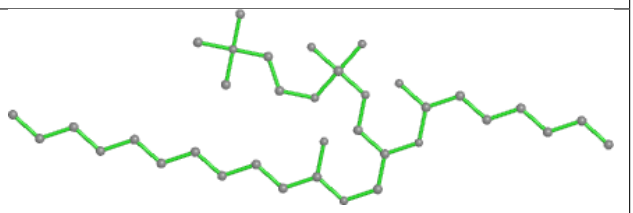
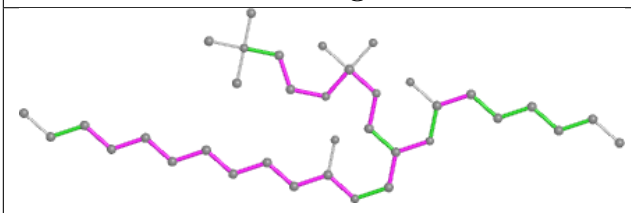


Bond angles



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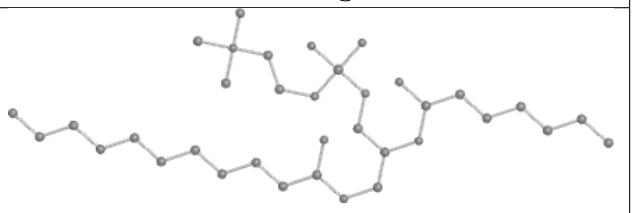
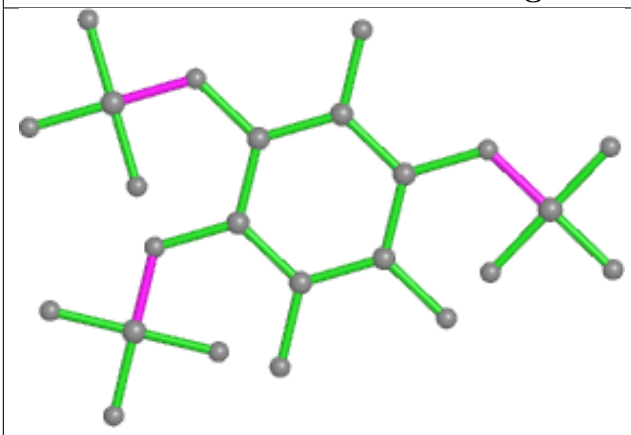


Rings

Ligand I3P C 2808



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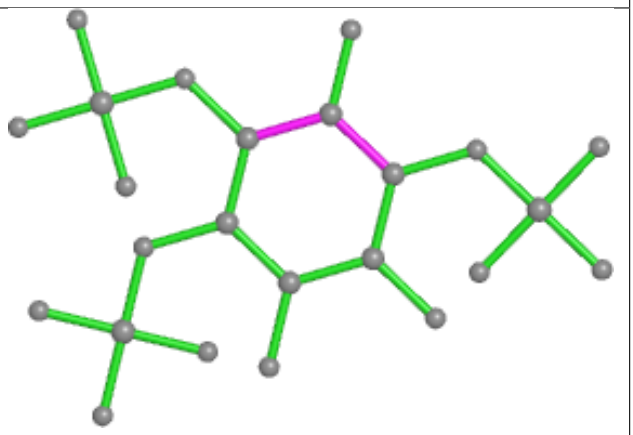
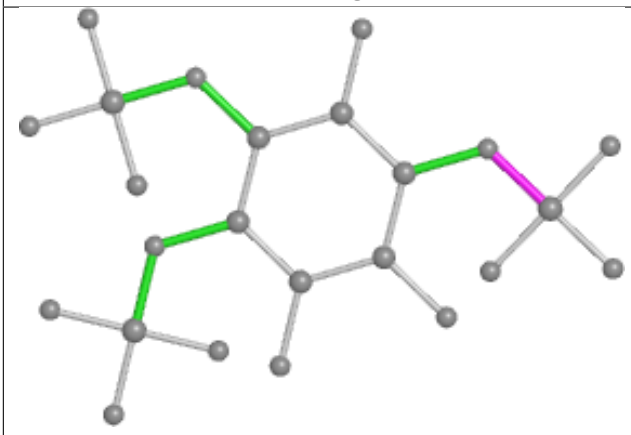


Bond angles



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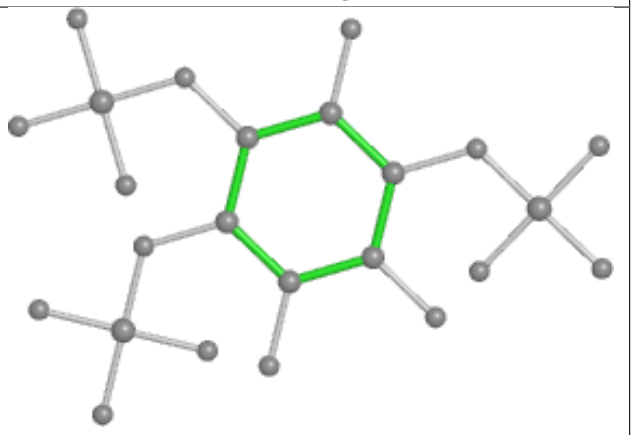
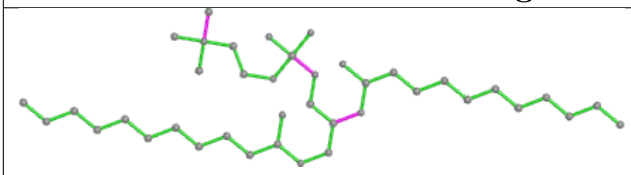


Rings

Ligand PLX A 2808



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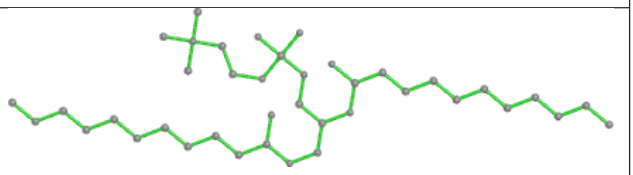
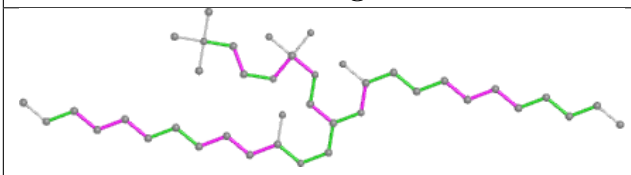


Bond angles



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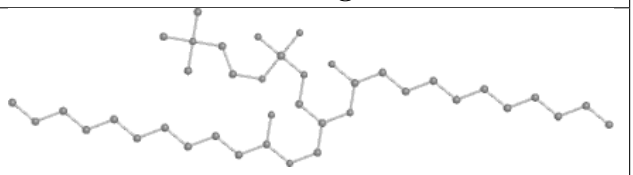
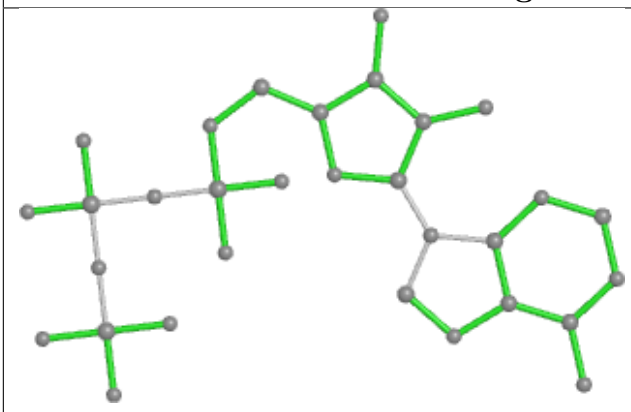
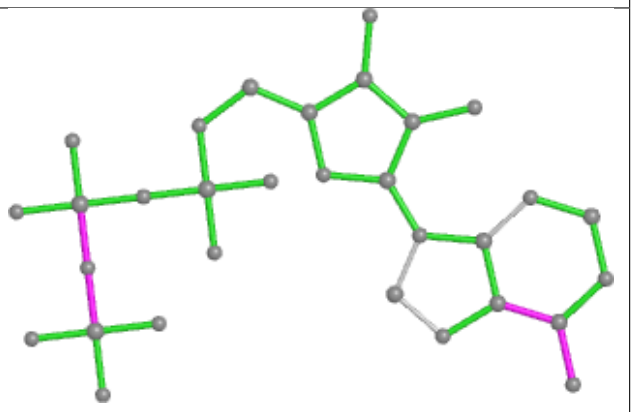


Rings

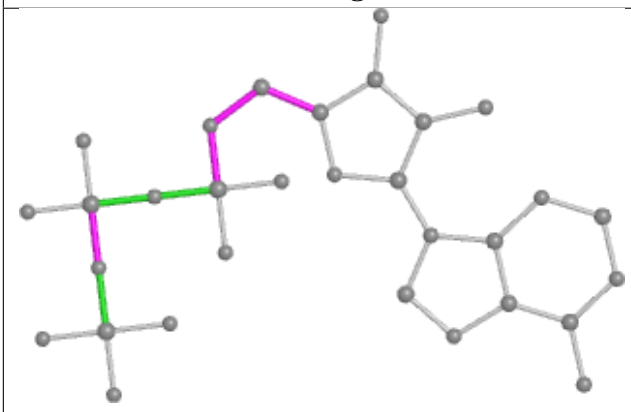
Ligand ATP A 2802



Bond lengths



Bond angles



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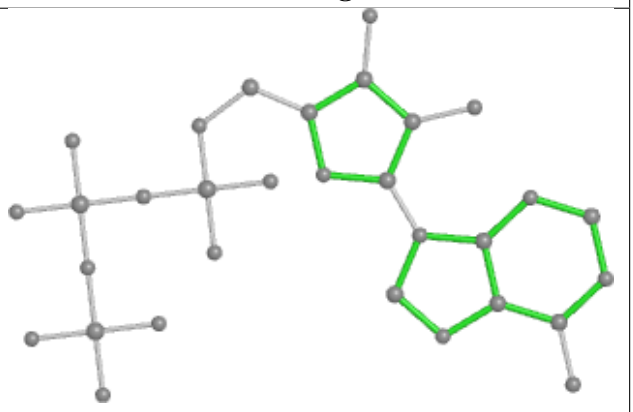
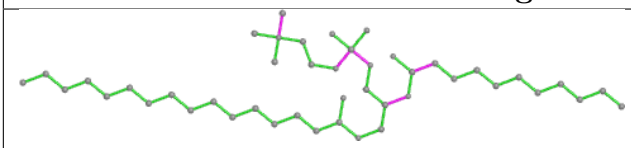
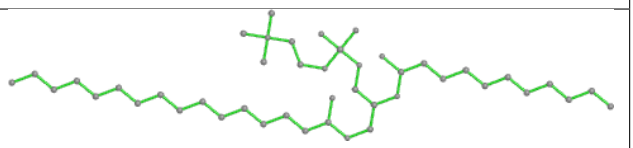


Rings

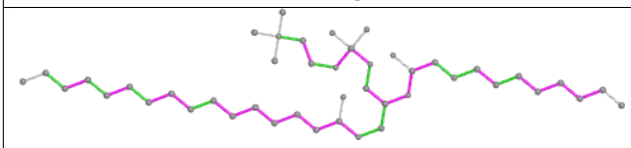
Ligand PLX D 2809



Bond lengths



Bond angles



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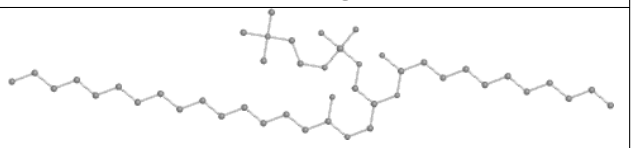
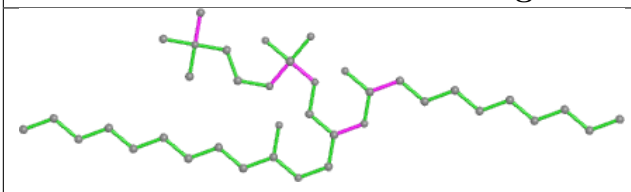
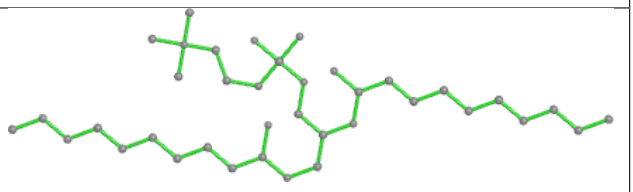
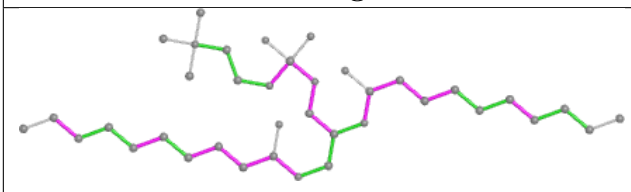
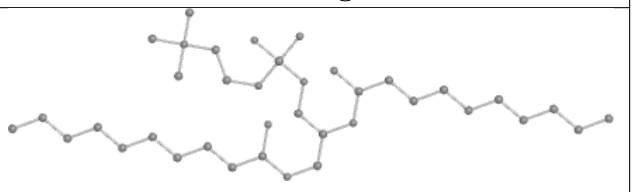
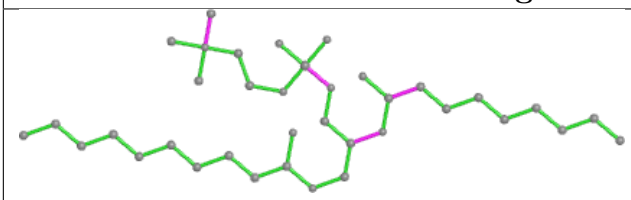
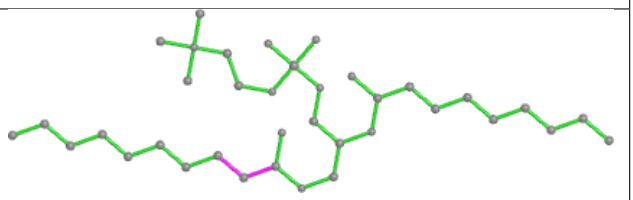
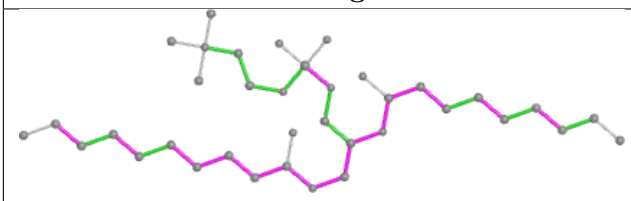
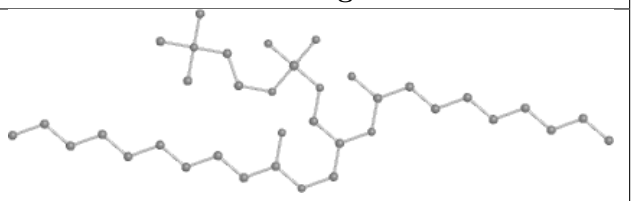
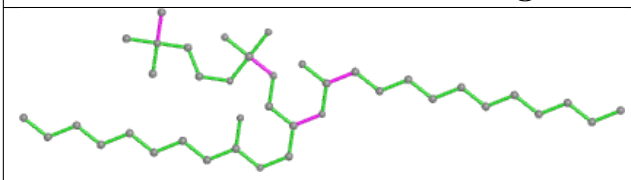
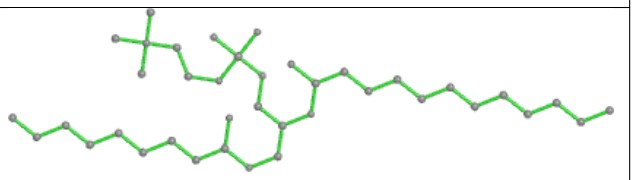
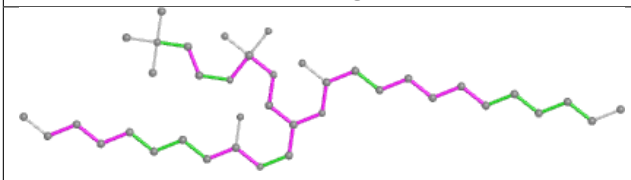
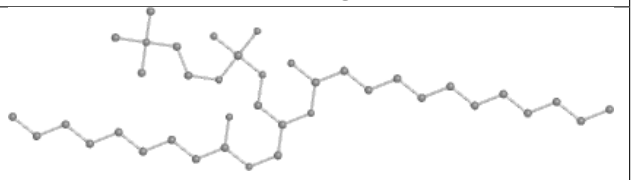


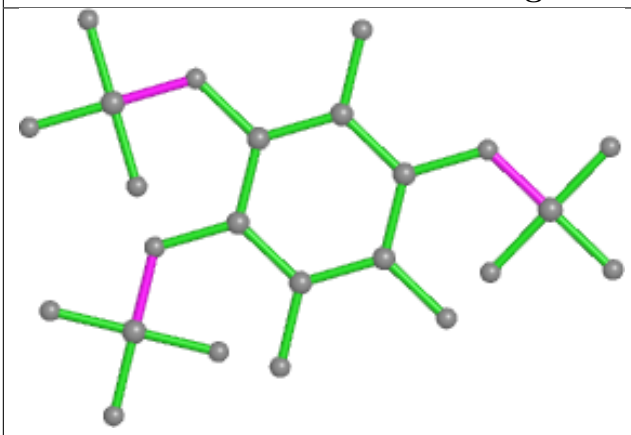
Rings

Ligand PLX A 2813	
 Bond lengths	 Bond angles
 Torsions	 Rings

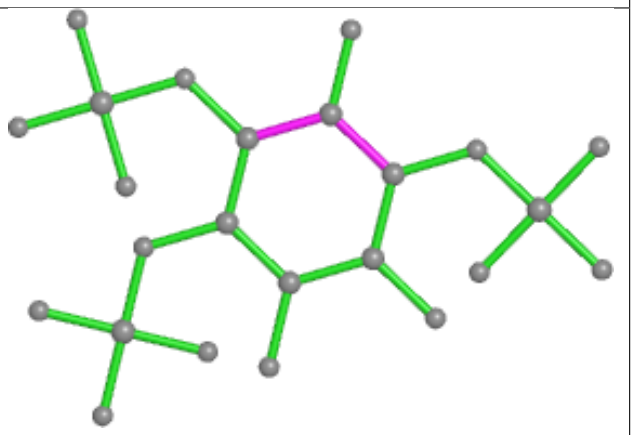
Ligand PLX A 2814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX B 2813	
 Bond lengths	 Bond angles
 Torsions	 Rings

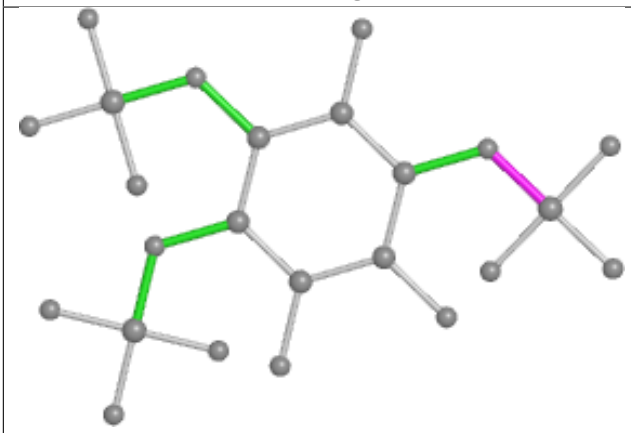
Ligand I3P B 2804



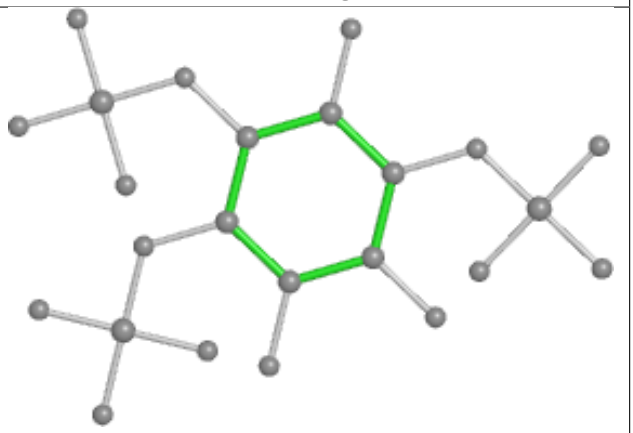
Bond lengths



Bond angles

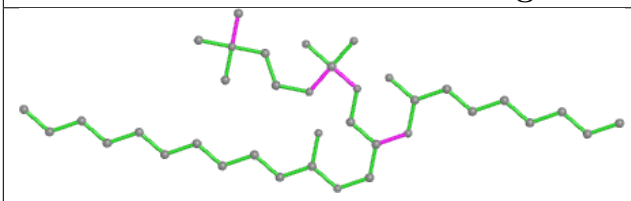


Torsions

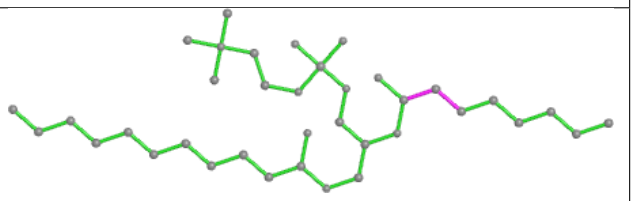


Rings

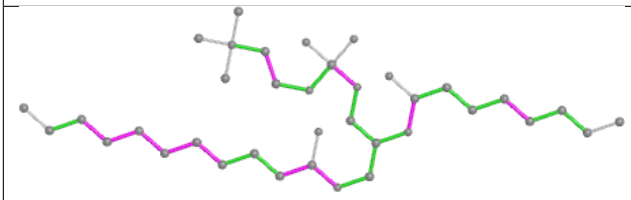
Ligand PLX B 2811



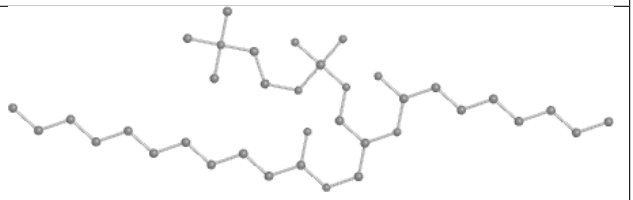
Bond lengths



Bond angles

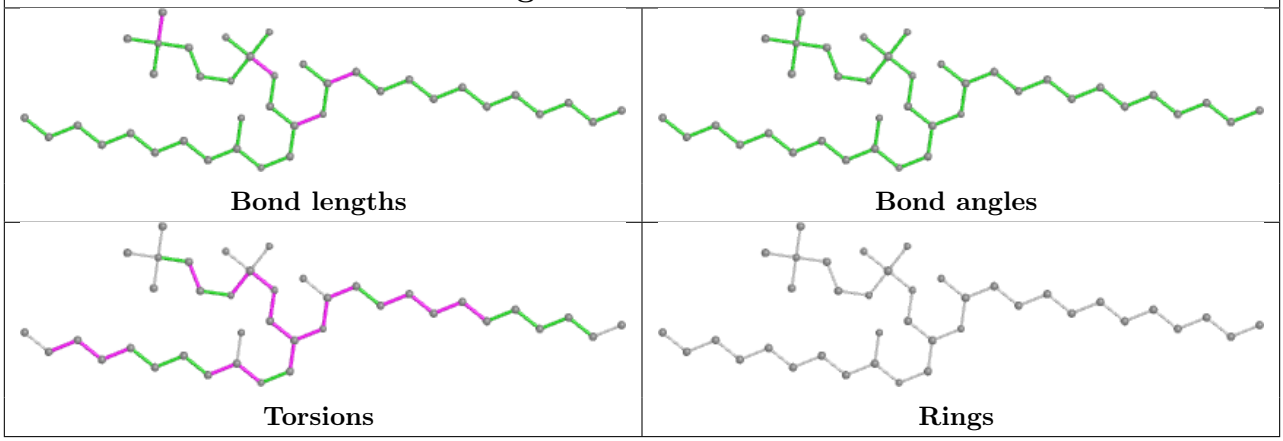


Torsions

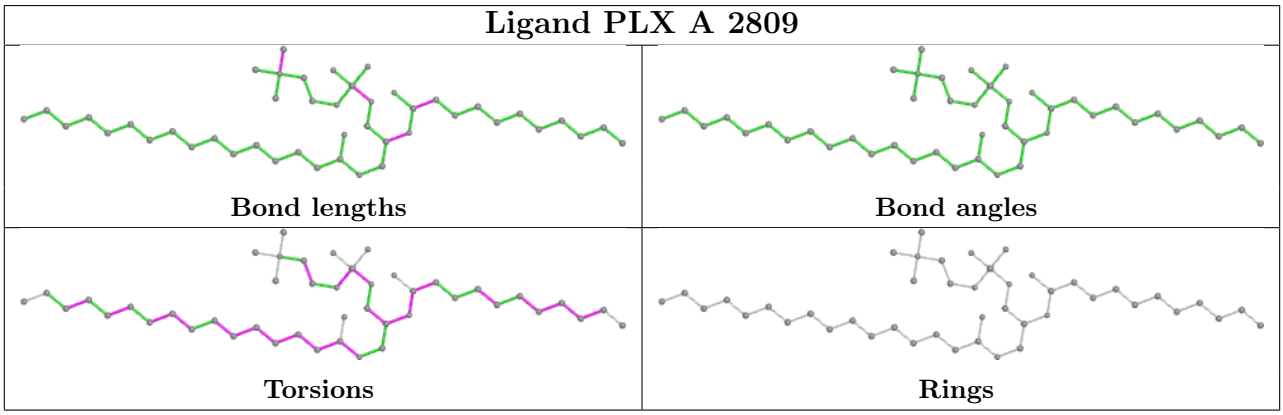


Rings

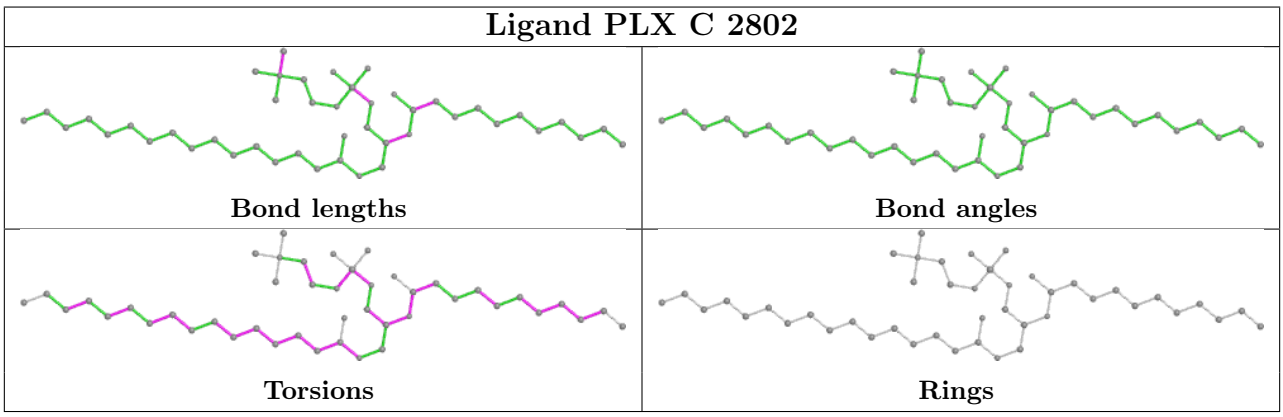
Ligand PLX C 2805



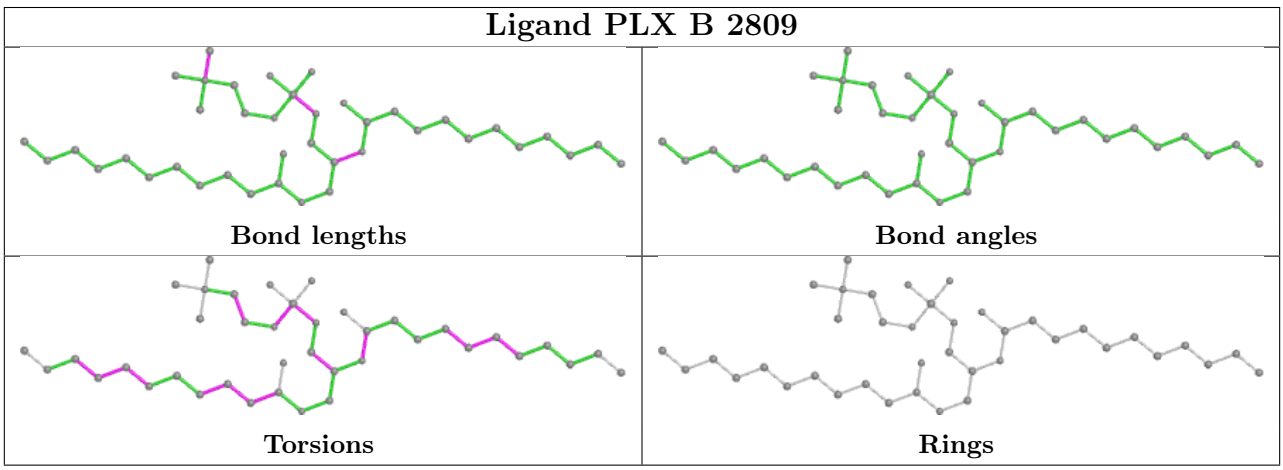
Ligand PLX A 2809



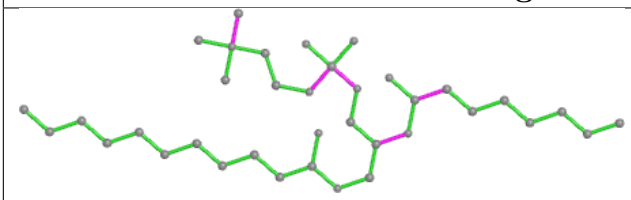
Ligand PLX C 2802



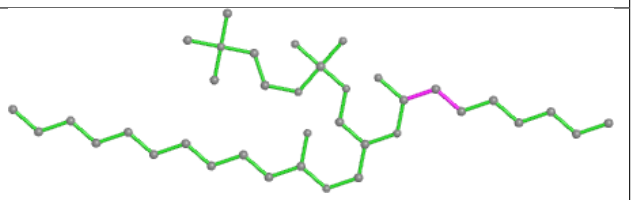
Ligand PLX B 2809



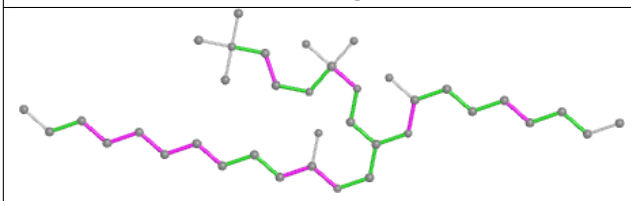
Ligand PLX D 2810



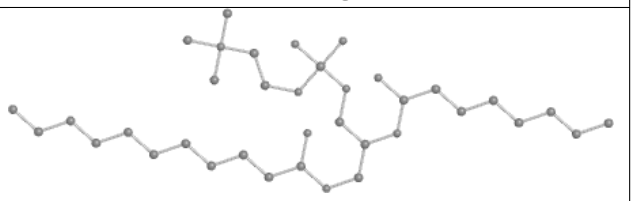
Bond lengths



Bond angles

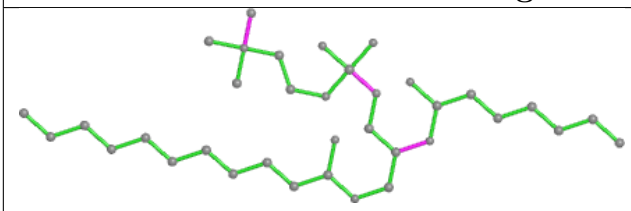


Torsions

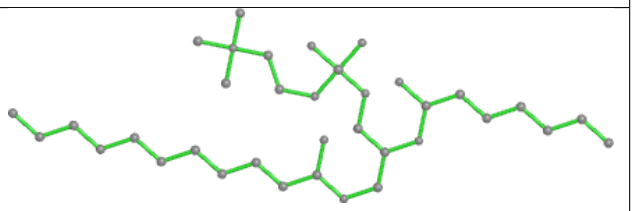


Rings

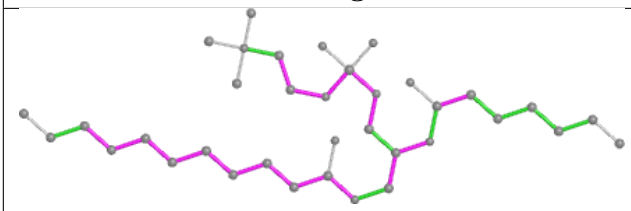
Ligand PLX C 2804



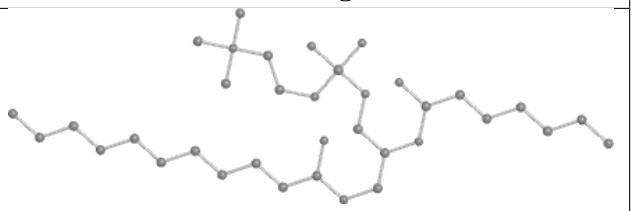
Bond lengths



Bond angles

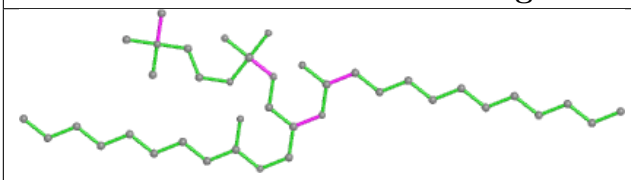


Torsions

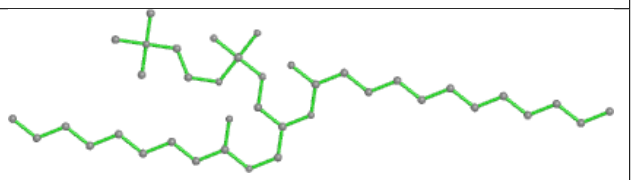


Rings

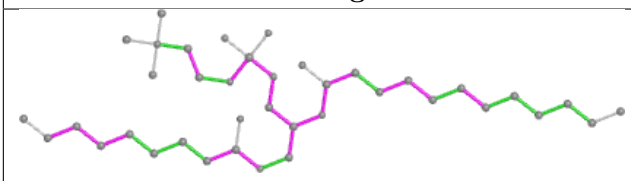
Ligand PLX D 2812



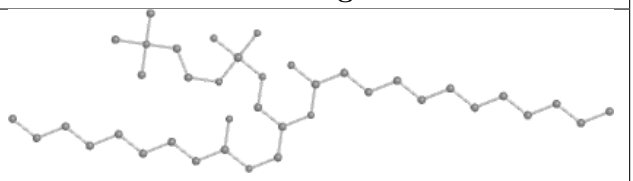
Bond lengths



Bond angles

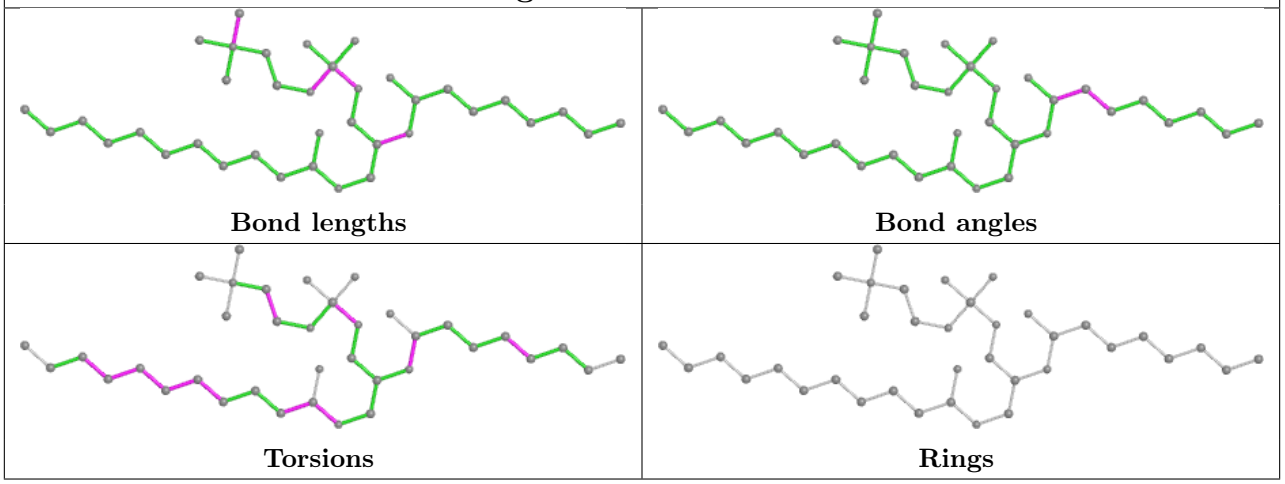


Torsions

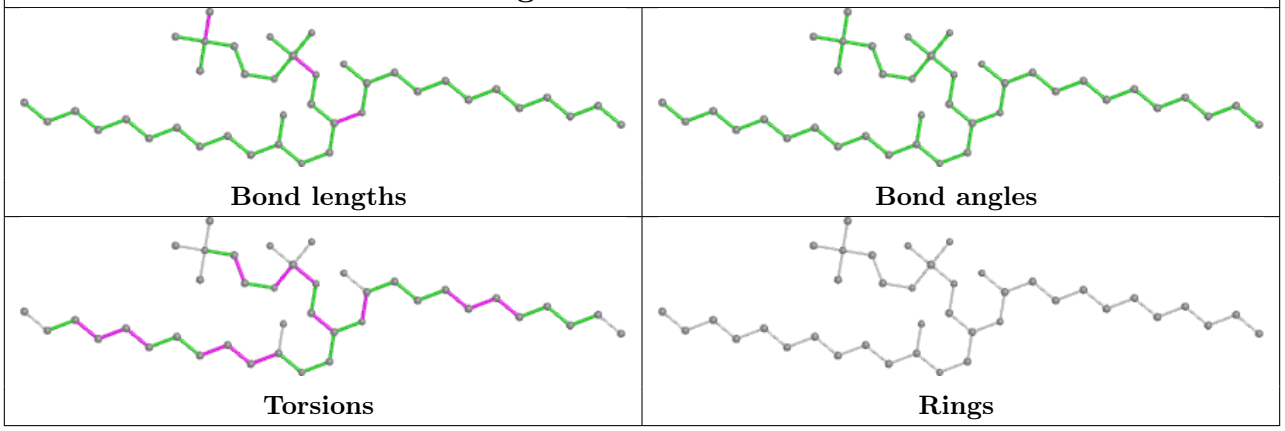


Rings

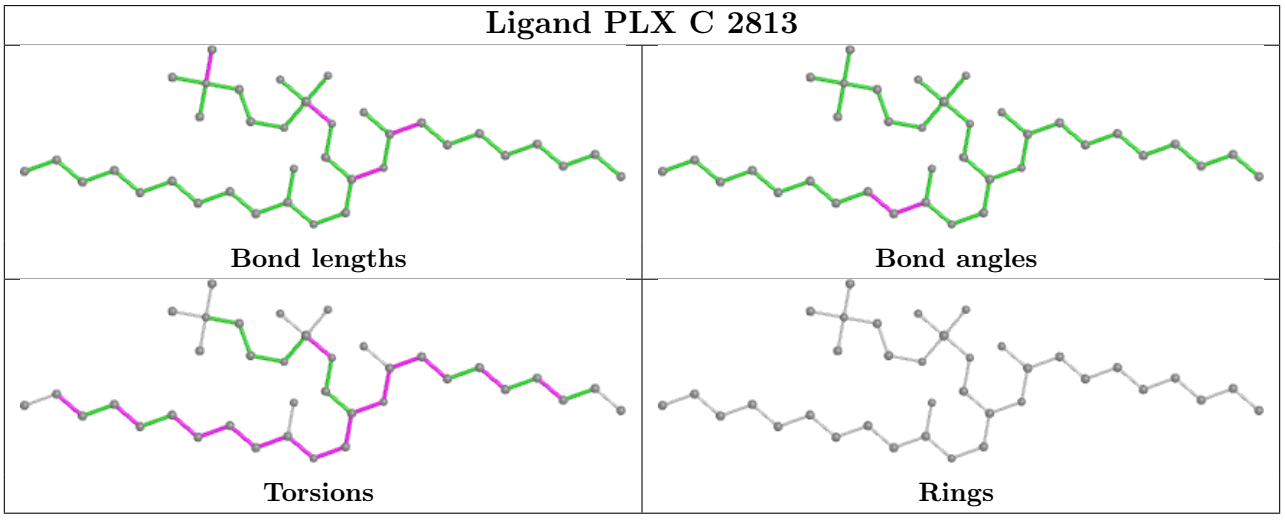
Ligand PLX A 2810



Ligand PLX C 2814



Ligand PLX C 2813



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

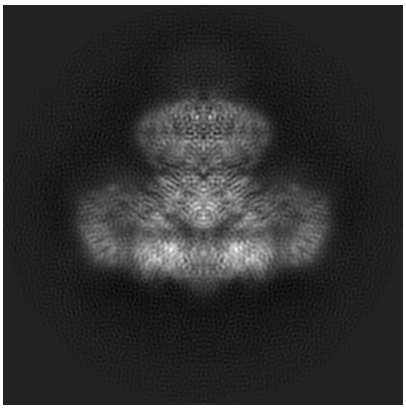
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27983. These allow visual inspection of the internal detail of the map and identification of artifacts.

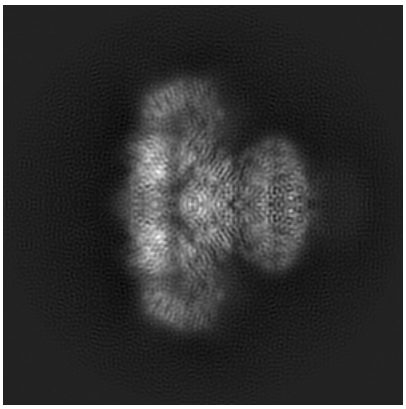
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

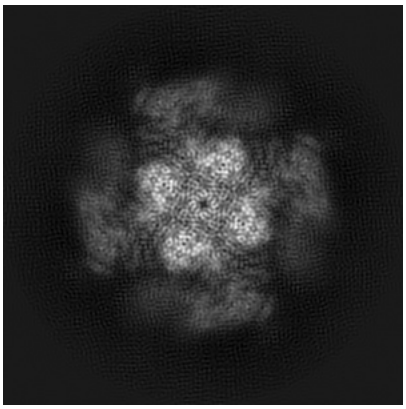
6.1.1 Primary map



X

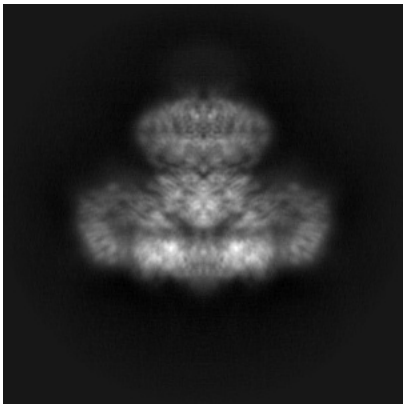


Y

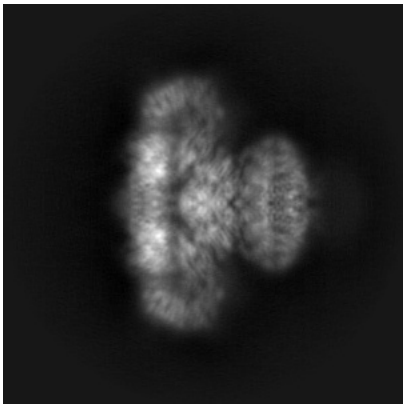


Z

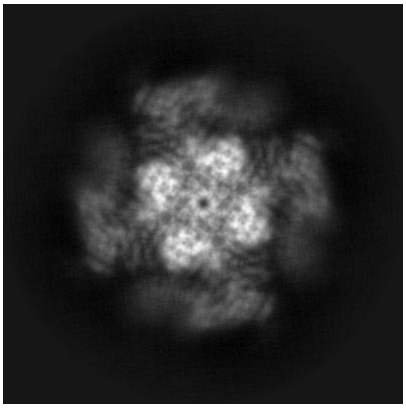
6.1.2 Raw map



X



Y

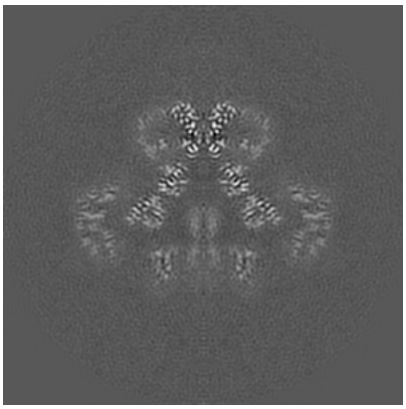


Z

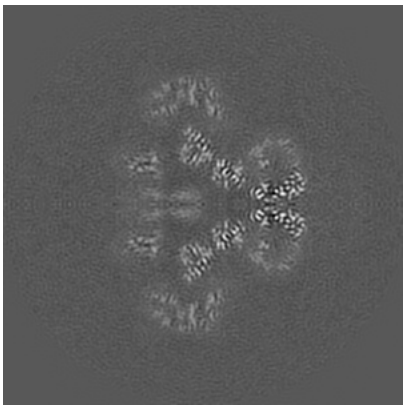
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

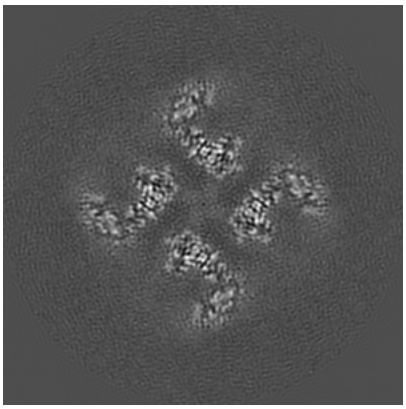
6.2.1 Primary map



X Index: 168

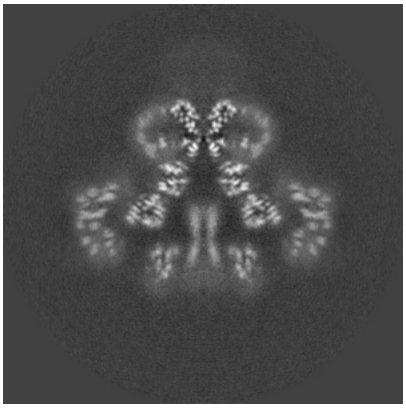


Y Index: 168

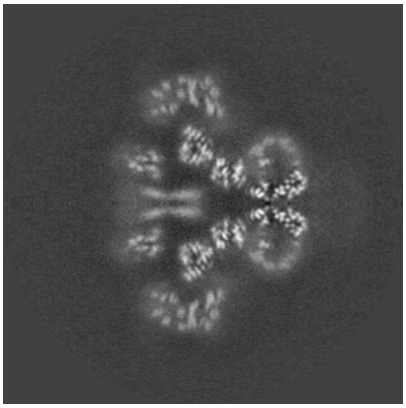


Z Index: 168

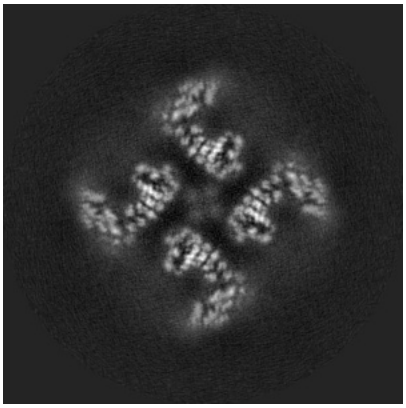
6.2.2 Raw map



X Index: 168



Y Index: 168

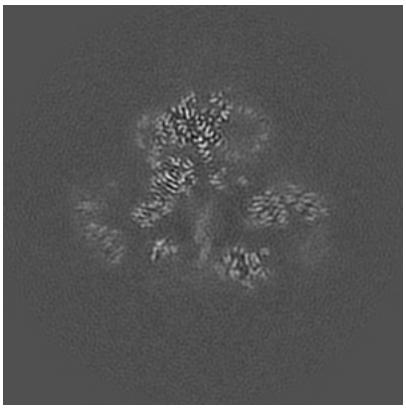


Z Index: 168

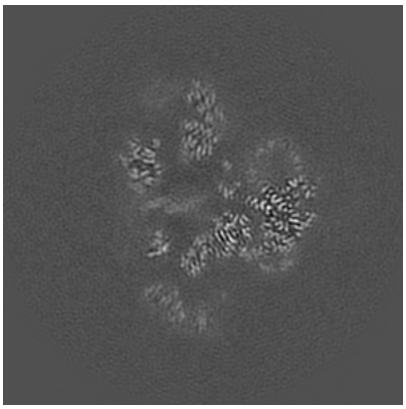
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

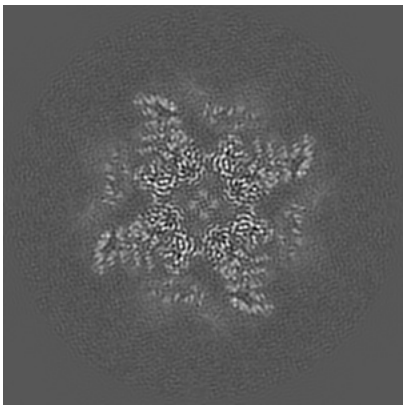
6.3.1 Primary map



X Index: 160

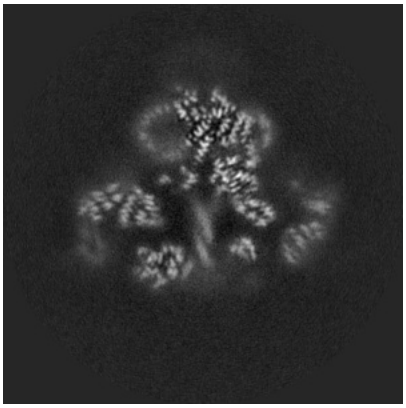


Y Index: 176

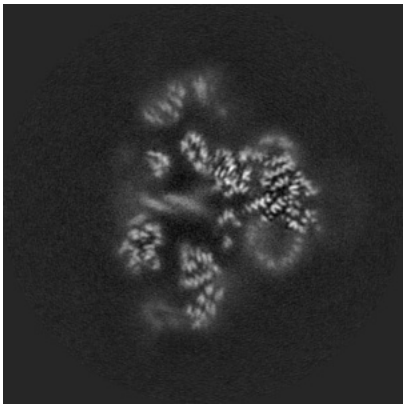


Z Index: 125

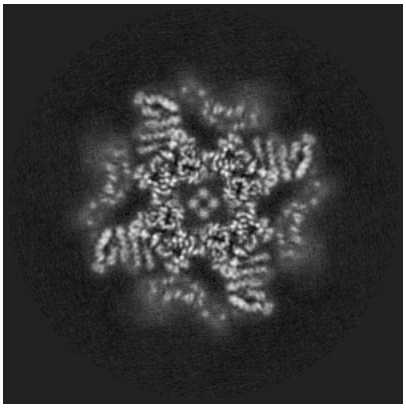
6.3.2 Raw map



X Index: 176



Y Index: 160

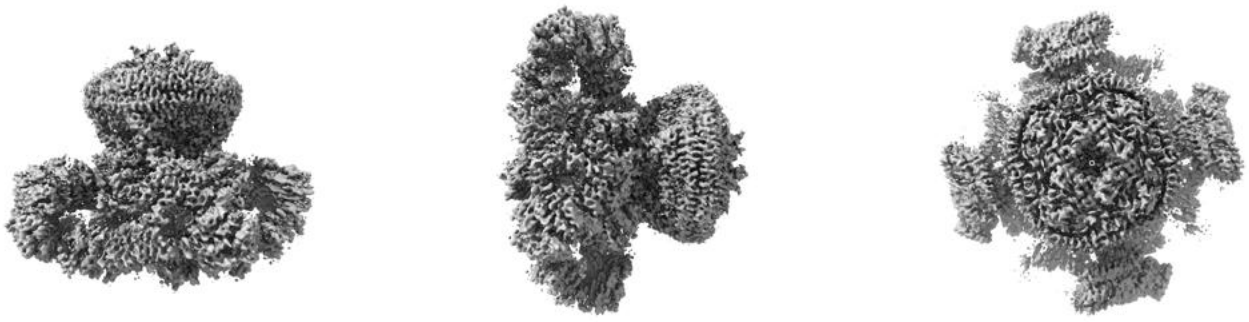


Z Index: 126

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

6.4.2 Raw map

X Y Z

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

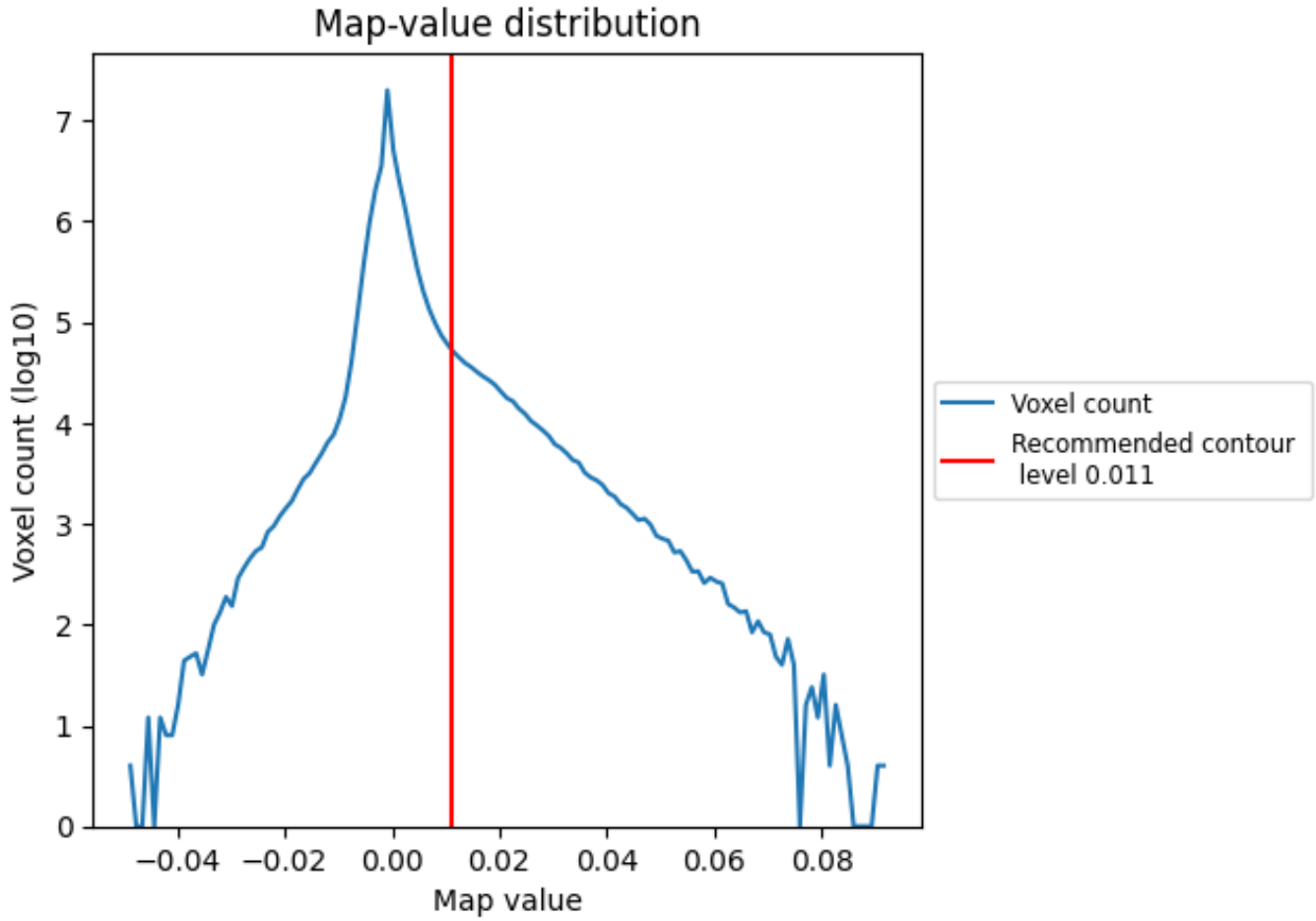
6.5 Mask visualisation (i)

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

7 Map analysis

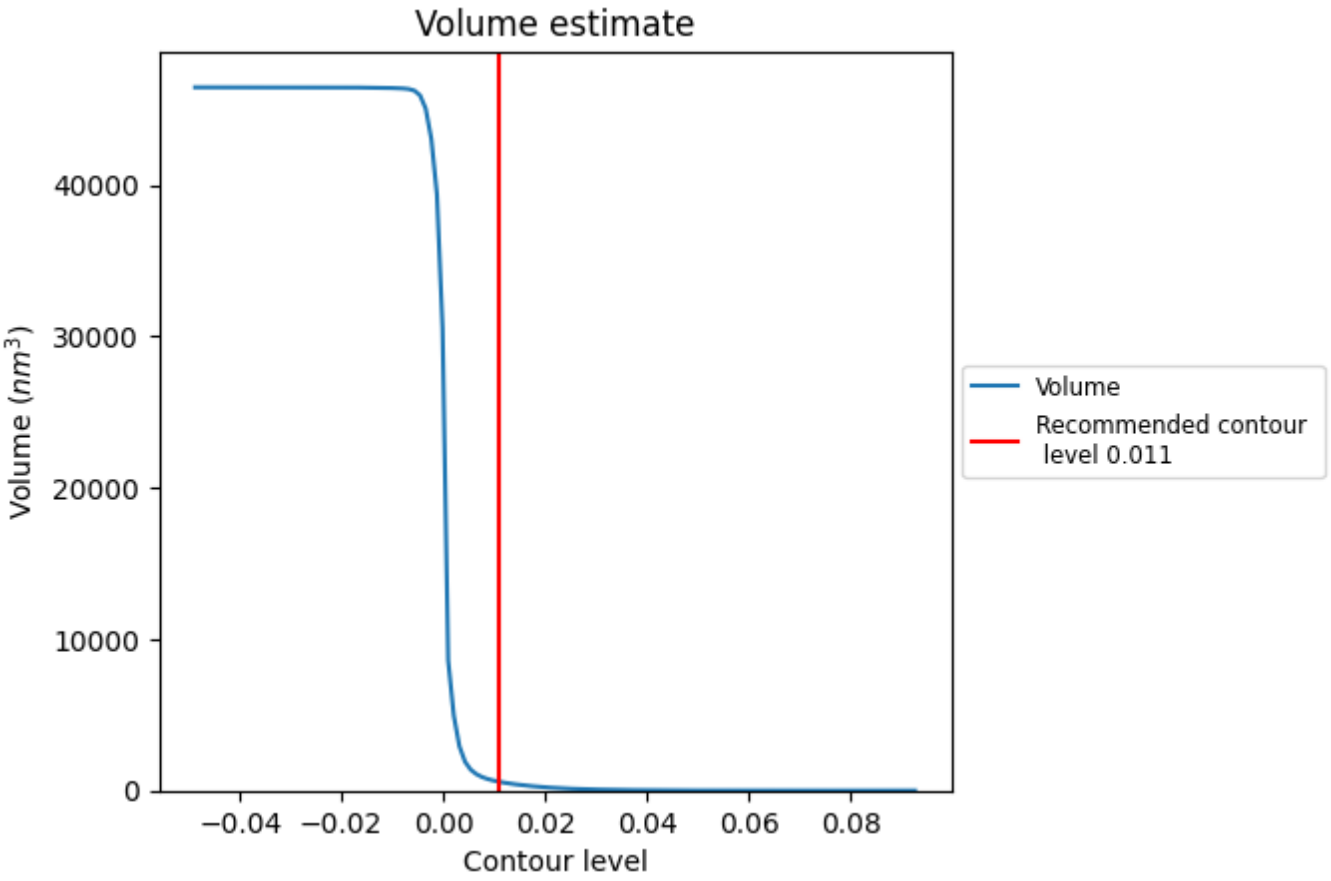
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

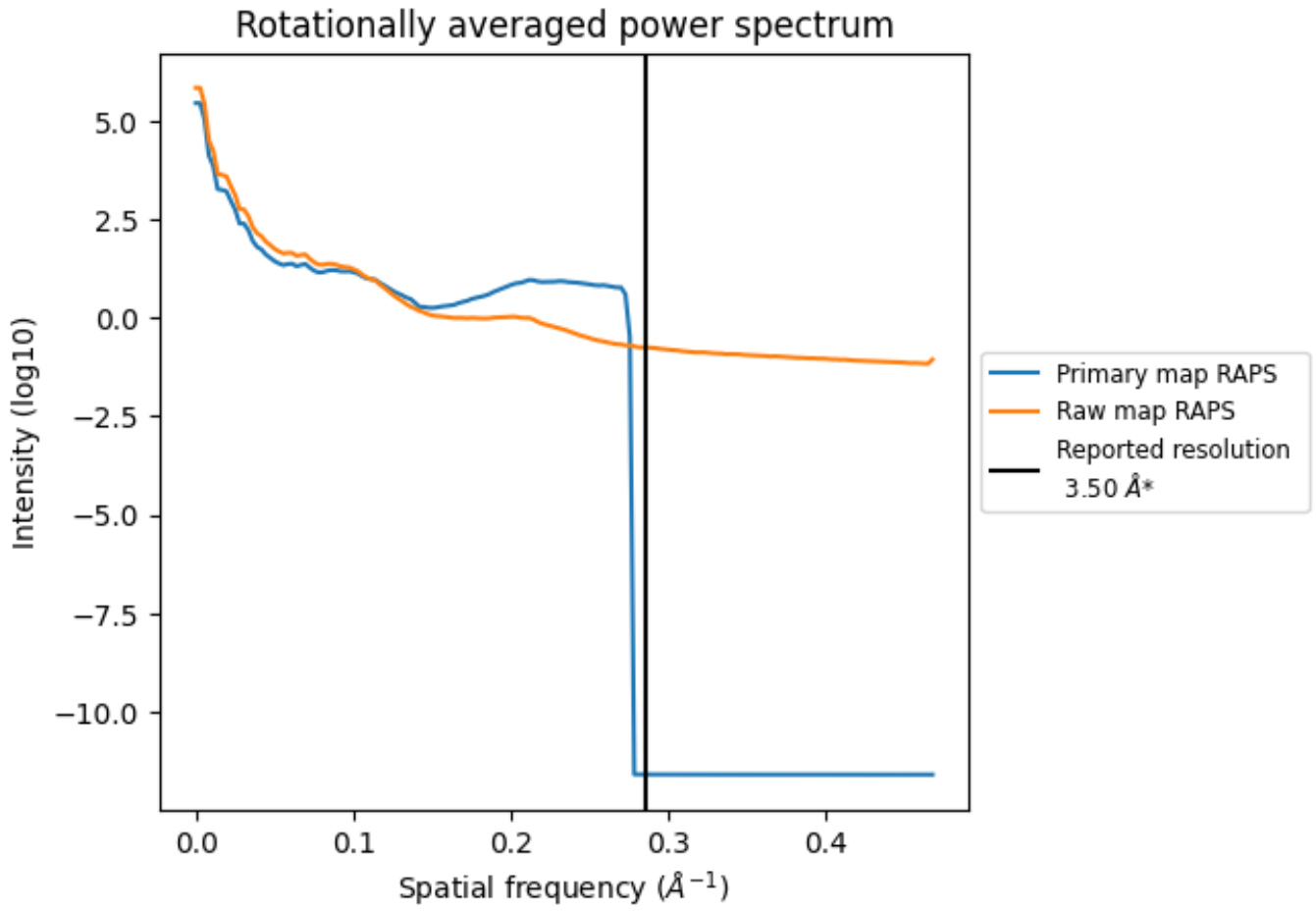
7.2 Volume estimate



The volume at the recommended contour level is 581 nm^3; this corresponds to an approximate mass of 525 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)

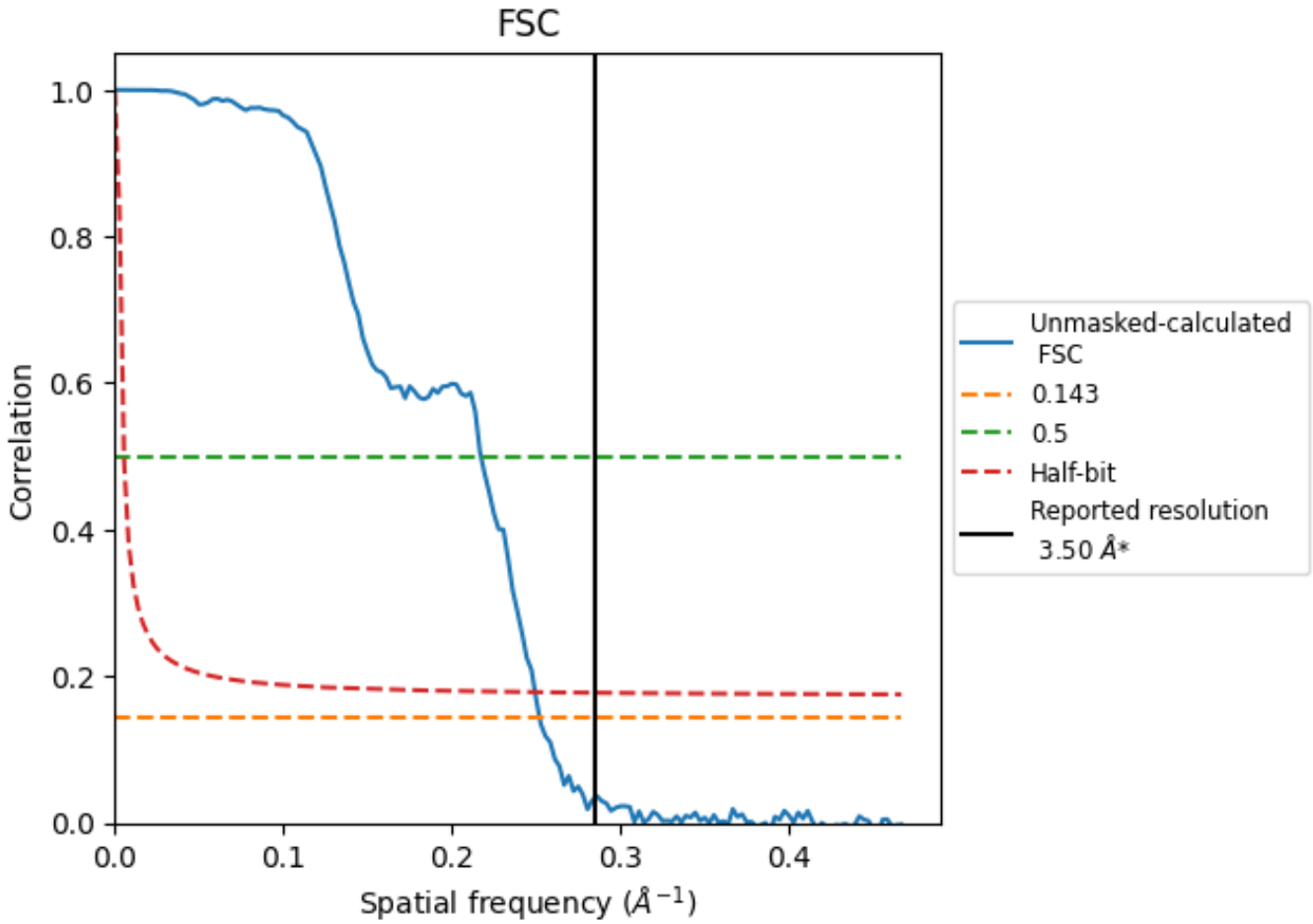


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

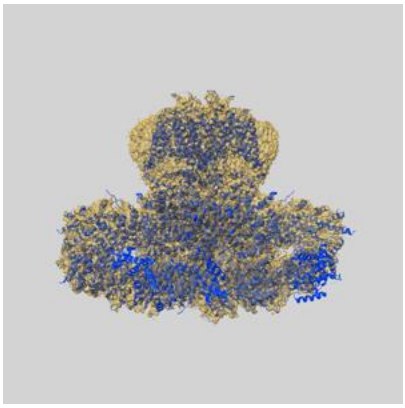
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	4.60	4.00

*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 3.96 differs from the reported value 3.5 by more than 10 %

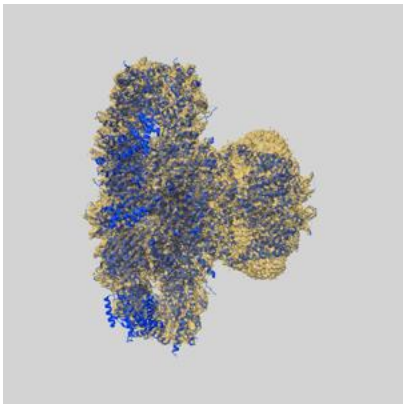
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27983 and PDB model 8EAR. Per-residue inclusion information can be found in section 3 on page 8.

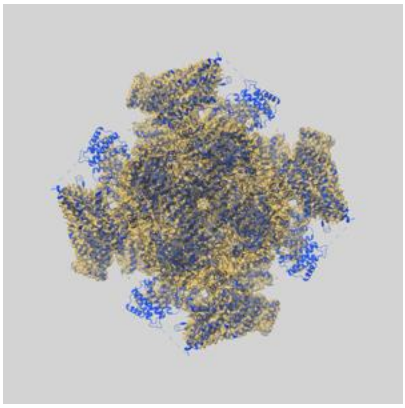
9.1 Map-model overlay



X



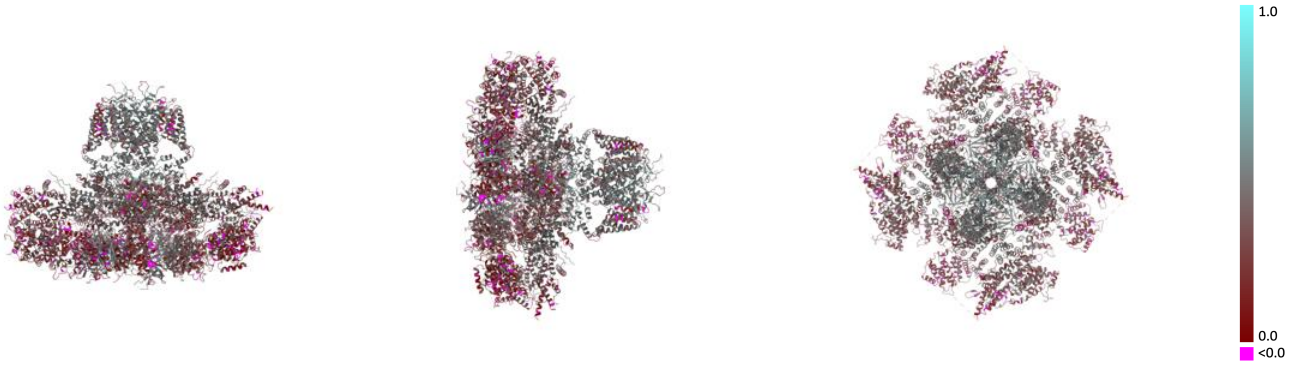
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

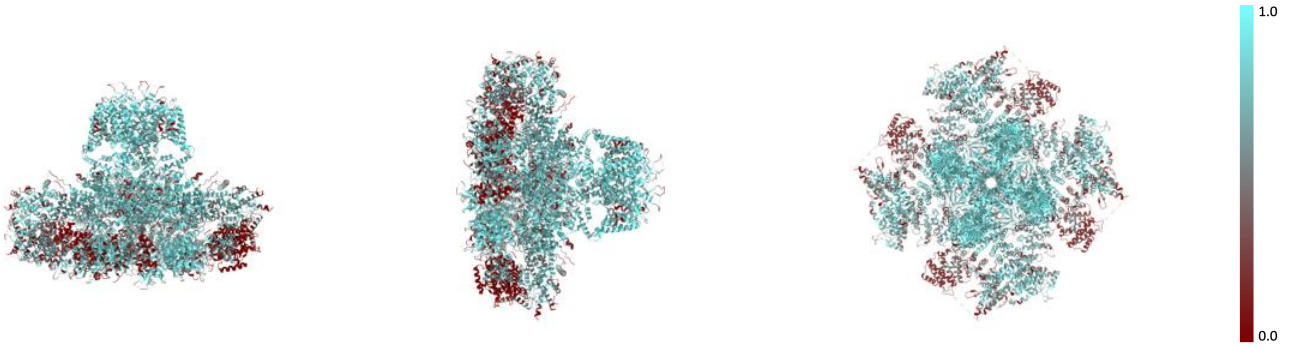
9.2 Q-score mapped to coordinate model (i)



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.

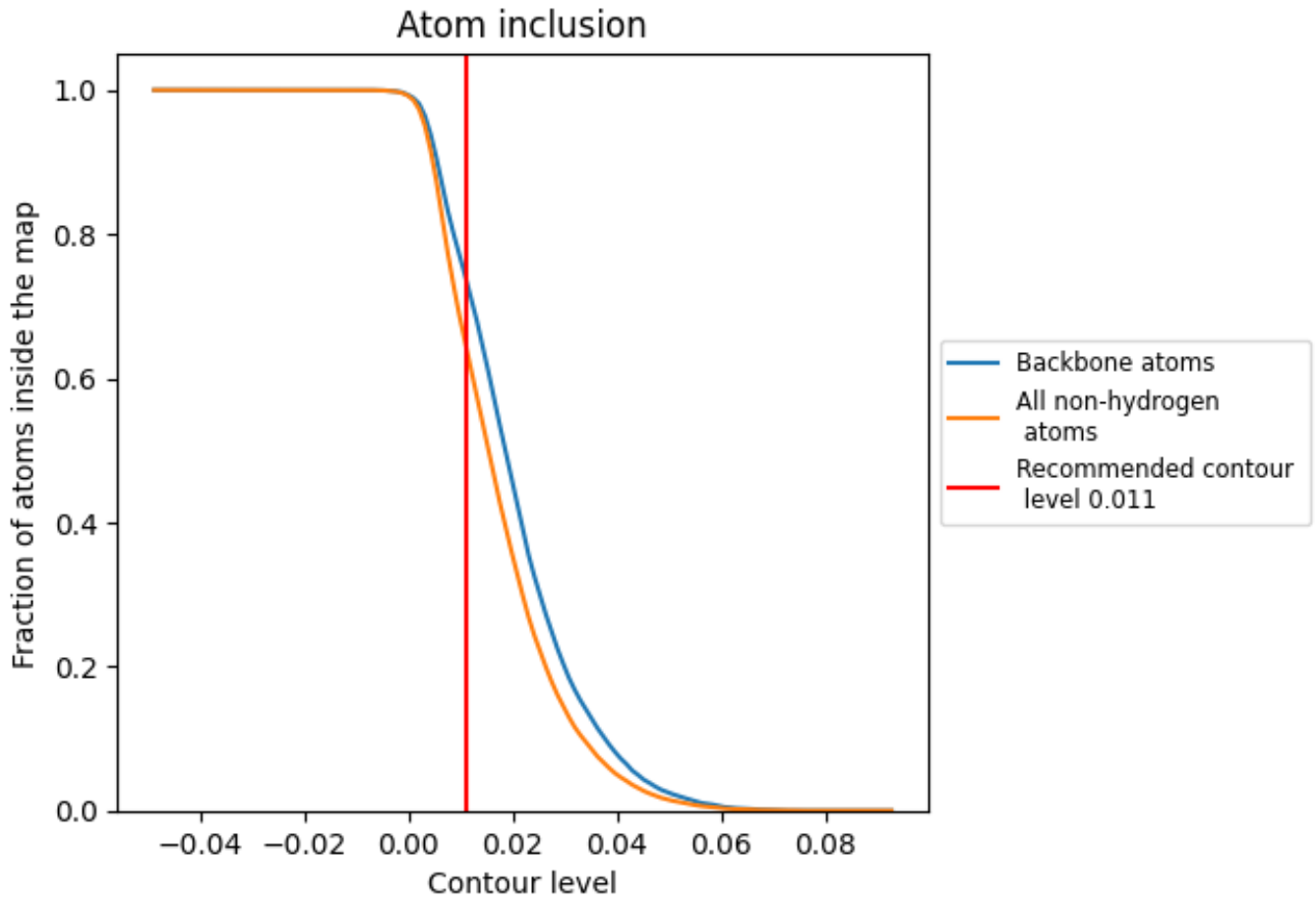
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6469	0.3500
A	0.6467	0.3500
B	0.6468	0.3500
C	0.6471	0.3500
D	0.6471	0.3500