Full wwPDB EM Validation Report

Mar 7, 2026 – 11:46 PM UTC

PDB ID	:	8IXN / pdb_00008ixn
EMDB ID	:	EMD-35799
Title	:	Curved structure of mPIEZO1-S2472E
Authors	:	Liu, S.; Yang, X.; Chen, X.; Li, X.; Xiao, B.
Deposited on	:	2023-04-01
Resolution	:	4.07 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

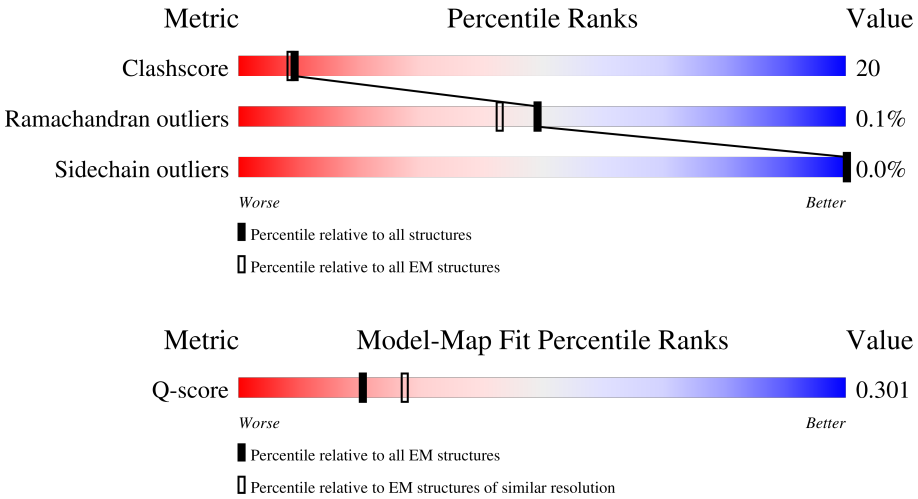
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.07 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6427 (3.58 - 4.57)

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	2547	19% 38% 15% 47%
1	C	2547	21% 37% 16% 47%
1	D	2547	11% 39% 14% 47%

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
3	PEE	A	2603	-	-	X	-
3	PEE	C	2603	-	-	X	-
3	PEE	D	2603	-	-	X	-
4	P5S	A	2604	-	-	X	-
4	P5S	C	2604	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30043 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.

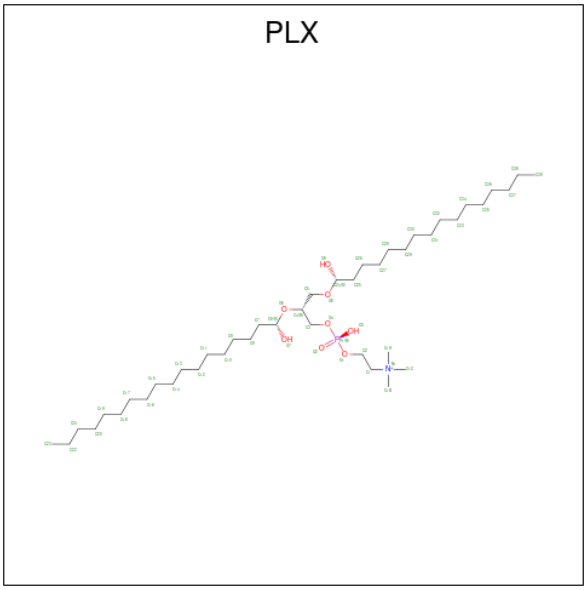
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1350	Total	C	N	O	S	0	0
			9804	6364	1661	1736	43		
1	A	1350	Total	C	N	O	S	0	0
			9802	6363	1660	1736	43		
1	D	1350	Total	C	N	O	S	0	0
			9810	6369	1661	1736	44		

There are 3 discrepancies between the modelled and reference sequences:

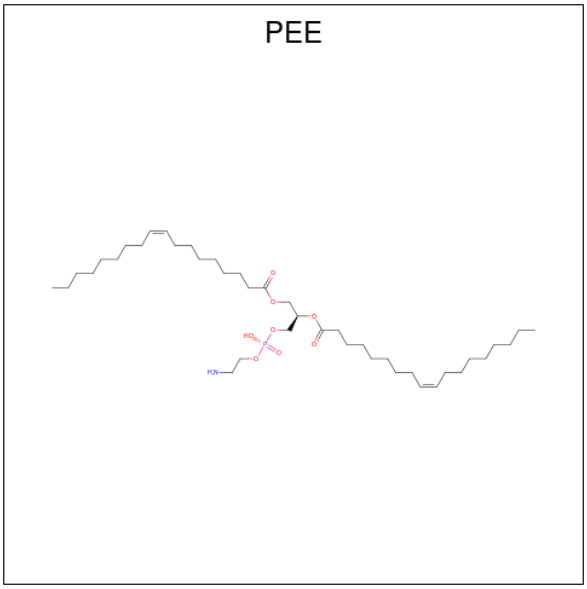
Chain	Residue	Modelled	Actual	Comment	Reference
C	2472	GLU	SER	engineered mutation	UNP E2JF22
A	2472	GLU	SER	engineered mutation	UNP E2JF22
D	2472	GLU	SER	engineered mutation	UNP E2JF22

- 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 (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



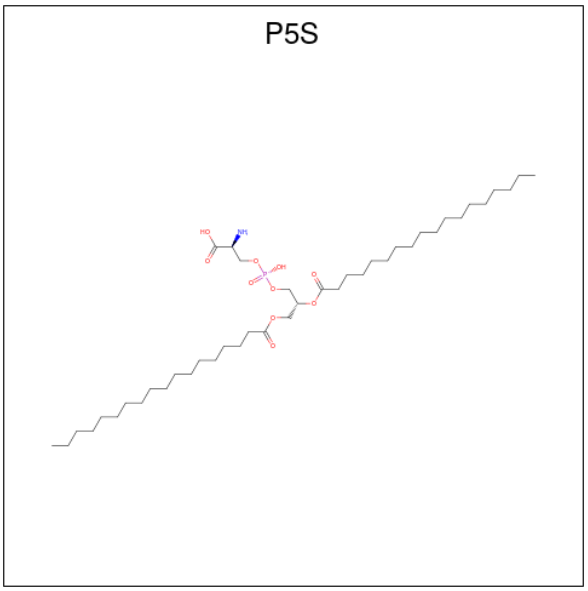
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	D	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



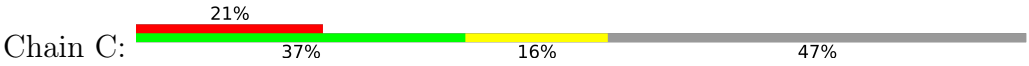
Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			54	42	1	10	1	
4	A	1	Total	C	N	O	P	0
			54	42	1	10	1	
4	D	1	Total	C	N	O	P	0
			54	42	1	10	1	

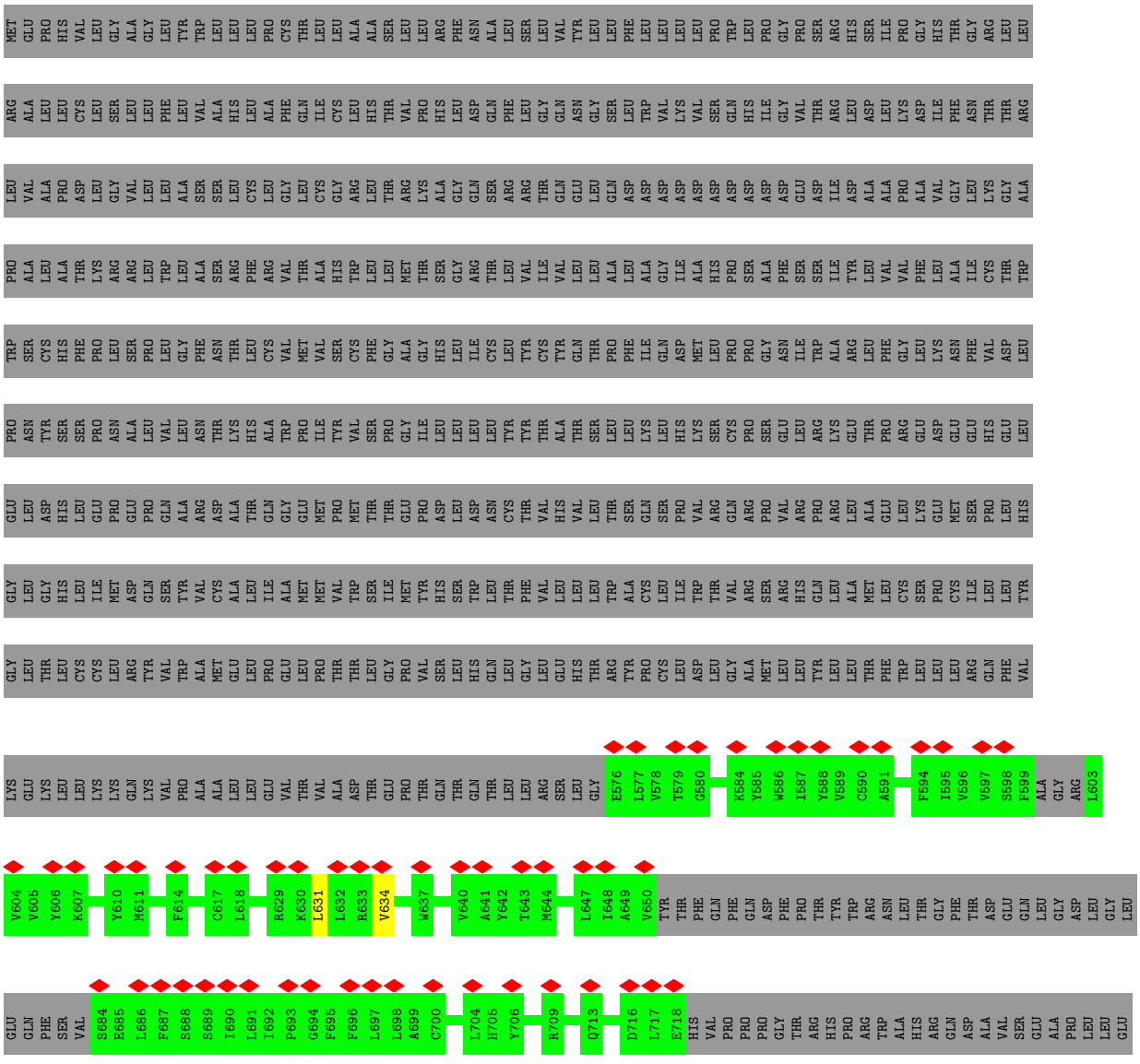
3 Residue-property plots (i)

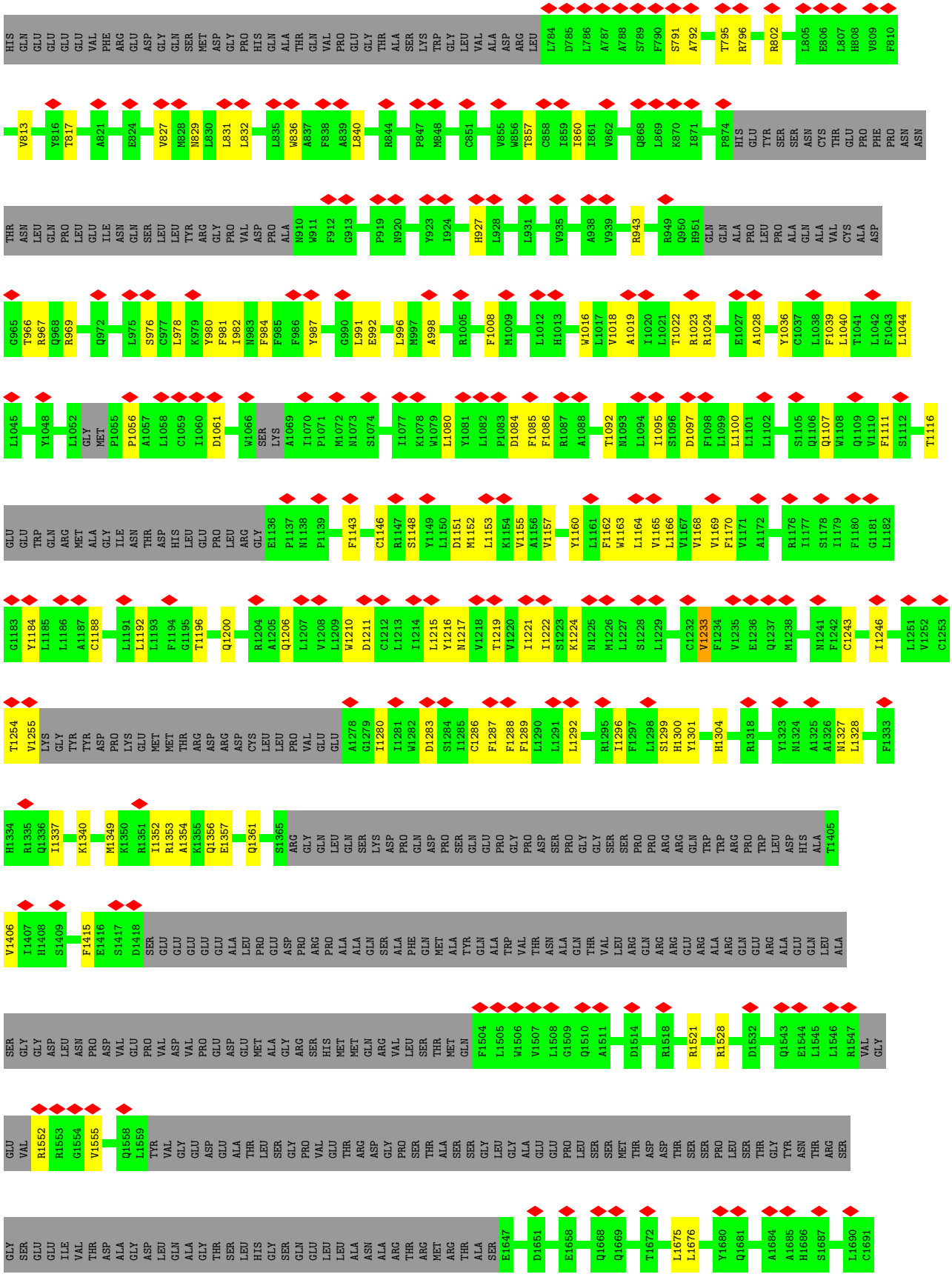
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

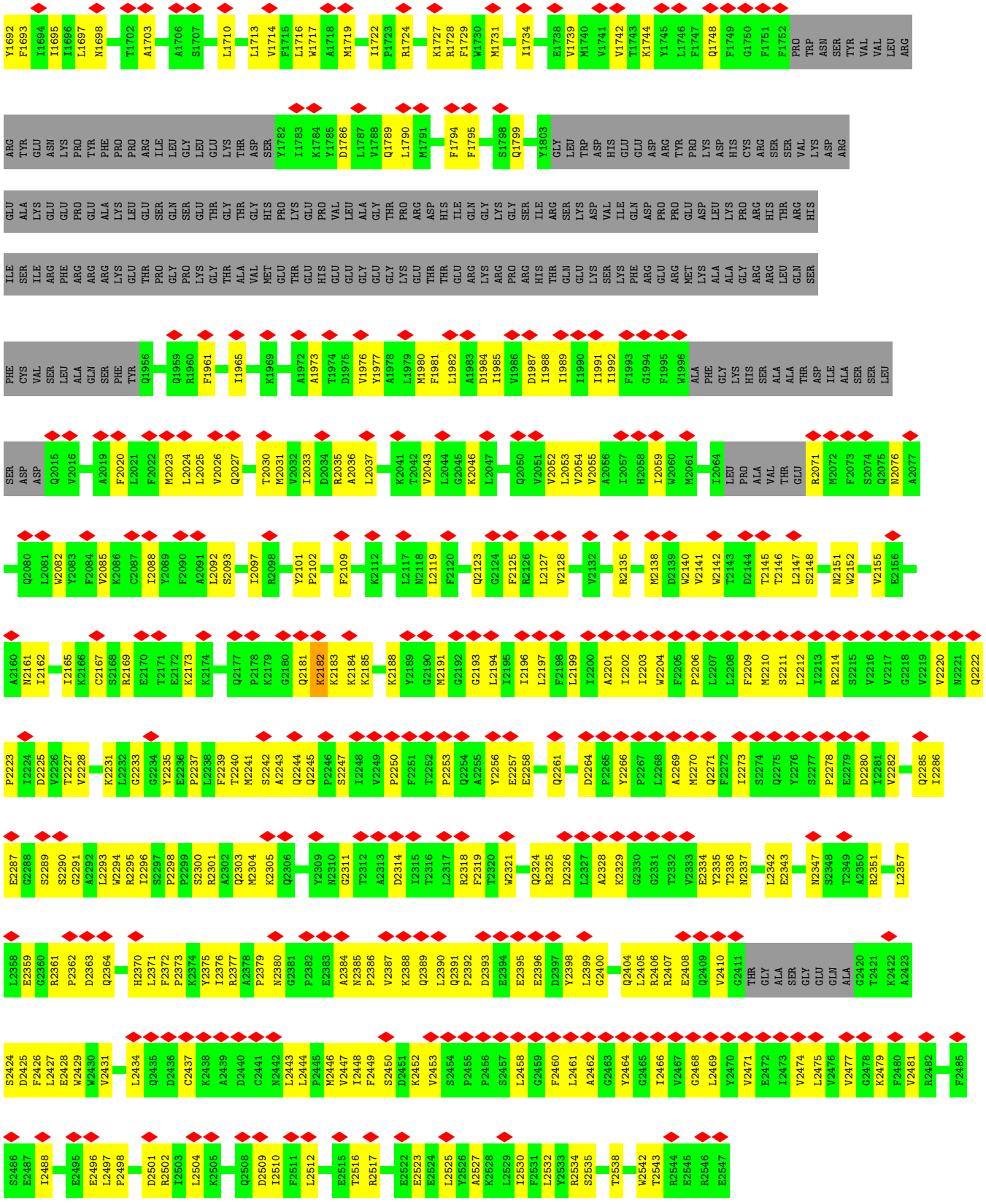
- Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain C:



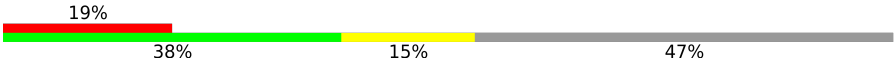


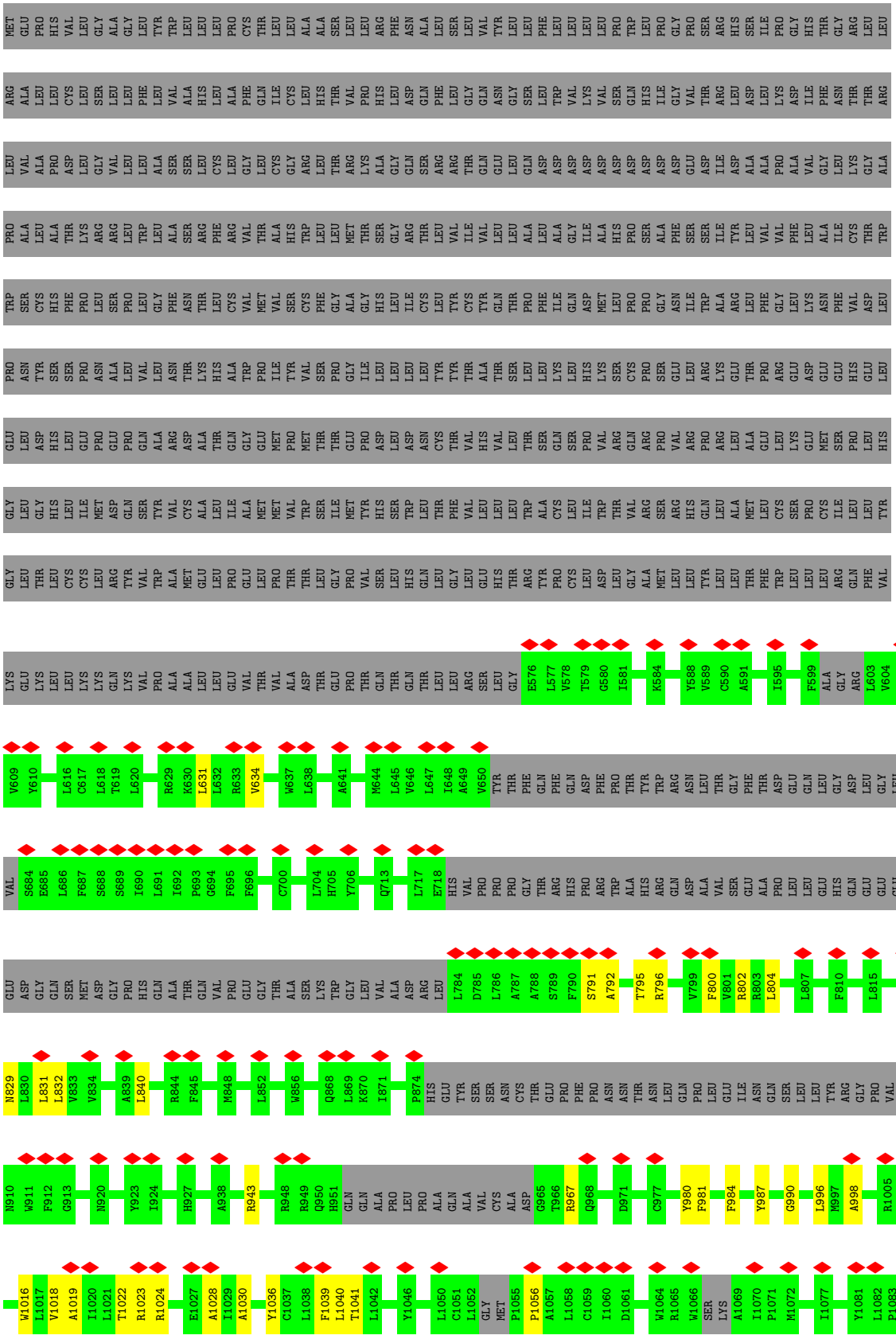

HIS GLN GLU GLU GLU GLU VAL PHE ARG GLU ASP GLY GLN SER MET ASP GLY PRO HIS GLN ALA THR GLN VAL PRO GLU GLY THR ALA SER LYS TRP GLY LEU VAL ALA ASP ARG LEU
L784 D785 L786 A787 A788 S789 F790 S791 A792 T795 R796 R802 L805 E806 L807 H808 V809 F810
V813 Y816 T817 A821 E824 V827 W828 N829 L830 L831 L832 L835 W836 A837 F838 A839 L840 R844 P847 M848 C851 V855 W856 T857 C858 I859 I860 I861 V862 Q868 L869 K870 I871 P874
HIS GLU TYR SER SER ASN CYS THR GLU PRO PHE PRO ASN ASN
THR ASN LEU GLN PRO LEU GLU ILE ASN GLN SER LEU LEU TYR ARG GLY PRO VAL ASP PRO ALA
N910 W911 P912 G913 P919 N920 Y923 I924 H927 L928 L931 V935 A938 V939 R943 R949 Q950 H951
GLN GLN ALA PRO LEU PRO ALA GLN ALA VAL CYS ALA ASP
G965 T966 R967 Q968 R969 Q972 L975 S976 C977 L978 K979 Y980 F981 I982 N983 F984 F985 F986 Y987 G990 L991 E992 L996 M997 A998 R1005 F1008 M1009 L1012 H1013 W1016 L1017 V1018 A1019 I1020 L1021 T1022 R1023 R1024 E1027 A1028 Y1036 C1037 L1038 F1039 L1040 T1041 L1042 F1043 L1044
L1045 Y1048 L1052 GLY MET P1055 P1056 A1057 L1058 C1059 I1060 D1061 W1066 SER LYS A1069 I1070 P1071 M1072 N1073 S1074 I1077 K1078 W1079 L1080 Y1081 L1082 P1083 D1084 F1085 F1086 R1087 A1088 T1092 N1093 L1094 I1095 S1096 D1097 F1098 L1099 L1100 L1101 L1102 S1105 Q1106 Q1107 W1108 Q1109 V1110 F1111 S1112 T1116
GLU GLU TRP GLN ARG MET ALA GLY ILE ASN THR ASP HIS LEU LEU GLU PRO LEU ARG CYS GLY E1136 P1137 N1138 P1139 F1143 C1146 R1147 S1148 Y1149 L1150 D1151 M1152 L1153 K1154 V1155 A1156 V1157 Y1160 L1161 F1162 W1163 L1164 V1165 L1166 V1167 V1168 V1169 F1170 V1171 A1172 R1176 I1177 S1178 I1179 F1180 G1181 L1182
G1183 Y1184 L1185 L1186 A1187 C1188 L1191 L1192 L1193 F1194 G1195 T1196 Q1200 R1204 A1205 Q1206 L1207 V1208 L1209 W1210 D1211 C1212 L1213 I1214 L1215 Y1216 N1217 V1218 T1219 V1220 I1221 I1222 S1223 K1224 N1225 M1226 L1227 S1228 L1229 C1232 V1233 F1234 V1235 E1236 Q1237 M1238 N1241 F1242 C1243 I1246 L1251 V1252 C1253
T1254 V1255 LYS GLY TYR TYR ASP PRO LYS GLU MET MET THR ARG ASP ARG ASP CYS LEU LEU PRO VAL GLU GLU A1278 G1279 I1280 I1281 W1282 D1283 S1284 I1285 C1286 F1287 F1288 F1289 L1290 L1291 L1292 R1295 I1296 F1297 L1298 S1299 H1300 Y1301 H1304 R1318 Y1323 N1324 A1325 A1326 N1327 L1328 F1333
H1334 R1335 Q1336 I1337 K1340 M1349 K1350 R1351 I1352 R1353 A1354 K1355 Q1356 E1357 Q1361 S1365 ARG GLY GLN LEU GLN SER LYS ASP PRO GLN ASP PRO SER GLN GLU PRO GLY PRO ASP SER PRO GLY GLY SER SER PRO PRO ARG ARG GLN TRP TRP ARG PRO TRP LEU ASP HIS ALA T1405
V1406 T1407 H1408 S1409 F1415 E1416 S1417 D1418 SER GLU GLU GLU GLU GLU ALA LEU PRO GLU ASP PRO ARG PRO ALA ALA GLN SER ALA PHE GLN MET ALA TYR GLN ALA TRP VAL THR ASN ALA GLN THR VAL LEU ARG GLN ARG ARG GLU ARG GLN GLU ARG ALA ARG GLN PRO TRP LEU ASP ARG ALA GLU GLN LEU ALA
SER GLY GLY ASP LEU ASN PRO ASP VAL GLU PRO VAL ASP VAL PRO GLU ASP GLU MET ALA GLY ARG SER HIS MET MET GLN ARG VAL LEU SER THR MET GLN F1504 L1505 W1506 V1507 L1508 G1509 Q1510 A1511 D1514 R1518 R1521 R1528 D1532 Q1543 E1544 L1545 L1546 R1547 VAL GLY
GLU VAL R1552 R1553 G1554 V1555 Q1558 L1559 TYR VAL GLY GLU ASP GLU ALA THR LEU SER GLY PRO VAL GLU THR ARG ASP GLY PRO SER THR ALA SER SER GLY LEU GLY ALA GLU GLU PRO LEU SER SER MET THR ASP ASP THR SER SER PRO LEU SER THR GLY TYR ASN THR ARG SER
GLY SER GLU GLU ILE VAL THR ASP ALA GLY ASP LEU GLN ALA GLY THR SER LEU HIS GLY SER GLN GLU LEU LEU ALA ASN ALA ARG THR MET ARG THR ALA SER E1647 D1651 E1658 Q1668 Q1669 T1672 L1675 L1676 Y1680 Q1681 A1684 A1685 H1686 S1687 L1690 C1691

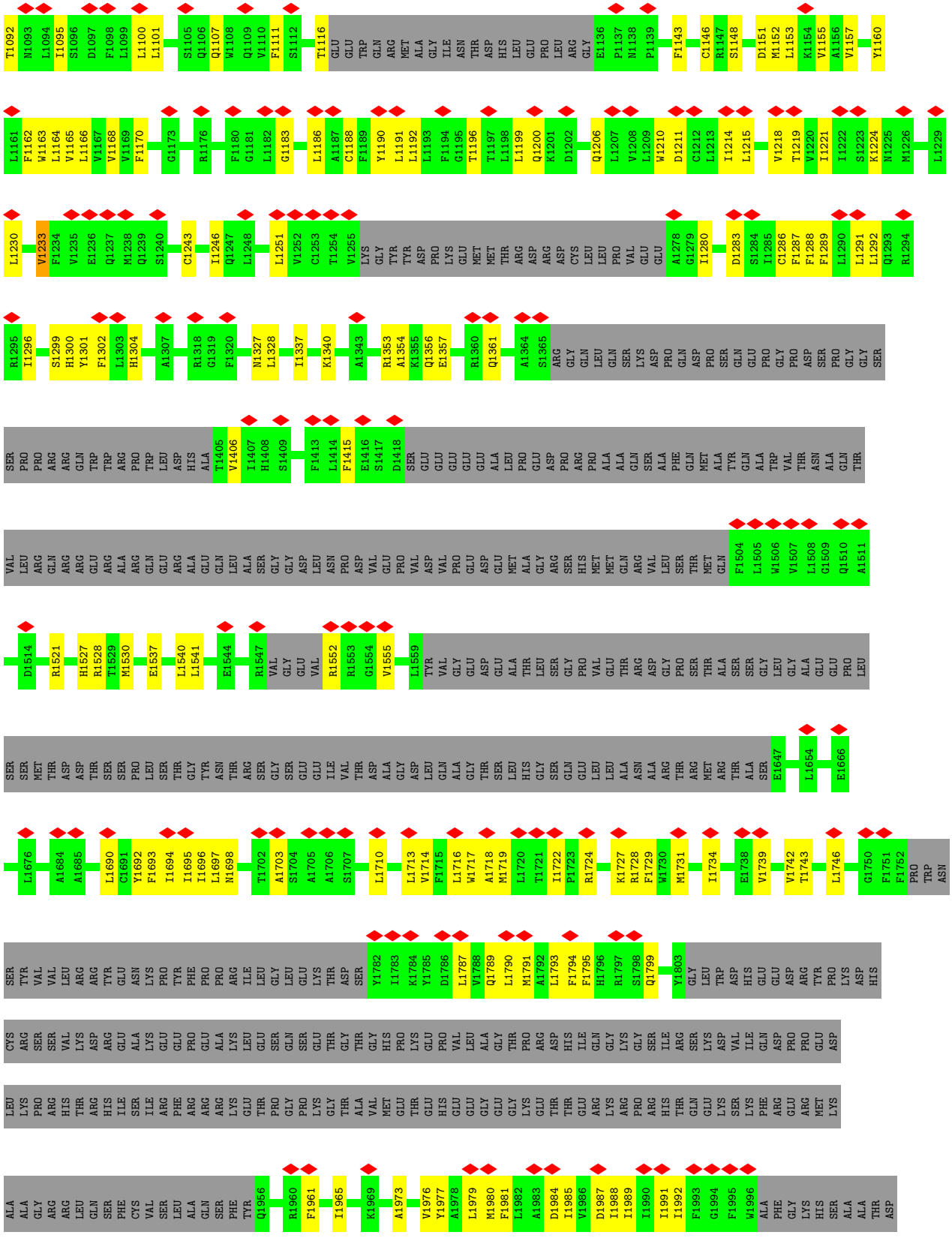


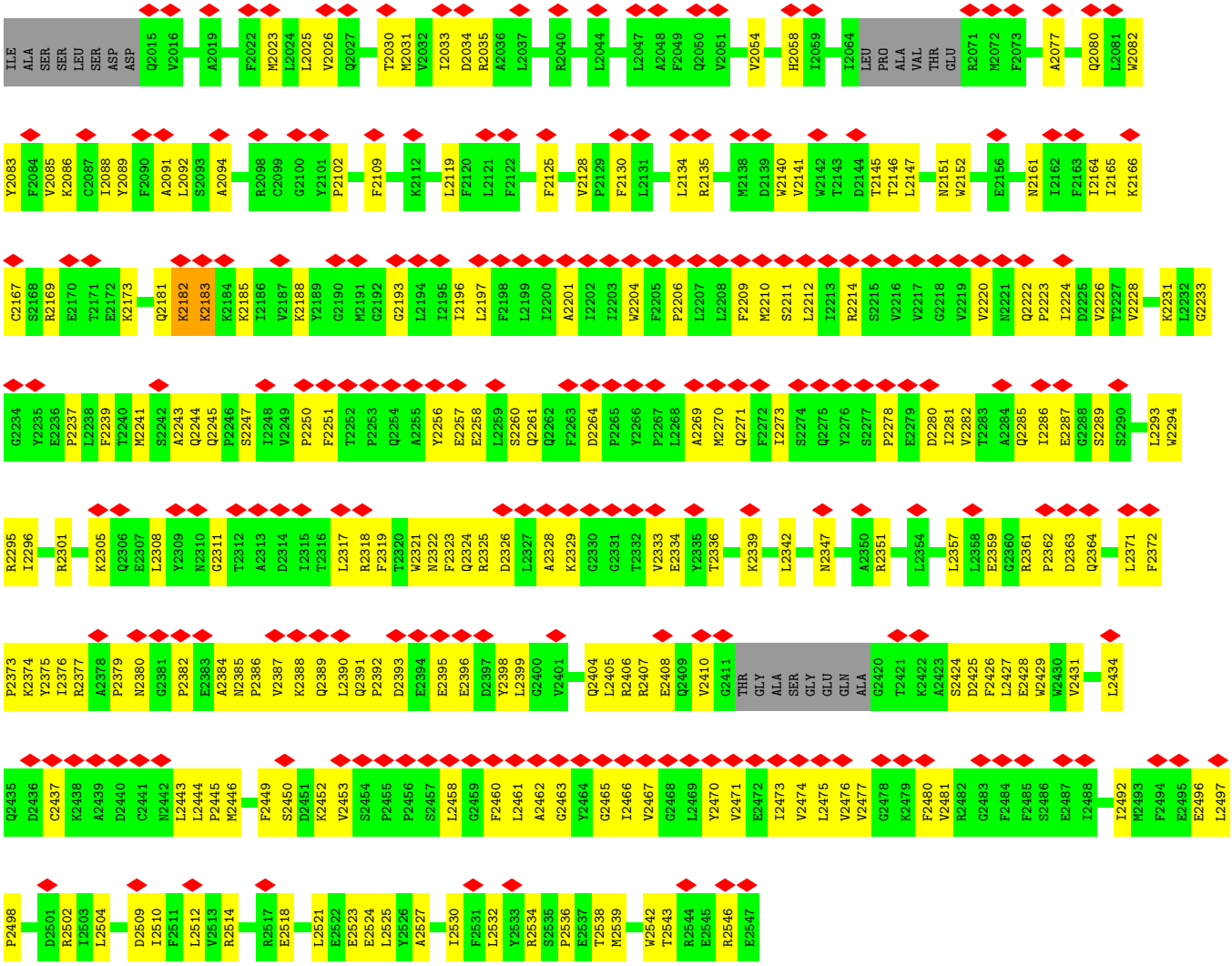
• Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain A:


19%
38%
15%
47%

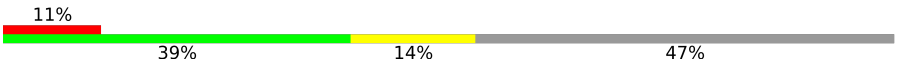

MET GLU PRO HIS VAL LEU GLY ALA GLY LEU TYR TRP LEU LEU LEU PRO CYS THR LEU LEU ALA ALA SER LEU LEU ARG PHE ASN ALA LEU SER LEU VAL TYR LEU LEU PHE LEU LEU PRO TRP LEU PRO GLY PRO SER ARG HIS SER ILE PRO GLY HIS THR GLY ARG LEU LEU
ARG ALA LEU LEU CYS LEU SER LEU LEU PHE LEU VAL ALA HIS LEU ALA PHE GLN ILE CYS LEU HIS THR VAL PRO HIS LEU ASP GLN PHE LEU GLY GLN ASN GLY SER LEU TRP VAL LYS VAL SER GLN HIS ILE GLY VAL THR ARG LEU ASP LEU LYS ASP ILE PHE ASN THR THR ARG
LEU VAL ALA PRO ASP LEU GLY VAL LEU LEU ALA SER SER LEU CYS LEU GLY LEU CYS GLY ARG LEU THR ARG LYS ALA GLY GLN SER ARG ARG THR GLN GLU LEU GLN ASP ASP ASP ASP ASP ASP ASP ASP ASP GLU ASP ILE ASP ALA ALA PRO ALA VAL GLY LEU LYS GLY ALA
PRO ALA LEU ALA THR LYS ARG ARG LEU TRP LEU LEU ALA SER ARG PHE ARG VAL THR ALA HIS TRP LEU LEU MET THR SER GLY ARG THR LEU VAL ILE VAL LEU LEU ALA LEU ALA GLY ILE ALA HIS PRO SER ALA PHE SER SER ILE TYR LEU VAL PHE LEU ALA ILE CYS THR TRP
TRP SER CYS HIS PHE PRO LEU SER PRO LEU GLY PHE ASN THR LEU CYS VAL MET VAL SER CYS PHE GLY ALA GLY HIS LEU ILE CYS LEU TYR CYS TYR GLN THR PRO PHE ILE GLN ASP MET LEU PRO PRO SER GLY ASN ILE TRP ALA ARG LEU PHE GLY LEU LYS ASN PHE VAL ASP LEU
PRO ASN TYR SER SER PRO ASN ALA LEU VAL LEU ASN THR LYS HIS ALA TRP PRO ILE TYR VAL SER PRO GLY ILE LEU LEU LEU LEU TYR TYR THR ALA THR SER LEU LEU LYS LEU HIS LYS SER CYS PRO PRO SER GLU LEU ARG LYS GLU THR PRO ARG GLU ASP GLU GLU LEU
GLU LEU ASP HIS LEU GLU PRO GLN ALA ARG ASP ALA THR GLN GLY GLU MET PRO MET THR THR GLU PRO ASP LEU ASP ASN CYS THR VAL HIS VAL LEU THR SER GLN LYS LEU SER PRO VAL ARG GLN ARG PRO VAL ARG PRO ARG LEU ALA GLU LEU LYS GLU MET SER PRO LEU HIS
GLY LEU GLY HIS LEU ILE MET ASP GLN SER TYR VAL CYS ALA LEU ILE ALA MET MET VAL TRP SER ILE MET TYR HIS SER TRP LEU THR PHE VAL LEU LEU LEU TRP ALA CYS LEU ILE TRP THR VAL ARG GLN ARG PRO VAL ARG ARG SER HIS GLN LEU ALA MET LEU LEU TYR
GLY LEU THR LEU CYS CYS LEU ARG TYR VAL TRP ALA MET GLU GLU PRO GLU LEU PRO THR THR LEU GLY PRO VAL SER LEU HIS GLN LEU GLY LEU GLU LEU THR ARG TYR PRO CYS LEU ASP LEU GLY ALA MET LEU LEU TYR LEU LEU LEU THR PHE TRP LEU LEU LEU ARG GLN PHE VAL
LYS GLU LYS LEU LEU LYS LYS GLN LYS VAL PRO ALA ALA LEU LEU GLU VAL THR VAL ALA ASP THR GLU PRO THR GLN THR GLN THR LEU LEU ARG SER LEU GLY E576 L577 V578 T579 G580 I581 K584 Y588 V589 C590 A591 I595 F599 ALA GLY ARG L603 V604 V605 Y606
V609 Y610 L616 C617 L618 T619 L620 R629 K630 I631 L632 R633 V634 W637 L638 A641 M644 L645 V646 L647 I648 A649 V650 TYR THR PHE GLN PHE GLN ASP PHE PRO THR TYR TRP ARG ASN LEU THR GLY PHE THR ASP GLU GLN LEU GLY ASP LEU LEU GLY LEU GLU GLN PHE SER
VAL S684 E685 L686 F687 S688 S689 I690 L691 I692 P693 G694 F695 F696 C700 L704 H705 Y706 Q713 L717 E718 HIS VAL PRO PRO PRO GLY THR ARG HIS PRO ARG TRP ALA HIS ARG GLN ASP ALA VAL SER GLU ALA PRO LEU LEU GLU HIS GLN GLU GLU GLU VAL PHE ARG
GLU ASP GLY GLN SER MET ASP GLY PRO HIS GLN ALA THR GLN VAL PRO GLU GLY THR ALA SER LYS TRP GLY LEU VAL ALA ASP ARG LEU L784 D785 L786 A787 A788 S789 F790 S791 A792 T795 R796 V799 F800 V801 R802 R803 L804 L807 F810 L815 L822 V827 M828
N829 L830 L831 L832 V833 V834 A839 L840 R844 F845 M848 L852 W856 Q868 L869 K870 I871 P874 HIS GLU TYR SER SER ASN CYS THR GLU PRO PHE PRO ASN ASN THR ASN LEU GLN PRO LEU GLU ILE ASN GLN SER LEU LEU TYR ARG GLY PRO VAL ASP PRO ALA
N910 W911 F912 G913 N920 Y923 I924 H927 A938 R943 R948 R949 Q950 H951 GLN GLN ALA PRO LEU PRO ALA GLN ALA VAL CYS ALA ASP G965 T966 R967 Q968 D971 C977 Y980 F981 F984 Y987 G990 L996 M997 A998 R1005 M1009 L1012
W1016 L1017 V1018 A1019 I1020 L1021 T1022 R1023 R1024 E1027 A1028 I1029 A1030 Y1036 C1037 L1038 F1039 L1040 T1041 L1042 Y1046 L1050 C1051 L1052 GLY MET P1055 P1056 A1057 L1058 C1059 I1060 D1061 W1064 R1065 W1066 SER LYS A1069 I1070 P1071 M1072 I1077 Y1081 L1082 P1083 D1084 F1085 F1086 R1087 A1088

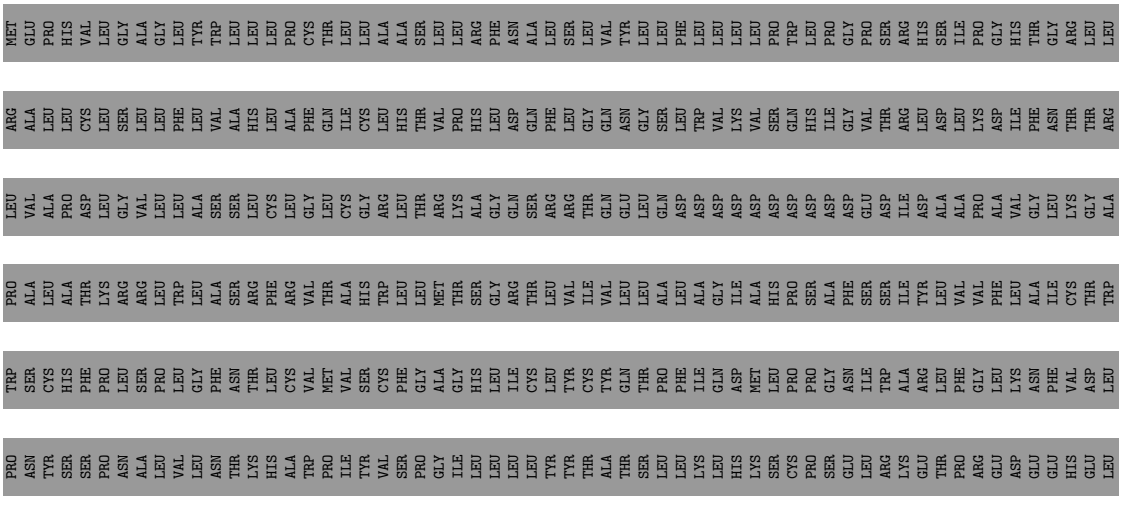

T1092 N1093 L1094 I1095 S1096 D1097 F1098 L1099 L1100 L1101 S1105 Q1106 Q1107 W1108 Q1109 V1110 F1111 S1112 T1116 GLU GLU TRP GLN ARG MET ALA GLY ILE ASN THR ASP HIS LEU GLU PRO LEU ARG GLY E1136 P1137 N1138 P1139 F1143 C1146 R1147 S1148 D1151 M1152 L1153 K1154 V1155 A1156 V1157 Y1160
L1161 F1162 W1163 L1164 V1165 L1166 V1167 V1168 V1169 F1170 G1173 R1176 F1180 G1181 L1182 G1183 L1186 A1187 C1188 F1189 Y1190 L1191 L1192 L1193 F1194 G1195 T1196 T1197 L1198 L1199 Q1200 K1201 D1202 Q1206 L1207 V1208 L1209 W1210 D1211 C1212 L1213 I1214 L1215 V1218 T1219 V1220 I1221 I1222 S1223 K1224 N1225 M1226 L1229
L1230 V1233 F1234 V1235 E1236 Q1237 M1238 Q1239 S1240 C1243 I1246 Q1247 L1248 L1251 V1252 C1253 T1254 V1255 LYS GLY TYR TYR ASP PRO LYS GLU MET MET THR ARG ASP ARG ASP CYS LEU LEU PRO VAL GLU GLU A1278 G1279 I1280 D1283 S1284 I1285 C1286 F1287 F1288 F1289 L1290 L1291 L1292 Q1293 R1294
R1295 I1296 S1299 H1300 Y1301 F1302 L1303 H1304 A1307 R1318 G1319 F1320 N1327 L1328 I1337 K1340 A1343 R1353 A1354 K1355 Q1356 E1357 R1360 Q1361 A1364 S1365 ARG GLY GLN LEU GLN SER LYS ASP PRO GLN ASP PRO SER GLN GLU PRO GLY PRO ASP SER PRO GLY GLY SER
SER PRO PRO ARG ARG GLN TRP TRP ARG PRO TRP LEU ASP HIS ALA T1405 V1406 I1407 H1408 S1409 F1413 L1414 F1415 E1416 S1417 D1418 SER GLU GLU GLU GLU GLU ALA LEU PRO GLU ASP PRO ARG PRO ALA ALA GLN SER ALA PHE GLN MET ALA TYR GLN ALA TRP VAL THR ASN ALA GLN THR
VAL LEU ARG GLN ARG ARG GLU ARG ALA ARG GLN GLU GLN ARG ALA GLU GLN LEU LEU ALA SER GLY GLY ASP LEU ASN PRO ASP SER VAL GLU PRO VAL ASP VAL PRO GLU ASP GLU MET ALA GLY ARG SER HIS MET MET GLN ARG VAL LEU SER THR MET GLN F1504 L1505 W1506 V1507 L1508 G1509 Q1510 A1511
D1514 R1521 H1527 R1528 T1529 M1530 E1537 L1540 L1541 E1544 R1547 VAL GLY GLU VAL R1552 R1553 G1554 V1555 L1559 TYR VAL GLY GLU ASP GLU ALA THR LEU SER GLY PRO VAL GLU THR ARG ASP GLY PRO SER THR ALA SER SER GLY LEU GLY ALA GLU GLU PRO LEU
SER SER MET THR ASP ASP THR SER SER PRO LEU SER THR GLY TYR ASN THR ARG SER GLY SER GLU GLU ILE VAL THR ASP ALA GLY ASP LEU GLN ALA GLY THR SER LEU HIS GLY SER GLN GLU LEU LEU ALA ASN ALA ARG THR ARG MET ARG THR ALA SER E1647 L1654 E1666
L1676 A1684 A1685 L1690 C1691 Y1692 F1693 I1694 I1695 I1696 I1697 N1698 T1702 A1703 S1704 A1705 A1706 S1707 L1710 L1713 V1714 F1715 L1716 W1717 A1718 M1719 L1720 T1721 I1722 P1723 R1724 K1727 R1728 F1729 W1730 M1731 I1734 E1738 V1739 V1742 T1743 L1746 G1750 F1751 F1752 PRO TRP ASN
SER TYR VAL VAL LEU ARG ARG TYR GLU ASN LYS PRO TYR PHE PRO PRO ARG ILE LEU GLY LEU GLU LYS THR ASP SER Y1782 I1783 K1784 Y1785 D1786 L1787 V1788 Q1789 L1790 M1791 A1792 L1793 F1794 F1795 H1796 R1797 S1798 Q1799 Y1803 GLY LEU TRP ASP HIS GLU GLU ASP ARG TYR PRO LYS ASP HIS
CYS ARG SER SER VAL LYS ASP ARG GLU ALA LYS GLU GLU PRO GLU ALA LYS LEU GLU SER GLN SER GLU THR GLY THR GLY HIS PRO LYS GLU PRO VAL LEU ALA GLY THR PRO ARG ASP HIS ILE ARG GLN GLY LYS GLY SER ILE ARG SER LYS ASP VAL ILE GLN ASP PRO PRO GLU ASP
LEU LYS PRO ARG HIS THR ARG HIS ILE SER ILE ARG PHE ARG ARG ARG LYS GLU THR PRO GLY PRO LYS GLY THR ALA VAL MET GLU THR GLU HIS GLU GLU GLY GLU GLY LYS GLU THR THR GLU ARG LYS ARG PRO ARG HIS THR GLN GLU LYS SER LYS PHE ARG GLU ARG MET LYS
ALA ALA GLY ARG ARG LEU GLN SER PHE CYS VAL SER LEU ALA GLN SER PHE TYR Q1956 R1960 F1961 I1965 K1969 A1973 V1976 Y1977 A1978 L1979 M1980 F1981 L1982 A1983 D1984 I1985 V1986 D1987 I1988 I1989 I1990 I1991 I1992 F1993 G1994 F1995 W1996 ALA PHE GLY LYS HIS SER ALA ALA THR ASP

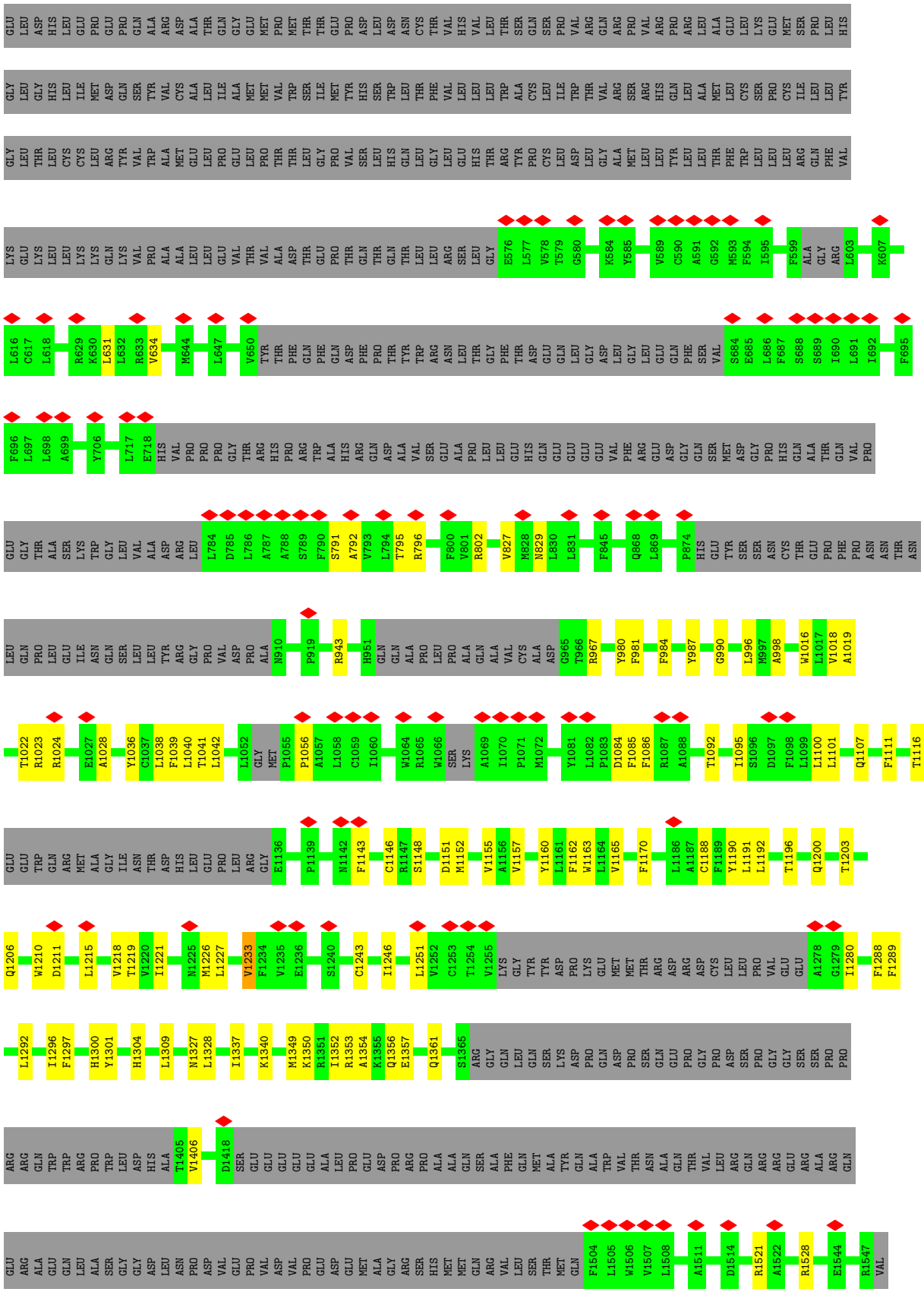


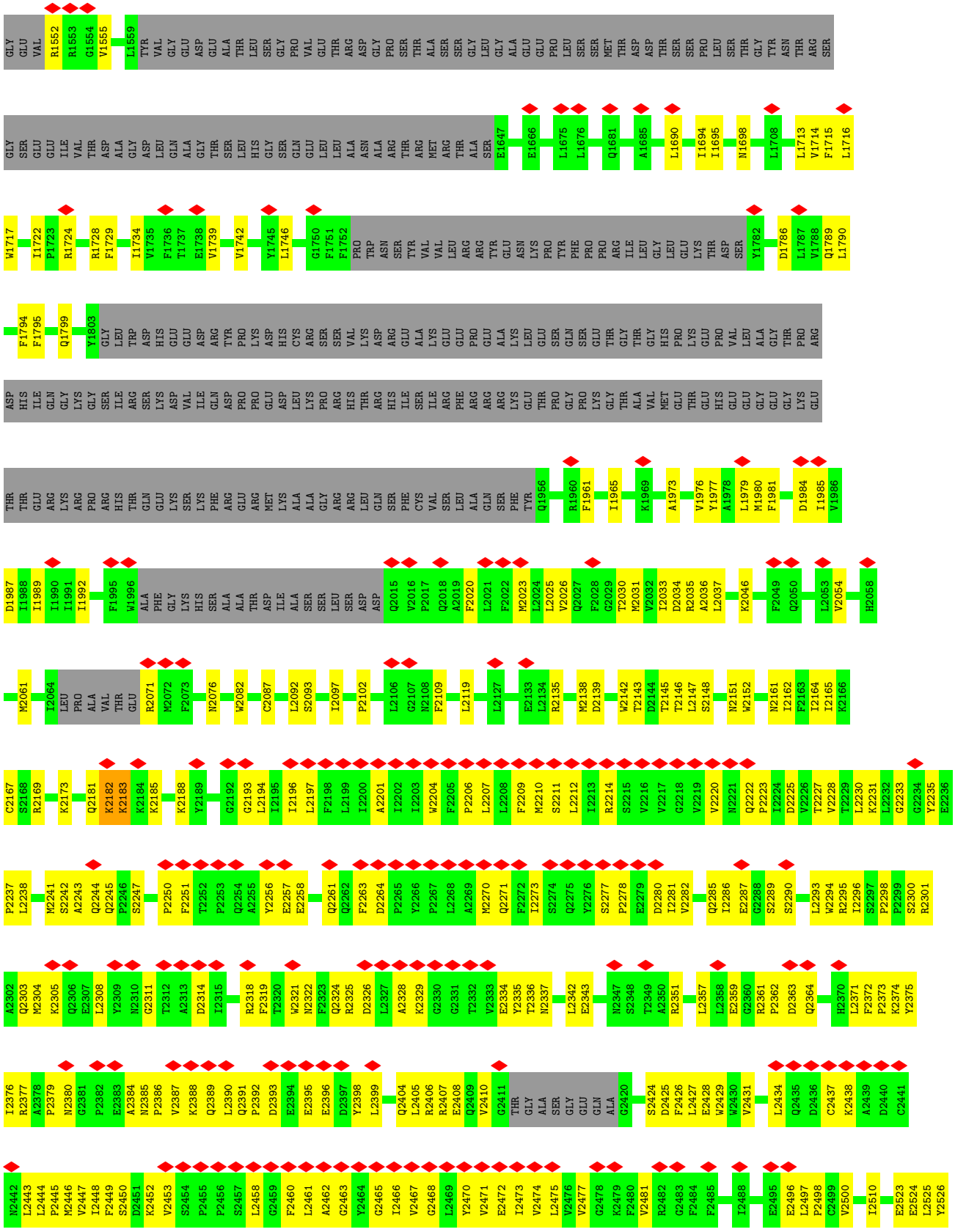
• Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain D:








GLY GLU VAL R1552 R1553 G1554 V1555 L1559 TYR VAL GLY GLU ASP GLU ALA THR LEU SER GLY PRO VAL GLU THR ARG ASP GLY PRO SER THR ALA SER SER GLY LEU GLY ALA GLU GLU PRO LEU SER SER MET THR ASP ASP THR SER SER PRO LEU SER THR GLY TYR ASN THR ARG SER
GLY SER GLU GLU ILE VAL THR ASP ALA GLY ASP LEU GLN ALA ALA GLY THR SER LEU HIS GLY SER GLN GLU LEU LEU ALA ASN ALA ARG THR ARG MET ARG THR ALA SER E1647 E1666 L1675 L1676 Q1681 A1685 L1690 I1694 I1695 N1698 L1708 L1713 V1714 F1715 L1716
W1717 I1722 P1723 R1724 R1728 F1729 I1734 V1735 F1736 T1737 E1738 V1739 V1742 Y1745 L1746 G1750 F1751 F1752 PRO TRP ASN SER TYR VAL VAL LEU ARG ARG TYR GLU ASN LYS PRO TYR PHE PRO PRO ARG ILE LEU GLY LEU GLU LYS THR ASP SER Y1762 D1786 L1787 V1788 Q1789 L1790
F1794 F1795 Q1799 Y1803 GLY LEU TRP ASP HIS GLU GLU ASP ARG TYR PRO LYS ASP HIS CYS ARG SER SER VAL LYS ASP ARG GLU ALA LYS LYS LEU GLU SER GLN SER GLU THR GLY THR GLY HIS PRO LYS GLU PRO VAL LEU ALA GLY THR PRO ARG
ASP HIS ILE GLN GLY LYS GLY SER ILE ARG SER LYS ASP VAL ILE GLN ASP PRO PRO GLU GLU ASP LEU LYS PRO ARG HIS THR ARG HIS ILE SER ILE ARG PHE ARG ARG ARG LYS GLU THR PRO GLY PRO LYS GLY THR ALA VAL MET GLU GLU THR GLU HIS GLU GLU GLY GLU GLY LYS GLU
THR THR GLU ARG LYS ARG PRO ARG HIS THR GLN GLU LYS SER LYS PHE ARG GLU ARG MET LYS ALA ALA GLY ARG ARG LEU GLN SER PHE CYS VAL SER LEU ALA GLN SER PHE TYR Q1956 R1960 F1961 I1965 K1969 A1973 V1976 Y1977 A1978 L1979 M1980 F1981 D1984 I1985 V1986
D1987 I1988 I1989 I1990 I1991 I1992 F1995 W1996 ALA PHE GLY LYS HIS SER ALA ALA THR ASP ILE ALA SER SER LEU SER ASP ASP Q2015 V2016 P2017 Q2018 A2019 P2020 L2021 P2022 M2023 L2024 L2025 V2026 Q2027 P2028 G2029 T2030 M2031 V2032 I2033 D2034 R2035 A2036 L2037 K2046 F2049 Q2050 L2053 V2054 H2058
M2061 I2064 LEU PRO ALA VAL THR GLU R2071 M2072 F2073 N2076 W2082 C2087 L2092 S2093 I2097 P2102 L2106 G2107 N2108 F2109 L2119 L2127 E2133 L2134 R2135 M2138 D2139 W2142 T2143 D2144 T2145 T2146 L2147 S2148 N2151 W2152 N2161 I2162 F2163 I2164 I2165 K2166
C2167 S2168 R2169 K2173 Q2181 K2182 K2183 K2184 K2185 K2188 Y2189 G2192 G2193 L2194 I2195 I2196 L2197 F2198 L2199 I2200 A2201 I2202 I2203 W2204 F2205 P2206 L2207 L2208 F2209 M2210 S2211 L2212 I2213 R2214 S2215 V2216 V2217 G2218 V2219 V2220 N2221 Q2222 P2223 I2224 D2225 V2226 T2227 V2228 T2229 L2230 K2231 L2232 G2233 G2234 Y2235 E2236
P2237 L2238 M2241 S2242 A2243 Q2244 Q2245 P2246 S2247 P2250 F2251 T2252 P2253 Q2254 A2255 Y2256 E2257 E2258 Q2261 Q2262 F2263 D2264 P2265 Y2266 P2267 L2268 A2269 M2270 Q2271 F2272 I2273 S2274 Q2275 Y2276 S2277 P2278 E2279 D2280 I2281 V2282 Q2285 I2286 E2287 G2288 S2289 S2290 L2293 W2294 R2295 I2296 S2297 P2298 P2299 S2300 R2301
A2302 Q2303 M2304 K2305 Q2306 E2307 L2308 Y2309 N2310 G2311 T2312 A2313 D2314 I2315 R2318 F2319 T2320 W2321 N2322 F2323 Q2324 R2325 D2326 L2327 A2328 K2329 G2330 G2331 T2332 V2333 E2334 Y2335 T2336 N2337 L2342 E2343 N2347 S2348 T2349 A2350 R2351 L2357 L2358 E2359 G2360 R2361 P2362 D2363 Q2364 H2370 L2371 F2372 P2373 K2374 Y2375
I2376 R2377 A2378 P2379 N2380 G2381 P2382 E2383 A2384 N2385 P2386 V2387 K2388 Q2389 L2390 Q2391 P2392 D2393 E2394 E2395 E2396 D2397 Y2398 L2399 Q2404 L2405 R2406 R2407 E2408 Q2409 V2410 G2411 THR GLY ALA SER GLY GLU GLN ALA G2420 S2424 D2425 F2426 L2427 E2428 W2429 W2430 V2431 L2434 Q2435 D2436 C2437 K2438 A2439 D2440 C2441
N2442 L2443 L2444 P2445 M2446 V2447 I2448 F2449 S2450 D2451 K2452 V2453 S2454 P2455 P2456 S2457 L2458 G2459 F2460 L2461 A2462 G2463 Y2464 G2465 I2466 V2467 G2468 L2469 Y2470 V2471 E2472 I2473 V2474 L2475 V2476 V2477 G2478 K2479 F2480 V2481 R2482 G2483 F2484 F2485 I2488 E2495 E2496 L2497 P2498 C2499 V2500 I2510 E2523 E2524 L2525 Y2526


L2529
I2530
Y2533
R2534
S2535
T2538
T2543
R2546
E2547

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	488709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	22.183	Depositor
Minimum map value	-9.040	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	8.23	Depositor
Map size (Å)	404.02722, 404.02722, 404.02722	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLX, P5S, PEE

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	0.20	0/9986	0.45	1/13618 (0.0%)
1	C	0.20	0/9990	0.46	1/13625 (0.0%)
1	D	0.19	0/9995	0.43	1/13630 (0.0%)
All	All	0.20	0/29971	0.45	3/40873 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1233	VAL	N-CA-C	-6.31	105.19	111.88
1	A	1233	VAL	N-CA-C	-6.23	105.28	111.88
1	D	1233	VAL	N-CA-C	-6.17	105.34	111.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9802	0	8926	380	0
1	C	9804	0	8928	414	0
1	D	9810	0	8942	346	0
2	A	104	0	176	14	0
2	C	104	0	176	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	104	0	176	14	0
3	A	51	0	82	60	0
3	C	51	0	82	72	0
3	D	51	0	82	64	0
4	A	54	0	80	24	0
4	C	54	0	80	25	0
4	D	54	0	80	17	0
All	All	30043	0	27810	1179	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 20.

All (1179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2109:PHE:HB2	3:D:2603:PEE:C5	1.55	1.34
1:A:1981:PHE:CE2	3:A:2603:PEE:H17	1.66	1.30
1:D:1981:PHE:CE2	3:D:2603:PEE:H17	1.77	1.17
1:C:1981:PHE:CD2	3:C:2603:PEE:H17	1.78	1.17
1:A:1981:PHE:CD2	3:A:2603:PEE:H13	1.82	1.13
1:A:1981:PHE:CD2	3:A:2603:PEE:H17	1.83	1.13
1:A:1989:ILE:HD11	3:A:2603:PEE:H37	1.19	1.12
1:A:1981:PHE:CE2	3:A:2603:PEE:C13	2.33	1.12
1:A:1153:LEU:CD1	4:A:2604:P5S:H49	1.80	1.11
1:D:1981:PHE:CD2	3:D:2603:PEE:H17	1.85	1.11
1:C:1989:ILE:HD11	3:C:2603:PEE:H37	1.20	1.11
1:D:1989:ILE:HD11	3:D:2603:PEE:H37	1.17	1.10
1:D:1989:ILE:CD1	3:D:2603:PEE:H37	1.81	1.10
1:C:1153:LEU:CD1	4:C:2604:P5S:H49	1.81	1.09
1:C:1981:PHE:CE2	3:C:2603:PEE:H17	1.87	1.09
1:A:1989:ILE:HD11	3:A:2603:PEE:C23	1.82	1.09
1:C:1989:ILE:HD11	3:C:2603:PEE:C23	1.83	1.08
1:A:1989:ILE:CD1	3:A:2603:PEE:H37	1.85	1.07
1:A:981:PHE:HZ	4:A:2604:P5S:H41A	1.18	1.06
1:D:1981:PHE:CD2	3:D:2603:PEE:H13	1.91	1.06
1:A:1153:LEU:HD12	4:A:2604:P5S:H46	1.33	1.05
1:A:1153:LEU:HD11	4:A:2604:P5S:H49	1.34	1.05
1:C:1989:ILE:CD1	3:C:2603:PEE:H37	1.85	1.05
1:D:2109:PHE:HB2	3:D:2603:PEE:H12	1.07	1.05
1:C:981:PHE:HZ	4:C:2604:P5S:H41A	1.19	1.04
1:A:1981:PHE:HE2	3:A:2603:PEE:C13	1.66	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1989:ILE:HD11	3:D:2603:PEE:C23	1.86	1.04
1:D:981:PHE:HZ	4:D:2604:P5S:H41A	1.20	1.04
1:C:1153:LEU:HD12	4:C:2604:P5S:H46	1.43	1.00
1:C:2109:PHE:CB	3:C:2603:PEE:H12	1.92	1.00
1:C:1153:LEU:HD11	4:C:2604:P5S:H49	1.41	1.00
3:C:2603:PEE:H40	3:C:2603:PEE:H81	1.44	0.99
1:A:1989:ILE:CD1	3:A:2603:PEE:C23	2.41	0.99
1:D:1981:PHE:CE2	3:D:2603:PEE:C13	2.44	0.99
1:D:2109:PHE:HB2	3:D:2603:PEE:H11	1.44	0.99
1:C:1989:ILE:CD1	3:C:2603:PEE:C23	2.40	0.99
1:D:1989:ILE:CD1	3:D:2603:PEE:C23	2.41	0.98
3:A:2603:PEE:H40	3:A:2603:PEE:H81	1.44	0.97
3:D:2603:PEE:H68	3:D:2603:PEE:C46	1.95	0.97
1:A:1981:PHE:HD2	3:A:2603:PEE:H13	1.27	0.97
1:D:2109:PHE:CB	3:D:2603:PEE:H12	1.95	0.96
3:C:2603:PEE:C46	3:C:2603:PEE:H68	1.95	0.96
3:D:2603:PEE:H40	3:D:2603:PEE:H81	1.44	0.96
3:A:2603:PEE:H68	3:A:2603:PEE:C46	1.95	0.95
1:C:1981:PHE:CD2	3:C:2603:PEE:H13	2.01	0.95
1:C:1981:PHE:CE2	3:C:2603:PEE:C13	2.50	0.94
1:A:1230:LEU:HD22	1:A:1251:LEU:HD22	1.49	0.94
3:A:2603:PEE:H68	3:A:2603:PEE:H82	1.48	0.94
3:D:2603:PEE:H68	3:D:2603:PEE:H82	1.48	0.93
1:A:1719:MET:HE2	1:A:2094:ALA:HB3	1.50	0.93
1:C:2109:PHE:CB	3:C:2603:PEE:C5	2.47	0.92
1:A:1163:TRP:HB3	2:A:2602:PLX:H282	1.50	0.92
3:D:2603:PEE:C46	3:D:2603:PEE:H40	2.00	0.92
1:C:1163:TRP:HB3	2:C:2602:PLX:H282	1.49	0.92
3:C:2603:PEE:H68	3:C:2603:PEE:H82	1.48	0.91
3:C:2603:PEE:H40	3:C:2603:PEE:C46	2.00	0.91
3:A:2603:PEE:H40	3:A:2603:PEE:C46	2.00	0.91
3:D:2603:PEE:H40	3:D:2603:PEE:C47	2.01	0.91
1:D:1981:PHE:HD2	3:D:2603:PEE:H13	1.31	0.91
3:C:2603:PEE:H40	3:C:2603:PEE:C47	2.01	0.90
3:C:2603:PEE:H68	3:C:2603:PEE:C47	2.02	0.90
3:A:2603:PEE:H40	3:A:2603:PEE:C47	2.01	0.90
1:D:2109:PHE:CB	3:D:2603:PEE:C5	2.49	0.90
3:A:2603:PEE:H68	3:A:2603:PEE:C47	2.02	0.90
3:D:2603:PEE:H68	3:D:2603:PEE:C47	2.02	0.90
1:C:981:PHE:CZ	4:C:2604:P5S:H41A	2.07	0.89
1:D:1981:PHE:HE2	3:D:2603:PEE:C13	1.81	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1981:PHE:CD2	3:A:2603:PEE:C11	2.54	0.89
1:C:1981:PHE:HD2	3:C:2603:PEE:H17	1.36	0.88
1:A:981:PHE:CZ	4:A:2604:P5S:H41A	2.07	0.88
1:D:1163:TRP:HB3	2:D:2602:PLX:H282	1.54	0.88
1:C:1981:PHE:CD2	3:C:2603:PEE:C13	2.56	0.87
1:D:981:PHE:CZ	4:D:2604:P5S:H41A	2.08	0.87
1:D:1157:VAL:HG11	4:D:2604:P5S:H21	1.57	0.87
1:A:1981:PHE:CE2	3:A:2603:PEE:C12	2.58	0.86
1:C:1981:PHE:HD2	3:C:2603:PEE:H13	1.40	0.86
1:A:1153:LEU:HD12	4:A:2604:P5S:C46	2.05	0.86
3:A:2603:PEE:H40	3:A:2603:PEE:C45	2.06	0.85
3:A:2603:PEE:H74	3:A:2603:PEE:H41	1.59	0.85
1:D:1157:VAL:HG21	4:D:2604:P5S:H44A	1.59	0.85
3:D:2603:PEE:H40	3:D:2603:PEE:C45	2.06	0.84
3:C:2603:PEE:H40	3:C:2603:PEE:C45	2.06	0.84
3:C:2603:PEE:H74	3:C:2603:PEE:H41	1.59	0.83
1:D:2321:TRP:HH2	1:D:2373:PRO:HG2	1.43	0.83
3:D:2603:PEE:H41	3:D:2603:PEE:H74	1.59	0.83
3:D:2603:PEE:H81	3:D:2603:PEE:C24	2.09	0.83
1:C:2321:TRP:HH2	1:C:2373:PRO:HG2	1.40	0.82
3:C:2603:PEE:H81	3:C:2603:PEE:C24	2.09	0.82
3:A:2603:PEE:H81	3:A:2603:PEE:C24	2.09	0.82
1:D:1981:PHE:CD2	3:D:2603:PEE:C11	2.62	0.82
1:C:1695:ILE:HD11	1:C:1710:LEU:HG	1.60	0.81
1:D:1981:PHE:CD2	3:D:2603:PEE:C13	2.64	0.81
1:C:1981:PHE:HE2	3:C:2603:PEE:C13	1.94	0.80
1:A:2031:MET:HE2	3:A:2603:PEE:H56	1.62	0.80
1:C:1153:LEU:HD12	4:C:2604:P5S:H49	1.64	0.79
1:A:2321:TRP:HH2	1:A:2373:PRO:HG2	1.47	0.79
3:C:2603:PEE:H68	3:C:2603:PEE:C45	2.12	0.78
3:D:2603:PEE:H68	3:D:2603:PEE:C45	2.12	0.78
1:C:1153:LEU:HD12	4:C:2604:P5S:C46	2.13	0.78
1:A:1719:MET:HE1	1:A:2091:ALA:HA	1.65	0.78
1:A:2109:PHE:CB	3:A:2603:PEE:H12	2.14	0.78
1:A:1981:PHE:CD2	3:A:2603:PEE:C13	2.61	0.78
1:A:2325:ARG:HD2	1:A:2334:GLU:HA	1.63	0.78
1:C:2185:LYS:O	1:C:2188:LYS:HB3	1.84	0.77
1:D:1981:PHE:HE2	3:D:2603:PEE:H17	1.38	0.77
1:C:1981:PHE:CD2	3:C:2603:PEE:C11	2.67	0.77
1:A:1157:VAL:HG11	4:A:2604:P5S:H44A	1.66	0.77
1:C:2410:VAL:HG23	1:D:2425:ASP:HA	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1979:LEU:HB3	1:A:2092:LEU:HD13	1.67	0.77
1:D:2294:TRP:HB3	1:D:2429:TRP:HA	1.67	0.77
1:C:1989:ILE:CD1	3:C:2603:PEE:H38	2.13	0.76
1:A:1981:PHE:CE2	3:A:2603:PEE:H16	2.20	0.76
1:A:1989:ILE:CD1	3:A:2603:PEE:H38	2.14	0.76
1:C:1157:VAL:HG11	4:C:2604:P5S:H23	1.67	0.76
1:C:1981:PHE:CD2	3:C:2603:PEE:C12	2.69	0.76
1:C:2425:ASP:HA	1:A:2410:VAL:HG23	1.67	0.76
1:A:1153:LEU:HD12	4:A:2604:P5S:H49	1.69	0.75
1:A:2294:TRP:HB3	1:A:2429:TRP:HA	1.67	0.75
1:C:1166:LEU:HD13	1:C:1192:LEU:HD12	1.69	0.74
1:C:2498:PRO:HD3	1:A:2534:ARG:HH22	1.49	0.74
1:A:2404:GLN:HB3	1:A:2431:VAL:HB	1.69	0.74
1:C:2138:MET:HE1	3:C:2603:PEE:H49	1.69	0.74
1:D:2380:ASN:HD21	1:D:2453:VAL:HA	1.52	0.74
1:C:2294:TRP:HB3	1:C:2429:TRP:HA	1.67	0.74
1:A:1695:ILE:HD11	1:A:1710:LEU:HG	1.70	0.74
1:C:1165:VAL:HG23	1:C:1289:PHE:HB3	1.69	0.74
1:D:1981:PHE:CE2	3:D:2603:PEE:C12	2.70	0.74
3:A:2603:PEE:H68	3:A:2603:PEE:C45	2.12	0.73
1:C:2380:ASN:HD21	1:C:2453:VAL:HA	1.52	0.73
1:C:2534:ARG:HH22	1:D:2498:PRO:HD3	1.54	0.73
1:A:2498:PRO:HD3	1:D:2534:ARG:HH22	1.52	0.73
1:A:2425:ASP:HA	1:D:2410:VAL:HG23	1.69	0.73
1:C:1984:ASP:HB3	1:C:2031:MET:HE2	1.70	0.73
1:A:1981:PHE:CD2	3:A:2603:PEE:C12	2.72	0.73
1:C:1722:ILE:HG22	1:C:1724:ARG:H	1.54	0.72
1:D:1981:PHE:HD2	3:D:2603:PEE:H17	1.53	0.72
1:D:2404:GLN:HB3	1:D:2431:VAL:HB	1.70	0.72
1:A:2380:ASN:HD21	1:A:2453:VAL:HA	1.53	0.72
1:C:1157:VAL:CG1	4:C:2604:P5S:H23	2.19	0.72
1:D:2325:ARG:HD2	1:D:2334:GLU:HA	1.72	0.71
1:A:2434:LEU:HB2	1:A:2437:CYS:HB3	1.72	0.71
1:C:1734:ILE:HG12	1:C:1794:PHE:CE1	2.25	0.71
1:D:2185:LYS:O	1:D:2188:LYS:HB3	1.90	0.71
1:C:966:THR:HG21	1:C:969:ARG:HH21	1.54	0.71
1:A:2374:LYS:NZ	1:A:2445:PRO:O	2.23	0.71
1:D:1989:ILE:CD1	3:D:2603:PEE:H38	2.19	0.71
1:A:2031:MET:HE2	3:A:2603:PEE:C35	2.20	0.71
1:A:2147:LEU:HB3	1:A:2151:ASN:HB2	1.71	0.71
1:C:1982:LEU:HD11	3:C:2603:PEE:H24	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1716:LEU:HD21	1:C:2054:VAL:HG11	1.73	0.70
1:D:2393:ASP:HB3	1:D:2396:GLU:HB2	1.73	0.70
1:D:1722:ILE:HG22	1:D:1724:ARG:H	1.56	0.70
1:A:1981:PHE:CE1	3:A:2603:PEE:H8	2.26	0.70
1:A:2393:ASP:HB3	1:A:2396:GLU:HB2	1.73	0.70
1:D:1984:ASP:HB3	1:D:2031:MET:HE2	1.72	0.70
1:A:1981:PHE:HE2	3:A:2603:PEE:C14	2.05	0.70
1:D:2147:LEU:HB3	1:D:2151:ASN:HB2	1.74	0.70
1:C:2138:MET:CE	3:C:2603:PEE:H49	2.23	0.69
1:C:2325:ARG:HD2	1:C:2334:GLU:HA	1.74	0.69
3:D:2603:PEE:H82	3:D:2603:PEE:C41	2.23	0.69
1:C:2109:PHE:CB	3:C:2603:PEE:H11	2.23	0.69
1:D:2461:LEU:HG	1:D:2462:ALA:H	1.57	0.69
1:C:2223:PRO:HA	1:C:2325:ARG:HA	1.73	0.69
1:A:1722:ILE:HG22	1:A:1724:ARG:H	1.56	0.69
1:C:1981:PHE:CE2	3:C:2603:PEE:C12	2.76	0.69
1:C:2393:ASP:HB3	1:C:2396:GLU:HB2	1.73	0.69
1:D:1981:PHE:CD2	3:D:2603:PEE:C12	2.75	0.69
1:C:2241:MET:HE1	1:C:2291:GLY:HA2	1.74	0.68
1:D:2228:VAL:HG23	1:D:2321:TRP:CD1	2.28	0.68
1:A:1166:LEU:HD13	1:A:1192:LEU:HG	1.75	0.68
4:D:2604:P5S:H56A	4:D:2604:P5S:H34A	1.75	0.68
1:C:1217:ASN:O	1:C:1221:ILE:HG12	1.93	0.68
4:C:2604:P5S:H56A	4:C:2604:P5S:H34A	1.75	0.68
1:A:1734:ILE:HG12	1:A:1794:PHE:CE1	2.29	0.68
1:C:2256:TYR:HB2	1:C:2278:PRO:HB3	1.74	0.68
1:A:2206:PRO:HG2	1:A:2470:TYR:HE1	1.59	0.68
1:D:2375:TYR:H	1:D:2391:GLN:HE22	1.41	0.68
1:D:2223:PRO:HA	1:D:2325:ARG:HA	1.76	0.68
3:A:2603:PEE:H82	3:A:2603:PEE:C41	2.23	0.67
1:D:2228:VAL:HG23	1:D:2321:TRP:HD1	1.59	0.67
1:D:1981:PHE:CE2	3:D:2603:PEE:H16	2.30	0.67
1:D:2256:TYR:HB2	1:D:2278:PRO:HB3	1.76	0.67
1:D:2434:LEU:HB2	1:D:2437:CYS:HB3	1.75	0.67
1:A:2256:TYR:HB2	1:A:2278:PRO:HB3	1.75	0.67
4:A:2604:P5S:H34A	4:A:2604:P5S:H56A	1.75	0.67
1:C:2188:LYS:HG3	1:A:2140:TRP:CH2	2.30	0.67
1:D:1016:TRP:CD1	1:D:1039:PHE:HZ	2.13	0.67
1:C:1714:VAL:HG22	1:C:1729:PHE:HZ	1.59	0.67
1:D:1200:GLN:HE22	1:D:1309:LEU:HB3	1.59	0.67
1:D:1734:ILE:HG12	1:D:1794:PHE:CE1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1160:TYR:HE1	2:C:2602:PLX:O2	1.77	0.66
1:A:1165:VAL:HG23	1:A:1289:PHE:HB3	1.76	0.66
1:A:2228:VAL:HG23	1:A:2321:TRP:CD1	2.30	0.66
1:D:1165:VAL:HG23	1:D:1289:PHE:HB3	1.77	0.66
1:C:1987:ASP:OD2	1:C:2027:GLN:NE2	2.28	0.66
1:C:2199:LEU:HG	1:A:2134:LEU:HD21	1.76	0.66
1:A:2109:PHE:CB	3:A:2603:PEE:C5	2.74	0.66
1:A:1537:GLU:O	1:A:1541:LEU:HG	1.96	0.66
1:A:2461:LEU:HG	1:A:2462:ALA:H	1.60	0.66
1:A:1016:TRP:CD1	1:A:1039:PHE:HZ	2.13	0.66
1:A:2243:ALA:HB1	1:A:2247:SER:HB2	1.77	0.66
1:D:2243:ALA:HB1	1:D:2247:SER:HB2	1.75	0.66
1:C:2228:VAL:HG23	1:C:2321:TRP:CD1	2.30	0.66
1:D:1799:GLN:HA	2:D:2602:PLX:H1C1	1.78	0.66
1:D:2206:PRO:HG2	1:D:2470:TYR:HE1	1.61	0.66
1:C:2244:GLN:HB2	1:D:2318:ARG:CZ	2.26	0.65
1:C:1016:TRP:CD1	1:C:1039:PHE:HZ	2.15	0.65
1:D:996:LEU:HD11	1:D:1288:PHE:HB2	1.77	0.65
3:D:2603:PEE:H74	3:D:2603:PEE:C25	2.26	0.65
1:A:2228:VAL:HG23	1:A:2321:TRP:HD1	1.62	0.65
1:D:1157:VAL:CG1	4:D:2604:P5S:H21	2.27	0.65
1:C:1728:ARG:CB	2:C:2601:PLX:O7	2.45	0.65
1:C:2228:VAL:HG23	1:C:2321:TRP:HD1	1.61	0.65
1:C:2250:PRO:HA	1:C:2282:VAL:HG12	1.79	0.65
1:A:2223:PRO:HA	1:A:2325:ARG:HA	1.77	0.65
1:C:1163:TRP:CB	2:C:2602:PLX:H282	2.26	0.64
1:A:1799:GLN:HA	2:A:2602:PLX:H1C1	1.79	0.64
3:C:2603:PEE:H82	3:C:2603:PEE:C41	2.23	0.64
1:C:2135:ARG:CZ	3:C:2603:PEE:O1P	2.45	0.64
3:C:2603:PEE:H74	3:C:2603:PEE:C25	2.26	0.64
1:C:1981:PHE:HE2	3:C:2603:PEE:C14	2.11	0.64
1:C:2227:THR:HG23	1:C:2324:GLN:HE22	1.63	0.64
3:A:2603:PEE:H74	3:A:2603:PEE:C25	2.26	0.64
1:C:1981:PHE:CE2	3:C:2603:PEE:H16	2.32	0.64
1:C:1982:LEU:CD1	3:C:2603:PEE:H24	2.27	0.64
1:C:2434:LEU:HB2	1:C:2437:CYS:HB3	1.80	0.64
1:D:2387:VAL:HG12	1:D:2390:LEU:H	1.63	0.64
1:C:1989:ILE:HD11	3:C:2603:PEE:H33	1.79	0.63
2:C:2602:PLX:O1	2:C:2602:PLX:H1A2	1.98	0.63
1:C:2373:PRO:HB3	1:C:2398:TYR:CE1	2.33	0.63
1:A:1981:PHE:HD2	3:A:2603:PEE:H17	1.58	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2135:ARG:CZ	3:D:2603:PEE:O1P	2.45	0.63
1:C:1799:GLN:HA	2:C:2602:PLX:H1C1	1.80	0.63
1:C:2460:PHE:HD1	1:C:2464:TYR:HE2	1.45	0.63
1:A:1981:PHE:HE2	3:A:2603:PEE:H17	1.25	0.63
1:D:2387:VAL:HG11	1:D:2390:LEU:HD23	1.80	0.63
1:A:2181:GLN:C	1:A:2183:LYS:H	2.06	0.63
1:D:1989:ILE:HD12	3:D:2603:PEE:H38	1.80	0.63
1:D:2227:THR:HG23	1:D:2324:GLN:HE22	1.63	0.63
2:D:2602:PLX:O1	2:D:2602:PLX:H1A2	1.98	0.63
1:C:2243:ALA:HB1	1:C:2247:SER:HB2	1.80	0.63
1:A:1153:LEU:CD1	4:A:2604:P5S:C49	2.67	0.63
2:A:2602:PLX:O1	2:A:2602:PLX:H1A2	1.98	0.63
1:D:2109:PHE:CB	3:D:2603:PEE:H11	2.23	0.63
1:A:2387:VAL:HG12	1:A:2390:LEU:H	1.64	0.63
1:D:1160:TYR:HE1	2:D:2602:PLX:O2	1.82	0.63
1:D:1799:GLN:HA	2:D:2602:PLX:C1C	2.28	0.62
1:C:817:THR:HG1	1:C:836:TRP:CD1	2.17	0.62
1:A:1296:ILE:HD11	4:A:2604:P5S:O18	1.99	0.62
1:A:1989:ILE:HD11	3:A:2603:PEE:H33	1.81	0.62
1:D:2250:PRO:HA	1:D:2282:VAL:HG12	1.81	0.62
1:A:1693:PHE:O	1:A:1697:LEU:HD23	2.00	0.62
1:D:1977:TYR:HA	1:D:1980:MET:HE3	1.80	0.62
4:C:2604:P5S:H48	4:C:2604:P5S:H26A	1.81	0.62
4:A:2604:P5S:H48	4:A:2604:P5S:H26A	1.81	0.62
1:D:1979:LEU:HB3	1:D:2092:LEU:HD13	1.82	0.62
1:D:1981:PHE:HE2	3:D:2603:PEE:C14	2.13	0.62
1:C:2240:THR:O	1:C:2241:MET:HE2	2.00	0.62
1:C:2210:MET:HE1	1:C:2466:ILE:HG23	1.81	0.61
1:C:2318:ARG:NH2	1:A:2245:GLN:HG2	2.15	0.61
1:C:1698:ASN:ND2	1:C:1786:ASP:OD1	2.29	0.61
1:A:2387:VAL:HG11	1:A:2390:LEU:HD23	1.82	0.61
1:C:2318:ARG:NH2	1:A:2244:GLN:HB2	2.16	0.61
1:A:2318:ARG:CZ	1:D:2244:GLN:HB2	2.31	0.61
1:C:1415:PHE:HE2	1:C:2532:LEU:HD12	1.65	0.61
1:C:1675:LEU:HG	1:C:1676:LEU:HD12	1.82	0.61
1:A:2250:PRO:HA	1:A:2282:VAL:HG12	1.81	0.61
1:A:2458:LEU:HB3	1:A:2461:LEU:HD13	1.81	0.61
1:C:2387:VAL:HG12	1:C:2390:LEU:H	1.65	0.61
1:D:1989:ILE:HD11	3:D:2603:PEE:H33	1.81	0.61
1:A:2318:ARG:NH2	1:D:2244:GLN:HB2	2.15	0.61
1:D:1296:ILE:HD11	4:D:2604:P5S:O18	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1980:MET:HB3	1:C:2092:LEU:HD11	1.83	0.61
1:C:1989:ILE:HD12	3:C:2603:PEE:H38	1.82	0.61
1:D:1352:ILE:HD11	1:D:2525:LEU:HD11	1.83	0.61
1:D:1795:PHE:HA	2:D:2602:PLX:H24	1.83	0.61
1:A:1727:LYS:O	1:A:1731:MET:HG2	2.01	0.61
1:A:2264:ASP:HA	1:A:2270:MET:SD	2.41	0.61
1:C:813:VAL:O	1:C:817:THR:HG23	2.01	0.60
1:A:2210:MET:HE1	1:A:2466:ILE:HG23	1.82	0.60
1:C:1296:ILE:HD11	4:C:2604:P5S:O18	2.00	0.60
1:A:1692:TYR:O	1:A:1695:ILE:HG22	2.01	0.60
1:D:802:ARG:HH21	1:D:943:ARG:HE	1.48	0.60
1:A:1160:TYR:HE1	2:A:2602:PLX:O2	1.83	0.60
3:A:2603:PEE:H40	3:A:2603:PEE:C44	2.31	0.60
1:D:1728:ARG:CB	2:D:2601:PLX:O7	2.49	0.60
1:C:1153:LEU:HD12	4:C:2604:P5S:C49	2.29	0.60
4:D:2604:P5S:H26A	4:D:2604:P5S:H48	1.81	0.60
1:A:1153:LEU:HD12	4:A:2604:P5S:C49	2.31	0.60
3:D:2603:PEE:H40	3:D:2603:PEE:C44	2.31	0.60
1:A:1152:MET:HA	1:A:1155:VAL:HG22	1.82	0.60
1:D:1019:ALA:O	1:D:1022:THR:OG1	2.20	0.60
1:D:2458:LEU:HB3	1:D:2461:LEU:HD13	1.83	0.60
1:C:1981:PHE:HD2	3:C:2603:PEE:C13	2.07	0.60
1:A:1799:GLN:HA	2:A:2602:PLX:C1C	2.32	0.60
1:A:2407:ARG:HB3	1:A:2426:PHE:HB3	1.84	0.60
1:D:2407:ARG:HB3	1:D:2426:PHE:HB3	1.84	0.60
1:C:2461:LEU:HG	1:C:2462:ALA:H	1.66	0.59
1:A:2023:MET:HA	1:A:2026:VAL:HG22	1.84	0.59
1:A:2377:ARG:HA	1:A:2449:PHE:HB2	1.83	0.59
1:D:1039:PHE:HA	1:D:1042:LEU:HD12	1.84	0.59
1:A:2058:HIS:NE2	1:A:2083:TYR:OH	2.35	0.59
3:C:2603:PEE:H40	3:C:2603:PEE:C44	2.31	0.59
1:A:2536:PRO:HA	1:A:2539:MET:HG2	1.84	0.59
1:D:2023:MET:HA	1:D:2026:VAL:HG12	1.84	0.59
1:C:2289:SER:HA	1:C:2431:VAL:HG13	1.85	0.59
1:C:2318:ARG:HH12	1:A:2245:GLN:H	1.51	0.59
1:C:2244:GLN:HB2	1:D:2318:ARG:NH2	2.16	0.59
1:A:1989:ILE:HD12	3:A:2603:PEE:H38	1.82	0.59
1:C:2407:ARG:HB3	1:C:2426:PHE:HB3	1.84	0.59
1:A:1357:GLU:O	1:A:1361:GLN:HG2	2.02	0.59
1:D:1715:PHE:HZ	1:D:2087:CYS:HG	1.49	0.59
1:D:1152:MET:HA	1:D:1155:VAL:HG12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2602:PLX:H271	2:D:2602:PLX:O8	2.03	0.59
1:A:802:ARG:HH21	1:A:943:ARG:HE	1.51	0.59
1:A:2181:GLN:O	1:A:2183:LYS:N	2.35	0.59
1:A:2377:ARG:HH12	1:A:2379:PRO:HB3	1.68	0.59
1:C:2375:TYR:H	1:C:2391:GLN:HE22	1.50	0.58
1:A:2373:PRO:HB3	1:A:2398:TYR:CE1	2.38	0.58
1:D:2377:ARG:HH12	1:D:2379:PRO:HB3	1.68	0.58
1:C:1799:GLN:HA	2:C:2602:PLX:C1C	2.33	0.58
2:A:2602:PLX:O8	2:A:2602:PLX:H271	2.03	0.58
2:C:2602:PLX:O8	2:C:2602:PLX:H271	2.03	0.58
1:A:1728:ARG:CB	2:A:2601:PLX:O7	2.51	0.58
1:C:2377:ARG:HA	1:C:2449:PHE:HB2	1.85	0.58
1:A:998:ALA:HA	1:A:1100:LEU:HD12	1.85	0.58
1:A:1991:ILE:HD11	1:A:2023:MET:HG3	1.85	0.58
1:A:2145:THR:HG21	1:A:2152:TRP:HZ3	1.67	0.58
1:D:2377:ARG:HA	1:D:2449:PHE:HB2	1.84	0.58
1:C:1092:THR:O	1:C:1095:ILE:HG22	2.03	0.58
1:A:1981:PHE:HD2	3:A:2603:PEE:C11	2.07	0.58
1:A:2379:PRO:HD2	1:A:2384:ALA:HA	1.85	0.58
1:A:2135:ARG:CZ	3:A:2603:PEE:O1P	2.51	0.58
1:D:1987:ASP:OD2	1:D:2082:TRP:NE1	2.36	0.58
1:D:2497:LEU:HD12	1:D:2543:THR:HG21	1.85	0.58
1:C:1693:PHE:O	1:C:1697:LEU:HD23	2.02	0.58
1:C:2035:ARG:NE	3:C:2603:PEE:O5	2.37	0.58
1:A:1980:MET:HB2	1:A:2089:TYR:CD1	2.39	0.58
1:A:2031:MET:CE	3:A:2603:PEE:H56	2.34	0.58
1:D:2145:THR:HG21	1:D:2152:TRP:CZ3	2.39	0.58
1:A:1795:PHE:HA	2:A:2602:PLX:H24	1.85	0.58
1:D:1203:THR:HA	1:D:1206:GLN:NE2	2.19	0.58
1:D:1357:GLU:O	1:D:1361:GLN:HG2	2.03	0.58
1:D:1985:ILE:O	1:D:1989:ILE:HG12	2.04	0.58
1:C:1357:GLU:O	1:C:1361:GLN:HG2	2.03	0.57
1:D:1716:LEU:HD21	1:D:2054:VAL:HG11	1.85	0.57
1:D:998:ALA:HA	1:D:1100:LEU:HD12	1.86	0.57
1:D:2357:LEU:HD21	1:D:2405:LEU:HB2	1.86	0.57
1:D:2377:ARG:HH21	1:D:2385:ASN:HD21	1.53	0.57
1:C:1008:PHE:CE2	1:C:1080:LEU:HD23	2.40	0.57
1:C:2357:LEU:HD21	1:C:2405:LEU:HB2	1.86	0.57
1:C:2497:LEU:HD12	1:C:2543:THR:HG21	1.85	0.57
1:D:1092:THR:O	1:D:1095:ILE:HG22	2.04	0.57
1:D:1981:PHE:CE1	3:D:2603:PEE:H8	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2145:THR:HG21	1:D:2152:TRP:HZ3	1.69	0.57
1:C:1352:ILE:HD11	1:C:2525:LEU:HD21	1.87	0.57
1:C:1152:MET:HA	1:C:1155:VAL:HG12	1.86	0.57
1:A:1981:PHE:CZ	3:A:2603:PEE:H8	2.38	0.57
1:D:2373:PRO:HB3	1:D:2398:TYR:CE1	2.39	0.57
1:C:1795:PHE:HA	2:C:2602:PLX:H24	1.87	0.57
1:A:2145:THR:HG22	1:A:2514:ARG:HD3	1.87	0.57
1:C:802:ARG:HH21	1:C:943:ARG:HE	1.50	0.57
1:D:1162:PHE:HE1	1:D:1210:TRP:HZ2	1.53	0.57
1:D:2379:PRO:HD2	1:D:2384:ALA:HA	1.86	0.57
1:C:1036:TYR:HA	1:C:1039:PHE:CE1	2.40	0.56
1:C:2025:LEU:HD23	1:D:2204:TRP:CZ2	2.40	0.56
1:A:1716:LEU:HD21	1:A:2054:VAL:HG11	1.86	0.56
1:D:1163:TRP:CB	2:D:2602:PLX:H282	2.32	0.56
1:C:1163:TRP:HB3	2:C:2602:PLX:C28	2.28	0.56
1:A:2497:LEU:HD12	1:A:2543:THR:HG21	1.86	0.56
1:D:2408:GLU:HB3	1:D:2427:LEU:HB2	1.85	0.56
1:C:1327:ASN:OD1	1:C:1328:LEU:N	2.38	0.56
1:A:2270:MET:HE3	1:A:2270:MET:HA	1.87	0.56
1:D:1714:VAL:HG22	1:D:1729:PHE:HZ	1.69	0.56
1:D:2231:LYS:NZ	1:D:2233:GLY:O	2.34	0.56
1:C:860:ILE:HD13	1:C:927:HIS:HE1	1.70	0.56
1:C:2325:ARG:HB2	1:C:2334:GLU:HG2	1.85	0.56
1:A:2357:LEU:HD21	1:A:2405:LEU:HB2	1.87	0.56
1:D:1206:GLN:HG3	1:D:1297:PHE:CE2	2.41	0.56
1:C:2181:GLN:C	1:C:2183:LYS:H	2.13	0.56
1:C:2318:ARG:CZ	1:A:2244:GLN:HB2	2.36	0.56
1:C:2509:ASP:HA	1:C:2512:LEU:HG	1.87	0.56
1:A:1092:THR:O	1:A:1095:ILE:HG22	2.05	0.56
1:D:1698:ASN:ND2	1:D:1786:ASP:OD1	2.35	0.56
1:D:2300:SER:O	1:D:2304:MET:HG2	2.06	0.56
1:C:2300:SER:O	1:C:2304:MET:HG2	2.05	0.56
1:A:2408:GLU:HB3	1:A:2427:LEU:HB2	1.87	0.56
1:C:998:ALA:HA	1:C:1100:LEU:HD12	1.87	0.56
1:C:2024:LEU:HD11	1:D:2204:TRP:HZ3	1.71	0.56
1:C:1981:PHE:CE1	3:C:2603:PEE:H8	2.40	0.56
1:C:1989:ILE:HD11	3:C:2603:PEE:C21	2.35	0.56
1:A:2377:ARG:HH21	1:A:2385:ASN:HD21	1.53	0.56
1:A:2342:LEU:HD13	1:A:2371:LEU:HD23	1.87	0.56
3:D:2603:PEE:H68	3:D:2603:PEE:H78	1.86	0.56
1:D:1327:ASN:OD1	1:D:1328:LEU:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1327:ASN:OD1	1:A:1328:LEU:N	2.39	0.55
1:A:1036:TYR:HA	1:A:1039:PHE:CE1	2.41	0.55
1:A:1714:VAL:HG22	1:A:1729:PHE:HZ	1.70	0.55
1:C:1981:PHE:HD2	3:C:2603:PEE:C11	2.11	0.55
1:C:2342:LEU:HD13	1:C:2371:LEU:HD23	1.88	0.55
1:C:2468:GLY:O	1:C:2471:VAL:HG12	2.07	0.55
1:A:1989:ILE:HD11	3:A:2603:PEE:C21	2.37	0.55
1:C:2245:GLN:HG2	1:D:2318:ARG:NH2	2.22	0.55
1:C:2298:PRO:HB3	1:C:2301:ARG:HH21	1.72	0.55
1:C:2408:GLU:HB3	1:C:2427:LEU:HB2	1.89	0.55
1:A:1985:ILE:O	1:A:1989:ILE:HG12	2.06	0.55
1:C:2377:ARG:HH12	1:C:2379:PRO:HB3	1.70	0.55
1:D:2285:GLN:HB3	1:D:2443:LEU:HD11	1.89	0.55
1:C:1056:PRO:HB3	1:C:1085:PHE:O	2.07	0.55
1:C:1987:ASP:OD2	1:C:2082:TRP:NE1	2.39	0.55
1:C:2191:MET:O	1:C:2194:LEU:HG	2.06	0.55
1:D:1036:TYR:HA	1:D:1039:PHE:CE1	2.42	0.55
4:C:2604:P5S:H24A	4:C:2604:P5S:H45	1.89	0.54
1:A:1987:ASP:OD2	1:A:2082:TRP:NE1	2.39	0.54
1:D:2119:LEU:HD12	1:D:2167:CYS:HB3	1.89	0.54
1:D:2135:ARG:HD2	3:D:2603:PEE:H2	1.87	0.54
1:C:2239:PHE:CZ	1:C:2241:MET:HG2	2.42	0.54
4:D:2604:P5S:H45	4:D:2604:P5S:H24A	1.89	0.54
1:C:984:PHE:HB3	1:C:987:TYR:HB3	1.89	0.54
1:C:2181:GLN:O	1:C:2183:LYS:N	2.40	0.54
1:A:2318:ARG:NH2	1:D:2245:GLN:HG2	2.22	0.54
1:C:2231:LYS:NZ	1:C:2233:GLY:O	2.34	0.54
1:C:2377:ARG:HH21	1:C:2385:ASN:HD21	1.56	0.54
1:A:984:PHE:HB3	1:A:987:TYR:HB3	1.90	0.54
1:A:2241:MET:HE2	1:A:2287:GLU:HB2	1.90	0.54
1:D:2305:LYS:HZ1	1:D:2359:GLU:HG3	1.73	0.54
1:C:2379:PRO:HD2	1:C:2384:ALA:HA	1.88	0.54
1:A:2031:MET:HE1	3:A:2603:PEE:H63	1.89	0.54
1:A:2182:LYS:O	1:A:2182:LYS:HD3	2.07	0.54
4:A:2604:P5S:H24A	4:A:2604:P5S:H45	1.89	0.54
1:D:2286:ILE:HG13	1:D:2444:LEU:HB2	1.90	0.54
1:D:2342:LEU:HD13	1:D:2371:LEU:HD23	1.87	0.54
1:D:2468:GLY:O	1:D:2471:VAL:HG12	2.07	0.54
1:C:1985:ILE:O	1:C:1989:ILE:HG12	2.07	0.54
1:C:2321:TRP:CH2	1:C:2373:PRO:HG2	2.32	0.54
1:D:2035:ARG:NE	3:D:2603:PEE:O5	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:HIS:HA	1:A:1530:MET:HE3	1.88	0.54
3:A:2603:PEE:H68	3:A:2603:PEE:H78	1.86	0.54
1:C:1352:ILE:HD12	1:C:2509:ASP:HB3	1.89	0.54
1:C:2030:THR:HA	1:C:2033:ILE:HG22	1.90	0.54
1:C:2135:ARG:HD2	3:C:2603:PEE:H2	1.89	0.54
1:A:1019:ALA:O	1:A:1022:THR:OG1	2.21	0.54
1:D:2325:ARG:HB2	1:D:2334:GLU:HG2	1.89	0.54
1:A:2471:VAL:O	1:A:2475:LEU:HG	2.08	0.54
1:C:1153:LEU:CD1	4:C:2604:P5S:C49	2.70	0.53
1:A:2119:LEU:HD12	1:A:2167:CYS:HB3	1.90	0.53
1:D:1170:PHE:HB2	1:D:1188:CYS:SG	2.47	0.53
1:D:1981:PHE:HD2	3:D:2603:PEE:C11	2.09	0.53
1:C:2183:LYS:HE2	1:A:2145:THR:C	2.33	0.53
1:C:2458:LEU:HB3	1:C:2461:LEU:HD13	1.91	0.53
1:A:2183:LYS:HB2	1:D:2146:THR:HA	1.90	0.53
1:C:1170:PHE:HB2	1:C:1188:CYS:SG	2.49	0.53
1:A:631:LEU:O	1:A:634:VAL:N	2.38	0.53
1:C:1982:LEU:HD13	3:C:2603:PEE:H23	1.91	0.53
1:C:2361:ARG:HB2	1:C:2362:PRO:HD2	1.90	0.53
4:C:2604:P5S:H54	4:C:2604:P5S:H32A	1.91	0.53
1:C:2043:VAL:HG12	1:C:2101:TYR:HD2	1.74	0.53
1:C:2188:LYS:HG3	1:A:2140:TRP:CZ3	2.43	0.53
1:A:2361:ARG:HB2	1:A:2362:PRO:HD2	1.90	0.53
1:C:2298:PRO:HD2	1:A:2429:TRP:CH2	2.43	0.53
4:A:2604:P5S:H54	4:A:2604:P5S:H32A	1.91	0.53
1:D:2194:LEU:O	1:D:2197:LEU:HG	2.09	0.53
1:A:1170:PHE:HB2	1:A:1188:CYS:SG	2.48	0.53
1:C:1157:VAL:HG11	4:C:2604:P5S:H44A	1.91	0.53
1:A:2285:GLN:HB3	1:A:2443:LEU:HD11	1.90	0.53
1:C:996:LEU:HD11	1:C:1288:PHE:HB2	1.91	0.52
1:C:2119:LEU:HD12	1:C:2167:CYS:HB3	1.90	0.52
3:C:2603:PEE:C45	3:C:2603:PEE:C41	2.86	0.52
1:D:984:PHE:HB3	1:D:987:TYR:HB3	1.92	0.52
1:D:1799:GLN:CA	2:D:2602:PLX:H1C1	2.38	0.52
1:D:2361:ARG:HB2	1:D:2362:PRO:HD2	1.90	0.52
1:D:2471:VAL:O	1:D:2475:LEU:HG	2.10	0.52
1:D:2535:SER:OG	1:D:2538:THR:OG1	2.27	0.52
1:C:2285:GLN:HB3	1:C:2443:LEU:HD11	1.91	0.52
1:A:1199:LEU:HD22	1:A:1302:PHE:HZ	1.74	0.52
1:A:2183:LYS:HD3	1:A:2183:LYS:C	2.35	0.52
1:A:2286:ILE:HG13	1:A:2444:LEU:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:LEU:O	1:C:634:VAL:N	2.38	0.52
1:C:1692:TYR:O	1:C:1695:ILE:HG22	2.09	0.52
3:A:2603:PEE:C45	3:A:2603:PEE:C41	2.85	0.52
1:D:2298:PRO:HB3	1:D:2301:ARG:HH21	1.75	0.52
1:C:1192:LEU:HB3	1:C:1794:PHE:CE2	2.45	0.52
1:A:2147:LEU:HD23	1:A:2151:ASN:HB3	1.91	0.52
1:C:1162:PHE:O	1:C:1165:VAL:HG12	2.10	0.52
1:A:2363:ASP:CG	1:A:2406:ARG:HH22	2.17	0.52
1:A:2445:PRO:O	1:A:2446:MET:HE2	2.09	0.52
3:A:2603:PEE:C45	3:A:2603:PEE:C24	2.85	0.52
1:C:1406:VAL:HG11	1:C:2523:GLU:HG3	1.90	0.52
1:C:2404:GLN:HB3	1:C:2431:VAL:HB	1.92	0.52
1:C:1019:ALA:O	1:C:1022:THR:OG1	2.23	0.52
1:A:1734:ILE:HG12	1:A:1794:PHE:HE1	1.75	0.52
3:C:2603:PEE:H68	3:C:2603:PEE:H78	1.86	0.52
1:A:2305:LYS:HZ1	1:A:2359:GLU:HG3	1.75	0.52
1:D:2037:LEU:HD23	1:D:2046:LYS:HA	1.91	0.52
2:C:2602:PLX:H291	2:C:2602:PLX:H6	1.93	0.51
1:A:1190:TYR:HD2	1:A:1191:LEU:HD22	1.75	0.51
1:A:2026:VAL:O	1:A:2030:THR:HG23	2.09	0.51
1:A:2324:GLN:HA	1:A:2334:GLU:O	2.10	0.51
1:C:1221:ILE:HD11	1:C:1283:ASP:HB3	1.90	0.51
1:C:2305:LYS:HZ1	1:C:2359:GLU:HG3	1.74	0.51
3:D:2603:PEE:C45	3:D:2603:PEE:C41	2.86	0.51
1:C:1219:THR:HA	1:C:1222:ILE:HG12	1.90	0.51
1:A:1988:ILE:O	1:A:1991:ILE:HG22	2.10	0.51
1:D:1162:PHE:O	1:D:1165:VAL:HG12	2.10	0.51
1:C:2162:ILE:HG22	1:C:2504:LEU:HD21	1.92	0.51
1:C:2183:LYS:NZ	1:A:2147:LEU:O	2.24	0.51
1:C:2527:ALA:HA	1:C:2530:ILE:HG22	1.93	0.51
2:D:2602:PLX:H6	2:D:2602:PLX:H291	1.92	0.51
1:C:1982:LEU:CD1	3:C:2603:PEE:C16	2.88	0.51
1:A:1406:VAL:HG11	1:A:2523:GLU:HG3	1.93	0.51
1:A:1713:LEU:O	1:A:1717:TRP:N	2.43	0.51
1:C:2271:GLN:HE22	1:C:2389:GLN:HE22	1.59	0.51
1:C:2286:ILE:HG13	1:C:2444:LEU:HB2	1.92	0.51
1:D:1989:ILE:HD11	3:D:2603:PEE:C21	2.41	0.51
1:D:2181:GLN:C	1:D:2183:LYS:H	2.18	0.51
2:A:2602:PLX:H291	2:A:2602:PLX:H6	1.93	0.51
1:D:1976:VAL:O	1:D:1976:VAL:HG13	2.11	0.51
1:C:2264:ASP:HA	1:C:2270:MET:SD	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2429:TRP:CH2	1:D:2298:PRO:HD2	2.46	0.51
1:D:2363:ASP:CG	1:D:2406:ARG:HH22	2.18	0.51
1:C:2387:VAL:HG11	1:C:2390:LEU:HD23	1.93	0.51
1:A:1743:THR:HA	1:A:1746:LEU:HG	1.92	0.51
1:C:2266:TYR:O	1:C:2270:MET:HG2	2.10	0.51
3:C:2603:PEE:C45	3:C:2603:PEE:C24	2.85	0.51
1:D:1157:VAL:HG22	4:D:2604:P5S:H23	1.94	0.51
4:D:2604:P5S:H28A	4:D:2604:P5S:H50	1.92	0.51
4:D:2604:P5S:H32A	4:D:2604:P5S:H54	1.91	0.51
1:A:2185:LYS:O	1:A:2188:LYS:HB3	2.11	0.50
1:A:2197:LEU:O	1:A:2201:ALA:N	2.40	0.50
1:D:1163:TRP:HB3	2:D:2602:PLX:C28	2.34	0.50
1:D:2138:MET:SD	1:D:2142:TRP:CD1	3.04	0.50
1:D:2294:TRP:CB	1:D:2429:TRP:HA	2.41	0.50
1:C:2471:VAL:O	1:C:2475:LEU:HG	2.11	0.50
1:A:996:LEU:HD11	1:A:1288:PHE:HB2	1.92	0.50
1:A:1107:GLN:O	1:A:1111:PHE:HB2	2.11	0.50
1:C:1008:PHE:CD2	1:C:1080:LEU:HD23	2.46	0.50
1:C:2363:ASP:CG	1:C:2406:ARG:HH22	2.18	0.50
4:C:2604:P5S:H50	4:C:2604:P5S:H28A	1.92	0.50
1:D:2197:LEU:O	1:D:2201:ALA:N	2.39	0.50
1:C:2146:THR:HG22	1:D:2181:GLN:HB3	1.94	0.50
1:A:1787:LEU:O	1:A:1791:MET:HG2	2.10	0.50
1:A:2509:ASP:HA	1:A:2512:LEU:HG	1.94	0.50
1:D:1190:TYR:HD2	1:D:1191:LEU:HD22	1.77	0.50
1:D:2321:TRP:CH2	1:D:2373:PRO:HG2	2.34	0.50
1:C:1044:LEU:HD13	1:C:1097:ASP:OD2	2.12	0.50
1:C:1734:ILE:HD11	1:C:1790:LEU:HD13	1.93	0.50
1:C:2085:VAL:O	1:C:2088:ILE:HG22	2.12	0.50
1:C:2294:TRP:CZ2	1:C:2296:ILE:HD12	2.46	0.50
1:D:1084:ASP:OD1	1:D:1086:PHE:N	2.44	0.50
1:D:2294:TRP:CZ2	1:D:2296:ILE:HD12	2.47	0.50
1:C:1107:GLN:O	1:C:1111:PHE:HB2	2.11	0.50
1:A:1163:TRP:HB3	2:A:2602:PLX:C28	2.32	0.50
4:A:2604:P5S:H50	4:A:2604:P5S:H28A	1.92	0.50
1:C:1981:PHE:HE2	3:C:2603:PEE:H20	1.75	0.50
1:D:1981:PHE:CZ	3:D:2603:PEE:H8	2.46	0.50
1:C:1036:TYR:CZ	1:C:1040:LEU:HD11	2.47	0.50
1:C:1713:LEU:O	1:C:1717:TRP:N	2.43	0.50
1:A:2222:GLN:H	1:A:2329:LYS:HE3	1.77	0.50
1:C:1521:ARG:HE	1:C:1528:ARG:NH1	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1991:ILE:CD1	1:A:2023:MET:HG3	2.42	0.50
1:A:2321:TRP:CH2	1:A:2373:PRO:HG2	2.37	0.49
1:D:1148:SER:OG	1:D:1151:ASP:OD2	2.24	0.49
1:C:2501:ASP:OD1	1:C:2502:ARG:N	2.44	0.49
1:A:1162:PHE:O	1:A:1165:VAL:HG12	2.12	0.49
1:A:2130:PHE:O	1:A:2134:LEU:HD12	2.12	0.49
1:D:1107:GLN:O	1:D:1111:PHE:HB2	2.11	0.49
1:D:1690:LEU:O	1:D:1694:ILE:HG12	2.12	0.49
1:C:2227:THR:HG22	1:C:2242:SER:HB3	1.93	0.49
1:C:2037:LEU:HD23	1:C:2046:LYS:HA	1.93	0.49
1:C:2151:ASN:O	1:C:2155:VAL:HG23	2.12	0.49
1:C:2271:GLN:NE2	1:C:2389:GLN:OE1	2.45	0.49
1:C:2389:GLN:O	1:C:2392:PRO:HD3	2.12	0.49
1:A:1211:ASP:HA	1:A:1214:ILE:HG12	1.94	0.49
1:A:1287:PHE:O	1:A:1291:LEU:HG	2.11	0.49
1:D:2135:ARG:NH2	3:D:2603:PEE:O1P	2.46	0.49
1:C:1289:PHE:HA	1:C:1292:LEU:HG	1.92	0.49
1:C:2245:GLN:H	1:D:2318:ARG:HH12	1.60	0.49
1:C:2377:ARG:NH1	1:C:2379:PRO:HB3	2.28	0.49
1:A:822:LEU:HD13	1:A:1092:THR:HA	1.95	0.49
1:D:631:LEU:O	1:D:634:VAL:N	2.37	0.49
1:C:1153:LEU:O	1:C:1157:VAL:HG22	2.13	0.49
1:C:1353:ARG:O	1:C:1356:GLN:HG3	2.13	0.49
1:C:2147:LEU:HB3	1:C:2151:ASN:HB2	1.95	0.49
1:C:2395:GLU:HA	1:C:2398:TYR:CD2	2.47	0.49
1:A:1163:TRP:CB	2:A:2602:PLX:H282	2.33	0.49
1:A:1246:ILE:HA	1:A:1251:LEU:CD1	2.41	0.49
1:D:2148:SER:HB3	1:D:2151:ASN:ND2	2.28	0.49
1:D:2377:ARG:NH1	1:D:2379:PRO:HB3	2.27	0.49
1:C:2183:LYS:NZ	1:A:2145:THR:OG1	2.46	0.49
1:C:2293:LEU:HB2	1:D:2295:ARG:HB2	1.95	0.49
1:C:2295:ARG:HB2	1:A:2293:LEU:HD12	1.94	0.49
1:C:1148:SER:OG	1:C:1151:ASP:OD2	2.22	0.49
1:C:1162:PHE:O	1:C:1166:LEU:HG	2.12	0.49
1:C:1695:ILE:HA	1:C:1789:GLN:HE21	1.77	0.49
1:C:1981:PHE:CE1	3:C:2603:PEE:H50	2.47	0.49
1:A:2318:ARG:HH12	1:D:2245:GLN:H	1.60	0.49
1:D:2535:SER:HG	1:D:2538:THR:HG1	1.61	0.49
1:A:1224:LYS:NZ	1:A:1280:ILE:HD13	2.27	0.49
1:A:1976:VAL:O	1:A:1976:VAL:HG13	2.13	0.49
1:A:1353:ARG:O	1:A:1356:GLN:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1695:ILE:HA	1:A:1789:GLN:HE21	1.77	0.49
1:D:1038:LEU:O	1:D:1041:THR:OG1	2.28	0.49
1:C:1243:CYS:HA	1:C:1246:ILE:HG12	1.94	0.48
1:C:2295:ARG:HB2	1:A:2293:LEU:HB2	1.95	0.48
1:A:1157:VAL:CG1	4:A:2604:P5S:H23	2.43	0.48
1:A:1521:ARG:HE	1:A:1528:ARG:NH1	2.11	0.48
1:A:2295:ARG:HB2	1:D:2293:LEU:HD12	1.96	0.48
1:D:2227:THR:HG22	1:D:2242:SER:HB3	1.94	0.48
1:D:2235:TYR:CD1	1:D:2304:MET:HE1	2.48	0.48
1:D:2389:GLN:O	1:D:2392:PRO:HD3	2.13	0.48
1:C:1734:ILE:HG12	1:C:1794:PHE:HE1	1.75	0.48
1:A:2231:LYS:NZ	1:A:2233:GLY:O	2.35	0.48
1:A:2496:GLU:HB2	1:D:2534:ARG:HE	1.78	0.48
1:C:2222:GLN:H	1:C:2329:LYS:HE3	1.76	0.48
1:C:2318:ARG:HH22	1:A:2245:GLN:HG2	1.78	0.48
3:C:2603:PEE:H40	3:C:2603:PEE:H77	1.95	0.48
1:A:2135:ARG:HD2	3:A:2603:PEE:H2	1.95	0.48
1:A:2239:PHE:CZ	1:A:2241:MET:HG2	2.49	0.48
1:A:2377:ARG:NH1	1:A:2379:PRO:HB3	2.27	0.48
1:A:2460:PHE:HD2	1:A:2465:GLY:HA3	1.78	0.48
1:D:1713:LEU:O	1:D:1717:TRP:N	2.46	0.48
1:D:2374:LYS:NZ	1:D:2445:PRO:O	2.39	0.48
1:C:969:ARG:HG2	1:C:976:SER:HB2	1.95	0.48
1:C:2135:ARG:NH2	3:C:2603:PEE:O1P	2.46	0.48
1:C:2517:ARG:HG3	1:C:2517:ARG:O	2.13	0.48
1:A:1023:ARG:HD3	1:A:1028:ALA:HB1	1.95	0.48
1:A:1036:TYR:CZ	1:A:1040:LEU:HD11	2.48	0.48
1:A:1337:ILE:HA	1:A:1340:LYS:HZ2	1.78	0.48
1:A:2492:ILE:O	1:A:2496:GLU:HG2	2.13	0.48
1:D:1992:ILE:HG21	3:D:2603:PEE:C27	2.42	0.48
1:C:1692:TYR:HA	1:C:1695:ILE:HG22	1.94	0.48
1:C:2194:LEU:O	1:C:2197:LEU:HG	2.12	0.48
1:C:2257:GLU:O	1:C:2261:GLN:OE1	2.31	0.48
1:A:2471:VAL:HA	1:A:2474:VAL:HG12	1.96	0.48
1:D:2375:TYR:HD1	1:D:2391:GLN:HE22	1.60	0.48
1:C:2245:GLN:HG2	1:D:2318:ARG:CZ	2.43	0.48
1:A:1146:CYS:HA	1:A:1151:ASP:HB3	1.94	0.48
1:D:1961:PHE:O	1:D:1965:ILE:HG12	2.14	0.48
3:D:2603:PEE:C45	3:D:2603:PEE:C24	2.85	0.48
1:C:1799:GLN:CA	2:C:2602:PLX:H1C1	2.43	0.48
1:D:2529:LEU:HD11	1:D:2533:TYR:HE2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2197:LEU:O	1:C:2201:ALA:N	2.41	0.48
1:A:1992:ILE:HG21	3:A:2603:PEE:C27	2.44	0.48
1:A:2407:ARG:HB3	1:A:2426:PHE:CG	2.49	0.48
1:D:1406:VAL:HG11	1:D:2523:GLU:HG3	1.94	0.48
1:D:2222:GLN:H	1:D:2329:LYS:HE3	1.78	0.48
1:D:2407:ARG:HB3	1:D:2426:PHE:CG	2.49	0.48
1:C:1146:CYS:HA	1:C:1151:ASP:HB3	1.95	0.48
1:C:2293:LEU:HD12	1:D:2295:ARG:HB2	1.95	0.48
1:C:2347:ASN:O	1:C:2347:ASN:ND2	2.47	0.48
1:A:1961:PHE:O	1:A:1965:ILE:HG12	2.13	0.48
1:D:1521:ARG:HE	1:D:1528:ARG:NH1	2.11	0.48
1:D:2135:ARG:HB2	3:D:2603:PEE:H48	1.95	0.48
1:D:2241:MET:HE3	1:D:2287:GLU:O	2.14	0.48
1:C:1961:PHE:O	1:C:1965:ILE:HG12	2.14	0.48
1:A:2295:ARG:HB2	1:D:2293:LEU:HB2	1.96	0.48
1:D:1023:ARG:HD3	1:D:1028:ALA:HB1	1.95	0.48
1:D:1143:PHE:HE1	1:D:1155:VAL:HA	1.79	0.48
1:C:2140:TRP:HD1	1:C:2152:TRP:CE3	2.32	0.47
1:C:2372:PHE:HD2	1:C:2400:GLY:HA2	1.78	0.47
3:C:2603:PEE:H82	3:C:2603:PEE:H75	1.66	0.47
1:A:2325:ARG:HB2	1:A:2334:GLU:HG2	1.95	0.47
1:C:2235:TYR:CD1	1:C:2304:MET:HE1	2.49	0.47
1:A:2389:GLN:O	1:A:2392:PRO:HD3	2.14	0.47
1:D:2241:MET:HE1	1:D:2290:SER:O	2.14	0.47
1:A:2311:GLY:O	1:A:2351:ARG:NH1	2.47	0.47
1:A:2477:VAL:O	1:A:2481:VAL:HG23	2.14	0.47
1:D:1353:ARG:O	1:D:1356:GLN:HG3	2.14	0.47
1:C:978:LEU:O	1:C:982:ILE:HG12	2.13	0.47
1:C:1143:PHE:HE1	1:C:1155:VAL:HA	1.79	0.47
1:C:2380:ASN:ND2	1:C:2453:VAL:HA	2.26	0.47
1:C:2407:ARG:HB3	1:C:2426:PHE:CG	2.49	0.47
1:A:2347:ASN:O	1:A:2347:ASN:ND2	2.47	0.47
1:D:2147:LEU:HD23	1:D:2151:ASN:HB3	1.95	0.47
1:D:2477:VAL:O	1:D:2481:VAL:HG23	2.15	0.47
1:C:1160:TYR:CE1	2:C:2602:PLX:O2	2.62	0.47
1:A:1287:PHE:CE2	1:A:1291:LEU:HD11	2.50	0.47
1:A:1734:ILE:HD11	1:A:1790:LEU:HD13	1.96	0.47
1:A:2224:ILE:HG12	1:A:2326:ASP:HA	1.96	0.47
1:D:2093:SER:O	1:D:2097:ILE:HG13	2.14	0.47
1:D:2447:VAL:O	1:D:2448:ILE:HD13	2.15	0.47
1:C:1985:ILE:HG21	3:C:2603:PEE:H26	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1521:ARG:O	1:A:1528:ARG:NH2	2.48	0.47
1:D:1036:TYR:CZ	1:D:1040:LEU:HD11	2.49	0.47
1:D:1695:ILE:HA	1:D:1789:GLN:HE21	1.80	0.47
1:C:1739:VAL:HA	1:C:1742:VAL:HG12	1.95	0.47
1:C:1982:LEU:HD13	3:C:2603:PEE:C16	2.45	0.47
1:C:2311:GLY:O	1:C:2351:ARG:NH1	2.48	0.47
1:C:2324:GLN:HA	1:C:2334:GLU:O	2.14	0.47
1:A:1799:GLN:CA	2:A:2602:PLX:H1C1	2.42	0.47
1:A:1985:ILE:HG21	3:A:2603:PEE:H26	1.95	0.47
1:A:2294:TRP:CZ2	1:A:2296:ILE:HD12	2.49	0.47
1:A:2473:ILE:HA	1:A:2476:VAL:HG22	1.97	0.47
1:D:1146:CYS:HA	1:D:1151:ASP:HB3	1.95	0.47
1:D:1218:VAL:HA	1:D:1221:ILE:HG22	1.97	0.47
1:D:2225:ASP:OD2	1:D:2324:GLN:NE2	2.48	0.47
1:D:2311:GLY:O	1:D:2351:ARG:NH1	2.47	0.47
1:C:1162:PHE:CE2	1:C:1166:LEU:HD11	2.50	0.47
1:C:1415:PHE:CE2	1:C:2532:LEU:HD12	2.47	0.47
1:C:1976:VAL:O	1:C:1976:VAL:HG13	2.15	0.47
1:C:2488:ILE:O	1:C:2488:ILE:HG13	2.14	0.47
1:C:2496:GLU:O	1:A:2534:ARG:NH2	2.48	0.47
1:A:831:LEU:HD12	1:A:832:LEU:N	2.30	0.47
1:C:1162:PHE:HE1	1:C:1210:TRP:CZ2	2.33	0.47
1:C:1337:ILE:HA	1:C:1340:LYS:HZ2	1.78	0.47
1:C:2211:SER:HA	1:C:2214:ARG:HE	1.80	0.47
1:A:1977:TYR:OH	1:A:2034:ASP:OD1	2.31	0.47
1:D:2036:ALA:HA	1:D:2142:TRP:CD1	2.49	0.47
1:C:2225:ASP:OD2	1:C:2324:GLN:NE2	2.47	0.47
1:D:1337:ILE:HA	1:D:1340:LYS:HZ2	1.79	0.47
1:D:1734:ILE:HG12	1:D:1794:PHE:HE1	1.75	0.47
1:C:1206:GLN:O	1:C:1210:TRP:HD1	1.98	0.46
1:C:1714:VAL:HG12	1:C:1719:MET:HE3	1.96	0.46
1:C:2183:LYS:O	1:C:2184:LYS:C	2.58	0.46
1:C:2477:VAL:O	1:C:2481:VAL:HG23	2.15	0.46
1:A:2280:ASP:OD2	1:A:2452:LYS:HE3	2.15	0.46
1:A:2326:ASP:HB3	1:A:2329:LYS:HB2	1.97	0.46
1:C:1061:ASP:HA	1:C:1085:PHE:CE1	2.50	0.46
1:C:2193:GLY:O	1:C:2196:ILE:HG12	2.15	0.46
1:A:1718:ALA:HB2	1:A:1729:PHE:CZ	2.50	0.46
1:A:2373:PRO:HB3	1:A:2398:TYR:CD1	2.51	0.46
1:D:1739:VAL:HA	1:D:1742:VAL:HG12	1.97	0.46
1:D:2181:GLN:O	1:D:2183:LYS:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1023:ARG:HD3	1:C:1028:ALA:HB1	1.96	0.46
1:C:1084:ASP:OD1	1:C:1086:PHE:N	2.46	0.46
1:A:1988:ILE:HA	1:A:1991:ILE:HG22	1.97	0.46
1:D:1734:ILE:HD11	1:D:1790:LEU:HD13	1.95	0.46
1:C:1980:MET:HB3	1:C:2092:LEU:CD1	2.44	0.46
1:A:2031:MET:CE	3:A:2603:PEE:C35	2.92	0.46
1:D:1206:GLN:O	1:D:1210:TRP:HD1	1.99	0.46
1:C:2141:VAL:HA	1:D:2188:LYS:NZ	2.30	0.46
1:A:1218:VAL:HA	1:A:1221:ILE:HG22	1.98	0.46
1:A:1233:VAL:HG12	1:A:1233:VAL:O	2.16	0.46
3:A:2603:PEE:H1	3:A:2603:PEE:O2P	2.16	0.46
1:D:2182:LYS:HG2	1:D:2185:LYS:HG3	1.96	0.46
1:D:2380:ASN:ND2	1:D:2453:VAL:HA	2.26	0.46
1:C:1233:VAL:HG12	1:C:1233:VAL:O	2.16	0.46
1:C:1992:ILE:HG21	3:C:2603:PEE:C27	2.46	0.46
1:C:2092:LEU:HD12	1:C:2093:SER:N	2.30	0.46
1:D:2342:LEU:HD22	1:D:2371:LEU:HG	1.97	0.46
1:C:1744:LYS:O	1:C:1748:GLN:HG2	2.16	0.46
1:A:1984:ASP:O	1:A:1988:ILE:HG12	2.16	0.46
1:D:2211:SER:HA	1:D:2214:ARG:HE	1.81	0.46
1:D:2271:GLN:HE22	1:D:2389:GLN:HE22	1.63	0.46
1:C:2286:ILE:CG1	1:C:2444:LEU:HB2	2.46	0.46
1:C:2301:ARG:HH12	1:C:2424:SER:CA	2.29	0.46
1:A:1056:PRO:HB3	1:A:1085:PHE:O	2.16	0.46
1:A:2166:LYS:HB2	1:A:2504:LEU:HD11	1.97	0.46
1:A:2321:TRP:HH2	1:A:2373:PRO:CG	2.24	0.46
1:D:2305:LYS:HD2	1:D:2305:LYS:HA	1.81	0.46
1:D:2460:PHE:HB3	1:D:2465:GLY:HA3	1.98	0.46
1:C:857:THR:HA	1:C:860:ILE:HG22	1.98	0.46
1:C:2372:PHE:HB2	1:C:2399:LEU:O	2.15	0.46
1:C:2468:GLY:O	1:C:2471:VAL:N	2.49	0.46
1:A:2030:THR:HA	1:A:2033:ILE:HG12	1.96	0.46
1:D:1246:ILE:HA	1:D:1251:LEU:CD1	2.46	0.46
1:D:2139:ASP:O	1:D:2143:THR:OG1	2.30	0.46
1:D:2319:PHE:CE2	1:D:2321:TRP:NE1	2.78	0.46
1:C:1024:ARG:HH12	1:C:1211:ASP:CG	2.24	0.46
1:C:2202:ILE:O	1:C:2206:PRO:HD3	2.16	0.46
1:C:2298:PRO:HD2	1:A:2429:TRP:CZ3	2.51	0.46
1:C:2532:LEU:HD11	1:C:2542:TRP:CD1	2.51	0.46
1:A:2085:VAL:O	1:A:2088:ILE:HG22	2.16	0.46
1:C:2280:ASP:OD2	1:C:2452:LYS:HE3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2376:ILE:HA	1:C:2386:PRO:HA	1.98	0.45
1:C:2534:ARG:HG3	1:D:2496:GLU:OE1	2.15	0.45
1:A:2361:ARG:HH11	1:A:2364:GLN:HG2	1.81	0.45
1:A:2463:GLY:H	1:A:2467:VAL:HG21	1.81	0.45
1:D:2280:ASP:OD2	1:D:2452:LYS:HE3	2.16	0.45
3:D:2603:PEE:H1	3:D:2603:PEE:O2P	2.16	0.45
1:C:2535:SER:OG	1:C:2538:THR:OG1	2.28	0.45
1:A:1153:LEU:HD12	4:A:2604:P5S:C48	2.46	0.45
1:D:1233:VAL:HG12	1:D:1233:VAL:O	2.15	0.45
1:D:2280:ASP:O	1:D:2450:SER:N	2.49	0.45
1:D:2405:LEU:HD11	1:D:2428:GLU:HB3	1.98	0.45
1:C:1162:PHE:HE1	1:C:1210:TRP:HZ2	1.62	0.45
1:C:1224:LYS:NZ	1:C:1280:ILE:HD13	2.31	0.45
1:C:2301:ARG:O	1:C:2304:MET:HB2	2.16	0.45
1:A:1084:ASP:OD1	1:A:1086:PHE:N	2.47	0.45
1:A:1692:TYR:HA	1:A:1695:ILE:HG22	1.98	0.45
1:A:2473:ILE:O	1:A:2477:VAL:HG12	2.17	0.45
1:D:2271:GLN:NE2	1:D:2389:GLN:OE1	2.48	0.45
1:D:2301:ARG:HH12	1:D:2424:SER:CA	2.29	0.45
1:C:2119:LEU:HD12	1:C:2167:CYS:CB	2.46	0.45
1:A:2308:LEU:HD22	1:A:2351:ARG:HG3	1.98	0.45
1:D:1280:ILE:HG22	1:D:1280:ILE:O	2.16	0.45
1:D:2324:GLN:HA	1:D:2334:GLU:O	2.17	0.45
1:C:2280:ASP:O	1:C:2450:SER:N	2.50	0.45
1:C:2305:LYS:HD2	1:C:2305:LYS:HA	1.81	0.45
3:C:2603:PEE:C24	3:C:2603:PEE:C44	2.95	0.45
1:A:2211:SER:HA	1:A:2214:ARG:HE	1.82	0.45
1:A:2271:GLN:NE2	1:A:2389:GLN:OE1	2.48	0.45
1:D:1296:ILE:CD1	4:D:2604:P5S:O18	2.65	0.45
1:A:1018:VAL:O	1:A:1022:THR:HG23	2.17	0.45
1:A:1215:LEU:O	1:A:1219:THR:HG23	2.17	0.45
1:A:1696:ILE:HD11	1:A:2083:TYR:CE2	2.52	0.45
1:A:2333:VAL:HG11	1:A:2382:PRO:HA	1.97	0.45
1:A:2375:TYR:CD2	1:A:2390:LEU:HB3	2.52	0.45
1:D:1215:LEU:O	1:D:1219:THR:HG23	2.17	0.45
1:D:2301:ARG:O	1:D:2304:MET:HB2	2.17	0.45
1:C:831:LEU:HD12	1:C:832:LEU:N	2.31	0.45
1:C:1192:LEU:HD23	1:C:1794:PHE:CD2	2.52	0.45
1:C:2204:TRP:CE2	1:A:2025:LEU:HD12	2.52	0.45
1:A:2280:ASP:O	1:A:2450:SER:N	2.50	0.45
1:D:2373:PRO:HB3	1:D:2398:TYR:CD1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2125:PHE:O	1:C:2128:VAL:HG12	2.17	0.45
1:C:2361:ARG:HH11	1:C:2364:GLN:HG2	1.81	0.45
1:C:2479:LYS:HE2	1:A:2480:PHE:CZ	2.52	0.45
1:A:1243:CYS:HA	1:A:1246:ILE:HG22	1.98	0.45
1:A:1739:VAL:HA	1:A:1742:VAL:HG12	1.99	0.45
1:A:2034:ASP:OD1	1:A:2035:ARG:N	2.49	0.45
1:A:2261:GLN:HA	1:A:2264:ASP:HB2	1.98	0.45
1:A:2510:ILE:HG12	1:A:2525:LEU:HB3	1.99	0.45
3:A:2603:PEE:H40	3:A:2603:PEE:H77	1.94	0.45
3:A:2603:PEE:C24	3:A:2603:PEE:C44	2.95	0.45
1:D:1162:PHE:HE1	1:D:1210:TRP:CZ2	2.34	0.45
3:D:2603:PEE:C25	3:D:2603:PEE:C44	2.95	0.45
1:C:2183:LYS:HG3	1:C:2184:LYS:HG2	1.99	0.45
1:C:2471:VAL:HA	1:C:2474:VAL:HG12	1.99	0.45
1:A:2405:LEU:HD11	1:A:2428:GLU:HB3	1.98	0.45
1:D:2119:LEU:HD12	1:D:2167:CYS:CB	2.46	0.45
1:D:2210:MET:HE1	1:D:2466:ILE:HG23	1.98	0.45
1:C:967:ARG:NH1	1:C:1116:THR:OG1	2.49	0.45
1:C:1981:PHE:CZ	3:C:2603:PEE:H8	2.52	0.45
1:C:2055:VAL:O	1:C:2059:ILE:HG12	2.17	0.45
1:D:2258:GLU:HA	1:D:2261:GLN:OE1	2.16	0.45
1:D:2321:TRP:HH2	1:D:2373:PRO:CG	2.22	0.45
1:C:1254:THR:HG23	1:C:1255:VAL:HG12	1.99	0.44
1:C:2294:TRP:CB	1:C:2429:TRP:HA	2.41	0.44
1:C:2325:ARG:NH1	1:C:2336:THR:OG1	2.47	0.44
1:A:2286:ILE:CG1	1:A:2444:LEU:HB2	2.46	0.44
1:A:2294:TRP:CB	1:A:2429:TRP:HA	2.41	0.44
1:A:2498:PRO:HD3	1:D:2534:ARG:NH2	2.26	0.44
1:D:2220:VAL:HG21	1:D:2280:ASP:HA	2.00	0.44
1:C:2318:ARG:CZ	1:A:2245:GLN:HG2	2.47	0.44
1:C:2319:PHE:CE2	1:C:2321:TRP:NE1	2.78	0.44
3:C:2603:PEE:H1	3:C:2603:PEE:O2P	2.16	0.44
1:A:1024:ARG:HH12	1:A:1211:ASP:CG	2.24	0.44
1:D:1301:TYR:HA	1:D:1304:HIS:CD2	2.53	0.44
1:D:2376:ILE:HA	1:D:2386:PRO:HA	1.99	0.44
1:C:1349:MET:HE2	1:C:1353:ARG:HH21	1.82	0.44
1:D:2325:ARG:NH1	1:D:2336:THR:OG1	2.47	0.44
1:C:2181:GLN:HB3	1:A:2146:THR:HG22	2.00	0.44
1:D:1243:CYS:HA	1:D:1246:ILE:HG22	1.99	0.44
1:D:2138:MET:HE2	1:D:2138:MET:HA	1.98	0.44
1:D:2263:PHE:O	1:D:2270:MET:HE3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1166:LEU:HB3	1:C:1192:LEU:HD11	1.99	0.44
1:C:2138:MET:HE1	3:C:2603:PEE:H54	1.98	0.44
1:A:2204:TRP:CH2	1:D:2025:LEU:HB2	2.52	0.44
1:A:2220:VAL:HG21	1:A:2280:ASP:HA	1.99	0.44
1:A:2258:GLU:HA	1:A:2261:GLN:OE1	2.18	0.44
1:D:792:ALA:O	1:D:796:ARG:HG2	2.17	0.44
1:D:1227:LEU:HD21	1:D:1251:LEU:HG	1.99	0.44
1:D:2193:GLY:HA2	1:D:2196:ILE:HG12	2.00	0.44
1:D:2324:GLN:HG3	1:D:2335:TYR:HD1	1.81	0.44
3:D:2603:PEE:C23	3:D:2603:PEE:H81	2.47	0.44
1:C:792:ALA:O	1:C:796:ARG:HG2	2.17	0.44
1:C:2182:LYS:O	1:C:2183:LYS:C	2.60	0.44
1:D:2162:ILE:HD11	1:D:2500:VAL:HB	1.99	0.44
1:D:2263:PHE:C	1:D:2270:MET:HE3	2.43	0.44
1:D:2286:ILE:CG1	1:D:2444:LEU:HB2	2.47	0.44
1:A:2125:PHE:O	1:A:2128:VAL:HG12	2.17	0.44
1:D:1024:ARG:HH12	1:D:1211:ASP:CG	2.25	0.44
1:D:1349:MET:HE2	1:D:1353:ARG:HH21	1.83	0.44
1:C:1018:VAL:O	1:C:1022:THR:HG23	2.18	0.44
1:A:792:ALA:O	1:A:796:ARG:HG2	2.17	0.44
1:A:1143:PHE:HA	1:A:1151:ASP:OD1	2.17	0.44
1:A:2301:ARG:HH12	1:A:2424:SER:CA	2.31	0.44
1:D:2031:MET:HA	1:D:2034:ASP:OD2	2.18	0.44
1:D:2395:GLU:HA	1:D:2398:TYR:CD2	2.52	0.44
3:D:2603:PEE:C24	3:D:2603:PEE:C44	2.95	0.44
1:C:1698:ASN:O	1:C:1703:ALA:HB3	2.18	0.44
1:C:1977:TYR:O	1:C:1980:MET:HG2	2.17	0.44
1:C:2375:TYR:H	1:C:2391:GLN:NE2	2.14	0.44
1:C:2407:ARG:HB3	1:C:2426:PHE:CD2	2.53	0.44
1:A:2145:THR:HG21	1:A:2152:TRP:CZ3	2.50	0.44
1:A:2395:GLU:HA	1:A:2398:TYR:CD2	2.53	0.44
1:A:2406:ARG:HA	1:A:2406:ARG:HD3	1.80	0.44
1:A:2521:LEU:O	1:A:2525:LEU:HD23	2.17	0.44
3:A:2603:PEE:C25	3:A:2603:PEE:C44	2.95	0.44
1:D:2361:ARG:HH11	1:D:2364:GLN:HG2	1.82	0.44
3:D:2603:PEE:C24	3:D:2603:PEE:H77	2.48	0.44
1:C:2324:GLN:HG3	1:C:2335:TYR:HD1	1.82	0.43
1:C:2405:LEU:HD11	1:C:2428:GLU:HB3	1.99	0.43
1:C:2534:ARG:NH2	1:D:2498:PRO:HD3	2.29	0.43
1:A:967:ARG:NH1	1:A:1116:THR:OG1	2.51	0.43
1:A:2182:LYS:O	1:A:2183:LYS:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2301:ARG:HH12	1:C:2424:SER:HA	1.82	0.43
3:C:2603:PEE:C25	3:C:2603:PEE:C44	2.95	0.43
1:A:1206:GLN:O	1:A:1210:TRP:HD1	2.01	0.43
1:D:1023:ARG:HB3	1:D:1028:ALA:HB3	1.99	0.43
1:D:2209:PHE:HD1	1:D:2212:LEU:HD21	1.84	0.43
1:D:2372:PHE:HB2	1:D:2399:LEU:O	2.19	0.43
1:D:2406:ARG:HA	1:D:2406:ARG:HD3	1.82	0.43
1:C:2220:VAL:HG21	1:C:2280:ASP:HA	2.00	0.43
1:A:2289:SER:HA	1:A:2431:VAL:HG13	2.00	0.43
1:A:2318:ARG:HH22	1:D:2245:GLN:HG2	1.83	0.43
1:A:2407:ARG:HB3	1:A:2426:PHE:CD2	2.53	0.43
1:A:2408:GLU:O	1:A:2426:PHE:HA	2.18	0.43
3:A:2603:PEE:C23	3:A:2603:PEE:H81	2.47	0.43
1:A:1300:HIS:CD2	4:A:2604:P5S:N	2.86	0.43
1:A:2231:LYS:HB3	1:A:2318:ARG:HB2	1.99	0.43
1:D:1157:VAL:CG2	4:D:2604:P5S:H23	2.48	0.43
1:D:1981:PHE:HD2	3:D:2603:PEE:C13	2.22	0.43
1:C:2204:TRP:CH2	1:A:2025:LEU:HB2	2.53	0.43
1:A:2496:GLU:O	1:D:2534:ARG:NH2	2.52	0.43
1:D:1160:TYR:CE1	2:D:2602:PLX:O2	2.67	0.43
1:D:2375:TYR:HD1	1:D:2391:GLN:NE2	2.15	0.43
1:D:2473:ILE:O	1:D:2477:VAL:HG12	2.18	0.43
1:C:1292:LEU:O	1:C:1296:ILE:HG12	2.18	0.43
1:C:2527:ALA:O	1:C:2530:ILE:HG22	2.18	0.43
1:A:2361:ARG:NH1	1:A:2364:GLN:HG2	2.34	0.43
1:A:2372:PHE:HB2	1:A:2399:LEU:O	2.19	0.43
2:A:2602:PLX:H202	2:A:2602:PLX:H171	1.90	0.43
1:D:967:ARG:NH1	1:D:1116:THR:OG1	2.51	0.43
1:C:1192:LEU:HD23	1:C:1794:PHE:CE2	2.53	0.43
1:C:2241:MET:CE	1:C:2291:GLY:HA2	2.47	0.43
1:C:2318:ARG:HH12	1:A:2245:GLN:N	2.13	0.43
1:C:2370:HIS:HB3	1:C:2398:TYR:O	2.18	0.43
1:A:1415:PHE:HE2	1:A:2532:LEU:HD13	1.83	0.43
1:A:2181:GLN:HB3	1:D:2146:THR:HG22	2.00	0.43
1:A:2376:ILE:HA	1:A:2386:PRO:HA	2.00	0.43
1:D:1018:VAL:O	1:D:1022:THR:HG23	2.18	0.43
1:C:967:ARG:HG2	1:C:980:TYR:CE1	2.54	0.43
3:C:2603:PEE:C24	3:C:2603:PEE:H77	2.48	0.43
1:A:1023:ARG:HB3	1:A:1028:ALA:HB3	2.00	0.43
1:A:2193:GLY:O	1:A:2196:ILE:HG12	2.17	0.43
1:A:2523:GLU:HG2	1:A:2524:GLU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1521:ARG:O	1:D:1528:ARG:NH2	2.50	0.43
1:D:2247:SER:O	1:D:2285:GLN:NE2	2.52	0.43
1:D:2257:GLU:O	1:D:2261:GLN:OE1	2.37	0.43
1:D:2471:VAL:HA	1:D:2474:VAL:HG12	2.00	0.43
1:D:2523:GLU:HG2	1:D:2524:GLU:N	2.34	0.43
1:C:2148:SER:HB3	1:C:2151:ASN:ND2	2.33	0.43
1:C:2444:LEU:HB3	1:C:2446:MET:HE2	2.00	0.43
1:C:2512:LEU:O	1:C:2516:THR:HG23	2.19	0.43
3:C:2603:PEE:C23	3:C:2603:PEE:H81	2.47	0.43
1:A:2257:GLU:O	1:A:2261:GLN:OE1	2.37	0.43
1:A:2271:GLN:HE22	1:A:2389:GLN:HE22	1.67	0.43
1:D:2261:GLN:HA	1:D:2264:ASP:HB2	2.01	0.43
1:C:2093:SER:O	1:C:2097:ILE:HG13	2.18	0.43
1:C:2123:GLN:O	1:C:2127:LEU:HG	2.19	0.43
1:C:2183:LYS:HD3	1:A:2146:THR:C	2.44	0.43
1:C:2202:ILE:HG23	1:C:2203:ILE:HG13	2.01	0.43
1:C:2231:LYS:HG3	1:C:2237:PRO:HA	2.01	0.43
1:A:1296:ILE:CD1	4:A:2604:P5S:O18	2.65	0.43
1:A:2161:ASN:O	1:A:2164:ILE:HG22	2.19	0.43
1:A:2182:LYS:HD3	1:A:2185:LYS:H	1.84	0.43
1:D:1350:LYS:HE3	1:D:1350:LYS:HB3	1.91	0.43
1:D:2301:ARG:HH12	1:D:2424:SER:HA	1.83	0.43
1:D:2407:ARG:HB3	1:D:2426:PHE:CD2	2.53	0.43
1:C:1521:ARG:O	1:C:1528:ARG:NH2	2.52	0.42
1:C:2052:VAL:HG13	1:C:2053:LEU:HD22	2.00	0.42
1:C:2227:THR:CG2	1:C:2324:GLN:HE22	2.32	0.42
1:C:2357:LEU:CD2	1:C:2405:LEU:HB2	2.48	0.42
1:A:1300:HIS:HD2	4:A:2604:P5S:N	2.16	0.42
1:A:1695:ILE:HD11	1:A:1710:LEU:CG	2.46	0.42
1:A:1980:MET:HB2	1:A:2089:TYR:HD1	1.83	0.42
1:A:2119:LEU:HD12	1:A:2167:CYS:CB	2.48	0.42
1:A:2326:ASP:C	1:A:2328:ALA:H	2.27	0.42
1:D:2161:ASN:O	1:D:2164:ILE:HG22	2.19	0.42
1:D:2445:PRO:O	1:D:2446:MET:HE2	2.19	0.42
1:C:2210:MET:HG3	1:C:2214:ARG:NH2	2.33	0.42
1:C:2220:VAL:O	1:C:2329:LYS:HD2	2.19	0.42
1:C:2468:GLY:O	1:C:2469:LEU:C	2.62	0.42
1:A:2342:LEU:HD22	1:A:2371:LEU:HG	2.00	0.42
1:D:1192:LEU:HB3	1:D:1794:PHE:CE2	2.54	0.42
1:C:1056:PRO:HA	1:C:1085:PHE:HB3	2.01	0.42
1:C:2375:TYR:HD1	1:C:2447:VAL:HB	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2206:PRO:O	1:D:2210:MET:HB2	2.19	0.42
1:D:2468:GLY:O	1:D:2471:VAL:N	2.53	0.42
1:C:2025:LEU:HD12	1:C:2026:VAL:N	2.34	0.42
1:C:2188:LYS:HE2	1:A:2141:VAL:O	2.19	0.42
1:C:2303:GLN:OE1	1:C:2304:MET:HE2	2.19	0.42
1:C:2388:LYS:NZ	1:C:2392:PRO:O	2.53	0.42
1:A:2183:LYS:HE3	1:D:2147:LEU:C	2.44	0.42
1:A:2247:SER:O	1:A:2285:GLN:NE2	2.51	0.42
1:A:2325:ARG:HB2	1:A:2334:GLU:HB3	2.01	0.42
4:A:2604:P5S:H51A	4:A:2604:P5S:H30	2.01	0.42
1:D:2357:LEU:CD2	1:D:2405:LEU:HB2	2.49	0.42
1:D:2388:LYS:NZ	1:D:2392:PRO:O	2.53	0.42
1:D:2407:ARG:HB3	1:D:2426:PHE:CB	2.49	0.42
3:D:2603:PEE:H38	3:D:2603:PEE:H43	1.83	0.42
1:C:1300:HIS:HD2	4:C:2604:P5S:N	2.18	0.42
1:C:1354:ALA:O	1:C:1357:GLU:HG3	2.19	0.42
1:A:967:ARG:HG2	1:A:980:TYR:CE1	2.53	0.42
1:A:2404:GLN:OE1	1:A:2406:ARG:NH2	2.53	0.42
1:D:2408:GLU:O	1:D:2426:PHE:HA	2.18	0.42
1:C:1157:VAL:HG12	4:C:2604:P5S:H23	1.96	0.42
1:C:1296:ILE:CD1	4:C:2604:P5S:O18	2.67	0.42
1:C:2020:PHE:HA	1:C:2023:MET:HE2	2.00	0.42
1:C:2169:ARG:O	1:C:2173:LYS:HG3	2.20	0.42
1:C:2408:GLU:O	1:C:2426:PHE:HA	2.18	0.42
1:A:1981:PHE:HE2	3:A:2603:PEE:H20	1.82	0.42
1:C:802:ARG:HH21	1:C:943:ARG:HH21	1.67	0.42
1:A:1537:GLU:O	1:A:1540:LEU:HG	2.20	0.42
1:A:2169:ARG:O	1:A:2173:LYS:HG3	2.20	0.42
3:A:2603:PEE:C24	3:A:2603:PEE:H77	2.48	0.42
1:D:2030:THR:HA	1:D:2033:ILE:HG22	2.00	0.42
1:D:2303:GLN:OE1	1:D:2304:MET:HE2	2.20	0.42
1:C:791:SER:O	1:C:795:THR:HG23	2.20	0.42
1:A:840:LEU:HD23	1:A:840:LEU:HA	1.90	0.42
1:A:1148:SER:OG	1:A:1151:ASP:OD2	2.20	0.42
1:A:1698:ASN:O	1:A:1703:ALA:HB3	2.20	0.42
1:A:2031:MET:HA	1:A:2034:ASP:OD2	2.20	0.42
1:A:2109:PHE:CB	3:A:2603:PEE:H11	2.48	0.42
1:A:2388:LYS:NZ	1:A:2392:PRO:O	2.52	0.42
1:A:2502:ARG:HH22	1:A:2546:ARG:CZ	2.33	0.42
1:D:827:VAL:C	1:D:829:ASN:H	2.27	0.42
1:D:967:ARG:HG2	1:D:980:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2438:LYS:HE2	1:D:2438:LYS:HB3	1.89	0.42
1:C:1169:VAL:HG22	1:C:1286:CYS:SG	2.60	0.42
1:C:1184:TYR:HE2	1:C:1283:ASP:OD1	2.03	0.42
1:C:1196:THR:O	1:C:1200:GLN:HG2	2.20	0.42
1:C:2145:THR:HG21	1:C:2152:TRP:CZ3	2.55	0.42
1:C:2287:GLU:HB3	1:C:2290:SER:HB3	2.02	0.42
1:A:1041:THR:HA	1:A:1101:LEU:HD11	2.02	0.42
1:A:1251:LEU:HD12	1:A:1251:LEU:H	1.84	0.42
1:A:2231:LYS:HG3	1:A:2237:PRO:HA	2.02	0.42
1:A:2318:ARG:CZ	1:D:2245:GLN:HG2	2.50	0.42
1:D:1041:THR:HA	1:D:1101:LEU:HD11	2.02	0.42
1:D:2231:LYS:HG3	1:D:2237:PRO:HA	2.02	0.42
1:D:2289:SER:HA	1:D:2431:VAL:HG13	2.01	0.42
1:D:2404:GLN:N	1:D:2431:VAL:O	2.52	0.42
1:D:2468:GLY:O	1:D:2472:GLU:OE1	2.37	0.42
3:D:2603:PEE:H82	3:D:2603:PEE:H75	1.66	0.42
1:C:1301:TYR:HA	1:C:1304:HIS:CD2	2.55	0.42
1:C:1989:ILE:HD13	3:C:2603:PEE:H37	1.92	0.42
1:C:2036:ALA:HA	1:C:2142:TRP:CD1	2.55	0.42
1:C:2261:GLN:HA	1:C:2264:ASP:HB2	2.01	0.42
1:C:2314:ASP:HB3	1:C:2343:GLU:CD	2.45	0.42
1:C:2447:VAL:O	1:C:2448:ILE:HD13	2.20	0.42
1:A:1170:PHE:CD1	1:A:1170:PHE:C	2.98	0.42
1:A:1183:GLY:HA2	1:A:1186:LEU:HG	2.02	0.42
1:A:1196:THR:O	1:A:1200:GLN:HG2	2.20	0.42
1:A:1353:ARG:NH2	1:A:2518:GLU:OE2	2.53	0.42
1:A:2082:TRP:O	1:A:2086:LYS:HG2	2.20	0.42
1:D:2169:ARG:O	1:D:2173:LYS:HG3	2.20	0.42
1:D:2361:ARG:NH1	1:D:2364:GLN:HG2	2.35	0.42
4:D:2604:P5S:H51A	4:D:2604:P5S:H30	2.01	0.42
1:C:1153:LEU:HD12	4:C:2604:P5S:C48	2.50	0.41
1:C:1300:HIS:CD2	4:C:2604:P5S:N	2.88	0.41
1:C:2209:PHE:HD1	1:C:2212:LEU:HD21	1.84	0.41
1:C:2342:LEU:HD22	1:C:2371:LEU:HG	2.01	0.41
1:A:791:SER:O	1:A:795:THR:HG23	2.20	0.41
1:A:1157:VAL:HG11	4:A:2604:P5S:H23	2.01	0.41
1:A:1973:ALA:O	1:A:2102:PRO:HB3	2.20	0.41
1:A:2322:ASN:OD1	1:A:2324:GLN:NE2	2.53	0.41
1:D:2256:TYR:OH	1:D:2273:ILE:O	2.31	0.41
1:C:2023:MET:HA	1:C:2026:VAL:HG22	2.02	0.41
1:C:2361:ARG:NH1	1:C:2364:GLN:HG2	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2370:HIS:HA	1:C:2399:LEU:C	2.45	0.41
1:A:1552:ARG:O	1:A:1555:VAL:HG22	2.20	0.41
1:A:1731:MET:HA	1:A:1734:ILE:HG22	2.03	0.41
1:A:1739:VAL:O	1:A:1743:THR:HG23	2.20	0.41
1:A:2058:HIS:CD2	1:A:2083:TYR:HH	2.38	0.41
1:A:2318:ARG:HD2	1:A:2318:ARG:HA	1.85	0.41
1:D:2220:VAL:O	1:D:2329:LYS:HD2	2.21	0.41
1:C:1164:LEU:O	1:C:1168:VAL:HG23	2.21	0.41
1:C:1981:PHE:CD1	3:C:2603:PEE:H8	2.55	0.41
1:C:2373:PRO:HB3	1:C:2398:TYR:CD1	2.54	0.41
4:C:2604:P5S:H51A	4:C:2604:P5S:H30	2.01	0.41
1:A:827:VAL:C	1:A:829:ASN:H	2.28	0.41
1:A:1192:LEU:HB3	1:A:1794:PHE:CE2	2.54	0.41
1:A:2357:LEU:HD23	1:A:2405:LEU:HD22	2.01	0.41
1:D:791:SER:O	1:D:795:THR:HG23	2.21	0.41
1:D:990:GLY:HA3	1:D:1107:GLN:OE1	2.20	0.41
1:D:1056:PRO:HA	1:D:1085:PHE:HB3	2.01	0.41
1:D:2161:ASN:O	1:D:2165:ILE:HG12	2.21	0.41
1:D:2210:MET:HG3	1:D:2214:ARG:CZ	2.50	0.41
1:C:996:LEU:HD22	1:C:1287:PHE:HE1	1.84	0.41
1:C:1727:LYS:O	1:C:1731:MET:HG2	2.20	0.41
1:C:1988:ILE:HA	1:C:1991:ILE:HG22	2.02	0.41
1:A:802:ARG:HH21	1:A:943:ARG:HH21	1.67	0.41
1:A:1280:ILE:HG13	1:A:1283:ASP:HB3	2.01	0.41
1:A:2301:ARG:HH12	1:A:2424:SER:HA	1.85	0.41
1:A:2319:PHE:CE2	1:A:2321:TRP:NE1	2.78	0.41
1:C:1023:ARG:HB3	1:C:1028:ALA:HB3	2.01	0.41
1:C:2530:ILE:HG13	1:D:2496:GLU:OE2	2.21	0.41
1:A:1243:CYS:O	1:A:1246:ILE:HG22	2.19	0.41
1:D:1552:ARG:O	1:D:1555:VAL:HG22	2.20	0.41
1:D:2207:LEU:O	1:D:2210:MET:HB3	2.21	0.41
1:D:2357:LEU:HD23	1:D:2405:LEU:HD22	2.02	0.41
1:C:1216:TYR:HA	1:C:1219:THR:HG22	2.02	0.41
1:A:2407:ARG:HB3	1:A:2426:PHE:CB	2.49	0.41
1:D:1746:LEU:HD23	1:D:1746:LEU:HA	1.90	0.41
1:D:2318:ARG:HA	1:D:2318:ARG:HD2	1.83	0.41
1:C:1977:TYR:OH	1:C:2035:ARG:HD2	2.21	0.41
1:C:2247:SER:O	1:C:2285:GLN:NE2	2.54	0.41
1:A:2251:PHE:CE2	1:A:2281:ILE:HG22	2.55	0.41
1:A:2325:ARG:NH1	1:A:2336:THR:OG1	2.49	0.41
1:D:1196:THR:O	1:D:1200:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1973:ALA:O	1:D:2102:PRO:HB3	2.20	0.41
1:D:1981:PHE:HE2	3:D:2603:PEE:H20	1.83	0.41
1:D:1985:ILE:HG21	3:D:2603:PEE:H26	2.01	0.41
1:C:1695:ILE:HA	1:C:1789:GLN:NE2	2.36	0.41
1:C:2326:ASP:C	1:C:2328:ALA:H	2.28	0.41
1:C:2380:ASN:ND2	1:C:2453:VAL:HG12	2.36	0.41
1:A:2209:PHE:HD1	1:A:2212:LEU:HD21	1.86	0.41
1:D:2314:ASP:HB3	1:D:2343:GLU:CD	2.46	0.41
1:D:2326:ASP:C	1:D:2328:ALA:H	2.28	0.41
1:C:967:ARG:H	1:C:967:ARG:HG3	1.64	0.41
1:C:981:PHE:HZ	4:C:2604:P5S:C41	2.09	0.41
1:C:991:LEU:HD12	1:C:992:GLU:N	2.36	0.41
1:C:1693:PHE:CE1	1:C:1697:LEU:HD21	2.56	0.41
1:C:1695:ILE:HD13	1:C:1714:VAL:HG21	2.03	0.41
1:C:1973:ALA:O	1:C:2102:PRO:HB3	2.20	0.41
1:C:2138:MET:HE1	3:C:2603:PEE:C34	2.51	0.41
1:C:2140:TRP:HD1	1:C:2152:TRP:CD2	2.39	0.41
1:C:2253:PRO:O	1:C:2256:TYR:HB3	2.21	0.41
1:C:2258:GLU:HA	1:C:2261:GLN:OE1	2.20	0.41
1:C:2269:ALA:O	1:C:2273:ILE:HG13	2.20	0.41
1:C:2357:LEU:HD23	1:C:2405:LEU:HD22	2.02	0.41
1:C:2404:GLN:N	1:C:2431:VAL:O	2.54	0.41
1:A:1160:TYR:CE1	2:A:2602:PLX:O2	2.68	0.41
1:A:1301:TYR:HA	1:A:1304:HIS:CD2	2.55	0.41
1:A:1690:LEU:O	1:A:1694:ILE:HG12	2.21	0.41
1:A:2161:ASN:O	1:A:2165:ILE:HG12	2.20	0.41
1:A:2317:LEU:HD12	1:A:2319:PHE:HB2	2.03	0.41
1:A:2536:PRO:O	1:A:2539:MET:HG2	2.21	0.41
4:A:2604:P5S:H2	4:A:2604:P5S:H39	1.48	0.41
1:D:1226:MET:SD	1:D:1227:LEU:N	2.94	0.41
1:D:1246:ILE:HA	1:D:1251:LEU:HD12	2.01	0.41
1:D:1292:LEU:O	1:D:1296:ILE:HG12	2.21	0.41
1:D:1300:HIS:HD2	4:D:2604:P5S:N	2.19	0.41
1:D:1300:HIS:CD2	4:D:2604:P5S:N	2.89	0.41
1:D:1354:ALA:O	1:D:1357:GLU:HG3	2.20	0.41
1:D:2071:ARG:O	1:D:2076:ASN:N	2.33	0.41
1:D:2227:THR:CG2	1:D:2324:GLN:HE22	2.32	0.41
1:D:2251:PHE:CE2	1:D:2281:ILE:HG22	2.56	0.41
2:D:2601:PLX:O1	2:D:2601:PLX:H1A2	2.21	0.41
3:D:2603:PEE:H82	3:D:2603:PEE:C40	2.51	0.41
1:C:827:VAL:C	1:C:829:ASN:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1552:ARG:O	1:C:1555:VAL:HG22	2.20	0.41
1:C:2141:VAL:O	1:D:2188:LYS:NZ	2.42	0.41
1:C:2510:ILE:HG12	1:C:2525:LEU:HB3	2.03	0.41
1:A:990:GLY:HA3	1:A:1107:GLN:OE1	2.21	0.41
1:A:1299:SER:HB2	1:A:1301:TYR:HD1	1.85	0.41
1:A:2226:VAL:HG23	1:A:2323:PHE:HD1	1.86	0.41
1:A:2339:LYS:HE3	1:A:2339:LYS:HB3	1.95	0.41
1:D:2230:LEU:HD23	1:D:2238:LEU:HB2	2.03	0.41
1:D:2308:LEU:HD22	1:D:2351:ARG:HG3	2.03	0.41
1:D:2322:ASN:HA	1:D:2337:ASN:HB3	2.03	0.41
1:D:2463:GLY:H	1:D:2467:VAL:HG21	1.86	0.41
1:D:2510:ILE:HG12	1:D:2525:LEU:HB3	2.03	0.41
1:C:840:LEU:HD23	1:C:840:LEU:HA	1.90	0.40
1:A:1164:LEU:O	1:A:1168:VAL:HG23	2.21	0.40
1:A:1292:LEU:O	1:A:1296:ILE:HG12	2.21	0.40
1:A:2257:GLU:O	1:A:2260:SER:HB2	2.20	0.40
1:A:2269:ALA:O	1:A:2273:ILE:HG13	2.21	0.40
1:A:2538:THR:O	1:A:2542:TRP:N	2.54	0.40
1:D:2277:SER:HB2	1:D:2278:PRO:HD2	2.03	0.40
1:C:2071:ARG:O	1:C:2076:ASN:N	2.33	0.40
1:C:2161:ASN:O	1:C:2165:ILE:HG12	2.21	0.40
1:C:2231:LYS:HZ1	1:C:2235:TYR:N	2.19	0.40
1:C:2253:PRO:O	1:C:2257:GLU:OE1	2.38	0.40
1:A:1030:ALA:HB2	1:A:1111:PHE:HE2	1.86	0.40
1:A:1168:VAL:HG12	1:A:1286:CYS:SG	2.61	0.40
1:A:1337:ILE:O	1:A:1340:LYS:HG2	2.21	0.40
1:A:2077:ALA:O	1:A:2080:GLN:HG2	2.22	0.40
1:D:2020:PHE:HA	1:D:2023:MET:HG2	2.04	0.40
1:D:2321:TRP:HZ3	1:D:2376:ILE:HD12	1.86	0.40
1:C:1211:ASP:O	1:C:1215:LEU:HG	2.21	0.40
1:C:1299:SER:HB2	1:C:1301:TYR:HD1	1.86	0.40
1:A:2527:ALA:HA	1:A:2530:ILE:HG22	2.03	0.40
1:D:2061:MET:N	1:D:2061:MET:SD	2.94	0.40
1:D:2380:ASN:ND2	1:D:2453:VAL:HG12	2.36	0.40
1:D:2526:TYR:O	1:D:2530:ILE:HG12	2.21	0.40
1:C:2135:ARG:HB2	3:C:2603:PEE:H48	2.03	0.40
1:C:2321:TRP:HZ3	1:C:2376:ILE:HD12	1.86	0.40
1:C:2321:TRP:O	1:C:2337:ASN:HA	2.22	0.40
2:C:2601:PLX:O1	2:C:2601:PLX:H1A2	2.21	0.40
3:C:2603:PEE:H82	3:C:2603:PEE:C40	2.51	0.40
1:A:1084:ASP:OD1	1:A:1087:ARG:N	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1354:ALA:O	1:A:1357:GLU:HG3	2.21	0.40
1:A:2318:ARG:HH12	1:D:2245:GLN:N	2.19	0.40
1:A:800:PHE:O	1:A:804:LEU:HG	2.22	0.40
1:A:1734:ILE:HD13	1:A:1793:LEU:HB2	2.03	0.40
1:A:2211:SER:HA	1:A:2214:ARG:HH21	1.87	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	1312/2547 (52%)	1241 (95%)	69 (5%)	2 (0%)	43	75
1	C	1312/2547 (52%)	1245 (95%)	66 (5%)	1 (0%)	48	81
1	D	1312/2547 (52%)	1241 (95%)	69 (5%)	2 (0%)	43	75
All	All	3936/7641 (52%)	3727 (95%)	204 (5%)	5 (0%)	49	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2182	LYS
1	A	2182	LYS
1	D	2182	LYS
1	A	2183	LYS
1	D	2183	LYS

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	869/2246 (39%)	868 (100%)	1 (0%)	88 89
1	C	870/2246 (39%)	870 (100%)	0	100 100
1	D	872/2246 (39%)	872 (100%)	0	100 100
All	All	2611/6738 (39%)	2610 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1300	HIS
1	C	1336	GLN
1	C	1344	GLN
1	C	1789	GLN
1	C	2058	HIS
1	C	2115	ASN
1	C	2222	GLN
1	C	2271	GLN
1	C	2285	GLN
1	C	2380	ASN
1	A	1300	HIS
1	A	1344	GLN
1	A	1748	GLN
1	A	1789	GLN
1	A	2115	ASN
1	A	2271	GLN
1	A	2285	GLN
1	A	2324	GLN
1	A	2380	ASN
1	D	1200	GLN
1	D	1300	HIS
1	D	1336	GLN
1	D	1344	GLN
1	D	1789	GLN
1	D	2058	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2115	ASN
1	D	2271	GLN
1	D	2285	GLN
1	D	2380	ASN
1	D	2391	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 oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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	A	2601	-	51,51,51	0.60	0	53,59,59	0.69	0
3	PEE	A	2603	-	50,50,50	1.20	7 (14%)	53,55,55	1.26	6 (11%)
2	PLX	D	2601	-	51,51,51	0.59	0	53,59,59	0.69	0
2	PLX	C	2601	-	51,51,51	0.59	0	53,59,59	0.69	0
4	P5S	A	2604	-	52,53,53	0.39	0	54,60,60	0.40	0
2	PLX	D	2602	-	51,51,51	0.64	0	53,59,59	0.71	1 (1%)
3	PEE	C	2603	-	50,50,50	1.20	7 (14%)	53,55,55	1.27	6 (11%)
3	PEE	D	2603	-	50,50,50	1.20	7 (14%)	53,55,55	1.27	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	P5S	C	2604	-	52,53,53	0.38	0	54,60,60	0.40	0
4	P5S	D	2604	-	52,53,53	0.39	0	54,60,60	0.40	0
2	PLX	C	2602	-	51,51,51	0.63	0	53,59,59	0.71	1 (1%)
2	PLX	A	2602	-	51,51,51	0.64	0	53,59,59	0.71	1 (1%)

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	A	2601	-	-	3/55/55/55	-
3	PEE	A	2603	-	-	27/54/54/54	-
2	PLX	D	2601	-	-	3/55/55/55	-
2	PLX	C	2601	-	-	3/55/55/55	-
4	P5S	A	2604	-	-	16/59/59/59	-
2	PLX	D	2602	-	-	9/55/55/55	-
3	PEE	C	2603	-	-	27/54/54/54	-
3	PEE	D	2603	-	-	27/54/54/54	-
4	P5S	C	2604	-	-	16/59/59/59	-
4	P5S	D	2604	-	-	16/59/59/59	-
2	PLX	C	2602	-	-	9/55/55/55	-
2	PLX	A	2602	-	-	9/55/55/55	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2603	PEE	C39-C38	3.77	1.53	1.31
3	A	2603	PEE	C39-C38	3.76	1.53	1.31
3	C	2603	PEE	C39-C38	3.76	1.53	1.31
3	A	2603	PEE	C18-C19	3.55	1.51	1.31
3	C	2603	PEE	C18-C19	3.55	1.51	1.31
3	D	2603	PEE	C18-C19	3.55	1.51	1.31
3	D	2603	PEE	P-O4P	3.13	1.71	1.59
3	C	2603	PEE	P-O4P	3.12	1.71	1.59
3	A	2603	PEE	P-O4P	3.12	1.71	1.59
3	A	2603	PEE	O3-C3	-2.74	1.39	1.45
3	C	2603	PEE	O3-C3	-2.73	1.39	1.45
3	D	2603	PEE	O3-C3	-2.73	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2603	PEE	O4P-C4	-2.43	1.35	1.44
3	C	2603	PEE	O4P-C4	-2.42	1.35	1.44
3	D	2603	PEE	O4P-C4	-2.41	1.35	1.44
3	C	2603	PEE	O3-C30	2.35	1.40	1.33
3	D	2603	PEE	O3-C30	2.34	1.40	1.33
3	A	2603	PEE	O3-C30	2.32	1.40	1.33
3	A	2603	PEE	O2-C2	-2.14	1.41	1.46
3	C	2603	PEE	O2-C2	-2.12	1.41	1.46
3	D	2603	PEE	O2-C2	-2.12	1.41	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2603	PEE	O2P-P-O1P	3.46	128.56	112.44
3	D	2603	PEE	O2P-P-O1P	3.46	128.56	112.44
3	A	2603	PEE	O2P-P-O1P	3.46	128.55	112.44
3	C	2603	PEE	C2-O2-C10	2.35	123.41	117.80
3	A	2603	PEE	C2-O2-C10	2.35	123.41	117.80
3	D	2603	PEE	C2-O2-C10	2.34	123.40	117.80
3	C	2603	PEE	O4P-P-O1P	-2.32	99.75	108.94
3	D	2603	PEE	O4P-P-O1P	-2.32	99.76	108.94
3	A	2603	PEE	O4P-P-O1P	-2.31	99.76	108.94
3	D	2603	PEE	C3-O3-C30	-2.25	108.89	117.12
3	C	2603	PEE	C3-O3-C30	-2.25	108.90	117.12
3	A	2603	PEE	C3-O3-C30	-2.25	108.90	117.12
3	A	2603	PEE	C12-C11-C10	-2.19	105.67	113.69
3	C	2603	PEE	C12-C11-C10	-2.19	105.68	113.69
3	D	2603	PEE	C12-C11-C10	-2.19	105.68	113.69
2	D	2602	PLX	C5-C4-C3	-2.14	106.80	111.78
2	C	2602	PLX	C5-C4-C3	-2.13	106.82	111.78
2	A	2602	PLX	C5-C4-C3	-2.13	106.82	111.78
3	D	2603	PEE	O2-C2-C1	2.07	115.78	108.34
3	C	2603	PEE	O2-C2-C1	2.07	115.77	108.34
3	A	2603	PEE	O2-C2-C1	2.07	115.77	108.34
3	D	2603	PEE	C37-C38-C39	-2.00	109.84	124.83

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2602	PLX	O7-C6-O6-C4
2	C	2602	PLX	C2-O1-P1-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	2602	PLX	C2-O1-P1-O2
2	A	2602	PLX	O7-C6-O6-C4
2	A	2602	PLX	C2-O1-P1-O4
2	A	2602	PLX	C2-O1-P1-O2
2	D	2602	PLX	O7-C6-O6-C4
2	D	2602	PLX	C2-O1-P1-O4
2	D	2602	PLX	C2-O1-P1-O2
3	C	2603	PEE	C2-C1-O3P-P
3	C	2603	PEE	C1-O3P-P-O4P
3	C	2603	PEE	C4-O4P-P-O3P
3	C	2603	PEE	C4-O4P-P-O1P
3	A	2603	PEE	C2-C1-O3P-P
3	A	2603	PEE	C1-O3P-P-O4P
3	A	2603	PEE	C4-O4P-P-O3P
3	A	2603	PEE	C4-O4P-P-O1P
3	D	2603	PEE	C2-C1-O3P-P
3	D	2603	PEE	C1-O3P-P-O4P
3	D	2603	PEE	C4-O4P-P-O3P
3	D	2603	PEE	C4-O4P-P-O1P
4	C	2604	P5S	O-C-CA-CB
4	C	2604	P5S	OXT-C-CA-CB
4	C	2604	P5S	CA-CB-OG-P12
4	C	2604	P5S	C3-O16-P12-OG
4	C	2604	P5S	C3-O16-P12-O15
4	C	2604	P5S	C39-C38-O37-C2
4	C	2604	P5S	O47-C38-O37-C2
4	A	2604	P5S	O-C-CA-CB
4	A	2604	P5S	OXT-C-CA-CB
4	A	2604	P5S	CA-CB-OG-P12
4	A	2604	P5S	C3-O16-P12-OG
4	A	2604	P5S	C3-O16-P12-O15
4	A	2604	P5S	C39-C38-O37-C2
4	A	2604	P5S	O47-C38-O37-C2
4	D	2604	P5S	O-C-CA-CB
4	D	2604	P5S	OXT-C-CA-CB
4	D	2604	P5S	CA-CB-OG-P12
4	D	2604	P5S	C3-O16-P12-OG
4	D	2604	P5S	C3-O16-P12-O15
4	D	2604	P5S	C39-C38-O37-C2
4	D	2604	P5S	O47-C38-O37-C2
3	C	2603	PEE	C31-C30-O3-C3
3	A	2603	PEE	C31-C30-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	2603	PEE	C31-C30-O3-C3
3	C	2603	PEE	C41-C42-C43-C44
3	A	2603	PEE	C41-C42-C43-C44
3	D	2603	PEE	C41-C42-C43-C44
3	C	2603	PEE	C11-C10-O2-C2
3	A	2603	PEE	C11-C10-O2-C2
3	D	2603	PEE	C11-C10-O2-C2
3	C	2603	PEE	O5-C30-O3-C3
3	A	2603	PEE	O5-C30-O3-C3
3	D	2603	PEE	O5-C30-O3-C3
3	C	2603	PEE	C1-C2-O2-C10
3	A	2603	PEE	C1-C2-O2-C10
3	D	2603	PEE	C1-C2-O2-C10
3	C	2603	PEE	C31-C32-C33-C34
3	A	2603	PEE	C31-C32-C33-C34
3	D	2603	PEE	C31-C32-C33-C34
3	C	2603	PEE	C17-C18-C19-C20
3	A	2603	PEE	C17-C18-C19-C20
3	D	2603	PEE	C17-C18-C19-C20
3	C	2603	PEE	C43-C44-C45-C46
3	A	2603	PEE	C43-C44-C45-C46
3	D	2603	PEE	C43-C44-C45-C46
3	C	2603	PEE	O4-C10-O2-C2
3	A	2603	PEE	O4-C10-O2-C2
3	D	2603	PEE	O4-C10-O2-C2
3	C	2603	PEE	C44-C45-C46-C47
3	A	2603	PEE	C44-C45-C46-C47
3	D	2603	PEE	C44-C45-C46-C47
3	A	2603	PEE	C14-C15-C16-C17
3	D	2603	PEE	C14-C15-C16-C17
3	C	2603	PEE	C14-C15-C16-C17
3	C	2603	PEE	C12-C13-C14-C15
3	A	2603	PEE	C12-C13-C14-C15
3	D	2603	PEE	C12-C13-C14-C15
3	C	2603	PEE	O2-C2-C3-O3
3	A	2603	PEE	O2-C2-C3-O3
3	D	2603	PEE	O2-C2-C3-O3
2	C	2602	PLX	C20-C21-C22-C23
2	D	2602	PLX	C20-C21-C22-C23
2	A	2602	PLX	C20-C21-C22-C23
4	C	2604	P5S	O19-C1-C2-C3
4	A	2604	P5S	O19-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	2604	P5S	O19-C1-C2-C3
2	C	2602	PLX	C13-C14-C15-C16
2	A	2602	PLX	C13-C14-C15-C16
2	D	2602	PLX	C13-C14-C15-C16
4	C	2604	P5S	C2-C3-O16-P12
4	A	2604	P5S	C2-C3-O16-P12
4	D	2604	P5S	C2-C3-O16-P12
3	C	2603	PEE	C42-C43-C44-C45
3	D	2603	PEE	C42-C43-C44-C45
3	A	2603	PEE	C42-C43-C44-C45
2	C	2602	PLX	C19-C20-C21-C22
2	A	2602	PLX	C19-C20-C21-C22
2	D	2602	PLX	C19-C20-C21-C22
3	C	2603	PEE	C15-C16-C17-C18
3	A	2603	PEE	C15-C16-C17-C18
3	D	2603	PEE	C15-C16-C17-C18
4	C	2604	P5S	O19-C1-C2-O37
4	A	2604	P5S	O19-C1-C2-O37
4	D	2604	P5S	O19-C1-C2-O37
4	C	2604	P5S	N-CA-CB-OG
4	A	2604	P5S	N-CA-CB-OG
4	D	2604	P5S	N-CA-CB-OG
3	C	2603	PEE	C38-C39-C40-C41
3	A	2603	PEE	C38-C39-C40-C41
3	D	2603	PEE	C38-C39-C40-C41
2	C	2601	PLX	C3-O4-P1-O2
2	A	2601	PLX	C3-O4-P1-O2
2	D	2601	PLX	C3-O4-P1-O2
3	C	2603	PEE	C1-O3P-P-O1P
3	A	2603	PEE	C1-O3P-P-O1P
3	D	2603	PEE	C1-O3P-P-O1P
4	C	2604	P5S	CB-OG-P12-O15
4	A	2604	P5S	CB-OG-P12-O15
4	D	2604	P5S	CB-OG-P12-O15
4	C	2604	P5S	O37-C2-C3-O16
4	A	2604	P5S	O37-C2-C3-O16
4	D	2604	P5S	O37-C2-C3-O16
3	D	2603	PEE	C13-C14-C15-C16
3	C	2603	PEE	C13-C14-C15-C16
3	A	2603	PEE	C13-C14-C15-C16
3	C	2603	PEE	C1-C2-C3-O3
3	A	2603	PEE	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	2603	PEE	C1-C2-C3-O3
3	C	2603	PEE	C40-C41-C42-C43
3	A	2603	PEE	C40-C41-C42-C43
3	D	2603	PEE	C40-C41-C42-C43
3	C	2603	PEE	C33-C34-C35-C36
3	D	2603	PEE	C33-C34-C35-C36
3	A	2603	PEE	C33-C34-C35-C36
2	C	2602	PLX	O8-C24-C25-C26
2	A	2602	PLX	O8-C24-C25-C26
2	D	2602	PLX	O8-C24-C25-C26
2	C	2601	PLX	O7-C6-C7-C8
2	A	2601	PLX	O7-C6-C7-C8
2	D	2601	PLX	O7-C6-C7-C8
4	C	2604	P5S	C1-C2-C3-O16
4	A	2604	P5S	C1-C2-C3-O16
4	D	2604	P5S	C1-C2-C3-O16
4	A	2604	P5S	C29-C30-C31-C32
4	D	2604	P5S	C29-C30-C31-C32
4	C	2604	P5S	C29-C30-C31-C32
2	C	2601	PLX	O4-C3-C4-C5
2	A	2601	PLX	O4-C3-C4-C5
2	D	2601	PLX	O4-C3-C4-C5
2	A	2602	PLX	C9-C10-C11-C12
2	C	2602	PLX	C9-C10-C11-C12
2	D	2602	PLX	C9-C10-C11-C12
4	C	2604	P5S	OXT-C-CA-N
4	A	2604	P5S	OXT-C-CA-N
4	D	2604	P5S	OXT-C-CA-N
2	C	2602	PLX	O9-C24-O8-C5
2	A	2602	PLX	O9-C24-O8-C5
2	D	2602	PLX	O9-C24-O8-C5
3	C	2603	PEE	O2-C10-C11-C12
3	A	2603	PEE	O2-C10-C11-C12
3	D	2603	PEE	O2-C10-C11-C12
3	C	2603	PEE	O4-C10-C11-C12
3	A	2603	PEE	O4-C10-C11-C12
3	D	2603	PEE	O4-C10-C11-C12

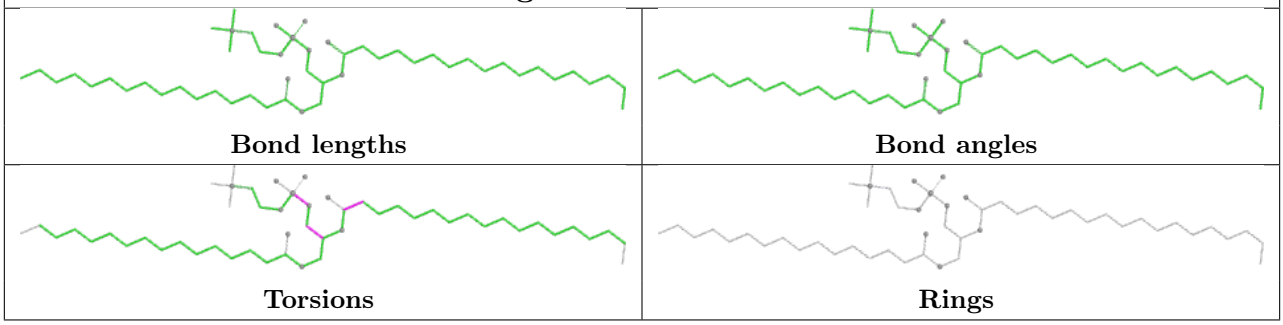
There are no ring outliers.

12 monomers are involved in 304 short contacts:

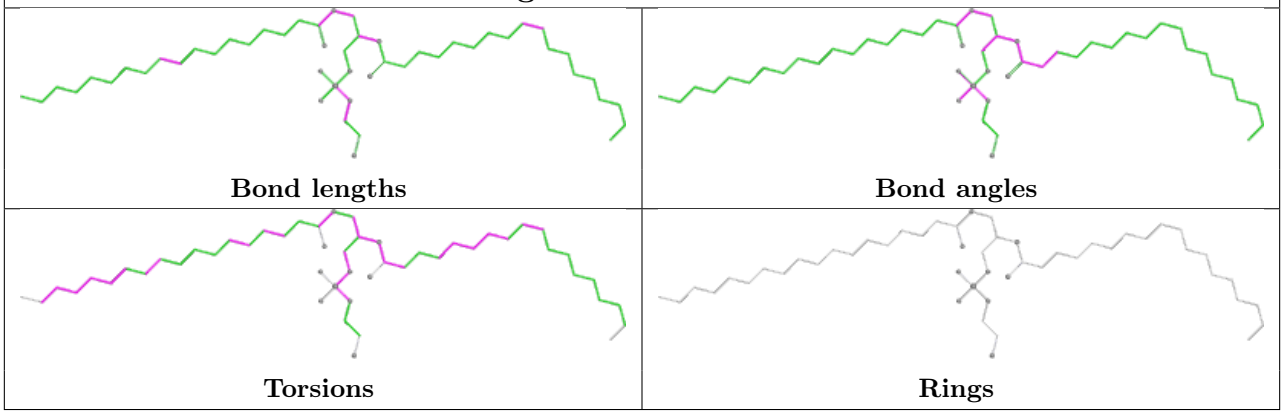
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	PLX	1	0
3	A	2603	PEE	60	0
2	D	2601	PLX	2	0
2	C	2601	PLX	2	0
4	A	2604	P5S	24	0
2	D	2602	PLX	12	0
3	C	2603	PEE	72	0
3	D	2603	PEE	64	0
4	C	2604	P5S	25	0
4	D	2604	P5S	17	0
2	C	2602	PLX	12	0
2	A	2602	PLX	13	0

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.

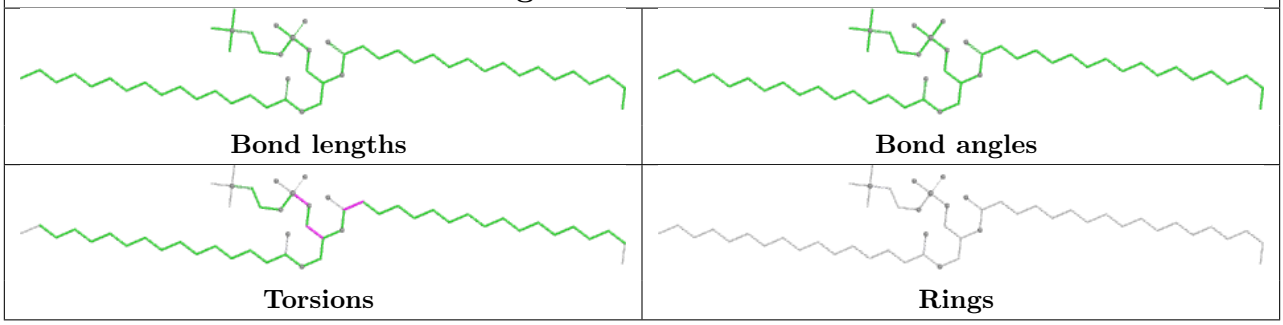
Ligand PLX A 2601



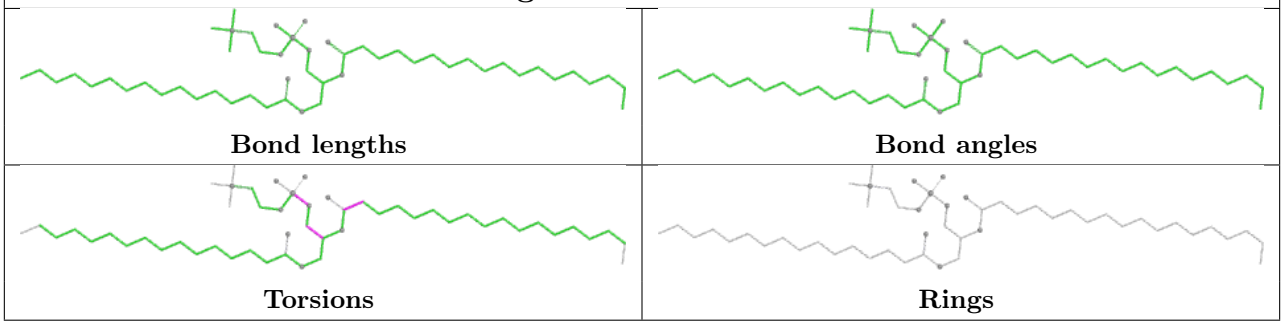
Ligand PEE A 2603



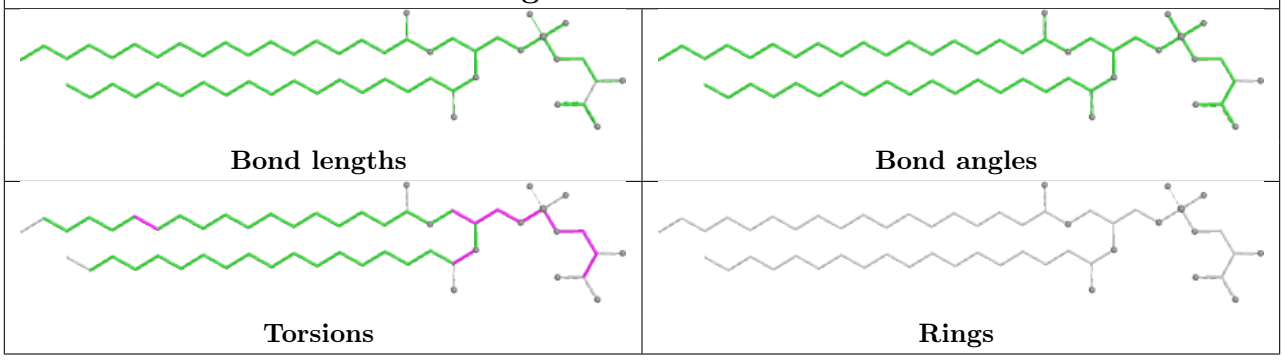
Ligand PLX D 2601



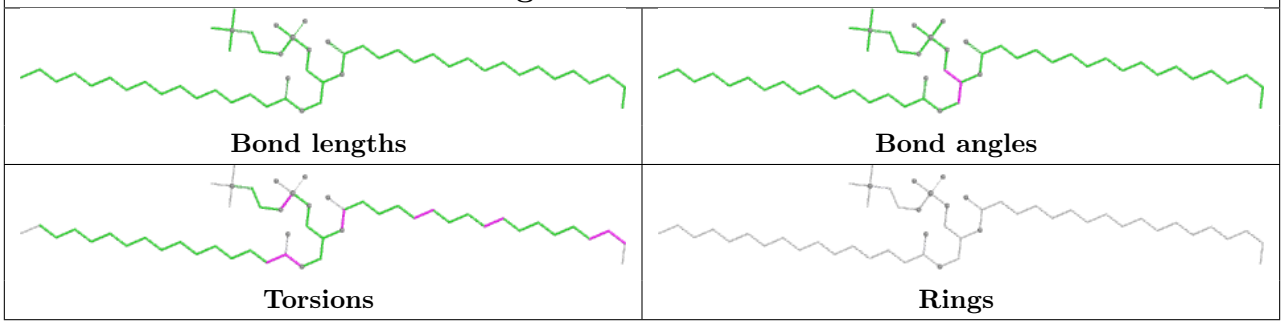
Ligand PLX C 2601



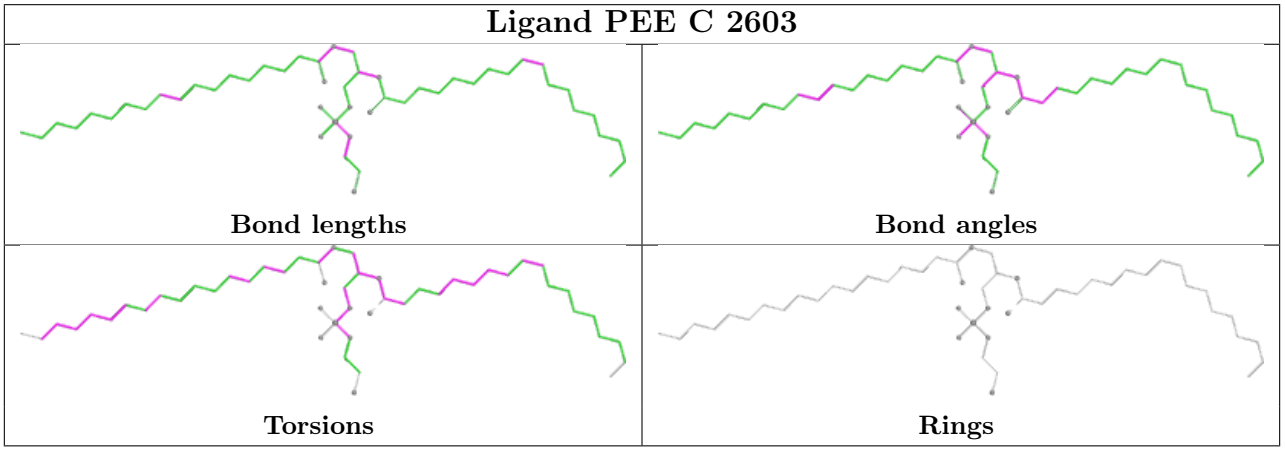
Ligand P5S A 2604



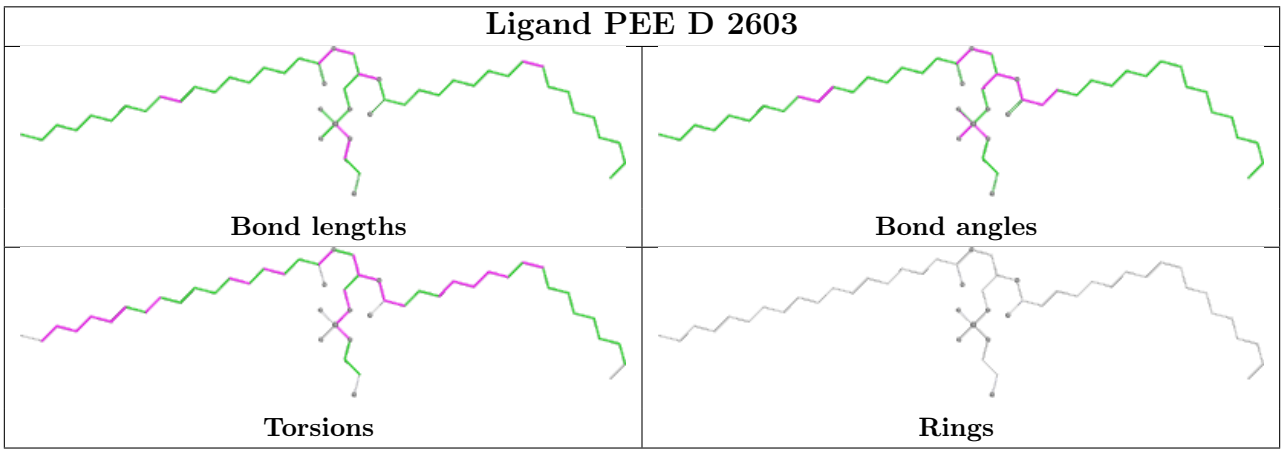
Ligand PLX D 2602



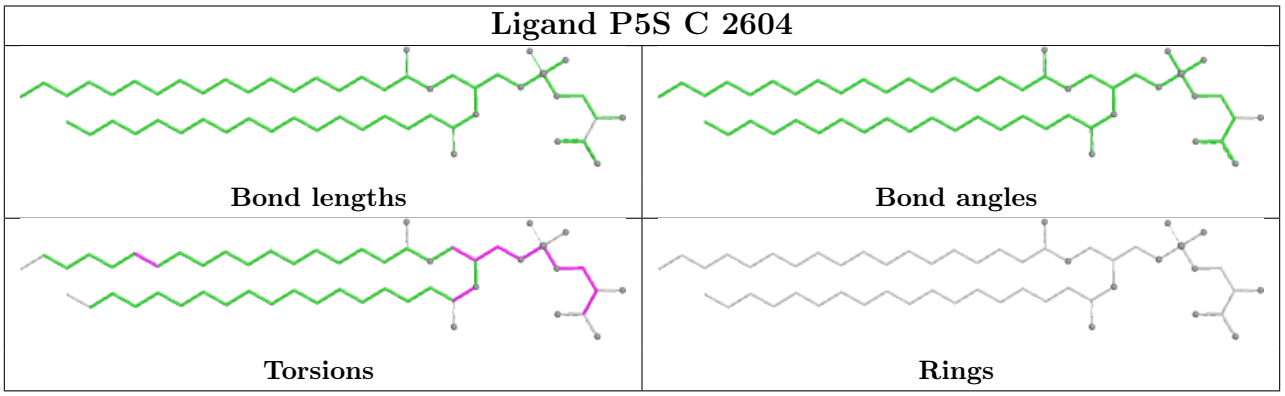
Ligand PEE C 2603

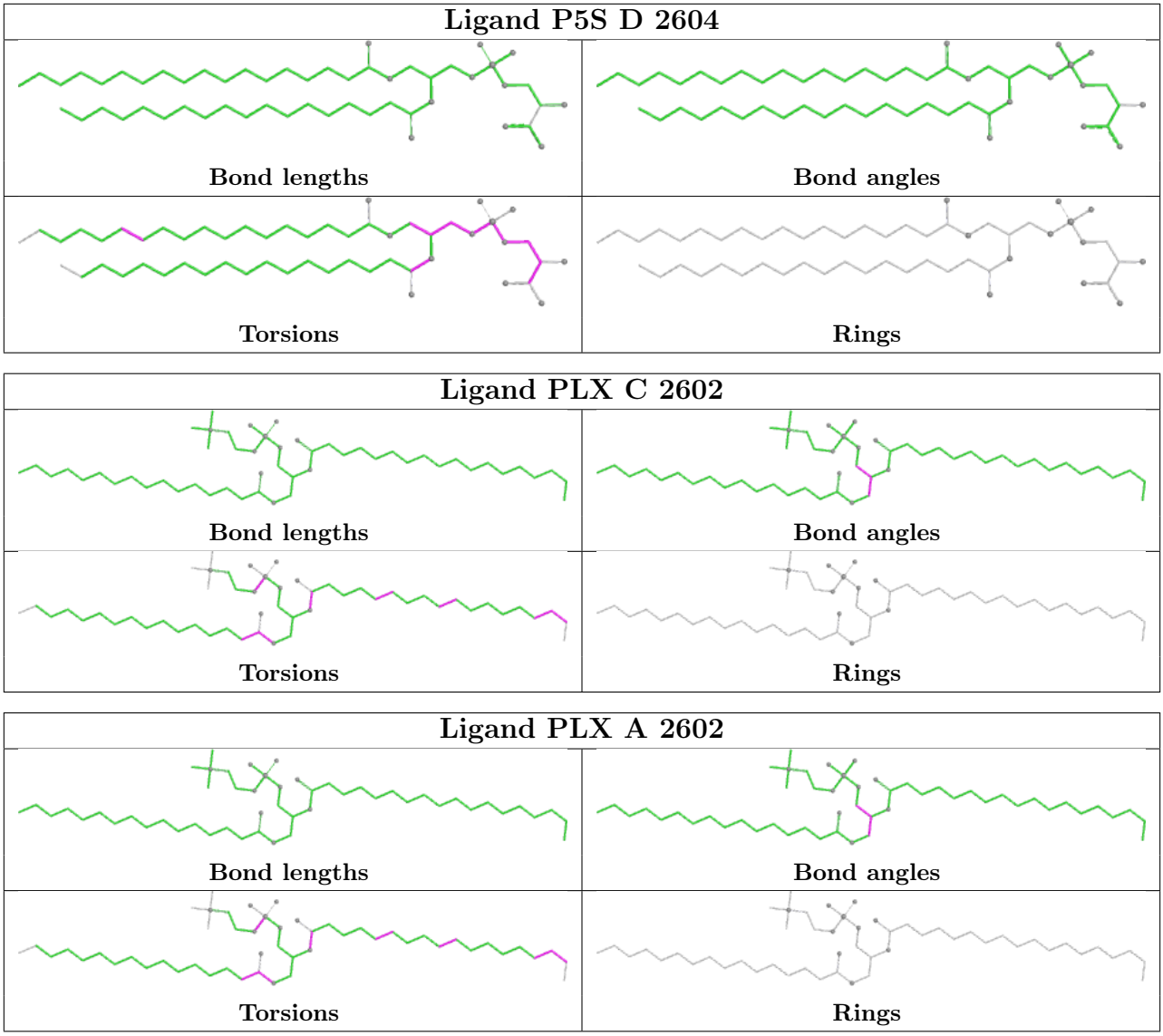


Ligand PEE D 2603



Ligand P5S C 2604





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.

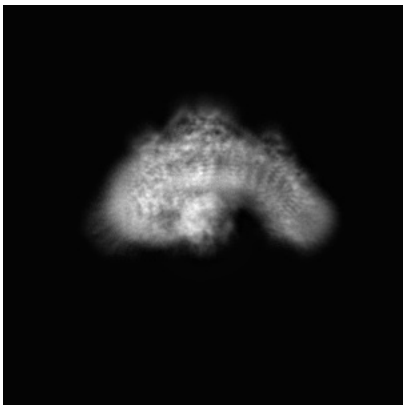
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35799. These allow visual inspection of the internal detail of the map and identification of artifacts.

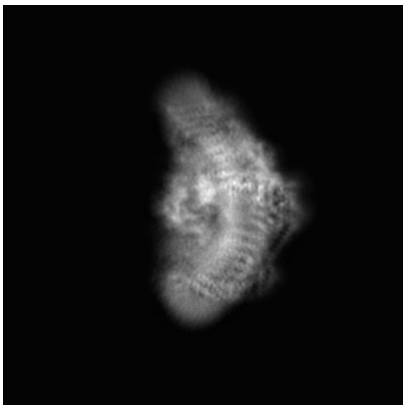
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

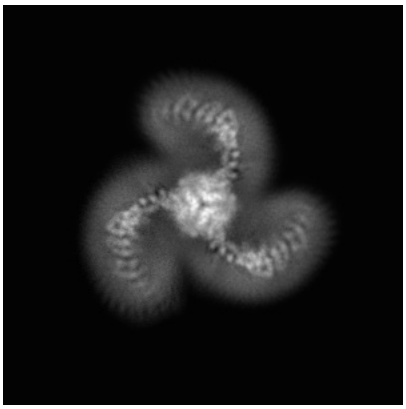
6.1.1 Primary map



X

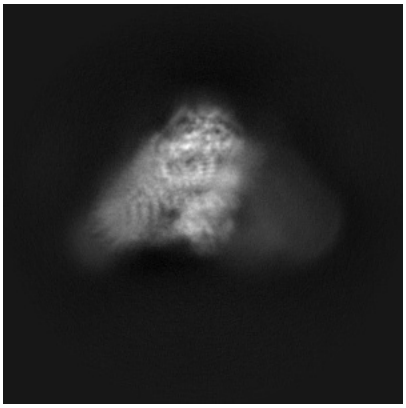


Y

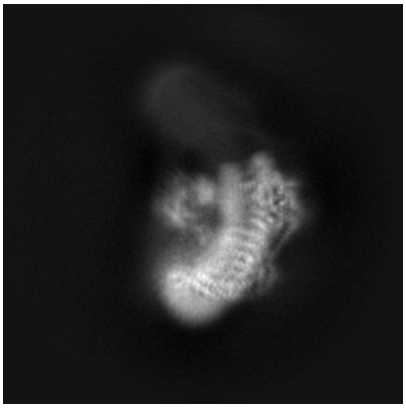


Z

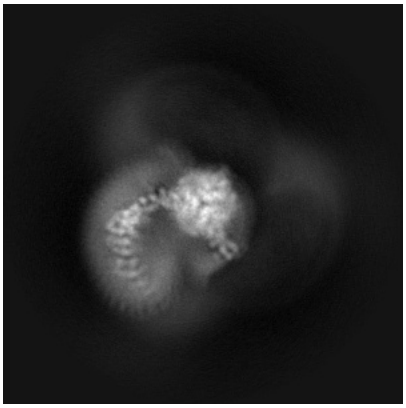
6.1.2 Raw map



X



Y

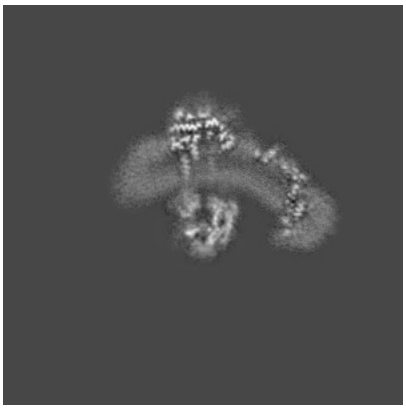


Z

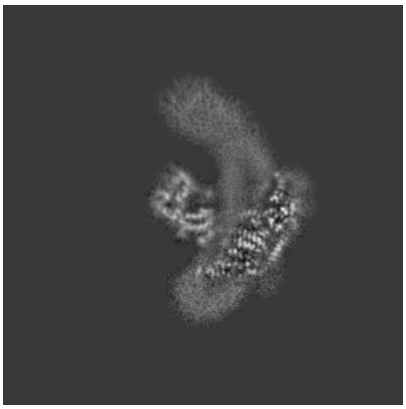
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

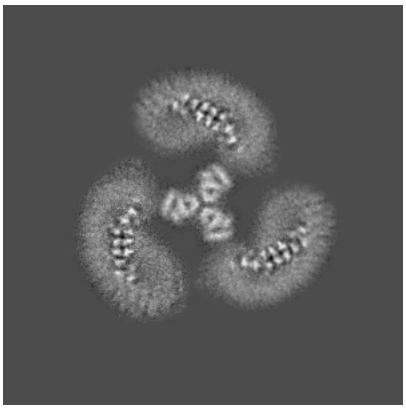
6.2.1 Primary map



X Index: 184

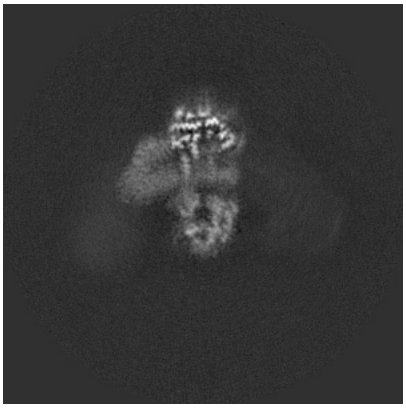


Y Index: 184

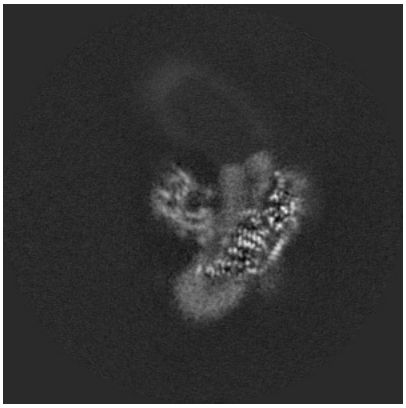


Z Index: 184

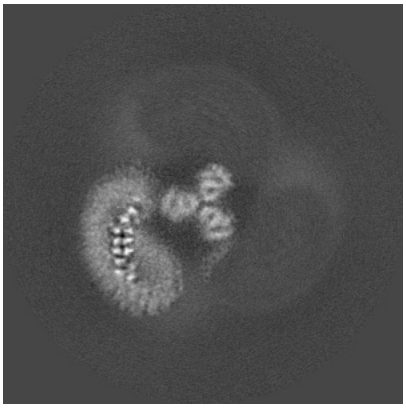
6.2.2 Raw map



X Index: 184



Y Index: 184

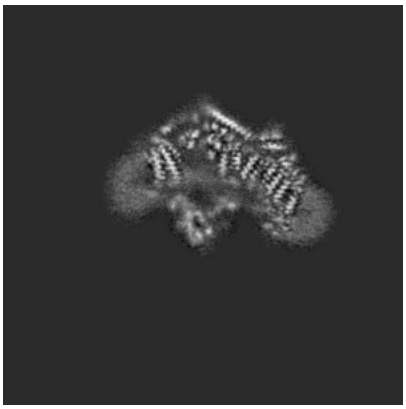


Z Index: 184

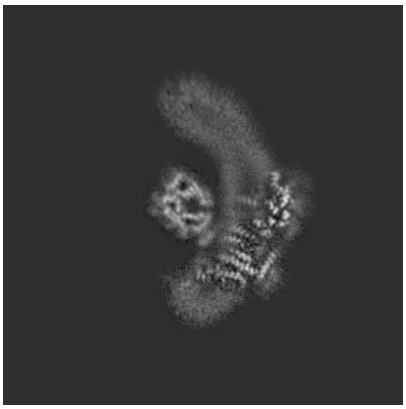
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

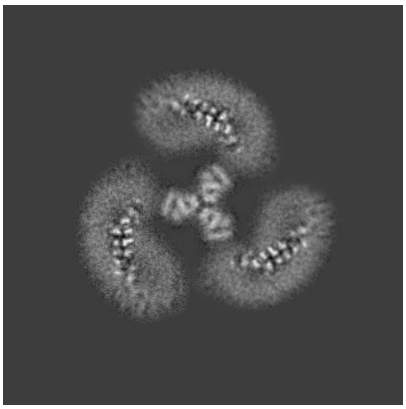
6.3.1 Primary map



X Index: 202

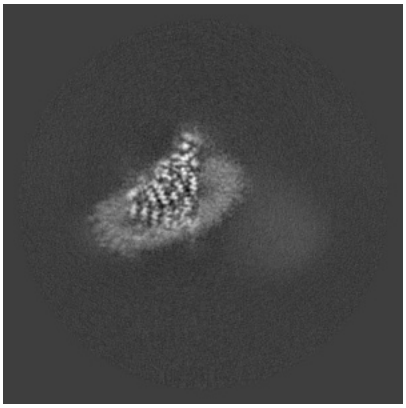


Y Index: 179

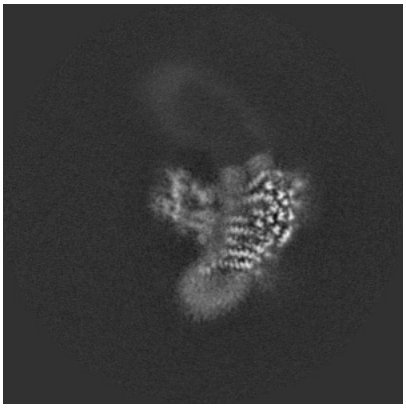


Z Index: 185

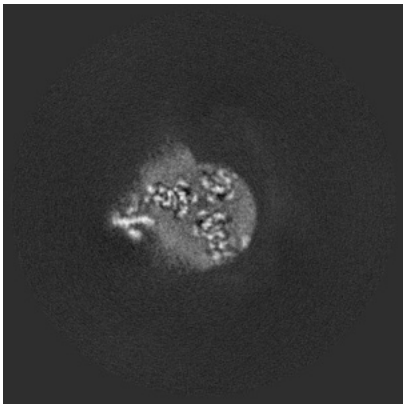
6.3.2 Raw map



X Index: 111



Y Index: 189

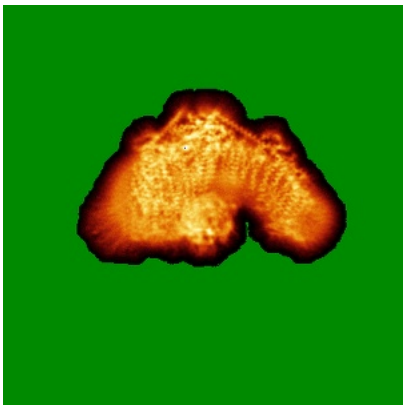


Z Index: 236

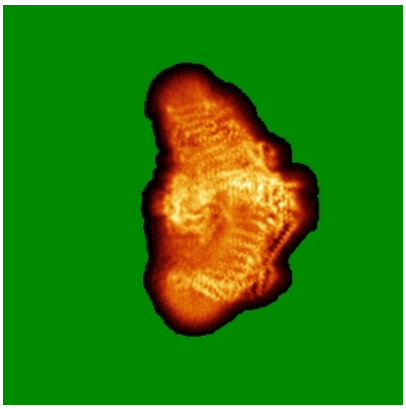
The images above show the largest variance slices of the map in three orthogonal directions.

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

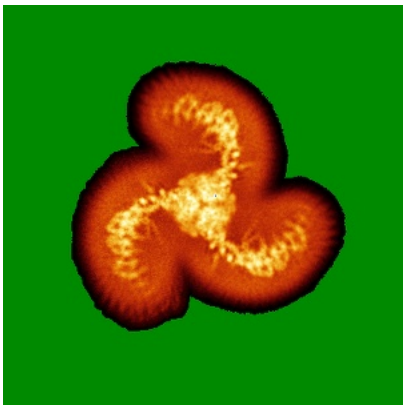
6.4.1 Primary map



X

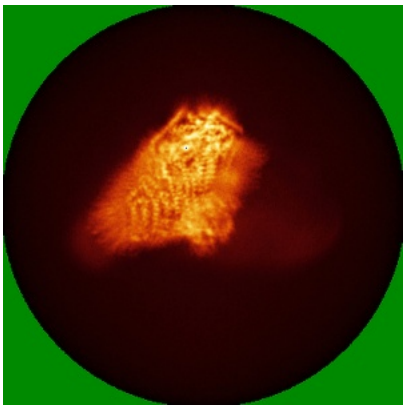


Y



Z

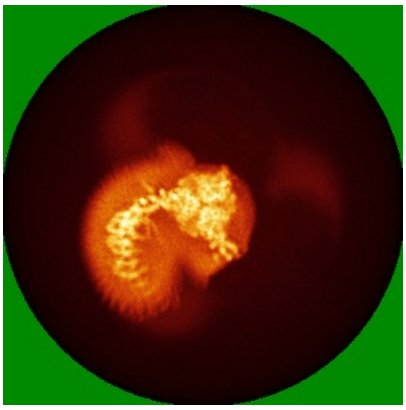
6.4.2 Raw map



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)

This section was not generated.

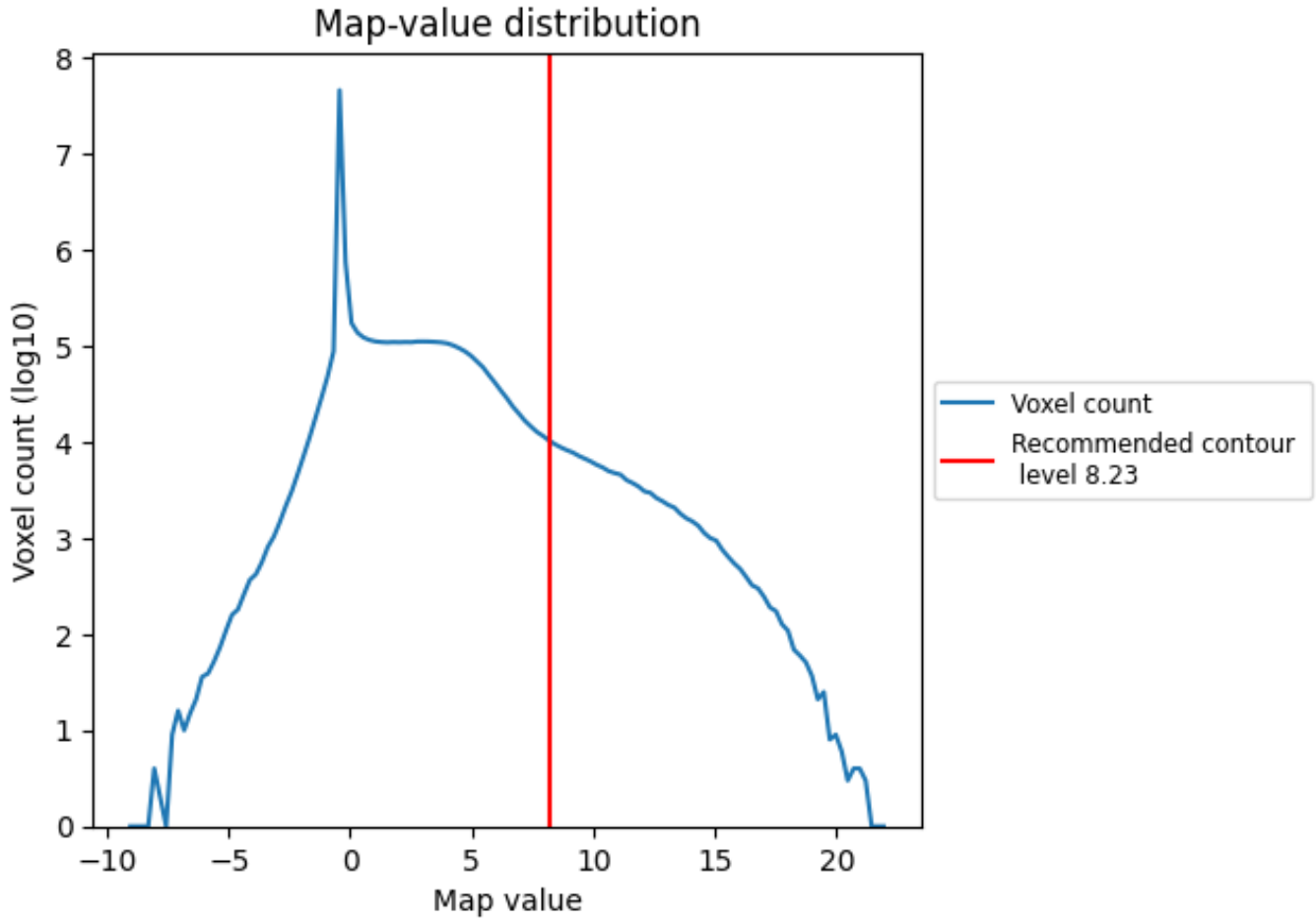
6.6 Mask visualisation (i)

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

7 Map analysis

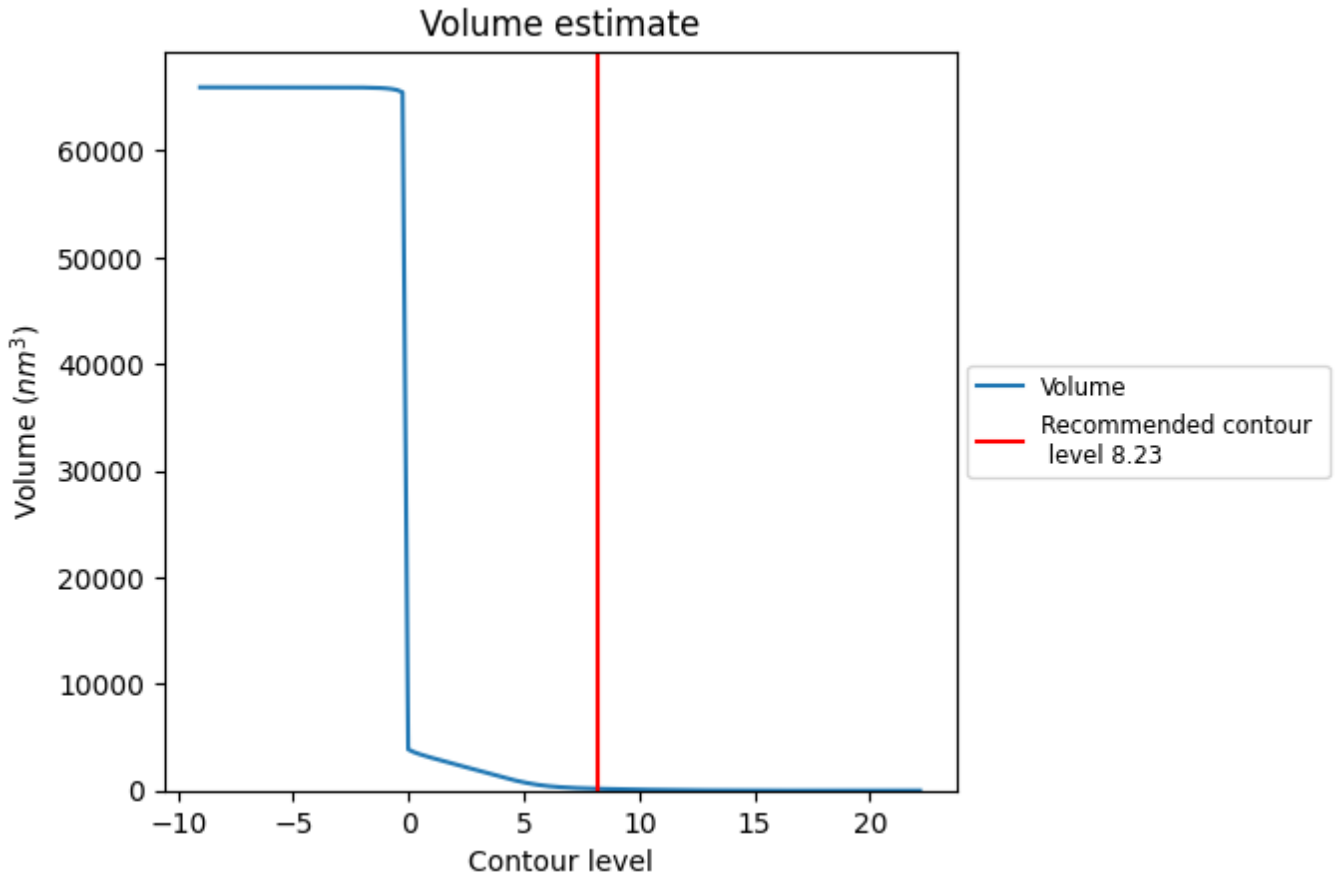
This section contains the results of statistical analysis of the map.

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.

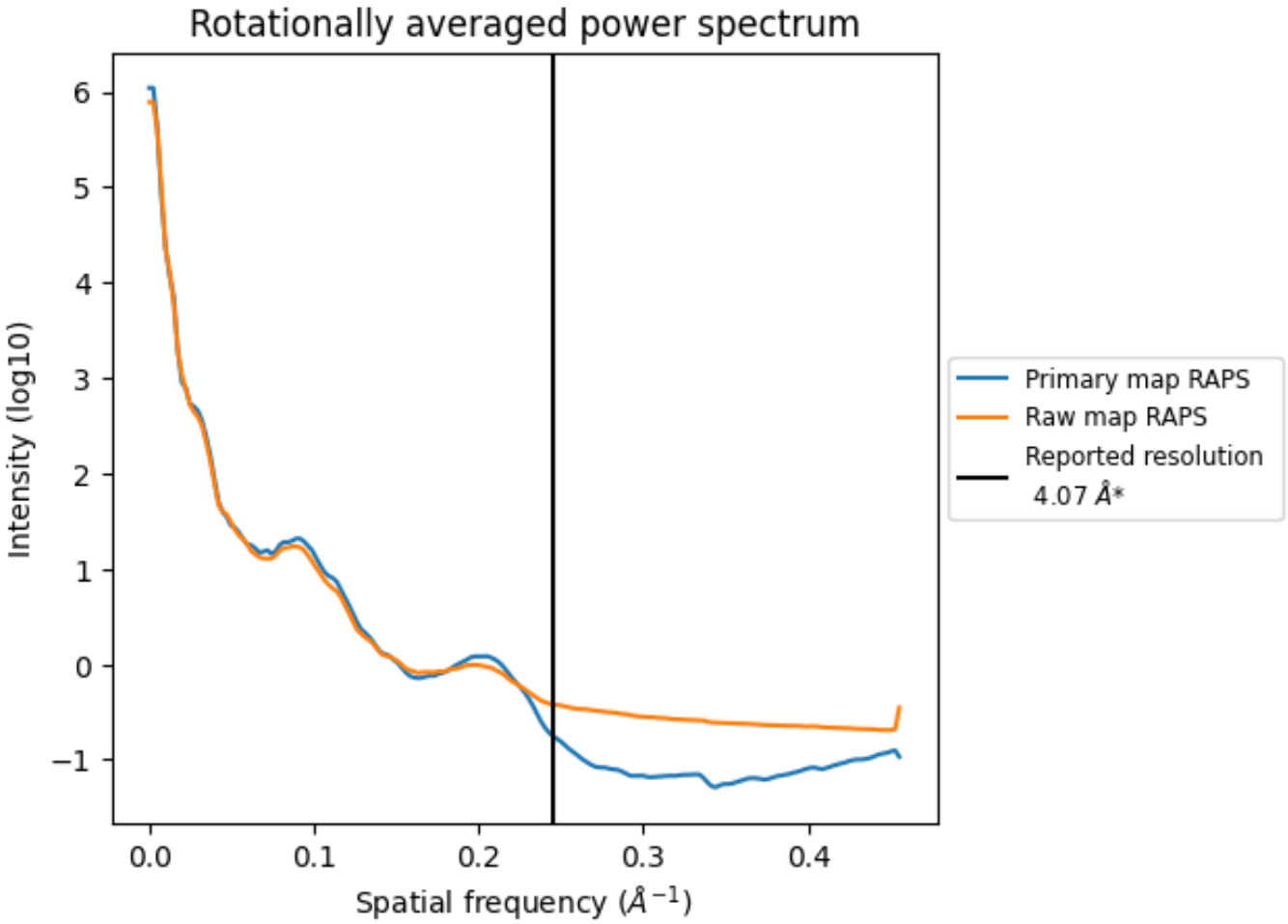
7.2 Volume estimate



The volume at the recommended contour level is 170 nm^3; this corresponds to an approximate mass of 154 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)

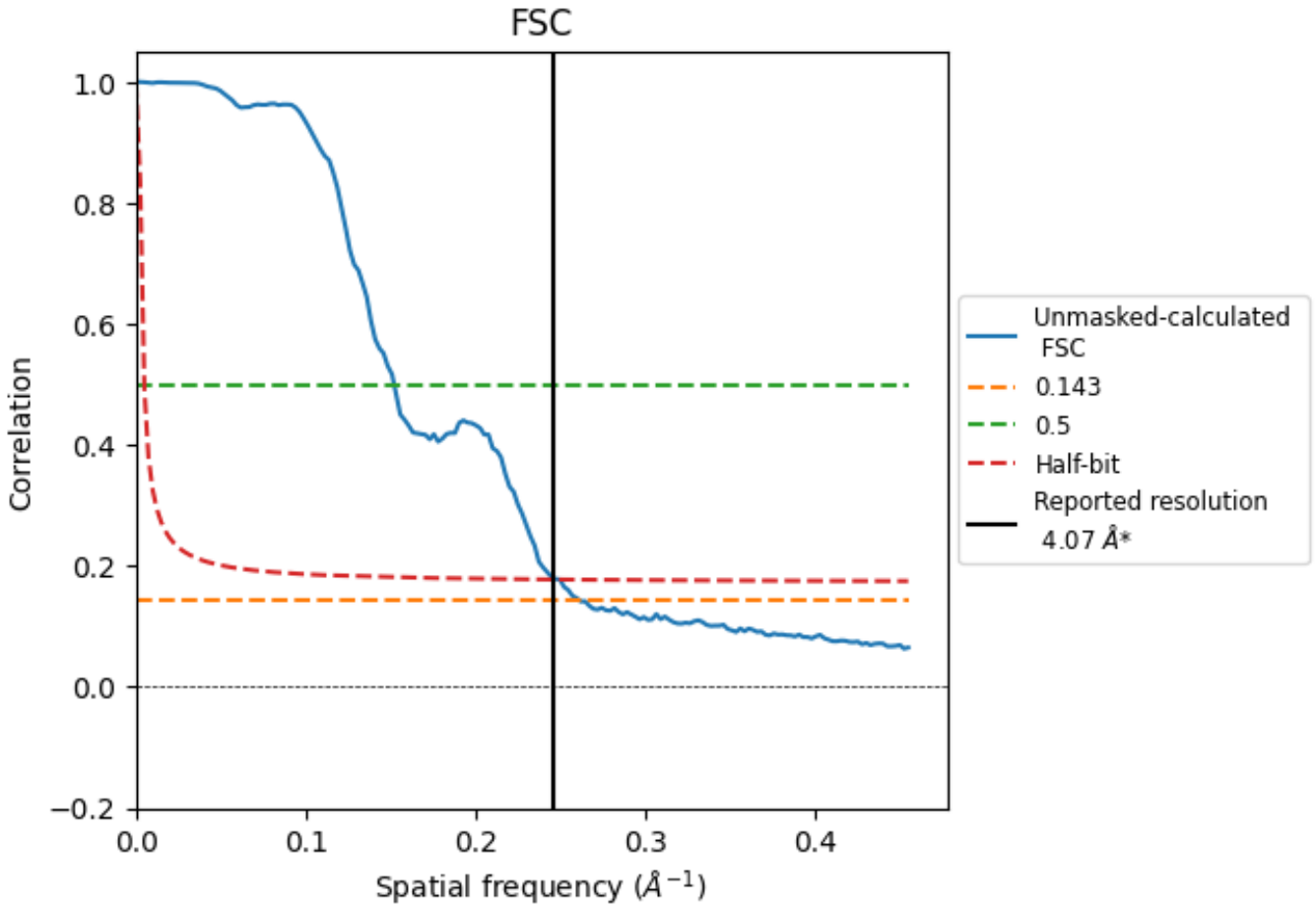


*Reported resolution corresponds to spatial frequency of 0.246 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.246 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	6.57	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

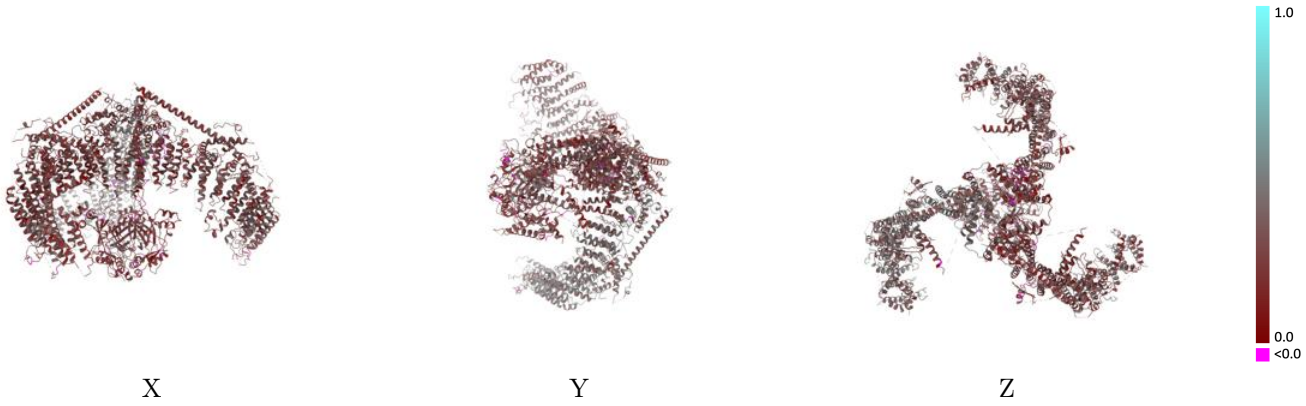
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35799 and PDB model 8IXN. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay

This section was not generated.

9.2 Q-score mapped to coordinate model

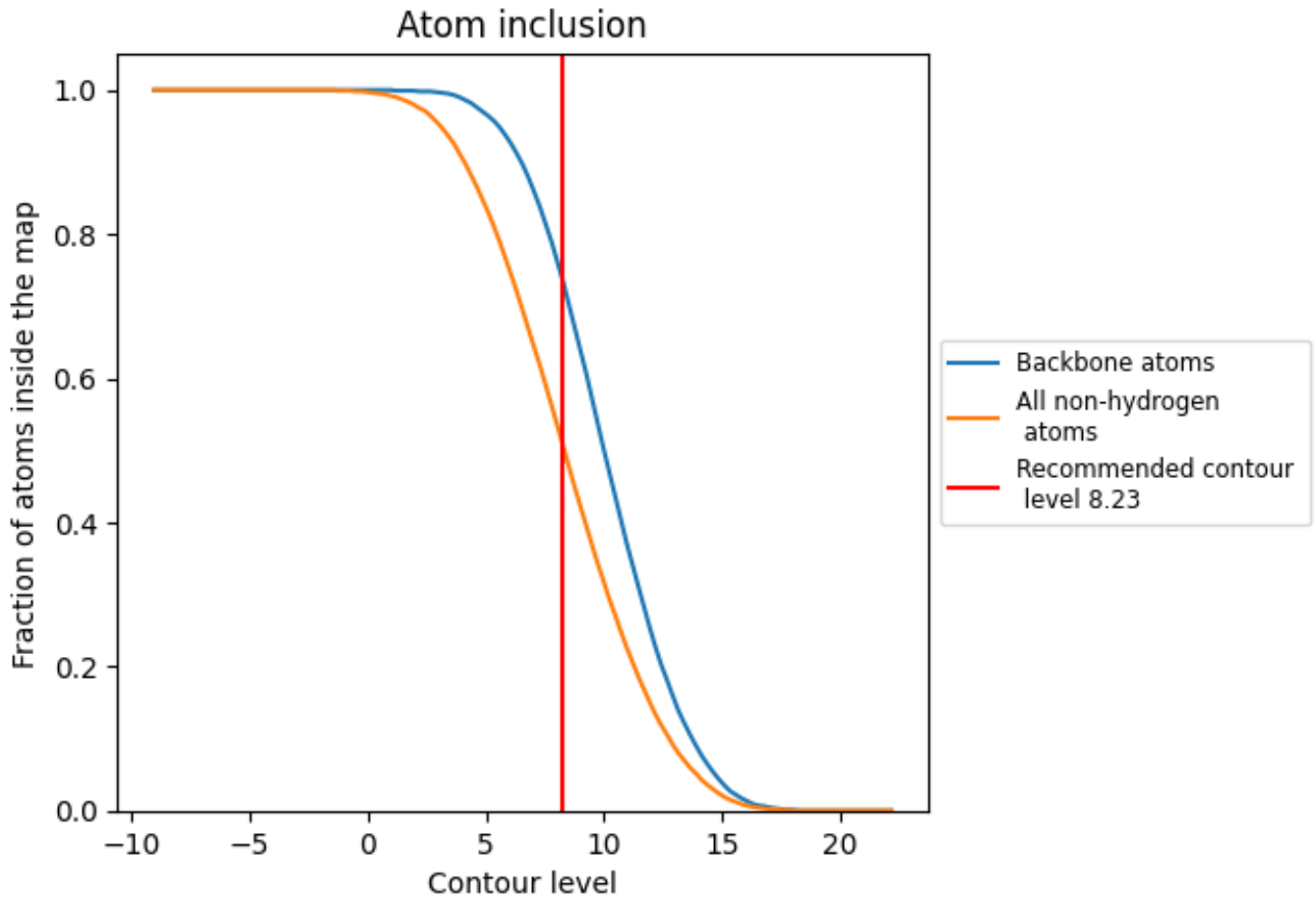


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 51% 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 (8.23) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.5120	0.3010
A	0.4980	0.2760
C	0.4770	0.2610
D	0.5600	0.3640