Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 12:41 AM EST

PDB ID	:	7LHE
EMDB ID	:	EMD-23337
Title	:	Structure of full-length IP3R1 channel reconstituted into lipid nanodisc in the apo-state
Authors	:	Baker, M.R.; Fan, G.; Baker, M.L.; Serysheva, I.I.
Deposited on	:	2021-01-22
Resolution	:	3.30 Å(reported)
Based on initial model	:	6MU2

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:

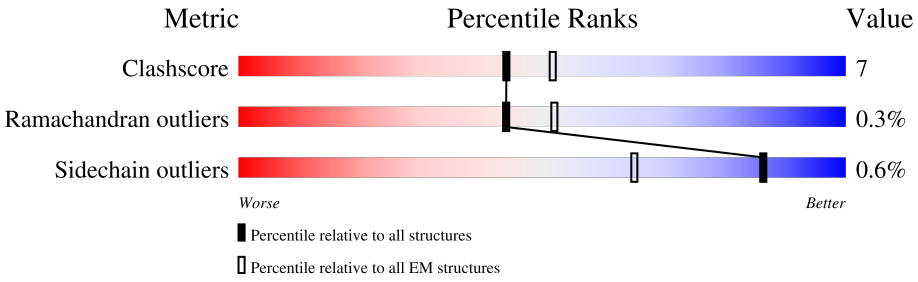
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	2734	18% 69% 14% • 16%
1	B	2734	18% 69% 14% • 16%
1	C	2734	18% 69% 14% • 16%
1	D	2734	18% 70% 14% • 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLX	A	2801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLX	A	2802	X	-	-	-
2	PLX	A	2803	X	-	-	-
2	PLX	A	2804	X	-	-	-
2	PLX	A	2806	X	-	-	-
2	PLX	A	2807	X	-	-	-
2	PLX	A	2808	X	-	-	-
2	PLX	B	2801	X	-	-	-
2	PLX	B	2802	X	-	-	-
2	PLX	B	2803	X	-	-	-
2	PLX	B	2804	X	-	-	-
2	PLX	B	2805	X	-	-	-
2	PLX	B	2806	X	-	-	-
2	PLX	B	2807	X	-	-	-
2	PLX	B	2808	X	-	-	-
2	PLX	C	2801	X	-	-	-
2	PLX	C	2802	X	-	-	-
2	PLX	C	2803	X	-	-	-
2	PLX	C	2804	X	-	-	-
2	PLX	C	2805	X	-	-	-
2	PLX	C	2807	X	-	-	-
2	PLX	C	2808	X	-	-	-
2	PLX	D	2801	X	-	-	-
2	PLX	D	2802	X	-	-	-
2	PLX	D	2803	X	-	-	-
2	PLX	D	2804	X	-	-	-
2	PLX	D	2806	X	-	-	-
2	PLX	D	2807	X	-	-	-

2 Entry composition

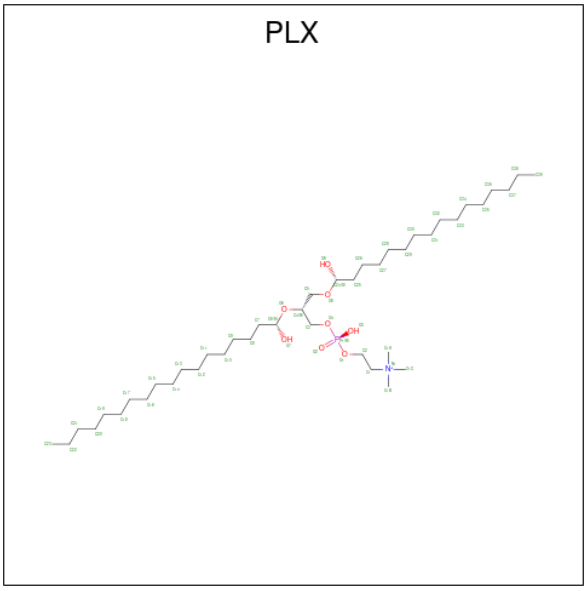
There are 3 unique types of molecules in this entry. The entry contains 73691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2298	Total	C	N	O	S	0	0
			18148	11558	3171	3309	110		
1	D	2298	Total	C	N	O	S	0	0
			18148	11558	3171	3309	110		
1	C	2298	Total	C	N	O	S	0	0
			18148	11558	3171	3309	110		
1	B	2298	Total	C	N	O	S	0	0
			18148	11558	3171	3309	110		

- Molecule 2 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: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			34	24	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
2	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	D	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	D	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	D	1	Total	C	N	O	P	0
			43	33	1	8	1	
2	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
2	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	B	1	Total	C	N	O	P	0
			46	36	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
2	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	B	1	Total	C	N	O	P	0
			34	24	1	8	1	
2	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	B	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

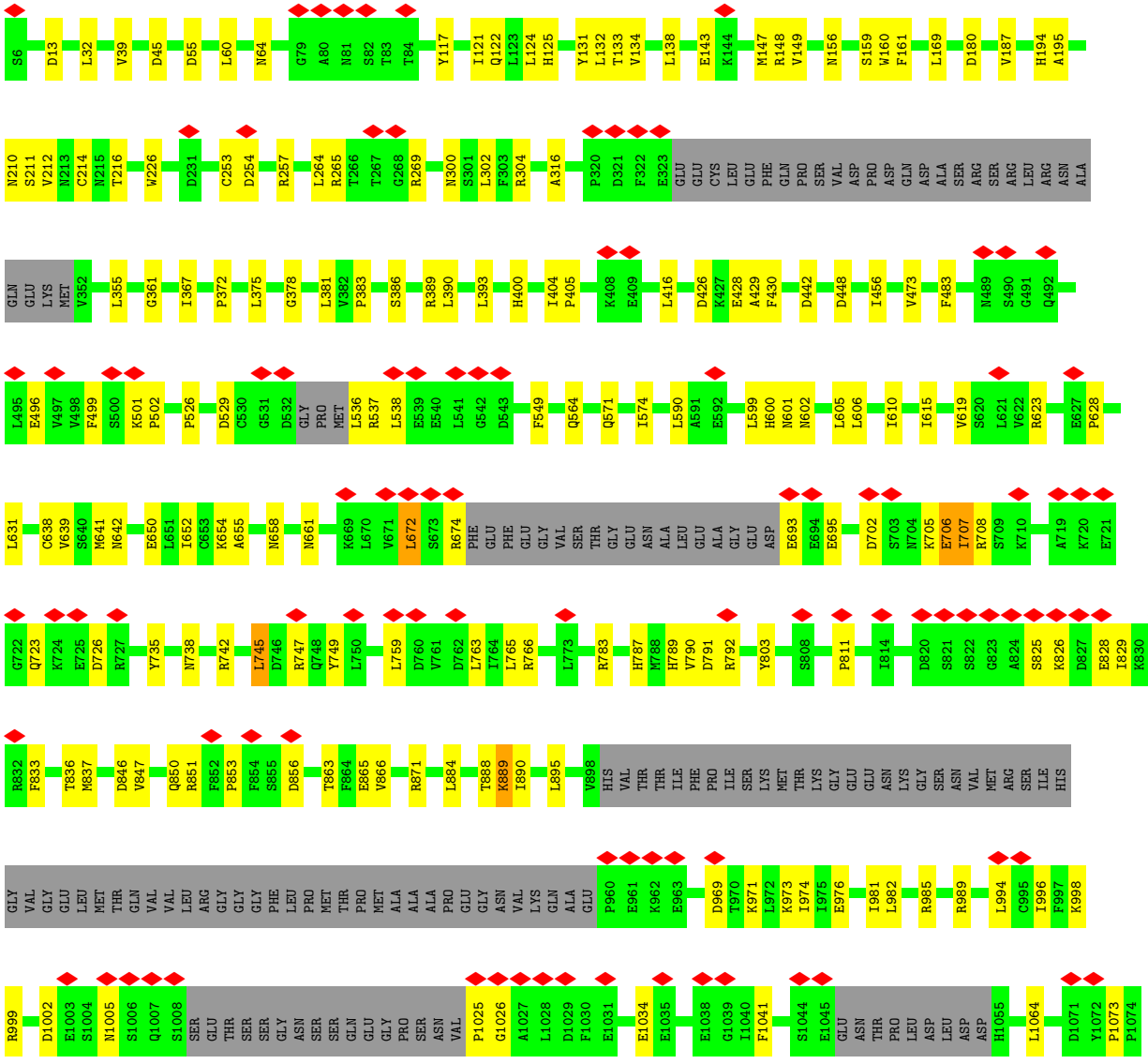
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	

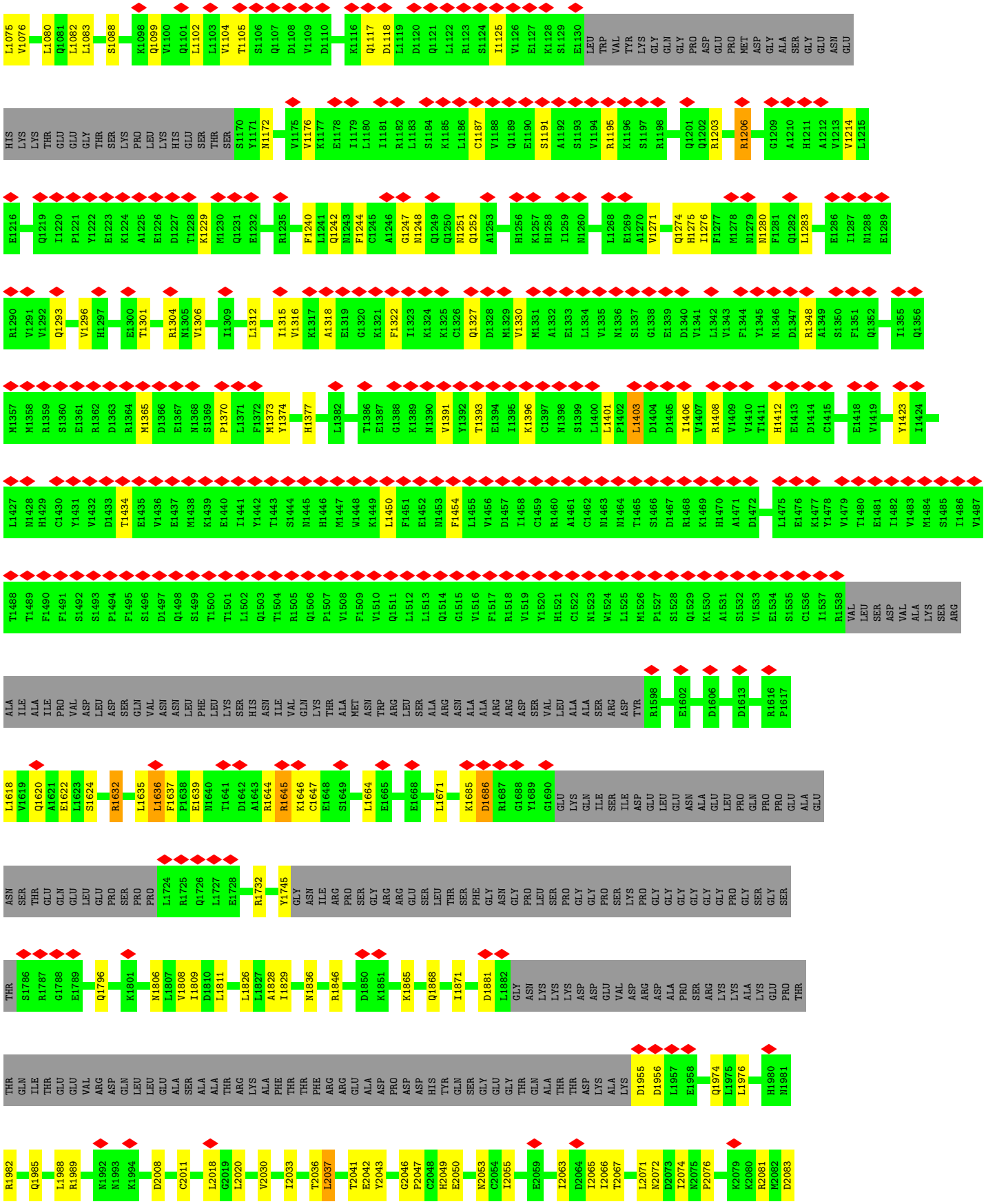
3 Residue-property plots (i)

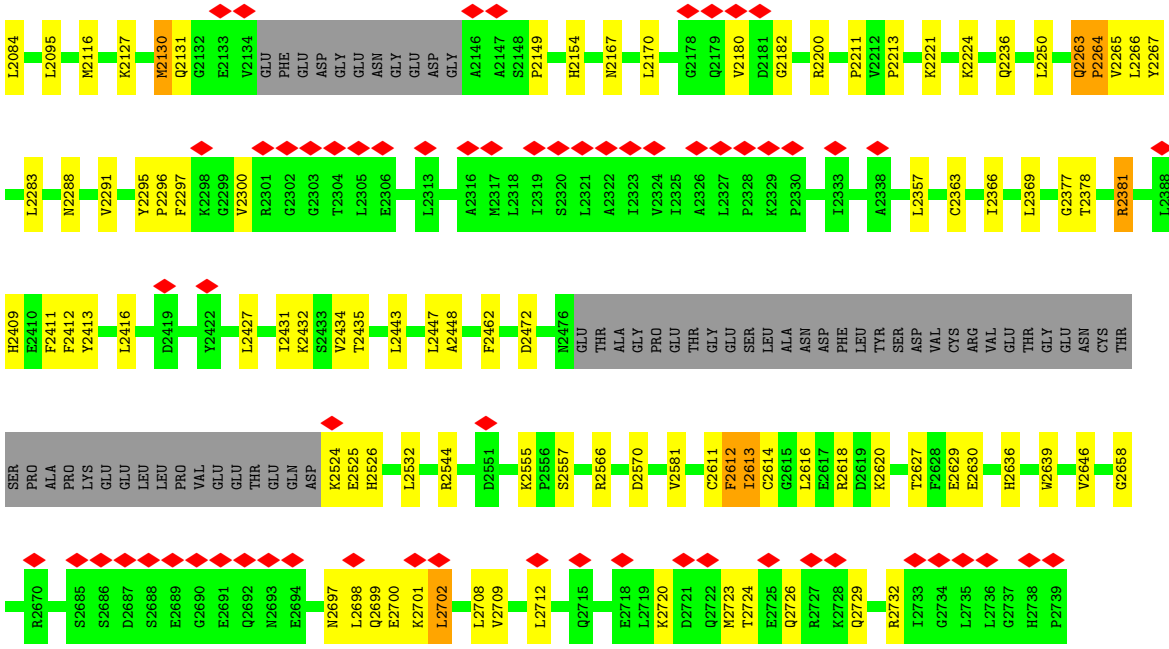
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

Chain A:

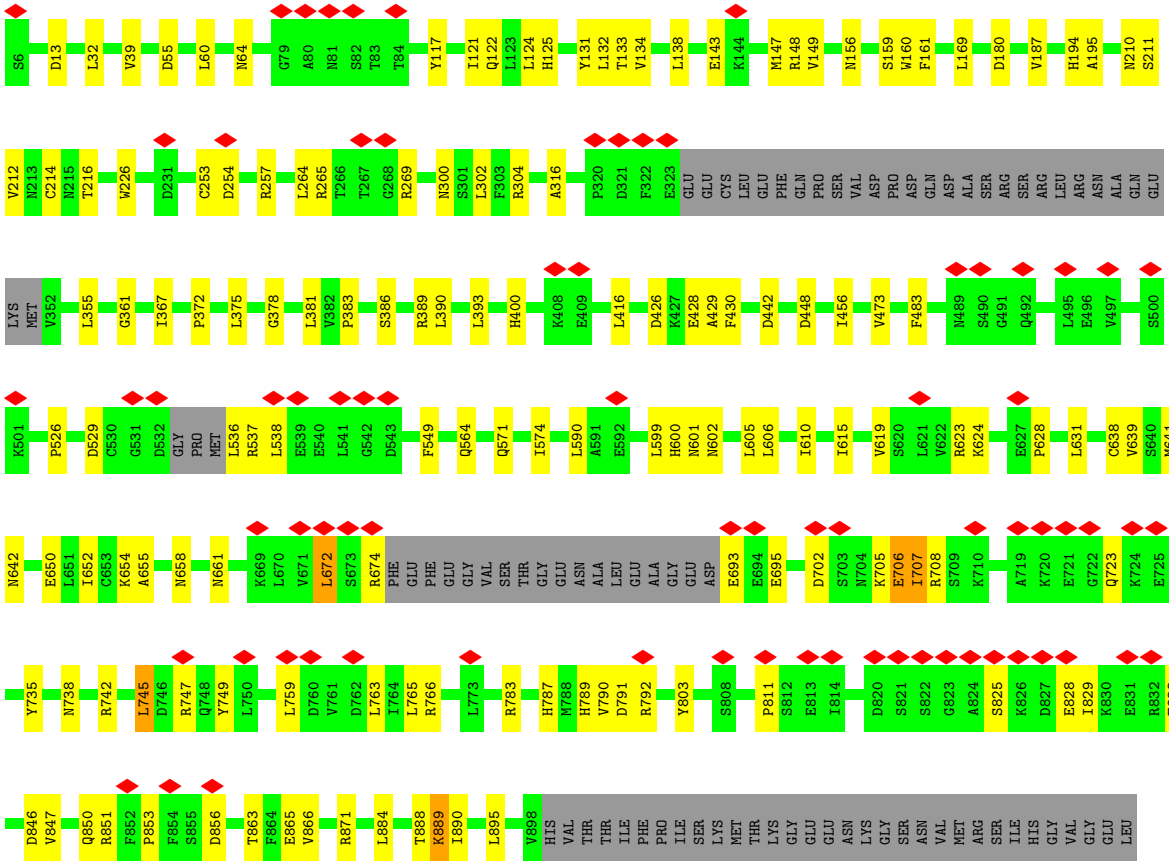


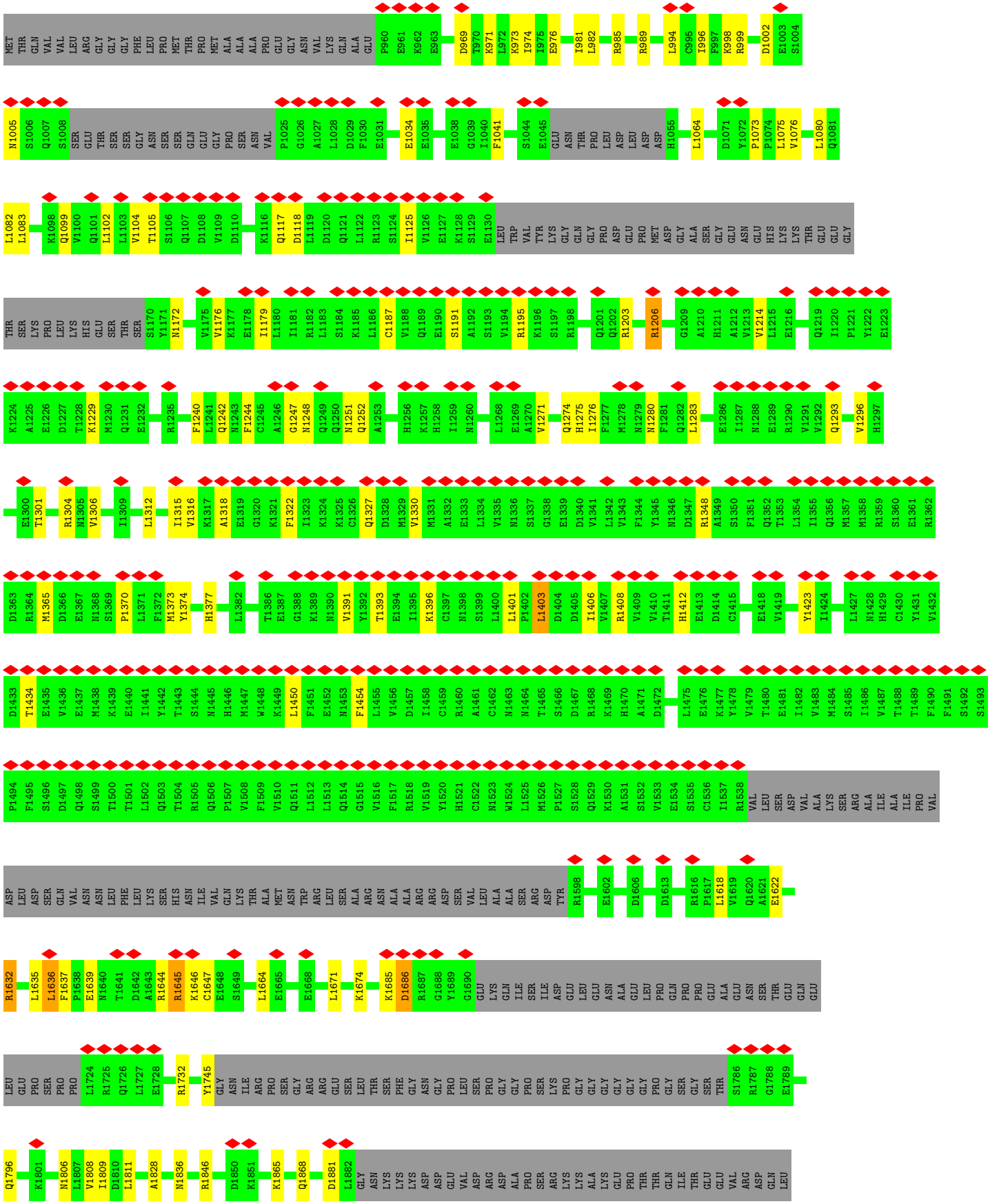

L1075 V1076 L1080 Q1081 L1082 L1083 S1088 K1098 Q1099 V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 D1109 D1110 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU
HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 V1175 V1176 K1177 E1178 I1179 L1180 I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 Q1201 Q1202 R1203 R1206 G1209 A1210 H1211 A1212 V1213 V1214 L1215
E1216 Q1219 I1220 P1221 Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 R1235 F1240 L1241 Q1242 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 H1256 K1257 H1258 I1259 N1260 L1268 E1269 A1270 V1271 Q1274 H1275 I1276 F1277 M1278 N1279 N1280 F1281 Q1282 L1283 E1286 I1287 N1288 E1289
R1290 V1291 V1292 Q1293 V1296 H1297 E1300 T1301 R1304 N1305 V1306 I1309 L1312 I1315 V1316 K1317 A1318 E1319 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 I1355 Q1356
M1357 M1358 R1359 S1360 E1361 R1362 D1363 R1364 M1365 D1366 E1367 N1368 S1369 P1370 L1371 F1372 M1373 Y1374 H1377 L1382 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 E1418 V1419 Y1423 I1424
L1427 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 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487
T1488 T1489 F1490 F1491 S1492 S1493 P1494 F1495 S1496 D1497 Q1498 S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG
ALA ILE ALA ILE PRO VAL ASP LEU ASP SER GLN VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 E1602 D1606 D1613 R1616 P1617
L1618 V1619 Q1620 A1621 E1622 L1623 S1624 R1632 L1635 L1636 F1637 P1638 E1639 N1640 T1641 D1642 A1643 R1644 R1645 K1646 C1647 E1648 S1649 L1664 E1665 E1668 L1671 K1685 D1686 R1687 G1688 Y1689 G1690 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 PRO PRO L1724 R1725 Q1726 L1727 E1728 R1732 Y1745 GLY ASN ILE 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 SER
THR S1786 R1787 G1788 E1789 Q1796 K1801 N1806 L1807 V1808 I1809 D1810 L1811 L1826 L1827 A1828 I1829 N1836 R1846 D1850 K1851 K1865 Q1868 I1871 D1881 L1882 GLY ASN LYS 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 LEU GLU ALA SER ALA ALA ALA THR ARG LYS ALA PHE THR THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 L1967 E1958 Q1974 L1975 L1976 H1980 N1981
R1982 Q1985 L1988 R1989 N1992 N1993 K1994 D2008 C2011 L2018 G2019 L2020 V2030 I2033 T2036 L2037 T2041 E2042 Y2043 G2046 P2047 C2048 H2049 E2050 N2053 C2054 I2055 E2059 I2063 D2064 I2065 I2066 T2067 L2071 N2072 D2073 I2074 N2075 P2076 K2079 K2080 R2081 M2082 D2083

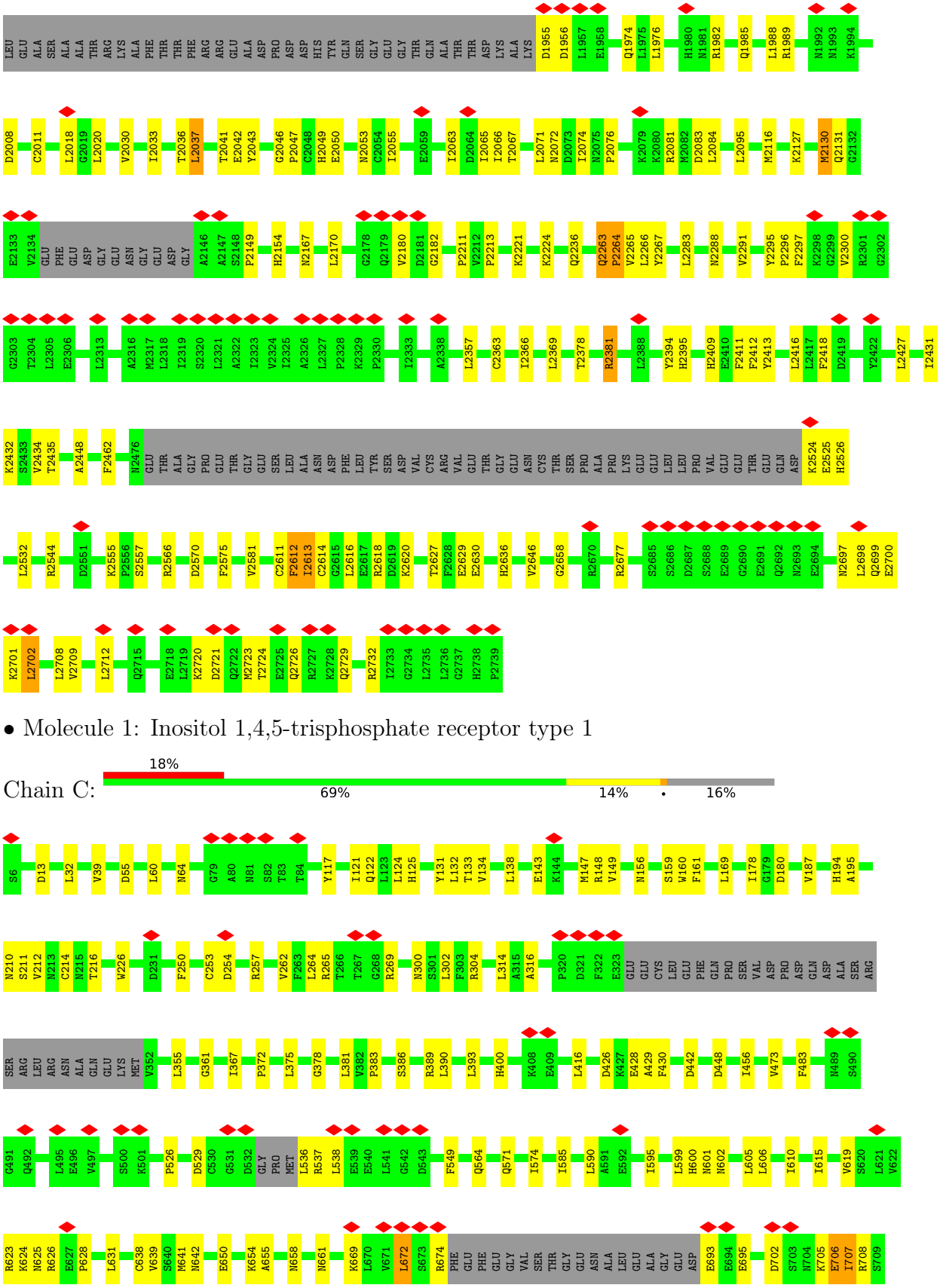


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain D:

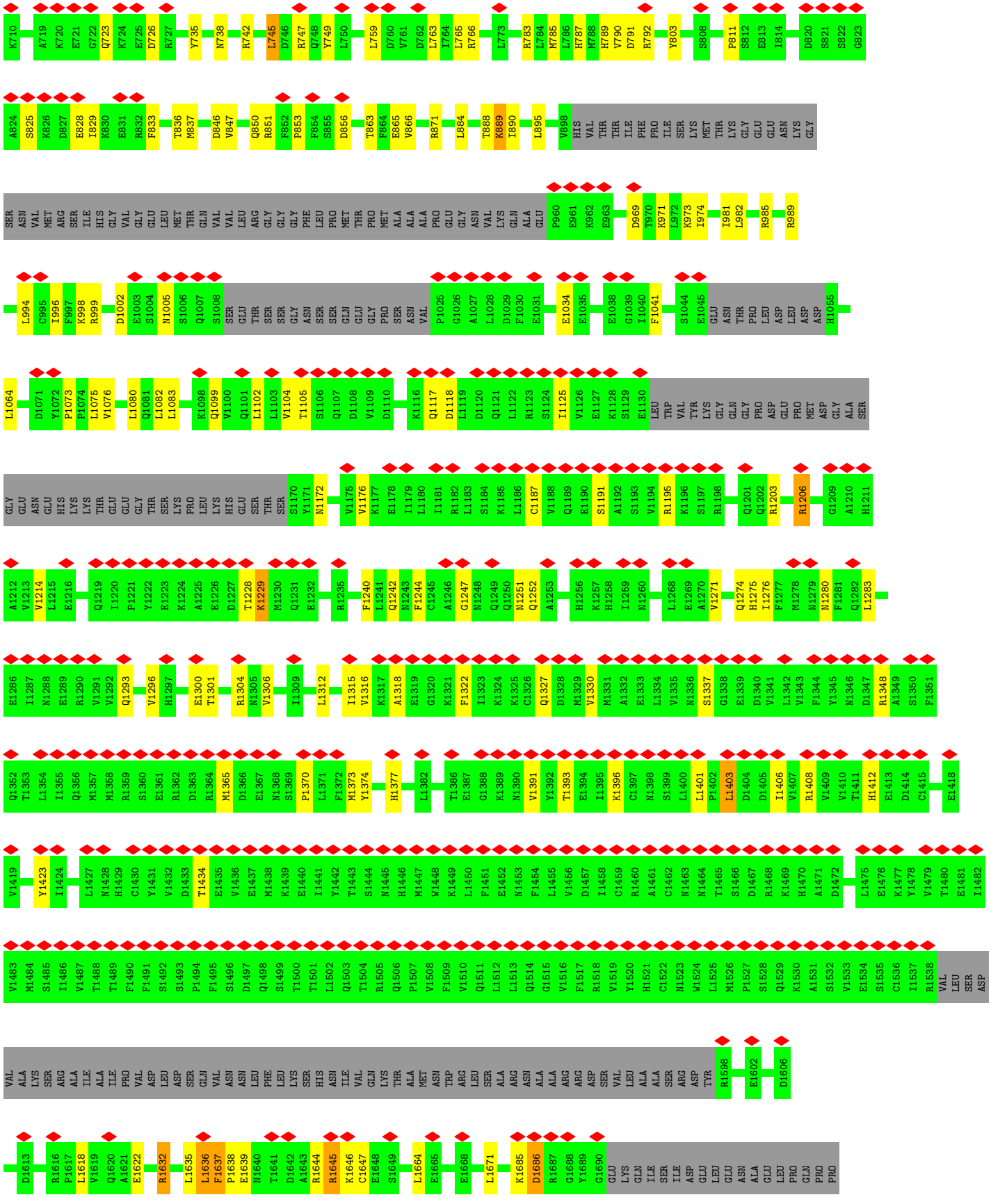



MET THR GLN VAL VAL LEU ARG GLY GLY GLY PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU
P960 E961 K962 E963 D969 T970 K971 L972 K973 I974 I975 E976 I981 L982 R985 R989 L994 C995 I996 F997 K998 R999 D1002 E1003 S1004
N1005 S1006 Q1007 S1008 SER GLU THR SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL P1025 G1026 A1027 L1028 D1029 F1030 E1031 E1034 E1035 E1038 G1039 I1040 F1041 S1044 E1045 GLU ASN THR PRO LEU ASP LEU ASP H1055 L1064 D1071 Y1072 P1073 P1074 L1075 V1076 L1080 Q1081
L1082 L1083 K1098 Q1099 V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 V1109 D1110 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY
THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 V1175 V1176 K1177 E1178 I1179 L1180 I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 Q1201 Q1202 R1203 R1206 G1209 A1210 H1211 A1212 V1213 V1214 L1215 E1216 Q1219 I1220 P1221 Y1222 E1223
K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 R1235 F1240 L1241 Q1242 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 H1256 K1257 H1258 I1259 N1260 L1268 E1269 A1270 V1271 Q1274 H1275 I1276 F1277 M1278 N1279 N1280 F1281 Q1282 L1283 E1286 I1287 N1288 E1289 R1290 V1291 V1292 Q1293 V1296 H1297
E1300 T1301 R1304 N1305 V1306 I1309 L1312 I1315 V1316 K1317 A1318 E1319 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 Y1374 H1377 L1382 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 E1418 V1419 Y1423 I1424 L1427 N1428 H1429 C1430 Y1431 V1432
D1433 T1434 E1435 V1436 D1437 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 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 F1491 S1492 S1493
P1494 F1495 S1496 D1497 Q1498 S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL
ASP LEU ASP SER GLN VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 E1602 D1606 D1613 R1616 P1617 L1618 V1619 Q1620 A1621 E1622
R1632 L1635 L1636 F1637 P1638 E1639 N1640 T1641 D1642 A1643 R1644 R1645 K1646 C1647 E1648 S1649 L1664 E1665 E1668 L1671 K1674 K1685 D1686 R1687 G1688 Y1689 G1690 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 PRO PRO L1724 R1725 Q1726 L1727 E1728 R1732 Y1745 GLY ASN ILE 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 SER THR S1786 R1787 G1788 E1789
Q1796 K1801 N1806 L1807 V1808 I1809 D1810 L1811 A1828 N1836 R1846 D1850 K1851 K1865 Q1868 D1881 L1882 GLY ASN LYS 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



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

Chain C: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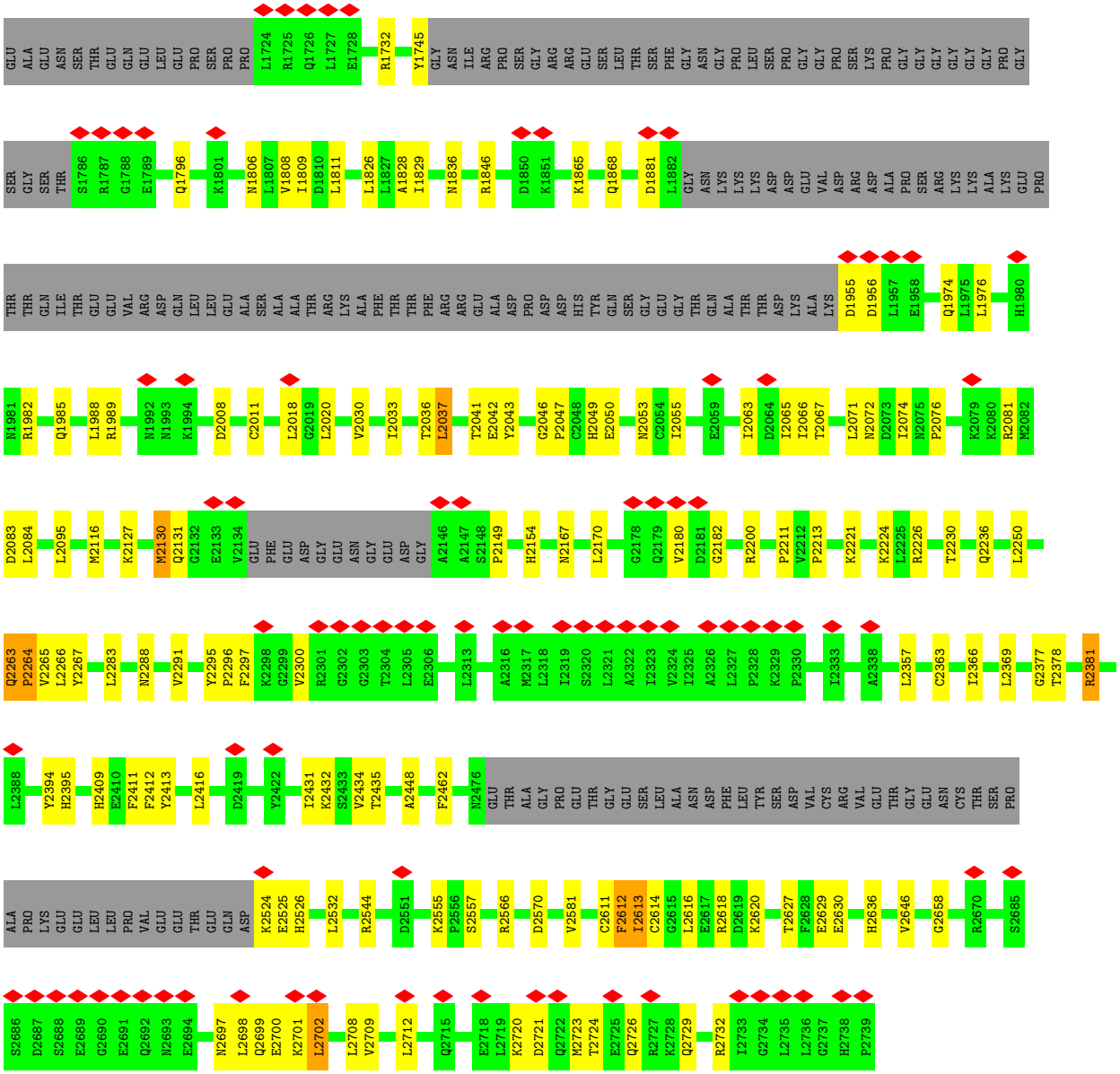
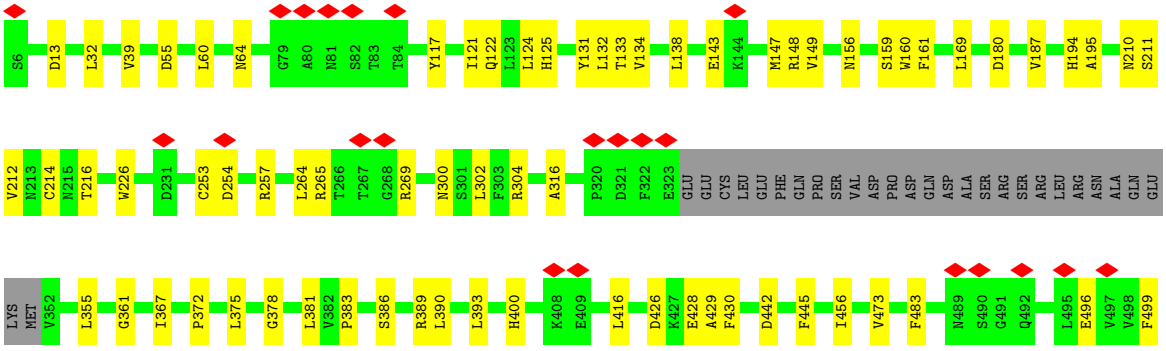
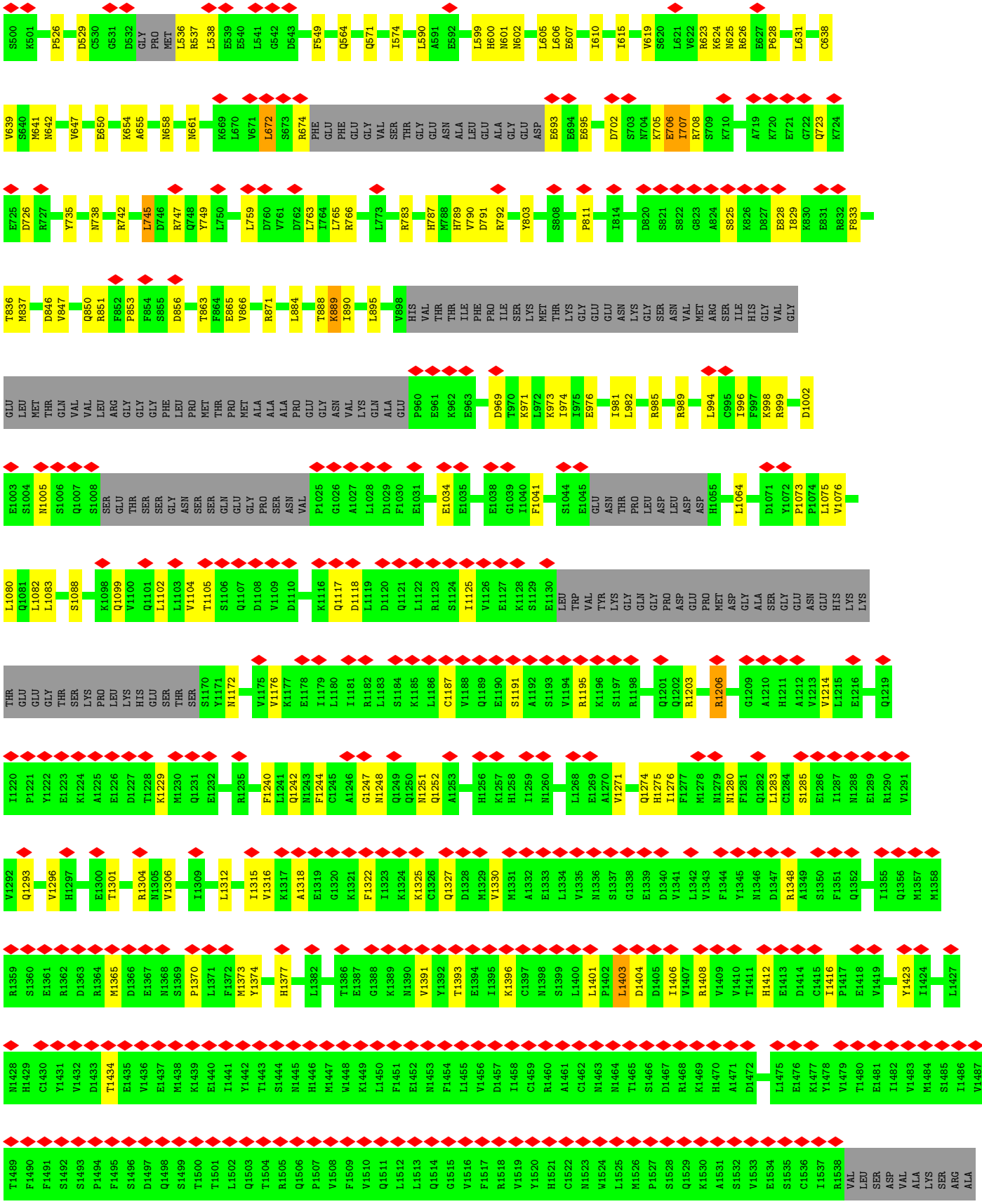
A824 S825 K826 D827 E828 I829 K830 E831 R832 F833 T836 M837 D846 V847 Q850 R851 F852 P853 F854 S855 D856 T863 F864 E865 V866 R871 L884 T888 K889 I890 L895 V898 HIS VAL THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY
SER ASN VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL 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 D969 T970 K971 L972 K973 I974 I981 L982 R985 R989
L994 C995 I996 F997 K998 R999 D1002 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 D1029 F1030 E1031 E1034 E1035 E1038 G1039 I1040 F1041 S1044 E1045 GLU ASN THR PRO LEU ASP LEU ASP ASP H1055
L1064 D1071 Y1072 P1073 P1074 L1075 V1076 L1080 Q1081 L1082 L1083 K1098 Q1099 V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 V1109 D1110 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER
GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 V1175 V1176 K1177 E1178 I1179 L1180 I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 Q1201 Q1202 R1203 R1206 G1209 A1210 H1211
A1212 V1213 V1214 L1215 E1216 Q1219 I1220 P1221 Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 R1235 F1240 L1241 Q1242 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 H1256 K1257 H1258 I1259 N1260 L1268 E1269 A1270 V1271 Q1274 H1275 I1276 F1277 M1278 N1279 N1280 F1281 Q1282 L1283
E1286 I1287 N1288 E1289 R1290 V1291 V1292 Q1293 V1296 H1297 E1300 T1301 R1304 N1305 V1306 I1309 L1312 I1315 V1316 K1317 A1318 E1319 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 Y1374 H1377 L1382 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 E1418
V1419 Y1423 I1424 L1427 N1428 H1429 C1430 Y1431 V1432 S1433 D1434 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 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482
V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 F1491 S1492 S1493 P1494 F1495 S1496 D1497 Q1498 S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP
VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP SER GLN VAL VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 E1602 D1606
D1613 R1616 P1617 L1618 V1619 Q1620 A1621 E1622 R1632 L1635 L1636 F1637 P1638 E1639 N1640 T1641 D1642 A1643 R1644 R1645 K1646 C1647 E1648 S1649 L1664 E1665 E1668 L1671 K1685 D1686 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO



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

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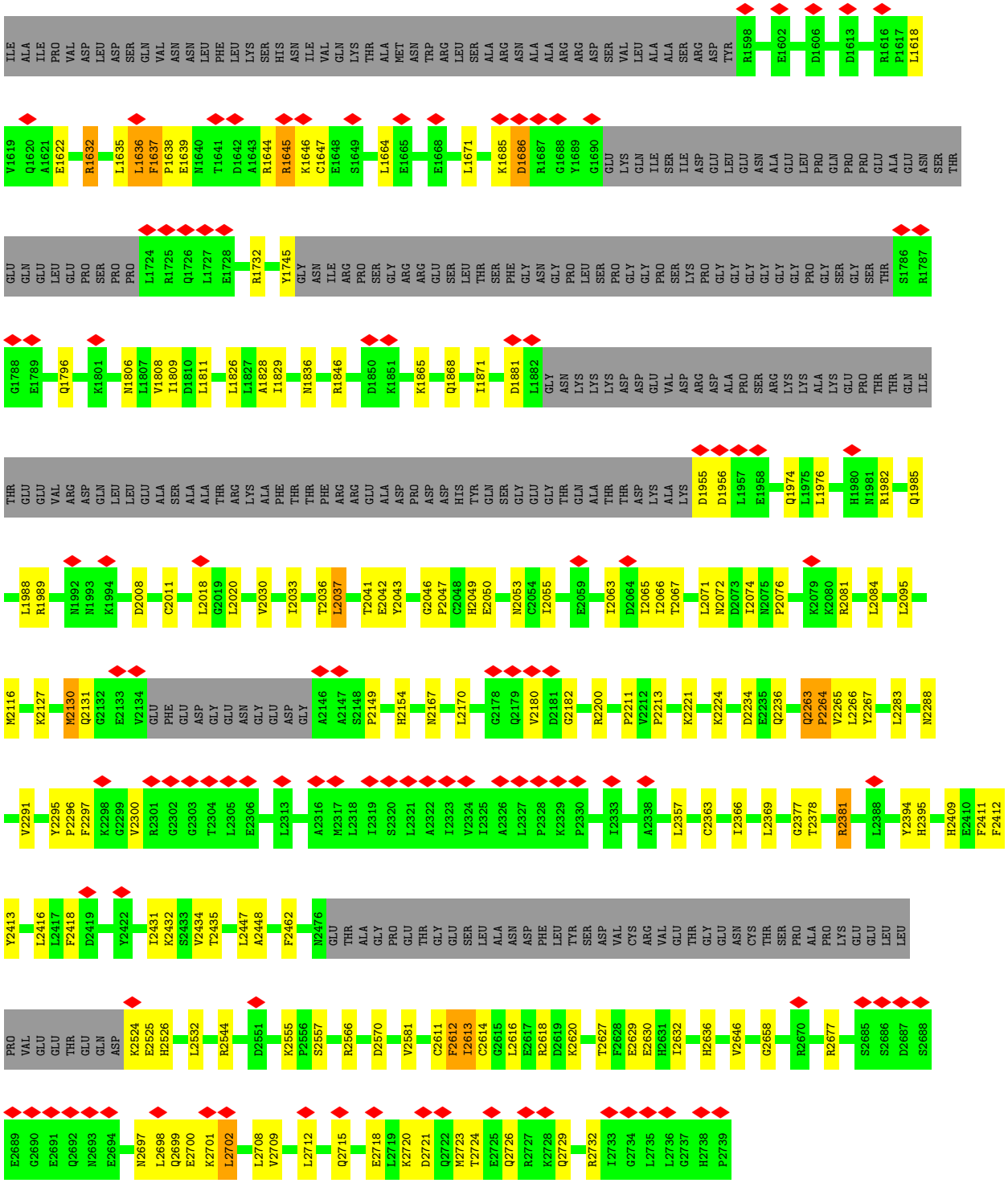
V639 S640 M641 N642 V647 E650 K654 A655 N658 N661 K669 L670 V671 L672 S673 R674 PHE GLU PHE GLU GLY VAL SER THR GLY GLU GLN ALA LEU GLU ALA GLY GLU ASP E693 E694 E695 D702 S703 N704 K705 E706 I707 R708 S709 K710 A719 K720 E721 G722 Q723 K724
E725 D726 R727 Y735 N738 R742 L745 D746 R747 G748 Y749 L750 L759 D760 V761 D762 L763 I764 L765 R766 L773 R783 H787 M788 H789 V790 D791 R792 Y803 S808 P811 I814 D820 S821 S822 G823 A824 S825 K826 D827 E828 I829 K830 E831 R832 F833
T836 M837 D846 V847 Q850 R851 F852 P853 F854 S855 D856 T863 F864 E865 V866 R871 L884 T888 K889 I890 L895 V898 HIS VAL 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 D969 T970 K971 L972 K973 I974 I975 E976 I981 L982 R985 R989 L994 C995 I996 F997 K998 R999 D1002
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 D1029 F1030 E1031 E1034 E1035 E1038 G1039 I1040 F1041 S1044 E1045 GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 L1064 D1071 Y1072 P1073 P1074 L1075 V1076
L1080 Q1081 L1082 L1083 S1088 K1098 Q1099 V1100 Q1101 L1102 L1103 V1104 T1105 S1106 Q1107 D1108 V1109 D1110 K1116 Q1117 D1118 L1119 D1120 Q1121 L1122 R1123 S1124 I1125 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY GLY ALA SER GLY GLU ASN GLU HIS LYS LYS
THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 V1175 V1176 K1177 E1178 I1179 L1180 I1181 R1182 L1183 S1184 K1185 L1186 C1187 V1188 Q1189 E1190 S1191 A1192 S1193 V1194 R1195 K1196 S1197 R1198 Q1201 Q1202 R1203 R1206 G1209 A1210 H1211 A1212 V1213 V1214 L1215 E1216 Q1219
I1220 P1221 Y1222 E1223 K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 R1235 F1240 L1241 Q1242 N1243 F1244 C1245 A1246 G1247 N1248 Q1249 Q1250 N1251 Q1252 A1253 H1256 K1257 H1258 I1259 N1260 L1268 E1269 A1270 V1271 Q1274 H1275 I1276 F1277 M1278 N1279 N1280 F1281 Q1282 L1283 C1284 S1285 E1286 I1287 N1288 E1289 R1290 V1291
V1292 Q1293 V1296 H1297 E1300 T1301 R1304 N1305 V1306 I1309 L1312 I1315 V1316 K1317 A1318 E1319 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 I1355 Q1356 M1357 M1358
R1359 S1360 E1361 R1362 D1363 R1364 M1365 D1366 E1367 N1368 S1369 P1370 L1371 F1372 M1373 Y1374 H1377 L1382 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 D1405 I1406 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 Y1423 I1424 L1427
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 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488
T1489 F1490 F1491 S1492 S1493 P1494 F1495 S1496 D1497 Q1498 S1499 T1500 T1501 L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	573723	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.754	Depositor
Minimum map value	-0.700	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.263	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/18460	0.64	19/24875 (0.1%)
1	B	0.28	0/18460	0.64	19/24875 (0.1%)
1	C	0.28	0/18460	0.64	19/24875 (0.1%)
1	D	0.28	0/18460	0.64	19/24875 (0.1%)
All	All	0.28	0/73840	0.64	76/99500 (0.1%)

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	7
1	B	0	7
1	C	0	7
1	D	0	7
All	All	0	28

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1403	LEU	CA-CB-CG	9.26	136.59	115.30
1	A	1403	LEU	CA-CB-CG	9.26	136.59	115.30
1	C	1403	LEU	CA-CB-CG	9.26	136.59	115.30
1	D	1403	LEU	CA-CB-CG	9.24	136.56	115.30
1	A	381	LEU	CA-CB-CG	8.48	134.80	115.30
1	D	381	LEU	CA-CB-CG	8.48	134.80	115.30
1	C	381	LEU	CA-CB-CG	8.48	134.80	115.30
1	B	381	LEU	CA-CB-CG	8.48	134.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	672	LEU	CA-CB-CG	7.64	132.86	115.30
1	A	672	LEU	CA-CB-CG	7.63	132.84	115.30
1	B	672	LEU	CA-CB-CG	7.63	132.84	115.30
1	D	672	LEU	CA-CB-CG	7.62	132.84	115.30
1	A	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	D	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	C	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	B	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	A	2702	LEU	CA-CB-CG	7.44	132.42	115.30
1	C	2702	LEU	CA-CB-CG	7.44	132.42	115.30
1	B	2702	LEU	CA-CB-CG	7.44	132.42	115.30
1	D	2702	LEU	CA-CB-CG	7.44	132.41	115.30
1	D	590	LEU	CA-CB-CG	6.83	131.00	115.30
1	B	590	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	590	LEU	CA-CB-CG	6.82	130.98	115.30
1	C	590	LEU	CA-CB-CG	6.82	130.98	115.30
1	C	994	LEU	CA-CB-CG	6.53	130.32	115.30
1	D	994	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	994	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	994	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	D	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	C	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	B	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	B	1636	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	1636	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	1636	LEU	CA-CB-CG	6.16	129.46	115.30
1	C	1636	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	1365	MET	CA-CB-CG	5.97	123.45	113.30
1	D	1365	MET	CA-CB-CG	5.97	123.45	113.30
1	D	2708	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	1365	MET	CA-CB-CG	5.97	123.45	113.30
1	B	2708	LEU	CA-CB-CG	5.97	129.03	115.30
1	C	1365	MET	CA-CB-CG	5.96	123.43	113.30
1	A	2708	LEU	CA-CB-CG	5.95	128.99	115.30
1	C	2708	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	599	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	599	LEU	CA-CB-CG	5.72	128.45	115.30
1	B	599	LEU	CA-CB-CG	5.70	128.42	115.30
1	C	599	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	1102	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	1102	LEU	CA-CB-CG	5.59	128.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1102	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	1102	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	2020	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	2020	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	2020	LEU	CA-CB-CG	5.56	128.09	115.30
1	D	2020	LEU	CA-CB-CG	5.55	128.07	115.30
1	D	2723	MET	CA-CB-CG	5.52	122.69	113.30
1	A	2723	MET	CA-CB-CG	5.52	122.69	113.30
1	B	2723	MET	CA-CB-CG	5.49	122.63	113.30
1	C	2723	MET	CA-CB-CG	5.49	122.62	113.30
1	C	132	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	132	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	132	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	132	LEU	CA-CB-CG	5.41	127.73	115.30
1	C	2130	MET	CA-CB-CG	5.22	122.17	113.30
1	A	2130	MET	CA-CB-CG	5.20	122.14	113.30
1	D	2130	MET	CA-CB-CG	5.20	122.14	113.30
1	B	2130	MET	CA-CB-CG	5.20	122.14	113.30
1	C	1401	LEU	CA-CB-CG	5.19	127.25	115.30
1	B	1401	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	1401	LEU	CA-CB-CG	5.19	127.23	115.30
1	D	1401	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	2037	LEU	CA-CB-CG	5.12	127.09	115.30
1	D	2037	LEU	CA-CB-CG	5.12	127.09	115.30
1	C	2037	LEU	CA-CB-CG	5.12	127.09	115.30
1	B	2037	LEU	CA-CB-CG	5.12	127.09	115.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1637	PHE	Peptide
1	A	2263	GLN	Peptide
1	A	2295	TYR	Peptide
1	A	2296	PRO	Peptide
1	A	2532	LEU	Peptide
1	A	706	GLU	Peptide
1	A	707	ILE	Peptide
1	B	1637	PHE	Peptide
1	B	2263	GLN	Peptide
1	B	2295	TYR	Peptide
1	B	2296	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	2532	LEU	Peptide
1	B	706	GLU	Peptide
1	B	707	ILE	Peptide
1	C	1637	PHE	Peptide
1	C	2263	GLN	Peptide
1	C	2295	TYR	Peptide
1	C	2296	PRO	Peptide
1	C	2532	LEU	Peptide
1	C	706	GLU	Peptide
1	C	707	ILE	Peptide
1	D	1637	PHE	Peptide
1	D	2263	GLN	Peptide
1	D	2295	TYR	Peptide
1	D	2296	PRO	Peptide
1	D	2532	LEU	Peptide
1	D	706	GLU	Peptide
1	D	707	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18148	0	17980	255	0
1	B	18148	0	17980	256	0
1	C	18148	0	17980	252	0
1	D	18148	0	17980	245	0
2	A	274	0	370	29	0
2	B	313	0	422	33	0
2	C	274	0	369	30	0
2	D	234	0	315	29	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	73691	0	73396	1013	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 7.

All (1013) 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:C:2409:HIS:CG	2:C:2804:PLX:H51	1.37	1.58
1:D:2409:HIS:CG	2:D:2803:PLX:H51	1.40	1.54
1:A:2409:HIS:CG	2:A:2803:PLX:H51	1.46	1.49
1:C:2409:HIS:CD2	2:C:2804:PLX:H51	1.49	1.46
1:B:2409:HIS:CG	2:B:2807:PLX:H51	1.49	1.43
1:D:2409:HIS:CD2	2:D:2803:PLX:H51	1.56	1.40
1:B:2409:HIS:CE1	2:B:2807:PLX:H51	1.60	1.36
1:B:2409:HIS:CD2	2:B:2807:PLX:H51	1.61	1.36
1:B:2462:PHE:CD2	2:B:2802:PLX:O9	1.79	1.35
1:A:2409:HIS:CD2	2:A:2803:PLX:H51	1.62	1.35
1:B:2409:HIS:CD2	2:B:2807:PLX:H32	1.63	1.32
1:A:2409:HIS:CD2	2:A:2803:PLX:H32	1.66	1.30
1:B:2409:HIS:ND1	2:B:2807:PLX:H51	1.48	1.28
1:A:2570:ASP:OD2	1:D:2544:ARG:NH2	1.69	1.26
1:D:2570:ASP:OD2	1:C:2544:ARG:NH2	1.68	1.25
1:B:2409:HIS:CG	2:B:2807:PLX:C5	2.17	1.24
1:C:2462:PHE:CD2	2:C:2807:PLX:O9	1.91	1.24
1:A:2462:PHE:CD2	2:A:2806:PLX:O9	1.91	1.24
1:A:2544:ARG:NH2	1:B:2570:ASP:OD2	1.68	1.23
1:C:2570:ASP:OD2	1:B:2544:ARG:NH2	1.68	1.23
1:D:2409:HIS:CD2	2:D:2803:PLX:H32	1.77	1.20
1:C:2409:HIS:CG	2:C:2804:PLX:C5	2.25	1.19
1:A:2409:HIS:CG	2:A:2803:PLX:C5	2.23	1.19
1:A:2409:HIS:ND1	2:A:2803:PLX:H51	1.57	1.17
1:A:2409:HIS:CE1	2:A:2803:PLX:H51	1.78	1.17
1:B:2462:PHE:CG	2:B:2802:PLX:O9	1.98	1.16
1:D:2409:HIS:CG	2:D:2803:PLX:C5	2.29	1.14
1:C:2409:HIS:CD2	2:C:2804:PLX:H32	1.84	1.11
1:B:2409:HIS:NE2	2:B:2807:PLX:H51	1.66	1.09
1:B:2409:HIS:CD2	2:B:2807:PLX:C3	2.39	1.05
1:B:2409:HIS:CD2	2:B:2807:PLX:C5	2.38	1.05
1:B:2409:HIS:CE1	2:B:2807:PLX:C5	2.42	1.03
1:A:2409:HIS:CD2	2:A:2803:PLX:C3	2.42	1.03
1:B:2409:HIS:ND1	2:B:2807:PLX:C5	2.21	1.01
1:A:2409:HIS:CD2	2:A:2803:PLX:C5	2.42	1.00
1:C:2409:HIS:CD2	2:C:2804:PLX:C5	2.40	0.99
1:D:2409:HIS:CD2	2:D:2803:PLX:C5	2.46	0.99
1:C:2462:PHE:CG	2:C:2807:PLX:O9	2.17	0.97
1:D:2409:HIS:ND1	2:D:2803:PLX:H51	1.79	0.97
1:A:2409:HIS:NE2	2:A:2803:PLX:H51	1.79	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:PHE:CG	2:A:2806:PLX:O9	2.17	0.96
1:C:2409:HIS:ND1	2:C:2804:PLX:H51	1.87	0.89
1:D:2409:HIS:CD2	2:D:2803:PLX:C3	2.55	0.89
1:A:2409:HIS:ND1	2:A:2803:PLX:C5	2.34	0.88
1:A:2409:HIS:CE1	2:A:2803:PLX:C5	2.56	0.88
1:B:2409:HIS:HD2	2:B:2807:PLX:H32	1.40	0.86
1:B:2409:HIS:CG	2:B:2807:PLX:H52	2.08	0.86
1:D:2409:HIS:CE1	2:D:2803:PLX:H51	2.10	0.86
1:C:2409:HIS:CD2	2:C:2804:PLX:C3	2.60	0.83
1:A:623:ARG:HH12	1:A:628:PRO:HA	1.44	0.83
1:A:2409:HIS:HD2	2:A:2803:PLX:H32	1.44	0.83
1:B:623:ARG:HH12	1:B:628:PRO:HA	1.44	0.83
1:D:623:ARG:HH12	1:D:628:PRO:HA	1.44	0.81
1:C:623:ARG:HH12	1:C:628:PRO:HA	1.44	0.81
1:D:2462:PHE:CD1	2:D:2806:PLX:O8	2.32	0.79
1:A:2409:HIS:NE2	2:A:2803:PLX:H32	1.98	0.79
1:D:2409:HIS:NE2	2:D:2803:PLX:H51	1.98	0.79
1:C:2409:HIS:CE1	2:C:2804:PLX:H51	2.19	0.77
1:B:2409:HIS:NE2	2:B:2807:PLX:H32	1.99	0.77
1:C:2409:HIS:NE2	2:C:2804:PLX:H51	2.00	0.76
1:A:2462:PHE:CE2	2:A:2806:PLX:O9	2.41	0.74
1:B:2462:PHE:CE2	2:B:2802:PLX:O9	2.41	0.73
1:C:2462:PHE:CE2	2:C:2807:PLX:O9	2.41	0.73
1:D:2462:PHE:CE1	2:D:2806:PLX:C24	2.52	0.71
1:D:2409:HIS:CE1	2:D:2803:PLX:C5	2.74	0.71
1:D:2409:HIS:HD2	2:D:2803:PLX:H32	1.49	0.71
1:D:212:VAL:HG23	1:D:214:CYS:H	1.57	0.70
1:D:1374:TYR:HA	1:D:1377:HIS:HB3	1.74	0.70
1:C:1374:TYR:HA	1:C:1377:HIS:HB3	1.74	0.70
1:C:2409:HIS:ND1	2:C:2804:PLX:C5	2.51	0.70
1:A:212:VAL:HG23	1:A:214:CYS:H	1.57	0.69
1:B:1315:ILE:HG23	1:B:1316:VAL:HG23	1.74	0.69
1:C:1315:ILE:HG23	1:C:1316:VAL:HG23	1.74	0.69
1:A:1315:ILE:HG23	1:A:1316:VAL:HG23	1.74	0.68
1:B:1374:TYR:HA	1:B:1377:HIS:HB3	1.74	0.68
1:A:1374:TYR:HA	1:A:1377:HIS:HB3	1.74	0.68
1:C:2614:CYS:SG	1:C:2636:HIS:CE1	2.87	0.68
1:D:2614:CYS:SG	1:D:2636:HIS:CE1	2.87	0.68
1:B:212:VAL:HG23	1:B:214:CYS:H	1.57	0.68
1:C:212:VAL:HG23	1:C:214:CYS:H	1.57	0.68
1:D:1315:ILE:HG23	1:D:1316:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2409:HIS:CE1	2:C:2804:PLX:C5	2.76	0.68
1:B:2614:CYS:SG	1:B:2636:HIS:CE1	2.87	0.68
1:D:1636:LEU:HA	1:D:1639:GLU:HB3	1.76	0.67
1:A:1636:LEU:HA	1:A:1639:GLU:HB3	1.76	0.67
1:A:2614:CYS:SG	1:A:2636:HIS:CE1	2.87	0.67
1:C:2409:HIS:HD2	2:C:2804:PLX:H32	1.54	0.67
1:D:2409:HIS:ND1	2:D:2803:PLX:C5	2.49	0.67
1:B:2411:PHE:O	1:B:2413:TYR:N	2.26	0.67
1:B:1636:LEU:HA	1:B:1639:GLU:HB3	1.76	0.67
1:A:2409:HIS:CG	2:A:2803:PLX:H52	2.25	0.67
1:C:1636:LEU:HA	1:C:1639:GLU:HB3	1.75	0.67
1:C:2411:PHE:O	1:C:2413:TYR:N	2.26	0.66
1:B:1796:GLN:OE1	1:B:1836:ASN:ND2	2.29	0.66
1:A:1796:GLN:OE1	1:A:1836:ASN:ND2	2.29	0.66
1:D:2462:PHE:CZ	2:D:2806:PLX:C24	2.71	0.66
1:D:1796:GLN:OE1	1:D:1836:ASN:ND2	2.29	0.65
1:C:133:THR:HG22	1:C:159:SER:HB3	1.78	0.65
1:C:1796:GLN:OE1	1:C:1836:ASN:ND2	2.29	0.65
1:B:133:THR:HG22	1:B:159:SER:HB3	1.78	0.65
1:A:1408:ARG:HH12	1:A:1423:TYR:HB3	1.62	0.65
1:D:1408:ARG:HH12	1:D:1423:TYR:HB3	1.62	0.65
1:C:1408:ARG:HH12	1:C:1423:TYR:HB3	1.62	0.65
1:B:1408:ARG:HH12	1:B:1423:TYR:HB3	1.62	0.65
1:D:133:THR:HG22	1:D:159:SER:HB3	1.78	0.64
1:A:133:THR:HG22	1:A:159:SER:HB3	1.78	0.64
1:A:2411:PHE:O	1:A:2413:TYR:N	2.26	0.64
1:C:2074:ILE:HG21	1:C:2081:ARG:HH22	1.62	0.64
1:B:2074:ILE:HG21	1:B:2081:ARG:HH22	1.62	0.64
1:D:2411:PHE:O	1:D:2413:TYR:N	2.26	0.64
1:A:1187:CYS:SG	1:A:1206:ARG:NH2	2.71	0.64
1:A:2264:PRO:HA	1:A:2267:TYR:HB3	1.80	0.64
1:B:134:VAL:HG22	1:B:149:VAL:HG12	1.80	0.64
1:A:2074:ILE:HG21	1:A:2081:ARG:HH22	1.62	0.64
1:D:1187:CYS:SG	1:D:1206:ARG:NH2	2.71	0.64
1:D:2409:HIS:NE2	2:D:2803:PLX:H32	2.13	0.64
1:C:1187:CYS:SG	1:C:1206:ARG:NH2	2.71	0.64
1:B:654:LYS:O	1:B:658:ASN:ND2	2.31	0.64
1:D:2074:ILE:HG21	1:D:2081:ARG:HH22	1.62	0.63
1:C:134:VAL:HG22	1:C:149:VAL:HG12	1.80	0.63
1:B:2264:PRO:HA	1:B:2267:TYR:HB3	1.80	0.63
1:A:654:LYS:O	1:A:658:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2264:PRO:HA	1:C:2267:TYR:HB3	1.80	0.63
1:B:1187:CYS:SG	1:B:1206:ARG:NH2	2.71	0.63
1:D:2264:PRO:HA	1:D:2267:TYR:HB3	1.80	0.63
1:A:134:VAL:HG22	1:A:149:VAL:HG12	1.80	0.63
1:D:2555:LYS:H	1:D:2566:ARG:HH22	1.47	0.62
1:D:134:VAL:HG22	1:D:149:VAL:HG12	1.80	0.62
1:C:847:VAL:HG13	1:C:851:ARG:HE	1.65	0.61
1:A:847:VAL:HG13	1:A:851:ARG:HE	1.65	0.61
1:D:2462:PHE:CE1	2:D:2806:PLX:O8	2.52	0.61
1:B:847:VAL:HG13	1:B:851:ARG:HE	1.65	0.61
1:C:2076:PRO:O	1:C:2081:ARG:NH1	2.34	0.61
1:B:2555:LYS:H	1:B:2566:ARG:HH22	1.47	0.61
1:B:2076:PRO:O	1:B:2081:ARG:NH1	2.34	0.61
1:A:1312:LEU:HA	1:A:1315:ILE:HG22	1.82	0.61
1:D:1312:LEU:HA	1:D:1315:ILE:HG22	1.82	0.60
1:B:1312:LEU:HA	1:B:1315:ILE:HG22	1.82	0.60
1:A:2221:LYS:HD3	1:A:2224:LYS:HD2	1.83	0.60
1:A:2555:LYS:H	1:A:2566:ARG:HH22	1.47	0.60
1:D:2076:PRO:O	1:D:2081:ARG:NH1	2.34	0.60
1:C:654:LYS:O	1:C:658:ASN:ND2	2.31	0.60
1:D:650:GLU:O	1:D:654:LYS:NZ	2.35	0.60
1:D:706:GLU:HG3	1:D:707:ILE:H	1.67	0.60
1:A:2076:PRO:O	1:A:2081:ARG:NH1	2.34	0.60
1:A:2618:ARG:NH2	1:A:2629:GLU:OE2	2.35	0.60
1:D:2616:LEU:HD12	1:D:2620:LYS:HG3	1.83	0.60
1:C:2555:LYS:H	1:C:2566:ARG:HH22	1.47	0.60
1:D:2011:CYS:HB3	1:D:2065:ILE:HD11	1.84	0.60
1:C:2221:LYS:HD3	1:C:2224:LYS:HD2	1.83	0.60
1:B:706:GLU:HG3	1:B:707:ILE:H	1.67	0.60
1:D:654:LYS:O	1:D:658:ASN:ND2	2.31	0.60
1:D:847:VAL:HG13	1:D:851:ARG:HE	1.65	0.60
1:D:1644:ARG:NH1	1:D:1647:CYS:SG	2.75	0.60
1:D:2221:LYS:HD3	1:D:2224:LYS:HD2	1.83	0.60
1:C:1312:LEU:HA	1:C:1315:ILE:HG22	1.82	0.60
1:B:650:GLU:O	1:B:654:LYS:NZ	2.35	0.60
1:A:1644:ARG:NH1	1:A:1647:CYS:SG	2.75	0.60
1:B:2616:LEU:HD12	1:B:2620:LYS:HG3	1.83	0.60
1:B:2618:ARG:NH2	1:B:2629:GLU:OE2	2.35	0.60
1:C:1644:ARG:NH1	1:C:1647:CYS:SG	2.75	0.59
1:B:602:ASN:HB3	1:B:605:LEU:HD12	1.84	0.59
1:B:1974:GLN:HG3	1:B:2042:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:GLU:O	1:C:654:LYS:NZ	2.35	0.59
1:C:706:GLU:HG3	1:C:707:ILE:H	1.67	0.59
1:B:828:GLU:HG3	1:B:829:ILE:HG23	1.84	0.59
1:A:2011:CYS:HB3	1:A:2065:ILE:HD11	1.84	0.59
1:D:1974:GLN:HG3	1:D:2042:GLU:HG3	1.84	0.59
1:C:2616:LEU:HD12	1:C:2620:LYS:HG3	1.83	0.59
1:A:765:LEU:HD11	1:A:836:THR:HG22	1.85	0.59
1:B:2221:LYS:HD3	1:B:2224:LYS:HD2	1.83	0.59
1:A:2616:LEU:HD12	1:A:2620:LYS:HG3	1.83	0.59
1:D:2618:ARG:NH2	1:D:2629:GLU:OE2	2.35	0.59
1:C:2618:ARG:NH2	1:C:2629:GLU:OE2	2.35	0.59
1:B:989:ARG:HD2	1:B:1041:PHE:HE1	1.67	0.59
1:B:1644:ARG:NH1	1:B:1647:CYS:SG	2.75	0.59
1:D:989:ARG:HD2	1:D:1041:PHE:HE1	1.67	0.59
1:B:996:ILE:HA	1:B:999:ARG:HG2	1.85	0.59
1:A:706:GLU:HG3	1:A:707:ILE:H	1.67	0.59
1:A:828:GLU:HG3	1:A:829:ILE:HG23	1.84	0.59
1:D:169:LEU:HD21	1:C:429:ALA:HB3	1.85	0.59
1:C:1974:GLN:HG3	1:C:2042:GLU:HG3	1.84	0.59
1:A:996:ILE:HA	1:A:999:ARG:HG2	1.85	0.59
1:B:2409:HIS:CD2	2:B:2807:PLX:C4	2.86	0.59
1:A:650:GLU:O	1:A:654:LYS:NZ	2.35	0.58
1:D:996:ILE:HA	1:D:999:ARG:HG2	1.85	0.58
1:C:996:ILE:HA	1:C:999:ARG:HG2	1.85	0.58
1:C:2524:LYS:HE2	1:C:2526:HIS:HB2	1.85	0.58
1:B:2524:LYS:HE2	1:B:2526:HIS:HB2	1.85	0.58
1:A:989:ARG:HD2	1:A:1041:PHE:HE1	1.67	0.58
1:D:765:LEU:HD11	1:D:836:THR:HG22	1.85	0.58
1:C:2011:CYS:HB3	1:C:2065:ILE:HD11	1.84	0.58
1:B:765:LEU:HD11	1:B:836:THR:HG22	1.85	0.58
1:D:602:ASN:HB3	1:D:605:LEU:HD12	1.84	0.58
1:D:759:LEU:HD13	1:D:763:LEU:HG	1.86	0.58
1:C:602:ASN:HB3	1:C:605:LEU:HD12	1.84	0.58
1:A:1974:GLN:HG3	1:A:2042:GLU:HG3	1.84	0.58
1:A:1982:ARG:HA	1:A:1985:GLN:HB3	1.86	0.58
1:C:765:LEU:HD11	1:C:836:THR:HG22	1.85	0.58
1:A:429:ALA:HB3	1:B:169:LEU:HD21	1.85	0.58
1:A:759:LEU:HD13	1:A:763:LEU:HG	1.86	0.58
1:C:828:GLU:HG3	1:C:829:ILE:HG23	1.84	0.58
1:C:1982:ARG:HA	1:C:1985:GLN:HB3	1.86	0.58
1:A:602:ASN:HB3	1:A:605:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2524:LYS:HE2	1:A:2526:HIS:HB2	1.85	0.58
1:D:2524:LYS:HE2	1:D:2526:HIS:HB2	1.85	0.58
1:C:169:LEU:HD21	1:B:429:ALA:HB3	1.85	0.58
1:B:790:VAL:O	1:B:792:ARG:NH1	2.37	0.58
1:B:2011:CYS:HB3	1:B:2065:ILE:HD11	1.84	0.58
1:D:1982:ARG:HA	1:D:1985:GLN:HB3	1.86	0.57
1:C:606:LEU:HD13	1:C:610:ILE:HD12	1.86	0.57
1:C:989:ARG:HD2	1:C:1041:PHE:HE1	1.67	0.57
1:D:606:LEU:HD13	1:D:610:ILE:HD12	1.86	0.57
1:A:790:VAL:O	1:A:792:ARG:NH1	2.37	0.57
1:C:790:VAL:O	1:C:792:ARG:NH1	2.37	0.57
1:B:846:ASP:OD2	1:B:850:GLN:NE2	2.37	0.57
1:A:143:GLU:OE1	1:A:210:ASN:ND2	2.38	0.57
1:D:828:GLU:HG3	1:D:829:ILE:HG23	1.84	0.57
1:D:846:ASP:OD2	1:D:850:GLN:NE2	2.37	0.57
1:C:1985:GLN:NE2	1:C:2043:TYR:O	2.38	0.57
1:A:1632:ARG:NH2	1:A:1635:LEU:O	2.38	0.57
1:C:846:ASP:OD2	1:C:850:GLN:NE2	2.37	0.57
1:C:2409:HIS:NE2	2:C:2804:PLX:H32	2.18	0.57
1:A:169:LEU:HD21	1:D:429:ALA:HB3	1.85	0.57
1:D:1985:GLN:NE2	1:D:2043:TYR:O	2.38	0.57
1:D:1632:ARG:NH2	1:D:1635:LEU:O	2.38	0.57
1:C:1808:VAL:HG11	1:C:1828:ALA:HB2	1.87	0.57
1:C:655:ALA:O	1:C:661:ASN:ND2	2.38	0.56
1:C:1632:ARG:NH2	1:C:1635:LEU:O	2.38	0.56
1:B:1982:ARG:HA	1:B:1985:GLN:HB3	1.86	0.56
1:A:537:ARG:HH12	1:A:549:PHE:HE2	1.54	0.56
1:A:846:ASP:OD2	1:A:850:GLN:NE2	2.37	0.56
1:D:790:VAL:O	1:D:792:ARG:NH1	2.37	0.56
1:D:1808:VAL:HG11	1:D:1828:ALA:HB2	1.87	0.56
1:C:143:GLU:OE1	1:C:210:ASN:ND2	2.38	0.56
1:C:537:ARG:HH12	1:C:549:PHE:HE2	1.54	0.56
1:C:759:LEU:HD13	1:C:763:LEU:HG	1.86	0.56
1:B:759:LEU:HD13	1:B:763:LEU:HG	1.86	0.56
1:B:1632:ARG:NH2	1:B:1635:LEU:O	2.38	0.56
1:A:606:LEU:HD13	1:A:610:ILE:HD12	1.86	0.56
1:D:537:ARG:HH12	1:D:549:PHE:HE2	1.54	0.56
1:C:571:GLN:HB3	1:C:605:LEU:HD11	1.88	0.56
1:B:143:GLU:OE1	1:B:210:ASN:ND2	2.38	0.56
1:B:606:LEU:HD13	1:B:610:ILE:HD12	1.86	0.56
1:B:1808:VAL:HG11	1:B:1828:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:GLN:HB3	1:D:605:LEU:HD11	1.88	0.56
1:B:537:ARG:HH12	1:B:549:PHE:HE2	1.54	0.56
1:A:571:GLN:HB3	1:A:605:LEU:HD11	1.88	0.56
1:D:143:GLU:OE1	1:D:210:ASN:ND2	2.38	0.55
1:D:655:ALA:O	1:D:661:ASN:ND2	2.38	0.55
1:C:13:ASP:OD1	1:C:226:TRP:N	2.40	0.55
1:B:1985:GLN:NE2	1:B:2043:TYR:O	2.38	0.55
1:A:888:THR:HG21	1:A:981:ILE:HD13	1.88	0.55
1:A:1985:GLN:NE2	1:A:2043:TYR:O	2.38	0.55
1:D:2418:PHE:HE2	2:D:2804:PLX:H301	1.72	0.55
2:D:2801:PLX:H251	2:D:2801:PLX:H72	1.89	0.55
1:C:888:THR:HG21	1:C:981:ILE:HD13	1.88	0.55
1:A:1808:VAL:HG11	1:A:1828:ALA:HB2	1.87	0.55
1:C:389:ARG:NH2	1:C:426:ASP:OD1	2.40	0.55
1:D:888:THR:HG21	1:D:981:ILE:HD13	1.88	0.55
1:B:264:LEU:HD12	1:B:416:LEU:HD21	1.89	0.55
1:A:304:ARG:NH1	1:A:361:GLY:O	2.40	0.55
1:A:389:ARG:NH2	1:A:426:ASP:OD1	2.40	0.55
1:C:304:ARG:NH1	1:C:361:GLY:O	2.40	0.55
1:B:389:ARG:NH2	1:B:426:ASP:OD1	2.40	0.55
1:B:655:ALA:O	1:B:661:ASN:ND2	2.38	0.55
1:A:2049:HIS:O	1:A:2053:ASN:ND2	2.40	0.55
1:D:389:ARG:NH2	1:D:426:ASP:OD1	2.40	0.55
1:C:2049:HIS:O	1:C:2053:ASN:ND2	2.40	0.55
1:B:2180:VAL:HG12	1:B:2182:GLY:H	1.72	0.55
1:D:2049:HIS:O	1:D:2053:ASN:ND2	2.40	0.55
1:C:264:LEU:HD12	1:C:416:LEU:HD21	1.89	0.55
1:C:2180:VAL:HG12	1:C:2182:GLY:H	1.72	0.55
1:B:571:GLN:HB3	1:B:605:LEU:HD11	1.88	0.54
2:C:2802:PLX:H72	2:C:2802:PLX:H251	1.89	0.54
1:B:304:ARG:NH1	1:B:361:GLY:O	2.40	0.54
1:B:2049:HIS:O	1:B:2053:ASN:ND2	2.40	0.54
1:D:2448:ALA:HB2	1:D:2581:VAL:HG11	1.89	0.54
1:A:655:ALA:O	1:A:661:ASN:ND2	2.38	0.54
1:A:2180:VAL:HG12	1:A:2182:GLY:H	1.72	0.54
1:D:264:LEU:HD12	1:D:416:LEU:HD21	1.89	0.54
1:D:304:ARG:NH1	1:D:361:GLY:O	2.40	0.54
1:B:888:THR:HG21	1:B:981:ILE:HD13	1.88	0.54
1:B:2418:PHE:HE2	2:B:2808:PLX:H301	1.72	0.54
1:A:13:ASP:OD1	1:A:226:TRP:N	2.40	0.54
2:B:2805:PLX:H72	2:B:2805:PLX:H251	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:CYS:SG	1:C:254:ASP:N	2.81	0.54
1:D:13:ASP:OD1	1:D:226:TRP:N	2.40	0.54
1:C:2283:LEU:HD11	1:C:2357:LEU:HD22	1.90	0.54
1:A:2409:HIS:CD2	2:A:2803:PLX:C4	2.90	0.54
1:D:253:CYS:SG	1:D:254:ASP:N	2.81	0.54
1:C:2448:ALA:HB2	1:C:2581:VAL:HG11	1.89	0.54
1:A:2448:ALA:HB2	1:A:2581:VAL:HG11	1.89	0.54
1:B:2283:LEU:HD11	1:B:2357:LEU:HD22	1.90	0.53
1:A:302:LEU:HB3	1:A:367:ILE:HD11	1.91	0.53
1:B:13:ASP:OD1	1:B:226:TRP:N	2.40	0.53
1:A:1073:PRO:HB2	1:A:1075:LEU:H	1.72	0.53
1:A:1306:VAL:HG21	1:A:1370:PRO:HD2	1.90	0.53
1:D:2180:VAL:HG12	1:D:2182:GLY:H	1.72	0.53
1:B:1306:VAL:HG21	1:B:1370:PRO:HD2	1.90	0.53
1:B:1989:ARG:HH21	1:B:2050:GLU:HG3	1.74	0.53
1:A:1989:ARG:HH21	1:A:2050:GLU:HG3	1.74	0.53
1:D:1073:PRO:HB2	1:D:1075:LEU:H	1.72	0.53
1:C:1989:ARG:HH21	1:C:2050:GLU:HG3	1.74	0.53
1:C:2409:HIS:CE1	2:C:2804:PLX:O8	2.61	0.53
1:A:264:LEU:HD12	1:A:416:LEU:HD21	1.89	0.53
1:A:982:LEU:HD23	1:A:985:ARG:HD3	1.91	0.53
1:C:674:ARG:NH1	1:C:693:GLU:O	2.42	0.53
1:B:1073:PRO:HB2	1:B:1075:LEU:H	1.72	0.53
1:D:2283:LEU:HD11	1:D:2357:LEU:HD22	1.90	0.53
1:B:302:LEU:HB3	1:B:367:ILE:HD11	1.91	0.53
1:A:702:ASP:OD2	1:A:708:ARG:NH2	2.42	0.53
1:A:2378:THR:HA	1:A:2381:ARG:HE	1.73	0.53
1:C:1073:PRO:HB2	1:C:1075:LEU:H	1.72	0.53
1:B:702:ASP:OD2	1:B:708:ARG:NH2	2.42	0.53
1:B:982:LEU:HD23	1:B:985:ARG:HD3	1.91	0.53
1:A:253:CYS:SG	1:A:254:ASP:N	2.81	0.53
1:A:2283:LEU:HD11	1:A:2357:LEU:HD22	1.90	0.53
1:D:302:LEU:HB3	1:D:367:ILE:HD11	1.91	0.53
1:D:2074:ILE:HG22	1:D:2076:PRO:HD2	1.91	0.53
1:C:1242:GLN:HE21	1:C:1275:HIS:HB3	1.73	0.53
1:B:1002:ASP:HA	1:B:1005:ASN:HB2	1.91	0.53
1:B:2074:ILE:HG22	1:B:2076:PRO:HD2	1.91	0.53
1:A:1002:ASP:HA	1:A:1005:ASN:HB2	1.91	0.53
1:A:1242:GLN:HE21	1:A:1275:HIS:HB3	1.73	0.53
1:A:1316:VAL:HG11	1:A:1330:VAL:HB	1.91	0.53
1:D:1316:VAL:HG11	1:D:1330:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1989:ARG:HH21	1:D:2050:GLU:HG3	1.74	0.53
1:C:982:LEU:HD23	1:C:985:ARG:HD3	1.91	0.53
1:C:2071:LEU:HD11	1:C:2116:MET:HG3	1.91	0.53
1:B:674:ARG:NH1	1:B:693:GLU:O	2.42	0.53
1:A:390:LEU:HD22	1:A:430:PHE:HZ	1.74	0.53
1:D:702:ASP:OD2	1:D:708:ARG:NH2	2.42	0.53
1:D:982:LEU:HD23	1:D:985:ARG:HD3	1.91	0.53
1:C:1306:VAL:HG21	1:C:1370:PRO:HD2	1.90	0.53
1:C:2074:ILE:HG22	1:C:2076:PRO:HD2	1.91	0.53
1:C:2378:THR:HA	1:C:2381:ARG:HE	1.73	0.53
1:B:253:CYS:SG	1:B:254:ASP:N	2.81	0.53
1:B:2448:ALA:HB2	1:B:2581:VAL:HG11	1.89	0.53
1:A:2071:LEU:HD11	1:A:2116:MET:HG3	1.91	0.52
1:D:811:PRO:HG3	1:D:998:LYS:HE2	1.92	0.52
1:D:1242:GLN:HE21	1:D:1275:HIS:HB3	1.73	0.52
1:D:1306:VAL:HG21	1:D:1370:PRO:HD2	1.90	0.52
1:D:2008:ASP:HA	1:D:2065:ILE:HD13	1.91	0.52
1:C:702:ASP:OD2	1:C:708:ARG:NH2	2.42	0.52
1:C:2008:ASP:HA	1:C:2065:ILE:HD13	1.91	0.52
1:B:811:PRO:HG3	1:B:998:LYS:HE2	1.92	0.52
1:B:2071:LEU:HD11	1:B:2116:MET:HG3	1.91	0.52
1:D:674:ARG:NH1	1:D:693:GLU:O	2.42	0.52
1:B:2008:ASP:HA	1:B:2065:ILE:HD13	1.91	0.52
1:D:2071:LEU:HD11	1:D:2116:MET:HG3	1.91	0.52
1:D:1002:ASP:HA	1:D:1005:ASN:HB2	1.91	0.52
1:D:1318:ALA:HA	1:D:1322:PHE:HB2	1.92	0.52
1:C:1316:VAL:HG11	1:C:1330:VAL:HB	1.91	0.52
1:A:811:PRO:HG3	1:A:998:LYS:HE2	1.92	0.52
1:A:1252:GLN:NE2	1:A:1276:ILE:O	2.43	0.52
1:A:2018:LEU:O	1:A:2072:ASN:ND2	2.43	0.52
1:C:302:LEU:HB3	1:C:367:ILE:HD11	1.91	0.52
1:C:2066:ILE:HG12	1:C:2095:LEU:HD22	1.91	0.52
1:B:390:LEU:HD22	1:B:430:PHE:HZ	1.74	0.52
1:B:1064:LEU:HD21	1:B:1082:LEU:HD23	1.92	0.52
1:D:2018:LEU:O	1:D:2072:ASN:ND2	2.43	0.52
1:D:2263:GLN:HB3	1:D:2266:LEU:HB3	1.92	0.52
1:D:2378:THR:HA	1:D:2381:ARG:HE	1.73	0.52
1:C:390:LEU:HD22	1:C:430:PHE:HZ	1.74	0.52
1:C:811:PRO:HG3	1:C:998:LYS:HE2	1.92	0.52
1:B:2378:THR:HA	1:B:2381:ARG:HE	1.73	0.52
1:A:674:ARG:NH1	1:A:693:GLU:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2074:ILE:HG22	1:A:2076:PRO:HD2	1.91	0.52
1:D:1809:ILE:HG21	1:D:1846:ARG:HG2	1.92	0.52
1:D:2066:ILE:HG12	1:D:2095:LEU:HD22	1.91	0.52
1:C:400:HIS:HB2	1:C:428:GLU:HG3	1.92	0.52
1:C:2263:GLN:HB3	1:C:2266:LEU:HB3	1.92	0.52
1:A:2066:ILE:HG12	1:A:2095:LEU:HD22	1.91	0.52
1:C:1064:LEU:HD21	1:C:1082:LEU:HD23	1.92	0.52
1:C:1809:ILE:HG21	1:C:1846:ARG:HG2	1.92	0.52
1:B:1242:GLN:HE21	1:B:1275:HIS:HB3	1.73	0.52
1:B:2066:ILE:HG12	1:B:2095:LEU:HD22	1.91	0.52
1:D:390:LEU:HD22	1:D:430:PHE:HZ	1.74	0.51
1:B:1316:VAL:HG11	1:B:1330:VAL:HB	1.91	0.51
1:A:1809:ILE:HG21	1:A:1846:ARG:HG2	1.92	0.51
1:A:2008:ASP:HA	1:A:2065:ILE:HD13	1.91	0.51
1:C:1252:GLN:NE2	1:C:1276:ILE:O	2.43	0.51
1:B:2018:LEU:O	1:B:2072:ASN:ND2	2.43	0.51
1:C:1318:ALA:HA	1:C:1322:PHE:HB2	1.92	0.51
1:B:2263:GLN:HB3	1:B:2266:LEU:HB3	1.92	0.51
1:B:2409:HIS:NE2	2:B:2807:PLX:C5	2.51	0.51
1:A:1064:LEU:HD21	1:A:1082:LEU:HD23	1.92	0.51
1:D:1252:GLN:NE2	1:D:1276:ILE:O	2.43	0.51
1:B:1252:GLN:NE2	1:B:1276:ILE:O	2.43	0.51
1:B:1809:ILE:HG21	1:B:1846:ARG:HG2	1.92	0.51
1:C:1002:ASP:HA	1:C:1005:ASN:HB2	1.91	0.51
1:C:2018:LEU:O	1:C:2072:ASN:ND2	2.43	0.51
1:B:400:HIS:HB2	1:B:428:GLU:HG3	1.92	0.51
1:A:1318:ALA:HA	1:A:1322:PHE:HB2	1.92	0.51
1:B:1125:ILE:HG22	1:B:1172:ASN:HB2	1.93	0.51
1:A:2263:GLN:HB3	1:A:2266:LEU:HB3	1.92	0.51
1:D:400:HIS:HB2	1:D:428:GLU:HG3	1.92	0.51
1:A:400:HIS:HB2	1:A:428:GLU:HG3	1.92	0.50
1:A:1064:LEU:HB3	1:A:1083:LEU:HD12	1.94	0.50
1:D:1064:LEU:HD21	1:D:1082:LEU:HD23	1.92	0.50
1:D:1064:LEU:HB3	1:D:1083:LEU:HD12	1.94	0.50
1:D:1125:ILE:HG22	1:D:1172:ASN:HB2	1.93	0.50
1:B:871:ARG:HD3	1:B:973:LYS:HE2	1.94	0.50
1:B:1064:LEU:HB3	1:B:1083:LEU:HD12	1.94	0.50
1:B:1318:ALA:HA	1:B:1322:PHE:HB2	1.92	0.50
1:C:1064:LEU:HB3	1:C:1083:LEU:HD12	1.94	0.50
1:A:871:ARG:HD3	1:A:973:LYS:HE2	1.94	0.50
1:C:871:ARG:HD3	1:C:973:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:871:ARG:HD3	1:D:973:LYS:HE2	1.94	0.49
1:D:2067:THR:OG1	1:D:2116:MET:SD	2.63	0.49
1:C:1125:ILE:HG22	1:C:1172:ASN:HB2	1.93	0.49
1:A:615:ILE:O	1:A:619:VAL:N	2.44	0.49
1:A:1125:ILE:HG22	1:A:1172:ASN:HB2	1.93	0.49
1:C:738:ASN:OD1	1:C:783:ARG:NH1	2.45	0.49
1:C:2613:ILE:H	1:C:2613:ILE:HD12	1.78	0.49
1:C:2213:PRO:HG2	1:C:2646:VAL:HG23	1.94	0.49
1:B:2067:THR:OG1	1:B:2116:MET:SD	2.63	0.49
1:A:2544:ARG:NH2	1:B:2570:ASP:CG	2.60	0.49
1:D:2213:PRO:HG2	1:D:2646:VAL:HG23	1.94	0.49
1:D:2627:THR:OG1	1:D:2630:GLU:OE1	2.31	0.49
1:D:738:ASN:OD1	1:D:783:ARG:NH1	2.45	0.49
1:D:783:ARG:NH2	1:D:865:GLU:OE2	2.46	0.49
1:D:863:THR:HA	1:D:866:VAL:HG12	1.95	0.49
1:D:2575:PHE:HD2	2:D:2807:PLX:C36	2.26	0.49
1:C:863:THR:HA	1:C:866:VAL:HG12	1.95	0.49
1:C:2131:GLN:HG2	1:C:2149:PRO:HG2	1.94	0.49
1:B:1191:SER:OG	1:B:1195:ARG:NH2	2.46	0.49
1:A:1191:SER:OG	1:A:1195:ARG:NH2	2.46	0.49
1:C:2067:THR:OG1	1:C:2116:MET:SD	2.63	0.49
1:B:194:HIS:HA	1:B:216:THR:HG21	1.94	0.49
1:A:738:ASN:OD1	1:A:783:ARG:NH1	2.45	0.49
2:A:2801:PLX:H72	2:A:2801:PLX:H251	1.94	0.49
1:D:2613:ILE:HD12	1:D:2613:ILE:H	1.78	0.49
1:C:971:LYS:HA	1:C:974:ILE:HG12	1.95	0.49
1:A:863:THR:HA	1:A:866:VAL:HG12	1.95	0.48
1:A:971:LYS:HA	1:A:974:ILE:HG12	1.95	0.48
1:D:2131:GLN:HG2	1:D:2149:PRO:HG2	1.94	0.48
1:A:194:HIS:HA	1:A:216:THR:HG21	1.94	0.48
1:A:783:ARG:NH2	1:A:865:GLU:OE2	2.46	0.48
1:D:194:HIS:HA	1:D:216:THR:HG21	1.94	0.48
1:B:2613:ILE:HD12	1:B:2613:ILE:H	1.78	0.48
1:A:1881:ASP:OD1	1:A:1881:ASP:N	2.46	0.48
1:A:2432:LYS:HA	1:A:2435:THR:HG22	1.96	0.48
1:D:1191:SER:OG	1:D:1195:ARG:NH2	2.46	0.48
1:C:194:HIS:HA	1:C:216:THR:HG21	1.94	0.48
1:B:600:HIS:CG	1:B:601:ASN:H	2.31	0.48
1:B:863:THR:HA	1:B:866:VAL:HG12	1.95	0.48
1:A:600:HIS:CG	1:A:601:ASN:H	2.31	0.48
1:A:2213:PRO:HG2	1:A:2646:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2613:ILE:HD12	1:A:2613:ILE:H	1.78	0.48
1:D:971:LYS:HA	1:D:974:ILE:HG12	1.95	0.48
1:D:2726:GLN:OE1	1:D:2729:GLN:NE2	2.47	0.48
1:C:600:HIS:CG	1:C:601:ASN:H	2.31	0.48
1:C:783:ARG:NH2	1:C:865:GLU:OE2	2.46	0.48
1:C:1191:SER:OG	1:C:1195:ARG:NH2	2.46	0.48
1:B:2131:GLN:HG2	1:B:2149:PRO:HG2	1.94	0.48
1:B:2213:PRO:HG2	1:B:2646:VAL:HG23	1.94	0.48
1:B:2726:GLN:OE1	1:B:2729:GLN:NE2	2.46	0.48
1:A:2726:GLN:OE1	1:A:2729:GLN:NE2	2.46	0.48
1:B:971:LYS:HA	1:B:974:ILE:HG12	1.95	0.48
1:B:2627:THR:OG1	1:B:2630:GLU:OE1	2.31	0.48
1:B:738:ASN:OD1	1:B:783:ARG:NH1	2.45	0.48
1:A:2131:GLN:HG2	1:A:2149:PRO:HG2	1.94	0.48
1:D:600:HIS:CG	1:D:601:ASN:H	2.31	0.48
1:B:783:ARG:NH2	1:B:865:GLU:OE2	2.46	0.48
1:B:856:ASP:OD1	1:B:856:ASP:N	2.47	0.48
1:D:2432:LYS:HA	1:D:2435:THR:HG22	1.96	0.48
1:C:138:LEU:HD23	1:C:148:ARG:HH22	1.79	0.48
1:D:2413:TYR:HA	1:D:2416:LEU:HG	1.96	0.47
1:C:2726:GLN:OE1	1:C:2729:GLN:NE2	2.46	0.47
1:B:702:ASP:OD1	1:B:702:ASP:N	2.47	0.47
1:A:138:LEU:HD23	1:A:148:ARG:HH22	1.79	0.47
1:D:456:ILE:HD13	1:D:473:VAL:HB	1.96	0.47
1:C:2409:HIS:CD2	2:C:2804:PLX:C4	2.97	0.47
1:B:1976:LEU:HD23	1:B:1988:LEU:HD11	1.96	0.47
1:A:702:ASP:OD1	1:A:702:ASP:N	2.47	0.47
1:C:2627:THR:OG1	1:C:2630:GLU:OE1	2.31	0.47
1:B:789:HIS:CD2	1:B:790:VAL:HG13	2.49	0.47
1:A:856:ASP:N	1:A:856:ASP:OD1	2.47	0.47
1:D:2724:THR:HG21	1:C:2720:LYS:NZ	2.29	0.47
1:C:789:HIS:CD2	1:C:790:VAL:HG13	2.49	0.47
1:C:2698:LEU:HA	1:C:2701:LYS:HE2	1.97	0.47
1:B:2432:LYS:HA	1:B:2435:THR:HG22	1.95	0.47
1:A:456:ILE:HD13	1:A:473:VAL:HB	1.96	0.47
1:A:2557:SER:O	1:A:2557:SER:OG	2.31	0.47
1:C:2413:TYR:HA	1:C:2416:LEU:HG	1.96	0.47
1:A:2627:THR:OG1	1:A:2630:GLU:OE1	2.31	0.47
1:A:2724:THR:HG21	1:D:2720:LYS:NZ	2.30	0.47
1:D:2698:LEU:HA	1:D:2701:LYS:HE2	1.97	0.47
1:C:64:ASN:HD22	1:C:122:GLN:HE21	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2697:ASN:O	1:B:2700:GLU:HG3	2.15	0.47
1:A:160:TRP:HE3	1:A:187:VAL:HG11	1.80	0.47
1:A:789:HIS:CD2	1:A:790:VAL:HG13	2.49	0.47
1:A:2697:ASN:O	1:A:2700:GLU:HG3	2.15	0.47
1:D:138:LEU:HD23	1:D:148:ARG:HH22	1.79	0.47
1:D:641:MET:HG3	1:D:642:ASN:H	1.80	0.47
1:D:789:HIS:CD2	1:D:790:VAL:HG13	2.49	0.47
1:C:1976:LEU:HD23	1:C:1988:LEU:HD11	1.96	0.47
1:C:2432:LYS:HA	1:C:2435:THR:HG22	1.96	0.47
1:B:1982:ARG:NH1	1:B:2047:PRO:O	2.48	0.47
1:D:160:TRP:HE3	1:D:187:VAL:HG11	1.80	0.47
1:D:1881:ASP:OD1	1:D:1881:ASP:N	2.46	0.47
1:C:856:ASP:OD1	1:C:856:ASP:N	2.47	0.47
1:B:456:ILE:HD13	1:B:473:VAL:HB	1.96	0.47
1:C:2724:THR:HG21	1:B:2720:LYS:NZ	2.29	0.47
1:B:2698:LEU:HA	1:B:2701:LYS:HE2	1.97	0.47
2:A:2803:PLX:H1A2	2:A:2803:PLX:H21	1.75	0.47
1:C:1982:ARG:NH1	1:C:2047:PRO:O	2.48	0.47
1:C:641:MET:HG3	1:C:642:ASN:H	1.80	0.46
1:A:147:MET:HB3	1:A:211:SER:HB3	1.98	0.46
1:D:64:ASN:HD22	1:D:122:GLN:HE21	1.63	0.46
1:D:117:TYR:OH	1:D:180:ASP:OD2	2.34	0.46
1:D:147:MET:HB3	1:D:211:SER:HB3	1.98	0.46
1:C:2697:ASN:O	1:C:2700:GLU:HG3	2.15	0.46
1:B:2413:TYR:HA	1:B:2416:LEU:HG	1.96	0.46
1:A:2413:TYR:HA	1:A:2416:LEU:HG	1.96	0.46
1:C:117:TYR:OH	1:C:180:ASP:OD2	2.34	0.46
1:C:2409:HIS:ND1	2:C:2804:PLX:O8	2.47	0.46
1:B:160:TRP:HE3	1:B:187:VAL:HG11	1.80	0.46
1:A:1301:THR:HB	1:B:138:LEU:HG	1.97	0.46
1:A:1976:LEU:HD23	1:A:1988:LEU:HD11	1.96	0.46
1:D:2409:HIS:CD2	2:D:2803:PLX:C4	2.97	0.46
1:C:160:TRP:HE3	1:C:187:VAL:HG11	1.80	0.46
1:C:1373:MET:O	1:C:1377:HIS:N	2.48	0.46
1:B:138:LEU:HD23	1:B:148:ARG:HH22	1.79	0.46
1:A:2698:LEU:HA	1:A:2701:LYS:HE2	1.97	0.46
1:B:147:MET:HB3	1:B:211:SER:HB3	1.98	0.46
1:C:316:ALA:HB2	1:C:355:LEU:HD23	1.98	0.46
1:C:456:ILE:HD13	1:C:473:VAL:HB	1.96	0.46
1:C:702:ASP:OD1	1:C:702:ASP:N	2.47	0.46
1:A:747:ARG:NH1	1:A:749:TYR:OH	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2618:ARG:HH21	1:B:2236:GLN:HG3	1.81	0.46
1:A:2720:LYS:NZ	1:B:2724:THR:HG21	2.30	0.46
1:C:1117:GLN:NE2	1:C:1118:ASP:OD1	2.49	0.46
1:C:2409:HIS:NE2	2:C:2804:PLX:C5	2.70	0.46
1:C:2570:ASP:CG	1:B:2544:ARG:NH2	2.61	0.46
2:C:2802:PLX:H252	2:C:2803:PLX:H72	1.97	0.46
1:A:1073:PRO:HG2	1:A:1076:VAL:H	1.81	0.46
1:D:1685:LYS:HG2	1:D:1686:ASP:H	1.81	0.46
1:D:2570:ASP:CG	1:C:2544:ARG:NH2	2.61	0.46
1:B:117:TYR:OH	1:B:180:ASP:OD2	2.34	0.46
1:B:745:LEU:HA	1:B:787:HIS:HB3	1.98	0.46
1:A:117:TYR:OH	1:A:180:ASP:OD2	2.34	0.46
1:D:889:LYS:HD2	1:D:890:ILE:HG23	1.98	0.46
1:D:1976:LEU:HD23	1:D:1988:LEU:HD11	1.96	0.46
1:D:2697:ASN:O	1:D:2700:GLU:HG3	2.15	0.46
2:D:2801:PLX:H252	2:D:2802:PLX:H72	1.96	0.46
1:C:138:LEU:HG	1:B:1301:THR:HB	1.98	0.46
1:C:147:MET:HB3	1:C:211:SER:HB3	1.98	0.46
1:C:745:LEU:HA	1:C:787:HIS:HB3	1.98	0.46
2:B:2805:PLX:H252	2:B:2806:PLX:H72	1.98	0.46
1:A:742:ARG:HA	1:A:745:LEU:HD23	1.98	0.46
1:A:1685:LYS:HG2	1:A:1686:ASP:H	1.81	0.46
1:D:1982:ARG:NH1	1:D:2047:PRO:O	2.48	0.46
1:C:1956:ASP:OD1	1:C:1956:ASP:N	2.49	0.46
1:B:747:ARG:NH1	1:B:749:TYR:OH	2.49	0.46
1:B:1117:GLN:NE2	1:B:1118:ASP:OD1	2.49	0.46
1:A:1125:ILE:HD12	1:A:1176:VAL:HG22	1.98	0.45
1:A:1373:MET:O	1:A:1377:HIS:N	2.48	0.45
1:A:2236:GLN:HG3	1:D:2618:ARG:HH21	1.81	0.45
1:D:316:ALA:HB2	1:D:355:LEU:HD23	1.98	0.45
1:C:1685:LYS:HG2	1:C:1686:ASP:H	1.81	0.45
1:C:2226:ARG:O	1:C:2230:THR:OG1	2.32	0.45
1:B:64:ASN:HD22	1:B:122:GLN:HE21	1.63	0.45
1:B:1125:ILE:HD12	1:B:1176:VAL:HG22	1.98	0.45
1:A:316:ALA:HB2	1:A:355:LEU:HD23	1.98	0.45
1:A:641:MET:HG3	1:A:642:ASN:H	1.80	0.45
1:A:889:LYS:HD2	1:A:890:ILE:HG23	1.98	0.45
1:D:39:VAL:HG21	1:D:195:ALA:HB1	1.98	0.45
1:D:856:ASP:OD1	1:D:856:ASP:N	2.47	0.45
1:C:889:LYS:HD2	1:C:890:ILE:HG23	1.98	0.45
1:B:889:LYS:HD2	1:B:890:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1073:PRO:HG2	1:B:1076:VAL:H	1.81	0.45
1:A:64:ASN:HD22	1:A:122:GLN:HE21	1.63	0.45
1:D:564:GLN:NE2	1:D:574:ILE:HD12	2.32	0.45
1:D:1956:ASP:N	1:D:1956:ASP:OD1	2.49	0.45
1:D:1117:GLN:NE2	1:D:1118:ASP:OD1	2.49	0.45
1:D:1327:GLN:HA	1:D:1330:VAL:HG12	1.99	0.45
1:C:1327:GLN:HA	1:C:1330:VAL:HG12	1.99	0.45
1:B:742:ARG:HA	1:B:745:LEU:HD23	1.98	0.45
1:B:1034:GLU:OE2	1:B:1732:ARG:NH1	2.50	0.45
1:B:1806:ASN:HA	1:B:1809:ILE:HG22	1.99	0.45
1:A:442:ASP:HB2	1:A:483:PHE:HE1	1.82	0.45
1:D:442:ASP:HB2	1:D:483:PHE:HE1	1.82	0.45
1:D:742:ARG:HA	1:D:745:LEU:HD23	1.98	0.45
1:D:1393:THR:HB	1:D:1396:LYS:HB3	1.99	0.45
1:B:641:MET:HG3	1:B:642:ASN:H	1.80	0.45
1:A:564:GLN:NE2	1:A:574:ILE:HD12	2.32	0.45
1:C:1393:THR:HB	1:C:1396:LYS:HB3	1.99	0.45
1:A:1393:THR:HB	1:A:1396:LYS:HB3	1.99	0.45
1:A:1982:ARG:NH1	1:A:2047:PRO:O	2.48	0.45
1:D:138:LEU:HG	1:C:1301:THR:HB	1.98	0.45
1:C:39:VAL:HG21	1:C:195:ALA:HB1	1.98	0.45
1:C:442:ASP:HB2	1:C:483:PHE:HE1	1.82	0.45
1:C:742:ARG:HA	1:C:745:LEU:HD23	1.98	0.45
1:C:1034:GLU:OE2	1:C:1732:ARG:NH1	2.50	0.45
1:C:1125:ILE:HD12	1:C:1176:VAL:HG22	1.98	0.45
1:C:2236:GLN:HG3	1:B:2618:ARG:HH21	1.81	0.45
2:C:2804:PLX:H21	2:C:2804:PLX:H1A2	1.77	0.45
1:B:2557:SER:O	1:B:2557:SER:OG	2.31	0.45
2:B:2802:PLX:H252	2:B:2802:PLX:H51	1.72	0.45
1:A:1034:GLU:OE2	1:A:1732:ARG:NH1	2.50	0.45
1:D:1080:LEU:HD22	1:D:1671:LEU:HD21	1.99	0.45
1:D:1806:ASN:HA	1:D:1809:ILE:HG22	1.99	0.45
1:D:2409:HIS:CE1	2:D:2803:PLX:O8	2.70	0.45
1:B:442:ASP:HB2	1:B:483:PHE:HE1	1.82	0.45
1:B:564:GLN:NE2	1:B:574:ILE:HD12	2.32	0.45
1:B:1881:ASP:OD1	1:B:1881:ASP:N	2.46	0.45
1:D:1034:GLU:OE2	1:D:1732:ARG:NH1	2.50	0.45
1:D:1073:PRO:HG2	1:D:1076:VAL:H	1.81	0.45
1:D:2288:ASN:HA	1:D:2291:VAL:HG12	1.99	0.45
1:B:372:PRO:HG2	1:B:375:LEU:HD23	1.99	0.45
1:B:628:PRO:HB2	1:B:735:TYR:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1327:GLN:HA	1:B:1330:VAL:HG12	1.99	0.45
1:A:745:LEU:HA	1:A:787:HIS:HB3	1.98	0.45
1:A:1327:GLN:HA	1:A:1330:VAL:HG12	1.99	0.45
1:D:747:ARG:NH1	1:D:749:TYR:OH	2.49	0.45
1:D:1125:ILE:HD12	1:D:1176:VAL:HG22	1.98	0.45
1:C:564:GLN:NE2	1:C:574:ILE:HD12	2.32	0.45
1:B:39:VAL:HG21	1:B:195:ALA:HB1	1.98	0.45
1:B:2288:ASN:HA	1:B:2291:VAL:HG12	1.99	0.45
1:A:1117:GLN:NE2	1:A:1118:ASP:OD1	2.49	0.44
1:D:372:PRO:HG2	1:D:375:LEU:HD23	1.99	0.44
1:C:1664:LEU:HD12	1:C:1811:LEU:HD12	2.00	0.44
1:B:1080:LEU:HD22	1:B:1671:LEU:HD21	1.99	0.44
1:B:1685:LYS:HG2	1:B:1686:ASP:H	1.81	0.44
1:A:138:LEU:HG	1:D:1301:THR:HB	1.98	0.44
1:D:745:LEU:HA	1:D:787:HIS:HB3	1.98	0.44
1:D:1955:ASP:OD1	1:D:1955:ASP:N	2.51	0.44
1:D:2236:GLN:HG3	1:C:2618:ARG:HH21	1.81	0.44
1:C:1881:ASP:N	1:C:1881:ASP:OD1	2.46	0.44
1:B:600:HIS:CD2	1:B:601:ASN:H	2.35	0.44
1:A:372:PRO:HG2	1:A:375:LEU:HD23	1.99	0.44
1:A:1080:LEU:HD22	1:A:1671:LEU:HD21	1.99	0.44
1:A:2409:HIS:NE2	2:A:2803:PLX:C5	2.61	0.44
1:D:600:HIS:CD2	1:D:601:ASN:H	2.35	0.44
1:D:2033:ILE:HA	1:D:2036:THR:HG22	2.00	0.44
2:D:2803:PLX:H1A2	2:D:2803:PLX:H21	1.77	0.44
1:C:372:PRO:HG2	1:C:375:LEU:HD23	1.99	0.44
1:C:2288:ASN:HA	1:C:2291:VAL:HG12	1.99	0.44
1:B:316:ALA:HB2	1:B:355:LEU:HD23	1.98	0.44
1:B:1664:LEU:HD12	1:B:1811:LEU:HD12	2.00	0.44
1:A:1806:ASN:HA	1:A:1809:ILE:HG22	1.99	0.44
1:D:1214:VAL:HG21	1:D:1240:PHE:HE2	1.83	0.44
1:C:526:PRO:HA	1:C:529:ASP:HB3	1.99	0.44
1:C:1806:ASN:HA	1:C:1809:ILE:HG22	1.99	0.44
2:C:2807:PLX:H1C2	2:C:2807:PLX:H21	1.79	0.44
1:B:1280:ASN:HD22	1:B:1283:LEU:HB2	1.83	0.44
1:B:1373:MET:O	1:B:1377:HIS:N	2.48	0.44
1:B:2167:ASN:HD22	1:B:2170:LEU:HB2	1.83	0.44
1:A:2288:ASN:HA	1:A:2291:VAL:HG12	1.99	0.44
1:D:1664:LEU:HD12	1:D:1811:LEU:HD12	2.00	0.44
1:D:1865:LYS:HD2	1:D:1868:GLN:HE21	1.83	0.44
1:B:1393:THR:HB	1:B:1396:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PRO:HA	1:A:529:ASP:HB3	1.99	0.44
1:A:600:HIS:CD2	1:A:601:ASN:H	2.35	0.44
1:A:628:PRO:HB2	1:A:735:TYR:HD2	1.82	0.44
1:D:194:HIS:CD2	1:D:212:VAL:HG22	2.53	0.44
1:C:600:HIS:CD2	1:C:601:ASN:H	2.35	0.44
1:C:1214:VAL:HG21	1:C:1240:PHE:HE2	1.83	0.44
1:C:1280:ASN:HD22	1:C:1283:LEU:HB2	1.83	0.44
1:C:2127:LYS:HA	1:C:2130:MET:SD	2.58	0.44
1:B:2033:ILE:HA	1:B:2036:THR:HG22	2.00	0.44
1:B:2127:LYS:HA	1:B:2130:MET:SD	2.58	0.44
1:A:2127:LYS:HA	1:A:2130:MET:SD	2.58	0.44
1:A:2729:GLN:HA	1:A:2732:ARG:HG3	2.00	0.44
1:D:628:PRO:HB2	1:D:735:TYR:HD2	1.82	0.44
1:C:1080:LEU:HD22	1:C:1671:LEU:HD21	1.99	0.44
1:C:2033:ILE:HA	1:C:2036:THR:HG22	2.00	0.44
1:A:39:VAL:HG21	1:A:195:ALA:HB1	1.98	0.44
1:A:2033:ILE:HA	1:A:2036:THR:HG22	2.00	0.44
1:A:2363:CYS:HA	1:A:2366:ILE:HG22	2.00	0.44
1:D:1373:MET:O	1:D:1377:HIS:N	2.48	0.44
1:C:194:HIS:CD2	1:C:212:VAL:HG22	2.53	0.44
1:C:615:ILE:O	1:C:619:VAL:N	2.44	0.44
1:B:1088:SER:O	1:B:1088:SER:OG	2.36	0.44
1:A:791:ASP:N	1:A:791:ASP:OD1	2.51	0.44
1:D:2127:LYS:HA	1:D:2130:MET:SD	2.58	0.44
1:C:791:ASP:N	1:C:791:ASP:OD1	2.51	0.44
1:C:2154:HIS:CD2	1:C:2211:PRO:HB3	2.53	0.44
1:B:2154:HIS:CD2	1:B:2211:PRO:HB3	2.53	0.44
1:A:194:HIS:CD2	1:A:212:VAL:HG22	2.53	0.43
1:A:1956:ASP:N	1:A:1956:ASP:OD1	2.49	0.43
1:D:884:LEU:HD12	1:D:981:ILE:HG22	2.00	0.43
1:C:133:THR:HG21	1:C:156:ASN:HB3	2.00	0.43
1:C:2037:LEU:O	1:C:2041:THR:HG23	2.18	0.43
2:C:2803:PLX:H1B2	2:C:2803:PLX:H21	1.73	0.43
2:C:2807:PLX:H252	2:C:2807:PLX:H51	1.87	0.43
1:B:1955:ASP:N	1:B:1955:ASP:OD1	2.51	0.43
1:B:2394:TYR:HB2	2:B:2808:PLX:H81	2.00	0.43
1:A:1408:ARG:O	1:A:1412:HIS:ND1	2.51	0.43
1:A:1865:LYS:HD2	1:A:1868:GLN:HE21	1.83	0.43
1:A:2067:THR:OG1	1:A:2116:MET:SD	2.63	0.43
2:A:2802:PLX:H262	2:A:2802:PLX:H291	1.67	0.43
1:D:300:ASN:ND2	1:D:378:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:PRO:HA	1:D:529:ASP:HB3	1.99	0.43
1:D:2394:TYR:HB2	2:D:2804:PLX:H81	2.01	0.43
1:C:1300:GLU:OE2	1:C:1337:SER:OG	2.30	0.43
1:A:1214:VAL:HG21	1:A:1240:PHE:HE2	1.83	0.43
1:D:791:ASP:OD1	1:D:791:ASP:N	2.51	0.43
1:B:2055:ILE:HG22	1:B:2063:ILE:HD11	2.01	0.43
1:A:1664:LEU:HD12	1:A:1811:LEU:HD12	2.00	0.43
1:D:1280:ASN:HD22	1:D:1283:LEU:HB2	1.83	0.43
1:D:1391:VAL:HG22	1:D:1434:THR:HG21	2.01	0.43
1:D:2363:CYS:HA	1:D:2366:ILE:HG22	2.00	0.43
1:D:2729:GLN:HA	1:D:2732:ARG:HG3	2.00	0.43
1:C:2055:ILE:HG22	1:C:2063:ILE:HD11	2.01	0.43
1:C:2083:ASP:OD1	1:C:2083:ASP:N	2.51	0.43
2:C:2807:PLX:H322	2:C:2807:PLX:H351	1.86	0.43
1:B:1865:LYS:HD2	1:B:1868:GLN:HE21	1.83	0.43
1:B:1956:ASP:OD1	1:B:1956:ASP:N	2.49	0.43
1:A:2167:ASN:HD22	1:A:2170:LEU:HB2	1.83	0.43
1:D:2154:HIS:CD2	1:D:2211:PRO:HB3	2.53	0.43
1:D:2167:ASN:HD22	1:D:2170:LEU:HB2	1.83	0.43
1:C:1073:PRO:HG2	1:C:1076:VAL:H	1.81	0.43
1:C:2729:GLN:HA	1:C:2732:ARG:HG3	2.00	0.43
1:B:194:HIS:CD2	1:B:212:VAL:HG22	2.53	0.43
1:B:969:ASP:O	1:B:973:LYS:HG2	2.19	0.43
1:A:300:ASN:ND2	1:A:378:GLY:O	2.51	0.43
1:D:2037:LEU:O	1:D:2041:THR:HG23	2.18	0.43
1:D:2677:ARG:HD3	1:D:2677:ARG:HA	1.87	0.43
1:C:672:LEU:HA	1:C:695:GLU:HG3	2.01	0.43
1:C:969:ASP:O	1:C:973:LYS:HG2	2.19	0.43
1:C:1865:LYS:HD2	1:C:1868:GLN:HE21	1.83	0.43
1:C:1955:ASP:OD1	1:C:1955:ASP:N	2.51	0.43
2:C:2807:PLX:H111	2:C:2808:PLX:H141	2.01	0.43
1:B:884:LEU:HD12	1:B:981:ILE:HG22	2.00	0.43
1:B:1408:ARG:O	1:B:1412:HIS:ND1	2.51	0.43
1:A:884:LEU:HD12	1:A:981:ILE:HG22	2.00	0.43
1:A:1955:ASP:OD1	1:A:1955:ASP:N	2.51	0.43
1:A:2154:HIS:CD2	1:A:2211:PRO:HB3	2.53	0.43
1:D:969:ASP:O	1:D:973:LYS:HG2	2.19	0.43
1:D:2055:ILE:HG22	1:D:2063:ILE:HD11	2.01	0.43
1:D:2083:ASP:N	1:D:2083:ASP:OD1	2.51	0.43
1:C:628:PRO:HB2	1:C:735:TYR:HD2	1.82	0.43
2:B:2802:PLX:H322	2:B:2802:PLX:H351	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2807:PLX:H292	2:B:2807:PLX:H321	1.84	0.43
1:A:133:THR:HG21	1:A:156:ASN:HB3	2.00	0.43
1:A:1203:ARG:HA	1:A:1206:ARG:HH11	1.84	0.43
1:A:1280:ASN:HD22	1:A:1283:LEU:HB2	1.83	0.43
1:D:803:TYR:HE2	1:D:1099:GLN:HG3	1.84	0.43
1:C:825:SER:HB2	1:C:829:ILE:HD11	2.01	0.43
1:C:1293:GLN:HA	1:C:1296:VAL:HG23	2.01	0.43
1:C:1391:VAL:HG22	1:C:1434:THR:HG21	2.01	0.43
1:B:526:PRO:HA	1:B:529:ASP:HB3	1.99	0.43
1:B:791:ASP:OD1	1:B:791:ASP:N	2.51	0.43
1:B:833:PHE:O	1:B:837:MET:HG2	2.19	0.43
1:B:1214:VAL:HG21	1:B:1240:PHE:HE2	1.83	0.43
1:B:1285:SER:O	1:B:1325:LYS:NZ	2.43	0.43
1:B:1391:VAL:HG22	1:B:1434:THR:HG21	2.01	0.43
1:B:2037:LEU:O	1:B:2041:THR:HG23	2.18	0.43
1:B:2263:GLN:O	1:B:2265:VAL:N	2.52	0.43
1:A:638:CYS:SG	1:A:639:VAL:HG23	2.59	0.43
1:A:1293:GLN:HA	1:A:1296:VAL:HG23	2.01	0.43
1:D:1408:ARG:O	1:D:1412:HIS:ND1	2.51	0.43
1:C:747:ARG:NH1	1:C:749:TYR:OH	2.49	0.43
1:C:747:ARG:NH2	1:C:792:ARG:HB2	2.34	0.43
1:C:803:TYR:HE2	1:C:1099:GLN:HG3	1.84	0.43
1:C:2394:TYR:HB2	2:C:2805:PLX:H81	2.01	0.43
2:C:2803:PLX:H291	2:C:2803:PLX:H262	1.65	0.43
1:B:672:LEU:HA	1:B:695:GLU:HG3	2.01	0.43
1:B:1203:ARG:HA	1:B:1206:ARG:HH11	1.84	0.43
1:B:2363:CYS:HA	1:B:2366:ILE:HG22	2.00	0.43
2:B:2806:PLX:H1B2	2:B:2806:PLX:H21	1.74	0.43
2:A:2806:PLX:H111	2:A:2807:PLX:H141	2.01	0.43
1:D:825:SER:HB2	1:D:829:ILE:HD11	2.01	0.43
1:D:833:PHE:O	1:D:837:MET:HG2	2.19	0.43
1:D:2263:GLN:O	1:D:2265:VAL:N	2.52	0.43
1:D:2409:HIS:NE2	2:D:2803:PLX:C5	2.72	0.43
1:C:2297:PHE:HA	1:C:2300:VAL:HG13	2.01	0.43
1:B:638:CYS:SG	1:B:639:VAL:HG23	2.59	0.43
1:B:1618:LEU:O	1:B:1622:GLU:HB2	2.19	0.43
1:A:969:ASP:O	1:A:973:LYS:HG2	2.19	0.42
1:A:2055:ILE:HG22	1:A:2063:ILE:HD11	2.01	0.42
1:A:2083:ASP:OD1	1:A:2083:ASP:N	2.51	0.42
1:A:2394:TYR:HB2	2:A:2804:PLX:H81	2.00	0.42
1:D:124:LEU:HD12	1:D:131:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ASN:ND2	1:C:378:GLY:O	2.51	0.42
1:C:2167:ASN:HD22	1:C:2170:LEU:HB2	1.83	0.42
1:B:803:TYR:HE2	1:B:1099:GLN:HG3	1.84	0.42
1:A:124:LEU:HD12	1:A:131:TYR:CZ	2.54	0.42
1:A:803:TYR:HE2	1:A:1099:GLN:HG3	1.84	0.42
1:A:2127:LYS:NZ	1:A:2149:PRO:O	2.51	0.42
1:A:2525:GLU:O	1:A:2526:HIS:ND1	2.53	0.42
1:D:638:CYS:SG	1:D:639:VAL:HG23	2.59	0.42
1:D:2699:GLN:HA	1:D:2702:LEU:HD23	2.01	0.42
1:C:1408:ARG:O	1:C:1412:HIS:ND1	2.51	0.42
1:C:1618:LEU:O	1:C:1622:GLU:HB2	2.19	0.42
1:C:2250:LEU:HD23	1:C:2250:LEU:HA	1.85	0.42
1:A:2030:VAL:HG11	1:A:2084:LEU:HG	2.01	0.42
1:A:2699:GLN:HA	1:A:2702:LEU:HD23	2.01	0.42
1:D:133:THR:HG21	1:D:156:ASN:HB3	2.00	0.42
1:C:884:LEU:HD12	1:C:981:ILE:HG22	2.00	0.42
1:B:1104:VAL:HG22	1:B:1105:THR:H	1.84	0.42
1:A:833:PHE:O	1:A:837:MET:HG2	2.19	0.42
1:D:747:ARG:NH2	1:D:792:ARG:HB2	2.34	0.42
1:B:133:THR:HG21	1:B:156:ASN:HB3	2.00	0.42
1:B:1632:ARG:HG3	1:B:1745:TYR:HE1	1.85	0.42
1:A:2037:LEU:O	1:A:2041:THR:HG23	2.18	0.42
1:D:672:LEU:HA	1:D:695:GLU:HG3	2.01	0.42
1:C:1104:VAL:HG22	1:C:1105:THR:H	1.84	0.42
1:C:2263:GLN:O	1:C:2265:VAL:N	2.52	0.42
1:B:300:ASN:ND2	1:B:378:GLY:O	2.51	0.42
1:B:895:LEU:HD21	1:B:974:ILE:HD11	2.02	0.42
1:B:2297:PHE:HA	1:B:2300:VAL:HG13	2.01	0.42
1:B:2525:GLU:O	1:B:2526:HIS:ND1	2.53	0.42
1:A:895:LEU:HD21	1:A:974:ILE:HD11	2.02	0.42
1:A:2046:GLY:HA2	1:A:2658:GLY:HA3	2.02	0.42
1:A:2263:GLN:O	1:A:2265:VAL:N	2.52	0.42
2:A:2806:PLX:H1C2	2:A:2806:PLX:H21	1.79	0.42
1:D:1618:LEU:O	1:D:1622:GLU:HB2	2.19	0.42
1:D:2046:GLY:HA2	1:D:2658:GLY:HA3	2.02	0.42
1:D:2721:ASP:O	1:D:2724:THR:OG1	2.31	0.42
1:C:638:CYS:SG	1:C:639:VAL:HG23	2.59	0.42
1:C:833:PHE:O	1:C:837:MET:HG2	2.19	0.42
1:C:2525:GLU:O	1:C:2526:HIS:ND1	2.53	0.42
1:B:55:ASP:O	1:B:125:HIS:NE2	2.53	0.42
1:B:124:LEU:HD12	1:B:131:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:ARG:NH2	1:B:792:ARG:HB2	2.34	0.42
1:B:2729:GLN:HA	1:B:2732:ARG:HG3	2.00	0.42
1:A:825:SER:HB2	1:A:829:ILE:HD11	2.01	0.42
1:A:2250:LEU:HD23	1:A:2250:LEU:HA	1.85	0.42
1:D:723:GLN:HB2	1:D:726:ASP:HB2	2.02	0.42
1:D:2297:PHE:HA	1:D:2300:VAL:HG13	2.01	0.42
1:C:60:LEU:HD12	1:C:121:ILE:HG12	2.02	0.42
1:C:2363:CYS:HA	1:C:2366:ILE:HG22	2.00	0.42
1:A:723:GLN:HB2	1:A:726:ASP:HB2	2.02	0.42
1:A:1391:VAL:HG22	1:A:1434:THR:HG21	2.01	0.42
1:D:615:ILE:O	1:D:619:VAL:N	2.44	0.42
1:D:624:LYS:HD2	1:D:624:LYS:HA	1.89	0.42
1:D:1203:ARG:HA	1:D:1206:ARG:HH11	1.84	0.42
1:D:2431:ILE:HA	1:D:2434:VAL:HG12	2.01	0.42
1:C:55:ASP:O	1:C:125:HIS:NE2	2.53	0.42
1:C:124:LEU:HD12	1:C:131:TYR:CZ	2.54	0.42
1:C:2699:GLN:HA	1:C:2702:LEU:HD23	2.01	0.42
1:B:536:LEU:HB3	1:B:538:LEU:HD23	2.02	0.42
1:B:1244:PHE:O	1:B:1251:ASN:ND2	2.53	0.42
1:B:1293:GLN:HA	1:B:1296:VAL:HG23	2.00	0.42
1:B:2409:HIS:CB	2:B:2807:PLX:H52	2.49	0.42
1:A:1244:PHE:O	1:A:1251:ASN:ND2	2.53	0.42
2:A:2803:PLX:H321	2:A:2803:PLX:H292	1.86	0.42
1:D:55:ASP:O	1:D:125:HIS:NE2	2.53	0.42
1:D:60:LEU:HD12	1:D:121:ILE:HG12	2.02	0.42
1:C:723:GLN:HB2	1:C:726:ASP:HB2	2.02	0.42
1:B:2699:GLN:HA	1:B:2702:LEU:HD23	2.01	0.42
1:A:1104:VAL:HG22	1:A:1105:THR:H	1.84	0.42
1:D:1104:VAL:HG22	1:D:1105:THR:H	1.84	0.42
1:D:1293:GLN:HA	1:D:1296:VAL:HG23	2.01	0.42
1:C:1203:ARG:HA	1:C:1206:ARG:HH11	1.84	0.42
1:C:2431:ILE:HA	1:C:2434:VAL:HG12	2.01	0.42
1:B:265:ARG:O	1:B:269:ARG:NH2	2.53	0.42
1:B:623:ARG:NH1	1:B:631:LEU:HB2	2.35	0.42
1:B:825:SER:HB2	1:B:829:ILE:HD11	2.01	0.42
2:B:2807:PLX:H1A2	2:B:2807:PLX:H21	1.76	0.42
1:A:672:LEU:HA	1:A:695:GLU:HG3	2.01	0.41
2:A:2802:PLX:H21	2:A:2802:PLX:H1B2	1.74	0.41
1:D:2525:GLU:O	1:D:2526:HIS:ND1	2.53	0.41
1:C:1271:VAL:HA	1:C:1274:GLN:HB3	2.02	0.41
1:B:2127:LYS:NZ	1:B:2149:PRO:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ARG:NH1	1:A:631:LEU:HB2	2.35	0.41
1:A:747:ARG:NH2	1:A:792:ARG:HB2	2.34	0.41
1:C:895:LEU:HD21	1:C:974:ILE:HD11	2.02	0.41
1:C:1632:ARG:HG3	1:C:1745:TYR:HE1	1.85	0.41
1:C:2200:ARG:HD3	1:C:2200:ARG:HA	1.89	0.41
1:C:2721:ASP:O	1:C:2724:THR:OG1	2.31	0.41
1:B:2030:VAL:HG11	1:B:2084:LEU:HG	2.01	0.41
1:B:2632:ILE:HD13	1:B:2632:ILE:HA	1.94	0.41
1:B:2721:ASP:O	1:B:2724:THR:OG1	2.31	0.41
2:B:2806:PLX:H291	2:B:2806:PLX:H262	1.66	0.41
1:A:1618:LEU:O	1:A:1622:GLU:HB2	2.19	0.41
1:A:1644:ARG:HA	1:A:1647:CYS:HB3	2.03	0.41
1:A:2297:PHE:HA	1:A:2300:VAL:HG13	2.01	0.41
1:D:1271:VAL:HA	1:D:1274:GLN:HB3	2.02	0.41
1:D:2614:CYS:SG	1:D:2616:LEU:HD23	2.61	0.41
1:C:623:ARG:NH1	1:C:631:LEU:HB2	2.35	0.41
1:C:1403:LEU:HG	1:C:1406:ILE:HB	2.03	0.41
1:B:723:GLN:HB2	1:B:726:ASP:HB2	2.02	0.41
1:B:1203:ARG:HH21	1:B:1247:GLY:H	1.68	0.41
1:B:1203:ARG:NH1	1:B:1248:ASN:OD1	2.54	0.41
1:A:1025:PRO:HB2	1:A:1026:GLY:H	1.64	0.41
1:A:1203:ARG:HH21	1:A:1247:GLY:H	1.68	0.41
1:A:2443:LEU:HD23	1:A:2443:LEU:HA	1.88	0.41
1:C:2369:LEU:HD21	1:C:2395:HIS:HB3	2.03	0.41
2:B:2802:PLX:H131	2:B:2802:PLX:H162	1.95	0.41
1:A:55:ASP:O	1:A:125:HIS:NE2	2.53	0.41
1:A:404:ILE:HA	1:A:405:PRO:HD3	1.95	0.41
1:A:1403:LEU:HG	1:A:1406:ILE:HB	2.03	0.41
1:A:2369:LEU:HD21	1:A:2395:HIS:HB3	2.03	0.41
1:D:265:ARG:O	1:D:269:ARG:NH2	2.53	0.41
1:D:623:ARG:NH1	1:D:631:LEU:HB2	2.35	0.41
1:D:1403:LEU:HG	1:D:1406:ILE:HB	2.03	0.41
1:D:2544:ARG:H	1:D:2544:ARG:HG2	1.72	0.41
1:C:2614:CYS:SG	1:C:2616:LEU:HD23	2.61	0.41
1:B:2409:HIS:CE1	2:B:2807:PLX:O8	2.71	0.41
2:B:2802:PLX:H111	2:B:2803:PLX:H141	2.02	0.41
1:A:1088:SER:O	1:A:1088:SER:OG	2.36	0.41
1:A:1271:VAL:HA	1:A:1274:GLN:HB3	2.02	0.41
1:A:2200:ARG:HD3	1:A:2200:ARG:HA	1.89	0.41
1:D:536:LEU:HB3	1:D:538:LEU:HD23	2.02	0.41
1:D:895:LEU:HD21	1:D:974:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1203:ARG:NH1	1:D:1248:ASN:OD1	2.54	0.41
1:D:2030:VAL:HG11	1:D:2084:LEU:HG	2.01	0.41
1:C:265:ARG:O	1:C:269:ARG:NH2	2.53	0.41
1:C:1244:PHE:O	1:C:1251:ASN:ND2	2.53	0.41
1:B:871:ARG:NH2	1:B:976:GLU:OE2	2.51	0.41
1:B:1271:VAL:HA	1:B:1274:GLN:HB3	2.03	0.41
1:A:122:GLN:OE1	1:A:159:SER:OG	2.30	0.41
1:A:300:ASN:HB2	1:B:2732:ARG:NH2	2.36	0.41
1:A:1203:ARG:NH1	1:A:1248:ASN:OD1	2.54	0.41
1:A:2377:GLY:O	1:A:2381:ARG:NE	2.54	0.41
1:D:1644:ARG:HA	1:D:1647:CYS:HB3	2.03	0.41
1:D:2611:CYS:SG	1:D:2612:PHE:N	2.94	0.41
2:D:2806:PLX:H1C2	2:D:2806:PLX:H21	1.82	0.41
1:C:785:MET:O	1:C:789:HIS:ND1	2.53	0.41
1:C:2709:VAL:O	1:C:2712:LEU:HG	2.21	0.41
1:A:265:ARG:O	1:A:269:ARG:NH2	2.53	0.41
1:A:383:PRO:HG2	1:A:386:SER:HB3	2.03	0.41
1:D:1203:ARG:HH21	1:D:1247:GLY:H	1.68	0.41
1:D:1632:ARG:HG3	1:D:1745:TYR:HE1	1.85	0.41
1:D:1674:LYS:HD2	1:D:1674:LYS:HA	1.90	0.41
1:D:2369:LEU:HD21	1:D:2395:HIS:HB3	2.03	0.41
1:C:2557:SER:O	1:C:2557:SER:OG	2.31	0.41
1:B:60:LEU:HD12	1:B:121:ILE:HG12	2.02	0.41
1:B:383:PRO:HG2	1:B:386:SER:HB3	2.03	0.41
1:B:1403:LEU:HG	1:B:1406:ILE:HB	2.03	0.41
1:B:1644:ARG:HA	1:B:1647:CYS:HB3	2.03	0.41
1:A:45:ASP:N	1:A:45:ASP:OD1	2.53	0.41
1:A:871:ARG:NH2	1:A:976:GLU:OE2	2.51	0.41
1:A:1632:ARG:HG3	1:A:1745:TYR:HE1	1.85	0.41
1:D:1244:PHE:O	1:D:1251:ASN:ND2	2.53	0.41
1:D:2575:PHE:CD2	2:D:2807:PLX:C36	3.03	0.41
2:D:2803:PLX:H292	2:D:2803:PLX:H321	1.79	0.41
1:C:536:LEU:HB3	1:C:538:LEU:HD23	2.02	0.41
1:C:585:ILE:HD11	1:C:595:ILE:HG21	2.03	0.41
1:C:2030:VAL:HG11	1:C:2084:LEU:HG	2.01	0.41
1:C:2611:CYS:SG	1:C:2612:PHE:N	2.94	0.41
1:C:2732:ARG:NH2	1:B:300:ASN:HB2	2.36	0.41
1:B:625:ASN:O	1:B:626:ARG:NE	2.51	0.41
1:B:1645:ARG:NH1	1:B:1646:LYS:HB2	2.36	0.41
1:B:1826:LEU:HD23	1:B:1829:ILE:HD12	2.03	0.41
1:B:2046:GLY:HA2	1:B:2658:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2377:GLY:O	1:B:2381:ARG:NE	2.54	0.41
1:A:60:LEU:HD12	1:A:121:ILE:HG12	2.02	0.41
1:A:2431:ILE:HA	1:A:2434:VAL:HG12	2.01	0.41
1:D:2557:SER:O	1:D:2557:SER:OG	2.31	0.41
1:C:383:PRO:HG2	1:C:386:SER:HB3	2.03	0.41
1:C:1645:ARG:NH1	1:C:1646:LYS:HB2	2.36	0.41
1:C:2046:GLY:HA2	1:C:2658:GLY:HA3	2.02	0.41
1:C:2377:GLY:O	1:C:2381:ARG:NE	2.54	0.41
1:B:32:LEU:HD23	1:B:445:PHE:HB2	2.03	0.41
1:B:2431:ILE:HA	1:B:2434:VAL:HG12	2.02	0.41
1:B:2611:CYS:SG	1:B:2612:PHE:N	2.94	0.41
1:B:2709:VAL:O	1:B:2712:LEU:HG	2.21	0.41
2:A:2804:PLX:H141	2:A:2804:PLX:H111	1.95	0.40
2:A:2806:PLX:H252	2:A:2806:PLX:H51	1.85	0.40
1:D:32:LEU:N	1:D:448:ASP:OD2	2.54	0.40
1:D:871:ARG:NH2	1:D:976:GLU:OE2	2.51	0.40
1:D:1179:ILE:HD12	1:D:1179:ILE:HA	1.92	0.40
1:D:1450:LEU:O	1:D:1454:PHE:HB2	2.22	0.40
1:C:32:LEU:N	1:C:448:ASP:OD2	2.55	0.40
1:C:250:PHE:HB2	1:C:262:VAL:HG22	2.03	0.40
1:A:121:ILE:HG22	1:A:161:PHE:HB2	2.03	0.40
1:A:496:GLU:HB3	1:A:499:PHE:HE2	1.86	0.40
1:A:501:LYS:HA	1:A:502:PRO:HD3	1.87	0.40
1:A:638:CYS:HB2	1:A:652:ILE:HD13	2.04	0.40
1:A:1450:LEU:O	1:A:1454:PHE:HB2	2.22	0.40
1:A:1645:ARG:NH1	1:A:1646:LYS:HB2	2.36	0.40
1:A:1826:LEU:HD23	1:A:1829:ILE:HD12	2.03	0.40
1:A:2614:CYS:SG	1:A:2616:LEU:HD23	2.61	0.40
1:D:121:ILE:HG22	1:D:161:PHE:HB2	2.03	0.40
1:D:638:CYS:HB2	1:D:652:ILE:HD13	2.04	0.40
1:C:1644:ARG:HA	1:C:1647:CYS:HB3	2.03	0.40
1:C:1826:LEU:HD23	1:C:1826:LEU:HA	1.86	0.40
1:B:121:ILE:HG22	1:B:161:PHE:HB2	2.03	0.40
1:B:607:GLU:HB3	1:B:647:VAL:HG11	2.03	0.40
1:B:615:ILE:O	1:B:619:VAL:N	2.44	0.40
1:B:2234:ASP:N	1:B:2234:ASP:OD1	2.55	0.40
1:A:1620:GLN:O	1:A:1624:SER:OG	2.30	0.40
1:A:2427:LEU:HD11	1:B:2447:LEU:HD22	2.03	0.40
1:A:2472:ASP:OD1	1:A:2472:ASP:N	2.55	0.40
1:D:1645:ARG:NH1	1:D:1646:LYS:HB2	2.36	0.40
1:C:121:ILE:HG22	1:C:161:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:ASN:O	1:C:626:ARG:NE	2.51	0.40
1:C:1203:ARG:HH21	1:C:1247:GLY:H	1.68	0.40
1:C:1826:LEU:HD23	1:C:1829:ILE:HD12	2.03	0.40
1:B:2369:LEU:HD21	1:B:2395:HIS:HB3	2.03	0.40
1:B:2677:ARG:HD3	1:B:2677:ARG:HA	1.87	0.40
1:A:32:LEU:N	1:A:448:ASP:OD2	2.55	0.40
1:A:2224:LYS:HG3	1:A:2639:TRP:CZ2	2.57	0.40
1:A:2611:CYS:SG	1:A:2612:PHE:N	2.94	0.40
1:A:2709:VAL:O	1:A:2712:LEU:HG	2.21	0.40
1:D:2732:ARG:NH2	1:C:300:ASN:HB2	2.36	0.40
1:C:178:ILE:HD13	1:C:178:ILE:HA	1.88	0.40
1:C:1637:PHE:HD1	1:C:1638:PRO:HD3	1.87	0.40
1:B:1404:ASP:O	1:B:1408:ARG:HG2	2.21	0.40
1:B:1416:ILE:HD13	1:B:1416:ILE:HA	1.93	0.40
1:B:1637:PHE:HD1	1:B:1638:PRO:HD3	1.87	0.40
1:B:1871:ILE:H	1:B:1871:ILE:HG12	1.69	0.40
1:B:2715:GLN:HA	1:B:2718:GLU:HG3	2.04	0.40
1:A:536:LEU:HB3	1:A:538:LEU:HD23	2.02	0.40
1:A:826:LYS:HD2	1:A:826:LYS:HA	1.90	0.40
1:A:1871:ILE:H	1:A:1871:ILE:HG12	1.69	0.40
1:A:2447:LEU:HD22	1:D:2427:LEU:HD11	2.03	0.40
1:D:383:PRO:HG2	1:D:386:SER:HB3	2.03	0.40
1:D:2709:VAL:O	1:D:2712:LEU:HG	2.21	0.40
1:C:314:LEU:HD12	1:C:314:LEU:HA	1.94	0.40
1:C:624:LYS:HD2	1:C:624:LYS:HA	1.89	0.40
1:C:669:LYS:HA	1:C:669:LYS:HD2	1.93	0.40
1:C:1228:THR:OG1	1:C:1229:LYS:N	2.53	0.40
1:B:496:GLU:HB3	1:B:499:PHE:HE2	1.87	0.40
1:B:624:LYS:HA	1:B:624:LYS:HD2	1.89	0.40
1:B:2200:ARG:HD3	1:B:2200:ARG:HA	1.89	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	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
1	B	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
1	C	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
1	D	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
All	All	9080/10936 (83%)	8072 (89%)	984 (11%)	24 (0%)	44	71

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2412	PHE
1	D	2412	PHE
1	C	2412	PHE
1	B	2412	PHE
1	A	2612	PHE
1	D	2612	PHE
1	C	2612	PHE
1	B	2612	PHE
1	A	393	LEU
1	A	2264	PRO
1	D	393	LEU
1	D	2264	PRO
1	C	393	LEU
1	C	2264	PRO
1	B	393	LEU
1	B	2264	PRO
1	A	853	PRO
1	D	853	PRO
1	C	853	PRO
1	B	853	PRO
1	A	2613	ILE
1	D	2613	ILE
1	C	2613	ILE
1	B	2613	ILE

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	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
1	B	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
1	C	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
1	D	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
All	All	7888/9776 (81%)	7844 (99%)	44 (1%)	86	91

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ARG
1	A	705	LYS
1	A	766	ARG
1	A	889	LYS
1	A	1206	ARG
1	A	1229	LYS
1	A	1304	ARG
1	A	1348	ARG
1	A	1632	ARG
1	A	1645	ARG
1	A	2381	ARG
1	D	257	ARG
1	D	705	LYS
1	D	766	ARG
1	D	889	LYS
1	D	1206	ARG
1	D	1229	LYS
1	D	1304	ARG
1	D	1348	ARG
1	D	1632	ARG
1	D	1645	ARG
1	D	2381	ARG
1	C	257	ARG
1	C	705	LYS
1	C	766	ARG
1	C	889	LYS
1	C	1206	ARG
1	C	1229	LYS
1	C	1304	ARG
1	C	1348	ARG

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Mol	Chain	Res	Type
1	C	1632	ARG
1	C	1645	ARG
1	C	2381	ARG
1	B	257	ARG
1	B	705	LYS
1	B	766	ARG
1	B	889	LYS
1	B	1206	ARG
1	B	1229	LYS
1	B	1304	ARG
1	B	1348	ARG
1	B	1632	ARG
1	B	1645	ARG
1	B	2381	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	122	GLN
1	A	1242	GLN
1	A	1252	GLN
1	A	1836	ASN
1	A	2053	ASN
1	A	2108	ASN
1	A	2729	GLN
1	D	103	ASN
1	D	122	GLN
1	D	1242	GLN
1	D	1252	GLN
1	D	1836	ASN
1	D	2053	ASN
1	D	2108	ASN
1	D	2729	GLN
1	C	103	ASN
1	C	122	GLN
1	C	1242	GLN
1	C	1252	GLN
1	C	1836	ASN
1	C	2053	ASN
1	C	2108	ASN
1	C	2729	GLN

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Mol	Chain	Res	Type
1	B	64	ASN
1	B	1242	GLN
1	B	1252	GLN
1	B	1836	ASN
1	B	2053	ASN
1	B	2108	ASN
1	B	2729	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 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLX	C	2805	-	38,38,51	1.95	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	B	2807	-	35,35,51	2.02	5 (14%)	39,43,59	1.71	5 (12%)
2	PLX	B	2804	-	39,39,51	1.91	4 (10%)	43,47,59	1.60	5 (11%)
2	PLX	B	2801	-	39,39,51	1.92	4 (10%)	43,47,59	1.61	5 (11%)
2	PLX	D	2803	-	35,35,51	2.01	4 (11%)	39,43,59	1.70	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PLX	C	2807	-	45,45,51	1.79	4 (8%)	49,53,59	1.57	5 (10%)
2	PLX	C	2808	-	42,42,51	1.86	4 (9%)	46,50,59	1.55	5 (10%)
2	PLX	D	2806	-	45,45,51	1.69	6 (13%)	49,53,59	1.66	6 (12%)
2	PLX	D	2802	-	35,35,51	2.02	4 (11%)	39,43,59	1.62	6 (15%)
2	PLX	A	2804	-	38,38,51	1.96	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	A	2808	-	39,39,51	1.92	4 (10%)	43,47,59	1.60	5 (11%)
2	PLX	B	2805	-	33,33,51	2.07	4 (12%)	37,41,59	1.73	5 (13%)
2	PLX	D	2804	-	38,38,51	1.96	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	A	2801	-	33,33,51	2.07	4 (12%)	37,41,59	1.72	5 (13%)
2	PLX	A	2807	-	42,42,51	1.86	4 (9%)	46,50,59	1.54	5 (10%)
2	PLX	B	2806	-	35,35,51	2.02	4 (11%)	39,43,59	1.62	6 (15%)
2	PLX	D	2807	-	42,42,51	1.86	4 (9%)	46,50,59	1.54	5 (10%)
2	PLX	C	2804	-	35,35,51	2.02	5 (14%)	39,43,59	1.69	5 (12%)
2	PLX	A	2802	-	35,35,51	2.02	4 (11%)	39,43,59	1.63	6 (15%)
2	PLX	B	2802	-	45,45,51	1.79	4 (8%)	49,53,59	1.51	5 (10%)
2	PLX	C	2802	-	33,33,51	2.07	4 (12%)	37,41,59	1.73	5 (13%)
2	PLX	D	2801	-	33,33,51	2.07	4 (12%)	37,41,59	1.73	5 (13%)
2	PLX	A	2803	-	35,35,51	2.02	4 (11%)	39,43,59	1.71	6 (15%)
2	PLX	B	2803	-	41,41,51	1.88	4 (9%)	45,49,59	1.56	5 (11%)
2	PLX	C	2803	-	35,35,51	2.02	4 (11%)	39,43,59	1.63	6 (15%)
2	PLX	C	2801	-	39,39,51	1.92	4 (10%)	43,47,59	1.60	5 (11%)
2	PLX	B	2808	-	38,38,51	1.96	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	A	2806	-	45,45,51	1.79	4 (8%)	49,53,59	1.56	5 (10%)

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
2	PLX	C	2805	-	3/3/5/5	23/42/42/55	-
2	PLX	B	2807	-	3/3/5/5	16/39/39/55	-
2	PLX	B	2804	-	3/3/5/5	22/43/43/55	-
2	PLX	B	2801	-	3/3/5/5	23/43/43/55	-
2	PLX	D	2803	-	3/3/5/5	21/39/39/55	-
2	PLX	C	2807	-	3/3/5/5	25/49/49/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	C	2808	-	3/3/5/5	25/46/46/55	-
2	PLX	D	2806	-	3/3/5/5	25/49/49/55	-
2	PLX	D	2802	-	3/3/5/5	19/39/39/55	-
2	PLX	A	2804	-	3/3/5/5	26/42/42/55	-
2	PLX	A	2808	-	3/3/5/5	20/43/43/55	-
2	PLX	B	2805	-	3/3/5/5	18/37/37/55	-
2	PLX	D	2804	-	3/3/5/5	24/42/42/55	-
2	PLX	A	2801	-	3/3/5/5	17/37/37/55	-
2	PLX	A	2807	-	3/3/5/5	25/46/46/55	-
2	PLX	B	2806	-	3/3/5/5	19/39/39/55	-
2	PLX	D	2807	-	3/3/5/5	26/46/46/55	-
2	PLX	C	2804	-	3/3/5/5	18/39/39/55	-
2	PLX	A	2802	-	3/3/5/5	19/39/39/55	-
2	PLX	B	2802	-	3/3/5/5	26/49/49/55	-
2	PLX	C	2802	-	3/3/5/5	18/37/37/55	-
2	PLX	D	2801	-	3/3/5/5	18/37/37/55	-
2	PLX	A	2803	-	3/3/5/5	17/39/39/55	-
2	PLX	B	2803	-	3/3/5/5	24/45/45/55	-
2	PLX	C	2803	-	3/3/5/5	19/39/39/55	-
2	PLX	C	2801	-	3/3/5/5	21/43/43/55	-
2	PLX	B	2808	-	3/3/5/5	24/42/42/55	-
2	PLX	A	2806	-	3/3/5/5	25/49/49/55	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2801	PLX	O7-C6	-7.25	1.18	1.39
2	C	2804	PLX	O7-C6	-7.24	1.18	1.39
2	C	2803	PLX	O7-C6	-7.24	1.18	1.39
2	B	2808	PLX	O7-C6	-7.23	1.18	1.39
2	C	2808	PLX	O7-C6	-7.23	1.18	1.39
2	B	2806	PLX	O7-C6	-7.22	1.18	1.39
2	A	2803	PLX	O7-C6	-7.22	1.18	1.39
2	C	2801	PLX	O7-C6	-7.22	1.18	1.39
2	A	2802	PLX	O7-C6	-7.22	1.18	1.39
2	A	2807	PLX	O7-C6	-7.22	1.18	1.39
2	B	2807	PLX	O7-C6	-7.22	1.18	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2808	PLX	O7-C6	-7.22	1.19	1.39
2	D	2804	PLX	O7-C6	-7.22	1.19	1.39
2	D	2802	PLX	O7-C6	-7.21	1.19	1.39
2	B	2805	PLX	O7-C6	-7.21	1.19	1.39
2	A	2804	PLX	O7-C6	-7.21	1.19	1.39
2	D	2807	PLX	O7-C6	-7.21	1.19	1.39
2	B	2804	PLX	O7-C6	-7.21	1.19	1.39
2	C	2802	PLX	O7-C6	-7.21	1.19	1.39
2	D	2803	PLX	O7-C6	-7.21	1.19	1.39
2	D	2801	PLX	O7-C6	-7.20	1.19	1.39
2	C	2805	PLX	O7-C6	-7.20	1.19	1.39
2	B	2803	PLX	O7-C6	-7.20	1.19	1.39
2	A	2801	PLX	O7-C6	-7.20	1.19	1.39
2	A	2806	PLX	O9-C24	-7.19	1.19	1.39
2	B	2802	PLX	O7-C6	-7.18	1.19	1.39
2	A	2806	PLX	O7-C6	-7.16	1.19	1.39
2	C	2807	PLX	O7-C6	-7.15	1.19	1.39
2	D	2804	PLX	O9-C24	-7.15	1.19	1.39
2	A	2804	PLX	O9-C24	-7.15	1.19	1.39
2	B	2808	PLX	O9-C24	-7.15	1.19	1.39
2	A	2802	PLX	O9-C24	-7.14	1.19	1.39
2	D	2802	PLX	O9-C24	-7.14	1.19	1.39
2	C	2807	PLX	O9-C24	-7.14	1.19	1.39
2	D	2806	PLX	O7-C6	-7.14	1.19	1.39
2	A	2807	PLX	O9-C24	-7.13	1.19	1.39
2	C	2805	PLX	O9-C24	-7.13	1.19	1.39
2	B	2803	PLX	O9-C24	-7.13	1.19	1.39
2	C	2808	PLX	O9-C24	-7.13	1.19	1.39
2	B	2802	PLX	O9-C24	-7.12	1.19	1.39
2	B	2806	PLX	O9-C24	-7.12	1.19	1.39
2	A	2803	PLX	O9-C24	-7.12	1.19	1.39
2	C	2803	PLX	O9-C24	-7.11	1.19	1.39
2	B	2807	PLX	O9-C24	-7.11	1.19	1.39
2	D	2801	PLX	O9-C24	-7.11	1.19	1.39
2	C	2804	PLX	O9-C24	-7.11	1.19	1.39
2	A	2801	PLX	O9-C24	-7.10	1.19	1.39
2	B	2805	PLX	O9-C24	-7.10	1.19	1.39
2	C	2802	PLX	O9-C24	-7.10	1.19	1.39
2	C	2801	PLX	O9-C24	-7.10	1.19	1.39
2	D	2807	PLX	O9-C24	-7.10	1.19	1.39
2	B	2801	PLX	O9-C24	-7.09	1.19	1.39
2	B	2804	PLX	O9-C24	-7.08	1.19	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2808	PLX	O9-C24	-7.08	1.19	1.39
2	D	2803	PLX	O9-C24	-7.08	1.19	1.39
2	D	2806	PLX	O9-C24	-5.27	1.24	1.39
2	A	2803	PLX	O6-C4	-3.41	1.40	1.44
2	B	2803	PLX	O6-C4	-3.35	1.40	1.44
2	A	2807	PLX	O6-C4	-3.33	1.40	1.44
2	B	2807	PLX	O6-C4	-3.33	1.40	1.44
2	C	2808	PLX	O6-C4	-3.31	1.40	1.44
2	D	2807	PLX	O6-C4	-3.31	1.40	1.44
2	C	2804	PLX	O6-C4	-3.22	1.40	1.44
2	A	2808	PLX	O6-C4	-3.20	1.40	1.44
2	A	2804	PLX	O6-C4	-3.20	1.40	1.44
2	B	2801	PLX	O6-C4	-3.19	1.40	1.44
2	D	2803	PLX	O6-C4	-3.19	1.40	1.44
2	C	2805	PLX	O6-C4	-3.17	1.40	1.44
2	B	2808	PLX	O6-C4	-3.17	1.40	1.44
2	D	2804	PLX	O6-C4	-3.16	1.40	1.44
2	B	2804	PLX	O6-C4	-3.15	1.40	1.44
2	C	2803	PLX	O6-C4	-3.14	1.40	1.44
2	C	2801	PLX	O6-C4	-3.13	1.40	1.44
2	D	2802	PLX	O6-C4	-3.11	1.40	1.44
2	A	2801	PLX	O6-C4	-3.07	1.40	1.44
2	B	2806	PLX	O6-C4	-3.07	1.40	1.44
2	D	2801	PLX	O6-C4	-3.06	1.40	1.44
2	A	2802	PLX	O6-C4	-3.06	1.40	1.44
2	B	2805	PLX	O6-C4	-3.05	1.40	1.44
2	C	2802	PLX	O6-C4	-3.02	1.40	1.44
2	A	2806	PLX	O6-C4	-2.97	1.40	1.44
2	C	2807	PLX	O6-C4	-2.93	1.40	1.44
2	B	2802	PLX	O6-C4	-2.87	1.40	1.44
2	D	2806	PLX	C25-C24	2.72	1.56	1.50
2	D	2806	PLX	C7-C6	2.49	1.56	1.50
2	D	2806	PLX	O6-C4	-2.24	1.41	1.44
2	C	2807	PLX	C7-C6	2.21	1.55	1.50
2	A	2806	PLX	C7-C6	2.20	1.55	1.50
2	A	2808	PLX	C7-C6	2.19	1.55	1.50
2	B	2802	PLX	C7-C6	2.19	1.55	1.50
2	A	2804	PLX	C7-C6	2.18	1.55	1.50
2	C	2805	PLX	C7-C6	2.17	1.55	1.50
2	D	2804	PLX	C7-C6	2.17	1.55	1.50
2	B	2804	PLX	C7-C6	2.16	1.55	1.50
2	C	2801	PLX	C7-C6	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2808	PLX	C7-C6	2.14	1.55	1.50
2	B	2801	PLX	C7-C6	2.14	1.55	1.50
2	A	2807	PLX	C7-C6	2.13	1.55	1.50
2	D	2801	PLX	C7-C6	2.13	1.55	1.50
2	B	2803	PLX	C7-C6	2.13	1.55	1.50
2	D	2807	PLX	C7-C6	2.12	1.55	1.50
2	D	2806	PLX	O8-C24	2.12	1.43	1.40
2	C	2802	PLX	C7-C6	2.11	1.55	1.50
2	C	2808	PLX	C7-C6	2.11	1.55	1.50
2	D	2803	PLX	C7-C6	2.10	1.55	1.50
2	C	2803	PLX	C7-C6	2.10	1.55	1.50
2	A	2801	PLX	C7-C6	2.09	1.55	1.50
2	C	2804	PLX	C7-C6	2.09	1.55	1.50
2	B	2805	PLX	C7-C6	2.08	1.55	1.50
2	A	2802	PLX	C7-C6	2.06	1.55	1.50
2	D	2802	PLX	C7-C6	2.06	1.55	1.50
2	A	2803	PLX	C7-C6	2.06	1.55	1.50
2	B	2806	PLX	C7-C6	2.05	1.55	1.50
2	B	2807	PLX	P1-O4	2.02	1.67	1.59
2	B	2807	PLX	C7-C6	2.01	1.55	1.50
2	C	2804	PLX	P1-O4	2.00	1.67	1.59

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2806	PLX	O9-C24-C25	7.26	122.58	109.12
2	C	2807	PLX	O9-C24-C25	6.48	121.13	109.12
2	A	2806	PLX	O9-C24-C25	6.45	121.08	109.12
2	D	2803	PLX	O9-C24-C25	6.02	120.28	109.12
2	C	2804	PLX	O9-C24-C25	5.98	120.20	109.12
2	A	2804	PLX	O7-C6-C7	5.95	120.14	109.12
2	D	2804	PLX	O7-C6-C7	5.94	120.13	109.12
2	B	2801	PLX	O9-C24-C25	5.93	120.11	109.12
2	B	2804	PLX	O9-C24-C25	5.93	120.11	109.12
2	A	2808	PLX	O9-C24-C25	5.92	120.10	109.12
2	C	2805	PLX	O7-C6-C7	5.92	120.09	109.12
2	B	2808	PLX	O7-C6-C7	5.92	120.08	109.12
2	B	2805	PLX	O9-C24-C25	5.91	120.08	109.12
2	D	2801	PLX	O9-C24-C25	5.91	120.07	109.12
2	D	2803	PLX	O7-C6-C7	5.90	120.05	109.12
2	C	2801	PLX	O9-C24-C25	5.89	120.04	109.12
2	C	2804	PLX	O7-C6-C7	5.89	120.04	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2802	PLX	O9-C24-C25	5.88	120.02	109.12
2	A	2801	PLX	O9-C24-C25	5.88	120.01	109.12
2	C	2807	PLX	O7-C6-C7	5.88	120.01	109.12
2	A	2803	PLX	O7-C6-C7	5.87	119.99	109.12
2	B	2805	PLX	O7-C6-C7	5.85	119.97	109.12
2	B	2807	PLX	O7-C6-C7	5.85	119.96	109.12
2	B	2807	PLX	O9-C24-C25	5.84	119.95	109.12
2	C	2802	PLX	O7-C6-C7	5.83	119.92	109.12
2	D	2801	PLX	O7-C6-C7	5.82	119.91	109.12
2	A	2806	PLX	O7-C6-C7	5.81	119.89	109.12
2	A	2801	PLX	O7-C6-C7	5.81	119.88	109.12
2	B	2801	PLX	O7-C6-C7	5.80	119.87	109.12
2	C	2808	PLX	O7-C6-C7	5.79	119.86	109.12
2	A	2807	PLX	O7-C6-C7	5.78	119.83	109.12
2	B	2802	PLX	O9-C24-C25	5.77	119.81	109.12
2	B	2803	PLX	O7-C6-C7	5.77	119.81	109.12
2	B	2804	PLX	O7-C6-C7	5.77	119.80	109.12
2	C	2801	PLX	O7-C6-C7	5.76	119.78	109.12
2	B	2808	PLX	O9-C24-C25	5.75	119.78	109.12
2	A	2808	PLX	O7-C6-C7	5.75	119.78	109.12
2	D	2807	PLX	O7-C6-C7	5.75	119.77	109.12
2	D	2804	PLX	O9-C24-C25	5.74	119.75	109.12
2	C	2805	PLX	O9-C24-C25	5.72	119.71	109.12
2	A	2804	PLX	O9-C24-C25	5.71	119.70	109.12
2	A	2803	PLX	O9-C24-C25	5.69	119.66	109.12
2	C	2808	PLX	O9-C24-C25	5.67	119.63	109.12
2	A	2807	PLX	O9-C24-C25	5.65	119.59	109.12
2	B	2803	PLX	O9-C24-C25	5.64	119.58	109.12
2	D	2807	PLX	O9-C24-C25	5.64	119.56	109.12
2	B	2802	PLX	O7-C6-C7	5.62	119.54	109.12
2	A	2802	PLX	O9-C24-C25	5.51	119.34	109.12
2	C	2803	PLX	O9-C24-C25	5.50	119.32	109.12
2	C	2803	PLX	O7-C6-C7	5.50	119.30	109.12
2	B	2806	PLX	O7-C6-C7	5.50	119.30	109.12
2	B	2806	PLX	O9-C24-C25	5.48	119.28	109.12
2	D	2802	PLX	O9-C24-C25	5.48	119.28	109.12
2	D	2802	PLX	O7-C6-C7	5.48	119.28	109.12
2	A	2802	PLX	O7-C6-C7	5.48	119.27	109.12
2	D	2806	PLX	O7-C6-C7	5.03	118.44	109.12
2	D	2806	PLX	C1B-N1-C1C	3.99	119.24	108.97
2	D	2806	PLX	C26-C25-C24	3.96	122.54	113.38
2	C	2807	PLX	C1B-N1-C1C	3.96	119.14	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2802	PLX	C1B-N1-C1C	3.95	119.13	108.97
2	A	2806	PLX	C1B-N1-C1C	3.94	119.10	108.97
2	A	2807	PLX	C1B-N1-C1C	3.85	118.87	108.97
2	B	2803	PLX	C1B-N1-C1C	3.85	118.86	108.97
2	A	2803	PLX	C1B-N1-C1C	3.85	118.86	108.97
2	D	2807	PLX	C1B-N1-C1C	3.83	118.82	108.97
2	C	2808	PLX	C1B-N1-C1C	3.82	118.79	108.97
2	B	2807	PLX	C1B-N1-C1C	3.80	118.75	108.97
2	A	2801	PLX	C1B-N1-C1C	3.80	118.74	108.97
2	C	2802	PLX	C1B-N1-C1C	3.80	118.73	108.97
2	D	2801	PLX	C1B-N1-C1C	3.79	118.72	108.97
2	B	2805	PLX	C1B-N1-C1C	3.78	118.70	108.97
2	C	2804	PLX	C1B-N1-C1C	3.75	118.62	108.97
2	D	2803	PLX	C1B-N1-C1C	3.75	118.62	108.97
2	C	2805	PLX	C1B-N1-C1C	3.72	118.54	108.97
2	D	2804	PLX	C1B-N1-C1C	3.72	118.53	108.97
2	B	2808	PLX	C1B-N1-C1C	3.71	118.52	108.97
2	A	2808	PLX	C1B-N1-C1C	3.70	118.48	108.97
2	A	2804	PLX	C1B-N1-C1C	3.70	118.47	108.97
2	B	2801	PLX	C1B-N1-C1C	3.68	118.43	108.97
2	B	2804	PLX	C1B-N1-C1C	3.67	118.42	108.97
2	C	2801	PLX	C1B-N1-C1C	3.66	118.39	108.97
2	C	2803	PLX	C1B-N1-C1C	3.65	118.35	108.97
2	A	2802	PLX	C1B-N1-C1C	3.64	118.33	108.97
2	D	2802	PLX	C1B-N1-C1C	3.64	118.33	108.97
2	B	2806	PLX	C1B-N1-C1C	3.63	118.32	108.97
2	C	2803	PLX	O8-C24-C25	3.58	120.61	109.49
2	B	2806	PLX	O8-C24-C25	3.58	120.60	109.49
2	A	2802	PLX	O8-C24-C25	3.57	120.58	109.49
2	D	2802	PLX	O8-C24-C25	3.57	120.58	109.49
2	D	2804	PLX	O8-C24-C25	3.57	120.57	109.49
2	C	2805	PLX	O8-C24-C25	3.57	120.56	109.49
2	B	2808	PLX	O8-C24-C25	3.57	120.56	109.49
2	A	2804	PLX	O8-C24-C25	3.55	120.53	109.49
2	B	2803	PLX	O8-C24-C25	3.55	120.50	109.49
2	D	2807	PLX	O8-C24-C25	3.54	120.49	109.49
2	C	2808	PLX	O8-C24-C25	3.53	120.44	109.49
2	A	2807	PLX	O8-C24-C25	3.52	120.42	109.49
2	C	2802	PLX	O8-C24-C25	3.38	119.97	109.49
2	A	2801	PLX	O8-C24-C25	3.37	119.95	109.49
2	D	2801	PLX	O8-C24-C25	3.37	119.95	109.49
2	B	2805	PLX	O8-C24-C25	3.36	119.93	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2802	PLX	O8-C24-C25	3.33	119.82	109.49
2	C	2801	PLX	O8-C24-C25	3.31	119.76	109.49
2	B	2801	PLX	O8-C24-C25	3.30	119.73	109.49
2	B	2804	PLX	O8-C24-C25	3.30	119.73	109.49
2	A	2808	PLX	O8-C24-C25	3.30	119.73	109.49
2	A	2806	PLX	O8-C24-C25	3.25	119.59	109.49
2	C	2807	PLX	O8-C24-C25	3.25	119.58	109.49
2	C	2804	PLX	O8-C24-C25	3.11	119.15	109.49
2	D	2803	PLX	O8-C24-C25	3.10	119.10	109.49
2	B	2807	PLX	O8-C24-C25	3.05	118.97	109.49
2	A	2803	PLX	O8-C24-C25	3.04	118.92	109.49
2	B	2802	PLX	O6-C6-C7	2.32	120.44	110.05
2	B	2804	PLX	O6-C6-C7	2.28	120.28	110.05
2	A	2808	PLX	O6-C6-C7	2.28	120.28	110.05
2	B	2801	PLX	O6-C6-C7	2.28	120.28	110.05
2	C	2804	PLX	O6-C6-C7	2.28	120.26	110.05
2	C	2801	PLX	O6-C6-C7	2.28	120.26	110.05
2	A	2806	PLX	O6-C6-C7	2.27	120.23	110.05
2	C	2807	PLX	O6-C6-C7	2.26	120.21	110.05
2	D	2806	PLX	O6-C6-C7	2.25	120.13	110.05
2	D	2807	PLX	O6-C6-C7	2.24	120.10	110.05
2	B	2803	PLX	O6-C6-C7	2.24	120.08	110.05
2	A	2807	PLX	O6-C6-C7	2.24	120.08	110.05
2	C	2808	PLX	O6-C6-C7	2.23	120.04	110.05
2	A	2803	PLX	O6-C6-C7	2.22	120.01	110.05
2	A	2801	PLX	O6-C6-C7	2.22	119.99	110.05
2	A	2804	PLX	O6-C6-C7	2.22	119.99	110.05
2	B	2805	PLX	O6-C6-C7	2.22	119.99	110.05
2	C	2805	PLX	O6-C6-C7	2.21	119.98	110.05
2	B	2808	PLX	O6-C6-C7	2.21	119.98	110.05
2	D	2803	PLX	O6-C6-C7	2.21	119.96	110.05
2	C	2802	PLX	O6-C6-C7	2.21	119.96	110.05
2	D	2804	PLX	O6-C6-C7	2.21	119.95	110.05
2	D	2801	PLX	O6-C6-C7	2.20	119.94	110.05
2	D	2802	PLX	O6-C6-C7	2.20	119.90	110.05
2	B	2807	PLX	O6-C6-C7	2.20	119.90	110.05
2	C	2803	PLX	O6-C6-C7	2.19	119.86	110.05
2	A	2802	PLX	O6-C6-C7	2.18	119.85	110.05
2	B	2806	PLX	O6-C6-C7	2.18	119.85	110.05
2	A	2802	PLX	C5-O8-C24	2.10	117.86	113.80
2	C	2803	PLX	C5-O8-C24	2.09	117.82	113.80
2	D	2802	PLX	C5-O8-C24	2.07	117.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2806	PLX	O8-C5-C4	2.07	115.90	110.90
2	B	2806	PLX	C5-O8-C24	2.07	117.79	113.80
2	A	2803	PLX	O8-C5-C4	-2.06	105.94	110.90

All (84) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2801	PLX	C24
2	A	2801	PLX	C4
2	A	2801	PLX	C6
2	A	2802	PLX	C24
2	A	2802	PLX	C4
2	A	2802	PLX	C6
2	A	2803	PLX	C24
2	A	2803	PLX	C4
2	A	2803	PLX	C6
2	A	2804	PLX	C24
2	A	2804	PLX	C4
2	A	2804	PLX	C6
2	A	2806	PLX	C24
2	A	2806	PLX	C4
2	A	2806	PLX	C6
2	A	2807	PLX	C24
2	A	2807	PLX	C4
2	A	2807	PLX	C6
2	A	2808	PLX	C24
2	A	2808	PLX	C4
2	A	2808	PLX	C6
2	D	2801	PLX	C24
2	D	2801	PLX	C4
2	D	2801	PLX	C6
2	D	2802	PLX	C24
2	D	2802	PLX	C4
2	D	2802	PLX	C6
2	D	2803	PLX	C24
2	D	2803	PLX	C4
2	D	2803	PLX	C6
2	D	2804	PLX	C24
2	D	2804	PLX	C4
2	D	2804	PLX	C6
2	D	2806	PLX	C24
2	D	2806	PLX	C4

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Mol	Chain	Res	Type	Atom
2	D	2806	PLX	C6
2	D	2807	PLX	C24
2	D	2807	PLX	C4
2	D	2807	PLX	C6
2	C	2801	PLX	C24
2	C	2801	PLX	C4
2	C	2801	PLX	C6
2	C	2802	PLX	C24
2	C	2802	PLX	C4
2	C	2802	PLX	C6
2	C	2803	PLX	C24
2	C	2803	PLX	C4
2	C	2803	PLX	C6
2	C	2804	PLX	C24
2	C	2804	PLX	C4
2	C	2804	PLX	C6
2	C	2805	PLX	C24
2	C	2805	PLX	C4
2	C	2805	PLX	C6
2	C	2807	PLX	C24
2	C	2807	PLX	C4
2	C	2807	PLX	C6
2	C	2808	PLX	C24
2	C	2808	PLX	C4
2	C	2808	PLX	C6
2	B	2801	PLX	C24
2	B	2801	PLX	C4
2	B	2801	PLX	C6
2	B	2802	PLX	C24
2	B	2802	PLX	C4
2	B	2802	PLX	C6
2	B	2803	PLX	C24
2	B	2803	PLX	C4
2	B	2803	PLX	C6
2	B	2804	PLX	C24
2	B	2804	PLX	C4
2	B	2804	PLX	C6
2	B	2805	PLX	C24
2	B	2805	PLX	C4
2	B	2805	PLX	C6
2	B	2806	PLX	C24
2	B	2806	PLX	C4

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Mol	Chain	Res	Type	Atom
2	B	2806	PLX	C6
2	B	2807	PLX	C24
2	B	2807	PLX	C4
2	B	2807	PLX	C6
2	B	2808	PLX	C24
2	B	2808	PLX	C4
2	B	2808	PLX	C6

All (603) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2801	PLX	O7-C6-C7-C8
2	A	2801	PLX	C3-O4-P1-O2
2	A	2801	PLX	C3-O4-P1-O3
2	A	2801	PLX	O9-C24-C25-C26
2	A	2802	PLX	O7-C6-O6-C4
2	A	2802	PLX	C3-O4-P1-O2
2	A	2802	PLX	C3-O4-P1-O3
2	A	2803	PLX	O7-C6-C7-C8
2	A	2803	PLX	O7-C6-O6-C4
2	A	2803	PLX	C3-O4-P1-O2
2	A	2803	PLX	C3-O4-P1-O3
2	A	2803	PLX	O9-C24-C25-C26
2	A	2804	PLX	O7-C6-O6-C4
2	A	2804	PLX	C3-O4-P1-O1
2	A	2804	PLX	C3-O4-P1-O2
2	A	2804	PLX	C3-O4-P1-O3
2	A	2804	PLX	C2-O1-P1-O2
2	A	2804	PLX	C25-C24-O8-C5
2	A	2804	PLX	O9-C24-C25-C26
2	A	2806	PLX	O7-C6-O6-C4
2	A	2806	PLX	C3-O4-P1-O2
2	A	2807	PLX	O7-C6-O6-C4
2	A	2807	PLX	C3-O4-P1-O3
2	A	2807	PLX	C25-C24-O8-C5
2	A	2807	PLX	O9-C24-C25-C26
2	A	2808	PLX	O7-C6-O6-C4
2	A	2808	PLX	C3-O4-P1-O1
2	A	2808	PLX	C3-O4-P1-O2
2	A	2808	PLX	C3-O4-P1-O3
2	A	2808	PLX	N1-C1-C2-O1
2	A	2808	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	D	2801	PLX	O7-C6-C7-C8
2	D	2801	PLX	C3-O4-P1-O2
2	D	2801	PLX	C3-O4-P1-O3
2	D	2801	PLX	O9-C24-C25-C26
2	D	2802	PLX	O7-C6-O6-C4
2	D	2802	PLX	C3-O4-P1-O2
2	D	2802	PLX	C3-O4-P1-O3
2	D	2803	PLX	O7-C6-C7-C8
2	D	2803	PLX	O7-C6-O6-C4
2	D	2803	PLX	C3-O4-P1-O2
2	D	2803	PLX	C3-O4-P1-O3
2	D	2803	PLX	O9-C24-C25-C26
2	D	2804	PLX	O7-C6-O6-C4
2	D	2804	PLX	C3-O4-P1-O1
2	D	2804	PLX	C3-O4-P1-O2
2	D	2804	PLX	C3-O4-P1-O3
2	D	2804	PLX	C2-O1-P1-O2
2	D	2804	PLX	C25-C24-O8-C5
2	D	2804	PLX	O9-C24-C25-C26
2	D	2806	PLX	O7-C6-O6-C4
2	D	2806	PLX	N1-C1-C2-O1
2	D	2807	PLX	O7-C6-O6-C4
2	D	2807	PLX	C3-O4-P1-O3
2	D	2807	PLX	C25-C24-O8-C5
2	D	2807	PLX	O9-C24-C25-C26
2	C	2801	PLX	O7-C6-O6-C4
2	C	2801	PLX	C3-O4-P1-O2
2	C	2801	PLX	C3-O4-P1-O3
2	C	2801	PLX	N1-C1-C2-O1
2	C	2801	PLX	O8-C24-C25-C26
2	C	2802	PLX	O7-C6-C7-C8
2	C	2802	PLX	C3-O4-P1-O2
2	C	2802	PLX	C3-O4-P1-O3
2	C	2802	PLX	O9-C24-C25-C26
2	C	2803	PLX	O7-C6-O6-C4
2	C	2803	PLX	C3-O4-P1-O2
2	C	2803	PLX	C3-O4-P1-O3
2	C	2804	PLX	O7-C6-C7-C8
2	C	2804	PLX	O7-C6-O6-C4
2	C	2804	PLX	C3-O4-P1-O2
2	C	2804	PLX	C3-O4-P1-O3
2	C	2804	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	C	2805	PLX	O7-C6-O6-C4
2	C	2805	PLX	C3-O4-P1-O1
2	C	2805	PLX	C3-O4-P1-O2
2	C	2805	PLX	C3-O4-P1-O3
2	C	2805	PLX	C2-O1-P1-O2
2	C	2805	PLX	C25-C24-O8-C5
2	C	2805	PLX	O9-C24-C25-C26
2	C	2807	PLX	O7-C6-O6-C4
2	C	2807	PLX	C3-O4-P1-O2
2	C	2808	PLX	O7-C6-O6-C4
2	C	2808	PLX	C3-O4-P1-O3
2	C	2808	PLX	C25-C24-O8-C5
2	C	2808	PLX	O9-C24-C25-C26
2	B	2801	PLX	O7-C6-O6-C4
2	B	2801	PLX	C3-O4-P1-O1
2	B	2801	PLX	C3-O4-P1-O2
2	B	2801	PLX	C3-O4-P1-O3
2	B	2801	PLX	N1-C1-C2-O1
2	B	2801	PLX	O8-C24-C25-C26
2	B	2802	PLX	O7-C6-O6-C4
2	B	2802	PLX	C3-O4-P1-O1
2	B	2802	PLX	C3-O4-P1-O2
2	B	2803	PLX	O7-C6-O6-C4
2	B	2803	PLX	C3-O4-P1-O1
2	B	2803	PLX	C3-O4-P1-O3
2	B	2803	PLX	C25-C24-O8-C5
2	B	2803	PLX	O9-C24-C25-C26
2	B	2804	PLX	O7-C6-O6-C4
2	B	2804	PLX	C3-O4-P1-O2
2	B	2804	PLX	C3-O4-P1-O3
2	B	2804	PLX	N1-C1-C2-O1
2	B	2804	PLX	O8-C24-C25-C26
2	B	2805	PLX	O7-C6-C7-C8
2	B	2805	PLX	C3-O4-P1-O2
2	B	2805	PLX	C3-O4-P1-O3
2	B	2805	PLX	O9-C24-C25-C26
2	B	2806	PLX	O7-C6-O6-C4
2	B	2806	PLX	C3-O4-P1-O2
2	B	2806	PLX	C3-O4-P1-O3
2	B	2807	PLX	O7-C6-C7-C8
2	B	2807	PLX	O7-C6-O6-C4
2	B	2807	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
2	B	2807	PLX	C3-O4-P1-O3
2	B	2807	PLX	O9-C24-C25-C26
2	B	2808	PLX	O7-C6-O6-C4
2	B	2808	PLX	C3-O4-P1-O1
2	B	2808	PLX	C3-O4-P1-O2
2	B	2808	PLX	C3-O4-P1-O3
2	B	2808	PLX	C2-O1-P1-O2
2	B	2808	PLX	C25-C24-O8-C5
2	B	2808	PLX	O9-C24-C25-C26
2	A	2802	PLX	C26-C27-C28-C29
2	D	2802	PLX	C26-C27-C28-C29
2	B	2806	PLX	C26-C27-C28-C29
2	A	2804	PLX	C11-C12-C13-C14
2	C	2803	PLX	C26-C27-C28-C29
2	D	2804	PLX	C11-C12-C13-C14
2	C	2805	PLX	C11-C12-C13-C14
2	B	2808	PLX	C11-C12-C13-C14
2	A	2807	PLX	O6-C4-C5-O8
2	C	2808	PLX	O6-C4-C5-O8
2	B	2803	PLX	O6-C4-C5-O8
2	A	2804	PLX	C2-C1-N1-C1A
2	D	2804	PLX	C2-C1-N1-C1A
2	C	2805	PLX	C2-C1-N1-C1A
2	B	2808	PLX	C2-C1-N1-C1A
2	B	2802	PLX	C30-C31-C32-C33
2	A	2801	PLX	C3-O4-P1-O1
2	A	2802	PLX	C3-O4-P1-O1
2	A	2803	PLX	C3-O4-P1-O1
2	A	2804	PLX	C2-O1-P1-O4
2	A	2807	PLX	C3-O4-P1-O1
2	D	2801	PLX	C3-O4-P1-O1
2	D	2802	PLX	C3-O4-P1-O1
2	D	2803	PLX	C3-O4-P1-O1
2	D	2804	PLX	C2-O1-P1-O4
2	D	2807	PLX	C3-O4-P1-O1
2	C	2801	PLX	C3-O4-P1-O1
2	C	2802	PLX	C3-O4-P1-O1
2	C	2803	PLX	C3-O4-P1-O1
2	C	2804	PLX	C3-O4-P1-O1
2	C	2805	PLX	C2-O1-P1-O4
2	C	2808	PLX	C3-O4-P1-O1
2	B	2804	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
2	B	2805	PLX	C3-O4-P1-O1
2	B	2806	PLX	C3-O4-P1-O1
2	B	2807	PLX	C3-O4-P1-O1
2	B	2808	PLX	C2-O1-P1-O4
2	C	2807	PLX	C30-C31-C32-C33
2	A	2806	PLX	C30-C31-C32-C33
2	A	2802	PLX	O6-C6-C7-C8
2	A	2802	PLX	O8-C24-C25-C26
2	D	2802	PLX	O6-C6-C7-C8
2	D	2806	PLX	O8-C24-C25-C26
2	C	2803	PLX	O6-C6-C7-C8
2	B	2802	PLX	O8-C24-C25-C26
2	B	2806	PLX	O6-C6-C7-C8
2	A	2807	PLX	C11-C12-C13-C14
2	C	2805	PLX	C9-C10-C11-C12
2	A	2804	PLX	C9-C10-C11-C12
2	D	2804	PLX	C25-C26-C27-C28
2	C	2805	PLX	C25-C26-C27-C28
2	B	2801	PLX	C9-C10-C11-C12
2	B	2803	PLX	C11-C12-C13-C14
2	B	2804	PLX	C9-C10-C11-C12
2	B	2808	PLX	C25-C26-C27-C28
2	A	2804	PLX	C25-C26-C27-C28
2	A	2808	PLX	C9-C10-C11-C12
2	D	2804	PLX	C9-C10-C11-C12
2	D	2807	PLX	C11-C12-C13-C14
2	C	2801	PLX	C9-C10-C11-C12
2	B	2808	PLX	C9-C10-C11-C12
2	D	2802	PLX	C11-C10-C9-C8
2	C	2808	PLX	C11-C12-C13-C14
2	B	2808	PLX	C11-C10-C9-C8
2	D	2804	PLX	C11-C10-C9-C8
2	C	2805	PLX	C11-C10-C9-C8
2	B	2806	PLX	C11-C10-C9-C8
2	C	2808	PLX	C11-C10-C9-C8
2	C	2808	PLX	C26-C27-C28-C29
2	B	2803	PLX	C11-C10-C9-C8
2	D	2807	PLX	O6-C4-C5-O8
2	A	2804	PLX	C11-C10-C9-C8
2	A	2807	PLX	C11-C10-C9-C8
2	A	2807	PLX	C26-C27-C28-C29
2	D	2807	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	D	2807	PLX	C27-C28-C29-C30
2	C	2803	PLX	C11-C10-C9-C8
2	A	2804	PLX	C26-C27-C28-C29
2	C	2801	PLX	C7-C8-C9-C10
2	B	2804	PLX	C7-C8-C9-C10
2	B	2808	PLX	C26-C27-C28-C29
2	A	2806	PLX	C26-C27-C28-C29
2	A	2807	PLX	C27-C28-C29-C30
2	D	2804	PLX	C26-C27-C28-C29
2	D	2806	PLX	C25-C26-C27-C28
2	D	2806	PLX	C35-C36-C37-C38
2	D	2807	PLX	C26-C27-C28-C29
2	C	2807	PLX	C26-C27-C28-C29
2	C	2808	PLX	C27-C28-C29-C30
2	B	2801	PLX	C7-C8-C9-C10
2	B	2803	PLX	C27-C28-C29-C30
2	A	2808	PLX	C7-C8-C9-C10
2	C	2804	PLX	C26-C27-C28-C29
2	A	2808	PLX	C11-C10-C9-C8
2	D	2806	PLX	C11-C10-C9-C8
2	C	2801	PLX	C11-C10-C9-C8
2	B	2801	PLX	C28-C29-C30-C31
2	B	2802	PLX	C26-C27-C28-C29
2	B	2803	PLX	C26-C27-C28-C29
2	B	2807	PLX	C9-C10-C11-C12
2	A	2801	PLX	C27-C28-C29-C30
2	A	2803	PLX	C9-C10-C11-C12
2	D	2801	PLX	C27-C28-C29-C30
2	D	2803	PLX	C9-C10-C11-C12
2	C	2804	PLX	C11-C10-C9-C8
2	C	2805	PLX	C26-C27-C28-C29
2	B	2801	PLX	C11-C10-C9-C8
2	B	2802	PLX	C35-C36-C37-C38
2	B	2804	PLX	C11-C10-C9-C8
2	B	2804	PLX	C28-C29-C30-C31
2	A	2804	PLX	C2-C1-N1-C1B
2	A	2802	PLX	C11-C10-C9-C8
2	A	2806	PLX	C11-C10-C9-C8
2	C	2802	PLX	C27-C28-C29-C30
2	C	2807	PLX	C11-C10-C9-C8
2	B	2805	PLX	C27-C28-C29-C30
2	A	2806	PLX	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	C	2807	PLX	C35-C36-C37-C38
2	D	2801	PLX	C26-C27-C28-C29
2	C	2802	PLX	C26-C27-C28-C29
2	C	2804	PLX	C9-C10-C11-C12
2	C	2808	PLX	C25-C26-C27-C28
2	B	2802	PLX	C11-C10-C9-C8
2	B	2805	PLX	C26-C27-C28-C29
2	B	2807	PLX	C11-C10-C9-C8
2	A	2801	PLX	C26-C27-C28-C29
2	A	2807	PLX	C25-C26-C27-C28
2	B	2802	PLX	C9-C10-C11-C12
2	A	2806	PLX	C9-C10-C11-C12
2	A	2803	PLX	C26-C27-C28-C29
2	D	2803	PLX	C11-C10-C9-C8
2	C	2807	PLX	C9-C10-C11-C12
2	D	2806	PLX	C28-C29-C30-C31
2	D	2806	PLX	C11-C12-C13-C14
2	B	2802	PLX	C11-C12-C13-C14
2	B	2804	PLX	C27-C28-C29-C30
2	D	2803	PLX	C26-C27-C28-C29
2	D	2806	PLX	C9-C10-C11-C12
2	A	2803	PLX	C11-C10-C9-C8
2	D	2807	PLX	C25-C26-C27-C28
2	B	2801	PLX	C27-C28-C29-C30
2	A	2808	PLX	C28-C29-C30-C31
2	C	2803	PLX	C27-C28-C29-C30
2	B	2803	PLX	C25-C26-C27-C28
2	D	2804	PLX	C2-C1-N1-C1B
2	C	2805	PLX	C2-C1-N1-C1B
2	B	2808	PLX	C2-C1-N1-C1B
2	A	2806	PLX	C11-C12-C13-C14
2	D	2802	PLX	C27-C28-C29-C30
2	C	2807	PLX	C11-C12-C13-C14
2	C	2801	PLX	C27-C28-C29-C30
2	B	2801	PLX	C11-C12-C13-C14
2	A	2808	PLX	C11-C12-C13-C14
2	C	2801	PLX	C11-C12-C13-C14
2	C	2801	PLX	C28-C29-C30-C31
2	B	2806	PLX	C27-C28-C29-C30
2	A	2808	PLX	C27-C28-C29-C30
2	B	2804	PLX	C11-C12-C13-C14
2	D	2806	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	A	2802	PLX	C27-C28-C29-C30
2	B	2802	PLX	C32-C33-C34-C35
2	D	2807	PLX	C10-C11-C12-C13
2	B	2807	PLX	C26-C27-C28-C29
2	C	2808	PLX	C10-C11-C12-C13
2	A	2807	PLX	C10-C11-C12-C13
2	B	2803	PLX	C10-C11-C12-C13
2	A	2806	PLX	O4-C3-C4-C5
2	A	2807	PLX	O4-C3-C4-C5
2	D	2806	PLX	O4-C3-C4-C5
2	D	2807	PLX	O4-C3-C4-C5
2	C	2807	PLX	O4-C3-C4-C5
2	C	2808	PLX	O4-C3-C4-C5
2	B	2802	PLX	O4-C3-C4-C5
2	B	2803	PLX	O4-C3-C4-C5
2	D	2803	PLX	C7-C8-C9-C10
2	B	2807	PLX	C7-C8-C9-C10
2	A	2801	PLX	C3-C4-C5-O8
2	A	2804	PLX	C3-C4-C5-O8
2	A	2807	PLX	C3-C4-C5-O8
2	D	2801	PLX	C25-C26-C27-C28
2	D	2803	PLX	C3-C4-C5-O8
2	D	2804	PLX	C3-C4-C5-O8
2	C	2804	PLX	C3-C4-C5-O8
2	C	2805	PLX	C3-C4-C5-O8
2	B	2803	PLX	C3-C4-C5-O8
2	B	2808	PLX	C3-C4-C5-O8
2	B	2805	PLX	C25-C26-C27-C28
2	A	2802	PLX	C4-C5-O8-C24
2	D	2802	PLX	C4-C5-O8-C24
2	C	2803	PLX	C4-C5-O8-C24
2	B	2806	PLX	C4-C5-O8-C24
2	A	2803	PLX	C10-C11-C12-C13
2	C	2802	PLX	C25-C26-C27-C28
2	C	2808	PLX	O6-C6-C7-C8
2	C	2804	PLX	C10-C11-C12-C13
2	C	2802	PLX	C9-C10-C11-C12
2	B	2801	PLX	C13-C14-C15-C16
2	D	2801	PLX	C9-C10-C11-C12
2	B	2805	PLX	C9-C10-C11-C12
2	D	2803	PLX	C10-C11-C12-C13
2	B	2804	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	A	2801	PLX	C9-C10-C11-C12
2	B	2807	PLX	C10-C11-C12-C13
2	A	2804	PLX	C14-C15-C16-C17
2	A	2808	PLX	C13-C14-C15-C16
2	D	2806	PLX	C14-C15-C16-C17
2	C	2801	PLX	C13-C14-C15-C16
2	D	2802	PLX	O4-C3-C4-O6
2	C	2803	PLX	O4-C3-C4-O6
2	B	2806	PLX	O4-C3-C4-O6
2	C	2804	PLX	C7-C8-C9-C10
2	D	2801	PLX	C11-C10-C9-C8
2	D	2804	PLX	C13-C14-C15-C16
2	A	2806	PLX	C13-C14-C15-C16
2	C	2807	PLX	C14-C15-C16-C17
2	C	2807	PLX	C13-C14-C15-C16
2	B	2802	PLX	C14-C15-C16-C17
2	A	2806	PLX	C14-C15-C16-C17
2	B	2808	PLX	C13-C14-C15-C16
2	A	2801	PLX	C11-C10-C9-C8
2	C	2802	PLX	C11-C10-C9-C8
2	B	2805	PLX	C11-C10-C9-C8
2	C	2805	PLX	C13-C14-C15-C16
2	C	2805	PLX	C14-C15-C16-C17
2	B	2808	PLX	C14-C15-C16-C17
2	D	2804	PLX	C14-C15-C16-C17
2	A	2801	PLX	C25-C26-C27-C28
2	A	2802	PLX	C9-C10-C11-C12
2	C	2808	PLX	C14-C15-C16-C17
2	A	2807	PLX	C14-C15-C16-C17
2	D	2807	PLX	C14-C15-C16-C17
2	B	2803	PLX	C14-C15-C16-C17
2	C	2803	PLX	C9-C10-C11-C12
2	C	2803	PLX	C30-C31-C32-C33
2	B	2803	PLX	C30-C31-C32-C33
2	B	2803	PLX	C29-C30-C31-C32
2	D	2803	PLX	C4-C3-O4-P1
2	C	2804	PLX	C4-C3-O4-P1
2	B	2807	PLX	C4-C3-O4-P1
2	D	2802	PLX	C9-C10-C11-C12
2	C	2808	PLX	C32-C33-C34-C35
2	A	2807	PLX	C32-C33-C34-C35
2	B	2806	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	D	2801	PLX	C3-C4-C5-O8
2	D	2807	PLX	C3-C4-C5-O8
2	C	2802	PLX	C3-C4-C5-O8
2	C	2808	PLX	C3-C4-C5-O8
2	B	2805	PLX	C3-C4-C5-O8
2	D	2807	PLX	C30-C31-C32-C33
2	A	2804	PLX	C13-C14-C15-C16
2	B	2806	PLX	C30-C31-C32-C33
2	D	2802	PLX	C30-C31-C32-C33
2	A	2802	PLX	O4-C3-C4-O6
2	D	2807	PLX	C29-C30-C31-C32
2	B	2802	PLX	O6-C4-C5-O8
2	A	2803	PLX	C4-C3-O4-P1
2	A	2807	PLX	C29-C30-C31-C32
2	C	2808	PLX	C29-C30-C31-C32
2	A	2802	PLX	C30-C31-C32-C33
2	B	2802	PLX	C13-C14-C15-C16
2	B	2802	PLX	C24-C25-C26-C27
2	A	2804	PLX	O6-C6-C7-C8
2	A	2806	PLX	O6-C6-C7-C8
2	A	2807	PLX	O6-C6-C7-C8
2	A	2808	PLX	O6-C6-C7-C8
2	D	2804	PLX	O6-C6-C7-C8
2	D	2807	PLX	O6-C6-C7-C8
2	C	2801	PLX	O6-C6-C7-C8
2	C	2805	PLX	O6-C6-C7-C8
2	C	2807	PLX	O6-C6-C7-C8
2	B	2801	PLX	O6-C6-C7-C8
2	B	2802	PLX	O6-C6-C7-C8
2	B	2803	PLX	O6-C6-C7-C8
2	B	2804	PLX	O6-C6-C7-C8
2	B	2808	PLX	O6-C6-C7-C8
2	A	2802	PLX	O4-C3-C4-C5
2	D	2802	PLX	O4-C3-C4-C5
2	C	2803	PLX	O4-C3-C4-C5
2	B	2806	PLX	O4-C3-C4-C5
2	A	2803	PLX	C7-C8-C9-C10
2	A	2807	PLX	C13-C14-C15-C16
2	B	2803	PLX	C13-C14-C15-C16
2	B	2802	PLX	C3-C4-C5-O8
2	A	2806	PLX	O4-C3-C4-O6
2	D	2806	PLX	O4-C3-C4-O6

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Mol	Chain	Res	Type	Atoms
2	C	2807	PLX	O4-C3-C4-O6
2	B	2802	PLX	O4-C3-C4-O6
2	D	2807	PLX	C13-C14-C15-C16
2	C	2808	PLX	C13-C14-C15-C16
2	A	2801	PLX	O6-C4-C5-O8
2	A	2804	PLX	O6-C4-C5-O8
2	A	2806	PLX	O6-C4-C5-O8
2	D	2801	PLX	O6-C4-C5-O8
2	D	2804	PLX	O6-C4-C5-O8
2	C	2802	PLX	O6-C4-C5-O8
2	C	2804	PLX	O6-C4-C5-O8
2	C	2805	PLX	O6-C4-C5-O8
2	C	2807	PLX	O6-C4-C5-O8
2	B	2805	PLX	O6-C4-C5-O8
2	B	2808	PLX	O6-C4-C5-O8
2	A	2804	PLX	C2-C1-N1-C1C
2	B	2801	PLX	C31-C32-C33-C34
2	A	2804	PLX	C24-C25-C26-C27
2	A	2806	PLX	C24-C25-C26-C27
2	D	2804	PLX	C24-C25-C26-C27
2	C	2805	PLX	C24-C25-C26-C27
2	C	2807	PLX	C24-C25-C26-C27
2	B	2808	PLX	C24-C25-C26-C27
2	A	2802	PLX	C6-C7-C8-C9
2	A	2802	PLX	C24-C25-C26-C27
2	C	2803	PLX	C24-C25-C26-C27
2	A	2806	PLX	C3-O4-P1-O1
2	C	2807	PLX	C3-O4-P1-O1
2	B	2801	PLX	C26-C27-C28-C29
2	A	2807	PLX	C3-O4-P1-O2
2	D	2807	PLX	C3-O4-P1-O2
2	C	2805	PLX	C2-C1-N1-C1C
2	C	2808	PLX	C3-O4-P1-O2
2	B	2803	PLX	C3-O4-P1-O2
2	B	2808	PLX	C2-C1-N1-C1C
2	B	2802	PLX	C28-C29-C30-C31
2	A	2801	PLX	C25-C24-O8-C5
2	A	2808	PLX	C25-C24-O8-C5
2	D	2801	PLX	C25-C24-O8-C5
2	C	2801	PLX	C25-C24-O8-C5
2	C	2802	PLX	C25-C24-O8-C5
2	B	2801	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
2	B	2804	PLX	C25-C24-O8-C5
2	B	2805	PLX	C25-C24-O8-C5
2	D	2802	PLX	C24-C25-C26-C27
2	B	2806	PLX	C24-C25-C26-C27
2	B	2807	PLX	C29-C30-C31-C32
2	C	2808	PLX	C30-C31-C32-C33
2	A	2807	PLX	O4-C3-C4-O6
2	A	2808	PLX	O4-C3-C4-O6
2	D	2807	PLX	O4-C3-C4-O6
2	C	2801	PLX	O4-C3-C4-O6
2	B	2801	PLX	O4-C3-C4-O6
2	B	2803	PLX	O4-C3-C4-O6
2	B	2804	PLX	O4-C3-C4-O6
2	A	2807	PLX	C30-C31-C32-C33
2	D	2804	PLX	C2-C1-N1-C1C
2	A	2801	PLX	N1-C1-C2-O1
2	A	2806	PLX	C3-C4-C5-O8
2	A	2806	PLX	N1-C1-C2-O1
2	D	2801	PLX	N1-C1-C2-O1
2	D	2806	PLX	C3-C4-C5-O8
2	C	2802	PLX	N1-C1-C2-O1
2	C	2807	PLX	C3-C4-C5-O8
2	C	2807	PLX	N1-C1-C2-O1
2	B	2802	PLX	N1-C1-C2-O1
2	B	2805	PLX	N1-C1-C2-O1
2	D	2806	PLX	O6-C4-C5-O8
2	C	2807	PLX	C25-C26-C27-C28
2	A	2806	PLX	O8-C24-C25-C26
2	D	2806	PLX	O6-C6-C7-C8
2	C	2807	PLX	O8-C24-C25-C26
2	D	2806	PLX	C13-C14-C15-C16
2	D	2807	PLX	C33-C34-C35-C36
2	D	2804	PLX	C27-C28-C29-C30
2	B	2808	PLX	C27-C28-C29-C30
2	D	2803	PLX	C29-C30-C31-C32
2	C	2804	PLX	C24-C25-C26-C27
2	A	2808	PLX	C4-C3-O4-P1
2	C	2801	PLX	C4-C3-O4-P1
2	B	2804	PLX	C4-C3-O4-P1
2	C	2808	PLX	O4-C3-C4-O6
2	A	2806	PLX	C25-C26-C27-C28
2	D	2803	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
2	A	2803	PLX	C2-O1-P1-O4
2	D	2803	PLX	C2-O1-P1-O4
2	D	2806	PLX	C3-O4-P1-O1
2	C	2804	PLX	C2-O1-P1-O4
2	B	2807	PLX	C2-O1-P1-O4
2	A	2803	PLX	C3-C4-C5-O8
2	D	2802	PLX	C6-C7-C8-C9
2	C	2803	PLX	C6-C7-C8-C9
2	D	2806	PLX	C26-C27-C28-C29
2	D	2806	PLX	C4-C3-O4-P1
2	B	2801	PLX	C4-C3-O4-P1
2	D	2806	PLX	C24-C25-C26-C27
2	D	2807	PLX	C24-C25-C26-C27
2	B	2806	PLX	C6-C7-C8-C9
2	D	2807	PLX	C32-C33-C34-C35
2	C	2808	PLX	C24-C25-C26-C27
2	B	2803	PLX	C6-C7-C8-C9
2	B	2807	PLX	C24-C25-C26-C27
2	A	2801	PLX	O4-C3-C4-O6
2	B	2801	PLX	C10-C11-C12-C13
2	A	2807	PLX	C6-C7-C8-C9
2	D	2803	PLX	C24-C25-C26-C27
2	D	2807	PLX	C6-C7-C8-C9
2	C	2808	PLX	C6-C7-C8-C9
2	B	2803	PLX	C24-C25-C26-C27
2	D	2802	PLX	O8-C24-C25-C26
2	C	2803	PLX	O8-C24-C25-C26
2	B	2806	PLX	O8-C24-C25-C26
2	B	2807	PLX	C30-C31-C32-C33
2	A	2803	PLX	C24-C25-C26-C27
2	A	2806	PLX	C6-C7-C8-C9
2	A	2807	PLX	C24-C25-C26-C27
2	C	2807	PLX	C6-C7-C8-C9
2	A	2807	PLX	C9-C10-C11-C12
2	B	2802	PLX	C25-C26-C27-C28
2	D	2803	PLX	C30-C31-C32-C33
2	A	2801	PLX	C6-C7-C8-C9
2	D	2801	PLX	C6-C7-C8-C9
2	B	2802	PLX	C6-C7-C8-C9
2	C	2804	PLX	C30-C31-C32-C33
2	D	2801	PLX	C5-C4-O6-C6
2	C	2802	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
2	B	2805	PLX	C5-C4-O6-C6
2	D	2802	PLX	C4-C3-O4-P1
2	C	2803	PLX	C4-C3-O4-P1
2	B	2806	PLX	C4-C3-O4-P1
2	B	2803	PLX	C9-C10-C11-C12
2	C	2801	PLX	C10-C11-C12-C13
2	D	2806	PLX	C30-C31-C32-C33
2	B	2804	PLX	C10-C11-C12-C13
2	C	2802	PLX	C6-C7-C8-C9
2	B	2805	PLX	C6-C7-C8-C9
2	C	2807	PLX	C32-C33-C34-C35
2	A	2808	PLX	C10-C11-C12-C13
2	D	2807	PLX	C9-C10-C11-C12
2	C	2808	PLX	C9-C10-C11-C12
2	A	2803	PLX	C30-C31-C32-C33
2	D	2806	PLX	C6-C7-C8-C9
2	A	2806	PLX	C32-C33-C34-C35
2	D	2803	PLX	C4-C5-O8-C24
2	C	2804	PLX	C4-C5-O8-C24
2	D	2801	PLX	O4-C3-C4-O6
2	C	2802	PLX	O4-C3-C4-O6
2	B	2805	PLX	O4-C3-C4-O6
2	D	2806	PLX	C27-C28-C29-C30
2	A	2808	PLX	O4-C3-C4-C5
2	C	2801	PLX	O4-C3-C4-C5
2	B	2801	PLX	O4-C3-C4-C5
2	B	2804	PLX	O4-C3-C4-C5
2	A	2802	PLX	C4-C3-O4-P1
2	C	2807	PLX	C33-C34-C35-C36
2	D	2803	PLX	C27-C28-C29-C30
2	A	2806	PLX	C33-C34-C35-C36
2	B	2802	PLX	C33-C34-C35-C36
2	A	2804	PLX	O4-C3-C4-O6
2	A	2803	PLX	C6-C7-C8-C9
2	A	2804	PLX	O4-C3-C4-C5
2	A	2808	PLX	O9-C24-C25-C26
2	C	2801	PLX	O9-C24-C25-C26
2	B	2801	PLX	O9-C24-C25-C26
2	B	2804	PLX	O9-C24-C25-C26
2	D	2801	PLX	C24-C25-C26-C27
2	C	2802	PLX	C24-C25-C26-C27
2	B	2805	PLX	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	B	2801	PLX	C12-C13-C14-C15
2	B	2804	PLX	C12-C13-C14-C15
2	B	2804	PLX	C26-C27-C28-C29
2	A	2806	PLX	C28-C29-C30-C31
2	A	2802	PLX	C2-O1-P1-O2
2	A	2804	PLX	C2-O1-P1-O3
2	A	2806	PLX	C2-O1-P1-O2
2	D	2802	PLX	C2-O1-P1-O2
2	D	2806	PLX	C3-O4-P1-O2
2	C	2803	PLX	C2-O1-P1-O2
2	C	2807	PLX	C2-O1-P1-O2
2	B	2802	PLX	C2-O1-P1-O2
2	B	2806	PLX	C2-O1-P1-O2
2	A	2801	PLX	O4-C3-C4-C5
2	D	2804	PLX	O4-C3-C4-C5
2	C	2805	PLX	O4-C3-C4-C5
2	B	2808	PLX	O4-C3-C4-C5
2	C	2807	PLX	C28-C29-C30-C31
2	A	2802	PLX	C25-C24-O8-C5
2	D	2802	PLX	C25-C24-O8-C5
2	C	2803	PLX	C25-C24-O8-C5
2	B	2802	PLX	C25-C24-O8-C5
2	B	2806	PLX	C25-C24-O8-C5
2	A	2804	PLX	C27-C28-C29-C30
2	C	2801	PLX	C26-C27-C28-C29
2	D	2803	PLX	C6-C7-C8-C9

There are no ring outliers.

24 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2805	PLX	1	0
2	B	2807	PLX	20	0
2	D	2803	PLX	18	0
2	C	2807	PLX	7	0
2	C	2808	PLX	1	0
2	D	2806	PLX	5	0
2	D	2802	PLX	1	0
2	A	2804	PLX	2	0
2	B	2805	PLX	2	0
2	D	2804	PLX	2	0
2	A	2801	PLX	1	0

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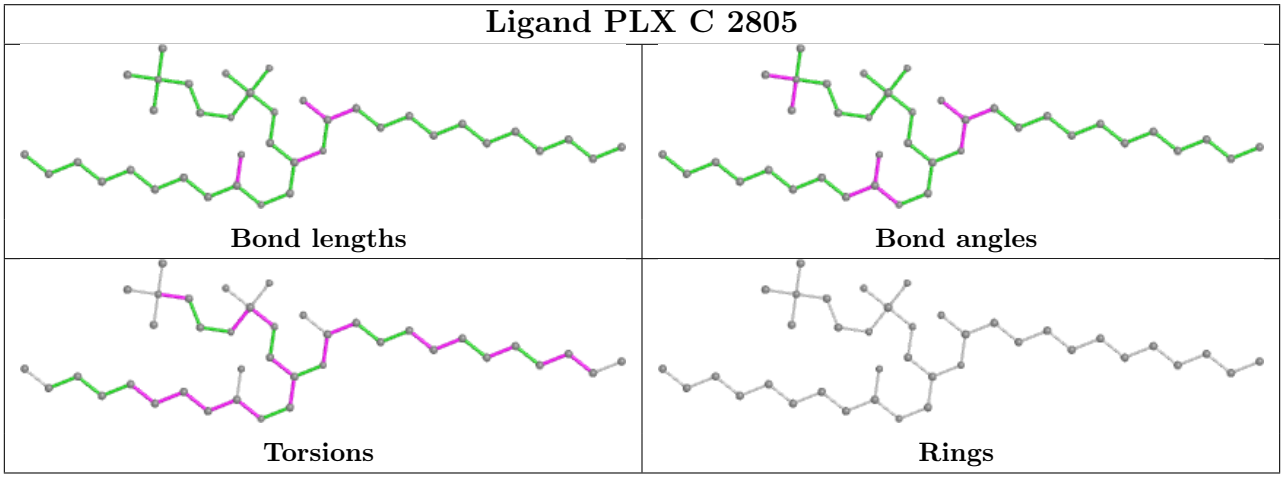
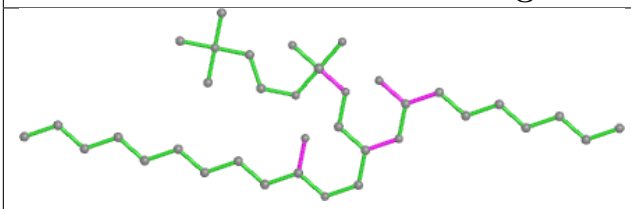
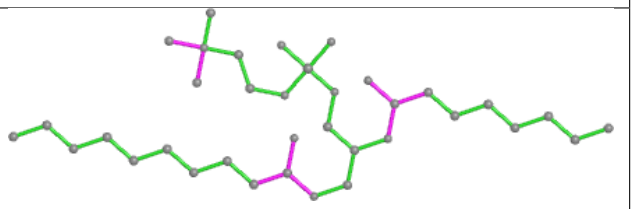
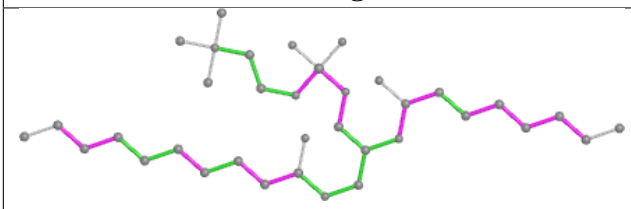
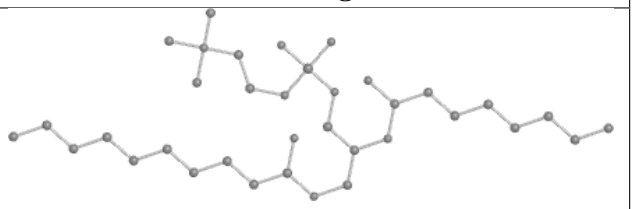
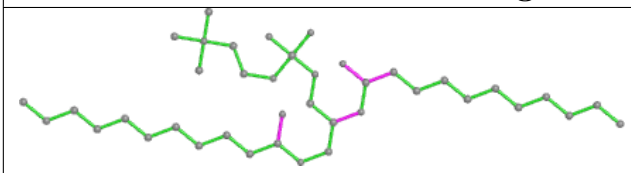
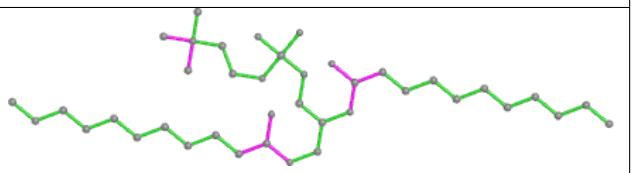
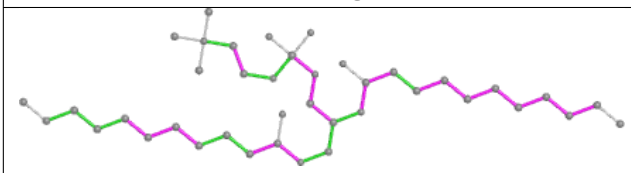
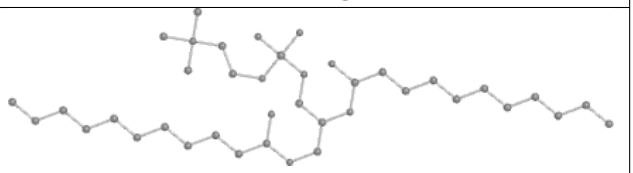
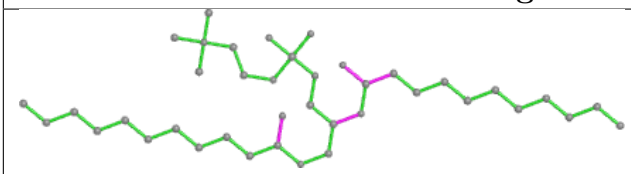
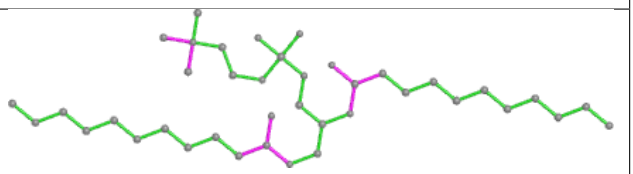
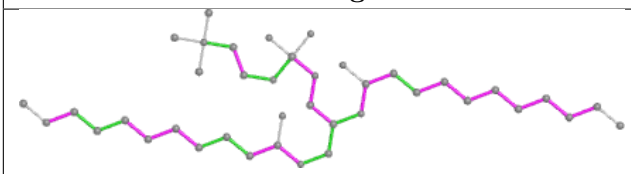
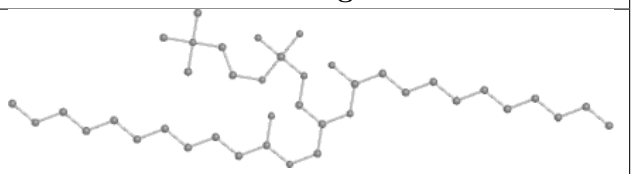
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2807	PLX	1	0
2	B	2806	PLX	3	0
2	D	2807	PLX	2	0
2	C	2804	PLX	18	0
2	A	2802	PLX	2	0
2	B	2802	PLX	7	0
2	C	2802	PLX	2	0
2	D	2801	PLX	2	0
2	A	2803	PLX	18	0
2	B	2803	PLX	1	0
2	C	2803	PLX	3	0
2	B	2808	PLX	2	0
2	A	2806	PLX	6	0

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.

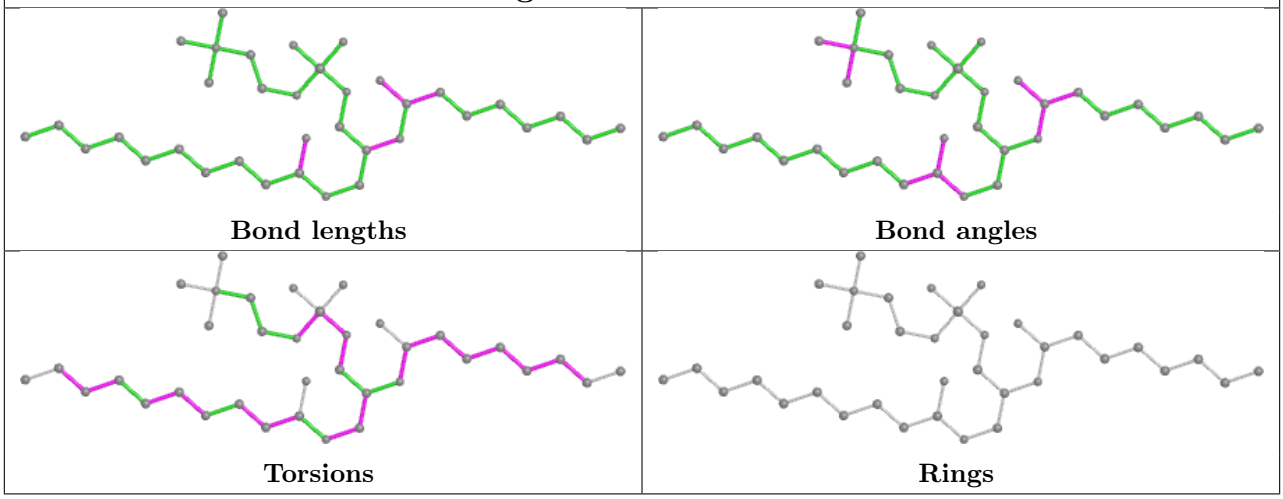


Ligand PLX B 2807	
 Bond lengths	 Bond angles
 Torsions	 Rings

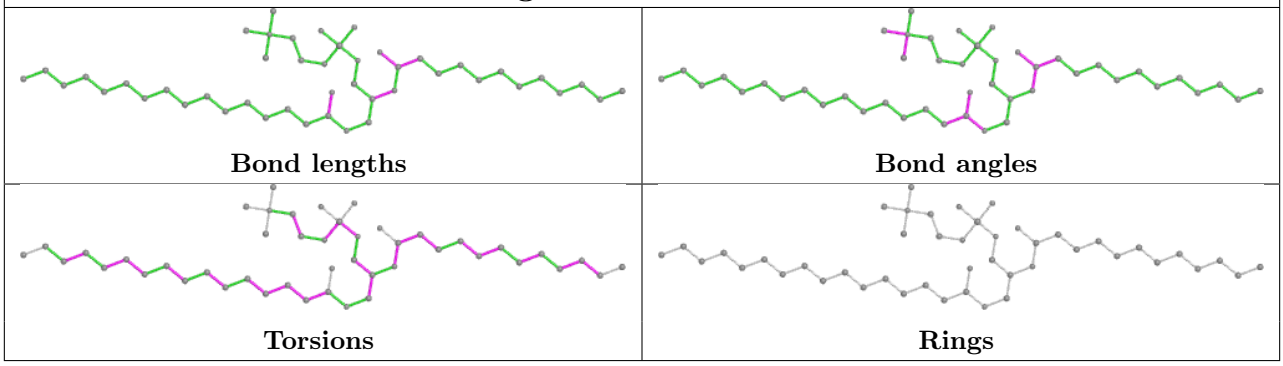
Ligand PLX B 2804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX B 2801	
 Bond lengths	 Bond angles
 Torsions	 Rings

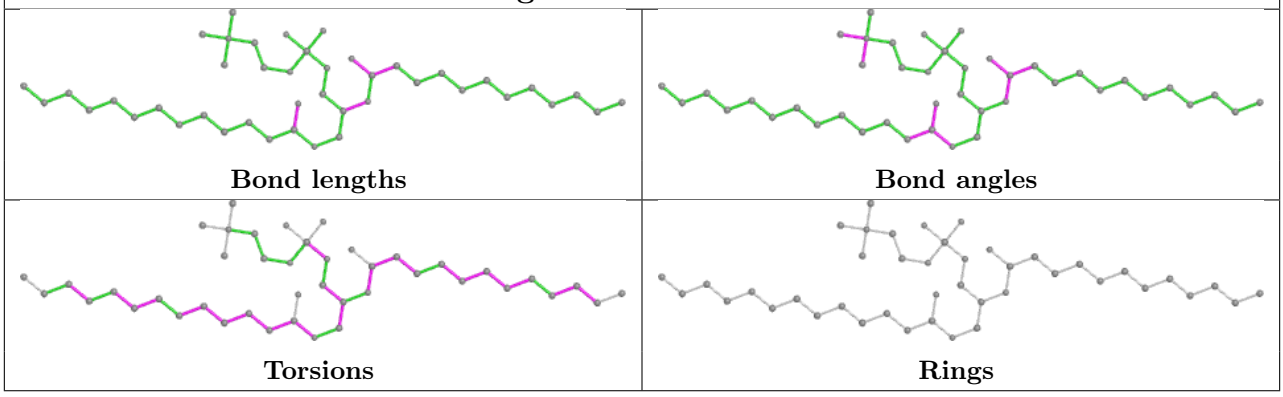
Ligand PLX D 2803



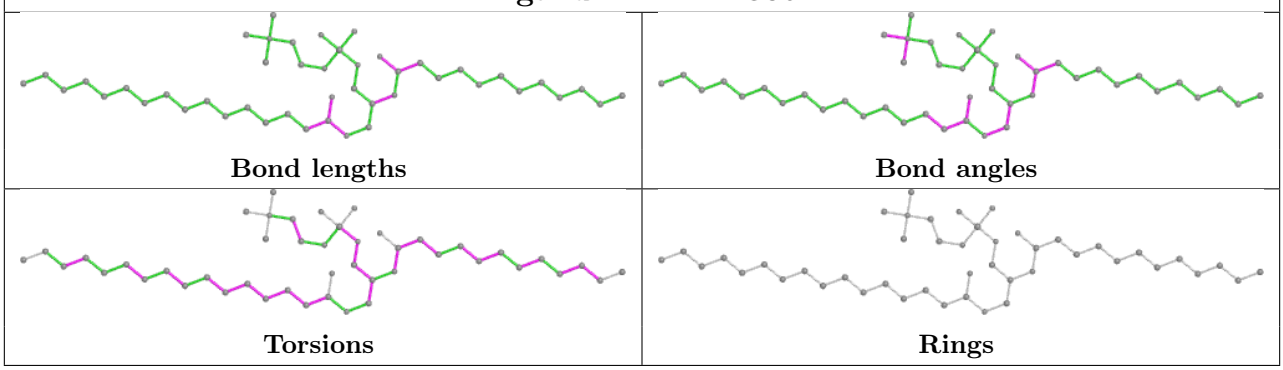
Ligand PLX C 2807



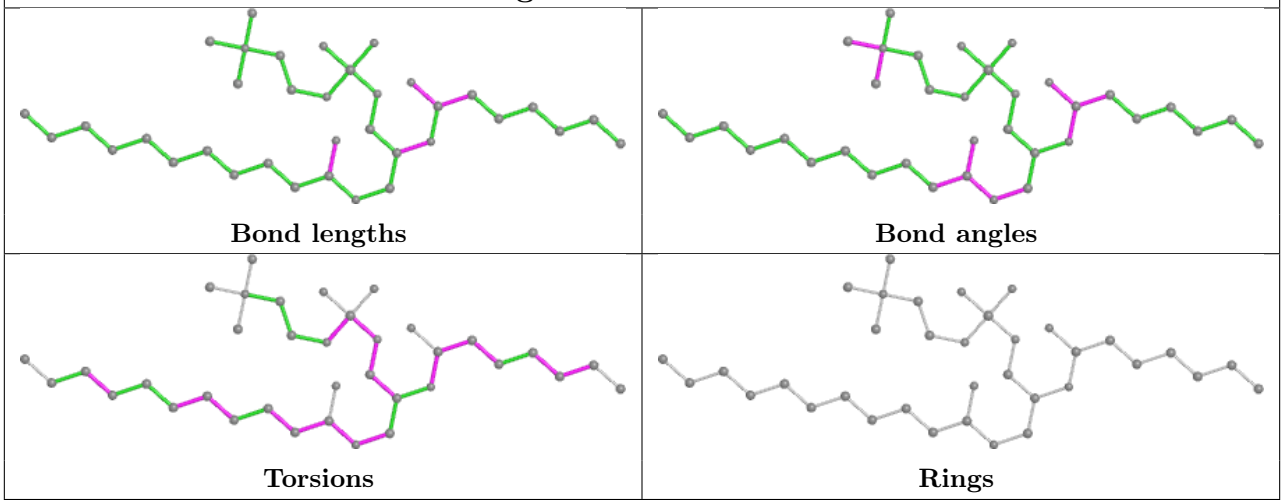
Ligand PLX C 2808



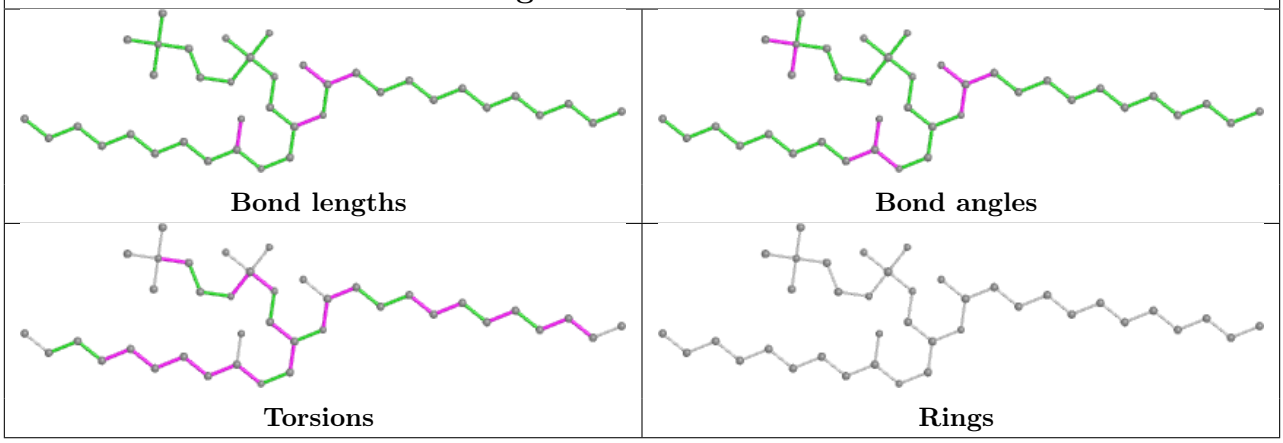
Ligand PLX D 2806



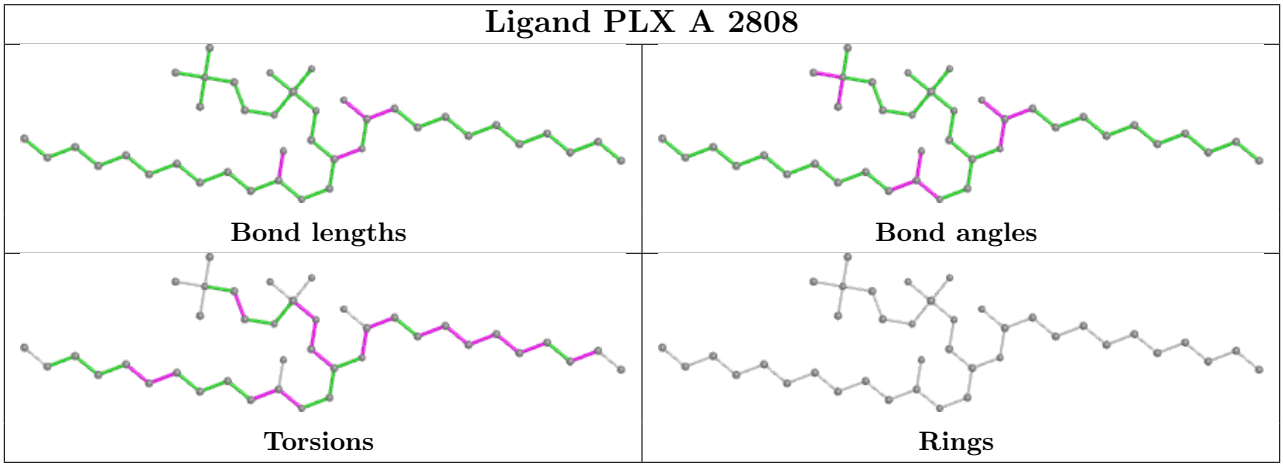
Ligand PLX D 2802



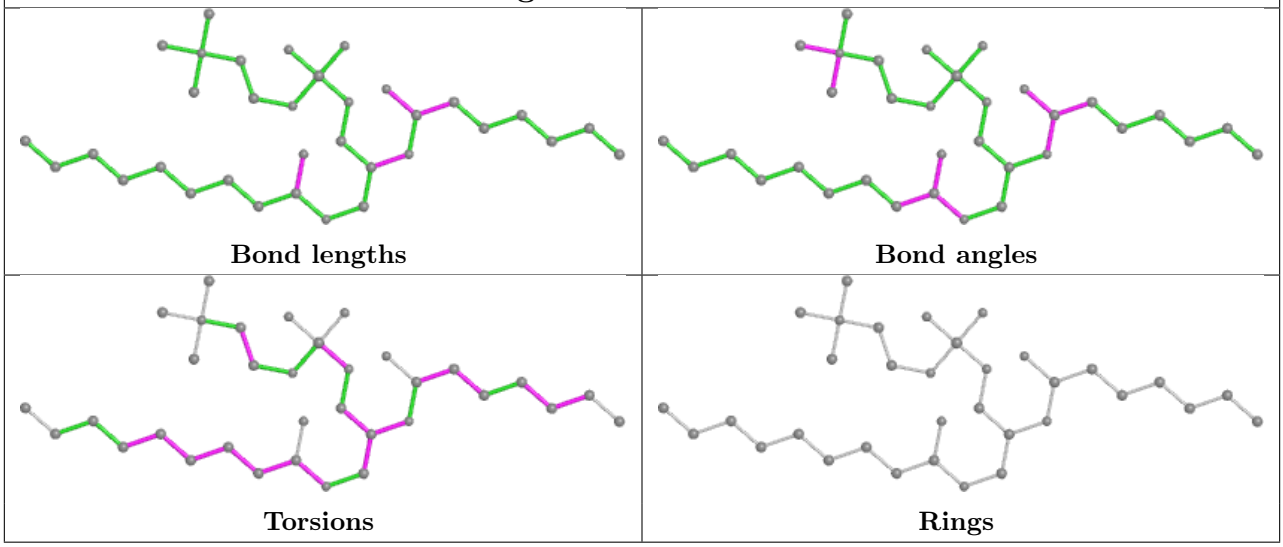
Ligand PLX A 2804



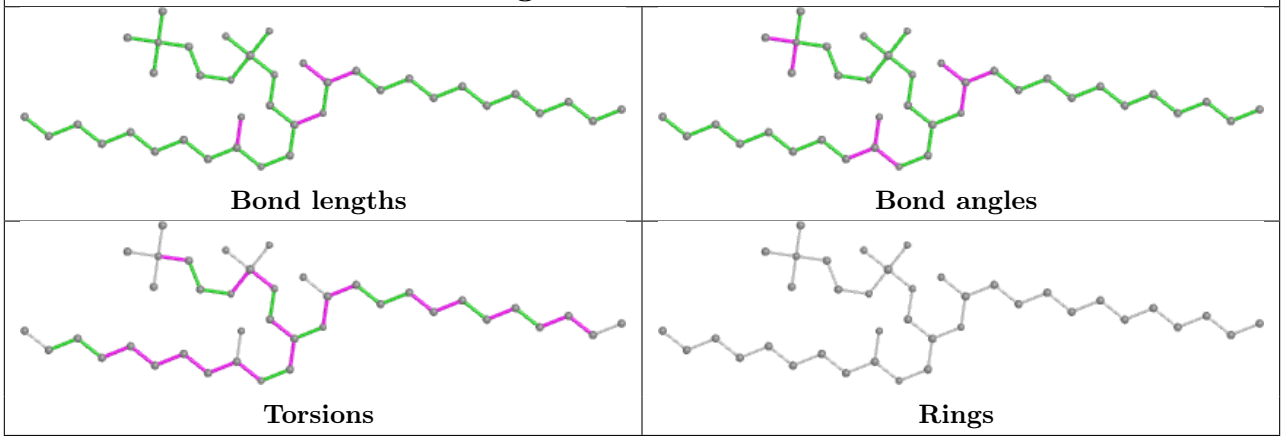
Ligand PLX A 2808



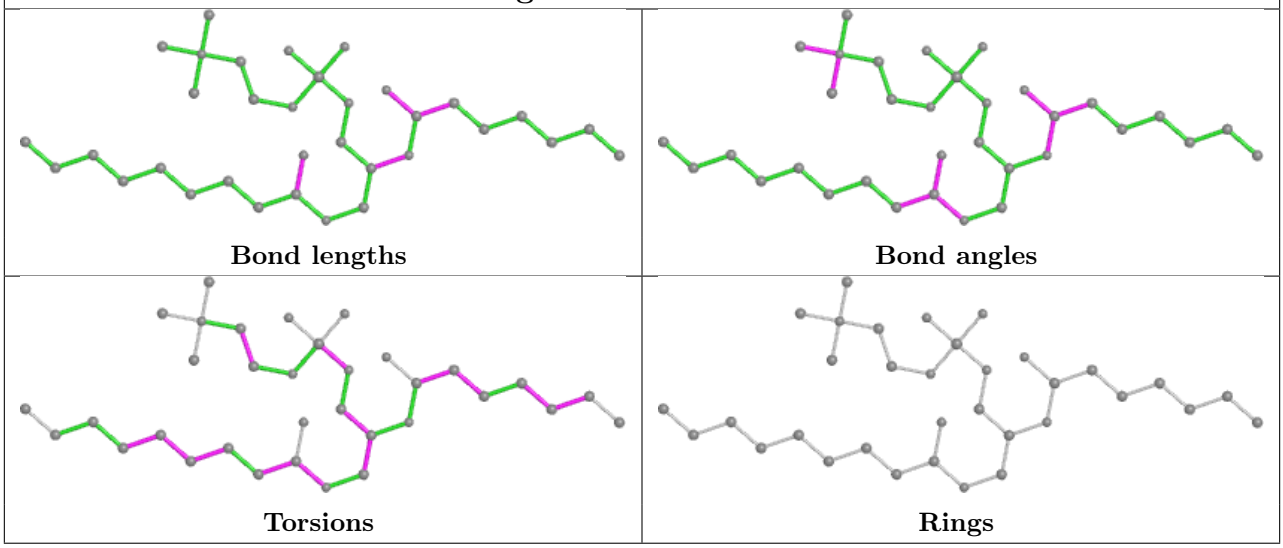
Ligand PLX B 2805



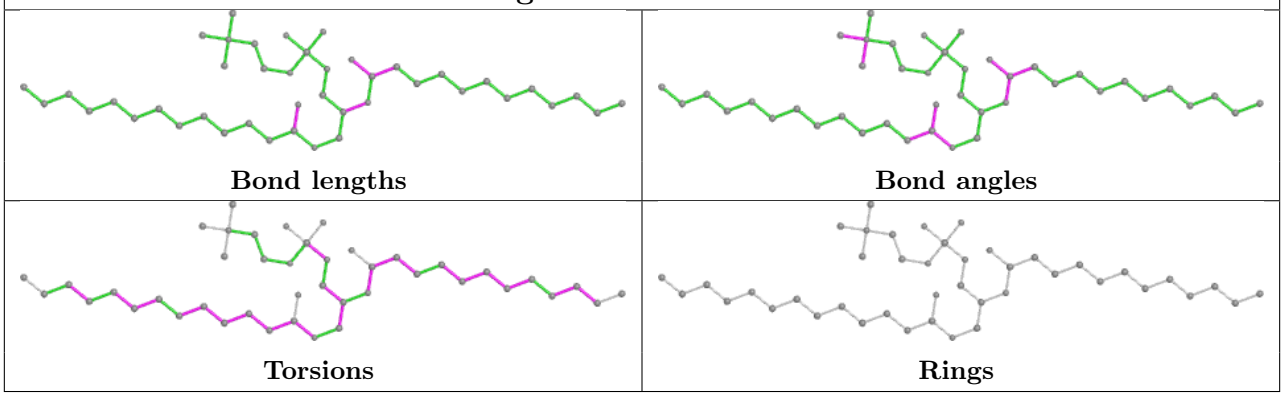
Ligand PLX D 2804



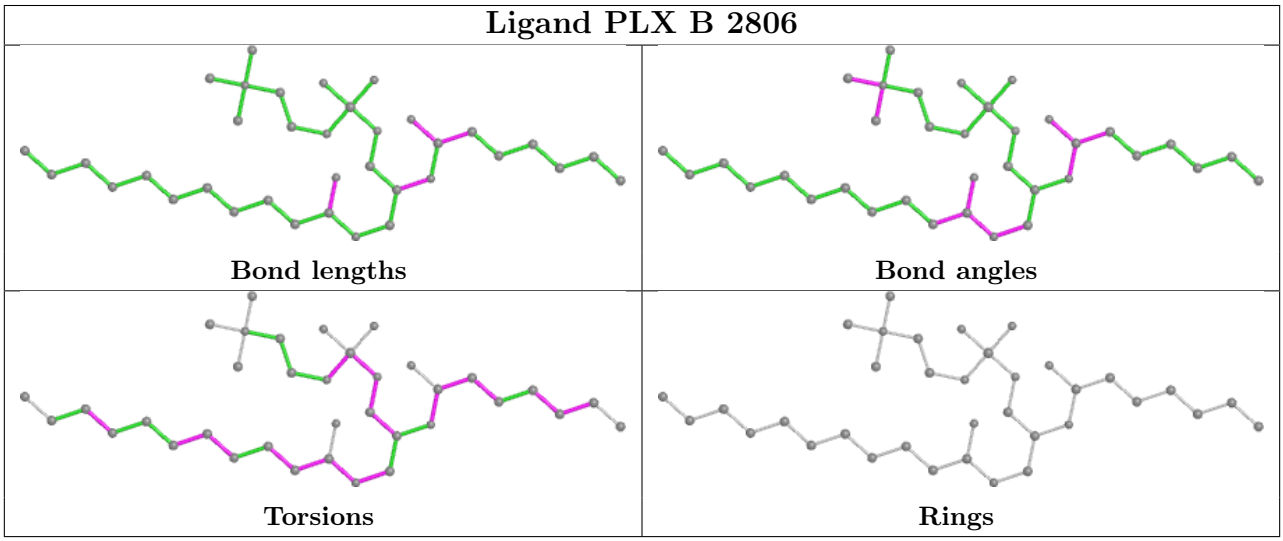
Ligand PLX A 2801



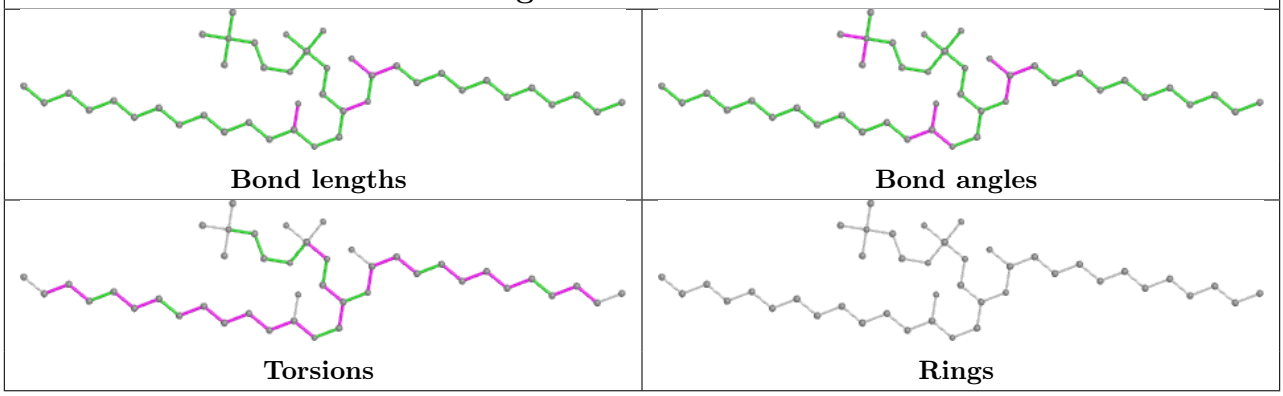
Ligand PLX A 2807



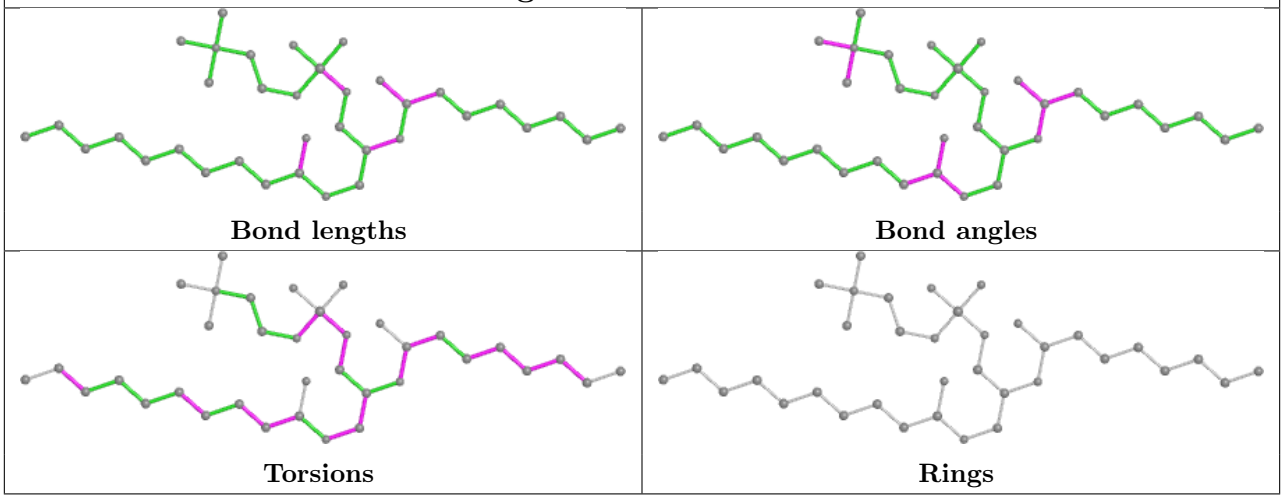
Ligand PLX B 2806



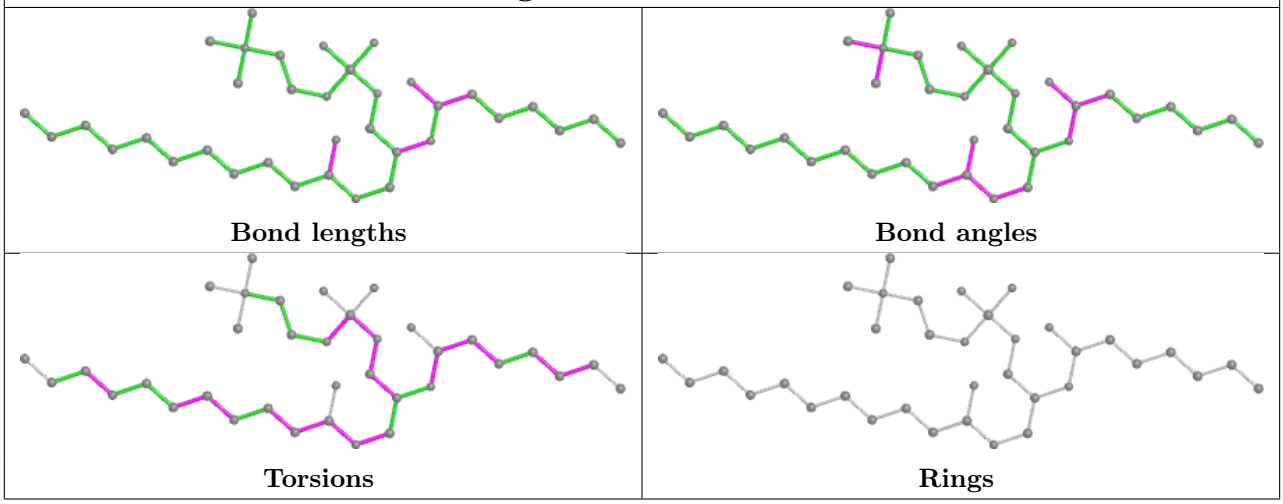
Ligand PLX D 2807



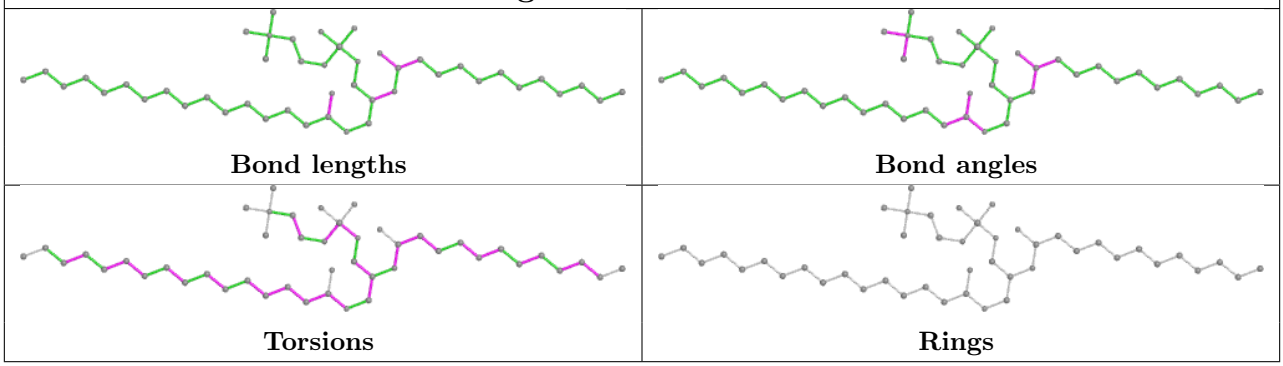
Ligand PLX C 2804



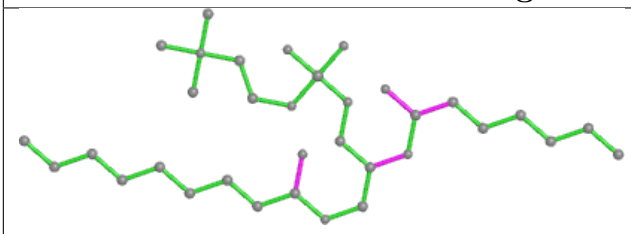
Ligand PLX A 2802

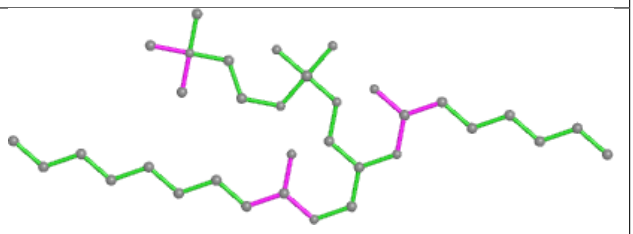


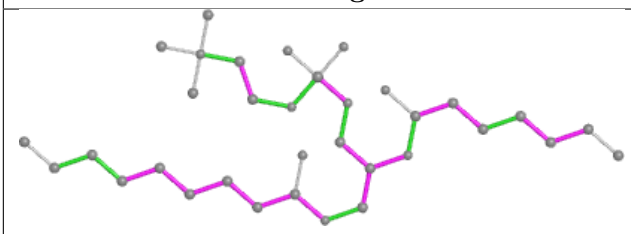
Ligand PLX B 2802

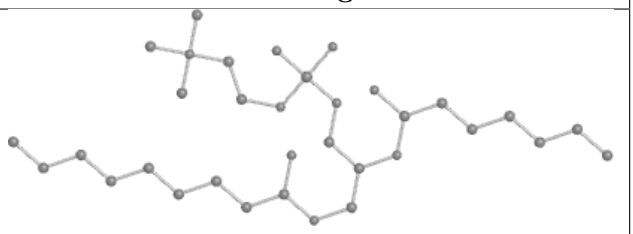


Ligand PLX C 2802

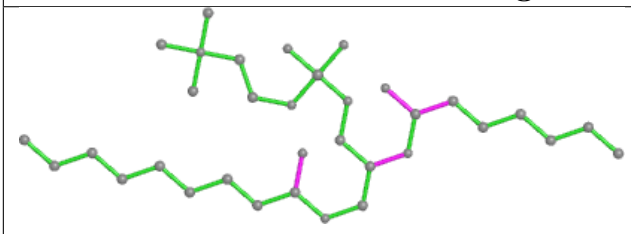

Bond lengths

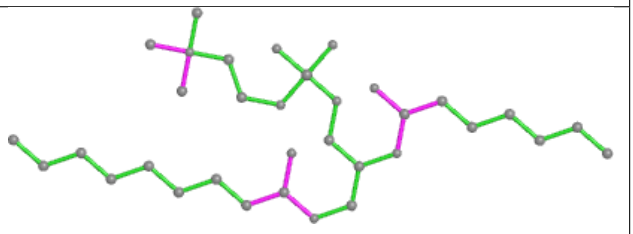

Bond angles

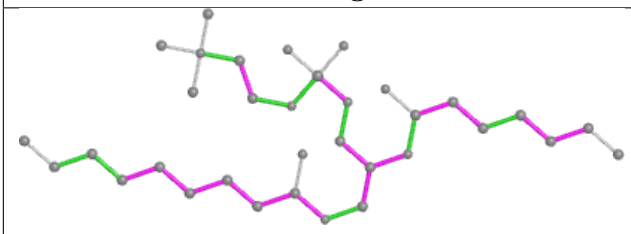

Torsions

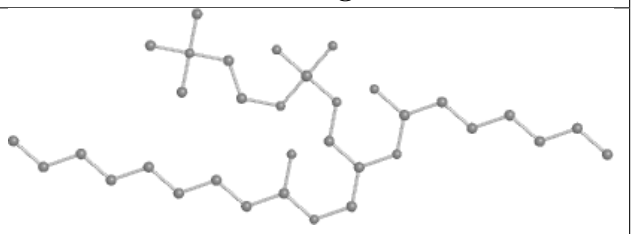

Rings

Ligand PLX D 2801

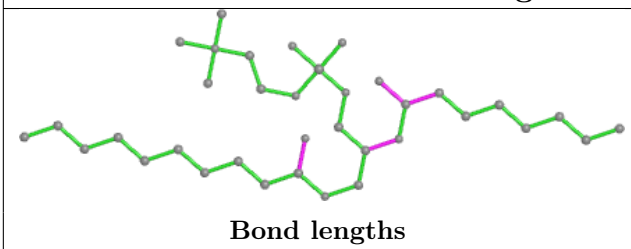

Bond lengths

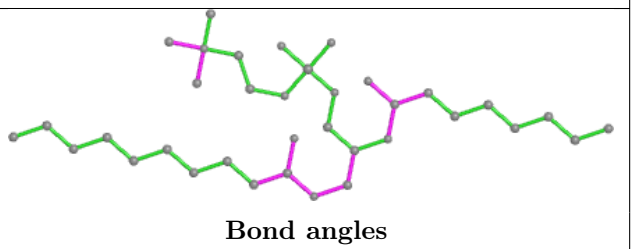

Bond angles

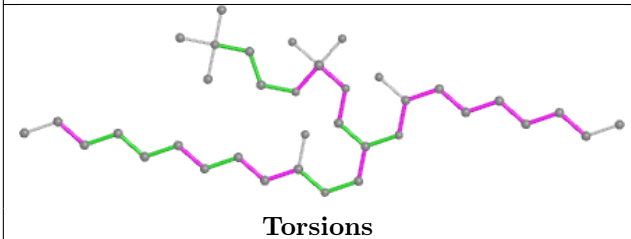

Torsions

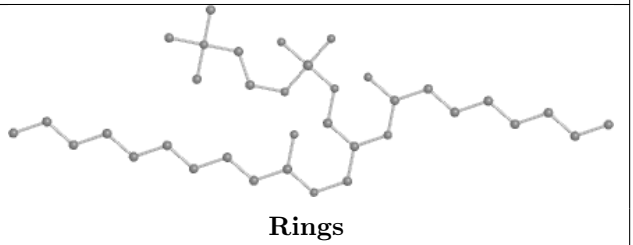

Rings

Ligand PLX A 2803

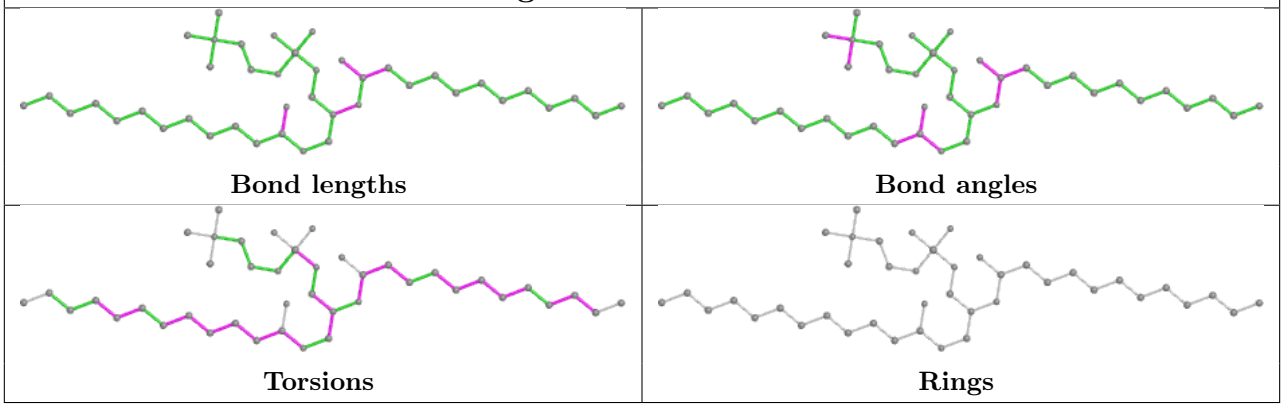

Bond lengths


Bond angles

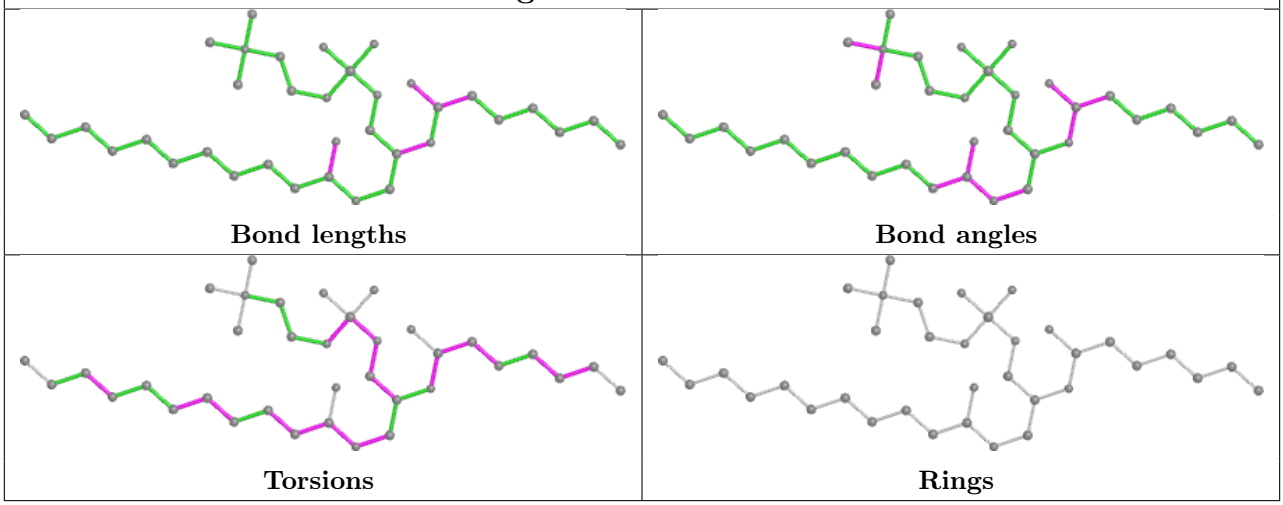

Torsions


Rings

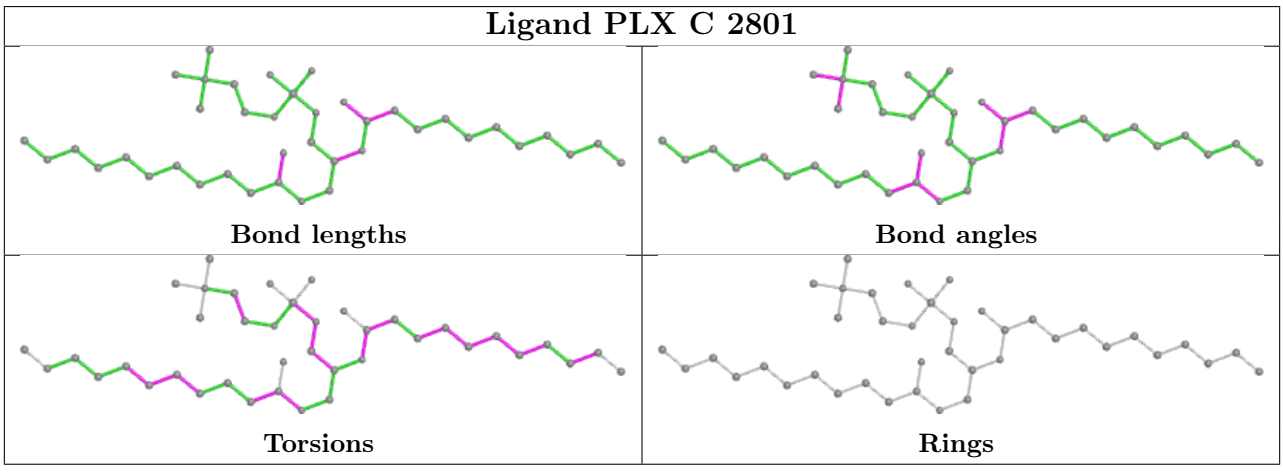
Ligand PLX B 2803

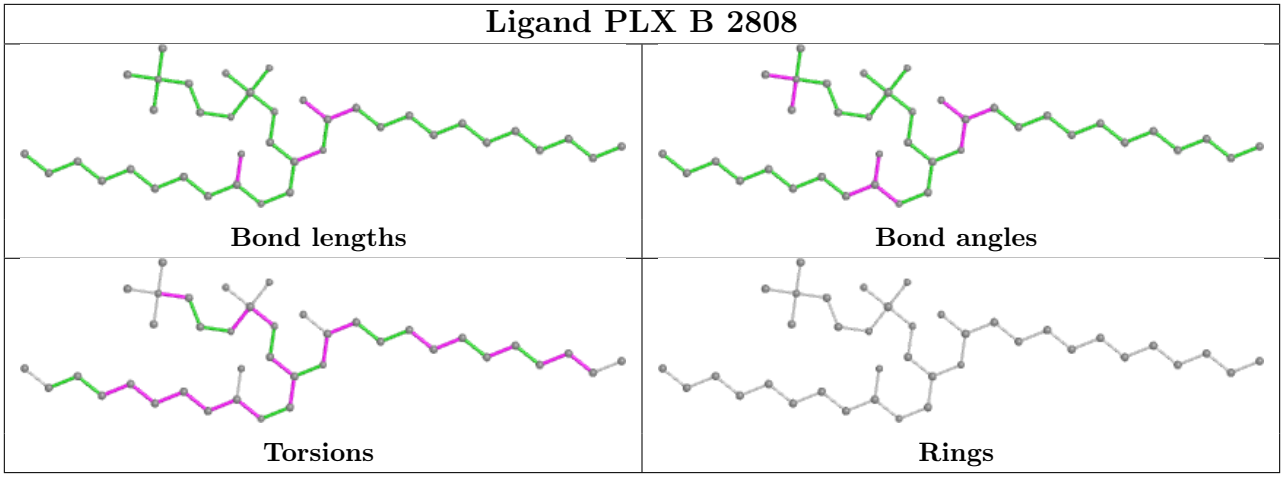


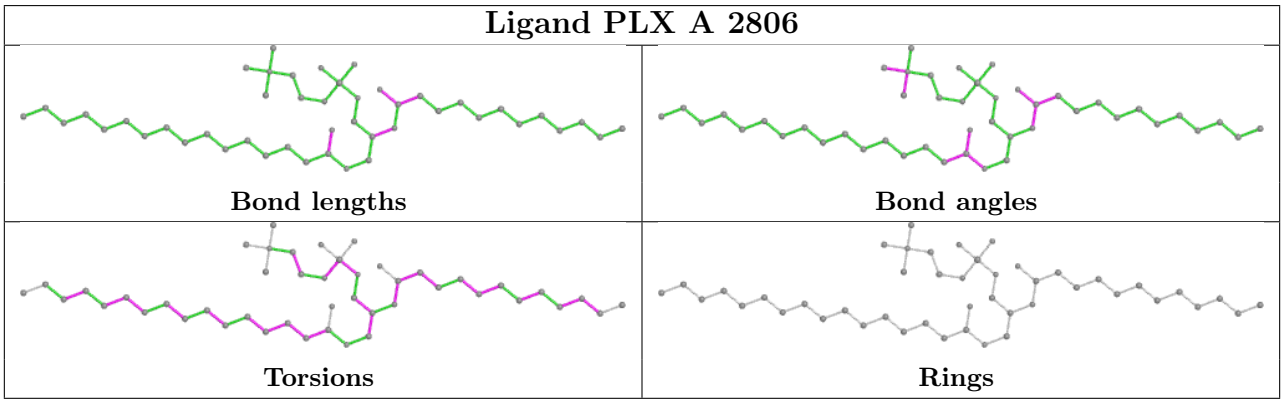
Ligand PLX C 2803



Ligand PLX C 2801







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

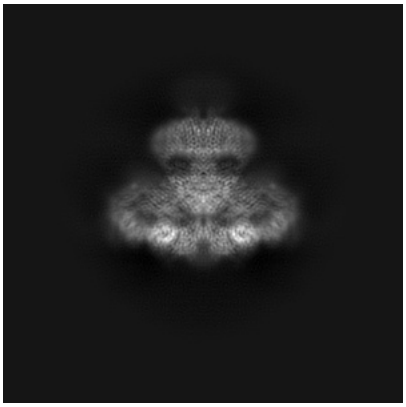
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23337. These allow visual inspection of the internal detail of the map and identification of artifacts.

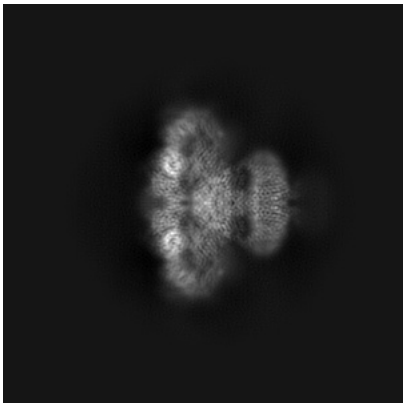
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

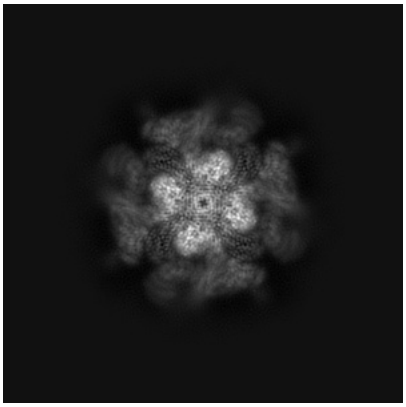
6.1.1 Primary map



X



Y

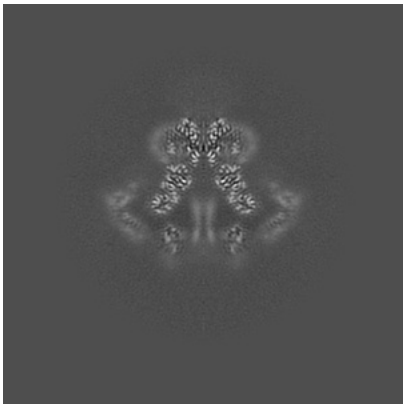


Z

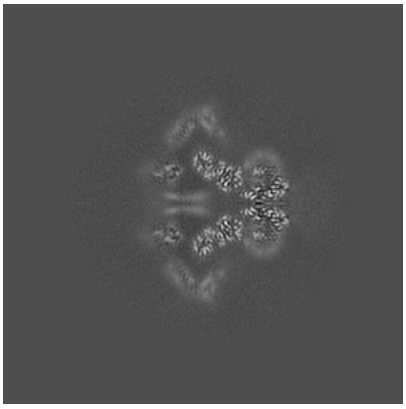
The images above show the map projected in three orthogonal directions.

6.2 Central slices

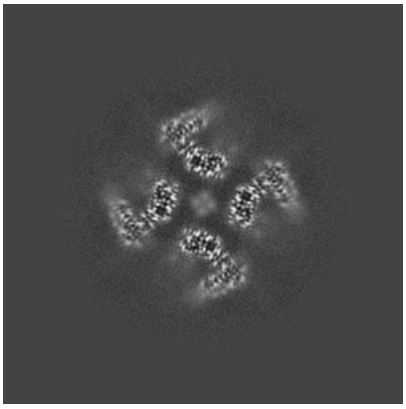
6.2.1 Primary map



X Index: 220



Y Index: 220

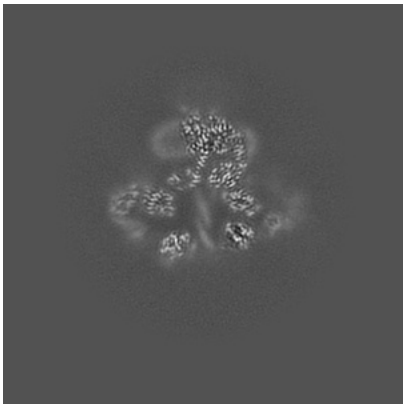


Z Index: 220

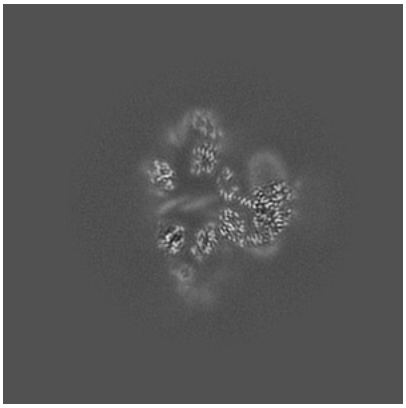
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

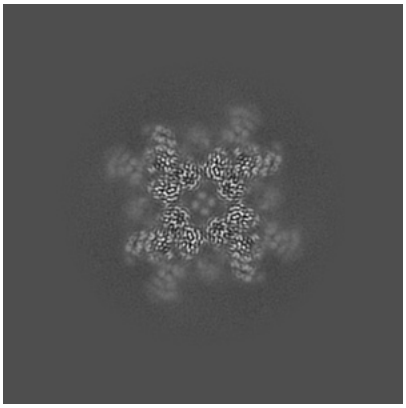
6.3.1 Primary map



X Index: 229



Y Index: 229

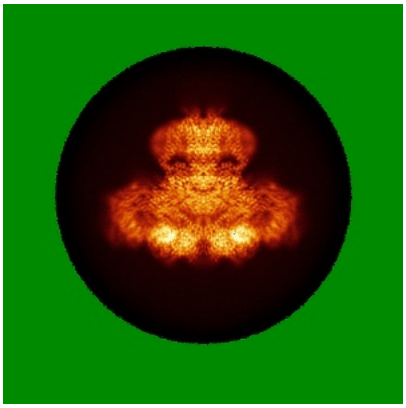


Z Index: 182

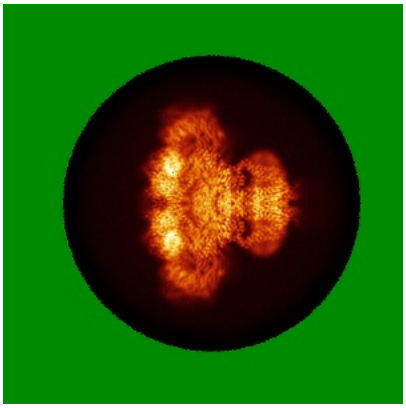
The images above show the largest variance slices of the map in three orthogonal directions.

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

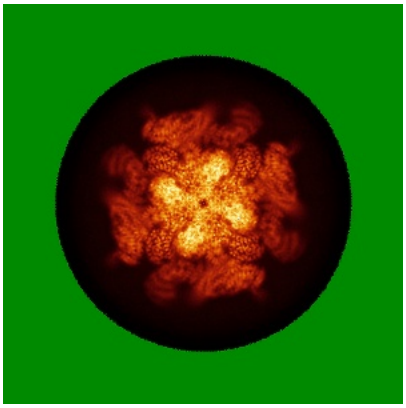
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

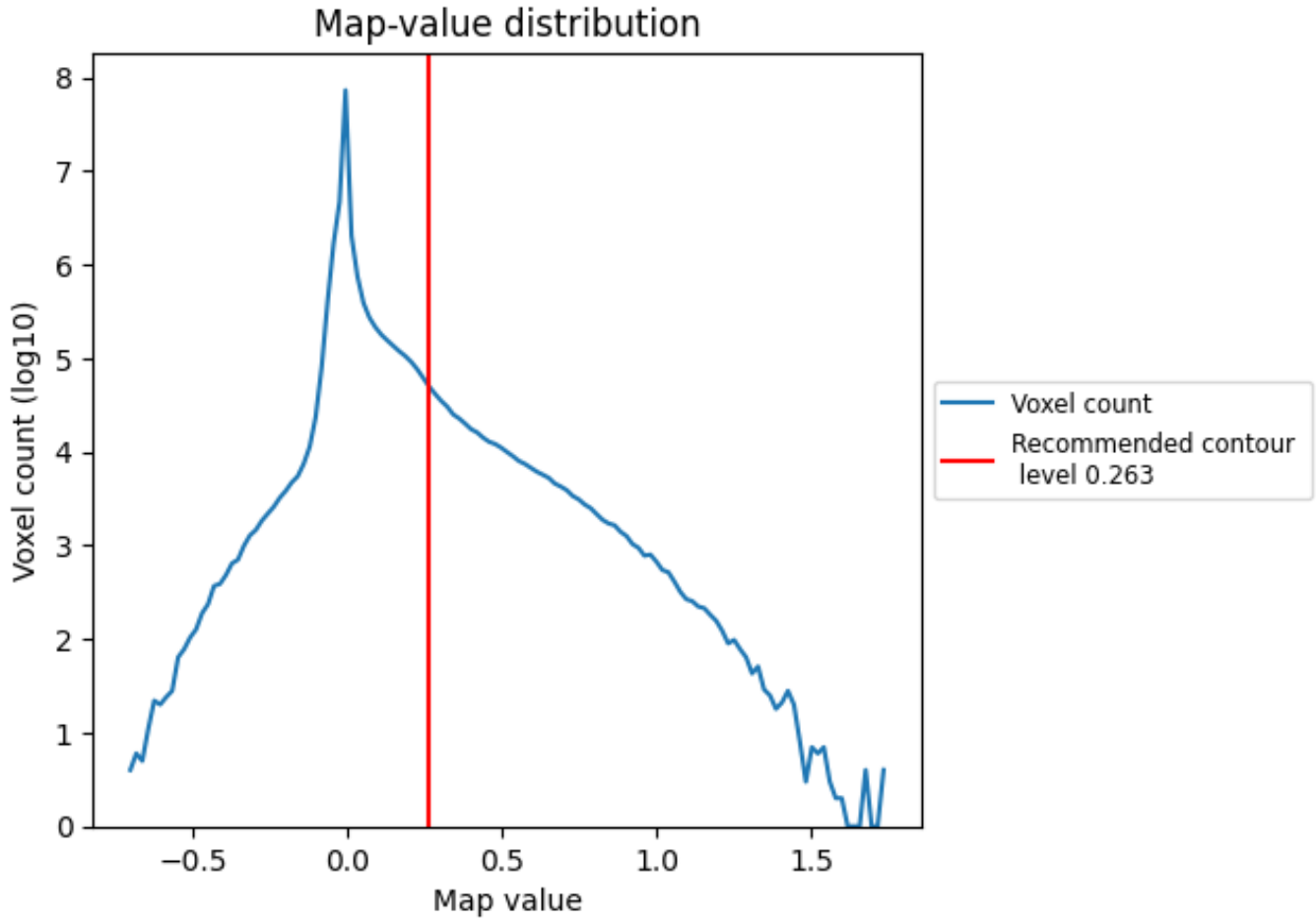
6.6 Mask visualisation (i)

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

7 Map analysis

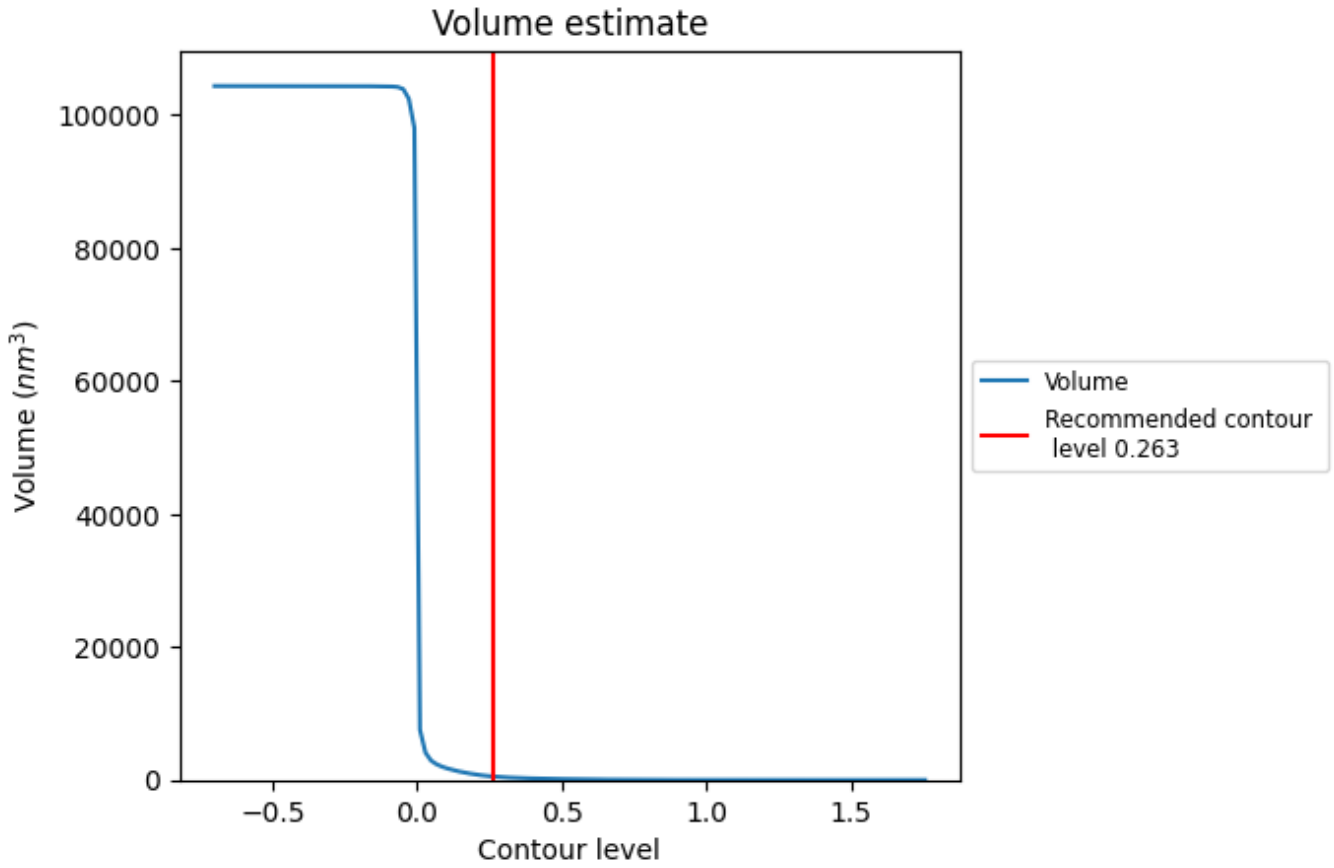
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

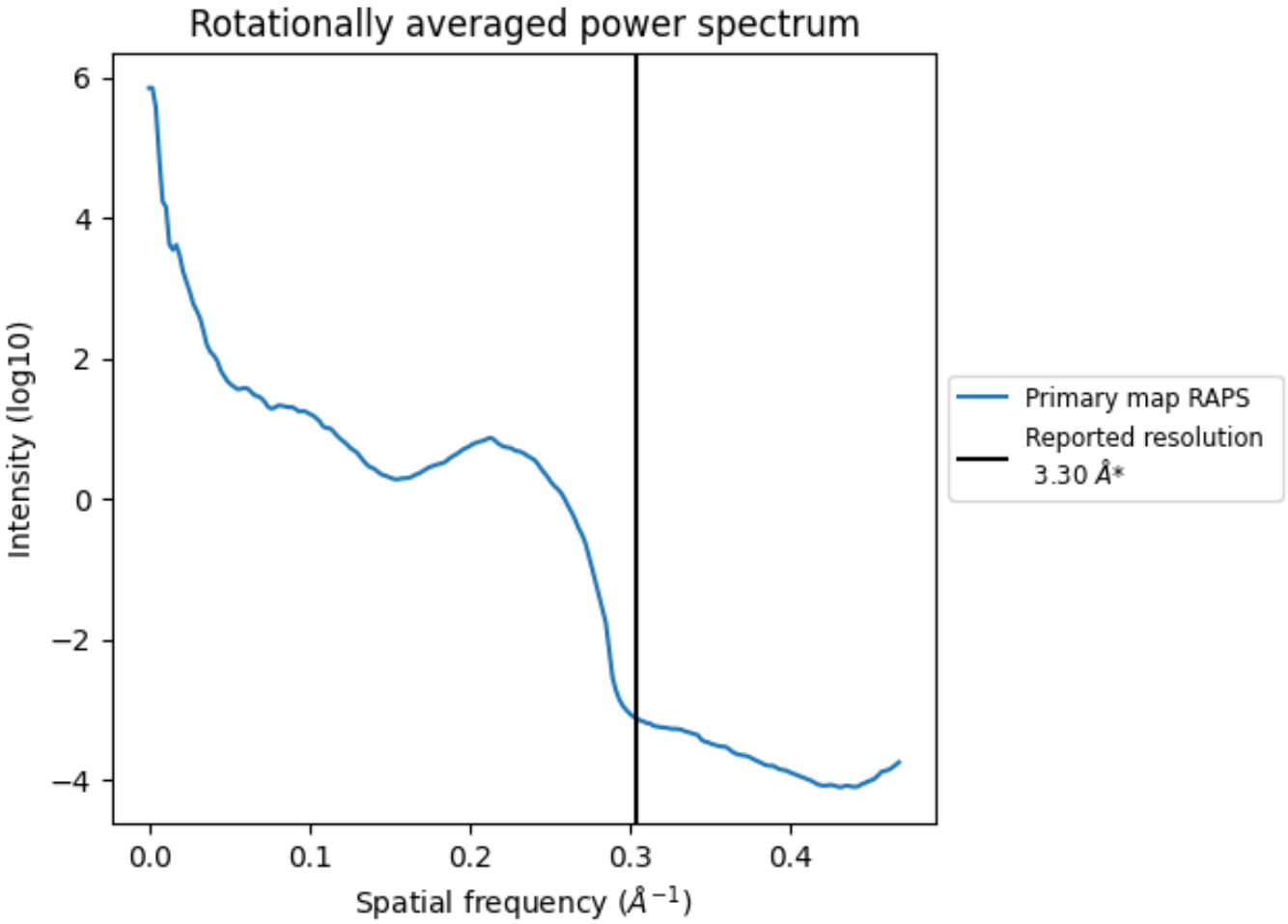
7.2 Volume estimate



The volume at the recommended contour level is 514 nm^3; this corresponds to an approximate mass of 464 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 0.303 $Å^{-1}$

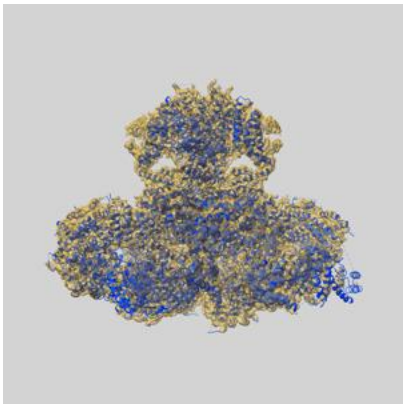
8 Fourier-Shell correlation

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

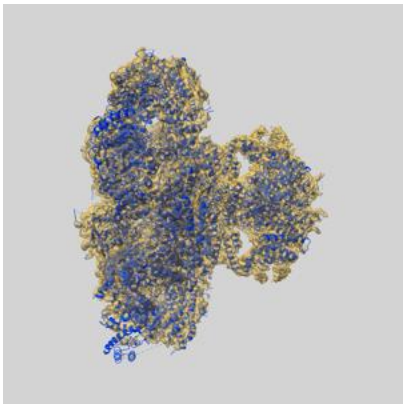
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23337 and PDB model 7LHE. Per-residue inclusion information can be found in section 3 on page 7.

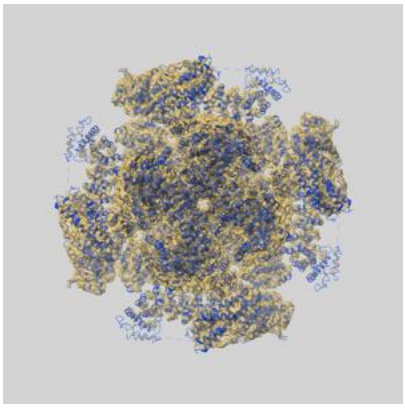
9.1 Map-model overlay



X



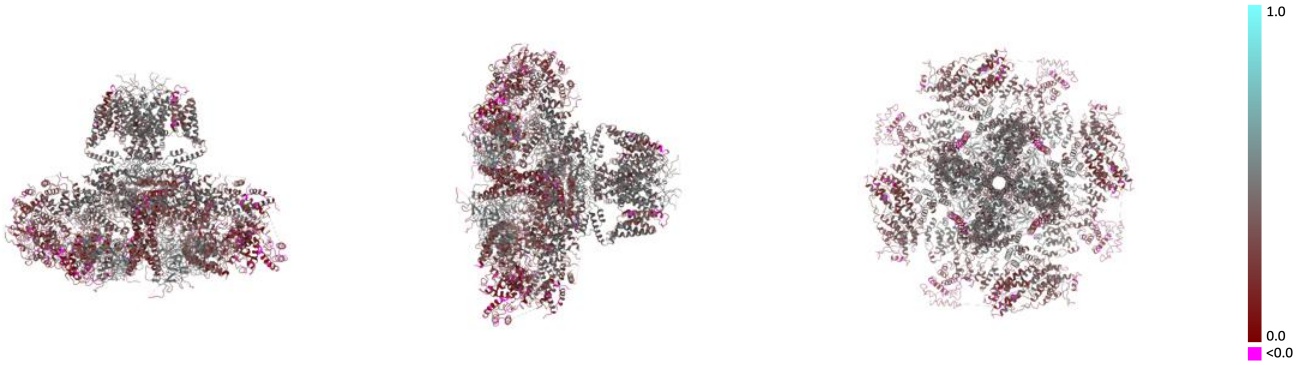
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.263 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.

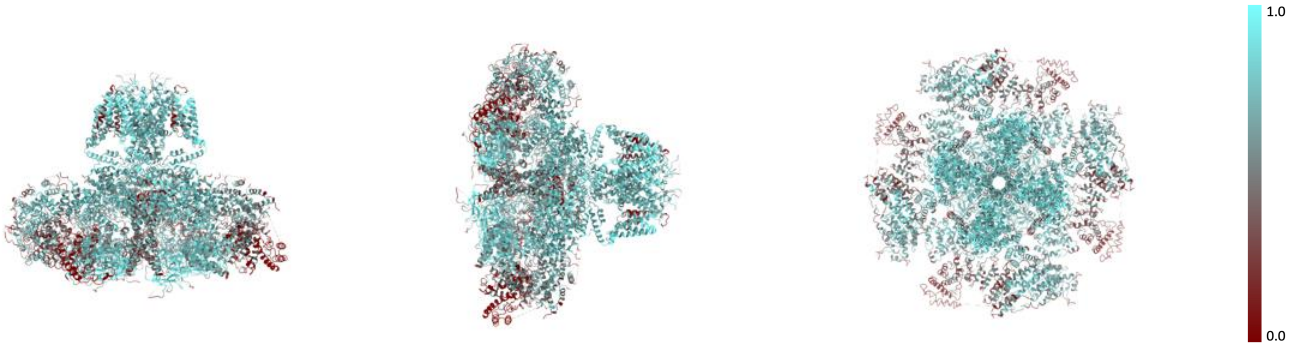
9.2 Q-score mapped to coordinate model (i)



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.

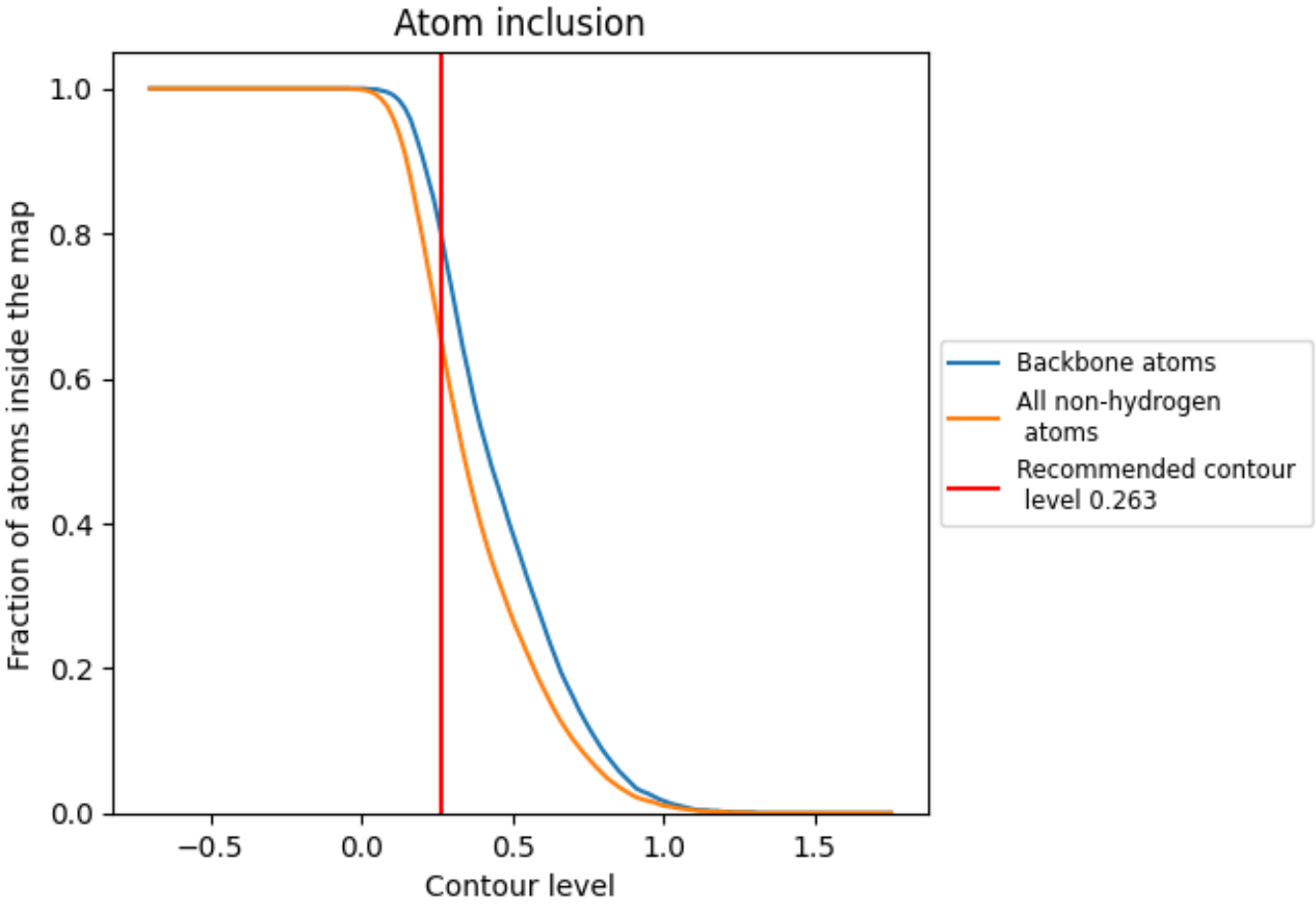
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.263).

9.4 Atom inclusion (i)



At the recommended contour level, 80% 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 (0.263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6540	0.3460
A	0.6540	0.3460
B	0.6540	0.3460
C	0.6540	0.3460
D	0.6540	0.3450