



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:45 AM UTC

PDB ID : 5JUL / pdb\_00005jul  
EMDB ID : EMD-8177  
Title : Near atomic structure of the Dark apoptosome  
Authors : Cheng, T.C.; Akey, I.V.; Yuan, S.; Yu, Z.; Ludtke, S.J.; Akey, C.W.  
Deposited on : 2016-05-10  
Resolution : 4.40 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](mailto: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:

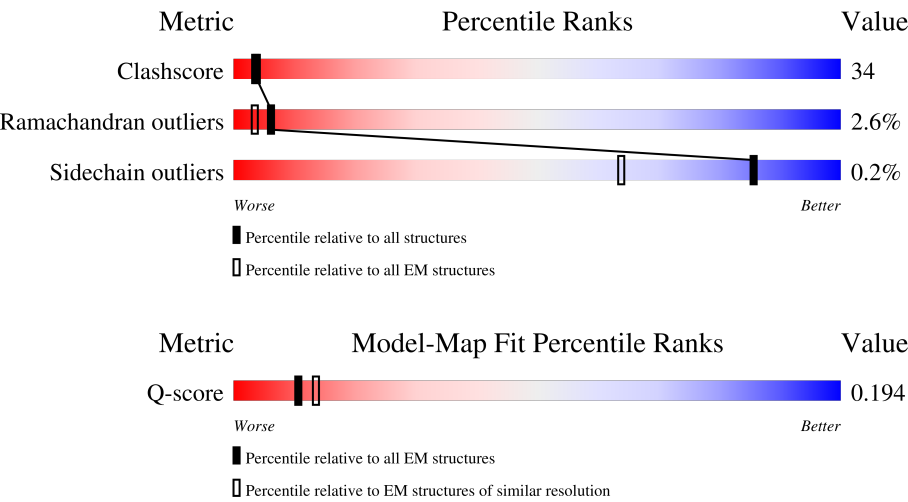
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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

The reported resolution of this entry is 4.40 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 3132 ( 3.91 - 4.90 )                                     |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 1440   | <div><div>45%</div><div><div></div><div></div><div></div><div></div></div><div>47%</div><div>35%</div><div>•</div><div>14%</div></div> |
| 1   | B     | 1440   | <div><div>45%</div><div><div></div><div></div><div></div><div></div></div><div>46%</div><div>37%</div><div>•</div><div>14%</div></div> |
| 1   | C     | 1440   | <div><div>45%</div><div><div></div><div></div><div></div><div></div></div><div>46%</div><div>36%</div><div>•</div><div>14%</div></div> |
| 1   | D     | 1440   | <div><div>45%</div><div><div></div><div></div><div></div><div></div></div><div>45%</div><div>37%</div><div>•</div><div>14%</div></div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |  |   |     |
|-----|-------|--------|------------------|--|---|-----|
| 1   | E     | 1440   | 45%              |  | • | 14% |
| 1   | F     | 1440   | 45%              |  | • | 14% |
| 1   | G     | 1440   | 45%              |  | • | 14% |
| 1   | H     | 1440   | 45%              |  | • | 14% |
| 1   | I     | 1440   | 45%              |  | • | 14% |
| 1   | J     | 1440   | 45%              |  | • | 14% |
| 1   | K     | 1440   | 45%              |  | • | 14% |
| 1   | L     | 1440   | 45%              |  | • | 14% |
| 1   | M     | 1440   | 45%              |  | • | 14% |
| 1   | N     | 1440   | 45%              |  | • | 14% |
| 1   | O     | 1440   | 45%              |  | • | 14% |
| 1   | P     | 1440   | 45%              |  | • | 14% |

## 2 Entry composition

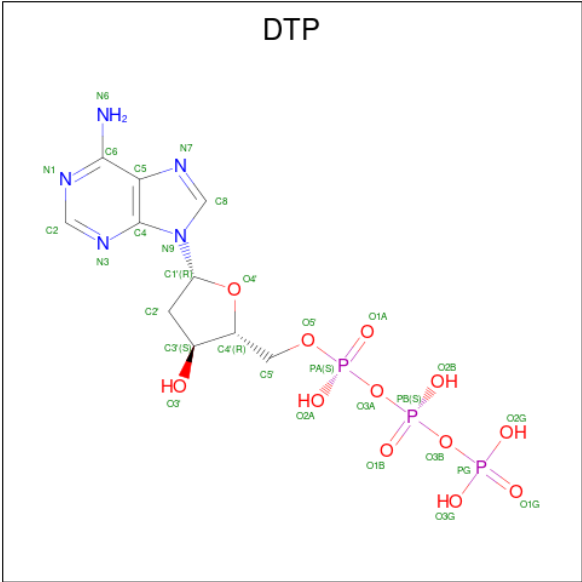
There are 2 unique types of molecules in this entry. The entry contains 161200 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Apaf-1 related killer DARK.

| Mol | Chain | Residues | Atoms          |           |           |           |        |         | AltConf | Trace |
|-----|-------|----------|----------------|-----------|-----------|-----------|--------|---------|---------|-------|
| 1   | A     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | B     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | C     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | D     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | E     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | F     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | G     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | H     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | I     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | J     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | K     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | L     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | M     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | N     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | O     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |
| 1   | P     | 1233     | Total<br>10045 | C<br>6434 | N<br>1698 | O<br>1860 | P<br>1 | S<br>52 | 0       | 0     |

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ )



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | I     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | L     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | M     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | N     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |

Continued on next page...

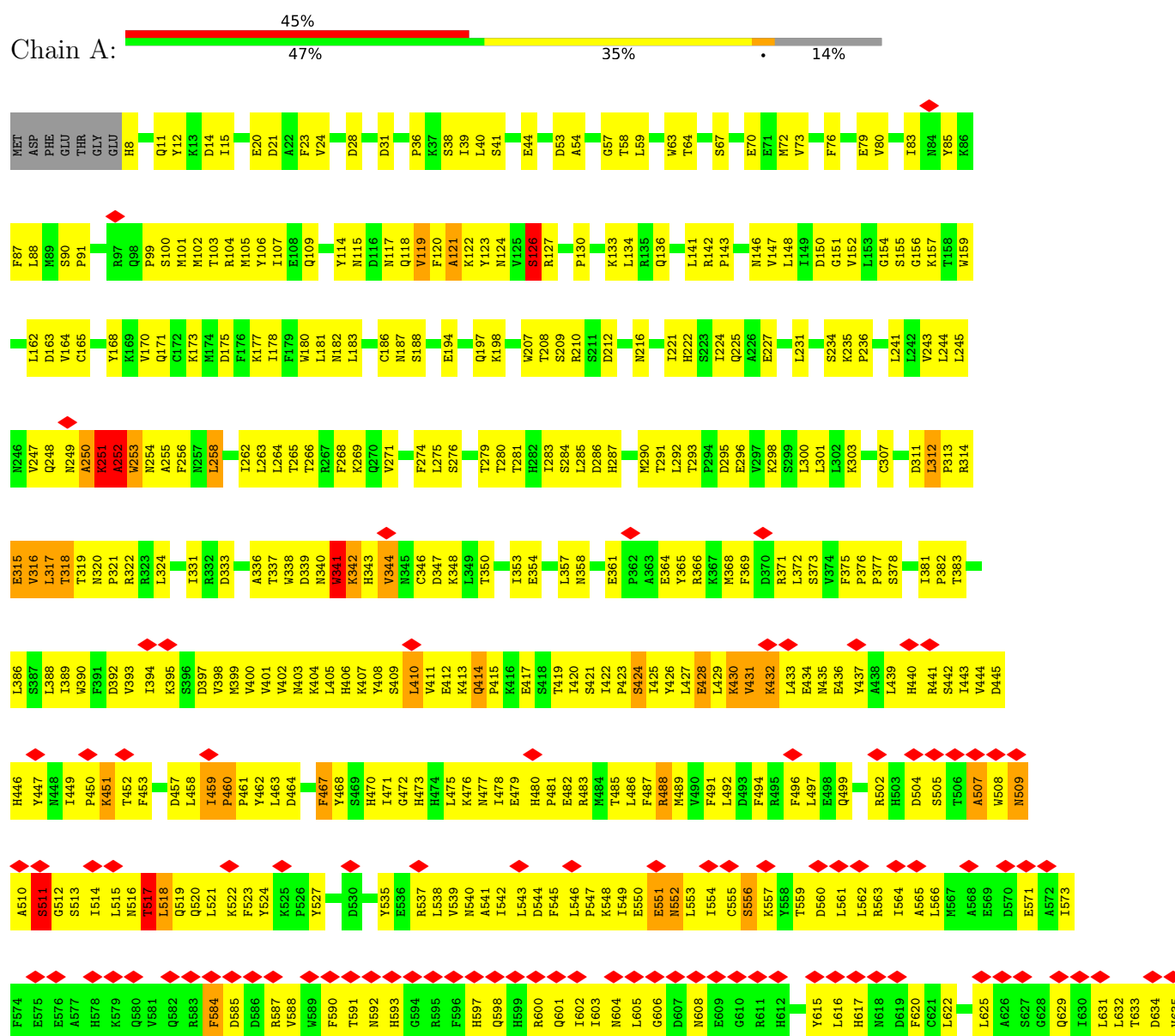
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | O     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |
| 2   | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |

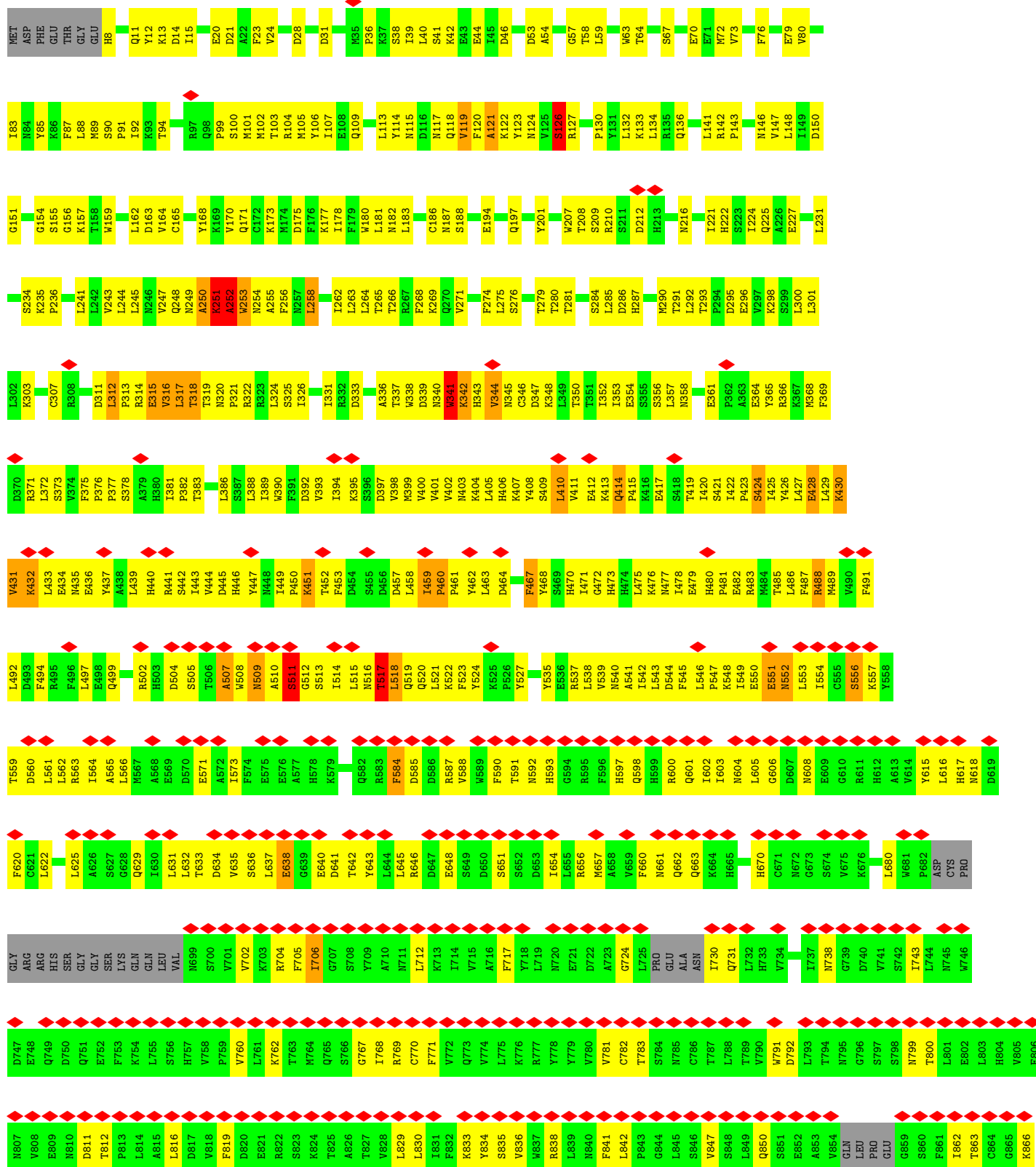
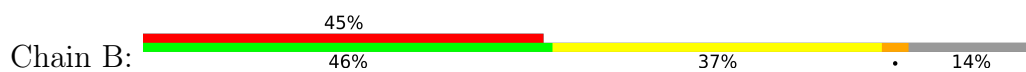
### 3 Residue-property plots

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.

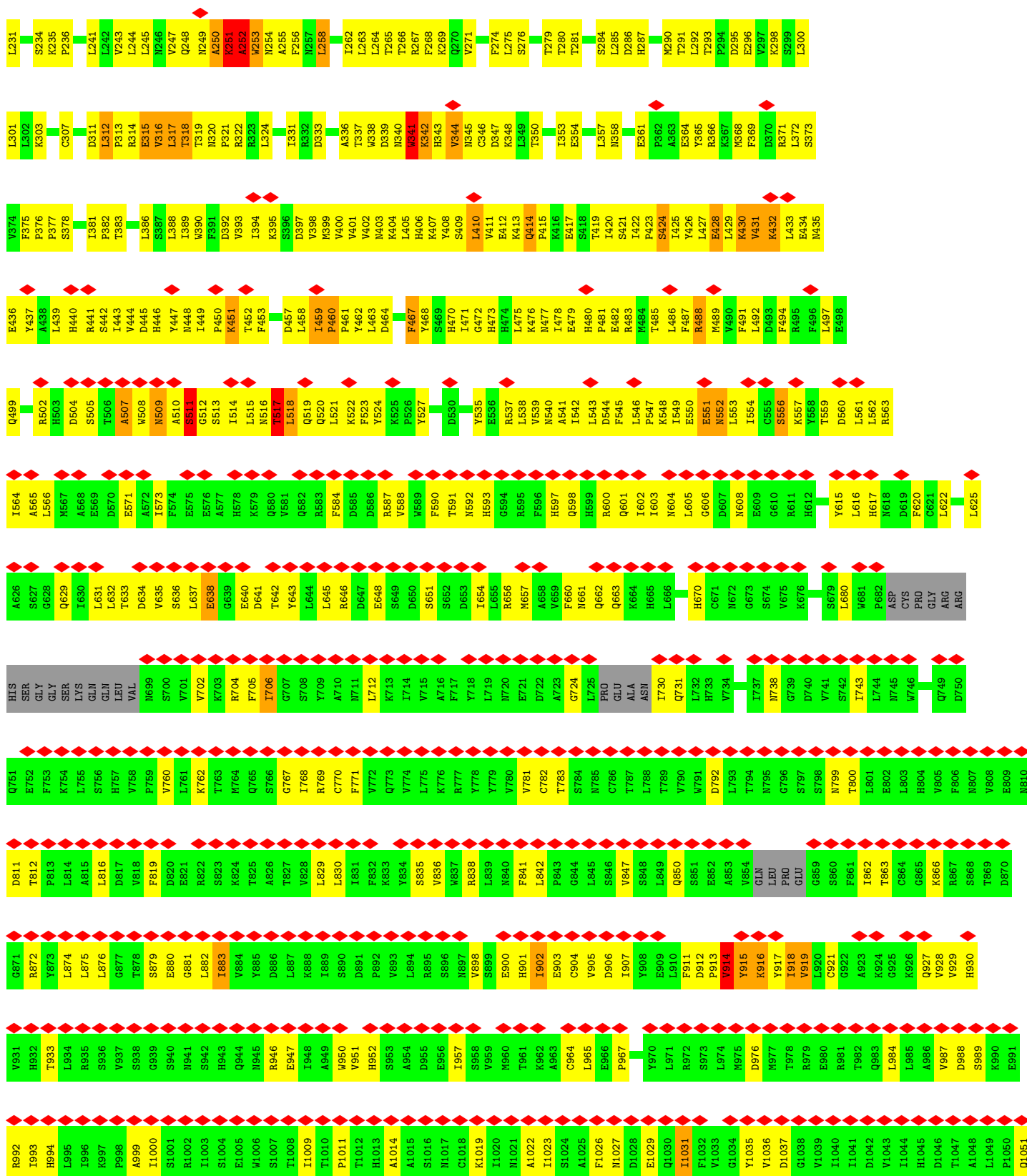
#### • Molecule 1: Apaf-1 related killer DARK



- Molecule 1: Apaf-1 related killer DARK



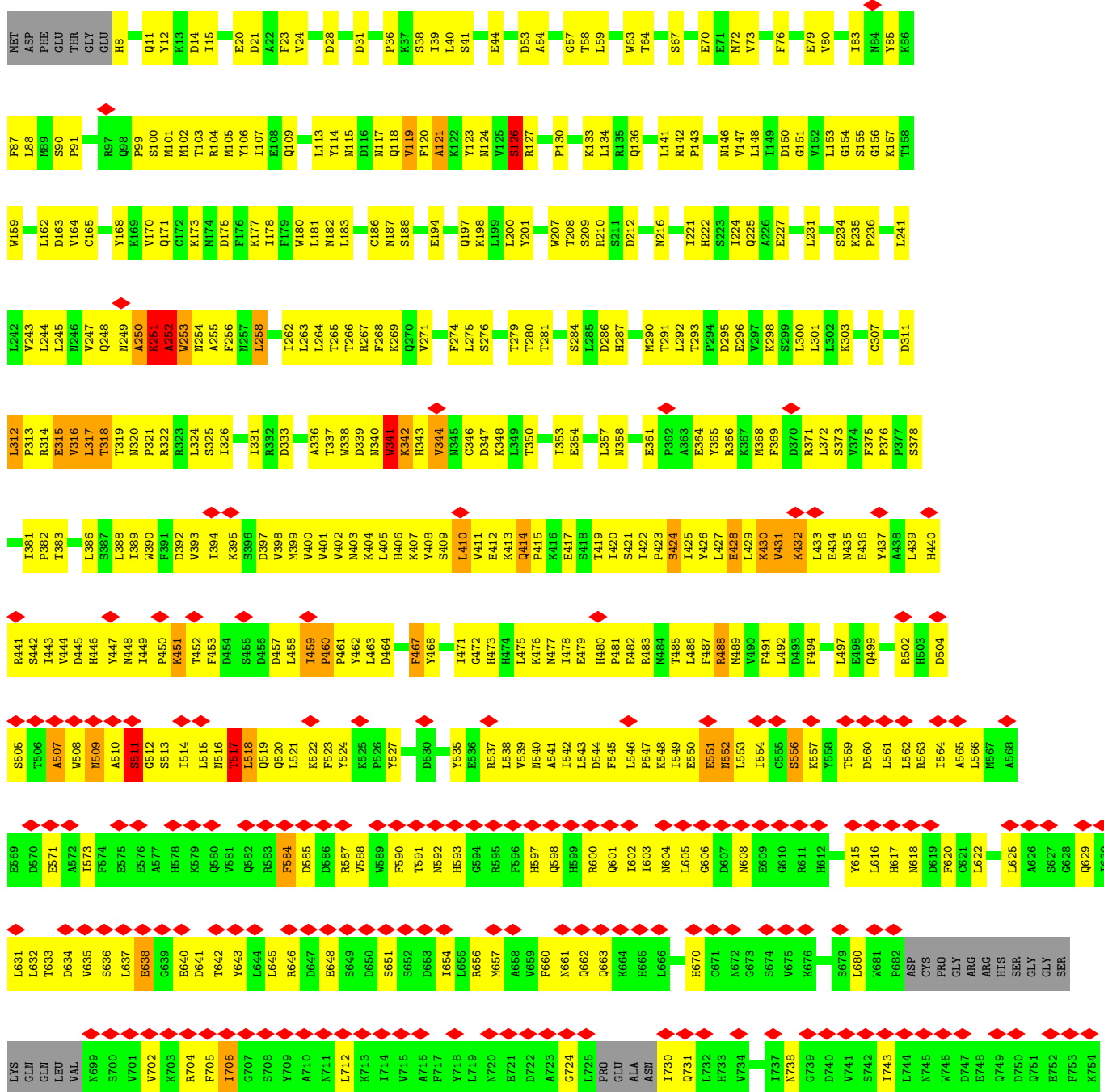






|     |       |       |       |       |       |      |      |      |      |      |      |      |
|-----|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|
| THR | L1225 | I1162 | V1102 | D1042 | T982  | C921 | L801 | V741 | L680 | N618 | K557 | L492 |
| GLN | Y1226 | I1163 | S1103 | V1043 | Q983  | G922 | E902 | S742 | W681 | D619 | Y558 | D493 |
| GLU | S1227 | D1164 | T1104 | I1044 | L984  | A923 | L803 | I743 | P682 | F620 | T559 | F494 |
| ALA | I1228 | V1165 | K1105 | H1045 | L985  | K924 | H804 | L744 | ASP  | C921 | D560 | R495 |
| VAL | E1229 | F1166 | A1106 | D1046 | A986  | K926 | V805 | N745 | PRD  | L622 | L561 | F496 |
| ASP | E1230 | R1167 | A1107 | T1047 | V987  | Q927 | F806 | N746 | GLY  | L625 | R562 | L497 |
| ALA | V1231 | L1168 | S1108 | A1048 | D988  | V928 | N807 | D747 | ARG  | A626 | I564 | Q499 |
| ALA | H1232 | I1169 | L1109 | P1049 | S989  | V929 | V808 | E748 | ARG  | S627 | A565 | R502 |
| ILE | F1170 | F1170 | Q1110 | P1050 | K990  | H930 | E809 | Q749 | SER  | Q628 | L566 | H503 |
| ALA | S1171 | E1111 | E1111 | Q1051 | E991  | V931 | N810 | D750 | GLY  | I630 | M567 | D504 |
| ASP | C1172 | G1112 | G1112 | Q1052 | R992  | H932 | D811 | E752 | SER  | I630 | A568 | S505 |
| ASP | N1173 | Q1113 | Q1113 | F1053 | I993  | T933 | T812 | F753 | LYS  | L631 | E569 | T506 |
| VAL | Q1174 | Y1114 | Y1114 | I1054 | H994  | L934 | P813 | E754 | GLN  | T632 | D570 | A507 |
| ASP | L1175 | I1115 | I1115 | E1055 | L995  | R935 | L814 | K754 | GLN  | T633 | E571 | V508 |
| VAL | R1176 | I1116 | I1116 | E1056 | I996  | S936 | A815 | L755 | LEU  | D634 | A572 | N509 |
| THR | Y1177 | L1117 | L1117 | P1057 | K997  | V937 | L816 | S756 | VAL  | V635 | I573 | A510 |
| PHE | F1241 | F1178 | F1118 | I1058 | P998  | S938 | D817 | H757 | N699 | S636 | F574 | S511 |
| VAL | F1241 | I1179 | S1119 | D1059 | A999  | Q939 | V818 | V758 | S700 | L637 | E576 | G512 |
| ALA | S1242 | I1180 | D1120 | Y1060 | I1000 | S940 | F819 | P759 | V701 | E638 | A577 | S513 |
| ASP | P1243 | C1181 | H1121 | I1061 | S1001 | N941 | D820 | L761 | K703 | G639 | H578 | I514 |
| GLU | C1244 | E1182 | G1122 | K1062 | I1002 | S942 | E821 | K762 | R704 | E640 | K579 | L515 |
| PHE | L1245 | E1183 | V1123 | Q1063 | I1003 | H943 | R822 | I763 | F705 | D641 | Q580 | N516 |
| HIS | K1246 | E1184 | C1124 | V1064 | S1004 | Q944 | S823 | H764 | I706 | T642 | V581 | T517 |
| VAL | L1247 | I1185 | I1125 | P1065 | E1005 | N945 | K824 | Q765 | G707 | Y643 | Q582 | L518 |
| ASN | L1248 | A1186 | L1126 | S1066 | I1006 | N946 | T825 | S766 | S708 | L644 | Q519 | Q520 |
| ARG | I1249 | I1187 | D1127 | N1067 | I1007 | E947 | A826 | S767 | V709 | R646 | Q520 | L521 |
| GLY | S1250 | Q1187 | I1068 | I1068 | I1008 | N948 | T827 | I768 | N711 | D647 | K522 | F523 |
| THR | C1251 | K1188 | I1128 | V1070 | I1009 | A949 | V828 | R769 | L712 | E648 | D586 | Y524 |
| ALA | A1252 | A1189 | A1129 | I1071 | I1010 | N950 | L829 | C770 | K713 | S649 | V588 | K525 |
| GLU | E1253 | K1190 | N1130 | A1072 | T1012 | H952 | T831 | V772 | I714 | S651 | F589 | P526 |
| LEU | Q1254 | I1191 | P1131 | S1072 | H1013 | S953 | K832 | Q773 | V715 | S652 | T591 | Y527 |
| ARG | L1255 | S1192 | S1132 | A1073 | H1014 | A954 | K833 | V774 | A716 | N592 | N592 | D530 |
| ASN | F1257 | L1194 | F1134 | H1074 | A1015 | D955 | Y834 | L775 | F717 | Y635 | H593 | Y635 |
| ASN | W1258 | V1195 | V1135 | S1075 | S1016 | E956 | S835 | L776 | L555 | L654 | G594 | E536 |
| ILE | T1261 | A1196 | K1136 | A1076 | S1016 | E956 | V836 | K776 | R656 | L654 | R537 | R537 |
| ARG | H1262 | T1197 | P1137 | Q1077 | N1017 | S958 | N837 | R777 | R656 | R657 | L538 | L538 |
| PRO | M1263 | D1198 | K1138 | K1078 | C1018 | S958 | R838 | V778 | E721 | A658 | V539 | N540 |
| LEU | R1264 | D1199 | D1139 | T1079 | C1018 | S958 | L839 | V779 | D722 | V859 | H597 | A541 |
| LEU | ASN   | G1200 | S1140 | V1080 | I1019 | N960 | N840 | V780 | A723 | F660 | Q598 | I542 |
| ALA | ASN   | T1201 | E1141 | F1081 | I1020 | T961 | N840 | V781 | G724 | N661 | H599 | L543 |
| CYS | M1202 | M1202 | E1142 | F1082 | A1022 | K962 | F841 | C782 | L725 | Q662 | R600 | D544 |
| VAL | L1203 | L1203 | Y1143 | Q1083 | I1023 | A963 | L842 | T783 | PRD  | Q663 | Q601 | F545 |
| PHE | A1204 | A1204 | I1144 | L1084 | S1024 | C964 | P843 | S784 | GLU  | K664 | I602 | L546 |
| VAL | M1205 | M1205 | V1145 | E1085 | A1025 | L965 | G844 | N785 | ALA  | H665 | I603 | P547 |
| GLY | G1206 | G1206 | G1146 | K1086 | F1026 | E966 | L845 | C786 | ASN  | L666 | N604 | K548 |
| ASN | F1207 | F1207 | F1147 | I1087 | N1027 | P967 | S846 | V787 | I730 | I667 | I549 | I549 |
| GLU | E1208 | E1208 | D1148 | D1088 | D1028 | Y970 | V847 | L788 | Q731 | G606 | L605 | E550 |
| ALA | N1209 | N1209 | L1149 | P1089 | E1029 | V970 | S848 | V789 | L732 | D607 | E551 | E551 |
| ARG | ARG   | ARG   | K1150 | L1090 | Q1030 | L971 | L849 | V790 | H733 | N608 | N552 | N552 |
| ARG | ARG   | ARG   | N1151 | Q1091 | I1031 | H972 | Q850 | V791 | V734 | E909 | L553 | L553 |
| HIS | L1212 | L1212 | S1152 | P1092 | F1032 | S973 | S851 | D792 | N672 | G610 | I554 | I554 |
| GLN | L1214 | L1214 | L1153 | N1093 | V1033 | L974 | E852 | L793 | G673 | G611 | C555 | C555 |
| GLN | F1215 | F1215 | L1154 | D1094 | G1034 | H975 | A853 | V794 | S674 | R611 | S556 | S556 |
| SER | N1219 | N1219 | F1155 | Q1095 | Y1035 | D976 | V854 | T796 | G739 | K676 | H612 | H612 |
| VAL | R1220 | R1220 | L1156 | V1096 | V1036 | H977 | GLN  | G796 | D740 | L877 | Y615 | Y615 |
| VAL | K1221 | K1221 | A1157 | P1097 | D1037 | T978 | LEU  | S797 | G675 | W678 | L616 | L616 |
| VAL | Q1222 | Q1222 | Y1158 | L1098 | G1038 | T979 | PRO  | S798 | S675 | S679 | H617 | H617 |
| ALA | L1224 | L1224 | E1159 | M1099 | V1039 | E980 | GLU  | N799 | G676 | S679 |      |      |

- Molecule 1: Apaf-1 related killer DARK

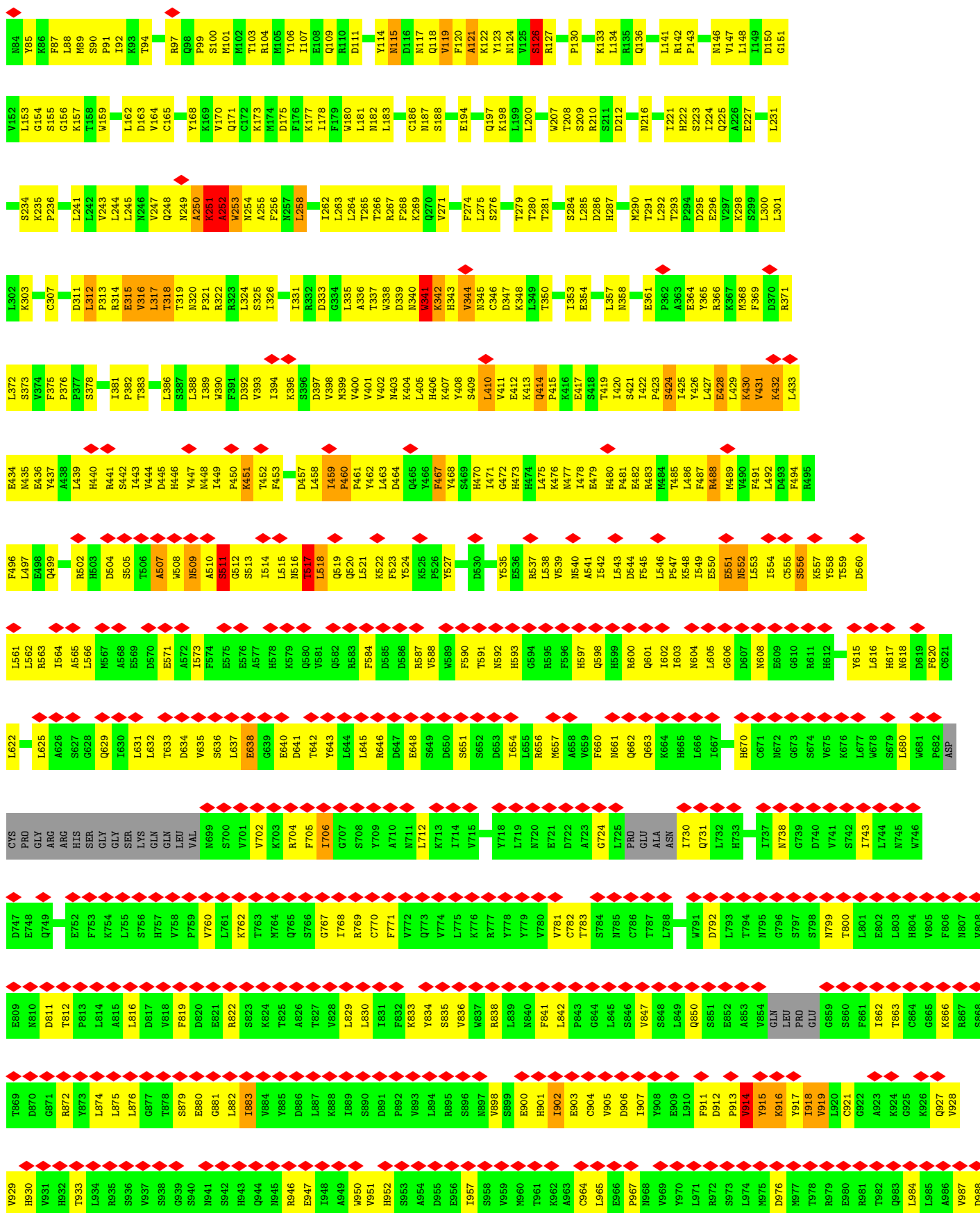


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |  |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|
| L1239 | L1240 | F1241 | S1242 | P1243 | C1244 | K1245 | L1246 | L1247 | L1248 | I1249 | S1250 | C1251 | A1252 | E1253 | Q1254 | L1255 | C1256 | F1257 | W1258 | T1261 | H1262 | M1263 | R1264 | ASN | ASN | GLN | LEU | GLU | GLU | ALA | ALA | CYS | VAL | LYS | ARG | ILE | VAL | ARG | GLY | ASN | GLU | PRO | GLN | LEU | GLU | ASP | ASP | THR | THR | ALA | ALA | ASP |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |  |
| ILE   | ASP   | VAL   | ASP   | VAL   | THR   | PHE   | VAL   | VAL   | ASP   | GLU   | PHE   | LEU   | PRO   | VAL   | VAL   | ASN   | ASN   | GLY   | THR   | ALA   | ALA   | PRO   | PRO   | LEU | TRP | ASP | VAL | THR | LYS | ARG | ASN | GLN | TYR | GLU | ASP | LEU | LEU | LYS | ASN | LEU | ARG | ILE | LEU | ASP | SER | PRO | GLY | GLN | ASP |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |  |
| LEU   | VAL   | GLU   | GLY   | ASN   | VAL   | GLY   | VAL   | ALA   | ALA   | THR   | ALA   | ALA   | PRO   | PRO   | GLU   | PRO   | PRO   | ASP   | ASP   | VAL   | THR   | GLN   | ASN   | ASN | PRO | VAL | THR | LEU | LEU | ILE | ASN | GLY | ASP | LEU | LEU | ALA | ALA | LYS | ASN | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU | GLU |  |

• Molecule 1: Apaf-1 related killer DARK



|     |     |     |     |     |     |     |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ASP | PHE | GLU | THR | GLY | GLU | H8 | Q11 | Y12 | K13 | L14 | I15 | E20 | D21 | A22 | F23 | V24 | D28 | D31 | P36 | K37 | S38 | I39 | L40 | S41 | K42 | E43 | E44 | I45 | D46 | D53 | A54 | G57 | T58 | L59 | W63 | T64 | S67 | E70 | E71 | M72 | V73 | F76 | E79 | V80 | I83 |
|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



|        |       |       |        |       |     |     |
|--------|-------|-------|--------|-------|-----|-----|
| SR89   | L1049 | L1109 | II189  | H1232 | ALA | GLY |
| K990   | P1050 | Q1110 | F1170  | E1233 | ALA | ALA |
| E991   | Q1051 | E1111 | S1171  | H1234 | PRO | ASP |
| R992   | Q1052 | G1112 | C1172  | C1235 | ILE | VAL |
| R993   | F1053 | G1113 | II173  | L1236 | ALA | VAL |
| H994   | I1054 | Y1114 | Q1174  | R1237 | ASP | GLY |
| L995   | E1055 | II115 | L1175  | Q1238 | ASP | ASN |
| T996   | E1056 | II116 | R1176  | L1239 | VAL | LEU |
| R997   | P1057 | II117 | Y1177  | L1240 | GLU | LEU |
| P998   | I1058 | F1118 | E1178  | F1241 | VAL | LVS |
| A999   | D1059 | S1119 | Q1179  | S1242 | THR | ASN |
| I1000  | Y1060 | D1120 | II180  | P1243 | PHE | GLY |
| S1001  | L1061 | II121 | C1181  | K1244 | VAL | GLY |
| R1002  | K1062 | G1122 | E1182  | K1245 | ALA | ALA |
| II1003 | Q1063 | V1123 | E1183  | L1246 | GLU | ARG |
| S1004  | V1064 | C1124 | E1184  | L1247 | PHE | LEU |
| E1005  | S1065 | II125 | II185  | L1248 | HIS | LEU |
| W1006  | P1066 | L1126 | II186  | I1249 | PRO | GLU |
| S1007  | N1067 | D1127 | Q1187  | S1250 | VAL | LEU |
| T1008  | I1068 | II128 | K1188  | C1251 | ARG | GLU |
| II1009 | L1069 | II129 | A1189  | A1252 | THR | ALA |
| T1010  | V1070 | M1130 | K1190  | E1253 | PRO | ALA |
| P1011  | A1071 | P1131 | II191  | Q1254 | GLU | PRO |
| T1012  | S1072 | S1132 | Y1192  | L1255 | TRP | ASP |
| H1013  | A1073 | II133 | S1193  | C1256 | TRP | PRO |
| A1014  | H1074 | F1134 | L1194  | F1257 | ASN | VAL |
| A1015  | S1075 | V1135 | V1195  | W1258 | THR | LEU |
| S1016  | A1076 | K1136 | A1196  | T1261 | GLY | ASP |
| W1017  | Q1077 | P1137 | T1197  | H1262 | ILE | ALA |
| C1018  | K1078 | K1138 | D1198  | M1263 | ASN | ASN |
| K1019  | T1079 | D1139 | G1199  | R1264 | ARG | TYR |
| II1020 | V1080 | S1140 | Q1200  | ASN   | PRO | GLU |
| A1021  | I1081 | E1141 | T1201  | GLN   | GLU | GLY |
| II1022 | F1082 | E1142 | M1202  | LEU   | LEU | ASP |
| II1023 | Q1083 | Y1143 | L1203  | GLU   | ALA | LEU |
| S1024  | L1084 | II144 | A1204  | ARG   | CYS | LYS |
| A1025  | E1085 | V1145 | M1205  | GLN   | VAL | ASN |
| F1026  | K1086 | G1146 | G1206  | LYS   | PHE | ARG |
| II1027 | I1087 | F1147 | F1207  | ILE   | VAL | ILE |
| D1028  | P1088 | L1148 | E1208  | ARG   | GLY | ASP |
| E1029  | L1089 | L1149 | M1209  | ARG   | ASN | SER |
| Q1030  | Q1090 | K1150 | L1212  | ARG   | ALA | PRO |
| II1031 | Q1091 | M1151 | E1213  | ARG   | GLN | MET |
| F1032  | P1092 | S1152 | L1214  | HIS   | GLN | GLN |
| V1033  | N1093 | L1153 | F1215  | LYS   | PHE | ASP |
| G1034  | D1094 | L1154 | A1216  | GLN   | THR | SER |
| Y1035  | Q1095 | F1155 | N1219  | HIS   | ASP | ASP |
| V1036  | W1096 | L1156 | R1220  | VAL   | THR | GLU |
| D1037  | P1097 | A1157 | Q1223  | THR   | GLN | ALA |
| G1038  | L1098 | Y1158 | L1224  | ASP   | GLY | ASP |
| V1039  | M1099 | E1159 | II1225 | ALA   | ASP | ALA |
| II1040 | M1100 | N1160 | Y1226  | VAL   | VAL | VAL |
| II1041 | D1101 | M1161 | S1227  | ASP   | ASP | ASP |
| D1042  | V1102 | II162 | II1228 | ASP   | ASP | ASP |
| V1043  | II103 | II163 | E1229  | ASP   | ASP | ASP |
| II1044 | T1104 | D1164 | E1230  | ASP   | ASP | ASP |
| H1045  | K1105 | V1165 | V1231  | ASP   | ASP | ASP |
| D1046  | Y1106 | F1166 |        |       |     |     |
| T1047  | A1107 | R1167 |        |       |     |     |
| A1048  | S1108 | L1168 |        |       |     |     |

• Molecule 1: Apaf-1 related killer DARK



|      |      |      |      |      |      |
|------|------|------|------|------|------|
| MET  | Y85  | Y168 | S155 | P236 | C307 |
| ASP  | K86  | Y169 | G156 | L241 | D311 |
| PHE  | T188 | Y170 | K157 | L242 | L312 |
| THR  | L88  | Y171 | W159 | V243 | P313 |
| GLY  | M89  | Y172 | L162 | L244 | R314 |
| GLU  | P91  | Y173 | D163 | L245 | E315 |
| H8   | T94  | Y174 | V164 | L246 | V316 |
| Q11  | R97  | Y175 | C165 | V247 | L317 |
| Y12  | Q98  | Y176 | Y168 | Q248 | T318 |
| K13  | P99  | Y177 | K169 | N249 | T319 |
| D14  | M101 | Y178 | V170 | A250 | N320 |
| I15  | M102 | Y179 | C171 | K251 | P321 |
| E20  | T103 | Y180 | Q172 | A252 | R322 |
| A22  | R104 | Y181 | M173 | W253 | R323 |
| F23  | M105 | Y182 | K174 | A254 | L324 |
| V24  | Y106 | Y183 | D175 | A255 | I331 |
| D28  | I107 | Y184 | F176 | F256 | R332 |
| D31  | E108 | Y185 | K177 | N257 | D333 |
| P36  | Q109 | Y186 | Y178 | L258 | A336 |
| R37  | Y114 | Y187 | W180 | I262 | T337 |
| S38  | N115 | Y188 | L181 | L263 | W338 |
| T39  | D116 | Y189 | N182 | L264 | D339 |
| L40  | N117 | Y190 | L183 | T265 | N340 |
| S41  | Q118 | Y191 | C186 | E267 | R341 |
| K42  | Y119 | Y192 | N187 | F268 | H343 |
| E43  | F120 | Y193 | S188 | K269 | N344 |
| E44  | A121 | Y194 | E194 | Q270 | N345 |
| I45  | K122 | Y195 | Q197 | F274 | C346 |
| D46  | Y123 | Y196 | K198 | L275 | D347 |
| D53  | V125 | Y197 | L199 | S276 | K348 |
| A54  | S126 | Y198 | L200 | F279 | I349 |
| R127 | R127 | Y199 | W207 | T280 | T350 |
| P130 | P130 | Y200 | T208 | T281 | I353 |
| K133 | K133 | Y201 | S209 | S284 | E354 |
| L134 | L134 | Y202 | R210 | L285 | L357 |
| R135 | R135 | Y203 | S211 | D286 | N358 |
| Q136 | Q136 | Y204 | D212 | H287 | E361 |
| L141 | L141 | Y205 | N216 | M290 | P362 |
| R142 | R142 | Y206 | I221 | T291 | A363 |
| P143 | P143 | Y207 | H222 | L292 | E364 |
| A144 | A144 | Y208 | S223 | T293 | Y365 |
| K145 | K145 | Y209 | D295 | P294 | K367 |
| N146 | N146 | Y210 | L296 | M368 | F369 |
| V147 | V147 | Y211 | Q225 | F369 | D370 |
| E227 | E227 | Y212 | A226 | R371 | L372 |
| L231 | L231 | Y213 | V297 | S373 | V374 |
| S234 | S234 | Y214 | S299 | F375 | P376 |
| K235 | K235 | Y215 | L300 | P377 |      |

|       |       |       |       |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|
| Q1113 | F1053 | I993  | H932  | R872 | T812 | E752 | GLY  | G628 | L566 | R502 | H440 | S378 |
| Y1114 | I1054 | H994  | T933  | H873 | P813 | F753 | GLY  | Q629 | H567 | H503 | R441 | I381 |
| I1115 | E1055 | L995  | L934  | L874 | L814 | K754 | LYS  | I630 | A568 | D504 | S442 | P382 |
| I1116 | E1056 | I996  | R935  | L875 | A815 | L755 | GLN  | L631 | E569 | S505 | I443 | T383 |
| F1117 | P1057 | K997  | S936  | L876 | L816 | S756 | LEU  | L632 | D570 | T506 | V444 |      |
| L1118 | I1058 | P998  | V937  | G877 | D817 | H757 | VAL  | T633 | E571 | A507 | H445 | L386 |
| S1119 | D1059 | A999  | S938  | T878 | V818 | H758 |      | D634 | I573 | W508 | H446 | S387 |
| D1120 | Y1060 | I1000 | G939  | S879 | F819 | P759 |      | V635 | F574 | N509 | I388 | L388 |
| H1121 | L1061 | S1001 | S940  | E880 | D820 | V760 |      | S636 | E575 | A510 | I389 | I389 |
| H1122 | K1062 | R1002 | S942  | C881 | E821 | L761 | V702 | L637 | E576 | S511 | V390 | V390 |
| V1123 | Q1063 | I1003 | S943  | L882 | R822 | K762 | K703 | E638 | A577 | G512 | F391 | F391 |
| C1124 | V1064 | S1004 | H943  | T883 | S823 | T763 | R704 | G639 | H578 | S513 | V393 | V393 |
| L1125 | S1065 | I1005 | Q944  | H884 | R824 | M764 | F705 | E640 | K579 | I514 | I394 | I394 |
| H1126 | P1066 | M1006 | H945  | H885 | T825 | Q765 | I706 | D641 | Q580 | L515 | K451 | K451 |
| D1127 | M1067 | S1007 | R946  | D886 | A826 | S766 | G707 | T642 | V581 | N516 | D457 | D457 |
| I1128 | I1068 | T1008 | E947  | L887 | T827 | G767 | L644 | L645 | Q582 | T517 | S455 | S455 |
| A1129 | L1069 | I1009 | I948  | R888 | H828 | R768 | S708 | L646 | R583 | L518 | D456 | D456 |
| V1130 | V1070 | T1010 | A949  | T889 | L829 | R769 | Y709 | R646 | Q519 | Q520 | L458 | L458 |
| P1131 | A1071 | P1011 | W950  | S890 | L830 | C770 | A710 | D647 | Q521 | K522 | P461 | P461 |
| S1132 | S1072 | T1012 | V951  | D891 | L831 | C771 | N711 | E648 | D585 | F523 | K404 | K404 |
| A1133 | A1073 | H1013 | H952  | P892 | F832 | F771 | L712 | S649 | D586 | Y524 | L405 | L405 |
| F1134 | H1074 | A1014 | S953  | H893 | K833 | V772 | K713 | D650 | V588 | K525 | H406 | H406 |
| V1135 | S1075 | A1015 | A954  | L894 | Y834 | Q773 | I714 | D651 | W589 | P526 | K407 | K407 |
| K1136 | A1076 | S1016 | D955  | L895 | S835 | V774 | T715 | S651 | F590 | Y527 | F467 | F467 |
| P1137 | Q1077 | N1017 | E956  | S896 | Y836 | L775 | A716 | D652 | T591 | S469 | S409 | S409 |
| K1138 | Q1078 | C1018 | N897  | H897 | H837 | K776 | F717 | D653 | N592 | H470 | V411 | V411 |
| D1139 | T1079 | K1019 | S958  | W898 | R838 | R777 | Y718 | I654 | H593 | E471 | E412 | E412 |
| S1140 | V1080 | I1020 | W959  | S899 | L839 | Y778 | L719 | L655 | G594 | Q414 | K413 | K413 |
| E1141 | I1081 | N1021 | M960  | H901 | R840 | V779 | N720 | M657 | R537 | P415 | P415 | P415 |
| E1142 | F1082 | A1022 | T961  | H901 | F841 | W780 | E721 | A658 | L538 | K476 | K416 | K416 |
| Y1143 | Q1083 | I1023 | K962  | I902 | L842 | V781 | D722 | W659 | V539 | I478 | E417 | E417 |
| L1144 | L1084 | S1024 | A963  | E903 | P843 | C782 | A723 | F660 | N540 | E479 | S418 | S418 |
| V1145 | E1085 | A1025 | C964  | C904 | H844 | C783 | G724 | N661 | L543 | H480 | I420 | I420 |
| G1146 | K1086 | F1026 | E966  | V905 | L845 | C786 | L725 | Q662 | D544 | E482 | I422 | I422 |
| F1147 | I1087 | N1027 | P967  | D906 | S846 | V787 | PRD  | Q663 | F545 | R483 | P423 | P423 |
| D1148 | P1088 | D1028 | P967  | I907 | Y847 | T787 | ALA  | K664 | L546 | M484 | S424 | S424 |
| L1149 | P1089 | E1029 | Q1030 | E909 | L849 | L788 | ASN  | H665 | P547 | T485 | I425 | I425 |
| K1150 | Q1091 | I1031 | L971  | F911 | Q850 | V790 | I730 | G670 | E551 | E428 | Y426 | Y426 |
| N1151 | F1032 | F1032 | R972  | D912 | S851 | W791 | Q731 | C671 | N552 | M489 | L427 | L427 |
| S1152 | P1092 | S1033 | S973  | P913 | E852 | D792 | L732 | N672 | L553 | V490 | K430 | K430 |
| L1153 | M1093 | G1034 | L974  | P914 | A853 | L793 | V734 | G673 | I554 | F491 | V431 | V431 |
| L1154 | D1094 | G1034 | L974  | Y915 | H854 | T794 | I737 | G674 | E554 | D493 | L433 | L433 |
| F1155 | Q1095 | V1035 | M975  | K916 | GLN  | W795 | N738 | V675 | C555 | F494 | E434 | E434 |
| L1156 | M1096 | V1036 | D976  | Y917 | LEU  | G796 | G739 | K676 | S566 | K495 | M435 | M435 |
| A1157 | P1097 | D1037 | M977  | Y917 | PRD  | V797 | T740 |      | K557 | F496 | E436 | E436 |
| Y1158 | L1098 | G1038 | T978  | V919 | GLU  | S797 | D740 | S679 | Y558 | T559 | Y437 | Y437 |
| M1159 | M1099 | V1039 | R979  | L920 | C859 | V798 | V741 | L880 | D560 | D560 | A438 | A438 |
| N1160 | M1100 | I1040 | E980  | C921 | S860 | W799 | S742 | W681 | L561 | L561 | Q499 | Q499 |
| N1161 | D1101 | I1041 | R981  | G922 | F861 | T800 | I743 | P682 | L562 | L562 |      |      |
| I1162 | V1102 | D1042 | T982  | A923 | L862 | L801 | L744 | ASP  | N618 | I564 |      |      |
| I1163 | S1103 | V1043 | Q983  | K924 | T863 | E802 | N745 | CYS  | D619 | S627 |      |      |
| D1164 | T1104 | I1044 | L984  | G925 | C864 | L803 | W746 | PRD  | F620 |      |      |      |
| V1165 | K1105 | H1045 | L985  | V928 | C865 | H804 | D747 | GLY  | C621 |      |      |      |
| F1166 | Y1106 | D1046 | A986  | Q927 | K866 | V805 | E748 | ARG  | L622 |      |      |      |
| R1167 | A1107 | T1047 | V987  | V928 | R867 | F806 | Q749 | ARG  | L625 |      |      |      |
| L1168 | S1108 | A1048 | D988  | V929 | S868 | N807 | D750 | HIS  | A626 |      |      |      |
| L1169 | L1109 | P1050 | S989  | H930 | T869 | E809 | Q751 | SER  | S627 |      |      |      |
| F1170 | Q1110 | Q1051 | K990  | H930 | D870 | E809 |      |      |      |      |      |      |
| S1171 | E1111 | Q1052 | E991  | D870 | G871 | N810 |      |      |      |      |      |      |
| C1172 | G1112 |       | R992  | G871 | D811 |      |      |      |      |      |      |      |

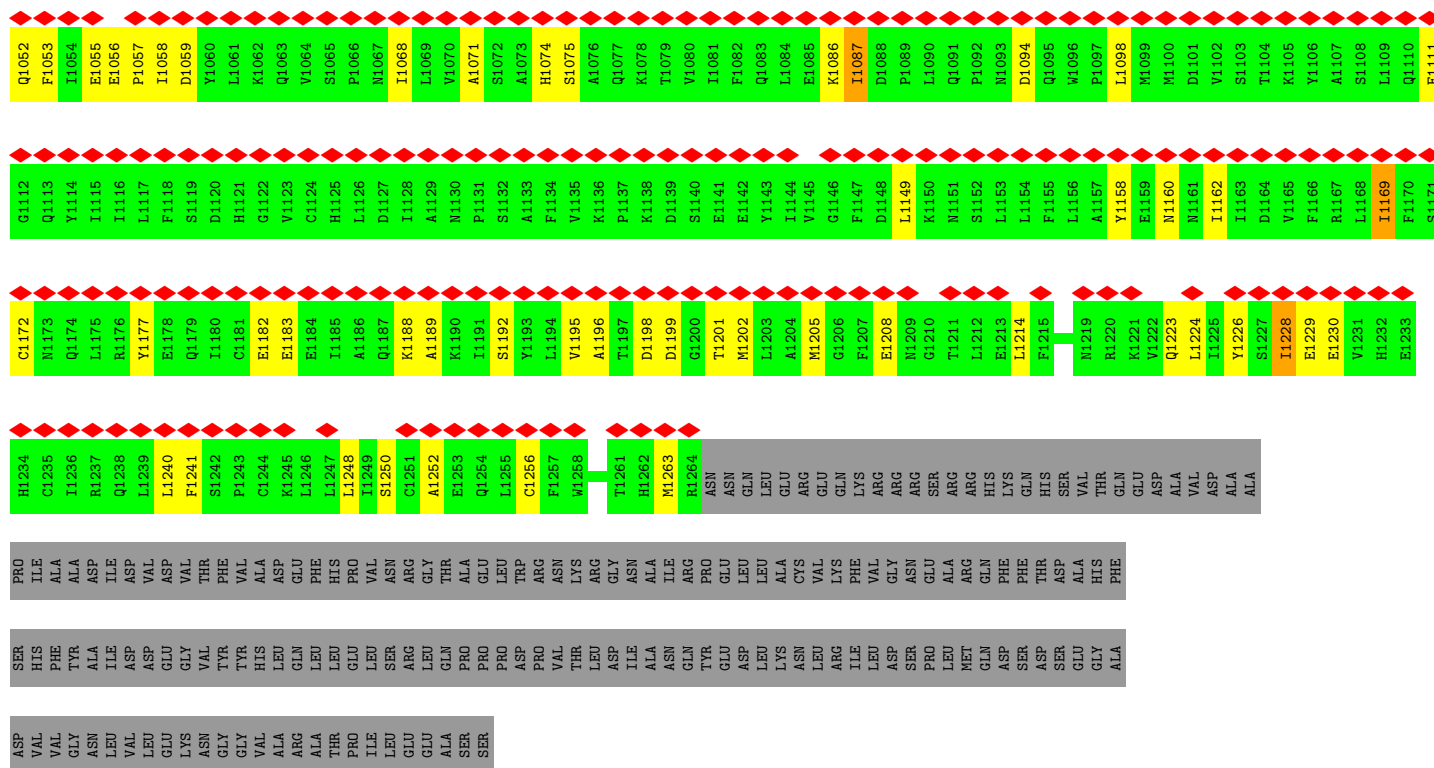


- Molecule 1: Apaf-1 related killer DARK

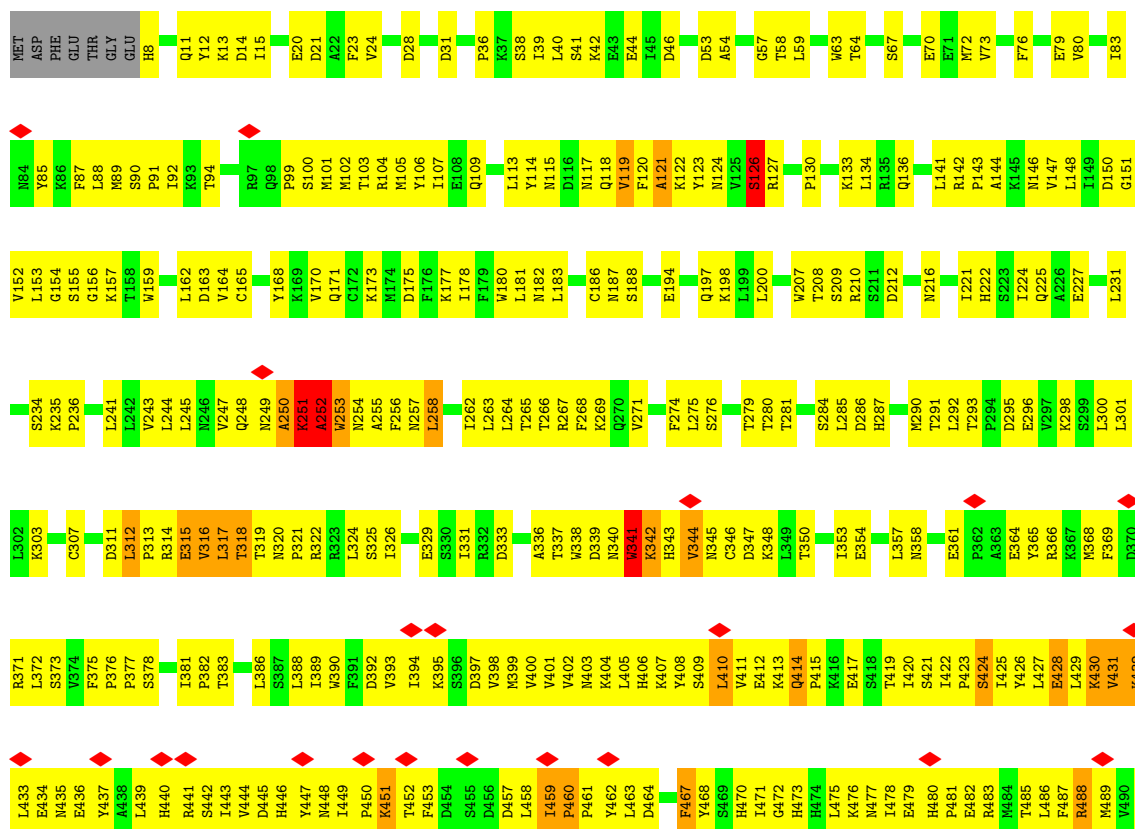






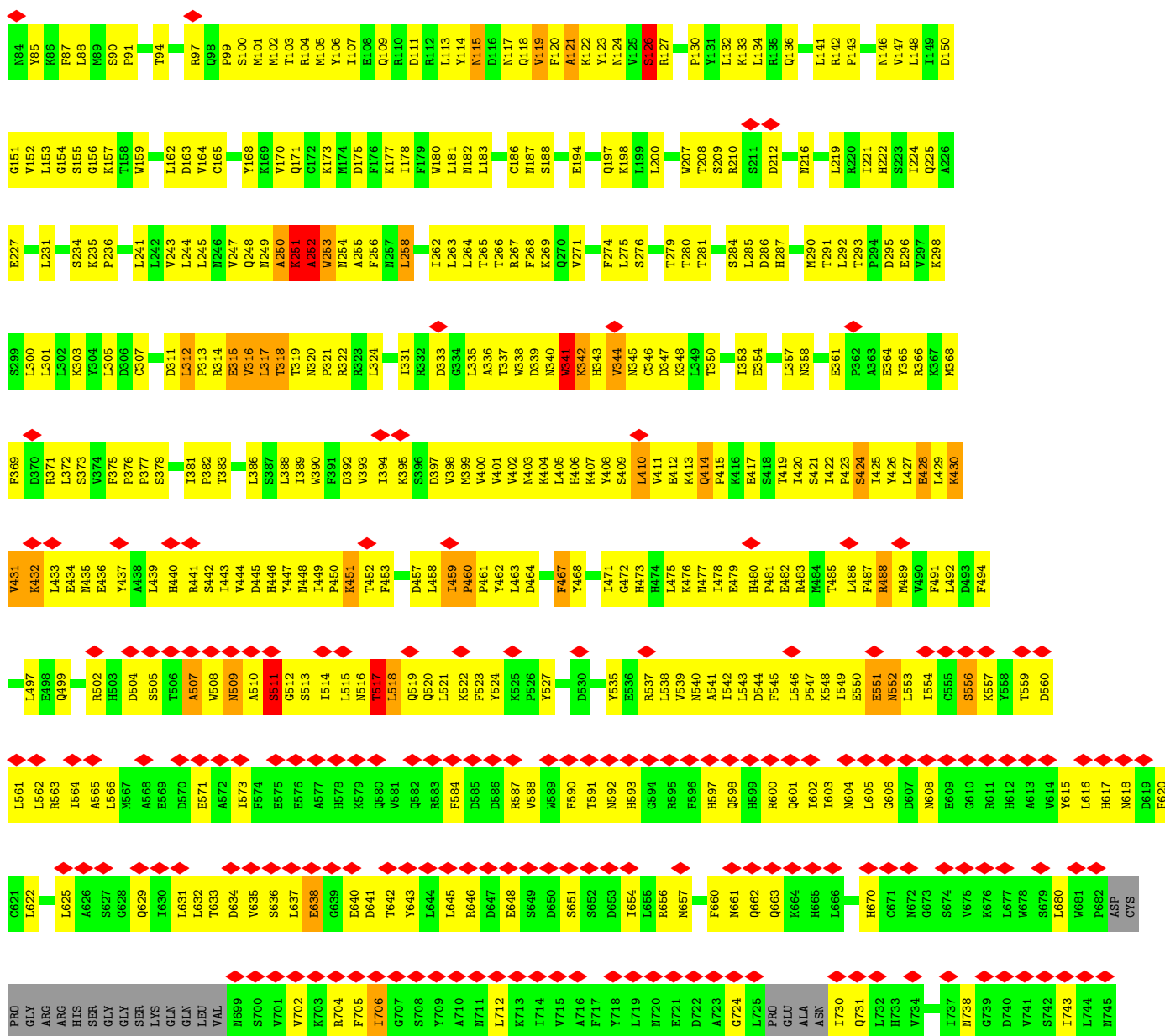
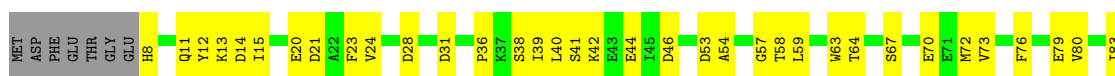


### • Molecule 1: Apaf-1 related killer DARK

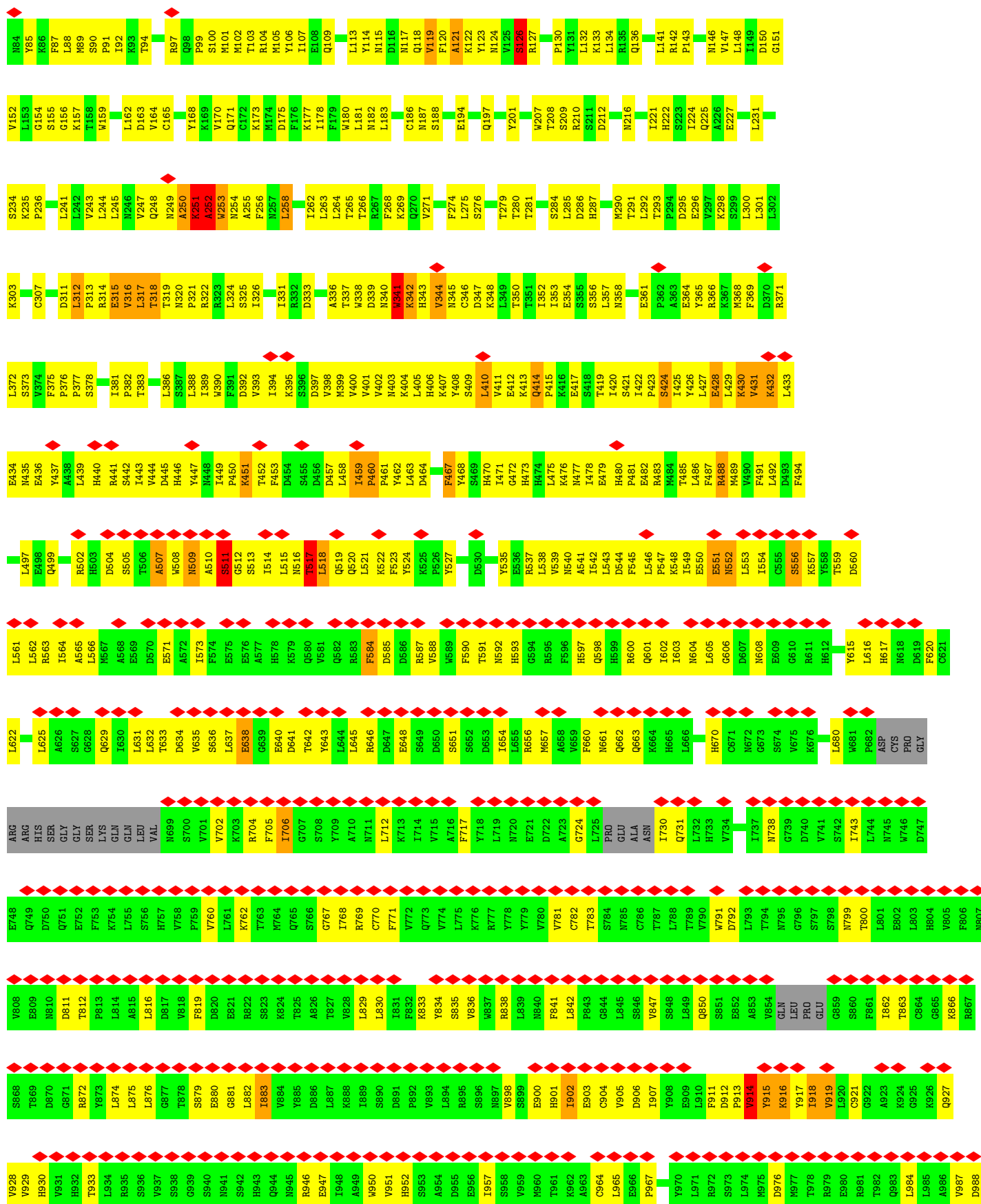


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| ALA   | VAL   | ASP   | ALA   | ALA   | PRO   | ILE   | ALA   | ASP   | ASP   | ILE   | ASP   | VAL   | ASP   | THR   | PHE   | VAL   | ALA   | ALA   | ASP   | GLU   | PHE   | HIS   | PRO   | VAL   | ASN   | ARG   | GLY   | THR   | ALA   | ALA   | GLU   | LEU   | LEU   | TRP   | ARG   | LYS   | ARG   | GLY   | ASN   | ALA   | ILE   | ARG   | PRO   | GLU   | LEU   | LEU   | ALA   | CYS   | VAL   | PHE   | VAL   | GLY   | ASN   | ARG   | ALA   | ARG   | GLN   | PHE   | PHE   |       |       |
| E1229 | E1230 | V1231 | H1232 | H1233 | H1234 | H1235 | C1236 | I1237 | Q1238 | L1239 | L1240 | F1241 | S1242 | P1243 | C1244 | K1245 | L1246 | L1247 | L1248 | L1249 | C1250 | C1251 | A1252 | E1253 | Q1254 | L1255 | F1256 | W1257 | T1258 | T1261 | H1262 | M1263 | R1264 | ASN   | ASN   | GLN   | LEU   | ALA   | CYS   | VAL   | LYS   | PHE   | VAL   | GLY   | ASN   | ARG   | ALA   | ARG   | GLN   | PHE   | PHE   |       |       |       |       |       |       |       |       |       |       |
| F1166 | R1167 | L1168 | I1169 | F1170 | S1171 | C1172 | N1173 | Q1174 | L1175 | R1176 | Y1177 | E1178 | Q1179 | I1180 | C1181 | E1182 | E1183 | E1184 | I1185 | A1186 | Q1187 | K1188 | A1189 | K1190 | I1191 | S1192 | Y1193 | L1194 | V1195 | A1196 | T1197 | D1198 | D1199 | G1200 | T1201 | M1202 | L1203 | A1204 | M1205 | G1206 | F1207 | E1208 | N1209 | L1210 | L1211 | L1212 | L1213 | L1214 | F1215 | R1216 | K1217 | Q1218 | L1219 | I1220 | K1221 | Q1222 | L1224 | I1225 | Y1226 | S1227 | I1228 |
| Y1106 | A1107 | S1108 | L1109 | Q1110 | E1111 | G1112 | Q1113 | Y1114 | I1115 | I1116 | L1117 | F1118 | S1119 | D1120 | H1121 | G1122 | V1123 | C1124 | H1125 | L1126 | D1127 | I1128 | A1129 | N1130 | P1131 | S1132 | A1133 | F1134 | V1135 | K1136 | P1137 | K1138 | D1139 | S1140 | E1141 | E1142 | Y1143 | I1144 | V1145 | G1146 | F1147 | L1148 | L1149 | K1150 | N1151 | S1152 | L1153 | L1154 | F1155 | L1156 | A1157 | Y1158 | E1159 | N1160 | N1161 | I1162 | T1163 | D1164 | V1165 |       |       |
| D1046 | T1047 | A1048 | L1049 | P1050 | Q1051 | Q1052 | F1053 | I1054 | E1055 | E1056 | P1057 | L1058 | D1059 | Y1060 | L1061 | K1062 | Q1063 | V1064 | S1065 | P1066 | M1067 | I1068 | L1069 | V1070 | A1071 | S1072 | A1073 | H1074 | S1075 | A1076 | Q1077 | K1078 | T1079 | V1080 | I1081 | F1082 | Q1083 | L1084 | E1085 | K1086 | I1087 | D1088 | P1089 | L1090 | Q1091 | P1092 | M1093 | D1094 | Q1095 | V1096 | P1097 | L1098 | M1099 | M1100 | D1101 | V1102 | S1103 | T1104 | K1105 |       |       |
| G865  | K866  | R867  | S868  | T869  | D870  | G871  | R872  | Y873  | L874  | L875  | L876  | G877  | T878  | S879  | E880  | G881  | L882  | L883  | V884  | Y885  | D886  | L887  | K888  | L889  | S890  | D891  | P892  | H893  | L894  | R895  | S896  | H897  | V898  | S899  | E900  | N901  | L902  | E903  | C904  | V905  | D906  | L907  | Y908  | E909  | L910  | F911  | D912  | P913  | V914  | Y915  | K916  | Y917  | L918  | P919  | L920  | C921  | G922  | A923  | K924  |       |       |
| H804  | V805  | F806  | N807  | V808  | E809  | N810  | D811  | T812  | P813  | L814  | A815  | L816  | D817  | V818  | F819  | D820  | E821  | R822  | S823  | K824  | T825  | A826  | T827  | V828  | L829  | L830  | L831  | Y834  | S835  | V836  | H837  | R838  | L839  | N840  | F841  | L842  | P843  | C844  | L845  | S846  | V847  | S848  | L849  | Q850  | S851  | D852  | A853  | V854  | L855  | P856  | L857  | G858  | S859  | S860  | F861  | T862  | T863  | C864  |       |       |       |
| I743  | L744  | N745  | V746  | D747  | E748  | Q749  | D750  | Q751  | E752  | F753  | K754  | L755  | S756  | H757  | V758  | P759  | V760  | L761  | K762  | T763  | H764  | Q765  | S766  | Q767  | I768  | R769  | C770  | F771  | V772  | Q773  | V774  | L775  | K776  | T777  | V778  | E779  | D780  | V781  | C782  | T783  | S784  | N785  | C786  | T787  | L788  | W791  | D792  | L793  | T794  | V795  | G796  | S797  | T798  | N799  | T800  | L801  | E802  | L803  |       |       |       |
| P882  | ASP   | CYS   | PRO   | GLY   | ARG   | HIS   | SER   | GLY   | GLY   | SER   | LYS   | GLN   | LEU   | VAL   | N699  | S700  | V701  | W702  | K703  | E840  | D841  | T842  | Y843  | L844  | L845  | R846  | D847  | E848  | S849  | L712  | K713  | I714  | V715  | A716  | F717  | L718  | L719  | N720  | E721  | D722  | A723  | G724  | L725  | P80   | GLU   | ALA   | ASN   | I730  | Q731  | L732  | H733  | V734  | I737  | N738  | G739  | D740  | V741  | S742  |       |       |       |
| F620  | C621  | L622  | L625  | A626  | S627  | G628  | Q629  | I630  | L631  | L632  | T633  | D634  | V635  | S636  | L637  | E638  | G639  | E640  | D641  | T642  | Y643  | L644  | L645  | R646  | D647  | E648  | S649  | L650  | S651  | S652  | D653  | I654  | R655  | M657  | V659  | F660  | N661  | Q662  | Q663  | K664  | H665  | L666  | I667  | H670  | C671  | N672  | G673  | S674  | K675  | L676  | L677  | W678  | S679  | L680  | W681  |       |       |       |       |       |       |
| T559  | D560  | L561  | L562  | R563  | I564  | A565  | L566  | M567  | A568  | E569  | D570  | E571  | A572  | I573  | F574  | E575  | E576  | A577  | H578  | K579  | Q580  | V581  | Q582  | L581  | Q583  | F584  | D585  | E586  | R587  | D588  | W589  | F590  | T591  | N592  | H593  | G594  | R595  | V596  | H597  | Q598  | H599  | R600  | Q601  | I602  | I603  | N604  | E605  | E606  | D607  | N608  | G609  | G610  | R611  | H612  | Y615  | L616  | H617  | N618  | D619  |       |       |
| F494  | R495  | F496  | L497  | E498  | Q499  | R502  | D504  | S505  | T506  | A507  | W508  | N509  | A510  | S511  | G512  | S513  | I514  | L515  | N516  | T517  | L518  | Q519  | Q520  | L521  | K522  | F523  | Y524  | K525  | P526  | Y527  | D530  | Y535  | E536  | R537  | L538  | V539  | N540  | A541  | I542  | L543  | D544  | F545  | L546  | P547  | K548  | I549  | E550  | E551  | N552  | L553  | I554  | C555  | S556  | K557  | Y558  |       |       |       |       |       |       |

- Molecule 1: Apaf-1 related killer DARK







|       |       |       |       |       |     |     |     |
|-------|-------|-------|-------|-------|-----|-----|-----|
| SR89  | L1049 | L1109 | II189 | V1231 | ASP | ALA | GLU |
| K990  | P1050 | Q1110 | F1170 | H1232 | ALA | HIS | GLY |
| E991  | Q1051 | E1111 | S1171 | E1233 | ALA | PHE | ALA |
| R992  | Q1052 | G1112 | C1172 | H1234 | PRO | SER | ASP |
| I993  | F1053 | G1113 | N1173 | I1235 | ILE | VAL | VAL |
| H994  | I1054 | Y1114 | Q1174 | I1236 | ALA | PHE | VAL |
| L995  | E1055 | I1115 | L1175 | R1237 | ASP | TYR | GLY |
| I996  | E1056 | I1116 | L1176 | Q1238 | ASP | ILE | ASN |
| R997  | P1057 | I1117 | R1177 | Q1239 | VAL | ASP | LEU |
| P998  | I1058 | F1118 | E1177 | L1240 | ASP | GLY | VAL |
| A999  | D1059 | S1119 | Q1179 | F1241 | THR | VAL | ASN |
| I1000 | Y1060 | D1120 | II180 | S1242 | PHE | GLY | GLY |
| S1001 | L1061 | G1121 | C1181 | P1243 | VAL | TYR | GLY |
| R1002 | K1062 | H1122 | E1182 | C1244 | ALA | VAL | VAL |
| I1003 | Q1063 | V1123 | E1183 | K1245 | ASP | ALA | ALA |
| S1004 | V1064 | C1124 | E1184 | L1246 | GLU | GLN | ARG |
| E1005 | S1065 | H1125 | II185 | L1247 | PHE | LEU | ALA |
| W1006 | P1066 | L1126 | II186 | L1248 | PRO | THR | THR |
| S1007 | N1067 | D1127 | Q1187 | I1249 | VAL | LEU | ILE |
| T1008 | I1068 | I1128 | K1188 | C1250 | ASN | SER | LEU |
| I1009 | L1069 | A1129 | A1189 | C1251 | ARG | ARG | GLU |
| T1010 | V1070 | M1130 | K1190 | A1252 | GLY | LEU | GLU |
| P1011 | A1071 | P1131 | II191 | E1253 | THR | GLN | ALA |
| T1012 | S1072 | S1132 | S1192 | E1254 | ALA | PRO | SER |
| H1013 | A1073 | A1133 | Y1193 | L1255 | LEU | PRO | ASP |
| A1014 | H1074 | F1134 | L1194 | C1256 | ARG | VAL | PRO |
| A1015 | S1075 | V1135 | V1195 | F1257 | LYS | THR | VAL |
| S1016 | Q1076 | K1136 | A1196 | W1258 | ASP | LEU | ASP |
| M1017 | Q1077 | P1137 | T1197 | T1261 | GLY | ILE | ILE |
| C1018 | K1078 | K1138 | D1198 | H1262 | ALA | ALA | ALA |
| K1019 | T1079 | D1139 | D1199 | M1263 | ILE | ASN | ASN |
| I1020 | I1080 | S1140 | G1200 | R1264 | ARG | TYR | GLN |
| N1021 | I1081 | E1141 | T1201 | ASN   | PRO | GLU | ASN |
| A1022 | F1082 | E1142 | M1202 | GLN   | LEU | LEU | GLN |
| I1023 | Q1083 | Y1143 | L1203 | ALA   | LEU | LEU | ALA |
| S1024 | L1084 | I1144 | A1204 | CYS   | VAL | LYS | ASN |
| A1025 | E1085 | V1145 | M1205 | ARG   | VAL | ARG | LEU |
| F1026 | K1086 | G1146 | G1206 | GLY   | PHE | ILE | ILE |
| N1027 | I1087 | F1147 | F1207 | LYS   | VAL | LEU | ASP |
| D1028 | P1088 | D1148 | E1208 | ARG   | GLY | ASP | ASN |
| E1029 | P1089 | L1149 | N1209 | ARG   | GLU | PRO | GLU |
| Q1030 | Q1090 | K1150 | L1212 | SER   | ALA | LEU | ALA |
| I1031 | Q1091 | M1151 | E1213 | ARG   | ALA | MET | GLN |
| F1032 | P1092 | S1152 | L1214 | ARG   | GLN | GLN | ASP |
| V1033 | N1093 | L1153 | F1215 | HIS   | PHE | ASP | SER |
| G1034 | D1094 | L1154 | A1216 | LYS   | THR | ASP | THR |
| Y1035 | Q1095 | F1155 | N1219 | HIS   | SER | SER | ASP |
| V1036 | W1096 | L1156 | R1220 | SER   | VAL | THR | VAL |
| D1037 | P1097 | A1157 | K1221 | THR   | GLN | GLN | GLN |
| G1038 | L1098 | Y1158 | Q1222 | GLN   | ASP | ASP | ASP |
| V1039 | M1099 | E1159 | Q1223 | ASP   | ALA | ALA | ALA |
| I1040 | M1100 | M1160 | L1224 | VAL   | VAL | VAL | VAL |
| I1041 | D1101 | M1161 | I1225 | VAL   | VAL | VAL | VAL |
| D1042 | V1102 | I1162 | Y1226 | VAL   | VAL | VAL | VAL |
| V1043 | S1103 | I1163 | I1227 | VAL   | VAL | VAL | VAL |
| I1044 | T1104 | D1164 | I1228 | VAL   | VAL | VAL | VAL |
| H1045 | K1105 | V1165 | I1229 | VAL   | VAL | VAL | VAL |
| D1046 | Y1106 | F1166 | E1230 | VAL   | VAL | VAL | VAL |
| T1047 | A1107 | R1167 |       | VAL   | VAL | VAL | VAL |
| A1048 | S1108 | L1168 |       | VAL   | VAL | VAL | VAL |

• Molecule 1: Apaf-1 related killer DARK



|     |     |      |      |      |
|-----|-----|------|------|------|
| MET | P87 | L162 | V946 | E315 |
| ASP | L88 | D163 | V247 | V316 |
| PHE | M89 | Q248 | N249 | L317 |
| GLU | S90 | T318 | A950 | T319 |
| THR | P91 | C165 | K251 | N320 |
| GLY |     |      | A952 | P321 |
| GLU |     |      | W253 | R322 |
| H8  |     |      | N254 | L324 |
| Q11 |     |      | A255 | I331 |
| Y12 |     |      | F256 | R332 |
| K13 |     |      | R257 | D333 |
| D14 |     |      | L258 | A336 |
| I15 |     |      | T262 | T337 |
| E20 |     |      | L263 | W338 |
| D21 |     |      | L264 | D339 |
| A22 |     |      | T265 | N340 |
| F23 |     |      | T266 | W341 |
| V24 |     |      | R267 | K342 |
| D28 |     |      | F268 | H343 |
| D31 |     |      | K269 | V344 |
| D36 |     |      | Q270 | N345 |
| P36 |     |      | V271 | C346 |
| R37 |     |      | F274 | D347 |
| S38 |     |      | L275 | K348 |
| I39 |     |      | S276 | L349 |
| L40 |     |      | T279 | T350 |
| S41 |     |      | T280 | I353 |
| E44 |     |      | H282 | E354 |
| D53 |     |      | T283 | L357 |
| A54 |     |      | S284 | N358 |
| G57 |     |      | L285 | E361 |
| T58 |     |      | D286 | P362 |
| L59 |     |      | H287 | A363 |
| W63 |     |      | M290 | E364 |
| T64 |     |      | T291 | Y365 |
| S67 |     |      | L292 | R366 |
| E70 |     |      | T293 | K367 |
| M72 |     |      | P294 | D295 |
| V73 |     |      | E296 | F297 |
| F76 |     |      | V297 | K298 |
| E79 |     |      | S299 | L300 |
| V80 |     |      | L301 | L302 |
| I83 |     |      | K303 | C307 |
| N84 |     |      | C307 | D311 |
| Y85 |     |      | D311 | L312 |
| K86 |     |      | L312 | P313 |
|     |     |      | T158 | L244 |
|     |     |      | W159 | L245 |

|       |       |       |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|
| D1120 | Y1060 | I1000 | G939 | F819 | F759 | VAL  | V635 | I573 | N509 | H446 | L386 |
| H1121 | L1061 | S1001 | S940 | D820 | V760 | N699 | S636 | F574 | A510 | Y447 | S387 |
| G1122 | K1062 | R1002 | N941 | E821 | L761 | S700 | L637 | E575 | S511 | N448 | L388 |
| V1123 | Q1063 | I1003 | S942 | R822 | K762 | V701 | E638 | E576 | G512 | I449 | L389 |
| C1124 | V1064 | S1004 | N943 | R823 | T763 | K703 | G639 | E577 | S513 | P450 | V390 |
| L1125 | P1065 | E1005 | H944 | K824 | V764 | R704 | E940 | H578 | I514 | K451 | D392 |
| L1126 | P1066 | V1006 | N945 | T825 | Q765 | R705 | D641 | K579 | L515 | T452 | V393 |
| D1127 | M1067 | V1007 | R946 | A826 | S766 | T706 | T642 | Q580 | N516 | F453 | I394 |
| I1128 | L1068 | T1008 | E947 | T827 | G767 | I706 | Y643 | V581 | T517 | D454 | K395 |
| A1129 | L1069 | I1009 | I948 | V828 | T768 | G707 | L644 | Q582 | L518 | S455 | S396 |
| M1130 | V1070 | T1010 | A949 | L829 | R769 | S708 | L645 | R583 | Q519 | D457 | D397 |
| P1131 | A1071 | P1011 | W950 | L830 | C770 | T709 | R646 | F584 | Q520 | L458 | V398 |
| S1132 | S1072 | H1012 | W951 | R831 | F771 | A710 | D647 | D585 | K522 | I459 | M399 |
| A1133 | A1073 | H1013 | H952 | K833 | V772 | N711 | E648 | D586 | F523 | P460 | V401 |
| F1134 | H1074 | A1014 | S953 | Y834 | Q773 | L712 | S649 | V588 | Y524 | P461 | V402 |
| V1135 | S1075 | A1015 | A954 | Y835 | V774 | K713 | D650 | W589 | K525 | Y462 | N403 |
| K1136 | A1076 | A1016 | D955 | S835 | L775 | T714 | S651 | F590 | P526 | K404 | K404 |
| P1137 | Q1077 | N1017 | E956 | V836 | L776 | T715 | S652 | T591 | Y527 | L463 | L405 |
| K1138 | Q1078 | C1018 | I957 | W837 | K777 | A716 | D653 | T592 | F467 | D464 | H406 |
| D1139 | T1079 | K1019 | S958 | R838 | R778 | F717 | T654 | N592 | Y468 | K407 | K407 |
| E1140 | V1080 | I1020 | W959 | L839 | V779 | Y718 | L655 | H593 | S469 | Y408 | Y408 |
| S1141 | I1081 | N1021 | N960 | W840 | V780 | L719 | R656 | Q594 | H470 | S409 | S409 |
| E1142 | F1082 | A1022 | T961 | F841 | W781 | N720 | M657 | R595 | I471 | V411 | V411 |
| Y1143 | Q1083 | I1023 | K962 | L842 | C782 | T721 | A658 | R596 | G472 | H412 | H412 |
| I1144 | L1084 | S1024 | A963 | R843 | T783 | A723 | V659 | Q598 | H474 | K413 | K413 |
| V1145 | E1085 | A1025 | C964 | L845 | S784 | G724 | F660 | H599 | L475 | P415 | P415 |
| K1086 | K1086 | F1026 | L965 | L846 | W785 | N661 | Q662 | L542 | K476 | K416 | K416 |
| I1087 | I1087 | N1027 | E966 | S846 | C786 | G725 | Q663 | L543 | N477 | E417 | E417 |
| D1148 | D1088 | D1028 | P967 | W847 | T787 | PHO  | K664 | R600 | E479 | S418 | S418 |
| L1149 | P1089 | I1029 | Y970 | S848 | L788 | GLU  | H665 | Q601 | H480 | T419 | T419 |
| K1150 | L1090 | Q1030 | N971 | L849 | V789 | ALA  | H666 | L605 | P481 | I420 | I420 |
| S1151 | Q1091 | I1031 | R972 | Q850 | W791 | I730 | H670 | E551 | S421 | I426 | I426 |
| S1152 | F1032 | D912  | D912 | S851 | D792 | L732 | C671 | N552 | I427 | Y426 | Y426 |
| L1153 | V1033 | P913  | S973 | E852 | L793 | H733 | H672 | L553 | L427 | F487 | F487 |
| L1154 | G1034 | Y914  | L974 | A853 | T794 | W734 | G673 | I554 | E428 | R488 | R488 |
| F1155 | Y1035 | Y915  | N975 | W854 | W795 |      | S674 | C555 | L429 | L429 | L429 |
| L1156 | V1036 | K916  | D976 | GLN  | G796 | I737 | V675 | S556 | K430 | K430 | K430 |
| A1157 | P1037 | Y917  | N977 | PRO  | G797 | N738 | K676 | K557 | V431 | V431 | V431 |
| Y1158 | L1098 | Y918  | T978 | GLU  | S797 | G739 |      | Y558 | K432 | K432 | K432 |
| E1159 | M1099 | V1039 | R979 | Q859 | S798 | D740 | S679 | T559 | L433 | L433 | L433 |
| N1160 | M1100 | I1040 | E980 | S860 | W799 | D741 | L680 | D560 | E434 | E434 | E434 |
| M1161 | D1101 | I1041 | R981 | F861 | T800 | V741 | W681 | L561 | N435 | N435 | N435 |
| Y1162 | V1102 | D1042 | T982 | T862 | L801 | I743 | P682 | L562 | Y437 | Y437 | Y437 |
| I1163 | S1103 | A923  | Q983 | T863 | E802 | L744 | ASP  | R563 | L439 | L439 | L439 |
| T1104 | T1104 | I1044 | G925 | C864 | L803 | N745 | CYS  | I564 | H440 | H440 | H440 |
| V1165 | K1105 | H1045 | Q927 | Q865 | H804 | W746 | PRO  | A565 | R441 | R441 | R441 |
| F1166 | V1106 | H1046 | Q928 | K866 | W805 | T747 | GLY  | L566 | D504 | D504 | D504 |
| R1167 | A1107 | T1047 | V928 | X867 | F806 | D748 | ARG  | M567 | S505 | S505 | S505 |
| S1108 | S1108 | L1048 | V929 | S868 | N807 | E748 | HIS  | A568 | T506 | T506 | T506 |
| L1168 | L1109 | L1049 | W931 | T869 | W808 | Q749 | SER  | E569 | A507 | A507 | A507 |
| I1169 | Q1050 | D870  | H932 | D870 | E809 | D750 | GLY  | D570 | W508 | W508 | W508 |
| F1170 | P1051 | Q1051 | H933 | C871 | E752 | Q751 | GLY  | E571 |      |      |      |
| C1171 | Q1051 | Q1051 | T933 | R872 | W811 | E753 | LYS  | A572 |      |      |      |
| M1173 | Q1052 | F1053 | L934 | R873 | T812 | K754 | GLN  |      |      |      |      |
| Q1174 | I1054 | I1054 | R935 | L874 | P813 | L755 | LEU  |      |      |      |      |
| L1175 | E1055 | E1055 | S936 | L875 | L814 | S756 |      |      |      |      |      |
| L1176 | I1115 | I1115 | V937 | L876 | L815 | H757 |      |      |      |      |      |
| Y1177 | L1117 | L1117 | S938 | C877 | L816 | W758 |      |      |      |      |      |
| E1178 | F1118 | F1118 | P998 | T878 | W817 |      |      |      |      |      |      |
| Q1179 | S1119 | D1059 | A999 |      | W818 |      |      |      |      |      |      |



- Molecule 1: Apaf-1 related killer DARK



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| RET  | ASP  | PHE  | GLU  | THR  | GLY  | GLU  | H8   | Q11  | Y12  | K13  | D14  | I15  | E20  | D21  | A22  | F23  | V24  | D28  | D31  | P36  | K37  | S38  | I39  | L40  | S41  | K42  | E43  | E44  | I45  | D46  | D53  | A54  | G57  | T58  | L59  | W63  | T64  | S67  | E70  | E71  | M72  | V73  | F76  | E79  | V80  | I83  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| N84  | Y85  | X86  | F87  | L88  | R89  | S90  | P91  | R97  | Q98  | P99  | S100 | M101 | M102 | T103 | R104 | M105 | I106 | I107 | E108 | Q109 | Y114 | N115 | D116 | M117 | Q118 | F119 | A121 | K122 | E123 | N124 | I125 | S126 | R127 | P130 | K133 | L134 | R135 | Q136 | L141 | R142 | P143 | N146 | V147 | L148 | I149 | D150 | G151 | G154 | S155 | G156 | K157 |      |      |      |      |      |      |      |      |      |      |      |      |
| T158 | W159 | L162 | D163 | V164 | C165 | Y168 | K169 | V170 | Q171 | K172 | K173 | M174 | D175 | F176 | K177 | L178 | F179 | W180 | E181 | N182 | L183 | C186 | M187 | S188 | E194 | Q197 | L200 | W207 | T208 | S209 | R210 | S211 | D212 | N216 | T221 | H222 | S223 | T224 | Q225 | A226 | E227 | L231 | S234 | K235 | P236 | L241 | L242 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| V243 | L244 | L245 | N246 | L247 | Q248 | N249 | A250 | K251 | A252 | K253 | N254 | A255 | F256 | N257 | L258 | L262 | L263 | L264 | T265 | T266 | K267 | F268 | K269 | V271 | F274 | L275 | S276 | T279 | T280 | T281 | S284 | L285 | H287 | N290 | T291 | L292 | T293 | F294 | D295 | E296 | V297 | K298 | L300 | L301 | L302 | K303 | C307 | D311 | L312 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| P313 | R314 | E315 | V316 | L317 | T318 | T319 | N320 | P321 | R322 | K323 | L324 | I331 | R332 | D333 | A336 | T337 | V338 | D339 | N340 | K341 | K342 | H343 | V344 | C346 | D347 | K348 | L349 | T350 | I353 | E354 | L357 | N358 | E361 | F362 | A363 | E364 | Y365 | R366 | F367 | M368 | D370 | L371 | L372 | S373 | V374 | F375 | P376 | F377 | S378 | I381 | P382 |      |      |      |      |      |      |      |      |      |      |      |      |
| T383 | L386 | S387 | L388 | I389 | W390 | F391 | D392 | P393 | R394 | K395 | S396 | D397 | V398 | M399 | V400 | T401 | V402 | N403 | K404 | L405 | H406 | K407 | Y408 | S409 | L410 | V411 | G412 | K413 | Q414 | P415 | K416 | E417 | S418 | T419 | I420 | S421 | I422 | P423 | S424 | I425 | E426 | L427 | E428 | L429 | K430 | V431 | K432 | L433 | E434 | N435 | E436 | Y437 | A438 | L439 | H440 | R441 | S442 | I443 |      |      |      |      |      |
| V444 | D445 | H446 | Y447 | N448 | I449 | P450 | K451 | T452 | F453 | D454 | D456 | L458 | L459 | Q520 | L521 | K522 | P461 | Y462 | D339 | E181 | D464 | F467 | Y468 | S469 | H470 | I471 | G472 | H473 | L474 | L475 | V476 | K477 | N477 | L478 | E479 | H480 | P481 | E482 | R483 | M484 | T485 | L486 | F487 | R488 | M489 | Y490 | F491 | L492 | D493 | F494 | R495 | L496 | L497 | E498 | Q499 | R502 | H503 | D504 | S505 |      |      |      |      |
| T506 | A507 | W508 | N509 | A510 | S511 | G512 | S513 | I514 | L515 | M516 | T517 | L518 | Q519 | Q520 | L521 | K522 | P461 | Y523 | Y524 | K525 | P526 | Y527 | D530 | Y535 | E536 | R537 | L538 | V539 | N540 | A541 | I542 | L543 | D544 | F545 | L546 | I547 | K548 | L549 | E550 | E551 | N552 | L553 | I554 | C555 | S556 | K557 | T558 | L559 | D560 | L561 | L562 | R563 | I564 | A565 | L566 | M567 | E568 | E569 |      |      |      |      |      |
| D570 | E571 | A572 | I573 | F574 | E575 | E576 | A577 | H578 | K579 | Q580 | V581 | Q582 | R583 | F584 | D585 | D586 | R587 | V588 | W589 | F590 | T591 | N592 | H593 | G594 | R595 | F596 | H597 | Q598 | H599 | R600 | Q601 | I602 | I603 | N604 | L605 | G606 | D607 | N608 | E609 | G610 | R611 | H612 | Y615 | L616 | H617 | N618 | D619 | F620 | G621 | L622 | L625 | A626 | S627 | G628 | Q629 | I630 | L631 |      |      |      |      |      |      |
| L632 | T633 | D634 | V635 | S636 | L637 | E638 | G639 | E640 | D641 | T642 | Y643 | L644 | L645 | R646 | D647 | E648 | S649 | D650 | S651 | S652 | D653 | L654 | L655 | M656 | A658 | V659 | F660 | N661 | Q662 | Q663 | K664 | H665 | L666 | I667 | H670 | C671 | N672 | G673 | S674 | V675 | K676 | L677 | W678 | S679 | L680 | W681 | P682 | ASP  | CYS  | PRO  | GLY  | ARG  | ARG  | HIS  | SER  | GLY  | GLY  |      |      |      |      |      |      |
| SER  | LYS  | GLN  | GLN  | LEU  | VAL  | N699 | S700 | V701 | W702 | K703 | R704 | F705 | I706 | G707 | S708 | Y709 | A710 | M711 | L712 | K713 | I714 | V715 | A716 | F717 | Y718 | L719 | M720 | E721 | D722 | A723 | G724 | L725 | PRO  | GLU  | ALA  | ASN  | I730 | Q731 | L732 | H733 | V734 | I737 | N738 | G739 | D740 | W741 | S742 | I743 | L744 | N745 | W746 | D747 | E748 | F805 | Q749 | D750 | Q751 | V808 | E809 | N810 | D811 | T812 | P813 |
| K754 | L755 | S756 | H757 | P758 | V759 | V760 | L761 | K762 | T763 | M764 | Q765 | S766 | G767 | I768 | R769 | C770 | F771 | V772 | Q773 | V774 | L775 | K776 | R777 | Y778 | Y779 | W780 | V781 | C782 | T783 | S784 | M785 | C786 | T787 | L788 | T789 | V790 | W791 | D792 | L793 | T794 | M795 | G796 | S797 | S798 | N799 | T800 | L801 | E802 | T803 | C804 | G805 | K806 | R807 | S808 | T809 | Q810 | D811 | T812 | P813 |      |      |      |      |
| L814 | A815 | L816 | D817 | V818 | P819 | D820 | E821 | R822 | S823 | K824 | T825 | A826 | T827 | V828 | L829 | L830 | L831 | F832 | K833 | Y834 | S835 | V836 | W837 | R838 | L839 | N840 | F841 | L842 | P843 | G844 | L845 | S846 | V847 | S848 | L849 | Q850 | S851 | E852 | A853 | V854 | GLN  | LEU  | PRO  | GLU  | G859 | S860 | F861 | L862 | T863 | C864 | G865 | K866 | R867 | S868 | T869 | Q870 | Q871 | R872 | Y873 |      |      |      |      |



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, D8                               | Depositor |
| Number of particles used             | 17769                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.8                                     | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 2400                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.222                                   | Depositor |
| Minimum map value                    | -0.151                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.03                                    | Depositor |
| Map size (Å)                         | 432.0, 432.0, 432.0                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.35, 1.35, 1.35                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | B     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | C     | 0.54         | 9/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | D     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | E     | 0.54         | 9/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | F     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | G     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | H     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | I     | 0.54         | 8/10231 (0.1%)    | 0.87        | 30/13873 (0.2%)   |
| 1   | J     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | K     | 0.54         | 9/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | L     | 0.54         | 9/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | M     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | N     | 0.54         | 9/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | O     | 0.54         | 7/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| 1   | P     | 0.54         | 8/10231 (0.1%)    | 0.87        | 31/13873 (0.2%)   |
| All | All   | 0.54         | 132/163696 (0.1%) | 0.87        | 495/221968 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 15                  |
| 1   | B     | 0                   | 15                  |
| 1   | C     | 0                   | 15                  |
| 1   | D     | 0                   | 15                  |
| 1   | E     | 0                   | 15                  |
| 1   | F     | 0                   | 15                  |
| 1   | G     | 0                   | 15                  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | H     | 0                   | 15                  |
| 1   | I     | 0                   | 15                  |
| 1   | J     | 0                   | 15                  |
| 1   | K     | 0                   | 15                  |
| 1   | L     | 0                   | 15                  |
| 1   | M     | 0                   | 15                  |
| 1   | N     | 0                   | 15                  |
| 1   | O     | 0                   | 15                  |
| 1   | P     | 0                   | 15                  |
| All | All   | 0                   | 240                 |

All (132) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 559 | THR  | C-N   | 11.28 | 1.49        | 1.33     |
| 1   | M     | 559 | THR  | C-N   | 11.28 | 1.49        | 1.33     |
| 1   | D     | 559 | THR  | C-N   | 11.27 | 1.49        | 1.33     |
| 1   | L     | 559 | THR  | C-N   | 11.26 | 1.49        | 1.33     |
| 1   | N     | 559 | THR  | C-N   | 11.26 | 1.49        | 1.33     |
| 1   | C     | 559 | THR  | C-N   | 11.24 | 1.49        | 1.33     |
| 1   | I     | 559 | THR  | C-N   | 11.23 | 1.49        | 1.33     |
| 1   | A     | 559 | THR  | C-N   | 11.22 | 1.49        | 1.33     |
| 1   | B     | 559 | THR  | C-N   | 11.21 | 1.49        | 1.33     |
| 1   | K     | 559 | THR  | C-N   | 11.20 | 1.49        | 1.33     |
| 1   | P     | 559 | THR  | C-N   | 11.20 | 1.49        | 1.33     |
| 1   | J     | 559 | THR  | C-N   | 11.20 | 1.49        | 1.33     |
| 1   | H     | 559 | THR  | C-N   | 11.19 | 1.49        | 1.33     |
| 1   | O     | 559 | THR  | C-N   | 11.19 | 1.49        | 1.33     |
| 1   | F     | 559 | THR  | C-N   | 11.17 | 1.49        | 1.33     |
| 1   | G     | 559 | THR  | C-N   | 11.17 | 1.49        | 1.33     |
| 1   | H     | 265 | THR  | C-N   | -7.81 | 1.23        | 1.33     |
| 1   | O     | 265 | THR  | C-N   | -7.81 | 1.23        | 1.33     |
| 1   | J     | 265 | THR  | C-N   | -7.81 | 1.23        | 1.33     |
| 1   | K     | 265 | THR  | C-N   | -7.80 | 1.23        | 1.33     |
| 1   | D     | 265 | THR  | C-N   | -7.80 | 1.23        | 1.33     |
| 1   | G     | 265 | THR  | C-N   | -7.79 | 1.23        | 1.33     |
| 1   | F     | 265 | THR  | C-N   | -7.78 | 1.23        | 1.33     |
| 1   | I     | 265 | THR  | C-N   | -7.78 | 1.23        | 1.33     |
| 1   | E     | 265 | THR  | C-N   | -7.77 | 1.23        | 1.33     |
| 1   | A     | 265 | THR  | C-N   | -7.77 | 1.23        | 1.33     |
| 1   | B     | 265 | THR  | C-N   | -7.77 | 1.23        | 1.33     |
| 1   | N     | 265 | THR  | C-N   | -7.75 | 1.23        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | L     | 265 | THR  | C-N   | -7.75 | 1.23        | 1.33     |
| 1   | P     | 265 | THR  | C-N   | -7.73 | 1.23        | 1.33     |
| 1   | C     | 265 | THR  | C-N   | -7.73 | 1.23        | 1.33     |
| 1   | M     | 265 | THR  | C-N   | -7.71 | 1.23        | 1.33     |
| 1   | K     | 250 | ALA  | CA-C  | -7.12 | 1.38        | 1.52     |
| 1   | G     | 250 | ALA  | CA-C  | -7.11 | 1.38        | 1.52     |
| 1   | B     | 250 | ALA  | CA-C  | -7.10 | 1.38        | 1.52     |
| 1   | M     | 250 | ALA  | CA-C  | -7.09 | 1.38        | 1.52     |
| 1   | O     | 250 | ALA  | CA-C  | -7.09 | 1.38        | 1.52     |
| 1   | E     | 250 | ALA  | CA-C  | -7.09 | 1.38        | 1.52     |
| 1   | N     | 250 | ALA  | CA-C  | -7.09 | 1.38        | 1.52     |
| 1   | A     | 250 | ALA  | CA-C  | -7.08 | 1.38        | 1.52     |
| 1   | D     | 250 | ALA  | CA-C  | -7.08 | 1.38        | 1.52     |
| 1   | J     | 250 | ALA  | CA-C  | -7.08 | 1.38        | 1.52     |
| 1   | C     | 250 | ALA  | CA-C  | -7.08 | 1.38        | 1.52     |
| 1   | P     | 250 | ALA  | CA-C  | -7.06 | 1.38        | 1.52     |
| 1   | H     | 250 | ALA  | CA-C  | -7.06 | 1.38        | 1.52     |
| 1   | L     | 250 | ALA  | CA-C  | -7.06 | 1.38        | 1.52     |
| 1   | F     | 250 | ALA  | CA-C  | -7.05 | 1.38        | 1.52     |
| 1   | I     | 250 | ALA  | CA-C  | -7.04 | 1.38        | 1.52     |
| 1   | P     | 250 | ALA  | CA-CB | -6.52 | 1.31        | 1.52     |
| 1   | J     | 250 | ALA  | CA-CB | -6.51 | 1.31        | 1.52     |
| 1   | F     | 250 | ALA  | CA-CB | -6.51 | 1.31        | 1.52     |
| 1   | L     | 250 | ALA  | CA-CB | -6.50 | 1.31        | 1.52     |
| 1   | B     | 250 | ALA  | CA-CB | -6.50 | 1.31        | 1.52     |
| 1   | E     | 250 | ALA  | CA-CB | -6.50 | 1.31        | 1.52     |
| 1   | C     | 250 | ALA  | CA-CB | -6.50 | 1.31        | 1.52     |
| 1   | A     | 250 | ALA  | CA-CB | -6.49 | 1.31        | 1.52     |
| 1   | H     | 250 | ALA  | CA-CB | -6.49 | 1.31        | 1.52     |
| 1   | G     | 250 | ALA  | CA-CB | -6.49 | 1.31        | 1.52     |
| 1   | I     | 250 | ALA  | CA-CB | -6.49 | 1.31        | 1.52     |
| 1   | M     | 250 | ALA  | CA-CB | -6.49 | 1.31        | 1.52     |
| 1   | O     | 250 | ALA  | CA-CB | -6.49 | 1.31        | 1.52     |
| 1   | K     | 250 | ALA  | CA-CB | -6.48 | 1.31        | 1.52     |
| 1   | D     | 250 | ALA  | CA-CB | -6.48 | 1.31        | 1.52     |
| 1   | N     | 250 | ALA  | CA-CB | -6.47 | 1.31        | 1.52     |
| 1   | O     | 414 | GLN  | C-N   | 5.83  | 1.47        | 1.33     |
| 1   | P     | 414 | GLN  | C-N   | 5.81  | 1.47        | 1.33     |
| 1   | D     | 414 | GLN  | C-N   | 5.81  | 1.47        | 1.33     |
| 1   | I     | 414 | GLN  | C-N   | 5.80  | 1.47        | 1.33     |
| 1   | F     | 414 | GLN  | C-N   | 5.80  | 1.47        | 1.33     |
| 1   | B     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |
| 1   | A     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |
| 1   | E     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |
| 1   | M     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |
| 1   | K     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |
| 1   | J     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |
| 1   | N     | 414 | GLN  | C-N   | 5.79  | 1.47        | 1.33     |
| 1   | C     | 414 | GLN  | C-N   | 5.77  | 1.47        | 1.33     |
| 1   | H     | 414 | GLN  | C-N   | 5.76  | 1.47        | 1.33     |
| 1   | L     | 414 | GLN  | C-N   | 5.76  | 1.47        | 1.33     |
| 1   | L     | 252 | ALA  | CA-CB | -5.53 | 1.34        | 1.52     |
| 1   | H     | 252 | ALA  | CA-CB | -5.53 | 1.34        | 1.52     |
| 1   | J     | 252 | ALA  | CA-CB | -5.51 | 1.34        | 1.52     |
| 1   | N     | 252 | ALA  | CA-CB | -5.51 | 1.34        | 1.52     |
| 1   | P     | 252 | ALA  | CA-CB | -5.51 | 1.34        | 1.52     |
| 1   | A     | 252 | ALA  | CA-CB | -5.51 | 1.34        | 1.52     |
| 1   | B     | 252 | ALA  | CA-CB | -5.50 | 1.34        | 1.52     |
| 1   | I     | 252 | ALA  | CA-CB | -5.50 | 1.34        | 1.52     |
| 1   | C     | 252 | ALA  | CA-CB | -5.50 | 1.34        | 1.52     |
| 1   | D     | 252 | ALA  | CA-CB | -5.50 | 1.34        | 1.52     |
| 1   | G     | 252 | ALA  | CA-CB | -5.50 | 1.34        | 1.52     |
| 1   | M     | 252 | ALA  | CA-CB | -5.49 | 1.34        | 1.52     |
| 1   | O     | 252 | ALA  | CA-CB | -5.49 | 1.34        | 1.52     |
| 1   | K     | 252 | ALA  | CA-CB | -5.49 | 1.34        | 1.52     |
| 1   | F     | 252 | ALA  | CA-CB | -5.49 | 1.34        | 1.52     |
| 1   | E     | 252 | ALA  | CA-CB | -5.49 | 1.34        | 1.52     |
| 1   | I     | 252 | ALA  | C-N   | 5.40  | 1.41        | 1.33     |
| 1   | B     | 252 | ALA  | C-N   | 5.39  | 1.41        | 1.33     |
| 1   | P     | 252 | ALA  | C-N   | 5.38  | 1.41        | 1.33     |
| 1   | E     | 252 | ALA  | C-N   | 5.37  | 1.41        | 1.33     |
| 1   | F     | 252 | ALA  | C-N   | 5.36  | 1.41        | 1.33     |
| 1   | C     | 252 | ALA  | C-N   | 5.35  | 1.41        | 1.33     |
| 1   | A     | 252 | ALA  | C-N   | 5.34  | 1.41        | 1.33     |
| 1   | J     | 252 | ALA  | C-N   | 5.34  | 1.41        | 1.33     |
| 1   | O     | 252 | ALA  | C-N   | 5.33  | 1.41        | 1.33     |
| 1   | G     | 252 | ALA  | C-N   | 5.32  | 1.41        | 1.33     |
| 1   | H     | 252 | ALA  | C-N   | 5.32  | 1.41        | 1.33     |
| 1   | L     | 252 | ALA  | C-N   | 5.31  | 1.41        | 1.33     |
| 1   | M     | 252 | ALA  | C-N   | 5.31  | 1.41        | 1.33     |
| 1   | D     | 252 | ALA  | C-N   | 5.31  | 1.41        | 1.33     |
| 1   | N     | 252 | ALA  | C-N   | 5.30  | 1.41        | 1.33     |
| 1   | K     | 252 | ALA  | C-N   | 5.28  | 1.41        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | K     | 1087 | ILE  | CA-CB | 5.18 | 1.59        | 1.55     |
| 1   | E     | 1087 | ILE  | CA-CB | 5.11 | 1.59        | 1.55     |
| 1   | A     | 1087 | ILE  | CA-CB | 5.09 | 1.59        | 1.55     |
| 1   | L     | 1087 | ILE  | CA-CB | 5.08 | 1.59        | 1.55     |
| 1   | B     | 1087 | ILE  | CA-CB | 5.07 | 1.59        | 1.55     |
| 1   | H     | 1087 | ILE  | CA-CB | 5.07 | 1.59        | 1.55     |
| 1   | I     | 1087 | ILE  | CA-CB | 5.07 | 1.59        | 1.55     |
| 1   | M     | 1087 | ILE  | CA-CB | 5.07 | 1.59        | 1.55     |
| 1   | C     | 1087 | ILE  | CA-CB | 5.06 | 1.59        | 1.55     |
| 1   | F     | 1087 | ILE  | CA-CB | 5.05 | 1.59        | 1.55     |
| 1   | J     | 1087 | ILE  | CA-CB | 5.05 | 1.59        | 1.55     |
| 1   | N     | 1087 | ILE  | CA-CB | 5.05 | 1.59        | 1.55     |
| 1   | L     | 291  | THR  | C-N   | 5.04 | 1.40        | 1.33     |
| 1   | K     | 291  | THR  | C-N   | 5.03 | 1.40        | 1.33     |
| 1   | P     | 1087 | ILE  | CA-CB | 5.03 | 1.59        | 1.55     |
| 1   | C     | 291  | THR  | C-N   | 5.03 | 1.40        | 1.33     |
| 1   | E     | 291  | THR  | C-N   | 5.02 | 1.40        | 1.33     |
| 1   | G     | 1087 | ILE  | CA-CB | 5.02 | 1.59        | 1.55     |
| 1   | D     | 1087 | ILE  | CA-CB | 5.01 | 1.59        | 1.55     |
| 1   | N     | 291  | THR  | C-N   | 5.01 | 1.40        | 1.33     |

All (495) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | L     | 414 | GLN  | O-C-N | 13.80  | 135.52      | 121.30   |
| 1   | I     | 414 | GLN  | O-C-N | 13.78  | 135.50      | 121.30   |
| 1   | P     | 414 | GLN  | O-C-N | 13.78  | 135.49      | 121.30   |
| 1   | C     | 414 | GLN  | O-C-N | 13.77  | 135.49      | 121.30   |
| 1   | K     | 414 | GLN  | O-C-N | 13.77  | 135.49      | 121.30   |
| 1   | F     | 414 | GLN  | O-C-N | 13.77  | 135.48      | 121.30   |
| 1   | J     | 414 | GLN  | O-C-N | 13.75  | 135.46      | 121.30   |
| 1   | A     | 414 | GLN  | O-C-N | 13.74  | 135.46      | 121.30   |
| 1   | N     | 414 | GLN  | O-C-N | 13.74  | 135.46      | 121.30   |
| 1   | G     | 414 | GLN  | O-C-N | 13.74  | 135.45      | 121.30   |
| 1   | M     | 414 | GLN  | O-C-N | 13.73  | 135.44      | 121.30   |
| 1   | E     | 414 | GLN  | O-C-N | 13.72  | 135.43      | 121.30   |
| 1   | O     | 414 | GLN  | O-C-N | 13.71  | 135.43      | 121.30   |
| 1   | B     | 414 | GLN  | O-C-N | 13.71  | 135.42      | 121.30   |
| 1   | D     | 414 | GLN  | O-C-N | 13.70  | 135.41      | 121.30   |
| 1   | H     | 414 | GLN  | O-C-N | 13.70  | 135.41      | 121.30   |
| 1   | M     | 559 | THR  | O-C-N | -10.75 | 110.42      | 122.03   |
| 1   | L     | 559 | THR  | O-C-N | -10.73 | 110.44      | 122.03   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | N     | 559 | THR  | O-C-N  | -10.73 | 110.44      | 122.03   |
| 1   | J     | 559 | THR  | O-C-N  | -10.71 | 110.46      | 122.03   |
| 1   | D     | 559 | THR  | O-C-N  | -10.71 | 110.46      | 122.03   |
| 1   | I     | 559 | THR  | O-C-N  | -10.71 | 110.47      | 122.03   |
| 1   | C     | 559 | THR  | O-C-N  | -10.71 | 110.47      | 122.03   |
| 1   | A     | 559 | THR  | O-C-N  | -10.70 | 110.48      | 122.03   |
| 1   | O     | 559 | THR  | O-C-N  | -10.70 | 110.48      | 122.03   |
| 1   | P     | 559 | THR  | O-C-N  | -10.69 | 110.48      | 122.03   |
| 1   | F     | 559 | THR  | O-C-N  | -10.69 | 110.48      | 122.03   |
| 1   | G     | 559 | THR  | O-C-N  | -10.68 | 110.49      | 122.03   |
| 1   | E     | 559 | THR  | O-C-N  | -10.68 | 110.49      | 122.03   |
| 1   | B     | 559 | THR  | O-C-N  | -10.67 | 110.51      | 122.03   |
| 1   | H     | 559 | THR  | O-C-N  | -10.66 | 110.52      | 122.03   |
| 1   | K     | 559 | THR  | O-C-N  | -10.65 | 110.52      | 122.03   |
| 1   | D     | 317 | LEU  | N-CA-C | 10.18  | 122.46      | 111.36   |
| 1   | P     | 317 | LEU  | N-CA-C | 10.18  | 122.46      | 111.36   |
| 1   | J     | 317 | LEU  | N-CA-C | 10.18  | 122.45      | 111.36   |
| 1   | N     | 317 | LEU  | N-CA-C | 10.18  | 122.46      | 111.36   |
| 1   | O     | 317 | LEU  | N-CA-C | 10.18  | 122.45      | 111.36   |
| 1   | G     | 317 | LEU  | N-CA-C | 10.17  | 122.45      | 111.36   |
| 1   | A     | 317 | LEU  | N-CA-C | 10.17  | 122.44      | 111.36   |
| 1   | E     | 317 | LEU  | N-CA-C | 10.16  | 122.44      | 111.36   |
| 1   | F     | 317 | LEU  | N-CA-C | 10.16  | 122.44      | 111.36   |
| 1   | B     | 317 | LEU  | N-CA-C | 10.16  | 122.44      | 111.36   |
| 1   | H     | 317 | LEU  | N-CA-C | 10.16  | 122.43      | 111.36   |
| 1   | L     | 317 | LEU  | N-CA-C | 10.14  | 122.42      | 111.36   |
| 1   | C     | 317 | LEU  | N-CA-C | 10.14  | 122.41      | 111.36   |
| 1   | M     | 317 | LEU  | N-CA-C | 10.13  | 122.41      | 111.36   |
| 1   | K     | 317 | LEU  | N-CA-C | 10.13  | 122.40      | 111.36   |
| 1   | I     | 317 | LEU  | N-CA-C | 10.10  | 122.36      | 111.36   |
| 1   | N     | 559 | THR  | CA-C-N | 9.79   | 140.24      | 121.54   |
| 1   | N     | 559 | THR  | C-N-CA | 9.79   | 140.24      | 121.54   |
| 1   | M     | 559 | THR  | CA-C-N | 9.78   | 140.23      | 121.54   |
| 1   | M     | 559 | THR  | C-N-CA | 9.78   | 140.23      | 121.54   |
| 1   | P     | 559 | THR  | CA-C-N | 9.78   | 140.23      | 121.54   |
| 1   | P     | 559 | THR  | C-N-CA | 9.78   | 140.23      | 121.54   |
| 1   | C     | 559 | THR  | CA-C-N | 9.77   | 140.20      | 121.54   |
| 1   | C     | 559 | THR  | C-N-CA | 9.77   | 140.20      | 121.54   |
| 1   | J     | 559 | THR  | CA-C-N | 9.77   | 140.20      | 121.54   |
| 1   | J     | 559 | THR  | C-N-CA | 9.77   | 140.20      | 121.54   |
| 1   | F     | 559 | THR  | CA-C-N | 9.77   | 140.20      | 121.54   |
| 1   | F     | 559 | THR  | C-N-CA | 9.77   | 140.20      | 121.54   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | I     | 559 | THR  | CA-C-N | 9.77 | 140.20      | 121.54   |
| 1   | I     | 559 | THR  | C-N-CA | 9.77 | 140.20      | 121.54   |
| 1   | L     | 559 | THR  | CA-C-N | 9.77 | 140.20      | 121.54   |
| 1   | L     | 559 | THR  | C-N-CA | 9.77 | 140.20      | 121.54   |
| 1   | K     | 559 | THR  | CA-C-N | 9.77 | 140.19      | 121.54   |
| 1   | K     | 559 | THR  | C-N-CA | 9.77 | 140.19      | 121.54   |
| 1   | A     | 559 | THR  | CA-C-N | 9.76 | 140.19      | 121.54   |
| 1   | A     | 559 | THR  | C-N-CA | 9.76 | 140.19      | 121.54   |
| 1   | O     | 559 | THR  | CA-C-N | 9.76 | 140.19      | 121.54   |
| 1   | O     | 559 | THR  | C-N-CA | 9.76 | 140.19      | 121.54   |
| 1   | B     | 559 | THR  | CA-C-N | 9.76 | 140.18      | 121.54   |
| 1   | B     | 559 | THR  | C-N-CA | 9.76 | 140.18      | 121.54   |
| 1   | D     | 559 | THR  | CA-C-N | 9.75 | 140.17      | 121.54   |
| 1   | D     | 559 | THR  | C-N-CA | 9.75 | 140.17      | 121.54   |
| 1   | G     | 559 | THR  | CA-C-N | 9.75 | 140.17      | 121.54   |
| 1   | G     | 559 | THR  | C-N-CA | 9.75 | 140.17      | 121.54   |
| 1   | H     | 559 | THR  | CA-C-N | 9.75 | 140.17      | 121.54   |
| 1   | H     | 559 | THR  | C-N-CA | 9.75 | 140.17      | 121.54   |
| 1   | E     | 559 | THR  | CA-C-N | 9.75 | 140.16      | 121.54   |
| 1   | E     | 559 | THR  | C-N-CA | 9.75 | 140.16      | 121.54   |
| 1   | L     | 918 | ILE  | N-CA-C | 8.46 | 120.01      | 108.17   |
| 1   | I     | 918 | ILE  | N-CA-C | 8.44 | 119.99      | 108.17   |
| 1   | P     | 918 | ILE  | N-CA-C | 8.44 | 119.99      | 108.17   |
| 1   | C     | 918 | ILE  | N-CA-C | 8.44 | 119.98      | 108.17   |
| 1   | D     | 918 | ILE  | N-CA-C | 8.44 | 119.98      | 108.17   |
| 1   | N     | 918 | ILE  | N-CA-C | 8.43 | 119.98      | 108.17   |
| 1   | B     | 918 | ILE  | N-CA-C | 8.43 | 119.97      | 108.17   |
| 1   | A     | 918 | ILE  | N-CA-C | 8.42 | 119.96      | 108.17   |
| 1   | F     | 918 | ILE  | N-CA-C | 8.42 | 119.96      | 108.17   |
| 1   | K     | 918 | ILE  | N-CA-C | 8.42 | 119.96      | 108.17   |
| 1   | M     | 918 | ILE  | N-CA-C | 8.42 | 119.96      | 108.17   |
| 1   | O     | 918 | ILE  | N-CA-C | 8.42 | 119.96      | 108.17   |
| 1   | G     | 918 | ILE  | N-CA-C | 8.41 | 119.94      | 108.17   |
| 1   | H     | 918 | ILE  | N-CA-C | 8.40 | 119.93      | 108.17   |
| 1   | J     | 918 | ILE  | N-CA-C | 8.40 | 119.93      | 108.17   |
| 1   | E     | 918 | ILE  | N-CA-C | 8.37 | 119.89      | 108.17   |
| 1   | K     | 460 | PRO  | N-CA-C | 7.90 | 119.03      | 110.58   |
| 1   | M     | 460 | PRO  | N-CA-C | 7.88 | 119.01      | 110.58   |
| 1   | I     | 460 | PRO  | N-CA-C | 7.87 | 119.00      | 110.58   |
| 1   | F     | 460 | PRO  | N-CA-C | 7.87 | 119.00      | 110.58   |
| 1   | D     | 460 | PRO  | N-CA-C | 7.86 | 118.99      | 110.58   |
| 1   | H     | 460 | PRO  | N-CA-C | 7.86 | 118.99      | 110.58   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 460 | PRO  | N-CA-C | 7.86  | 118.99      | 110.58   |
| 1   | A     | 460 | PRO  | N-CA-C | 7.86  | 118.98      | 110.58   |
| 1   | O     | 460 | PRO  | N-CA-C | 7.85  | 118.98      | 110.58   |
| 1   | P     | 460 | PRO  | N-CA-C | 7.85  | 118.98      | 110.58   |
| 1   | L     | 460 | PRO  | N-CA-C | 7.85  | 118.98      | 110.58   |
| 1   | C     | 460 | PRO  | N-CA-C | 7.85  | 118.98      | 110.58   |
| 1   | J     | 460 | PRO  | N-CA-C | 7.85  | 118.98      | 110.58   |
| 1   | N     | 460 | PRO  | N-CA-C | 7.85  | 118.98      | 110.58   |
| 1   | G     | 460 | PRO  | N-CA-C | 7.83  | 118.95      | 110.58   |
| 1   | E     | 460 | PRO  | N-CA-C | 7.81  | 118.93      | 110.58   |
| 1   | M     | 460 | PRO  | O-C-N  | 7.11  | 124.49      | 121.15   |
| 1   | C     | 460 | PRO  | O-C-N  | 7.09  | 124.48      | 121.15   |
| 1   | I     | 460 | PRO  | O-C-N  | 7.06  | 124.47      | 121.15   |
| 1   | N     | 460 | PRO  | O-C-N  | 7.04  | 124.46      | 121.15   |
| 1   | J     | 460 | PRO  | O-C-N  | 7.02  | 124.45      | 121.15   |
| 1   | P     | 460 | PRO  | O-C-N  | 7.01  | 124.45      | 121.15   |
| 1   | L     | 460 | PRO  | O-C-N  | 7.00  | 124.44      | 121.15   |
| 1   | A     | 460 | PRO  | O-C-N  | 6.99  | 124.44      | 121.15   |
| 1   | D     | 460 | PRO  | O-C-N  | 6.98  | 124.43      | 121.15   |
| 1   | H     | 460 | PRO  | O-C-N  | 6.98  | 124.43      | 121.15   |
| 1   | K     | 460 | PRO  | O-C-N  | 6.97  | 124.42      | 121.15   |
| 1   | O     | 460 | PRO  | O-C-N  | 6.92  | 124.40      | 121.15   |
| 1   | E     | 460 | PRO  | O-C-N  | 6.92  | 124.40      | 121.15   |
| 1   | G     | 460 | PRO  | O-C-N  | 6.92  | 124.40      | 121.15   |
| 1   | F     | 460 | PRO  | O-C-N  | 6.91  | 124.40      | 121.15   |
| 1   | B     | 460 | PRO  | O-C-N  | 6.91  | 124.40      | 121.15   |
| 1   | C     | 252 | ALA  | CA-C-N | -6.81 | 108.53      | 121.54   |
| 1   | C     | 252 | ALA  | C-N-CA | -6.81 | 108.53      | 121.54   |
| 1   | B     | 252 | ALA  | CA-C-N | -6.80 | 108.55      | 121.54   |
| 1   | B     | 252 | ALA  | C-N-CA | -6.80 | 108.55      | 121.54   |
| 1   | E     | 252 | ALA  | CA-C-N | -6.80 | 108.55      | 121.54   |
| 1   | E     | 252 | ALA  | C-N-CA | -6.80 | 108.55      | 121.54   |
| 1   | G     | 252 | ALA  | CA-C-N | -6.80 | 108.55      | 121.54   |
| 1   | G     | 252 | ALA  | C-N-CA | -6.80 | 108.55      | 121.54   |
| 1   | I     | 252 | ALA  | CA-C-N | -6.80 | 108.56      | 121.54   |
| 1   | I     | 252 | ALA  | C-N-CA | -6.80 | 108.56      | 121.54   |
| 1   | A     | 252 | ALA  | CA-C-N | -6.79 | 108.56      | 121.54   |
| 1   | A     | 252 | ALA  | C-N-CA | -6.79 | 108.56      | 121.54   |
| 1   | O     | 252 | ALA  | CA-C-N | -6.79 | 108.56      | 121.54   |
| 1   | O     | 252 | ALA  | C-N-CA | -6.79 | 108.56      | 121.54   |
| 1   | D     | 252 | ALA  | CA-C-N | -6.79 | 108.56      | 121.54   |
| 1   | D     | 252 | ALA  | C-N-CA | -6.79 | 108.56      | 121.54   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 252 | ALA  | CA-C-N  | -6.79 | 108.57      | 121.54   |
| 1   | K     | 252 | ALA  | C-N-CA  | -6.79 | 108.57      | 121.54   |
| 1   | P     | 252 | ALA  | CA-C-N  | -6.79 | 108.57      | 121.54   |
| 1   | P     | 252 | ALA  | C-N-CA  | -6.79 | 108.57      | 121.54   |
| 1   | F     | 252 | ALA  | CA-C-N  | -6.79 | 108.57      | 121.54   |
| 1   | F     | 252 | ALA  | C-N-CA  | -6.79 | 108.57      | 121.54   |
| 1   | N     | 252 | ALA  | CA-C-N  | -6.79 | 108.57      | 121.54   |
| 1   | N     | 252 | ALA  | C-N-CA  | -6.79 | 108.57      | 121.54   |
| 1   | H     | 252 | ALA  | CA-C-N  | -6.79 | 108.57      | 121.54   |
| 1   | H     | 252 | ALA  | C-N-CA  | -6.79 | 108.57      | 121.54   |
| 1   | M     | 252 | ALA  | CA-C-N  | -6.79 | 108.57      | 121.54   |
| 1   | M     | 252 | ALA  | C-N-CA  | -6.79 | 108.57      | 121.54   |
| 1   | J     | 252 | ALA  | CA-C-N  | -6.79 | 108.58      | 121.54   |
| 1   | J     | 252 | ALA  | C-N-CA  | -6.79 | 108.58      | 121.54   |
| 1   | L     | 252 | ALA  | CA-C-N  | -6.77 | 108.60      | 121.54   |
| 1   | L     | 252 | ALA  | C-N-CA  | -6.77 | 108.60      | 121.54   |
| 1   | E     | 517 | THR  | N-CA-C  | 6.60  | 124.86      | 110.80   |
| 1   | J     | 517 | THR  | N-CA-C  | 6.60  | 124.86      | 110.80   |
| 1   | F     | 517 | THR  | N-CA-C  | 6.59  | 124.84      | 110.80   |
| 1   | D     | 517 | THR  | N-CA-C  | 6.58  | 124.82      | 110.80   |
| 1   | L     | 517 | THR  | N-CA-C  | 6.58  | 124.82      | 110.80   |
| 1   | A     | 517 | THR  | N-CA-C  | 6.58  | 124.82      | 110.80   |
| 1   | C     | 517 | THR  | N-CA-C  | 6.58  | 124.80      | 110.80   |
| 1   | K     | 517 | THR  | N-CA-C  | 6.58  | 124.81      | 110.80   |
| 1   | I     | 517 | THR  | N-CA-C  | 6.57  | 124.80      | 110.80   |
| 1   | B     | 517 | THR  | N-CA-C  | 6.56  | 124.78      | 110.80   |
| 1   | H     | 517 | THR  | N-CA-C  | 6.56  | 124.78      | 110.80   |
| 1   | N     | 517 | THR  | N-CA-C  | 6.56  | 124.77      | 110.80   |
| 1   | P     | 517 | THR  | N-CA-C  | 6.56  | 124.77      | 110.80   |
| 1   | M     | 517 | THR  | N-CA-C  | 6.56  | 124.77      | 110.80   |
| 1   | O     | 517 | THR  | N-CA-C  | 6.56  | 124.77      | 110.80   |
| 1   | G     | 517 | THR  | N-CA-C  | 6.55  | 124.76      | 110.80   |
| 1   | K     | 507 | ALA  | CB-CA-C | -6.46 | 108.10      | 115.79   |
| 1   | J     | 507 | ALA  | CB-CA-C | -6.45 | 108.11      | 115.79   |
| 1   | H     | 507 | ALA  | CB-CA-C | -6.44 | 108.13      | 115.79   |
| 1   | H     | 291 | THR  | N-CA-C  | 6.44  | 119.38      | 107.99   |
| 1   | P     | 507 | ALA  | CB-CA-C | -6.43 | 108.13      | 115.79   |
| 1   | L     | 507 | ALA  | CB-CA-C | -6.43 | 108.14      | 115.79   |
| 1   | A     | 507 | ALA  | CB-CA-C | -6.43 | 108.14      | 115.79   |
| 1   | F     | 507 | ALA  | CB-CA-C | -6.43 | 108.14      | 115.79   |
| 1   | D     | 507 | ALA  | CB-CA-C | -6.43 | 108.14      | 115.79   |
| 1   | E     | 507 | ALA  | CB-CA-C | -6.42 | 108.14      | 115.79   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | I     | 507 | ALA  | CB-CA-C | -6.42 | 108.14      | 115.79   |
| 1   | G     | 507 | ALA  | CB-CA-C | -6.42 | 108.15      | 115.79   |
| 1   | N     | 291 | THR  | N-CA-C  | 6.42  | 119.35      | 107.99   |
| 1   | D     | 291 | THR  | N-CA-C  | 6.42  | 119.35      | 107.99   |
| 1   | E     | 291 | THR  | N-CA-C  | 6.42  | 119.35      | 107.99   |
| 1   | I     | 291 | THR  | N-CA-C  | 6.42  | 119.34      | 107.99   |
| 1   | O     | 291 | THR  | N-CA-C  | 6.42  | 119.34      | 107.99   |
| 1   | M     | 507 | ALA  | CB-CA-C | -6.41 | 108.16      | 115.79   |
| 1   | O     | 507 | ALA  | CB-CA-C | -6.41 | 108.16      | 115.79   |
| 1   | C     | 507 | ALA  | CB-CA-C | -6.41 | 108.16      | 115.79   |
| 1   | N     | 507 | ALA  | CB-CA-C | -6.41 | 108.16      | 115.79   |
| 1   | P     | 291 | THR  | N-CA-C  | 6.41  | 119.33      | 107.99   |
| 1   | G     | 291 | THR  | N-CA-C  | 6.41  | 119.33      | 107.99   |
| 1   | B     | 507 | ALA  | CB-CA-C | -6.40 | 108.17      | 115.79   |
| 1   | K     | 291 | THR  | N-CA-C  | 6.40  | 119.32      | 107.99   |
| 1   | F     | 291 | THR  | N-CA-C  | 6.40  | 119.32      | 107.99   |
| 1   | C     | 291 | THR  | N-CA-C  | 6.40  | 119.32      | 107.99   |
| 1   | A     | 291 | THR  | N-CA-C  | 6.39  | 119.31      | 107.99   |
| 1   | B     | 291 | THR  | N-CA-C  | 6.39  | 119.30      | 107.99   |
| 1   | M     | 291 | THR  | N-CA-C  | 6.39  | 119.30      | 107.99   |
| 1   | J     | 291 | THR  | N-CA-C  | 6.39  | 119.29      | 107.99   |
| 1   | L     | 291 | THR  | N-CA-C  | 6.36  | 119.25      | 107.99   |
| 1   | H     | 964 | CYS  | CB-CA-C | -6.10 | 109.53      | 116.54   |
| 1   | G     | 964 | CYS  | CB-CA-C | -6.09 | 109.53      | 116.54   |
| 1   | N     | 964 | CYS  | CB-CA-C | -6.09 | 109.53      | 116.54   |
| 1   | B     | 964 | CYS  | CB-CA-C | -6.08 | 109.54      | 116.54   |
| 1   | E     | 964 | CYS  | CB-CA-C | -6.08 | 109.55      | 116.54   |
| 1   | K     | 964 | CYS  | CB-CA-C | -6.08 | 109.55      | 116.54   |
| 1   | F     | 964 | CYS  | CB-CA-C | -6.08 | 109.55      | 116.54   |
| 1   | M     | 964 | CYS  | CB-CA-C | -6.08 | 109.55      | 116.54   |
| 1   | L     | 964 | CYS  | CB-CA-C | -6.07 | 109.56      | 116.54   |
| 1   | A     | 964 | CYS  | CB-CA-C | -6.07 | 109.56      | 116.54   |
| 1   | D     | 964 | CYS  | CB-CA-C | -6.07 | 109.56      | 116.54   |
| 1   | P     | 964 | CYS  | CB-CA-C | -6.06 | 109.57      | 116.54   |
| 1   | I     | 964 | CYS  | CB-CA-C | -6.06 | 109.57      | 116.54   |
| 1   | O     | 964 | CYS  | CB-CA-C | -6.06 | 109.57      | 116.54   |
| 1   | J     | 964 | CYS  | CB-CA-C | -6.06 | 109.57      | 116.54   |
| 1   | C     | 964 | CYS  | CB-CA-C | -6.06 | 109.58      | 116.54   |
| 1   | A     | 509 | ASN  | N-CA-C  | 5.90  | 118.42      | 109.63   |
| 1   | J     | 509 | ASN  | N-CA-C  | 5.90  | 118.42      | 109.63   |
| 1   | E     | 509 | ASN  | N-CA-C  | 5.89  | 118.40      | 109.63   |
| 1   | G     | 509 | ASN  | N-CA-C  | 5.89  | 118.40      | 109.63   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | O     | 509  | ASN  | N-CA-C  | 5.89  | 118.40      | 109.63   |
| 1   | H     | 509  | ASN  | N-CA-C  | 5.88  | 118.39      | 109.63   |
| 1   | I     | 509  | ASN  | N-CA-C  | 5.88  | 118.39      | 109.63   |
| 1   | M     | 509  | ASN  | N-CA-C  | 5.88  | 118.38      | 109.63   |
| 1   | C     | 509  | ASN  | N-CA-C  | 5.87  | 118.38      | 109.63   |
| 1   | L     | 509  | ASN  | N-CA-C  | 5.87  | 118.38      | 109.63   |
| 1   | B     | 467  | PHE  | N-CA-C  | 5.87  | 117.67      | 111.28   |
| 1   | N     | 509  | ASN  | N-CA-C  | 5.87  | 118.37      | 109.63   |
| 1   | H     | 467  | PHE  | N-CA-C  | 5.87  | 117.67      | 111.28   |
| 1   | K     | 509  | ASN  | N-CA-C  | 5.87  | 118.37      | 109.63   |
| 1   | B     | 509  | ASN  | N-CA-C  | 5.86  | 118.37      | 109.63   |
| 1   | C     | 467  | PHE  | N-CA-C  | 5.86  | 117.67      | 111.28   |
| 1   | P     | 509  | ASN  | N-CA-C  | 5.86  | 118.37      | 109.63   |
| 1   | J     | 467  | PHE  | N-CA-C  | 5.86  | 117.67      | 111.28   |
| 1   | F     | 509  | ASN  | N-CA-C  | 5.85  | 118.35      | 109.63   |
| 1   | D     | 509  | ASN  | N-CA-C  | 5.85  | 118.35      | 109.63   |
| 1   | I     | 467  | PHE  | N-CA-C  | 5.85  | 117.66      | 111.28   |
| 1   | M     | 467  | PHE  | N-CA-C  | 5.84  | 117.65      | 111.28   |
| 1   | L     | 467  | PHE  | N-CA-C  | 5.84  | 117.65      | 111.28   |
| 1   | P     | 467  | PHE  | N-CA-C  | 5.84  | 117.65      | 111.28   |
| 1   | A     | 1052 | GLN  | CB-CA-C | -5.83 | 109.31      | 117.23   |
| 1   | K     | 467  | PHE  | N-CA-C  | 5.82  | 117.63      | 111.28   |
| 1   | F     | 1052 | GLN  | CB-CA-C | -5.82 | 109.31      | 117.23   |
| 1   | G     | 467  | PHE  | N-CA-C  | 5.82  | 117.62      | 111.28   |
| 1   | D     | 467  | PHE  | N-CA-C  | 5.82  | 117.62      | 111.28   |
| 1   | A     | 467  | PHE  | N-CA-C  | 5.82  | 117.62      | 111.28   |
| 1   | E     | 1052 | GLN  | CB-CA-C | -5.81 | 109.32      | 117.23   |
| 1   | I     | 1052 | GLN  | CB-CA-C | -5.81 | 109.33      | 117.23   |
| 1   | N     | 467  | PHE  | N-CA-C  | 5.81  | 117.61      | 111.28   |
| 1   | E     | 704  | ARG  | CB-CA-C | -5.81 | 109.89      | 116.63   |
| 1   | B     | 1052 | GLN  | CB-CA-C | -5.80 | 109.34      | 117.23   |
| 1   | F     | 467  | PHE  | N-CA-C  | 5.80  | 117.60      | 111.28   |
| 1   | J     | 1052 | GLN  | CB-CA-C | -5.80 | 109.35      | 117.23   |
| 1   | F     | 704  | ARG  | CB-CA-C | -5.79 | 109.91      | 116.63   |
| 1   | H     | 1052 | GLN  | CB-CA-C | -5.79 | 109.35      | 117.23   |
| 1   | K     | 1052 | GLN  | CB-CA-C | -5.79 | 109.35      | 117.23   |
| 1   | E     | 467  | PHE  | N-CA-C  | 5.79  | 117.59      | 111.28   |
| 1   | G     | 1052 | GLN  | CB-CA-C | -5.79 | 109.36      | 117.23   |
| 1   | L     | 1052 | GLN  | CB-CA-C | -5.79 | 109.36      | 117.23   |
| 1   | N     | 1052 | GLN  | CB-CA-C | -5.79 | 109.36      | 117.23   |
| 1   | O     | 467  | PHE  | N-CA-C  | 5.79  | 117.59      | 111.28   |
| 1   | O     | 1052 | GLN  | CB-CA-C | -5.79 | 109.36      | 117.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C     | 1052 | GLN  | CB-CA-C | -5.78 | 109.36      | 117.23   |
| 1   | P     | 1052 | GLN  | CB-CA-C | -5.78 | 109.37      | 117.23   |
| 1   | D     | 704  | ARG  | CB-CA-C | -5.77 | 109.94      | 116.63   |
| 1   | C     | 704  | ARG  | CB-CA-C | -5.76 | 109.94      | 116.63   |
| 1   | M     | 1052 | GLN  | CB-CA-C | -5.76 | 109.39      | 117.23   |
| 1   | G     | 704  | ARG  | CB-CA-C | -5.76 | 109.95      | 116.63   |
| 1   | D     | 1052 | GLN  | CB-CA-C | -5.76 | 109.40      | 117.23   |
| 1   | I     | 704  | ARG  | CB-CA-C | -5.76 | 109.95      | 116.63   |
| 1   | A     | 704  | ARG  | CB-CA-C | -5.75 | 109.95      | 116.63   |
| 1   | M     | 704  | ARG  | CB-CA-C | -5.75 | 109.96      | 116.63   |
| 1   | O     | 704  | ARG  | CB-CA-C | -5.75 | 109.96      | 116.63   |
| 1   | P     | 584  | PHE  | CB-CA-C | -5.75 | 108.94      | 115.79   |
| 1   | J     | 704  | ARG  | CB-CA-C | -5.75 | 109.96      | 116.63   |
| 1   | G     | 584  | PHE  | CB-CA-C | -5.75 | 108.95      | 115.79   |
| 1   | H     | 584  | PHE  | CB-CA-C | -5.74 | 108.96      | 115.79   |
| 1   | B     | 704  | ARG  | CB-CA-C | -5.74 | 109.97      | 116.63   |
| 1   | C     | 584  | PHE  | CB-CA-C | -5.74 | 108.96      | 115.79   |
| 1   | M     | 584  | PHE  | CB-CA-C | -5.74 | 108.96      | 115.79   |
| 1   | K     | 704  | ARG  | CB-CA-C | -5.74 | 109.97      | 116.63   |
| 1   | O     | 584  | PHE  | CB-CA-C | -5.74 | 108.96      | 115.79   |
| 1   | P     | 704  | ARG  | CB-CA-C | -5.73 | 109.98      | 116.63   |
| 1   | H     | 704  | ARG  | CB-CA-C | -5.73 | 109.99      | 116.63   |
| 1   | A     | 584  | PHE  | CB-CA-C | -5.72 | 108.98      | 115.79   |
| 1   | N     | 584  | PHE  | CB-CA-C | -5.72 | 108.98      | 115.79   |
| 1   | L     | 704  | ARG  | CB-CA-C | -5.72 | 109.99      | 116.63   |
| 1   | B     | 584  | PHE  | CB-CA-C | -5.72 | 108.98      | 115.79   |
| 1   | J     | 584  | PHE  | CB-CA-C | -5.72 | 108.98      | 115.79   |
| 1   | K     | 584  | PHE  | CB-CA-C | -5.72 | 108.99      | 115.79   |
| 1   | F     | 584  | PHE  | CB-CA-C | -5.71 | 109.00      | 115.79   |
| 1   | E     | 584  | PHE  | CB-CA-C | -5.71 | 109.00      | 115.79   |
| 1   | D     | 584  | PHE  | CB-CA-C | -5.71 | 109.00      | 115.79   |
| 1   | N     | 704  | ARG  | CB-CA-C | -5.70 | 110.02      | 116.63   |
| 1   | I     | 584  | PHE  | CB-CA-C | -5.70 | 109.01      | 115.79   |
| 1   | L     | 584  | PHE  | CB-CA-C | -5.70 | 109.01      | 115.79   |
| 1   | H     | 1205 | MET  | N-CA-C  | 5.67  | 115.76      | 108.34   |
| 1   | B     | 1205 | MET  | N-CA-C  | 5.66  | 115.75      | 108.34   |
| 1   | D     | 1205 | MET  | N-CA-C  | 5.66  | 115.75      | 108.34   |
| 1   | L     | 1205 | MET  | N-CA-C  | 5.65  | 115.75      | 108.34   |
| 1   | C     | 1205 | MET  | N-CA-C  | 5.64  | 115.72      | 108.34   |
| 1   | I     | 1205 | MET  | N-CA-C  | 5.64  | 115.72      | 108.34   |
| 1   | O     | 1205 | MET  | N-CA-C  | 5.63  | 115.72      | 108.34   |
| 1   | A     | 1205 | MET  | N-CA-C  | 5.63  | 115.71      | 108.34   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | G     | 1205 | MET  | N-CA-C | 5.63  | 115.71      | 108.34   |
| 1   | N     | 1205 | MET  | N-CA-C | 5.63  | 115.71      | 108.34   |
| 1   | K     | 1205 | MET  | N-CA-C | 5.62  | 115.71      | 108.34   |
| 1   | J     | 1205 | MET  | N-CA-C | 5.62  | 115.70      | 108.34   |
| 1   | F     | 1205 | MET  | N-CA-C | 5.62  | 115.69      | 108.34   |
| 1   | M     | 1205 | MET  | N-CA-C | 5.62  | 115.70      | 108.34   |
| 1   | E     | 1205 | MET  | N-CA-C | 5.60  | 115.68      | 108.34   |
| 1   | P     | 1205 | MET  | N-CA-C | 5.59  | 115.66      | 108.34   |
| 1   | G     | 451  | LYS  | O-C-N  | 5.42  | 129.38      | 122.33   |
| 1   | I     | 451  | LYS  | O-C-N  | 5.42  | 129.37      | 122.33   |
| 1   | E     | 451  | LYS  | O-C-N  | 5.41  | 129.36      | 122.33   |
| 1   | D     | 451  | LYS  | O-C-N  | 5.40  | 129.35      | 122.33   |
| 1   | F     | 451  | LYS  | O-C-N  | 5.40  | 129.35      | 122.33   |
| 1   | A     | 451  | LYS  | O-C-N  | 5.38  | 129.33      | 122.33   |
| 1   | L     | 451  | LYS  | O-C-N  | 5.38  | 129.32      | 122.33   |
| 1   | N     | 451  | LYS  | O-C-N  | 5.38  | 129.32      | 122.33   |
| 1   | K     | 451  | LYS  | O-C-N  | 5.37  | 129.31      | 122.33   |
| 1   | P     | 451  | LYS  | O-C-N  | 5.37  | 129.31      | 122.33   |
| 1   | B     | 451  | LYS  | O-C-N  | 5.37  | 129.31      | 122.33   |
| 1   | J     | 451  | LYS  | O-C-N  | 5.36  | 129.29      | 122.33   |
| 1   | C     | 451  | LYS  | O-C-N  | 5.36  | 129.29      | 122.33   |
| 1   | M     | 451  | LYS  | O-C-N  | 5.36  | 129.29      | 122.33   |
| 1   | P     | 312  | LEU  | CA-C-N | -5.34 | 114.46      | 119.85   |
| 1   | P     | 312  | LEU  | C-N-CA | -5.34 | 114.46      | 119.85   |
| 1   | L     | 312  | LEU  | CA-C-N | -5.33 | 114.46      | 119.85   |
| 1   | L     | 312  | LEU  | C-N-CA | -5.33 | 114.46      | 119.85   |
| 1   | O     | 451  | LYS  | O-C-N  | 5.33  | 129.27      | 122.33   |
| 1   | M     | 312  | LEU  | CA-C-N | -5.33 | 114.46      | 119.85   |
| 1   | M     | 312  | LEU  | C-N-CA | -5.33 | 114.46      | 119.85   |
| 1   | H     | 451  | LYS  | O-C-N  | 5.33  | 129.26      | 122.33   |
| 1   | N     | 312  | LEU  | CA-C-N | -5.32 | 114.48      | 119.85   |
| 1   | N     | 312  | LEU  | C-N-CA | -5.32 | 114.48      | 119.85   |
| 1   | F     | 312  | LEU  | CA-C-N | -5.31 | 114.48      | 119.85   |
| 1   | F     | 312  | LEU  | C-N-CA | -5.31 | 114.48      | 119.85   |
| 1   | K     | 312  | LEU  | CA-C-N | -5.30 | 114.50      | 119.85   |
| 1   | K     | 312  | LEU  | C-N-CA | -5.30 | 114.50      | 119.85   |
| 1   | C     | 312  | LEU  | CA-C-N | -5.30 | 114.50      | 119.85   |
| 1   | C     | 312  | LEU  | C-N-CA | -5.30 | 114.50      | 119.85   |
| 1   | D     | 312  | LEU  | CA-C-N | -5.29 | 114.50      | 119.85   |
| 1   | D     | 312  | LEU  | C-N-CA | -5.29 | 114.50      | 119.85   |
| 1   | A     | 312  | LEU  | CA-C-N | -5.29 | 114.50      | 119.85   |
| 1   | A     | 312  | LEU  | C-N-CA | -5.29 | 114.50      | 119.85   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 459 | ILE  | CA-C-N | 5.29  | 123.47      | 119.66   |
| 1   | B     | 459 | ILE  | C-N-CA | 5.29  | 123.47      | 119.66   |
| 1   | I     | 312 | LEU  | CA-C-N | -5.28 | 114.52      | 119.85   |
| 1   | I     | 312 | LEU  | C-N-CA | -5.28 | 114.52      | 119.85   |
| 1   | J     | 312 | LEU  | CA-C-N | -5.28 | 114.52      | 119.85   |
| 1   | J     | 312 | LEU  | C-N-CA | -5.28 | 114.52      | 119.85   |
| 1   | G     | 312 | LEU  | CA-C-N | -5.27 | 114.52      | 119.85   |
| 1   | G     | 312 | LEU  | C-N-CA | -5.27 | 114.52      | 119.85   |
| 1   | F     | 459 | ILE  | CA-C-N | 5.27  | 123.45      | 119.66   |
| 1   | F     | 459 | ILE  | C-N-CA | 5.27  | 123.45      | 119.66   |
| 1   | E     | 312 | LEU  | CA-C-N | -5.27 | 114.53      | 119.85   |
| 1   | E     | 312 | LEU  | C-N-CA | -5.27 | 114.53      | 119.85   |
| 1   | B     | 312 | LEU  | CA-C-N | -5.26 | 114.53      | 119.85   |
| 1   | B     | 312 | LEU  | C-N-CA | -5.26 | 114.53      | 119.85   |
| 1   | P     | 459 | ILE  | CA-C-N | 5.26  | 123.45      | 119.66   |
| 1   | P     | 459 | ILE  | C-N-CA | 5.26  | 123.45      | 119.66   |
| 1   | H     | 312 | LEU  | CA-C-N | -5.25 | 114.55      | 119.85   |
| 1   | H     | 312 | LEU  | C-N-CA | -5.25 | 114.55      | 119.85   |
| 1   | O     | 312 | LEU  | CA-C-N | -5.25 | 114.55      | 119.85   |
| 1   | O     | 312 | LEU  | C-N-CA | -5.25 | 114.55      | 119.85   |
| 1   | D     | 459 | ILE  | CA-C-N | 5.25  | 123.44      | 119.66   |
| 1   | D     | 459 | ILE  | C-N-CA | 5.25  | 123.44      | 119.66   |
| 1   | O     | 459 | ILE  | CA-C-N | 5.24  | 123.43      | 119.66   |
| 1   | O     | 459 | ILE  | C-N-CA | 5.24  | 123.43      | 119.66   |
| 1   | A     | 459 | ILE  | CA-C-N | 5.24  | 123.43      | 119.66   |
| 1   | A     | 459 | ILE  | C-N-CA | 5.24  | 123.43      | 119.66   |
| 1   | I     | 459 | ILE  | CA-C-N | 5.23  | 123.42      | 119.66   |
| 1   | I     | 459 | ILE  | C-N-CA | 5.23  | 123.42      | 119.66   |
| 1   | J     | 459 | ILE  | CA-C-N | 5.22  | 123.42      | 119.66   |
| 1   | J     | 459 | ILE  | C-N-CA | 5.22  | 123.42      | 119.66   |
| 1   | L     | 459 | ILE  | CA-C-N | 5.22  | 123.42      | 119.66   |
| 1   | L     | 459 | ILE  | C-N-CA | 5.22  | 123.42      | 119.66   |
| 1   | N     | 459 | ILE  | CA-C-N | 5.22  | 123.42      | 119.66   |
| 1   | N     | 459 | ILE  | C-N-CA | 5.22  | 123.42      | 119.66   |
| 1   | C     | 459 | ILE  | CA-C-N | 5.21  | 123.41      | 119.66   |
| 1   | C     | 459 | ILE  | C-N-CA | 5.21  | 123.41      | 119.66   |
| 1   | H     | 459 | ILE  | CA-C-N | 5.21  | 123.41      | 119.66   |
| 1   | H     | 459 | ILE  | C-N-CA | 5.21  | 123.41      | 119.66   |
| 1   | E     | 459 | ILE  | CA-C-N | 5.20  | 123.41      | 119.66   |
| 1   | E     | 459 | ILE  | C-N-CA | 5.20  | 123.41      | 119.66   |
| 1   | G     | 459 | ILE  | CA-C-N | 5.19  | 123.40      | 119.66   |
| 1   | G     | 459 | ILE  | C-N-CA | 5.19  | 123.40      | 119.66   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | M     | 459 | ILE  | CA-C-N | 5.18  | 123.39      | 119.66   |
| 1   | M     | 459 | ILE  | C-N-CA | 5.18  | 123.39      | 119.66   |
| 1   | I     | 341 | TRP  | N-CA-C | 5.17  | 121.81      | 110.80   |
| 1   | M     | 341 | TRP  | N-CA-C | 5.17  | 121.81      | 110.80   |
| 1   | C     | 341 | TRP  | N-CA-C | 5.16  | 121.78      | 110.80   |
| 1   | K     | 459 | ILE  | CA-C-N | 5.15  | 123.37      | 119.66   |
| 1   | K     | 459 | ILE  | C-N-CA | 5.15  | 123.37      | 119.66   |
| 1   | O     | 341 | TRP  | N-CA-C | 5.15  | 121.77      | 110.80   |
| 1   | A     | 341 | TRP  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | D     | 341 | TRP  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | N     | 341 | TRP  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | E     | 341 | TRP  | N-CA-C | 5.14  | 121.74      | 110.80   |
| 1   | I     | 702 | VAL  | N-CA-C | -5.14 | 107.74      | 112.83   |
| 1   | J     | 341 | TRP  | N-CA-C | 5.14  | 121.75      | 110.80   |
| 1   | H     | 341 | TRP  | N-CA-C | 5.14  | 121.74      | 110.80   |
| 1   | K     | 341 | TRP  | N-CA-C | 5.14  | 121.74      | 110.80   |
| 1   | F     | 702 | VAL  | N-CA-C | -5.13 | 107.75      | 112.83   |
| 1   | L     | 341 | TRP  | N-CA-C | 5.13  | 121.73      | 110.80   |
| 1   | F     | 341 | TRP  | N-CA-C | 5.12  | 121.72      | 110.80   |
| 1   | K     | 702 | VAL  | N-CA-C | -5.12 | 107.76      | 112.83   |
| 1   | B     | 341 | TRP  | N-CA-C | 5.12  | 121.71      | 110.80   |
| 1   | G     | 341 | TRP  | N-CA-C | 5.12  | 121.72      | 110.80   |
| 1   | P     | 341 | TRP  | N-CA-C | 5.12  | 121.71      | 110.80   |
| 1   | E     | 702 | VAL  | N-CA-C | -5.11 | 107.77      | 112.83   |
| 1   | E     | 126 | SER  | CA-C-N | 5.11  | 131.29      | 121.54   |
| 1   | E     | 126 | SER  | C-N-CA | 5.11  | 131.29      | 121.54   |
| 1   | P     | 702 | VAL  | N-CA-C | -5.10 | 107.78      | 112.83   |
| 1   | I     | 126 | SER  | CA-C-N | 5.10  | 131.28      | 121.54   |
| 1   | I     | 126 | SER  | C-N-CA | 5.10  | 131.28      | 121.54   |
| 1   | N     | 702 | VAL  | N-CA-C | -5.10 | 107.78      | 112.83   |
| 1   | G     | 126 | SER  | CA-C-N | 5.10  | 131.27      | 121.54   |
| 1   | G     | 126 | SER  | C-N-CA | 5.10  | 131.27      | 121.54   |
| 1   | A     | 702 | VAL  | N-CA-C | -5.09 | 107.79      | 112.83   |
| 1   | B     | 126 | SER  | CA-C-N | 5.09  | 131.27      | 121.54   |
| 1   | B     | 126 | SER  | C-N-CA | 5.09  | 131.27      | 121.54   |
| 1   | J     | 126 | SER  | CA-C-N | 5.09  | 131.27      | 121.54   |
| 1   | J     | 126 | SER  | C-N-CA | 5.09  | 131.27      | 121.54   |
| 1   | O     | 126 | SER  | CA-C-N | 5.09  | 131.27      | 121.54   |
| 1   | O     | 126 | SER  | C-N-CA | 5.09  | 131.27      | 121.54   |
| 1   | D     | 126 | SER  | CA-C-N | 5.09  | 131.26      | 121.54   |
| 1   | D     | 126 | SER  | C-N-CA | 5.09  | 131.26      | 121.54   |
| 1   | D     | 702 | VAL  | N-CA-C | -5.09 | 107.79      | 112.83   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 126 | SER  | CA-C-N | 5.09  | 131.26      | 121.54   |
| 1   | F     | 126 | SER  | C-N-CA | 5.09  | 131.26      | 121.54   |
| 1   | G     | 702 | VAL  | N-CA-C | -5.09 | 107.79      | 112.83   |
| 1   | K     | 126 | SER  | CA-C-N | 5.09  | 131.26      | 121.54   |
| 1   | K     | 126 | SER  | C-N-CA | 5.09  | 131.26      | 121.54   |
| 1   | O     | 702 | VAL  | N-CA-C | -5.09 | 107.79      | 112.83   |
| 1   | A     | 126 | SER  | CA-C-N | 5.09  | 131.26      | 121.54   |
| 1   | A     | 126 | SER  | C-N-CA | 5.09  | 131.26      | 121.54   |
| 1   | E     | 342 | LYS  | N-CA-C | -5.09 | 99.97       | 110.80   |
| 1   | J     | 702 | VAL  | N-CA-C | -5.09 | 107.79      | 112.83   |
| 1   | L     | 126 | SER  | CA-C-N | 5.09  | 131.26      | 121.54   |
| 1   | L     | 126 | SER  | C-N-CA | 5.09  | 131.26      | 121.54   |
| 1   | L     | 702 | VAL  | N-CA-C | -5.09 | 107.79      | 112.83   |
| 1   | P     | 126 | SER  | CA-C-N | 5.09  | 131.25      | 121.54   |
| 1   | P     | 126 | SER  | C-N-CA | 5.09  | 131.25      | 121.54   |
| 1   | D     | 342 | LYS  | N-CA-C | -5.08 | 99.97       | 110.80   |
| 1   | H     | 126 | SER  | CA-C-N | 5.08  | 131.25      | 121.54   |
| 1   | H     | 126 | SER  | C-N-CA | 5.08  | 131.25      | 121.54   |
| 1   | H     | 702 | VAL  | N-CA-C | -5.08 | 107.80      | 112.83   |
| 1   | O     | 342 | LYS  | N-CA-C | -5.08 | 99.98       | 110.80   |
| 1   | K     | 342 | LYS  | N-CA-C | -5.08 | 99.98       | 110.80   |
| 1   | C     | 126 | SER  | CA-C-N | 5.08  | 131.23      | 121.54   |
| 1   | C     | 126 | SER  | C-N-CA | 5.08  | 131.23      | 121.54   |
| 1   | G     | 342 | LYS  | N-CA-C | -5.08 | 99.99       | 110.80   |
| 1   | C     | 702 | VAL  | N-CA-C | -5.07 | 107.81      | 112.83   |
| 1   | P     | 342 | LYS  | N-CA-C | -5.07 | 100.00      | 110.80   |
| 1   | C     | 342 | LYS  | N-CA-C | -5.07 | 100.01      | 110.80   |
| 1   | A     | 342 | LYS  | N-CA-C | -5.07 | 100.01      | 110.80   |
| 1   | B     | 702 | VAL  | N-CA-C | -5.07 | 107.81      | 112.83   |
| 1   | L     | 342 | LYS  | N-CA-C | -5.06 | 100.01      | 110.80   |
| 1   | M     | 126 | SER  | CA-C-N | 5.06  | 131.21      | 121.54   |
| 1   | M     | 126 | SER  | C-N-CA | 5.06  | 131.21      | 121.54   |
| 1   | B     | 342 | LYS  | N-CA-C | -5.06 | 100.02      | 110.80   |
| 1   | E     | 881 | GLY  | N-CA-C | -5.06 | 109.10      | 114.67   |
| 1   | I     | 342 | LYS  | N-CA-C | -5.06 | 100.02      | 110.80   |
| 1   | D     | 881 | GLY  | N-CA-C | -5.06 | 109.10      | 114.67   |
| 1   | M     | 702 | VAL  | N-CA-C | -5.06 | 107.82      | 112.83   |
| 1   | H     | 342 | LYS  | N-CA-C | -5.06 | 100.03      | 110.80   |
| 1   | N     | 342 | LYS  | N-CA-C | -5.06 | 100.03      | 110.80   |
| 1   | N     | 126 | SER  | CA-C-N | 5.06  | 131.20      | 121.54   |
| 1   | N     | 126 | SER  | C-N-CA | 5.06  | 131.20      | 121.54   |
| 1   | J     | 881 | GLY  | N-CA-C | -5.05 | 109.11      | 114.67   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 342 | LYS  | N-CA-C | -5.05 | 100.04      | 110.80   |
| 1   | B     | 881 | GLY  | N-CA-C | -5.05 | 109.12      | 114.67   |
| 1   | J     | 342 | LYS  | N-CA-C | -5.05 | 100.05      | 110.80   |
| 1   | A     | 881 | GLY  | N-CA-C | -5.04 | 109.13      | 114.67   |
| 1   | H     | 881 | GLY  | N-CA-C | -5.04 | 109.13      | 114.67   |
| 1   | K     | 881 | GLY  | N-CA-C | -5.04 | 109.13      | 114.67   |
| 1   | M     | 342 | LYS  | N-CA-C | -5.04 | 100.07      | 110.80   |
| 1   | G     | 881 | GLY  | N-CA-C | -5.04 | 109.13      | 114.67   |
| 1   | C     | 881 | GLY  | N-CA-C | -5.03 | 109.13      | 114.67   |
| 1   | M     | 881 | GLY  | N-CA-C | -5.02 | 109.14      | 114.67   |
| 1   | N     | 881 | GLY  | N-CA-C | -5.01 | 109.16      | 114.67   |
| 1   | O     | 881 | GLY  | N-CA-C | -5.01 | 109.16      | 114.67   |
| 1   | P     | 881 | GLY  | N-CA-C | -5.01 | 109.16      | 114.67   |
| 1   | F     | 881 | GLY  | N-CA-C | -5.00 | 109.17      | 114.67   |
| 1   | L     | 881 | GLY  | N-CA-C | -5.00 | 109.17      | 114.67   |

There are no chirality outliers.

All (240) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 115 | ASN  | Peptide   |
| 1   | A     | 123 | TYR  | Peptide   |
| 1   | A     | 126 | SER  | Peptide   |
| 1   | A     | 143 | PRO  | Peptide   |
| 1   | A     | 236 | PRO  | Peptide   |
| 1   | A     | 251 | APK  | Mainchain |
| 1   | A     | 252 | ALA  | Mainchain |
| 1   | A     | 428 | GLU  | Mainchain |
| 1   | A     | 431 | VAL  | Peptide   |
| 1   | A     | 488 | ARG  | Peptide   |
| 1   | A     | 511 | SER  | Peptide   |
| 1   | A     | 551 | GLU  | Peptide   |
| 1   | A     | 552 | ASN  | Peptide   |
| 1   | A     | 556 | SER  | Peptide   |
| 1   | A     | 8   | HIS  | Peptide   |
| 1   | B     | 115 | ASN  | Peptide   |
| 1   | B     | 123 | TYR  | Peptide   |
| 1   | B     | 126 | SER  | Peptide   |
| 1   | B     | 143 | PRO  | Peptide   |
| 1   | B     | 236 | PRO  | Peptide   |
| 1   | B     | 251 | APK  | Mainchain |
| 1   | B     | 252 | ALA  | Mainchain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 428 | GLU  | Mainchain |
| 1   | B     | 431 | VAL  | Peptide   |
| 1   | B     | 488 | ARG  | Peptide   |
| 1   | B     | 511 | SER  | Peptide   |
| 1   | B     | 551 | GLU  | Peptide   |
| 1   | B     | 552 | ASN  | Peptide   |
| 1   | B     | 556 | SER  | Peptide   |
| 1   | B     | 8   | HIS  | Peptide   |
| 1   | C     | 115 | ASN  | Peptide   |
| 1   | C     | 123 | TYR  | Peptide   |
| 1   | C     | 126 | SER  | Peptide   |
| 1   | C     | 143 | PRO  | Peptide   |
| 1   | C     | 236 | PRO  | Peptide   |
| 1   | C     | 251 | APK  | Mainchain |
| 1   | C     | 252 | ALA  | Mainchain |
| 1   | C     | 428 | GLU  | Mainchain |
| 1   | C     | 431 | VAL  | Peptide   |
| 1   | C     | 488 | ARG  | Peptide   |
| 1   | C     | 511 | SER  | Peptide   |
| 1   | C     | 551 | GLU  | Peptide   |
| 1   | C     | 552 | ASN  | Peptide   |
| 1   | C     | 556 | SER  | Peptide   |
| 1   | C     | 8   | HIS  | Peptide   |
| 1   | D     | 115 | ASN  | Peptide   |
| 1   | D     | 123 | TYR  | Peptide   |
| 1   | D     | 126 | SER  | Peptide   |
| 1   | D     | 143 | PRO  | Peptide   |
| 1   | D     | 236 | PRO  | Peptide   |
| 1   | D     | 251 | APK  | Mainchain |
| 1   | D     | 252 | ALA  | Mainchain |
| 1   | D     | 428 | GLU  | Mainchain |
| 1   | D     | 431 | VAL  | Peptide   |
| 1   | D     | 488 | ARG  | Peptide   |
| 1   | D     | 511 | SER  | Peptide   |
| 1   | D     | 551 | GLU  | Peptide   |
| 1   | D     | 552 | ASN  | Peptide   |
| 1   | D     | 556 | SER  | Peptide   |
| 1   | D     | 8   | HIS  | Peptide   |
| 1   | E     | 115 | ASN  | Peptide   |
| 1   | E     | 123 | TYR  | Peptide   |
| 1   | E     | 126 | SER  | Peptide   |
| 1   | E     | 143 | PRO  | Peptide   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | E     | 236 | PRO  | Peptide   |
| 1   | E     | 251 | APK  | Mainchain |
| 1   | E     | 252 | ALA  | Mainchain |
| 1   | E     | 428 | GLU  | Mainchain |
| 1   | E     | 431 | VAL  | Peptide   |
| 1   | E     | 488 | ARG  | Peptide   |
| 1   | E     | 511 | SER  | Peptide   |
| 1   | E     | 551 | GLU  | Peptide   |
| 1   | E     | 552 | ASN  | Peptide   |
| 1   | E     | 556 | SER  | Peptide   |
| 1   | E     | 8   | HIS  | Peptide   |
| 1   | F     | 115 | ASN  | Peptide   |
| 1   | F     | 123 | TYR  | Peptide   |
| 1   | F     | 126 | SER  | Peptide   |
| 1   | F     | 143 | PRO  | Peptide   |
| 1   | F     | 236 | PRO  | Peptide   |
| 1   | F     | 251 | APK  | Mainchain |
| 1   | F     | 252 | ALA  | Mainchain |
| 1   | F     | 428 | GLU  | Mainchain |
| 1   | F     | 431 | VAL  | Peptide   |
| 1   | F     | 488 | ARG  | Peptide   |
| 1   | F     | 511 | SER  | Peptide   |
| 1   | F     | 551 | GLU  | Peptide   |
| 1   | F     | 552 | ASN  | Peptide   |
| 1   | F     | 556 | SER  | Peptide   |
| 1   | F     | 8   | HIS  | Peptide   |
| 1   | G     | 115 | ASN  | Peptide   |
| 1   | G     | 123 | TYR  | Peptide   |
| 1   | G     | 126 | SER  | Peptide   |
| 1   | G     | 143 | PRO  | Peptide   |
| 1   | G     | 236 | PRO  | Peptide   |
| 1   | G     | 251 | APK  | Mainchain |
| 1   | G     | 252 | ALA  | Mainchain |
| 1   | G     | 428 | GLU  | Mainchain |
| 1   | G     | 431 | VAL  | Peptide   |
| 1   | G     | 488 | ARG  | Peptide   |
| 1   | G     | 511 | SER  | Peptide   |
| 1   | G     | 551 | GLU  | Peptide   |
| 1   | G     | 552 | ASN  | Peptide   |
| 1   | G     | 556 | SER  | Peptide   |
| 1   | G     | 8   | HIS  | Peptide   |
| 1   | H     | 115 | ASN  | Peptide   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | H     | 123 | TYR  | Peptide   |
| 1   | H     | 126 | SER  | Peptide   |
| 1   | H     | 143 | PRO  | Peptide   |
| 1   | H     | 236 | PRO  | Peptide   |
| 1   | H     | 251 | APK  | Mainchain |
| 1   | H     | 252 | ALA  | Mainchain |
| 1   | H     | 428 | GLU  | Mainchain |
| 1   | H     | 431 | VAL  | Peptide   |
| 1   | H     | 488 | ARG  | Peptide   |
| 1   | H     | 511 | SER  | Peptide   |
| 1   | H     | 551 | GLU  | Peptide   |
| 1   | H     | 552 | ASN  | Peptide   |
| 1   | H     | 556 | SER  | Peptide   |
| 1   | H     | 8   | HIS  | Peptide   |
| 1   | I     | 115 | ASN  | Peptide   |
| 1   | I     | 123 | TYR  | Peptide   |
| 1   | I     | 126 | SER  | Peptide   |
| 1   | I     | 143 | PRO  | Peptide   |
| 1   | I     | 236 | PRO  | Peptide   |
| 1   | I     | 251 | APK  | Mainchain |
| 1   | I     | 252 | ALA  | Mainchain |
| 1   | I     | 428 | GLU  | Mainchain |
| 1   | I     | 431 | VAL  | Peptide   |
| 1   | I     | 488 | ARG  | Peptide   |
| 1   | I     | 511 | SER  | Peptide   |
| 1   | I     | 551 | GLU  | Peptide   |
| 1   | I     | 552 | ASN  | Peptide   |
| 1   | I     | 556 | SER  | Peptide   |
| 1   | I     | 8   | HIS  | Peptide   |
| 1   | J     | 115 | ASN  | Peptide   |
| 1   | J     | 123 | TYR  | Peptide   |
| 1   | J     | 126 | SER  | Peptide   |
| 1   | J     | 143 | PRO  | Peptide   |
| 1   | J     | 236 | PRO  | Peptide   |
| 1   | J     | 251 | APK  | Mainchain |
| 1   | J     | 252 | ALA  | Mainchain |
| 1   | J     | 428 | GLU  | Mainchain |
| 1   | J     | 431 | VAL  | Peptide   |
| 1   | J     | 488 | ARG  | Peptide   |
| 1   | J     | 511 | SER  | Peptide   |
| 1   | J     | 551 | GLU  | Peptide   |
| 1   | J     | 552 | ASN  | Peptide   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | J     | 556 | SER  | Peptide   |
| 1   | J     | 8   | HIS  | Peptide   |
| 1   | K     | 115 | ASN  | Peptide   |
| 1   | K     | 123 | TYR  | Peptide   |
| 1   | K     | 126 | SER  | Peptide   |
| 1   | K     | 143 | PRO  | Peptide   |
| 1   | K     | 236 | PRO  | Peptide   |
| 1   | K     | 251 | APK  | Mainchain |
| 1   | K     | 252 | ALA  | Mainchain |
| 1   | K     | 428 | GLU  | Mainchain |
| 1   | K     | 431 | VAL  | Peptide   |
| 1   | K     | 488 | ARG  | Peptide   |
| 1   | K     | 511 | SER  | Peptide   |
| 1   | K     | 551 | GLU  | Peptide   |
| 1   | K     | 552 | ASN  | Peptide   |
| 1   | K     | 556 | SER  | Peptide   |
| 1   | K     | 8   | HIS  | Peptide   |
| 1   | L     | 115 | ASN  | Peptide   |
| 1   | L     | 123 | TYR  | Peptide   |
| 1   | L     | 126 | SER  | Peptide   |
| 1   | L     | 143 | PRO  | Peptide   |
| 1   | L     | 236 | PRO  | Peptide   |
| 1   | L     | 251 | APK  | Mainchain |
| 1   | L     | 252 | ALA  | Mainchain |
| 1   | L     | 428 | GLU  | Mainchain |
| 1   | L     | 431 | VAL  | Peptide   |
| 1   | L     | 488 | ARG  | Peptide   |
| 1   | L     | 511 | SER  | Peptide   |
| 1   | L     | 551 | GLU  | Peptide   |
| 1   | L     | 552 | ASN  | Peptide   |
| 1   | L     | 556 | SER  | Peptide   |
| 1   | L     | 8   | HIS  | Peptide   |
| 1   | M     | 115 | ASN  | Peptide   |
| 1   | M     | 123 | TYR  | Peptide   |
| 1   | M     | 126 | SER  | Peptide   |
| 1   | M     | 143 | PRO  | Peptide   |
| 1   | M     | 236 | PRO  | Peptide   |
| 1   | M     | 251 | APK  | Mainchain |
| 1   | M     | 252 | ALA  | Mainchain |
| 1   | M     | 428 | GLU  | Mainchain |
| 1   | M     | 431 | VAL  | Peptide   |
| 1   | M     | 488 | ARG  | Peptide   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | M     | 511 | SER  | Peptide   |
| 1   | M     | 551 | GLU  | Peptide   |
| 1   | M     | 552 | ASN  | Peptide   |
| 1   | M     | 556 | SER  | Peptide   |
| 1   | M     | 8   | HIS  | Peptide   |
| 1   | N     | 115 | ASN  | Peptide   |
| 1   | N     | 123 | TYR  | Peptide   |
| 1   | N     | 126 | SER  | Peptide   |
| 1   | N     | 143 | PRO  | Peptide   |
| 1   | N     | 236 | PRO  | Peptide   |
| 1   | N     | 251 | APK  | Mainchain |
| 1   | N     | 252 | ALA  | Mainchain |
| 1   | N     | 428 | GLU  | Mainchain |
| 1   | N     | 431 | VAL  | Peptide   |
| 1   | N     | 488 | ARG  | Peptide   |
| 1   | N     | 511 | SER  | Peptide   |
| 1   | N     | 551 | GLU  | Peptide   |
| 1   | N     | 552 | ASN  | Peptide   |
| 1   | N     | 556 | SER  | Peptide   |
| 1   | N     | 8   | HIS  | Peptide   |
| 1   | O     | 115 | ASN  | Peptide   |
| 1   | O     | 123 | TYR  | Peptide   |
| 1   | O     | 126 | SER  | Peptide   |
| 1   | O     | 143 | PRO  | Peptide   |
| 1   | O     | 236 | PRO  | Peptide   |
| 1   | O     | 251 | APK  | Mainchain |
| 1   | O     | 252 | ALA  | Mainchain |
| 1   | O     | 428 | GLU  | Mainchain |
| 1   | O     | 431 | VAL  | Peptide   |
| 1   | O     | 488 | ARG  | Peptide   |
| 1   | O     | 511 | SER  | Peptide   |
| 1   | O     | 551 | GLU  | Peptide   |
| 1   | O     | 552 | ASN  | Peptide   |
| 1   | O     | 556 | SER  | Peptide   |
| 1   | O     | 8   | HIS  | Peptide   |
| 1   | P     | 115 | ASN  | Peptide   |
| 1   | P     | 123 | TYR  | Peptide   |
| 1   | P     | 126 | SER  | Peptide   |
| 1   | P     | 143 | PRO  | Peptide   |
| 1   | P     | 236 | PRO  | Peptide   |
| 1   | P     | 251 | APK  | Mainchain |
| 1   | P     | 252 | ALA  | Mainchain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | P     | 428 | GLU  | Mainchain |
| 1   | P     | 431 | VAL  | Peptide   |
| 1   | P     | 488 | ARG  | Peptide   |
| 1   | P     | 511 | SER  | Peptide   |
| 1   | P     | 551 | GLU  | Peptide   |
| 1   | P     | 552 | ASN  | Peptide   |
| 1   | P     | 556 | SER  | Peptide   |
| 1   | P     | 8   | HIS  | Peptide   |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 10045 | 0        | 10046    | 695     | 0            |
| 1   | B     | 10045 | 0        | 10046    | 708     | 0            |
| 1   | C     | 10045 | 0        | 10046    | 708     | 0            |
| 1   | D     | 10045 | 0        | 10046    | 719     | 0            |
| 1   | E     | 10045 | 0        | 10046    | 696     | 0            |
| 1   | F     | 10045 | 0        | 10046    | 720     | 0            |
| 1   | G     | 10045 | 0        | 10046    | 706     | 0            |
| 1   | H     | 10045 | 0        | 10046    | 682     | 0            |
| 1   | I     | 10045 | 0        | 10046    | 697     | 0            |
| 1   | J     | 10045 | 0        | 10046    | 693     | 0            |
| 1   | K     | 10045 | 0        | 10046    | 721     | 0            |
| 1   | L     | 10045 | 0        | 10046    | 715     | 0            |
| 1   | M     | 10045 | 0        | 10045    | 700     | 0            |
| 1   | N     | 10045 | 0        | 10046    | 690     | 0            |
| 1   | O     | 10045 | 0        | 10046    | 687     | 0            |
| 1   | P     | 10045 | 0        | 10046    | 694     | 0            |
| 2   | A     | 30    | 0        | 9        | 6       | 0            |
| 2   | B     | 30    | 0        | 9        | 6       | 0            |
| 2   | C     | 30    | 0        | 9        | 6       | 0            |
| 2   | D     | 30    | 0        | 9        | 6       | 0            |
| 2   | E     | 30    | 0        | 9        | 6       | 0            |
| 2   | F     | 30    | 0        | 9        | 6       | 0            |
| 2   | G     | 30    | 0        | 9        | 6       | 0            |
| 2   | H     | 30    | 0        | 9        | 6       | 0            |
| 2   | I     | 30    | 0        | 9        | 6       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | J     | 30     | 0        | 9        | 6       | 0            |
| 2   | K     | 30     | 0        | 9        | 6       | 0            |
| 2   | L     | 30     | 0        | 9        | 6       | 0            |
| 2   | M     | 30     | 0        | 9        | 6       | 0            |
| 2   | N     | 30     | 0        | 9        | 6       | 0            |
| 2   | O     | 30     | 0        | 9        | 6       | 0            |
| 2   | P     | 30     | 0        | 9        | 6       | 0            |
| All | All   | 161200 | 0        | 160879   | 11007   | 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 34.

All (11007) 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:I:875:LEU:HD11 | 1:I:911:PHE:CE2 | 1.25                     | 1.72              |
| 1:E:875:LEU:HD11 | 1:E:911:PHE:CE2 | 1.25                     | 1.72              |
| 1:J:875:LEU:HD11 | 1:J:911:PHE:CE2 | 1.25                     | 1.71              |
| 1:F:875:LEU:HD11 | 1:F:911:PHE:CE2 | 1.25                     | 1.71              |
| 1:C:875:LEU:HD11 | 1:C:911:PHE:CE2 | 1.25                     | 1.71              |
| 1:D:875:LEU:HD11 | 1:D:911:PHE:CE2 | 1.25                     | 1.70              |
| 1:K:875:LEU:HD11 | 1:K:911:PHE:CE2 | 1.25                     | 1.70              |
| 1:L:875:LEU:HD11 | 1:L:911:PHE:CE2 | 1.25                     | 1.69              |
| 1:B:875:LEU:HD11 | 1:B:911:PHE:CE2 | 1.25                     | 1.67              |
| 1:C:875:LEU:CD1  | 1:C:911:PHE:CE2 | 1.77                     | 1.67              |
| 1:P:875:LEU:HD11 | 1:P:911:PHE:CE2 | 1.25                     | 1.67              |
| 1:G:875:LEU:HD11 | 1:G:911:PHE:CE2 | 1.25                     | 1.67              |
| 1:M:875:LEU:HD11 | 1:M:911:PHE:CE2 | 1.25                     | 1.67              |
| 1:H:875:LEU:CD1  | 1:H:911:PHE:CE2 | 1.77                     | 1.66              |
| 1:B:875:LEU:CD1  | 1:B:911:PHE:CE2 | 1.77                     | 1.66              |
| 1:O:875:LEU:CD1  | 1:O:911:PHE:CE2 | 1.77                     | 1.66              |
| 1:N:875:LEU:CD1  | 1:N:911:PHE:CE2 | 1.77                     | 1.66              |
| 1:M:875:LEU:CD1  | 1:M:911:PHE:CE2 | 1.77                     | 1.66              |
| 1:I:518:LEU:HD22 | 1:I:643:TYR:CD1 | 1.32                     | 1.65              |
| 1:F:518:LEU:HD22 | 1:F:643:TYR:CD1 | 1.32                     | 1.65              |
| 1:L:875:LEU:CD1  | 1:L:911:PHE:CE2 | 1.77                     | 1.65              |
| 1:J:518:LEU:HD22 | 1:J:643:TYR:CD1 | 1.32                     | 1.64              |
| 1:G:518:LEU:HD22 | 1:G:643:TYR:CD1 | 1.32                     | 1.63              |
| 1:P:518:LEU:HD22 | 1:P:643:TYR:CD1 | 1.32                     | 1.63              |
| 1:E:518:LEU:HD22 | 1:E:643:TYR:CD1 | 1.32                     | 1.63              |
| 1:O:875:LEU:HD11 | 1:O:911:PHE:CE2 | 1.25                     | 1.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:H:875:LEU:HD11 | 1:H:911:PHE:CE2 | 1.25                     | 1.62              |
| 1:B:518:LEU:HD22 | 1:B:643:TYR:CD1 | 1.32                     | 1.61              |
| 1:D:875:LEU:CD1  | 1:D:911:PHE:CE2 | 1.77                     | 1.61              |
| 1:A:875:LEU:CD1  | 1:A:911:PHE:CE2 | 1.77                     | 1.61              |
| 1:M:518:LEU:HD22 | 1:M:643:TYR:CD1 | 1.32                     | 1.61              |
| 1:K:518:LEU:HD22 | 1:K:643:TYR:CD1 | 1.32                     | 1.60              |
| 1:K:875:LEU:CD1  | 1:K:911:PHE:CE2 | 1.77                     | 1.60              |
| 1:F:875:LEU:HD11 | 1:F:911:PHE:CD2 | 1.36                     | 1.60              |
| 1:G:875:LEU:HD11 | 1:G:911:PHE:CD2 | 1.36                     | 1.60              |
| 1:D:518:LEU:HD22 | 1:D:643:TYR:CD1 | 1.32                     | 1.60              |
| 1:L:518:LEU:HD22 | 1:L:643:TYR:CD1 | 1.32                     | 1.60              |
| 1:P:875:LEU:HD11 | 1:P:911:PHE:CD2 | 1.36                     | 1.60              |
| 1:C:518:LEU:HD22 | 1:C:643:TYR:CD1 | 1.32                     | 1.59              |
| 1:I:875:LEU:HD11 | 1:I:911:PHE:CD2 | 1.36                     | 1.59              |
| 1:E:875:LEU:HD11 | 1:E:911:PHE:CD2 | 1.36                     | 1.59              |
| 1:H:875:LEU:HD11 | 1:H:911:PHE:CD2 | 1.36                     | 1.59              |
| 1:N:518:LEU:HD22 | 1:N:643:TYR:CD1 | 1.32                     | 1.59              |
| 1:O:875:LEU:HD11 | 1:O:911:PHE:CD2 | 1.36                     | 1.59              |
| 1:J:875:LEU:HD11 | 1:J:911:PHE:CD2 | 1.36                     | 1.59              |
| 1:O:875:LEU:CD1  | 1:O:911:PHE:HE2 | 1.08                     | 1.59              |
| 1:A:518:LEU:HD22 | 1:A:643:TYR:CD1 | 1.32                     | 1.58              |
| 1:H:875:LEU:CD1  | 1:H:911:PHE:HE2 | 1.08                     | 1.58              |
| 1:N:875:LEU:HD11 | 1:N:911:PHE:CE2 | 1.25                     | 1.58              |
| 1:G:875:LEU:CD1  | 1:G:911:PHE:HE2 | 1.08                     | 1.58              |
| 1:P:875:LEU:CD1  | 1:P:911:PHE:HE2 | 1.08                     | 1.58              |
| 1:H:518:LEU:HD22 | 1:H:643:TYR:CD1 | 1.32                     | 1.58              |
| 1:A:875:LEU:HD11 | 1:A:911:PHE:CE2 | 1.25                     | 1.58              |
| 1:D:875:LEU:HD11 | 1:D:911:PHE:CD2 | 1.36                     | 1.57              |
| 1:O:518:LEU:HD22 | 1:O:643:TYR:CD1 | 1.32                     | 1.57              |
| 1:E:875:LEU:CD1  | 1:E:911:PHE:CE2 | 1.77                     | 1.57              |
| 1:F:875:LEU:CD1  | 1:F:911:PHE:CE2 | 1.77                     | 1.57              |
| 1:K:875:LEU:HD11 | 1:K:911:PHE:CD2 | 1.36                     | 1.57              |
| 1:N:875:LEU:HD11 | 1:N:911:PHE:CD2 | 1.36                     | 1.57              |
| 1:A:875:LEU:HD11 | 1:A:911:PHE:CD2 | 1.36                     | 1.57              |
| 1:J:875:LEU:CD1  | 1:J:911:PHE:CE2 | 1.77                     | 1.56              |
| 1:G:875:LEU:CD1  | 1:G:911:PHE:CE2 | 1.77                     | 1.56              |
| 1:P:875:LEU:CD1  | 1:P:911:PHE:CE2 | 1.77                     | 1.56              |
| 1:B:875:LEU:HD11 | 1:B:911:PHE:CD2 | 1.36                     | 1.55              |
| 1:M:875:LEU:HD11 | 1:M:911:PHE:CD2 | 1.36                     | 1.55              |
| 1:N:875:LEU:CD1  | 1:N:911:PHE:HE2 | 1.08                     | 1.55              |
| 1:F:875:LEU:CD1  | 1:F:911:PHE:HE2 | 1.08                     | 1.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:I:875:LEU:CD1  | 1:I:911:PHE:CE2 | 1.77                     | 1.55              |
| 1:A:875:LEU:CD1  | 1:A:911:PHE:HE2 | 1.08                     | 1.54              |
| 1:I:875:LEU:CD1  | 1:I:911:PHE:HE2 | 1.08                     | 1.54              |
| 1:L:875:LEU:HD11 | 1:L:911:PHE:CD2 | 1.36                     | 1.54              |
| 1:C:875:LEU:HD11 | 1:C:911:PHE:CD2 | 1.36                     | 1.53              |
| 1:K:875:LEU:CD1  | 1:K:911:PHE:HE2 | 1.08                     | 1.51              |
| 1:E:875:LEU:CD1  | 1:E:911:PHE:HE2 | 1.08                     | 1.50              |
| 1:D:875:LEU:CD1  | 1:D:911:PHE:HE2 | 1.08                     | 1.50              |
| 1:J:875:LEU:CD1  | 1:J:911:PHE:HE2 | 1.08                     | 1.50              |
| 1:M:875:LEU:CD1  | 1:M:911:PHE:HE2 | 1.08                     | 1.50              |
| 1:C:875:LEU:CD1  | 1:C:911:PHE:HE2 | 1.08                     | 1.50              |
| 1:B:875:LEU:CD1  | 1:B:911:PHE:HE2 | 1.08                     | 1.49              |
| 1:L:875:LEU:CD1  | 1:L:911:PHE:HE2 | 1.08                     | 1.49              |
| 1:B:313:PRO:CB   | 1:B:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:C:313:PRO:CB   | 1:C:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:J:313:PRO:CB   | 1:J:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:L:313:PRO:CB   | 1:L:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:M:313:PRO:CB   | 1:M:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:D:313:PRO:CB   | 1:D:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:E:313:PRO:CB   | 1:E:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:K:313:PRO:CB   | 1:K:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:F:313:PRO:CB   | 1:F:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:I:313:PRO:CB   | 1:I:338:TRP:HZ2 | 1.39                     | 1.36              |
| 1:A:313:PRO:CB   | 1:A:338:TRP:HZ2 | 1.39                     | 1.35              |
| 1:G:313:PRO:CB   | 1:G:338:TRP:HZ2 | 1.39                     | 1.35              |
| 1:N:313:PRO:CB   | 1:N:338:TRP:HZ2 | 1.39                     | 1.35              |
| 1:P:313:PRO:CB   | 1:P:338:TRP:HZ2 | 1.39                     | 1.35              |
| 1:H:313:PRO:CB   | 1:H:338:TRP:HZ2 | 1.39                     | 1.35              |
| 1:O:313:PRO:CB   | 1:O:338:TRP:HZ2 | 1.39                     | 1.35              |
| 1:B:633:THR:HG21 | 1:B:642:THR:O   | 1.20                     | 1.35              |
| 1:F:389:ILE:HD13 | 1:F:446:HIS:NE2 | 1.42                     | 1.35              |
| 1:I:389:ILE:HD13 | 1:I:446:HIS:NE2 | 1.42                     | 1.35              |
| 1:M:633:THR:HG21 | 1:M:642:THR:O   | 1.20                     | 1.35              |
| 1:N:518:LEU:CD2  | 1:N:643:TYR:HD1 | 1.40                     | 1.34              |
| 1:P:518:LEU:CD2  | 1:P:643:TYR:HD1 | 1.40                     | 1.34              |
| 1:A:518:LEU:CD2  | 1:A:643:TYR:HD1 | 1.40                     | 1.34              |
| 1:G:518:LEU:CD2  | 1:G:643:TYR:HD1 | 1.40                     | 1.34              |
| 1:B:518:LEU:CD2  | 1:B:643:TYR:HD1 | 1.40                     | 1.34              |
| 1:G:633:THR:HG21 | 1:G:642:THR:O   | 1.20                     | 1.34              |
| 1:H:389:ILE:HD13 | 1:H:446:HIS:NE2 | 1.42                     | 1.34              |
| 1:M:518:LEU:CD2  | 1:M:643:TYR:HD1 | 1.40                     | 1.34              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:H:518:LEU:CD2  | 1:H:643:TYR:HD1 | 1.40                     | 1.34              |
| 1:L:389:ILE:HD13 | 1:L:446:HIS:NE2 | 1.42                     | 1.34              |
| 1:O:389:ILE:HD13 | 1:O:446:HIS:NE2 | 1.42                     | 1.34              |
| 1:P:633:THR:HG21 | 1:P:642:THR:O   | 1.20                     | 1.34              |
| 1:F:248:GLN:OE1  | 1:F:268:PHE:CE2 | 1.81                     | 1.33              |
| 1:I:248:GLN:OE1  | 1:I:268:PHE:CE2 | 1.81                     | 1.33              |
| 1:J:389:ILE:HD13 | 1:J:446:HIS:NE2 | 1.42                     | 1.33              |
| 1:O:518:LEU:CD2  | 1:O:643:TYR:HD1 | 1.40                     | 1.33              |
| 1:G:248:GLN:OE1  | 1:G:268:PHE:CE2 | 1.81                     | 1.33              |
| 1:P:248:GLN:OE1  | 1:P:268:PHE:CE2 | 1.81                     | 1.33              |
| 1:B:248:GLN:OE1  | 1:B:268:PHE:CE2 | 1.81                     | 1.33              |
| 1:C:248:GLN:OE1  | 1:C:268:PHE:CE2 | 1.81                     | 1.33              |
| 1:D:389:ILE:HD13 | 1:D:446:HIS:NE2 | 1.42                     | 1.33              |
| 1:E:389:ILE:HD13 | 1:E:446:HIS:NE2 | 1.42                     | 1.33              |
| 1:M:248:GLN:OE1  | 1:M:268:PHE:CE2 | 1.81                     | 1.33              |
| 1:C:389:ILE:HD13 | 1:C:446:HIS:NE2 | 1.42                     | 1.33              |
| 1:O:633:THR:HG21 | 1:O:642:THR:O   | 1.20                     | 1.33              |
| 1:D:518:LEU:CD2  | 1:D:643:TYR:HD1 | 1.40                     | 1.33              |
| 1:K:389:ILE:HD13 | 1:K:446:HIS:NE2 | 1.42                     | 1.33              |
| 1:K:518:LEU:CD2  | 1:K:643:TYR:HD1 | 1.40                     | 1.33              |
| 1:L:248:GLN:OE1  | 1:L:268:PHE:CE2 | 1.81                     | 1.32              |
| 1:E:518:LEU:CD2  | 1:E:643:TYR:HD1 | 1.40                     | 1.32              |
| 1:J:518:LEU:CD2  | 1:J:643:TYR:HD1 | 1.40                     | 1.32              |
| 1:O:248:GLN:OE1  | 1:O:268:PHE:HE2 | 1.06                     | 1.32              |
| 1:B:389:ILE:HD13 | 1:B:446:HIS:NE2 | 1.42                     | 1.32              |
| 1:C:518:LEU:CD2  | 1:C:643:TYR:HD1 | 1.40                     | 1.32              |
| 1:H:633:THR:HG21 | 1:H:642:THR:O   | 1.20                     | 1.32              |
| 1:L:518:LEU:CD2  | 1:L:643:TYR:HD1 | 1.40                     | 1.32              |
| 1:B:462:TYR:CE2  | 1:B:494:PHE:HE1 | 1.47                     | 1.32              |
| 1:M:389:ILE:HD13 | 1:M:446:HIS:NE2 | 1.42                     | 1.32              |
| 1:M:462:TYR:CE2  | 1:M:494:PHE:HE1 | 1.47                     | 1.32              |
| 1:N:462:TYR:CE2  | 1:N:494:PHE:HE1 | 1.47                     | 1.32              |
| 1:A:462:TYR:CE2  | 1:A:494:PHE:HE1 | 1.47                     | 1.32              |
| 1:E:248:GLN:OE1  | 1:E:268:PHE:CE2 | 1.81                     | 1.32              |
| 1:H:248:GLN:OE1  | 1:H:268:PHE:HE2 | 1.06                     | 1.32              |
| 1:C:462:TYR:CE2  | 1:C:494:PHE:HE1 | 1.47                     | 1.31              |
| 1:J:248:GLN:OE1  | 1:J:268:PHE:CE2 | 1.81                     | 1.31              |
| 1:N:248:GLN:OE1  | 1:N:268:PHE:HE2 | 1.06                     | 1.31              |
| 1:A:248:GLN:OE1  | 1:A:268:PHE:CE2 | 1.81                     | 1.31              |
| 1:I:518:LEU:CD2  | 1:I:643:TYR:HD1 | 1.40                     | 1.31              |
| 1:O:248:GLN:OE1  | 1:O:268:PHE:CE2 | 1.81                     | 1.31              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:H:248:GLN:OE1  | 1:H:268:PHE:CE2 | 1.81                     | 1.31              |
| 1:N:248:GLN:OE1  | 1:N:268:PHE:CE2 | 1.81                     | 1.31              |
| 1:O:462:TYR:CE2  | 1:O:494:PHE:HE1 | 1.47                     | 1.31              |
| 1:P:248:GLN:OE1  | 1:P:268:PHE:HE2 | 1.06                     | 1.31              |
| 1:D:462:TYR:CE2  | 1:D:494:PHE:HE1 | 1.47                     | 1.31              |
| 1:F:518:LEU:CD2  | 1:F:643:TYR:HD1 | 1.40                     | 1.31              |
| 1:H:462:TYR:CE2  | 1:H:494:PHE:HE1 | 1.47                     | 1.31              |
| 1:K:462:TYR:CE2  | 1:K:494:PHE:HE1 | 1.47                     | 1.31              |
| 1:L:462:TYR:CE2  | 1:L:494:PHE:HE1 | 1.47                     | 1.31              |
| 1:A:248:GLN:OE1  | 1:A:268:PHE:HE2 | 1.06                     | 1.31              |
| 1:G:389:ILE:HD13 | 1:G:446:HIS:NE2 | 1.42                     | 1.31              |
| 1:G:248:GLN:OE1  | 1:G:268:PHE:HE2 | 1.06                     | 1.30              |
| 1:I:462:TYR:CE2  | 1:I:494:PHE:HE1 | 1.47                     | 1.30              |
| 1:G:462:TYR:CE2  | 1:G:494:PHE:HE1 | 1.47                     | 1.30              |
| 1:K:248:GLN:OE1  | 1:K:268:PHE:CE2 | 1.81                     | 1.30              |
| 1:P:389:ILE:HD13 | 1:P:446:HIS:NE2 | 1.42                     | 1.30              |
| 1:P:462:TYR:CE2  | 1:P:494:PHE:HE1 | 1.47                     | 1.30              |
| 1:A:633:THR:HG21 | 1:A:642:THR:O   | 1.20                     | 1.30              |
| 1:D:248:GLN:OE1  | 1:D:268:PHE:CE2 | 1.81                     | 1.30              |
| 1:E:462:TYR:CE2  | 1:E:494:PHE:HE1 | 1.47                     | 1.30              |
| 1:N:389:ILE:HD13 | 1:N:446:HIS:NE2 | 1.42                     | 1.30              |
| 1:F:462:TYR:CE2  | 1:F:494:PHE:HE1 | 1.47                     | 1.30              |
| 1:I:248:GLN:OE1  | 1:I:268:PHE:HE2 | 1.06                     | 1.30              |
| 1:J:462:TYR:CE2  | 1:J:494:PHE:HE1 | 1.47                     | 1.30              |
| 1:A:389:ILE:HD13 | 1:A:446:HIS:NE2 | 1.42                     | 1.30              |
| 1:M:248:GLN:OE1  | 1:M:268:PHE:HE2 | 1.06                     | 1.30              |
| 1:J:248:GLN:OE1  | 1:J:268:PHE:HE2 | 1.06                     | 1.29              |
| 1:N:633:THR:HG21 | 1:N:642:THR:O   | 1.20                     | 1.29              |
| 1:B:248:GLN:OE1  | 1:B:268:PHE:HE2 | 1.06                     | 1.29              |
| 1:L:248:GLN:OE1  | 1:L:268:PHE:HE2 | 1.06                     | 1.29              |
| 1:F:248:GLN:OE1  | 1:F:268:PHE:HE2 | 1.06                     | 1.29              |
| 1:K:248:GLN:OE1  | 1:K:268:PHE:HE2 | 1.06                     | 1.29              |
| 1:E:248:GLN:OE1  | 1:E:268:PHE:HE2 | 1.06                     | 1.28              |
| 1:C:248:GLN:OE1  | 1:C:268:PHE:HE2 | 1.06                     | 1.28              |
| 1:D:248:GLN:OE1  | 1:D:268:PHE:HE2 | 1.06                     | 1.28              |
| 1:D:633:THR:HG21 | 1:D:642:THR:O   | 1.20                     | 1.28              |
| 1:K:633:THR:HG21 | 1:K:642:THR:O   | 1.20                     | 1.27              |
| 1:D:313:PRO:CA   | 1:D:338:TRP:HZ2 | 1.48                     | 1.27              |
| 1:E:633:THR:HG21 | 1:E:642:THR:O   | 1.20                     | 1.27              |
| 1:F:633:THR:HG21 | 1:F:642:THR:O   | 1.20                     | 1.27              |
| 1:I:633:THR:HG21 | 1:I:642:THR:O   | 1.20                     | 1.27              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:K:313:PRO:CA   | 1:K:338:TRP:HZ2 | 1.48                     | 1.27              |
| 1:J:313:PRO:CA   | 1:J:338:TRP:HZ2 | 1.48                     | 1.27              |
| 1:J:633:THR:HG21 | 1:J:642:THR:O   | 1.20                     | 1.27              |
| 1:O:313:PRO:CA   | 1:O:338:TRP:HZ2 | 1.48                     | 1.27              |
| 1:C:633:THR:HG21 | 1:C:642:THR:O   | 1.20                     | 1.26              |
| 1:E:313:PRO:CA   | 1:E:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:H:313:PRO:CA   | 1:H:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:N:313:PRO:CA   | 1:N:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:A:313:PRO:CA   | 1:A:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:C:313:PRO:CA   | 1:C:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:I:313:PRO:CA   | 1:I:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:L:313:PRO:CA   | 1:L:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:F:313:PRO:CA   | 1:F:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:G:313:PRO:CA   | 1:G:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:P:313:PRO:CA   | 1:P:338:TRP:HZ2 | 1.48                     | 1.26              |
| 1:L:633:THR:HG21 | 1:L:642:THR:O   | 1.20                     | 1.25              |
| 1:M:313:PRO:CA   | 1:M:338:TRP:HZ2 | 1.48                     | 1.25              |
| 1:B:313:PRO:CA   | 1:B:338:TRP:HZ2 | 1.48                     | 1.25              |
| 1:B:121:ALA:HB1  | 1:C:276:SER:CB  | 1.67                     | 1.23              |
| 1:L:212:ASP:OD2  | 1:M:209:SER:OG  | 1.57                     | 1.23              |
| 1:B:508:TRP:CA   | 1:B:606:GLY:HA3 | 1.70                     | 1.22              |
| 1:L:508:TRP:CA   | 1:L:606:GLY:HA3 | 1.70                     | 1.22              |
| 1:M:508:TRP:CA   | 1:M:606:GLY:HA3 | 1.70                     | 1.22              |
| 1:C:508:TRP:CA   | 1:C:606:GLY:HA3 | 1.70                     | 1.22              |
| 1:E:508:TRP:CA   | 1:E:606:GLY:HA3 | 1.70                     | 1.22              |
| 1:I:508:TRP:CA   | 1:I:606:GLY:HA3 | 1.70                     | 1.22              |
| 1:J:508:TRP:CA   | 1:J:606:GLY:HA3 | 1.70                     | 1.22              |
| 1:A:508:TRP:CA   | 1:A:606:GLY:HA3 | 1.70                     | 1.21              |
| 1:D:508:TRP:CA   | 1:D:606:GLY:HA3 | 1.70                     | 1.21              |
| 1:K:508:TRP:CA   | 1:K:606:GLY:HA3 | 1.70                     | 1.21              |
| 1:N:508:TRP:CA   | 1:N:606:GLY:HA3 | 1.70                     | 1.21              |
| 1:F:508:TRP:CA   | 1:F:606:GLY:HA3 | 1.70                     | 1.21              |
| 1:P:508:TRP:CA   | 1:P:606:GLY:HA3 | 1.70                     | 1.21              |
| 1:B:313:PRO:HA   | 1:B:338:TRP:CZ2 | 1.77                     | 1.20              |
| 1:G:508:TRP:CA   | 1:G:606:GLY:HA3 | 1.70                     | 1.20              |
| 1:M:313:PRO:HA   | 1:M:338:TRP:CZ2 | 1.77                     | 1.20              |
| 1:A:313:PRO:HA   | 1:A:338:TRP:CZ2 | 1.77                     | 1.20              |
| 1:C:313:PRO:HA   | 1:C:338:TRP:CZ2 | 1.77                     | 1.20              |
| 1:D:251:APK:O    | 1:D:253:TRP:N   | 1.75                     | 1.20              |
| 1:H:508:TRP:CA   | 1:H:606:GLY:HA3 | 1.70                     | 1.20              |
| 1:K:251:APK:O    | 1:K:253:TRP:N   | 1.75                     | 1.20              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:313:PRO:HA  | 1:L:338:TRP:CZ2 | 1.77                     | 1.20              |
| 1:N:313:PRO:HA  | 1:N:338:TRP:CZ2 | 1.77                     | 1.20              |
| 1:O:508:TRP:CA  | 1:O:606:GLY:HA3 | 1.70                     | 1.20              |
| 1:D:313:PRO:HA  | 1:D:338:TRP:CZ2 | 1.77                     | 1.20              |
| 1:I:313:PRO:CA  | 1:I:338:TRP:CZ2 | 2.25                     | 1.20              |
| 1:L:276:SER:HB3 | 1:M:121:ALA:HB1 | 1.20                     | 1.20              |
| 1:F:313:PRO:CA  | 1:F:338:TRP:CZ2 | 2.25                     | 1.19              |
| 1:H:313:PRO:CA  | 1:H:338:TRP:CZ2 | 2.25                     | 1.19              |
| 1:I:313:PRO:HA  | 1:I:338:TRP:CZ2 | 1.77                     | 1.19              |
| 1:N:251:APK:O   | 1:N:253:TRP:N   | 1.75                     | 1.19              |
| 1:A:251:APK:O   | 1:A:253:TRP:N   | 1.75                     | 1.19              |
| 1:F:251:APK:O   | 1:F:253:TRP:N   | 1.75                     | 1.19              |
| 1:F:313:PRO:HA  | 1:F:338:TRP:CZ2 | 1.77                     | 1.19              |
| 1:J:313:PRO:CB  | 1:J:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:K:313:PRO:HA  | 1:K:338:TRP:CZ2 | 1.77                     | 1.19              |
| 1:O:313:PRO:CA  | 1:O:338:TRP:CZ2 | 2.25                     | 1.19              |
| 1:C:313:PRO:CB  | 1:C:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:E:313:PRO:CB  | 1:E:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:G:251:APK:O   | 1:G:253:TRP:N   | 1.75                     | 1.19              |
| 1:L:313:PRO:CB  | 1:L:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:A:313:PRO:CB  | 1:A:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:G:313:PRO:HA  | 1:G:338:TRP:CZ2 | 1.77                     | 1.19              |
| 1:H:251:APK:O   | 1:H:253:TRP:N   | 1.75                     | 1.19              |
| 1:J:251:APK:O   | 1:J:253:TRP:N   | 1.75                     | 1.19              |
| 1:N:313:PRO:CB  | 1:N:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:O:313:PRO:HA  | 1:O:338:TRP:CZ2 | 1.77                     | 1.19              |
| 1:P:251:APK:O   | 1:P:253:TRP:N   | 1.75                     | 1.19              |
| 1:P:313:PRO:CB  | 1:P:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:E:251:APK:O   | 1:E:253:TRP:N   | 1.75                     | 1.19              |
| 1:E:313:PRO:CA  | 1:E:338:TRP:CZ2 | 2.25                     | 1.19              |
| 1:F:313:PRO:CB  | 1:F:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:G:313:PRO:CB  | 1:G:338:TRP:CZ2 | 2.26                     | 1.19              |
| 1:I:251:APK:O   | 1:I:253:TRP:N   | 1.75                     | 1.19              |
| 1:J:313:PRO:HA  | 1:J:338:TRP:CZ2 | 1.77                     | 1.19              |
| 1:O:251:APK:O   | 1:O:253:TRP:N   | 1.75                     | 1.19              |
| 1:P:313:PRO:HA  | 1:P:338:TRP:CZ2 | 1.77                     | 1.19              |
| 1:C:251:APK:O   | 1:C:253:TRP:N   | 1.75                     | 1.18              |
| 1:H:313:PRO:HA  | 1:H:338:TRP:CZ2 | 1.77                     | 1.18              |
| 1:J:313:PRO:CA  | 1:J:338:TRP:CZ2 | 2.25                     | 1.18              |
| 1:M:313:PRO:CB  | 1:M:338:TRP:CZ2 | 2.26                     | 1.18              |
| 1:N:313:PRO:CA  | 1:N:338:TRP:CZ2 | 2.25                     | 1.18              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:313:PRO:CA   | 1:A:338:TRP:CZ2 | 2.25                     | 1.18              |
| 1:B:313:PRO:CB   | 1:B:338:TRP:CZ2 | 2.26                     | 1.18              |
| 1:E:313:PRO:HA   | 1:E:338:TRP:CZ2 | 1.77                     | 1.18              |
| 1:I:313:PRO:CB   | 1:I:338:TRP:CZ2 | 2.26                     | 1.18              |
| 1:B:251:APK:O    | 1:B:253:TRP:N   | 1.75                     | 1.17              |
| 1:C:313:PRO:CA   | 1:C:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:D:313:PRO:CB   | 1:D:338:TRP:CZ2 | 2.26                     | 1.17              |
| 1:D:313:PRO:CA   | 1:D:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:G:313:PRO:CA   | 1:G:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:K:313:PRO:CB   | 1:K:338:TRP:CZ2 | 2.26                     | 1.17              |
| 1:K:313:PRO:CA   | 1:K:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:L:251:APK:O    | 1:L:253:TRP:N   | 1.75                     | 1.17              |
| 1:M:251:APK:O    | 1:M:253:TRP:N   | 1.75                     | 1.17              |
| 1:B:313:PRO:CA   | 1:B:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:L:313:PRO:CA   | 1:L:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:M:313:PRO:CA   | 1:M:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:P:313:PRO:CA   | 1:P:338:TRP:CZ2 | 2.25                     | 1.17              |
| 1:C:209:SER:OG   | 1:D:212:ASP:OD2 | 1.62                     | 1.17              |
| 1:G:508:TRP:HA   | 1:G:606:GLY:CA  | 1.75                     | 1.17              |
| 1:P:508:TRP:HA   | 1:P:606:GLY:CA  | 1.75                     | 1.17              |
| 1:H:313:PRO:CB   | 1:H:338:TRP:CZ2 | 2.26                     | 1.17              |
| 1:N:389:ILE:HD13 | 1:N:446:HIS:CE1 | 1.80                     | 1.17              |
| 1:O:313:PRO:CB   | 1:O:338:TRP:CZ2 | 2.26                     | 1.17              |
| 1:A:389:ILE:HD13 | 1:A:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:E:389:ILE:HD13 | 1:E:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:F:508:TRP:HA   | 1:F:606:GLY:CA  | 1.75                     | 1.16              |
| 1:G:442:SER:O    | 1:G:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:H:442:SER:O    | 1:H:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:I:508:TRP:HA   | 1:I:606:GLY:CA  | 1.75                     | 1.16              |
| 1:J:389:ILE:HD13 | 1:J:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:O:442:SER:O    | 1:O:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:P:442:SER:O    | 1:P:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:F:389:ILE:HD13 | 1:F:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:O:508:TRP:HA   | 1:O:606:GLY:CA  | 1.75                     | 1.16              |
| 1:H:508:TRP:HA   | 1:H:606:GLY:CA  | 1.75                     | 1.16              |
| 1:O:389:ILE:HD13 | 1:O:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:A:442:SER:O    | 1:A:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:B:442:SER:O    | 1:B:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:E:209:SER:OG   | 1:F:212:ASP:OD2 | 1.63                     | 1.16              |
| 1:E:508:TRP:HA   | 1:E:606:GLY:CA  | 1.75                     | 1.16              |
| 1:H:389:ILE:HD13 | 1:H:446:HIS:CE1 | 1.80                     | 1.16              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:K:389:ILE:HD13 | 1:K:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:M:442:SER:O    | 1:M:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:B:389:ILE:HD13 | 1:B:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:D:389:ILE:HD13 | 1:D:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:I:389:ILE:HD13 | 1:I:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:J:508:TRP:HA   | 1:J:606:GLY:CA  | 1.75                     | 1.16              |
| 1:M:389:ILE:HD13 | 1:M:446:HIS:CE1 | 1.80                     | 1.16              |
| 1:N:442:SER:O    | 1:N:446:HIS:CD2 | 1.98                     | 1.16              |
| 1:O:276:SER:HB3  | 1:P:121:ALA:HB1 | 1.24                     | 1.16              |
| 1:B:508:TRP:HA   | 1:B:606:GLY:CA  | 1.75                     | 1.15              |
| 1:C:442:SER:O    | 1:C:446:HIS:CD2 | 1.98                     | 1.15              |
| 1:C:508:TRP:HA   | 1:C:606:GLY:CA  | 1.75                     | 1.15              |
| 1:D:508:TRP:HA   | 1:D:606:GLY:CA  | 1.75                     | 1.15              |
| 1:K:276:SER:HB3  | 1:L:121:ALA:HB1 | 1.23                     | 1.15              |
| 1:F:442:SER:O    | 1:F:446:HIS:CD2 | 1.98                     | 1.15              |
| 1:I:442:SER:O    | 1:I:446:HIS:CD2 | 1.98                     | 1.15              |
| 1:K:508:TRP:HA   | 1:K:606:GLY:CA  | 1.75                     | 1.15              |
| 1:L:508:TRP:HA   | 1:L:606:GLY:CA  | 1.75                     | 1.15              |
| 1:M:508:TRP:HA   | 1:M:606:GLY:CA  | 1.75                     | 1.15              |
| 1:K:442:SER:O    | 1:K:446:HIS:CD2 | 1.98                     | 1.15              |
| 1:L:442:SER:O    | 1:L:446:HIS:CD2 | 1.98                     | 1.15              |
| 1:D:442:SER:O    | 1:D:446:HIS:CD2 | 1.98                     | 1.15              |
| 1:G:389:ILE:HD13 | 1:G:446:HIS:CE1 | 1.80                     | 1.15              |
| 1:N:508:TRP:HA   | 1:N:606:GLY:CA  | 1.75                     | 1.15              |
| 1:P:389:ILE:HD13 | 1:P:446:HIS:CE1 | 1.80                     | 1.15              |
| 1:A:508:TRP:HA   | 1:A:606:GLY:CA  | 1.75                     | 1.15              |
| 1:A:276:SER:HB3  | 1:H:121:ALA:HB1 | 1.21                     | 1.14              |
| 1:E:442:SER:O    | 1:E:446:HIS:CD2 | 1.98                     | 1.14              |
| 1:G:121:ALA:HB1  | 1:H:276:SER:HB3 | 1.21                     | 1.14              |
| 1:J:442:SER:O    | 1:J:446:HIS:CD2 | 1.98                     | 1.14              |
| 1:L:389:ILE:HD13 | 1:L:446:HIS:CE1 | 1.80                     | 1.14              |
| 1:F:633:THR:CG2  | 1:F:642:THR:O   | 1.96                     | 1.14              |
| 1:G:633:THR:CG2  | 1:G:642:THR:O   | 1.96                     | 1.14              |
| 1:M:276:SER:HB3  | 1:N:121:ALA:HB1 | 1.21                     | 1.14              |
| 1:P:633:THR:CG2  | 1:P:642:THR:O   | 1.96                     | 1.14              |
| 1:I:633:THR:CG2  | 1:I:642:THR:O   | 1.96                     | 1.14              |
| 1:C:389:ILE:HD13 | 1:C:446:HIS:CE1 | 1.80                     | 1.13              |
| 1:N:276:SER:HB3  | 1:O:121:ALA:HB1 | 1.19                     | 1.13              |
| 1:A:633:THR:CG2  | 1:A:642:THR:O   | 1.96                     | 1.13              |
| 1:N:633:THR:CG2  | 1:N:642:THR:O   | 1.96                     | 1.13              |
| 1:D:121:ALA:HB1  | 1:E:276:SER:HB3 | 1.14                     | 1.12              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:622:LEU:HB2 | 1:F:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:I:622:LEU:HB2 | 1:I:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:N:622:LEU:HB2 | 1:N:634:ASP:HB2 | 1.31                     | 1.13              |
| 1:H:622:LEU:HB2 | 1:H:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:A:622:LEU:HB2 | 1:A:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:E:622:LEU:HB2 | 1:E:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:O:622:LEU:HB2 | 1:O:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:H:633:THR:CG2 | 1:H:642:THR:O   | 1.96                     | 1.12              |
| 1:J:622:LEU:HB2 | 1:J:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:P:622:LEU:HB2 | 1:P:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:A:378:SER:H   | 1:A:422:ILE:CD1 | 1.63                     | 1.12              |
| 1:B:633:THR:CG2 | 1:B:642:THR:O   | 1.96                     | 1.12              |
| 1:E:504:ASP:OD1 | 1:E:608:ASN:ND2 | 1.83                     | 1.12              |
| 1:G:622:LEU:HB2 | 1:G:634:ASP:HB2 | 1.31                     | 1.12              |
| 1:J:504:ASP:OD1 | 1:J:608:ASN:ND2 | 1.83                     | 1.12              |
| 1:K:633:THR:CG2 | 1:K:642:THR:O   | 1.96                     | 1.12              |
| 1:O:633:THR:CG2 | 1:O:642:THR:O   | 1.96                     | 1.12              |
| 1:D:633:THR:CG2 | 1:D:642:THR:O   | 1.96                     | 1.12              |
| 1:H:378:SER:H   | 1:H:422:ILE:CD1 | 1.63                     | 1.12              |
| 1:J:633:THR:CG2 | 1:J:642:THR:O   | 1.96                     | 1.12              |
| 1:M:633:THR:CG2 | 1:M:642:THR:O   | 1.96                     | 1.12              |
| 1:N:378:SER:H   | 1:N:422:ILE:CD1 | 1.63                     | 1.12              |
| 1:O:378:SER:H   | 1:O:422:ILE:CD1 | 1.63                     | 1.12              |
| 1:B:378:SER:H   | 1:B:422:ILE:CD1 | 1.63                     | 1.11              |
| 1:E:633:THR:CG2 | 1:E:642:THR:O   | 1.96                     | 1.11              |
| 1:G:378:SER:H   | 1:G:422:ILE:CD1 | 1.63                     | 1.11              |
| 1:N:504:ASP:OD1 | 1:N:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:O:504:ASP:OD1 | 1:O:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:A:504:ASP:OD1 | 1:A:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:C:633:THR:CG2 | 1:C:642:THR:O   | 1.96                     | 1.11              |
| 1:D:504:ASP:OD1 | 1:D:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:E:462:TYR:CE2 | 1:E:494:PHE:CE1 | 2.39                     | 1.11              |
| 1:F:462:TYR:CE2 | 1:F:494:PHE:CE1 | 2.39                     | 1.11              |
| 1:F:504:ASP:OD1 | 1:F:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:H:504:ASP:OD1 | 1:H:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:I:462:TYR:CE2 | 1:I:494:PHE:CE1 | 2.39                     | 1.11              |
| 1:J:462:TYR:CE2 | 1:J:494:PHE:CE1 | 2.39                     | 1.11              |
| 1:K:504:ASP:OD1 | 1:K:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:M:378:SER:H   | 1:M:422:ILE:CD1 | 1.63                     | 1.11              |
| 1:P:378:SER:H   | 1:P:422:ILE:CD1 | 1.63                     | 1.11              |
| 1:I:504:ASP:OD1 | 1:I:608:ASN:ND2 | 1.83                     | 1.11              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:L:633:THR:CG2 | 1:L:642:THR:O   | 1.96                     | 1.11              |
| 1:I:276:SER:HB3 | 1:J:121:ALA:HB1 | 1.21                     | 1.11              |
| 1:L:504:ASP:OD1 | 1:L:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:B:504:ASP:OD1 | 1:B:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:C:378:SER:H   | 1:C:422:ILE:CD1 | 1.63                     | 1.11              |
| 1:F:378:SER:H   | 1:F:422:ILE:CD1 | 1.63                     | 1.11              |
| 1:I:314:ARG:O   | 1:I:315:GLU:HG3 | 1.51                     | 1.11              |
| 1:L:622:LEU:HB2 | 1:L:634:ASP:HB2 | 1.31                     | 1.11              |
| 1:M:504:ASP:OD1 | 1:M:608:ASN:ND2 | 1.83                     | 1.11              |
| 1:E:314:ARG:O   | 1:E:315:GLU:HG3 | 1.51                     | 1.10              |
| 1:F:314:ARG:O   | 1:F:315:GLU:HG3 | 1.51                     | 1.10              |
| 1:H:314:ARG:O   | 1:H:315:GLU:HG3 | 1.51                     | 1.10              |
| 1:I:378:SER:H   | 1:I:422:ILE:CD1 | 1.63                     | 1.10              |
| 1:J:314:ARG:O   | 1:J:315:GLU:HG3 | 1.51                     | 1.10              |
| 1:K:378:SER:H   | 1:K:422:ILE:CD1 | 1.63                     | 1.10              |
| 1:L:378:SER:H   | 1:L:422:ILE:CD1 | 1.63                     | 1.10              |
| 1:L:462:TYR:CE2 | 1:L:494:PHE:CE1 | 2.39                     | 1.10              |
| 1:C:504:ASP:OD1 | 1:C:608:ASN:ND2 | 1.83                     | 1.10              |
| 1:D:378:SER:H   | 1:D:422:ILE:CD1 | 1.63                     | 1.10              |
| 1:E:378:SER:H   | 1:E:422:ILE:CD1 | 1.63                     | 1.10              |
| 1:J:378:SER:H   | 1:J:422:ILE:CD1 | 1.63                     | 1.10              |
| 1:O:314:ARG:O   | 1:O:315:GLU:HG3 | 1.51                     | 1.10              |
| 1:C:462:TYR:CE2 | 1:C:494:PHE:CE1 | 2.39                     | 1.10              |
| 1:M:622:LEU:HB2 | 1:M:634:ASP:HB2 | 1.31                     | 1.10              |
| 1:C:622:LEU:HB2 | 1:C:634:ASP:HB2 | 1.31                     | 1.10              |
| 1:K:462:TYR:CE2 | 1:K:494:PHE:CE1 | 2.39                     | 1.10              |
| 1:K:622:LEU:HB2 | 1:K:634:ASP:HB2 | 1.31                     | 1.10              |
| 1:P:504:ASP:OD1 | 1:P:608:ASN:ND2 | 1.83                     | 1.10              |
| 1:D:462:TYR:CE2 | 1:D:494:PHE:CE1 | 2.39                     | 1.10              |
| 1:D:622:LEU:HB2 | 1:D:634:ASP:HB2 | 1.31                     | 1.10              |
| 1:G:462:TYR:CE2 | 1:G:494:PHE:CE1 | 2.39                     | 1.10              |
| 1:A:462:TYR:CE2 | 1:A:494:PHE:CE1 | 2.39                     | 1.09              |
| 1:B:462:TYR:CE2 | 1:B:494:PHE:CE1 | 2.38                     | 1.09              |
| 1:B:622:LEU:HB2 | 1:B:634:ASP:HB2 | 1.31                     | 1.09              |
| 1:F:14:ASP:OD2  | 1:G:142:ARG:NH1 | 1.83                     | 1.09              |
| 1:G:314:ARG:O   | 1:G:315:GLU:HG3 | 1.51                     | 1.09              |
| 1:G:504:ASP:OD1 | 1:G:608:ASN:ND2 | 1.83                     | 1.09              |
| 1:H:462:TYR:CE2 | 1:H:494:PHE:CE1 | 2.39                     | 1.09              |
| 1:K:314:ARG:O   | 1:K:315:GLU:HG3 | 1.51                     | 1.09              |
| 1:M:462:TYR:CE2 | 1:M:494:PHE:CE1 | 2.39                     | 1.09              |
| 1:N:462:TYR:CE2 | 1:N:494:PHE:CE1 | 2.38                     | 1.09              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:462:TYR:CE2  | 1:O:494:PHE:CE1 | 2.39                     | 1.09              |
| 1:P:314:ARG:O    | 1:P:315:GLU:HG3 | 1.51                     | 1.09              |
| 1:P:462:TYR:CE2  | 1:P:494:PHE:CE1 | 2.38                     | 1.09              |
| 1:C:462:TYR:CZ   | 1:C:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:D:314:ARG:O    | 1:D:315:GLU:HG3 | 1.51                     | 1.09              |
| 1:O:462:TYR:CZ   | 1:O:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:D:462:TYR:CZ   | 1:D:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:G:462:TYR:CZ   | 1:G:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:H:462:TYR:CZ   | 1:H:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:L:462:TYR:CZ   | 1:L:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:P:462:TYR:CZ   | 1:P:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:K:462:TYR:CZ   | 1:K:494:PHE:CE1 | 2.41                     | 1.09              |
| 1:O:378:SER:N    | 1:O:422:ILE:CD1 | 2.16                     | 1.09              |
| 1:A:314:ARG:O    | 1:A:315:GLU:HG3 | 1.51                     | 1.09              |
| 1:B:378:SER:N    | 1:B:422:ILE:CD1 | 2.16                     | 1.09              |
| 1:H:378:SER:N    | 1:H:422:ILE:CD1 | 2.16                     | 1.09              |
| 1:M:378:SER:N    | 1:M:422:ILE:CD1 | 2.16                     | 1.09              |
| 1:E:121:ALA:HB1  | 1:F:276:SER:HB3 | 1.09                     | 1.08              |
| 1:I:121:ALA:HB1  | 1:P:276:SER:HB3 | 1.27                     | 1.08              |
| 1:N:314:ARG:O    | 1:N:315:GLU:HG3 | 1.51                     | 1.08              |
| 1:B:462:TYR:CZ   | 1:B:494:PHE:CE1 | 2.41                     | 1.08              |
| 1:N:462:TYR:CZ   | 1:N:494:PHE:CE1 | 2.41                     | 1.08              |
| 1:A:378:SER:N    | 1:A:422:ILE:CD1 | 2.16                     | 1.08              |
| 1:A:462:TYR:CZ   | 1:A:494:PHE:CE1 | 2.41                     | 1.08              |
| 1:F:462:TYR:CZ   | 1:F:494:PHE:CE1 | 2.41                     | 1.08              |
| 1:G:313:PRO:HB3  | 1:G:338:TRP:CZ2 | 1.88                     | 1.08              |
| 1:M:462:TYR:CZ   | 1:M:494:PHE:CE1 | 2.41                     | 1.08              |
| 1:P:313:PRO:HB3  | 1:P:338:TRP:CZ2 | 1.88                     | 1.08              |
| 1:C:378:SER:N    | 1:C:422:ILE:CD1 | 2.16                     | 1.08              |
| 1:J:276:SER:HB3  | 1:K:121:ALA:HB1 | 1.14                     | 1.08              |
| 1:N:378:SER:N    | 1:N:422:ILE:CD1 | 2.16                     | 1.08              |
| 1:A:313:PRO:HB3  | 1:A:338:TRP:CZ2 | 1.88                     | 1.08              |
| 1:E:378:SER:N    | 1:E:422:ILE:CD1 | 2.16                     | 1.08              |
| 1:J:378:SER:N    | 1:J:422:ILE:CD1 | 2.16                     | 1.08              |
| 1:J:462:TYR:CZ   | 1:J:494:PHE:CE1 | 2.41                     | 1.08              |
| 1:L:875:LEU:HD13 | 1:L:911:PHE:CE2 | 1.64                     | 1.08              |
| 1:N:313:PRO:HB3  | 1:N:338:TRP:CZ2 | 1.88                     | 1.08              |
| 1:A:121:ALA:HB1  | 1:B:276:SER:HB3 | 1.34                     | 1.07              |
| 1:E:462:TYR:CZ   | 1:E:494:PHE:CE1 | 2.41                     | 1.07              |
| 1:G:378:SER:N    | 1:G:422:ILE:CD1 | 2.16                     | 1.07              |
| 1:I:462:TYR:CZ   | 1:I:494:PHE:CE1 | 2.41                     | 1.07              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:378:SER:N    | 1:L:422:ILE:CD1  | 2.16                     | 1.07              |
| 1:F:378:SER:N    | 1:F:422:ILE:CD1  | 2.16                     | 1.07              |
| 1:L:314:ARG:O    | 1:L:315:GLU:HG3  | 1.51                     | 1.07              |
| 1:P:378:SER:N    | 1:P:422:ILE:CD1  | 2.16                     | 1.07              |
| 1:I:378:SER:N    | 1:I:422:ILE:CD1  | 2.16                     | 1.07              |
| 1:B:314:ARG:O    | 1:B:315:GLU:HG3  | 1.51                     | 1.07              |
| 1:H:313:PRO:HB3  | 1:H:338:TRP:CZ2  | 1.88                     | 1.07              |
| 1:O:313:PRO:HB3  | 1:O:338:TRP:CZ2  | 1.88                     | 1.07              |
| 1:D:378:SER:N    | 1:D:422:ILE:CD1  | 2.16                     | 1.07              |
| 1:K:378:SER:N    | 1:K:422:ILE:CD1  | 2.16                     | 1.07              |
| 1:M:314:ARG:O    | 1:M:315:GLU:HG3  | 1.51                     | 1.07              |
| 1:C:314:ARG:O    | 1:C:315:GLU:HG3  | 1.51                     | 1.06              |
| 1:I:373:SER:CB   | 1:I:433:LEU:HD12 | 1.85                     | 1.06              |
| 1:F:373:SER:CB   | 1:F:433:LEU:HD12 | 1.85                     | 1.06              |
| 1:K:313:PRO:HB3  | 1:K:338:TRP:CZ2  | 1.88                     | 1.06              |
| 1:B:373:SER:CB   | 1:B:433:LEU:HD12 | 1.85                     | 1.06              |
| 1:C:313:PRO:HA   | 1:C:338:TRP:CH2  | 1.90                     | 1.06              |
| 1:D:313:PRO:HB3  | 1:D:338:TRP:CZ2  | 1.88                     | 1.06              |
| 1:E:875:LEU:HD13 | 1:E:911:PHE:CE2  | 1.64                     | 1.06              |
| 1:F:313:PRO:HB3  | 1:F:338:TRP:CZ2  | 1.88                     | 1.06              |
| 1:G:373:SER:CB   | 1:G:433:LEU:HD12 | 1.85                     | 1.06              |
| 1:H:313:PRO:HA   | 1:H:338:TRP:CH2  | 1.90                     | 1.06              |
| 1:J:313:PRO:HB3  | 1:J:338:TRP:CZ2  | 1.88                     | 1.06              |
| 1:M:373:SER:CB   | 1:M:433:LEU:HD12 | 1.85                     | 1.06              |
| 1:O:313:PRO:HA   | 1:O:338:TRP:CH2  | 1.90                     | 1.06              |
| 1:A:373:SER:CB   | 1:A:433:LEU:HD12 | 1.85                     | 1.06              |
| 1:C:313:PRO:HB3  | 1:C:338:TRP:CZ2  | 1.88                     | 1.06              |
| 1:G:313:PRO:HA   | 1:G:338:TRP:CH2  | 1.90                     | 1.06              |
| 1:L:313:PRO:HA   | 1:L:338:TRP:CH2  | 1.90                     | 1.06              |
| 1:P:313:PRO:HA   | 1:P:338:TRP:CH2  | 1.90                     | 1.06              |
| 1:P:373:SER:CB   | 1:P:433:LEU:HD12 | 1.85                     | 1.06              |
| 1:C:373:SER:CB   | 1:C:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:E:313:PRO:HB3  | 1:E:338:TRP:CZ2  | 1.88                     | 1.05              |
| 1:L:313:PRO:HB3  | 1:L:338:TRP:CZ2  | 1.88                     | 1.05              |
| 1:N:373:SER:CB   | 1:N:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:A:313:PRO:HA   | 1:A:338:TRP:CH2  | 1.90                     | 1.05              |
| 1:E:373:SER:CB   | 1:E:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:I:313:PRO:HA   | 1:I:338:TRP:CH2  | 1.90                     | 1.05              |
| 1:I:313:PRO:HB3  | 1:I:338:TRP:CZ2  | 1.88                     | 1.05              |
| 1:J:373:SER:CB   | 1:J:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:J:875:LEU:HD13 | 1:J:911:PHE:CE2  | 1.64                     | 1.05              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:313:PRO:HA   | 1:N:338:TRP:CH2  | 1.90                     | 1.05              |
| 1:D:313:PRO:HA   | 1:D:338:TRP:CH2  | 1.90                     | 1.05              |
| 1:D:373:SER:CB   | 1:D:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:F:313:PRO:HA   | 1:F:338:TRP:CH2  | 1.90                     | 1.05              |
| 1:K:373:SER:CB   | 1:K:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:L:373:SER:CB   | 1:L:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:J:313:PRO:HA   | 1:J:338:TRP:CH2  | 1.90                     | 1.05              |
| 1:K:313:PRO:HA   | 1:K:338:TRP:CH2  | 1.91                     | 1.05              |
| 1:E:313:PRO:HA   | 1:E:338:TRP:CH2  | 1.90                     | 1.05              |
| 1:F:916:LYS:HE2  | 1:G:1177:TYR:HE2 | 1.22                     | 1.05              |
| 1:H:373:SER:CB   | 1:H:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:O:373:SER:CB   | 1:O:433:LEU:HD12 | 1.85                     | 1.05              |
| 1:G:378:SER:N    | 1:G:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:P:378:SER:N    | 1:P:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:B:313:PRO:HA   | 1:B:338:TRP:CH2  | 1.90                     | 1.04              |
| 1:C:378:SER:N    | 1:C:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:N:462:TYR:CZ   | 1:N:494:PHE:HE1  | 1.76                     | 1.04              |
| 1:K:378:SER:N    | 1:K:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:L:378:SER:N    | 1:L:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:M:313:PRO:HA   | 1:M:338:TRP:CH2  | 1.91                     | 1.04              |
| 1:D:378:SER:N    | 1:D:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:E:378:SER:N    | 1:E:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:I:378:SER:N    | 1:I:422:ILE:HD12 | 1.73                     | 1.04              |
| 1:A:378:SER:N    | 1:A:422:ILE:HD12 | 1.73                     | 1.03              |
| 1:B:313:PRO:HB3  | 1:B:338:TRP:CZ2  | 1.88                     | 1.03              |
| 1:D:209:SER:OG   | 1:E:212:ASP:OD2  | 1.76                     | 1.03              |
| 1:J:378:SER:N    | 1:J:422:ILE:HD12 | 1.73                     | 1.03              |
| 1:M:313:PRO:HB3  | 1:M:338:TRP:CZ2  | 1.88                     | 1.03              |
| 1:C:508:TRP:HA   | 1:C:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:F:509:ASN:HD21 | 1:F:632:LEU:HD13 | 1.23                     | 1.03              |
| 1:G:509:ASN:HD21 | 1:G:632:LEU:HD13 | 1.23                     | 1.03              |
| 1:N:378:SER:N    | 1:N:422:ILE:HD12 | 1.73                     | 1.03              |
| 1:O:509:ASN:HD21 | 1:O:632:LEU:HD13 | 1.23                     | 1.03              |
| 1:P:509:ASN:HD21 | 1:P:632:LEU:HD13 | 1.23                     | 1.03              |
| 1:B:508:TRP:HA   | 1:B:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:F:378:SER:N    | 1:F:422:ILE:HD12 | 1.73                     | 1.03              |
| 1:H:508:TRP:HA   | 1:H:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:H:509:ASN:HD21 | 1:H:632:LEU:HD13 | 1.23                     | 1.03              |
| 1:O:508:TRP:HA   | 1:O:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:L:508:TRP:HA   | 1:L:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:M:508:TRP:HA   | 1:M:606:GLY:HA3  | 1.03                     | 1.03              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:508:TRP:HA   | 1:N:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:A:508:TRP:HA   | 1:A:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:A:875:LEU:HD13 | 1:A:911:PHE:CE2  | 1.64                     | 1.03              |
| 1:F:508:TRP:HA   | 1:F:606:GLY:HA3  | 1.04                     | 1.03              |
| 1:I:508:TRP:HA   | 1:I:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:I:509:ASN:HD21 | 1:I:632:LEU:HD13 | 1.23                     | 1.03              |
| 1:P:508:TRP:HA   | 1:P:606:GLY:HA3  | 1.03                     | 1.03              |
| 1:D:508:TRP:HA   | 1:D:606:GLY:HA3  | 1.03                     | 1.02              |
| 1:E:509:ASN:HD21 | 1:E:632:LEU:HD13 | 1.23                     | 1.02              |
| 1:G:508:TRP:HA   | 1:G:606:GLY:HA3  | 1.03                     | 1.02              |
| 1:N:509:ASN:HD21 | 1:N:632:LEU:HD13 | 1.23                     | 1.02              |
| 1:A:509:ASN:HD21 | 1:A:632:LEU:HD13 | 1.23                     | 1.02              |
| 1:E:557:LYS:HB3  | 1:E:1226:TYR:CZ  | 1.95                     | 1.02              |
| 1:J:557:LYS:HB3  | 1:J:1226:TYR:CZ  | 1.95                     | 1.02              |
| 1:K:508:TRP:HA   | 1:K:606:GLY:HA3  | 1.03                     | 1.02              |
| 1:B:557:LYS:HB3  | 1:B:1226:TYR:CZ  | 1.95                     | 1.02              |
| 1:C:557:LYS:HB3  | 1:C:1226:TYR:CZ  | 1.95                     | 1.02              |
| 1:E:508:TRP:HA   | 1:E:606:GLY:HA3  | 1.03                     | 1.02              |
| 1:J:508:TRP:HA   | 1:J:606:GLY:HA3  | 1.03                     | 1.02              |
| 1:J:509:ASN:HD21 | 1:J:632:LEU:HD13 | 1.23                     | 1.02              |
| 1:L:557:LYS:HB3  | 1:L:1226:TYR:CZ  | 1.95                     | 1.02              |
| 1:M:557:LYS:HB3  | 1:M:1226:TYR:CZ  | 1.95                     | 1.02              |
| 1:N:875:LEU:HD13 | 1:N:911:PHE:CE2  | 1.64                     | 1.02              |
| 1:C:121:ALA:HB1  | 1:D:276:SER:HB3  | 1.39                     | 1.02              |
| 1:F:121:ALA:HB1  | 1:G:276:SER:HB3  | 1.41                     | 1.02              |
| 1:E:121:ALA:HB1  | 1:F:276:SER:CB   | 1.90                     | 1.01              |
| 1:G:209:SER:OG   | 1:H:212:ASP:OD2  | 1.77                     | 1.01              |
| 1:I:557:LYS:HB3  | 1:I:1226:TYR:CZ  | 1.95                     | 1.01              |
| 1:L:509:ASN:HD21 | 1:L:632:LEU:HD13 | 1.23                     | 1.01              |
| 1:A:389:ILE:CD1  | 1:A:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:F:557:LYS:HB3  | 1:F:1226:TYR:CZ  | 1.95                     | 1.01              |
| 1:N:389:ILE:CD1  | 1:N:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:C:389:ILE:CD1  | 1:C:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:D:389:ILE:CD1  | 1:D:446:HIS:NE2  | 2.24                     | 1.01              |
| 1:G:389:ILE:CD1  | 1:G:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:K:389:ILE:CD1  | 1:K:446:HIS:NE2  | 2.24                     | 1.01              |
| 1:L:389:ILE:CD1  | 1:L:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:P:389:ILE:CD1  | 1:P:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:B:378:SER:N    | 1:B:422:ILE:HD12 | 1.73                     | 1.01              |
| 1:D:509:ASN:HD21 | 1:D:632:LEU:HD13 | 1.23                     | 1.01              |
| 1:E:389:ILE:CD1  | 1:E:446:HIS:NE2  | 2.24                     | 1.01              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:389:ILE:CD1  | 1:H:446:HIS:NE2  | 2.24                     | 1.01              |
| 1:H:557:LYS:HB3  | 1:H:1226:TYR:CZ  | 1.95                     | 1.01              |
| 1:J:389:ILE:CD1  | 1:J:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:K:557:LYS:HB3  | 1:K:1226:TYR:CZ  | 1.95                     | 1.01              |
| 1:M:378:SER:N    | 1:M:422:ILE:HD12 | 1.73                     | 1.01              |
| 1:M:509:ASN:HD21 | 1:M:632:LEU:HD13 | 1.23                     | 1.01              |
| 1:O:557:LYS:HB3  | 1:O:1226:TYR:CZ  | 1.95                     | 1.01              |
| 1:B:509:ASN:HD21 | 1:B:632:LEU:HD13 | 1.23                     | 1.01              |
| 1:D:557:LYS:HB3  | 1:D:1226:TYR:CZ  | 1.95                     | 1.01              |
| 1:O:389:ILE:CD1  | 1:O:446:HIS:NE2  | 2.23                     | 1.01              |
| 1:G:875:LEU:HD13 | 1:G:911:PHE:CE2  | 1.64                     | 1.00              |
| 1:K:509:ASN:HD21 | 1:K:632:LEU:HD13 | 1.23                     | 1.00              |
| 1:P:557:LYS:HB3  | 1:P:1226:TYR:CZ  | 1.95                     | 1.00              |
| 1:F:875:LEU:HD13 | 1:F:911:PHE:CE2  | 1.64                     | 1.00              |
| 1:G:557:LYS:HB3  | 1:G:1226:TYR:CZ  | 1.95                     | 1.00              |
| 1:I:389:ILE:CD1  | 1:I:446:HIS:NE2  | 2.24                     | 1.00              |
| 1:A:557:LYS:HB3  | 1:A:1226:TYR:CZ  | 1.95                     | 1.00              |
| 1:F:389:ILE:CD1  | 1:F:446:HIS:NE2  | 2.23                     | 1.00              |
| 1:C:509:ASN:HD21 | 1:C:632:LEU:HD13 | 1.23                     | 1.00              |
| 1:N:557:LYS:HB3  | 1:N:1226:TYR:CZ  | 1.95                     | 1.00              |
| 1:O:378:SER:N    | 1:O:422:ILE:HD12 | 1.73                     | 1.00              |
| 1:P:875:LEU:HD13 | 1:P:911:PHE:CE2  | 1.64                     | 1.00              |
| 1:H:378:SER:N    | 1:H:422:ILE:HD12 | 1.73                     | 1.00              |
| 1:H:875:LEU:HD13 | 1:H:911:PHE:CE2  | 1.64                     | 1.00              |
| 1:M:875:LEU:CD1  | 1:M:911:PHE:CD2  | 2.23                     | 1.00              |
| 1:I:212:ASP:OD2  | 1:J:209:SER:OG   | 1.80                     | 1.00              |
| 1:I:875:LEU:CD1  | 1:I:911:PHE:CD2  | 2.24                     | 1.00              |
| 1:F:518:LEU:CD2  | 1:F:643:TYR:CD1  | 2.27                     | 0.99              |
| 1:I:875:LEU:HD13 | 1:I:911:PHE:CE2  | 1.64                     | 0.99              |
| 1:B:389:ILE:CD1  | 1:B:446:HIS:NE2  | 2.23                     | 0.99              |
| 1:D:875:LEU:HD13 | 1:D:911:PHE:CE2  | 1.64                     | 0.99              |
| 1:J:462:TYR:CZ   | 1:J:494:PHE:HE1  | 1.76                     | 0.99              |
| 1:M:389:ILE:CD1  | 1:M:446:HIS:NE2  | 2.23                     | 0.99              |
| 1:O:875:LEU:HD13 | 1:O:911:PHE:CE2  | 1.64                     | 0.99              |
| 1:E:462:TYR:CZ   | 1:E:494:PHE:HE1  | 1.76                     | 0.99              |
| 1:I:462:TYR:CZ   | 1:I:494:PHE:HE1  | 1.76                     | 0.99              |
| 1:D:462:TYR:CZ   | 1:D:494:PHE:HE1  | 1.76                     | 0.99              |
| 1:K:875:LEU:HD13 | 1:K:911:PHE:CE2  | 1.64                     | 0.99              |
| 1:C:462:TYR:CZ   | 1:C:494:PHE:HE1  | 1.76                     | 0.99              |
| 1:B:121:ALA:HB1  | 1:C:276:SER:HB3  | 1.02                     | 0.99              |
| 1:H:251:APK:C    | 1:H:253:TRP:N    | 2.26                     | 0.99              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:212:ASP:OD2  | 1:N:209:SER:OG   | 1.80                     | 0.99              |
| 1:O:251:APK:C    | 1:O:253:TRP:N    | 2.26                     | 0.99              |
| 1:D:313:PRO:HG3  | 1:D:338:TRP:HE1  | 1.28                     | 0.99              |
| 1:K:462:TYR:CZ   | 1:K:494:PHE:HE1  | 1.76                     | 0.99              |
| 1:N:212:ASP:OD2  | 1:O:209:SER:OG   | 1.79                     | 0.99              |
| 1:N:251:APK:C    | 1:N:253:TRP:N    | 2.26                     | 0.99              |
| 1:B:462:TYR:CZ   | 1:B:494:PHE:HE1  | 1.76                     | 0.98              |
| 1:G:251:APK:C    | 1:G:253:TRP:N    | 2.26                     | 0.98              |
| 1:K:313:PRO:HG3  | 1:K:338:TRP:HE1  | 1.28                     | 0.98              |
| 1:L:462:TYR:CZ   | 1:L:494:PHE:HE1  | 1.76                     | 0.98              |
| 1:P:251:APK:C    | 1:P:253:TRP:N    | 2.26                     | 0.98              |
| 1:A:251:APK:C    | 1:A:253:TRP:N    | 2.26                     | 0.98              |
| 1:A:298:LYS:HG3  | 1:A:312:LEU:HD12 | 1.44                     | 0.98              |
| 1:F:313:PRO:HG3  | 1:F:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:F:462:TYR:CZ   | 1:F:494:PHE:HE1  | 1.76                     | 0.98              |
| 1:I:518:LEU:CD2  | 1:I:643:TYR:CD1  | 2.27                     | 0.98              |
| 1:I:313:PRO:HG3  | 1:I:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:N:298:LYS:HG3  | 1:N:312:LEU:HD12 | 1.44                     | 0.98              |
| 1:B:313:PRO:HG3  | 1:B:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:H:298:LYS:HG3  | 1:H:312:LEU:HD12 | 1.44                     | 0.98              |
| 1:L:313:PRO:HG3  | 1:L:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:M:313:PRO:HG3  | 1:M:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:M:462:TYR:CZ   | 1:M:494:PHE:HE1  | 1.76                     | 0.98              |
| 1:C:313:PRO:HG3  | 1:C:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:I:301:LEU:HD21 | 1:I:313:PRO:HG2  | 1.45                     | 0.98              |
| 1:J:251:APK:C    | 1:J:253:TRP:N    | 2.26                     | 0.98              |
| 1:O:298:LYS:HG3  | 1:O:312:LEU:HD12 | 1.44                     | 0.98              |
| 1:E:251:APK:C    | 1:E:253:TRP:N    | 2.26                     | 0.98              |
| 1:M:251:APK:C    | 1:M:253:TRP:N    | 2.26                     | 0.98              |
| 1:A:462:TYR:CZ   | 1:A:494:PHE:HE1  | 1.76                     | 0.98              |
| 1:F:301:LEU:HD21 | 1:F:313:PRO:HG2  | 1.45                     | 0.98              |
| 1:J:313:PRO:HG3  | 1:J:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:A:508:TRP:CE3  | 1:A:927:GLN:O    | 2.17                     | 0.98              |
| 1:B:251:APK:C    | 1:B:253:TRP:N    | 2.26                     | 0.98              |
| 1:D:251:APK:C    | 1:D:253:TRP:N    | 2.26                     | 0.98              |
| 1:E:313:PRO:HG3  | 1:E:338:TRP:NE1  | 1.79                     | 0.98              |
| 1:E:509:ASN:ND2  | 1:E:632:LEU:HD13 | 1.79                     | 0.98              |
| 1:F:509:ASN:ND2  | 1:F:632:LEU:HD13 | 1.79                     | 0.98              |
| 1:K:298:LYS:HG3  | 1:K:312:LEU:HD12 | 1.44                     | 0.98              |
| 1:N:508:TRP:CE3  | 1:N:927:GLN:O    | 2.17                     | 0.98              |
| 1:A:313:PRO:HG3  | 1:A:338:TRP:NE1  | 1.79                     | 0.98              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:508:TRP:CE3  | 1:B:927:GLN:O    | 2.17                     | 0.98              |
| 1:E:508:TRP:CE3  | 1:E:927:GLN:O    | 2.17                     | 0.98              |
| 1:K:251:APK:C    | 1:K:253:TRP:N    | 2.26                     | 0.98              |
| 1:K:317:LEU:O    | 1:K:318:THR:OG1  | 1.82                     | 0.98              |
| 1:M:508:TRP:CE3  | 1:M:927:GLN:O    | 2.17                     | 0.98              |
| 1:D:298:LYS:HG3  | 1:D:312:LEU:HD12 | 1.44                     | 0.97              |
| 1:D:317:LEU:O    | 1:D:318:THR:OG1  | 1.82                     | 0.97              |
| 1:G:462:TYR:CZ   | 1:G:494:PHE:HE1  | 1.76                     | 0.97              |
| 1:J:317:LEU:O    | 1:J:318:THR:OG1  | 1.82                     | 0.97              |
| 1:J:508:TRP:CE3  | 1:J:927:GLN:O    | 2.17                     | 0.97              |
| 1:J:509:ASN:ND2  | 1:J:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:K:508:TRP:CE3  | 1:K:927:GLN:O    | 2.17                     | 0.97              |
| 1:N:313:PRO:HG3  | 1:N:338:TRP:NE1  | 1.79                     | 0.97              |
| 1:P:462:TYR:CZ   | 1:P:494:PHE:HE1  | 1.76                     | 0.97              |
| 1:B:298:LYS:HG3  | 1:B:312:LEU:HD12 | 1.44                     | 0.97              |
| 1:D:508:TRP:CE3  | 1:D:927:GLN:O    | 2.17                     | 0.97              |
| 1:D:509:ASN:ND2  | 1:D:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:H:462:TYR:CZ   | 1:H:494:PHE:HE1  | 1.76                     | 0.97              |
| 1:I:509:ASN:ND2  | 1:I:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:P:509:ASN:ND2  | 1:P:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:E:317:LEU:O    | 1:E:318:THR:OG1  | 1.82                     | 0.97              |
| 1:G:509:ASN:ND2  | 1:G:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:H:508:TRP:CE3  | 1:H:927:GLN:O    | 2.17                     | 0.97              |
| 1:M:298:LYS:HG3  | 1:M:312:LEU:HD12 | 1.44                     | 0.97              |
| 1:E:637:LEU:O    | 1:E:638:GLU:HB2  | 1.65                     | 0.97              |
| 1:G:792:ASP:OD2  | 1:G:799:ASN:ND2  | 1.98                     | 0.97              |
| 1:K:313:PRO:HG3  | 1:K:338:TRP:NE1  | 1.79                     | 0.97              |
| 1:K:509:ASN:ND2  | 1:K:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:O:508:TRP:CE3  | 1:O:927:GLN:O    | 2.17                     | 0.97              |
| 1:P:792:ASP:OD2  | 1:P:799:ASN:ND2  | 1.98                     | 0.97              |
| 1:D:313:PRO:HG3  | 1:D:338:TRP:NE1  | 1.79                     | 0.97              |
| 1:G:301:LEU:HD21 | 1:G:313:PRO:HG2  | 1.45                     | 0.97              |
| 1:I:508:TRP:CE3  | 1:I:927:GLN:O    | 2.17                     | 0.97              |
| 1:J:301:LEU:HD21 | 1:J:313:PRO:HG2  | 1.45                     | 0.97              |
| 1:J:637:LEU:O    | 1:J:638:GLU:HB2  | 1.65                     | 0.97              |
| 1:B:792:ASP:OD2  | 1:B:799:ASN:ND2  | 1.98                     | 0.97              |
| 1:L:251:APK:C    | 1:L:253:TRP:N    | 2.26                     | 0.97              |
| 1:M:792:ASP:OD2  | 1:M:799:ASN:ND2  | 1.98                     | 0.97              |
| 1:O:462:TYR:CZ   | 1:O:494:PHE:HE1  | 1.76                     | 0.97              |
| 1:O:509:ASN:ND2  | 1:O:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:P:301:LEU:HD21 | 1:P:313:PRO:HG2  | 1.45                     | 0.97              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:373:SER:HB3  | 1:P:433:LEU:HD12 | 1.46                     | 0.97              |
| 1:A:875:LEU:CD1  | 1:A:911:PHE:CD2  | 2.23                     | 0.97              |
| 1:E:301:LEU:HD21 | 1:E:313:PRO:HG2  | 1.45                     | 0.97              |
| 1:F:508:TRP:CE3  | 1:F:927:GLN:O    | 2.17                     | 0.97              |
| 1:G:298:LYS:HG3  | 1:G:312:LEU:HD12 | 1.44                     | 0.97              |
| 1:G:373:SER:HB3  | 1:G:433:LEU:HD12 | 1.46                     | 0.97              |
| 1:H:313:PRO:HG3  | 1:H:338:TRP:NE1  | 1.79                     | 0.97              |
| 1:P:298:LYS:HG3  | 1:P:312:LEU:HD12 | 1.44                     | 0.97              |
| 1:F:373:SER:HB3  | 1:F:433:LEU:HD12 | 1.46                     | 0.97              |
| 1:F:637:LEU:O    | 1:F:638:GLU:HB2  | 1.65                     | 0.97              |
| 1:G:313:PRO:HG3  | 1:G:338:TRP:NE1  | 1.79                     | 0.97              |
| 1:H:509:ASN:ND2  | 1:H:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:I:373:SER:HB3  | 1:I:433:LEU:HD12 | 1.46                     | 0.97              |
| 1:L:508:TRP:CE3  | 1:L:927:GLN:O    | 2.17                     | 0.97              |
| 1:P:313:PRO:HG3  | 1:P:338:TRP:NE1  | 1.79                     | 0.97              |
| 1:C:509:ASN:ND2  | 1:C:632:LEU:HD13 | 1.79                     | 0.97              |
| 1:I:251:APK:C    | 1:I:253:TRP:N    | 2.26                     | 0.97              |
| 1:P:313:PRO:HG3  | 1:P:338:TRP:HE1  | 1.28                     | 0.97              |
| 1:C:251:APK:C    | 1:C:253:TRP:N    | 2.26                     | 0.97              |
| 1:G:313:PRO:HG3  | 1:G:338:TRP:HE1  | 1.29                     | 0.97              |
| 1:I:298:LYS:HG3  | 1:I:312:LEU:HD12 | 1.44                     | 0.97              |
| 1:M:313:PRO:HG3  | 1:M:338:TRP:HE1  | 1.28                     | 0.97              |
| 1:O:313:PRO:HG3  | 1:O:338:TRP:NE1  | 1.79                     | 0.97              |
| 1:O:373:SER:HB3  | 1:O:433:LEU:HD12 | 1.46                     | 0.97              |
| 1:A:317:LEU:O    | 1:A:318:THR:OG1  | 1.82                     | 0.96              |
| 1:B:313:PRO:HG3  | 1:B:338:TRP:HE1  | 1.28                     | 0.96              |
| 1:C:508:TRP:CE3  | 1:C:927:GLN:O    | 2.17                     | 0.96              |
| 1:D:792:ASP:OD2  | 1:D:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:L:509:ASN:ND2  | 1:L:632:LEU:HD13 | 1.79                     | 0.96              |
| 1:N:317:LEU:O    | 1:N:318:THR:OG1  | 1.82                     | 0.96              |
| 1:N:792:ASP:OD2  | 1:N:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:A:451:LYS:HD3  | 1:A:486:LEU:HD21 | 1.47                     | 0.96              |
| 1:A:792:ASP:OD2  | 1:A:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:B:509:ASN:ND2  | 1:B:632:LEU:HD13 | 1.79                     | 0.96              |
| 1:F:251:APK:C    | 1:F:253:TRP:N    | 2.26                     | 0.96              |
| 1:K:792:ASP:OD2  | 1:K:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:L:313:PRO:HG3  | 1:L:338:TRP:HE1  | 1.28                     | 0.96              |
| 1:N:451:LYS:HD3  | 1:N:486:LEU:HD21 | 1.47                     | 0.96              |
| 1:A:313:PRO:HG3  | 1:A:338:TRP:HE1  | 1.28                     | 0.96              |
| 1:E:313:PRO:HG3  | 1:E:338:TRP:HE1  | 1.28                     | 0.96              |
| 1:E:373:SER:HB3  | 1:E:433:LEU:HD12 | 1.46                     | 0.96              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:317:LEU:O    | 1:H:318:THR:OG1  | 1.82                     | 0.96              |
| 1:I:637:LEU:O    | 1:I:638:GLU:HB2  | 1.65                     | 0.96              |
| 1:J:313:PRO:HG3  | 1:J:338:TRP:HE1  | 1.28                     | 0.96              |
| 1:N:509:ASN:ND2  | 1:N:632:LEU:HD13 | 1.79                     | 0.96              |
| 1:O:317:LEU:O    | 1:O:318:THR:OG1  | 1.82                     | 0.96              |
| 1:P:502:ARG:HB3  | 1:P:516:ASN:OD1  | 1.66                     | 0.96              |
| 1:G:502:ARG:HB3  | 1:G:516:ASN:OD1  | 1.66                     | 0.96              |
| 1:L:518:LEU:CD2  | 1:L:643:TYR:CD1  | 2.27                     | 0.96              |
| 1:A:509:ASN:ND2  | 1:A:632:LEU:HD13 | 1.79                     | 0.96              |
| 1:B:301:LEU:HD21 | 1:B:313:PRO:HG2  | 1.45                     | 0.96              |
| 1:D:508:TRP:O    | 1:D:606:GLY:N    | 1.98                     | 0.96              |
| 1:E:792:ASP:OD2  | 1:E:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:F:298:LYS:HG3  | 1:F:312:LEU:HD12 | 1.44                     | 0.96              |
| 1:H:373:SER:HB3  | 1:H:433:LEU:HD12 | 1.46                     | 0.96              |
| 1:J:373:SER:HB3  | 1:J:433:LEU:HD12 | 1.46                     | 0.96              |
| 1:J:792:ASP:OD2  | 1:J:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:K:508:TRP:O    | 1:K:606:GLY:N    | 1.98                     | 0.96              |
| 1:M:509:ASN:ND2  | 1:M:632:LEU:HD13 | 1.79                     | 0.96              |
| 1:N:313:PRO:HG3  | 1:N:338:TRP:HE1  | 1.28                     | 0.96              |
| 1:P:508:TRP:CE3  | 1:P:927:GLN:O    | 2.17                     | 0.96              |
| 1:L:276:SER:CB   | 1:M:121:ALA:HB1  | 1.95                     | 0.96              |
| 1:N:875:LEU:CD1  | 1:N:911:PHE:CD2  | 2.24                     | 0.96              |
| 1:D:373:SER:HB3  | 1:D:433:LEU:HD12 | 1.46                     | 0.96              |
| 1:G:508:TRP:CE3  | 1:G:927:GLN:O    | 2.17                     | 0.96              |
| 1:K:637:LEU:O    | 1:K:638:GLU:HB2  | 1.65                     | 0.96              |
| 1:M:301:LEU:HD21 | 1:M:313:PRO:HG2  | 1.45                     | 0.96              |
| 1:A:502:ARG:HB3  | 1:A:516:ASN:OD1  | 1.66                     | 0.96              |
| 1:C:301:LEU:HD21 | 1:C:313:PRO:HG2  | 1.45                     | 0.96              |
| 1:C:502:ARG:HB3  | 1:C:516:ASN:OD1  | 1.66                     | 0.96              |
| 1:D:637:LEU:O    | 1:D:638:GLU:HB2  | 1.65                     | 0.96              |
| 1:H:792:ASP:OD2  | 1:H:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:L:317:LEU:O    | 1:L:318:THR:OG1  | 1.82                     | 0.96              |
| 1:L:792:ASP:OD2  | 1:L:799:ASN:ND2  | 1.98                     | 0.96              |
| 1:N:373:SER:HB3  | 1:N:433:LEU:HD12 | 1.46                     | 0.96              |
| 1:C:298:LYS:HG3  | 1:C:312:LEU:HD12 | 1.44                     | 0.96              |
| 1:C:508:TRP:O    | 1:C:606:GLY:N    | 1.98                     | 0.96              |
| 1:H:451:LYS:HD3  | 1:H:486:LEU:HD21 | 1.47                     | 0.96              |
| 1:H:502:ARG:HB3  | 1:H:516:ASN:OD1  | 1.66                     | 0.96              |
| 1:O:502:ARG:HB3  | 1:O:516:ASN:OD1  | 1.66                     | 0.96              |
| 1:A:301:LEU:HD21 | 1:A:313:PRO:HG2  | 1.45                     | 0.96              |
| 1:B:875:LEU:HD13 | 1:B:911:PHE:CE2  | 1.64                     | 0.96              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:317:LEU:O    | 1:I:318:THR:OG1  | 1.82                     | 0.96              |
| 1:M:451:LYS:HD3  | 1:M:486:LEU:HD21 | 1.47                     | 0.96              |
| 1:N:502:ARG:HB3  | 1:N:516:ASN:OD1  | 1.66                     | 0.96              |
| 1:N:505:SER:HG   | 1:N:513:SER:HG   | 1.02                     | 0.96              |
| 1:B:451:LYS:HD3  | 1:B:486:LEU:HD21 | 1.47                     | 0.95              |
| 1:C:313:PRO:HG3  | 1:C:338:TRP:HE1  | 1.28                     | 0.95              |
| 1:C:317:LEU:O    | 1:C:318:THR:OG1  | 1.82                     | 0.95              |
| 1:G:451:LYS:HD3  | 1:G:486:LEU:HD21 | 1.47                     | 0.95              |
| 1:G:508:TRP:O    | 1:G:606:GLY:N    | 1.99                     | 0.95              |
| 1:H:313:PRO:HG3  | 1:H:338:TRP:HE1  | 1.28                     | 0.95              |
| 1:O:451:LYS:HD3  | 1:O:486:LEU:HD21 | 1.47                     | 0.95              |
| 1:O:792:ASP:OD2  | 1:O:799:ASN:ND2  | 1.98                     | 0.95              |
| 1:P:451:LYS:HD3  | 1:P:486:LEU:HD21 | 1.47                     | 0.95              |
| 1:P:508:TRP:O    | 1:P:606:GLY:N    | 1.98                     | 0.95              |
| 1:A:373:SER:HB3  | 1:A:433:LEU:HD12 | 1.46                     | 0.95              |
| 1:D:502:ARG:HB3  | 1:D:516:ASN:OD1  | 1.66                     | 0.95              |
| 1:F:792:ASP:OD2  | 1:F:799:ASN:ND2  | 1.98                     | 0.95              |
| 1:K:502:ARG:HB3  | 1:K:516:ASN:OD1  | 1.66                     | 0.95              |
| 1:L:378:SER:H    | 1:L:422:ILE:HD12 | 1.27                     | 0.95              |
| 1:L:508:TRP:O    | 1:L:606:GLY:N    | 1.98                     | 0.95              |
| 1:O:314:ARG:O    | 1:O:315:GLU:CG   | 2.14                     | 0.95              |
| 1:G:317:LEU:O    | 1:G:318:THR:OG1  | 1.82                     | 0.95              |
| 1:H:314:ARG:O    | 1:H:315:GLU:CG   | 2.15                     | 0.95              |
| 1:K:373:SER:HB3  | 1:K:433:LEU:HD12 | 1.46                     | 0.95              |
| 1:L:314:ARG:O    | 1:L:315:GLU:CG   | 2.14                     | 0.95              |
| 1:N:301:LEU:HD21 | 1:N:313:PRO:HG2  | 1.45                     | 0.95              |
| 1:B:373:SER:HB3  | 1:B:433:LEU:HD12 | 1.46                     | 0.95              |
| 1:B:378:SER:H    | 1:B:422:ILE:HD12 | 1.27                     | 0.95              |
| 1:C:378:SER:H    | 1:C:422:ILE:HD12 | 1.27                     | 0.95              |
| 1:C:792:ASP:OD2  | 1:C:799:ASN:ND2  | 1.98                     | 0.95              |
| 1:F:505:SER:HG   | 1:F:513:SER:HG   | 1.06                     | 0.95              |
| 1:J:508:TRP:O    | 1:J:606:GLY:N    | 1.98                     | 0.95              |
| 1:M:378:SER:H    | 1:M:422:ILE:HD12 | 1.27                     | 0.95              |
| 1:P:317:LEU:O    | 1:P:318:THR:OG1  | 1.82                     | 0.95              |
| 1:C:875:LEU:HD13 | 1:C:911:PHE:CE2  | 1.64                     | 0.95              |
| 1:E:508:TRP:O    | 1:E:606:GLY:N    | 1.98                     | 0.95              |
| 1:M:373:SER:HB3  | 1:M:433:LEU:HD12 | 1.46                     | 0.95              |
| 1:O:508:TRP:O    | 1:O:606:GLY:N    | 1.99                     | 0.95              |
| 1:C:314:ARG:O    | 1:C:315:GLU:CG   | 2.15                     | 0.95              |
| 1:E:314:ARG:O    | 1:E:315:GLU:CG   | 2.14                     | 0.95              |
| 1:H:508:TRP:O    | 1:H:606:GLY:N    | 1.99                     | 0.95              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:314:ARG:O    | 1:I:315:GLU:CG   | 2.15                     | 0.95              |
| 1:L:298:LYS:HG3  | 1:L:312:LEU:HD12 | 1.44                     | 0.95              |
| 1:L:502:ARG:HB3  | 1:L:516:ASN:OD1  | 1.66                     | 0.95              |
| 1:M:875:LEU:HD13 | 1:M:911:PHE:CE2  | 1.64                     | 0.95              |
| 1:O:313:PRO:HG3  | 1:O:338:TRP:HE1  | 1.28                     | 0.95              |
| 1:O:637:LEU:O    | 1:O:638:GLU:HB2  | 1.65                     | 0.95              |
| 1:B:314:ARG:O    | 1:B:315:GLU:CG   | 2.14                     | 0.95              |
| 1:D:518:LEU:CD2  | 1:D:643:TYR:CD1  | 2.27                     | 0.95              |
| 1:F:314:ARG:O    | 1:F:315:GLU:CG   | 2.15                     | 0.95              |
| 1:F:502:ARG:HB3  | 1:F:516:ASN:OD1  | 1.66                     | 0.95              |
| 1:F:508:TRP:O    | 1:F:606:GLY:N    | 1.98                     | 0.95              |
| 1:I:792:ASP:OD2  | 1:I:799:ASN:ND2  | 1.98                     | 0.95              |
| 1:M:314:ARG:O    | 1:M:315:GLU:CG   | 2.15                     | 0.95              |
| 1:F:317:LEU:O    | 1:F:318:THR:OG1  | 1.82                     | 0.95              |
| 1:I:508:TRP:O    | 1:I:606:GLY:N    | 1.98                     | 0.95              |
| 1:J:314:ARG:O    | 1:J:315:GLU:CG   | 2.14                     | 0.95              |
| 1:K:378:SER:H    | 1:K:422:ILE:HD12 | 1.27                     | 0.95              |
| 1:C:518:LEU:CD2  | 1:C:643:TYR:CD1  | 2.27                     | 0.95              |
| 1:E:298:LYS:HG3  | 1:E:312:LEU:HD12 | 1.44                     | 0.95              |
| 1:G:637:LEU:O    | 1:G:638:GLU:HB2  | 1.65                     | 0.95              |
| 1:H:637:LEU:O    | 1:H:638:GLU:HB2  | 1.65                     | 0.95              |
| 1:L:301:LEU:HD21 | 1:L:313:PRO:HG2  | 1.45                     | 0.95              |
| 1:L:637:LEU:O    | 1:L:638:GLU:HB2  | 1.65                     | 0.95              |
| 1:M:317:LEU:O    | 1:M:318:THR:OG1  | 1.82                     | 0.95              |
| 1:A:508:TRP:O    | 1:A:606:GLY:N    | 1.98                     | 0.94              |
| 1:B:317:LEU:O    | 1:B:318:THR:OG1  | 1.82                     | 0.94              |
| 1:C:373:SER:HB3  | 1:C:433:LEU:HD12 | 1.46                     | 0.94              |
| 1:I:209:SER:OG   | 1:P:212:ASP:OD2  | 1.81                     | 0.94              |
| 1:J:502:ARG:HB3  | 1:J:516:ASN:OD1  | 1.66                     | 0.94              |
| 1:K:314:ARG:O    | 1:K:315:GLU:CG   | 2.15                     | 0.94              |
| 1:N:508:TRP:O    | 1:N:606:GLY:N    | 1.98                     | 0.94              |
| 1:N:637:LEU:O    | 1:N:638:GLU:HB2  | 1.65                     | 0.94              |
| 1:C:14:ASP:OD2   | 1:D:142:ARG:NH1  | 2.00                     | 0.94              |
| 1:D:314:ARG:O    | 1:D:315:GLU:CG   | 2.15                     | 0.94              |
| 1:D:378:SER:H    | 1:D:422:ILE:HD12 | 1.27                     | 0.94              |
| 1:J:212:ASP:OD2  | 1:K:209:SER:OG   | 1.85                     | 0.94              |
| 1:J:378:SER:H    | 1:J:422:ILE:HD12 | 1.27                     | 0.94              |
| 1:K:518:LEU:CD2  | 1:K:643:TYR:CD1  | 2.27                     | 0.94              |
| 1:M:508:TRP:O    | 1:M:606:GLY:N    | 1.98                     | 0.94              |
| 1:A:505:SER:HG   | 1:A:513:SER:HG   | 1.05                     | 0.94              |
| 1:B:508:TRP:O    | 1:B:606:GLY:N    | 1.98                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:502:ARG:HB3  | 1:E:516:ASN:OD1  | 1.66                     | 0.94              |
| 1:G:314:ARG:O    | 1:G:315:GLU:CG   | 2.15                     | 0.94              |
| 1:J:276:SER:CB   | 1:K:121:ALA:HB1  | 1.98                     | 0.94              |
| 1:L:373:SER:HB3  | 1:L:433:LEU:HD12 | 1.46                     | 0.94              |
| 1:P:314:ARG:O    | 1:P:315:GLU:CG   | 2.14                     | 0.94              |
| 1:P:637:LEU:O    | 1:P:638:GLU:HB2  | 1.65                     | 0.94              |
| 1:A:637:LEU:O    | 1:A:638:GLU:HB2  | 1.65                     | 0.94              |
| 1:B:502:ARG:HB3  | 1:B:516:ASN:OD1  | 1.66                     | 0.94              |
| 1:F:451:LYS:HD3  | 1:F:486:LEU:HD21 | 1.47                     | 0.94              |
| 1:E:518:LEU:CD2  | 1:E:643:TYR:CD1  | 2.27                     | 0.94              |
| 1:H:301:LEU:HD21 | 1:H:313:PRO:HG2  | 1.45                     | 0.94              |
| 1:H:463:LEU:HD22 | 1:H:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:H:518:LEU:CD2  | 1:H:643:TYR:CD1  | 2.27                     | 0.94              |
| 1:I:502:ARG:HB3  | 1:I:516:ASN:OD1  | 1.66                     | 0.94              |
| 1:M:502:ARG:HB3  | 1:M:516:ASN:OD1  | 1.66                     | 0.94              |
| 1:J:298:LYS:HG3  | 1:J:312:LEU:HD12 | 1.44                     | 0.94              |
| 1:N:314:ARG:O    | 1:N:315:GLU:CG   | 2.15                     | 0.94              |
| 1:N:378:SER:H    | 1:N:422:ILE:HD12 | 1.27                     | 0.94              |
| 1:O:463:LEU:HD22 | 1:O:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:C:451:LYS:HD3  | 1:C:486:LEU:HD21 | 1.47                     | 0.94              |
| 1:E:875:LEU:CD1  | 1:E:911:PHE:CD2  | 2.23                     | 0.94              |
| 1:I:451:LYS:HD3  | 1:I:486:LEU:HD21 | 1.47                     | 0.94              |
| 1:K:301:LEU:HD21 | 1:K:313:PRO:HG2  | 1.45                     | 0.94              |
| 1:A:314:ARG:O    | 1:A:315:GLU:CG   | 2.14                     | 0.94              |
| 1:A:378:SER:H    | 1:A:422:ILE:HD12 | 1.27                     | 0.94              |
| 1:A:557:LYS:O    | 1:A:1226:TYR:OH  | 1.86                     | 0.94              |
| 1:B:463:LEU:HD22 | 1:B:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:E:378:SER:H    | 1:E:422:ILE:HD12 | 1.27                     | 0.94              |
| 1:F:463:LEU:HD22 | 1:F:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:F:916:LYS:CE   | 1:G:1177:TYR:HE2 | 1.81                     | 0.94              |
| 1:H:557:LYS:O    | 1:H:1226:TYR:OH  | 1.86                     | 0.94              |
| 1:I:378:SER:H    | 1:I:422:ILE:HD12 | 1.27                     | 0.94              |
| 1:I:463:LEU:HD22 | 1:I:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:N:557:LYS:O    | 1:N:1226:TYR:OH  | 1.86                     | 0.94              |
| 1:O:557:LYS:O    | 1:O:1226:TYR:OH  | 1.86                     | 0.94              |
| 1:P:557:LYS:O    | 1:P:1226:TYR:OH  | 1.86                     | 0.94              |
| 1:D:547:PRO:HB3  | 1:D:603:ILE:HG13 | 1.50                     | 0.94              |
| 1:G:557:LYS:O    | 1:G:1226:TYR:OH  | 1.86                     | 0.94              |
| 1:M:463:LEU:HD22 | 1:M:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:M:637:LEU:O    | 1:M:638:GLU:HB2  | 1.65                     | 0.94              |
| 1:O:301:LEU:HD21 | 1:O:313:PRO:HG2  | 1.45                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:637:LEU:O    | 1:C:638:GLU:HB2  | 1.65                     | 0.94              |
| 1:J:518:LEU:CD2  | 1:J:643:TYR:CD1  | 2.27                     | 0.94              |
| 1:J:875:LEU:CD1  | 1:J:911:PHE:CD2  | 2.23                     | 0.94              |
| 1:K:463:LEU:HD22 | 1:K:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:N:463:LEU:HD22 | 1:N:467:PHE:CE2  | 2.03                     | 0.94              |
| 1:O:518:LEU:CD2  | 1:O:643:TYR:CD1  | 2.27                     | 0.94              |
| 1:B:557:LYS:O    | 1:B:1226:TYR:OH  | 1.86                     | 0.93              |
| 1:B:637:LEU:O    | 1:B:638:GLU:HB2  | 1.65                     | 0.93              |
| 1:B:875:LEU:CD1  | 1:B:911:PHE:CD2  | 2.23                     | 0.93              |
| 1:K:451:LYS:HD3  | 1:K:486:LEU:HD21 | 1.47                     | 0.93              |
| 1:K:547:PRO:HB3  | 1:K:603:ILE:HG13 | 1.51                     | 0.93              |
| 1:A:463:LEU:HD22 | 1:A:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:D:301:LEU:HD21 | 1:D:313:PRO:HG2  | 1.45                     | 0.93              |
| 1:D:463:LEU:HD22 | 1:D:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:M:557:LYS:O    | 1:M:1226:TYR:OH  | 1.86                     | 0.93              |
| 1:D:451:LYS:HD3  | 1:D:486:LEU:HD21 | 1.47                     | 0.93              |
| 1:G:463:LEU:HD22 | 1:G:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:B:518:LEU:CD2  | 1:B:643:TYR:CD1  | 2.27                     | 0.93              |
| 1:C:463:LEU:HD22 | 1:C:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:L:451:LYS:HD3  | 1:L:486:LEU:HD21 | 1.47                     | 0.93              |
| 1:O:378:SER:H    | 1:O:422:ILE:HD12 | 1.27                     | 0.93              |
| 1:P:463:LEU:HD22 | 1:P:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:M:518:LEU:CD2  | 1:M:643:TYR:CD1  | 2.27                     | 0.93              |
| 1:E:463:LEU:HD22 | 1:E:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:F:547:PRO:HB3  | 1:F:603:ILE:HG13 | 1.50                     | 0.93              |
| 1:I:505:SER:HG   | 1:I:513:SER:HG   | 1.02                     | 0.93              |
| 1:O:212:ASP:OD2  | 1:P:209:SER:OG   | 1.85                     | 0.93              |
| 1:P:378:SER:H    | 1:P:422:ILE:HD12 | 1.27                     | 0.93              |
| 1:B:547:PRO:HB3  | 1:B:603:ILE:HG13 | 1.50                     | 0.93              |
| 1:F:545:PHE:CZ   | 1:F:565:ALA:HA   | 2.04                     | 0.93              |
| 1:I:545:PHE:CZ   | 1:I:565:ALA:HA   | 2.04                     | 0.93              |
| 1:I:557:LYS:O    | 1:I:1226:TYR:OH  | 1.86                     | 0.93              |
| 1:L:463:LEU:HD22 | 1:L:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:F:378:SER:H    | 1:F:422:ILE:HD12 | 1.27                     | 0.93              |
| 1:F:557:LYS:O    | 1:F:1226:TYR:OH  | 1.86                     | 0.93              |
| 1:G:547:PRO:HB3  | 1:G:603:ILE:HG13 | 1.51                     | 0.93              |
| 1:M:547:PRO:HB3  | 1:M:603:ILE:HG13 | 1.51                     | 0.93              |
| 1:P:547:PRO:HB3  | 1:P:603:ILE:HG13 | 1.51                     | 0.93              |
| 1:A:875:LEU:HD13 | 1:A:911:PHE:HE2  | 0.76                     | 0.93              |
| 1:G:378:SER:H    | 1:G:422:ILE:HD12 | 1.27                     | 0.93              |
| 1:H:378:SER:H    | 1:H:422:ILE:HD12 | 1.27                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:451:LYS:HD3  | 1:J:486:LEU:HD21 | 1.47                     | 0.93              |
| 1:J:463:LEU:HD22 | 1:J:467:PHE:CE2  | 2.03                     | 0.93              |
| 1:N:875:LEU:HD13 | 1:N:911:PHE:HE2  | 0.76                     | 0.93              |
| 1:P:545:PHE:CZ   | 1:P:565:ALA:HA   | 2.04                     | 0.93              |
| 1:E:451:LYS:HD3  | 1:E:486:LEU:HD21 | 1.47                     | 0.93              |
| 1:E:545:PHE:CZ   | 1:E:565:ALA:HA   | 2.04                     | 0.93              |
| 1:C:557:LYS:O    | 1:C:1226:TYR:OH  | 1.86                     | 0.92              |
| 1:D:121:ALA:HB1  | 1:E:276:SER:CB   | 1.99                     | 0.92              |
| 1:G:545:PHE:CZ   | 1:G:565:ALA:HA   | 2.04                     | 0.92              |
| 1:H:875:LEU:CD1  | 1:H:911:PHE:CD2  | 2.24                     | 0.92              |
| 1:I:547:PRO:HB3  | 1:I:603:ILE:HG13 | 1.51                     | 0.92              |
| 1:A:483:ARG:O    | 1:A:487:PHE:N    | 2.03                     | 0.92              |
| 1:E:875:LEU:HD13 | 1:E:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:J:545:PHE:CZ   | 1:J:565:ALA:HA   | 2.04                     | 0.92              |
| 1:B:875:LEU:HD11 | 1:B:911:PHE:HD2  | 1.34                     | 0.92              |
| 1:D:312:LEU:HD23 | 1:D:313:PRO:N    | 1.85                     | 0.92              |
| 1:D:483:ARG:O    | 1:D:487:PHE:N    | 2.03                     | 0.92              |
| 1:E:333:ASP:OD2  | 1:F:403:ASN:ND2  | 2.01                     | 0.92              |
| 1:J:875:LEU:HD13 | 1:J:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:K:483:ARG:O    | 1:K:487:PHE:N    | 2.03                     | 0.92              |
| 1:M:875:LEU:HD11 | 1:M:911:PHE:HD2  | 1.34                     | 0.92              |
| 1:N:483:ARG:O    | 1:N:487:PHE:N    | 2.03                     | 0.92              |
| 1:B:382:PRO:HA   | 1:B:419:THR:HG22 | 1.52                     | 0.92              |
| 1:B:875:LEU:HD13 | 1:B:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:F:875:LEU:HD13 | 1:F:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:J:547:PRO:HB3  | 1:J:603:ILE:HG13 | 1.50                     | 0.92              |
| 1:K:312:LEU:HD23 | 1:K:313:PRO:N    | 1.85                     | 0.92              |
| 1:O:382:PRO:HA   | 1:O:419:THR:HG22 | 1.52                     | 0.92              |
| 1:O:545:PHE:CZ   | 1:O:565:ALA:HA   | 2.04                     | 0.92              |
| 1:B:545:PHE:CZ   | 1:B:565:ALA:HA   | 2.04                     | 0.92              |
| 1:H:382:PRO:HA   | 1:H:419:THR:HG22 | 1.52                     | 0.92              |
| 1:I:875:LEU:HD13 | 1:I:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:L:312:LEU:HD23 | 1:L:313:PRO:N    | 1.85                     | 0.92              |
| 1:M:483:ARG:O    | 1:M:487:PHE:N    | 2.03                     | 0.92              |
| 1:M:545:PHE:CZ   | 1:M:565:ALA:HA   | 2.04                     | 0.92              |
| 1:A:382:PRO:HA   | 1:A:419:THR:HG22 | 1.52                     | 0.92              |
| 1:B:483:ARG:O    | 1:B:487:PHE:N    | 2.03                     | 0.92              |
| 1:C:312:LEU:HD23 | 1:C:313:PRO:N    | 1.85                     | 0.92              |
| 1:D:545:PHE:CZ   | 1:D:565:ALA:HA   | 2.04                     | 0.92              |
| 1:E:312:LEU:HD23 | 1:E:313:PRO:N    | 1.85                     | 0.92              |
| 1:H:545:PHE:CZ   | 1:H:565:ALA:HA   | 2.04                     | 0.92              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:875:LEU:HD13 | 1:H:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:M:382:PRO:HA   | 1:M:419:THR:HG22 | 1.52                     | 0.92              |
| 1:M:875:LEU:HD13 | 1:M:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:N:312:LEU:HD23 | 1:N:313:PRO:CD   | 2.00                     | 0.92              |
| 1:O:875:LEU:CD1  | 1:O:911:PHE:CD2  | 2.23                     | 0.92              |
| 1:O:875:LEU:HD13 | 1:O:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:A:312:LEU:HD23 | 1:A:313:PRO:CD   | 2.00                     | 0.92              |
| 1:B:312:LEU:HD23 | 1:B:313:PRO:N    | 1.85                     | 0.92              |
| 1:E:547:PRO:HB3  | 1:E:603:ILE:HG13 | 1.50                     | 0.92              |
| 1:G:382:PRO:HA   | 1:G:419:THR:HG22 | 1.52                     | 0.92              |
| 1:H:547:PRO:HB3  | 1:H:603:ILE:HG13 | 1.50                     | 0.92              |
| 1:I:313:PRO:HG3  | 1:I:338:TRP:HE1  | 1.28                     | 0.92              |
| 1:L:557:LYS:O    | 1:L:1226:TYR:OH  | 1.86                     | 0.92              |
| 1:P:382:PRO:HA   | 1:P:419:THR:HG22 | 1.52                     | 0.92              |
| 1:B:312:LEU:HD23 | 1:B:313:PRO:CD   | 2.00                     | 0.92              |
| 1:C:547:PRO:HB3  | 1:C:603:ILE:HG13 | 1.50                     | 0.92              |
| 1:F:916:LYS:HE2  | 1:G:1177:TYR:CE2 | 2.04                     | 0.92              |
| 1:H:483:ARG:O    | 1:H:487:PHE:N    | 2.03                     | 0.92              |
| 1:J:312:LEU:HD23 | 1:J:313:PRO:N    | 1.85                     | 0.92              |
| 1:K:545:PHE:CZ   | 1:K:565:ALA:HA   | 2.04                     | 0.92              |
| 1:M:312:LEU:HD23 | 1:M:313:PRO:CD   | 2.00                     | 0.92              |
| 1:O:547:PRO:HB3  | 1:O:603:ILE:HG13 | 1.50                     | 0.92              |
| 1:B:209:SER:OG   | 1:C:212:ASP:OD2  | 1.87                     | 0.92              |
| 1:C:545:PHE:CZ   | 1:C:565:ALA:HA   | 2.04                     | 0.92              |
| 1:D:875:LEU:HD13 | 1:D:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:K:505:SER:HG   | 1:K:513:SER:HG   | 1.04                     | 0.92              |
| 1:K:557:LYS:HB3  | 1:K:1226:TYR:CE1 | 2.05                     | 0.92              |
| 1:K:875:LEU:HD13 | 1:K:911:PHE:HE2  | 0.76                     | 0.92              |
| 1:L:557:LYS:HB3  | 1:L:1226:TYR:CE1 | 2.05                     | 0.92              |
| 1:M:312:LEU:HD23 | 1:M:313:PRO:N    | 1.85                     | 0.92              |
| 1:O:483:ARG:O    | 1:O:487:PHE:N    | 2.03                     | 0.92              |
| 1:F:875:LEU:CD1  | 1:F:911:PHE:CD2  | 2.23                     | 0.92              |
| 1:N:382:PRO:HA   | 1:N:419:THR:HG22 | 1.52                     | 0.92              |
| 1:O:312:LEU:HD23 | 1:O:313:PRO:CD   | 2.00                     | 0.92              |
| 1:A:212:ASP:OD2  | 1:H:209:SER:OG   | 1.87                     | 0.91              |
| 1:C:312:LEU:HD23 | 1:C:313:PRO:CD   | 2.00                     | 0.91              |
| 1:D:557:LYS:HB3  | 1:D:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:G:518:LEU:CD2  | 1:G:643:TYR:CD1  | 2.27                     | 0.91              |
| 1:J:483:ARG:O    | 1:J:487:PHE:N    | 2.03                     | 0.91              |
| 1:J:557:LYS:HB3  | 1:J:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:L:483:ARG:O    | 1:L:487:PHE:N    | 2.03                     | 0.91              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:545:PHE:CZ   | 1:L:565:ALA:HA   | 2.04                     | 0.91              |
| 1:C:557:LYS:HB3  | 1:C:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:E:557:LYS:HB3  | 1:E:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:H:312:LEU:HD23 | 1:H:313:PRO:CD   | 2.00                     | 0.91              |
| 1:J:557:LYS:O    | 1:J:1226:TYR:OH  | 1.86                     | 0.91              |
| 1:L:875:LEU:HD13 | 1:L:911:PHE:HE2  | 0.76                     | 0.91              |
| 1:N:545:PHE:CZ   | 1:N:565:ALA:HA   | 2.04                     | 0.91              |
| 1:O:557:LYS:HB3  | 1:O:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:C:875:LEU:HD13 | 1:C:911:PHE:HE2  | 0.76                     | 0.91              |
| 1:E:483:ARG:O    | 1:E:487:PHE:N    | 2.03                     | 0.91              |
| 1:G:483:ARG:O    | 1:G:487:PHE:N    | 2.03                     | 0.91              |
| 1:H:557:LYS:HB3  | 1:H:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:L:312:LEU:HD23 | 1:L:313:PRO:CD   | 2.00                     | 0.91              |
| 1:P:483:ARG:O    | 1:P:487:PHE:N    | 2.03                     | 0.91              |
| 1:A:545:PHE:CZ   | 1:A:565:ALA:HA   | 2.04                     | 0.91              |
| 1:B:121:ALA:CB   | 1:C:276:SER:HB3  | 1.97                     | 0.91              |
| 1:B:557:LYS:HB3  | 1:B:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:C:382:PRO:HA   | 1:C:419:THR:HG22 | 1.52                     | 0.91              |
| 1:C:483:ARG:O    | 1:C:487:PHE:N    | 2.03                     | 0.91              |
| 1:E:557:LYS:O    | 1:E:1226:TYR:OH  | 1.86                     | 0.91              |
| 1:F:382:PRO:HA   | 1:F:419:THR:HG22 | 1.52                     | 0.91              |
| 1:F:483:ARG:O    | 1:F:487:PHE:N    | 2.03                     | 0.91              |
| 1:K:453:PHE:CZ   | 1:K:460:PRO:HB3  | 2.06                     | 0.91              |
| 1:L:382:PRO:HA   | 1:L:419:THR:HG22 | 1.52                     | 0.91              |
| 1:M:557:LYS:HB3  | 1:M:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:P:518:LEU:CD2  | 1:P:643:TYR:CD1  | 2.27                     | 0.91              |
| 1:A:557:LYS:HB3  | 1:A:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:D:453:PHE:CZ   | 1:D:460:PRO:HB3  | 2.06                     | 0.91              |
| 1:F:313:PRO:HG3  | 1:F:338:TRP:HE1  | 1.28                     | 0.91              |
| 1:H:518:LEU:O    | 1:H:522:LYS:N    | 2.04                     | 0.91              |
| 1:K:222:HIS:CG   | 1:L:198:LYS:HZ1  | 1.89                     | 0.91              |
| 1:N:557:LYS:HB3  | 1:N:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:O:518:LEU:O    | 1:O:522:LYS:N    | 2.04                     | 0.91              |
| 1:I:483:ARG:O    | 1:I:487:PHE:N    | 2.03                     | 0.91              |
| 1:B:453:PHE:CZ   | 1:B:460:PRO:HB3  | 2.06                     | 0.91              |
| 1:F:312:LEU:HD23 | 1:F:313:PRO:N    | 1.85                     | 0.91              |
| 1:I:312:LEU:HD23 | 1:I:313:PRO:N    | 1.85                     | 0.91              |
| 1:I:518:LEU:O    | 1:I:522:LYS:N    | 2.04                     | 0.91              |
| 1:K:557:LYS:O    | 1:K:1226:TYR:OH  | 1.86                     | 0.91              |
| 1:L:547:PRO:HB3  | 1:L:603:ILE:HG13 | 1.50                     | 0.91              |
| 1:M:453:PHE:CZ   | 1:M:460:PRO:HB3  | 2.06                     | 0.91              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:382:PRO:HA   | 1:D:419:THR:HG22 | 1.52                     | 0.91              |
| 1:D:557:LYS:O    | 1:D:1226:TYR:OH  | 1.86                     | 0.91              |
| 1:F:518:LEU:O    | 1:F:522:LYS:N    | 2.04                     | 0.91              |
| 1:B:518:LEU:O    | 1:B:522:LYS:N    | 2.04                     | 0.91              |
| 1:G:453:PHE:CZ   | 1:G:460:PRO:HB3  | 2.06                     | 0.91              |
| 1:I:382:PRO:HA   | 1:I:419:THR:HG22 | 1.52                     | 0.91              |
| 1:M:518:LEU:O    | 1:M:522:LYS:N    | 2.04                     | 0.91              |
| 1:A:312:LEU:HD23 | 1:A:313:PRO:N    | 1.85                     | 0.91              |
| 1:C:875:LEU:HD11 | 1:C:911:PHE:HD2  | 1.35                     | 0.91              |
| 1:I:557:LYS:HB3  | 1:I:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:K:382:PRO:HA   | 1:K:419:THR:HG22 | 1.52                     | 0.91              |
| 1:N:312:LEU:HD23 | 1:N:313:PRO:N    | 1.85                     | 0.91              |
| 1:O:508:TRP:C    | 1:O:606:GLY:HA3  | 1.96                     | 0.91              |
| 1:P:557:LYS:HB3  | 1:P:1226:TYR:CE1 | 2.05                     | 0.91              |
| 1:G:312:LEU:HD23 | 1:G:313:PRO:N    | 1.85                     | 0.90              |
| 1:H:508:TRP:C    | 1:H:606:GLY:HA3  | 1.97                     | 0.90              |
| 1:P:312:LEU:HD23 | 1:P:313:PRO:N    | 1.85                     | 0.90              |
| 1:P:453:PHE:CZ   | 1:P:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:D:518:LEU:O    | 1:D:522:LYS:N    | 2.04                     | 0.90              |
| 1:G:557:LYS:HB3  | 1:G:1226:TYR:CE1 | 2.05                     | 0.90              |
| 1:G:875:LEU:CD1  | 1:G:911:PHE:CD2  | 2.23                     | 0.90              |
| 1:A:453:PHE:CZ   | 1:A:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:E:382:PRO:HA   | 1:E:419:THR:HG22 | 1.52                     | 0.90              |
| 1:K:518:LEU:O    | 1:K:522:LYS:N    | 2.04                     | 0.90              |
| 1:L:557:LYS:HE3  | 1:L:1224:LEU:O   | 1.72                     | 0.90              |
| 1:N:518:LEU:O    | 1:N:522:LYS:N    | 2.04                     | 0.90              |
| 1:N:547:PRO:HB3  | 1:N:603:ILE:HG13 | 1.50                     | 0.90              |
| 1:P:312:LEU:HD23 | 1:P:313:PRO:CD   | 2.00                     | 0.90              |
| 1:P:557:LYS:HE3  | 1:P:1224:LEU:O   | 1.72                     | 0.90              |
| 1:A:518:LEU:O    | 1:A:522:LYS:N    | 2.04                     | 0.90              |
| 1:C:518:LEU:O    | 1:C:522:LYS:N    | 2.04                     | 0.90              |
| 1:E:557:LYS:HE3  | 1:E:1224:LEU:O   | 1.72                     | 0.90              |
| 1:F:312:LEU:HD23 | 1:F:313:PRO:CD   | 2.00                     | 0.90              |
| 1:F:508:TRP:C    | 1:F:606:GLY:HA3  | 1.97                     | 0.90              |
| 1:G:312:LEU:HD23 | 1:G:313:PRO:CD   | 2.00                     | 0.90              |
| 1:J:557:LYS:HE3  | 1:J:1224:LEU:O   | 1.72                     | 0.90              |
| 1:N:453:PHE:CZ   | 1:N:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:D:312:LEU:HD23 | 1:D:313:PRO:CD   | 2.00                     | 0.90              |
| 1:E:508:TRP:C    | 1:E:606:GLY:HA3  | 1.96                     | 0.90              |
| 1:F:557:LYS:HB3  | 1:F:1226:TYR:CE1 | 2.05                     | 0.90              |
| 1:G:518:LEU:O    | 1:G:522:LYS:N    | 2.04                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:557:LYS:HE3  | 1:G:1224:LEU:O   | 1.72                     | 0.90              |
| 1:H:453:PHE:CZ   | 1:H:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:I:453:PHE:CZ   | 1:I:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:J:508:TRP:C    | 1:J:606:GLY:HA3  | 1.97                     | 0.90              |
| 1:O:453:PHE:CZ   | 1:O:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:P:875:LEU:CD1  | 1:P:911:PHE:CD2  | 2.24                     | 0.90              |
| 1:A:547:PRO:HB3  | 1:A:603:ILE:HG13 | 1.50                     | 0.90              |
| 1:C:557:LYS:HE3  | 1:C:1224:LEU:O   | 1.72                     | 0.90              |
| 1:E:518:LEU:O    | 1:E:522:LYS:N    | 2.04                     | 0.90              |
| 1:I:312:LEU:HD23 | 1:I:313:PRO:CD   | 2.00                     | 0.90              |
| 1:I:508:TRP:C    | 1:I:606:GLY:HA3  | 1.96                     | 0.90              |
| 1:J:382:PRO:HA   | 1:J:419:THR:HG22 | 1.52                     | 0.90              |
| 1:M:508:TRP:C    | 1:M:606:GLY:HA3  | 1.96                     | 0.90              |
| 1:P:518:LEU:O    | 1:P:522:LYS:N    | 2.04                     | 0.90              |
| 1:B:508:TRP:C    | 1:B:606:GLY:HA3  | 1.97                     | 0.90              |
| 1:G:875:LEU:HD13 | 1:G:911:PHE:HE2  | 0.76                     | 0.90              |
| 1:K:312:LEU:HD23 | 1:K:313:PRO:CD   | 2.00                     | 0.90              |
| 1:H:312:LEU:HD23 | 1:H:313:PRO:N    | 1.85                     | 0.90              |
| 1:J:312:LEU:HD23 | 1:J:313:PRO:CD   | 2.00                     | 0.90              |
| 1:J:518:LEU:O    | 1:J:522:LYS:N    | 2.04                     | 0.90              |
| 1:L:518:LEU:O    | 1:L:522:LYS:N    | 2.04                     | 0.90              |
| 1:N:557:LYS:HE3  | 1:N:1224:LEU:O   | 1.72                     | 0.90              |
| 1:O:312:LEU:HD23 | 1:O:313:PRO:N    | 1.85                     | 0.90              |
| 1:C:453:PHE:CZ   | 1:C:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:F:916:LYS:CE   | 1:G:1177:TYR:CE2 | 2.55                     | 0.90              |
| 1:P:508:TRP:C    | 1:P:606:GLY:HA3  | 1.96                     | 0.90              |
| 1:A:557:LYS:HE3  | 1:A:1224:LEU:O   | 1.72                     | 0.90              |
| 1:E:312:LEU:HD23 | 1:E:313:PRO:CD   | 2.00                     | 0.90              |
| 1:F:453:PHE:CZ   | 1:F:460:PRO:HB3  | 2.06                     | 0.90              |
| 1:G:508:TRP:C    | 1:G:606:GLY:HA3  | 1.96                     | 0.90              |
| 1:H:557:LYS:HE3  | 1:H:1224:LEU:O   | 1.72                     | 0.90              |
| 1:P:875:LEU:HD13 | 1:P:911:PHE:HE2  | 0.76                     | 0.90              |
| 1:L:508:TRP:C    | 1:L:606:GLY:HA3  | 1.97                     | 0.89              |
| 1:O:557:LYS:HE3  | 1:O:1224:LEU:O   | 1.72                     | 0.89              |
| 1:B:557:LYS:HE3  | 1:B:1224:LEU:O   | 1.72                     | 0.89              |
| 1:C:508:TRP:C    | 1:C:606:GLY:HA3  | 1.97                     | 0.89              |
| 1:E:453:PHE:CZ   | 1:E:460:PRO:HB3  | 2.06                     | 0.89              |
| 1:J:453:PHE:CZ   | 1:J:460:PRO:HB3  | 2.06                     | 0.89              |
| 1:L:453:PHE:CZ   | 1:L:460:PRO:HB3  | 2.06                     | 0.89              |
| 1:A:508:TRP:C    | 1:A:606:GLY:HA3  | 1.97                     | 0.89              |
| 1:M:557:LYS:HE3  | 1:M:1224:LEU:O   | 1.72                     | 0.89              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:333:ASP:OD2  | 1:C:403:ASN:ND2 | 2.04                     | 0.89              |
| 1:M:252:ALA:O    | 1:M:253:TRP:C   | 2.15                     | 0.89              |
| 1:N:508:TRP:C    | 1:N:606:GLY:HA3 | 1.96                     | 0.89              |
| 1:B:252:ALA:O    | 1:B:253:TRP:C   | 2.15                     | 0.89              |
| 1:I:276:SER:CB   | 1:J:121:ALA:HB1 | 2.03                     | 0.89              |
| 1:A:518:LEU:CD2  | 1:A:643:TYR:CD1 | 2.27                     | 0.89              |
| 1:J:504:ASP:HB3  | 1:J:509:ASN:O   | 1.73                     | 0.89              |
| 1:A:252:ALA:O    | 1:A:253:TRP:C   | 2.15                     | 0.89              |
| 1:B:504:ASP:HB3  | 1:B:509:ASN:O   | 1.73                     | 0.89              |
| 1:C:505:SER:HG   | 1:C:513:SER:HG  | 1.12                     | 0.89              |
| 1:G:121:ALA:HB1  | 1:H:276:SER:CB  | 2.03                     | 0.89              |
| 1:I:557:LYS:HE3  | 1:I:1224:LEU:O  | 1.72                     | 0.89              |
| 1:J:252:ALA:O    | 1:J:253:TRP:C   | 2.15                     | 0.89              |
| 1:E:252:ALA:O    | 1:E:253:TRP:C   | 2.15                     | 0.89              |
| 1:I:504:ASP:HB3  | 1:I:509:ASN:O   | 1.73                     | 0.89              |
| 1:M:504:ASP:HB3  | 1:M:509:ASN:O   | 1.73                     | 0.89              |
| 1:N:518:LEU:CD2  | 1:N:643:TYR:CD1 | 2.27                     | 0.89              |
| 1:E:504:ASP:HB3  | 1:E:509:ASN:O   | 1.73                     | 0.88              |
| 1:H:504:ASP:HB3  | 1:H:509:ASN:O   | 1.73                     | 0.88              |
| 1:K:557:LYS:HE3  | 1:K:1224:LEU:O  | 1.72                     | 0.88              |
| 1:N:252:ALA:O    | 1:N:253:TRP:C   | 2.15                     | 0.88              |
| 1:O:504:ASP:HB3  | 1:O:509:ASN:O   | 1.73                     | 0.88              |
| 1:F:504:ASP:HB3  | 1:F:509:ASN:O   | 1.73                     | 0.88              |
| 1:C:875:LEU:CD1  | 1:C:911:PHE:CD2 | 2.23                     | 0.88              |
| 1:G:914:VAL:HG13 | 1:G:917:TYR:O   | 1.73                     | 0.88              |
| 1:K:222:HIS:CG   | 1:L:198:LYS:NZ  | 2.41                     | 0.88              |
| 1:H:914:VAL:HG13 | 1:H:917:TYR:O   | 1.74                     | 0.88              |
| 1:P:914:VAL:HG13 | 1:P:917:TYR:O   | 1.74                     | 0.88              |
| 1:D:252:ALA:O    | 1:D:253:TRP:C   | 2.15                     | 0.88              |
| 1:D:557:LYS:HE3  | 1:D:1224:LEU:O  | 1.72                     | 0.88              |
| 1:E:914:VAL:HG13 | 1:E:917:TYR:O   | 1.74                     | 0.88              |
| 1:F:557:LYS:HE3  | 1:F:1224:LEU:O  | 1.72                     | 0.88              |
| 1:J:914:VAL:HG13 | 1:J:917:TYR:O   | 1.73                     | 0.88              |
| 1:K:504:ASP:HB3  | 1:K:509:ASN:O   | 1.73                     | 0.88              |
| 1:O:914:VAL:HG13 | 1:O:917:TYR:O   | 1.74                     | 0.88              |
| 1:B:914:VAL:HG13 | 1:B:917:TYR:O   | 1.73                     | 0.88              |
| 1:K:252:ALA:O    | 1:K:253:TRP:C   | 2.15                     | 0.88              |
| 1:K:508:TRP:C    | 1:K:606:GLY:HA3 | 1.97                     | 0.88              |
| 1:M:914:VAL:HG13 | 1:M:917:TYR:O   | 1.73                     | 0.88              |
| 1:P:505:SER:HG   | 1:P:513:SER:HG  | 1.16                     | 0.88              |
| 1:C:252:ALA:O    | 1:C:253:TRP:C   | 2.15                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:508:TRP:C    | 1:D:606:GLY:HA3 | 1.97                     | 0.88              |
| 1:K:875:LEU:HD11 | 1:K:911:PHE:HD2 | 1.35                     | 0.88              |
| 1:N:276:SER:CB   | 1:O:121:ALA:HB1 | 2.02                     | 0.88              |
| 1:D:504:ASP:HB3  | 1:D:509:ASN:O   | 1.73                     | 0.88              |
| 1:L:505:SER:HG   | 1:L:513:SER:HG  | 1.12                     | 0.88              |
| 1:L:875:LEU:CD1  | 1:L:911:PHE:CD2 | 2.24                     | 0.88              |
| 1:M:276:SER:CB   | 1:N:121:ALA:HB1 | 2.03                     | 0.88              |
| 1:D:875:LEU:HD11 | 1:D:911:PHE:HD2 | 1.35                     | 0.88              |
| 1:G:504:ASP:HB3  | 1:G:509:ASN:O   | 1.73                     | 0.88              |
| 1:G:633:THR:HG21 | 1:G:642:THR:C   | 1.99                     | 0.88              |
| 1:L:442:SER:O    | 1:L:446:HIS:HD2 | 1.57                     | 0.88              |
| 1:P:504:ASP:HB3  | 1:P:509:ASN:O   | 1.73                     | 0.88              |
| 1:F:633:THR:HG21 | 1:F:642:THR:C   | 1.99                     | 0.87              |
| 1:G:505:SER:HG   | 1:G:513:SER:HG  | 1.16                     | 0.87              |
| 1:I:633:THR:HG21 | 1:I:642:THR:C   | 1.99                     | 0.87              |
| 1:L:252:ALA:O    | 1:L:253:TRP:C   | 2.15                     | 0.87              |
| 1:P:633:THR:HG21 | 1:P:642:THR:C   | 1.99                     | 0.87              |
| 1:A:504:ASP:HB3  | 1:A:509:ASN:O   | 1.73                     | 0.87              |
| 1:D:509:ASN:HD21 | 1:D:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:H:442:SER:O    | 1:H:446:HIS:HD2 | 1.57                     | 0.87              |
| 1:K:509:ASN:HD21 | 1:K:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:N:504:ASP:HB3  | 1:N:509:ASN:O   | 1.73                     | 0.87              |
| 1:C:442:SER:O    | 1:C:446:HIS:HD2 | 1.57                     | 0.87              |
| 1:G:509:ASN:HD21 | 1:G:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:H:633:THR:HG21 | 1:H:642:THR:C   | 1.99                     | 0.87              |
| 1:N:914:VAL:HG13 | 1:N:917:TYR:O   | 1.74                     | 0.87              |
| 1:O:442:SER:O    | 1:O:446:HIS:HD2 | 1.57                     | 0.87              |
| 1:P:509:ASN:HD21 | 1:P:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:C:504:ASP:HB3  | 1:C:509:ASN:O   | 1.73                     | 0.87              |
| 1:E:633:THR:HG21 | 1:E:642:THR:C   | 1.99                     | 0.87              |
| 1:J:505:SER:HG   | 1:J:513:SER:HG  | 1.17                     | 0.87              |
| 1:L:914:VAL:HG13 | 1:L:917:TYR:O   | 1.73                     | 0.87              |
| 1:N:509:ASN:HD21 | 1:N:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:O:633:THR:HG21 | 1:O:642:THR:C   | 1.99                     | 0.87              |
| 1:A:509:ASN:HD21 | 1:A:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:B:509:ASN:HD21 | 1:B:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:B:633:THR:HG21 | 1:B:642:THR:C   | 1.99                     | 0.87              |
| 1:F:509:ASN:HD21 | 1:F:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:F:914:VAL:HG13 | 1:F:917:TYR:O   | 1.74                     | 0.87              |
| 1:I:509:ASN:HD21 | 1:I:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:J:633:THR:HG21 | 1:J:642:THR:C   | 1.99                     | 0.87              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:252:ALA:O    | 1:O:253:TRP:C   | 2.15                     | 0.87              |
| 1:A:914:VAL:HG13 | 1:A:917:TYR:O   | 1.74                     | 0.87              |
| 1:H:252:ALA:O    | 1:H:253:TRP:C   | 2.15                     | 0.87              |
| 1:M:509:ASN:HD21 | 1:M:632:LEU:CD1 | 1.88                     | 0.87              |
| 1:M:633:THR:HG21 | 1:M:642:THR:C   | 1.99                     | 0.87              |
| 1:L:504:ASP:HB3  | 1:L:509:ASN:O   | 1.73                     | 0.87              |
| 1:N:875:LEU:HD11 | 1:N:911:PHE:HD2 | 1.34                     | 0.87              |
| 1:J:442:SER:O    | 1:J:446:HIS:HD2 | 1.57                     | 0.87              |
| 1:D:914:VAL:HG13 | 1:D:917:TYR:O   | 1.74                     | 0.86              |
| 1:E:442:SER:O    | 1:E:446:HIS:HD2 | 1.57                     | 0.86              |
| 1:I:914:VAL:HG13 | 1:I:917:TYR:O   | 1.74                     | 0.86              |
| 1:C:914:VAL:HG13 | 1:C:917:TYR:O   | 1.73                     | 0.86              |
| 1:F:442:SER:O    | 1:F:446:HIS:HD2 | 1.57                     | 0.86              |
| 1:L:509:ASN:HD21 | 1:L:632:LEU:CD1 | 1.88                     | 0.86              |
| 1:P:252:ALA:O    | 1:P:253:TRP:C   | 2.15                     | 0.86              |
| 1:G:252:ALA:O    | 1:G:253:TRP:C   | 2.15                     | 0.86              |
| 1:H:509:ASN:HD21 | 1:H:632:LEU:CD1 | 1.88                     | 0.86              |
| 1:K:914:VAL:HG13 | 1:K:917:TYR:O   | 1.74                     | 0.86              |
| 1:N:633:THR:HG21 | 1:N:642:THR:C   | 1.99                     | 0.86              |
| 1:A:633:THR:HG21 | 1:A:642:THR:C   | 1.99                     | 0.86              |
| 1:A:875:LEU:HD11 | 1:A:911:PHE:HD2 | 1.35                     | 0.86              |
| 1:D:633:THR:HG21 | 1:D:642:THR:C   | 1.99                     | 0.86              |
| 1:O:509:ASN:HD21 | 1:O:632:LEU:CD1 | 1.88                     | 0.86              |
| 1:C:509:ASN:HD21 | 1:C:632:LEU:CD1 | 1.88                     | 0.86              |
| 1:C:633:THR:HG21 | 1:C:642:THR:C   | 1.99                     | 0.86              |
| 1:E:509:ASN:HD21 | 1:E:632:LEU:CD1 | 1.88                     | 0.86              |
| 1:K:633:THR:HG21 | 1:K:642:THR:C   | 1.99                     | 0.86              |
| 1:F:252:ALA:O    | 1:F:253:TRP:C   | 2.15                     | 0.86              |
| 1:I:442:SER:O    | 1:I:446:HIS:HD2 | 1.57                     | 0.86              |
| 1:I:252:ALA:O    | 1:I:253:TRP:C   | 2.15                     | 0.86              |
| 1:J:403:ASN:ND2  | 1:K:333:ASP:OD2 | 2.09                     | 0.86              |
| 1:J:509:ASN:HD21 | 1:J:632:LEU:CD1 | 1.88                     | 0.86              |
| 1:L:633:THR:HG21 | 1:L:642:THR:C   | 1.99                     | 0.85              |
| 1:A:276:SER:CB   | 1:H:121:ALA:HB1 | 2.04                     | 0.85              |
| 1:E:505:SER:HG   | 1:E:513:SER:HG  | 1.18                     | 0.85              |
| 1:G:875:LEU:HD11 | 1:G:911:PHE:HD2 | 1.34                     | 0.85              |
| 1:H:505:SER:HG   | 1:H:513:SER:HG  | 1.06                     | 0.85              |
| 1:O:276:SER:CB   | 1:P:121:ALA:HB1 | 2.06                     | 0.85              |
| 1:P:875:LEU:HD11 | 1:P:911:PHE:HD2 | 1.35                     | 0.85              |
| 1:D:298:LYS:HG3  | 1:D:312:LEU:CD1 | 2.07                     | 0.85              |
| 1:K:298:LYS:HG3  | 1:K:312:LEU:CD1 | 2.07                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:442:SER:O    | 1:N:446:HIS:HD2  | 1.58                     | 0.85              |
| 1:L:633:THR:HG21 | 1:L:643:TYR:HA   | 1.59                     | 0.85              |
| 1:B:298:LYS:HG3  | 1:B:312:LEU:CD1  | 2.07                     | 0.85              |
| 1:C:633:THR:HG21 | 1:C:643:TYR:HA   | 1.59                     | 0.85              |
| 1:F:633:THR:HG21 | 1:F:643:TYR:HA   | 1.59                     | 0.85              |
| 1:G:298:LYS:HG3  | 1:G:312:LEU:CD1  | 2.07                     | 0.85              |
| 1:I:633:THR:HG21 | 1:I:643:TYR:HA   | 1.59                     | 0.85              |
| 1:P:298:LYS:HG3  | 1:P:312:LEU:CD1  | 2.07                     | 0.85              |
| 1:E:633:THR:HG21 | 1:E:643:TYR:HA   | 1.59                     | 0.85              |
| 1:F:300:LEU:HD13 | 2:F:1501:DTP:H2  | 1.59                     | 0.85              |
| 1:I:389:ILE:HD13 | 1:I:446:HIS:HE2  | 1.42                     | 0.85              |
| 1:I:463:LEU:HD22 | 1:I:467:PHE:CD2  | 2.12                     | 0.85              |
| 1:J:633:THR:HG21 | 1:J:643:TYR:HA   | 1.59                     | 0.85              |
| 1:M:298:LYS:HG3  | 1:M:312:LEU:CD1  | 2.07                     | 0.85              |
| 1:A:442:SER:O    | 1:A:446:HIS:HD2  | 1.57                     | 0.84              |
| 1:E:463:LEU:HD22 | 1:E:467:PHE:CD2  | 2.12                     | 0.84              |
| 1:I:300:LEU:HD13 | 2:I:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:P:442:SER:O    | 1:P:446:HIS:HD2  | 1.57                     | 0.84              |
| 1:A:298:LYS:HG3  | 1:A:312:LEU:CD1  | 2.07                     | 0.84              |
| 1:F:389:ILE:HD13 | 1:F:446:HIS:HE2  | 1.42                     | 0.84              |
| 1:F:463:LEU:HD22 | 1:F:467:PHE:CD2  | 2.12                     | 0.84              |
| 1:I:298:LYS:HG3  | 1:I:312:LEU:CD1  | 2.07                     | 0.84              |
| 1:N:298:LYS:HG3  | 1:N:312:LEU:CD1  | 2.07                     | 0.84              |
| 1:O:505:SER:HG   | 1:O:513:SER:HG   | 1.08                     | 0.84              |
| 1:D:633:THR:HG21 | 1:D:643:TYR:HA   | 1.59                     | 0.84              |
| 1:F:298:LYS:HG3  | 1:F:312:LEU:CD1  | 2.07                     | 0.84              |
| 1:J:463:LEU:HD22 | 1:J:467:PHE:CD2  | 2.12                     | 0.84              |
| 1:K:300:LEU:HD13 | 2:K:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:D:389:ILE:HD13 | 1:D:446:HIS:HE2  | 1.42                     | 0.84              |
| 1:K:389:ILE:HD13 | 1:K:446:HIS:HE2  | 1.42                     | 0.84              |
| 1:K:633:THR:HG21 | 1:K:643:TYR:HA   | 1.59                     | 0.84              |
| 1:L:300:LEU:HD13 | 2:L:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:O:298:LYS:HG3  | 1:O:312:LEU:CD1  | 2.07                     | 0.84              |
| 1:C:300:LEU:HD13 | 2:C:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:D:300:LEU:HD13 | 2:D:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:D:463:LEU:HD22 | 1:D:467:PHE:CD2  | 2.12                     | 0.84              |
| 1:E:492:LEU:CD2  | 1:E:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:J:492:LEU:CD2  | 1:J:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:K:463:LEU:HD22 | 1:K:467:PHE:CD2  | 2.12                     | 0.84              |
| 1:P:492:LEU:CD2  | 1:P:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:A:633:THR:HG21 | 1:A:643:TYR:HA   | 1.59                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:134:LEU:HD22 | 1:G:164:VAL:HG11 | 1.60                     | 0.84              |
| 1:G:442:SER:O    | 1:G:446:HIS:HD2  | 1.57                     | 0.84              |
| 1:G:492:LEU:CD2  | 1:G:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:H:298:LYS:HG3  | 1:H:312:LEU:CD1  | 2.07                     | 0.84              |
| 1:N:633:THR:HG21 | 1:N:643:TYR:HA   | 1.59                     | 0.84              |
| 1:E:300:LEU:HD13 | 2:E:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:E:875:LEU:HD11 | 1:E:911:PHE:HD2  | 1.35                     | 0.84              |
| 1:G:300:LEU:HD13 | 2:G:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:J:875:LEU:HD11 | 1:J:911:PHE:HD2  | 1.34                     | 0.84              |
| 1:M:492:LEU:CD2  | 1:M:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:O:134:LEU:HD22 | 1:O:164:VAL:HG11 | 1.59                     | 0.84              |
| 1:P:134:LEU:HD22 | 1:P:164:VAL:HG11 | 1.60                     | 0.84              |
| 1:B:492:LEU:CD2  | 1:B:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:J:300:LEU:HD13 | 2:J:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:M:505:SER:HG   | 1:M:513:SER:HG   | 1.21                     | 0.84              |
| 1:P:300:LEU:HD13 | 2:P:1501:DTP:H2  | 1.60                     | 0.84              |
| 1:D:492:LEU:CD2  | 1:D:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:G:633:THR:HG21 | 1:G:643:TYR:HA   | 1.59                     | 0.84              |
| 1:H:134:LEU:HD22 | 1:H:164:VAL:HG11 | 1.60                     | 0.84              |
| 1:H:389:ILE:HD13 | 1:H:446:HIS:HE2  | 1.42                     | 0.84              |
| 1:K:492:LEU:CD2  | 1:K:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:L:492:LEU:CD2  | 1:L:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:N:389:ILE:HD13 | 1:N:446:HIS:HE2  | 1.42                     | 0.84              |
| 1:O:492:LEU:CD2  | 1:O:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:A:389:ILE:HD13 | 1:A:446:HIS:HE2  | 1.42                     | 0.84              |
| 1:A:492:LEU:CD2  | 1:A:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:B:389:ILE:HD13 | 1:B:446:HIS:HE2  | 1.42                     | 0.84              |
| 1:B:442:SER:O    | 1:B:446:HIS:HD2  | 1.57                     | 0.84              |
| 1:C:492:LEU:CD2  | 1:C:562:LEU:HD23 | 2.08                     | 0.84              |
| 1:E:298:LYS:HG3  | 1:E:312:LEU:CD1  | 2.07                     | 0.84              |
| 1:K:249:ASN:HB2  | 1:K:252:ALA:HB2  | 1.60                     | 0.84              |
| 1:O:633:THR:HG21 | 1:O:643:TYR:HA   | 1.59                     | 0.84              |
| 1:A:463:LEU:HD22 | 1:A:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:B:300:LEU:HD13 | 2:B:1501:DTP:H2  | 1.59                     | 0.83              |
| 1:D:249:ASN:HB2  | 1:D:252:ALA:HB2  | 1.60                     | 0.83              |
| 1:F:492:LEU:CD2  | 1:F:562:LEU:HD23 | 2.08                     | 0.83              |
| 1:H:492:LEU:CD2  | 1:H:562:LEU:HD23 | 2.08                     | 0.83              |
| 1:N:492:LEU:CD2  | 1:N:562:LEU:HD23 | 2.08                     | 0.83              |
| 1:P:633:THR:HG21 | 1:P:643:TYR:HA   | 1.59                     | 0.83              |
| 1:F:134:LEU:HD22 | 1:F:164:VAL:HG11 | 1.60                     | 0.83              |
| 1:G:249:ASN:HB2  | 1:G:252:ALA:HB2  | 1.60                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:134:LEU:HD22 | 1:I:164:VAL:HG11 | 1.60                     | 0.83              |
| 1:M:389:ILE:HD13 | 1:M:446:HIS:HE2  | 1.42                     | 0.83              |
| 1:M:463:LEU:HD22 | 1:M:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:N:463:LEU:HD22 | 1:N:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:P:249:ASN:HB2  | 1:P:252:ALA:HB2  | 1.60                     | 0.83              |
| 1:B:463:LEU:HD22 | 1:B:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:C:298:LYS:HG3  | 1:C:312:LEU:CD1  | 2.07                     | 0.83              |
| 1:H:548:LYS:HZ2  | 1:H:601:GLN:HA   | 1.43                     | 0.83              |
| 1:H:633:THR:HG21 | 1:H:643:TYR:HA   | 1.59                     | 0.83              |
| 1:I:492:LEU:CD2  | 1:I:562:LEU:HD23 | 2.08                     | 0.83              |
| 1:J:298:LYS:HG3  | 1:J:312:LEU:CD1  | 2.07                     | 0.83              |
| 1:O:389:ILE:HD13 | 1:O:446:HIS:HE2  | 1.42                     | 0.83              |
| 1:O:548:LYS:HZ2  | 1:O:601:GLN:HA   | 1.43                     | 0.83              |
| 1:B:505:SER:HG   | 1:B:513:SER:HG   | 1.22                     | 0.83              |
| 1:E:378:SER:CA   | 1:E:422:ILE:HD12 | 2.09                     | 0.83              |
| 1:F:875:LEU:HD11 | 1:F:911:PHE:HD2  | 1.35                     | 0.83              |
| 1:H:463:LEU:HD22 | 1:H:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:I:249:ASN:HB2  | 1:I:252:ALA:HB2  | 1.60                     | 0.83              |
| 1:L:298:LYS:HG3  | 1:L:312:LEU:CD1  | 2.07                     | 0.83              |
| 1:L:463:LEU:HD22 | 1:L:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:M:300:LEU:HD13 | 2:M:1501:DTP:H2  | 1.60                     | 0.83              |
| 1:C:463:LEU:HD22 | 1:C:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:J:378:SER:CA   | 1:J:422:ILE:HD12 | 2.09                     | 0.83              |
| 1:P:463:LEU:HD22 | 1:P:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:F:249:ASN:HB2  | 1:F:252:ALA:HB2  | 1.60                     | 0.83              |
| 1:G:463:LEU:HD22 | 1:G:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:H:875:LEU:HD11 | 1:H:911:PHE:HD2  | 1.35                     | 0.83              |
| 1:O:875:LEU:HD11 | 1:O:911:PHE:HD2  | 1.35                     | 0.83              |
| 1:E:194:GLU:OE2  | 1:F:216:ASN:ND2  | 2.10                     | 0.83              |
| 1:K:442:SER:O    | 1:K:446:HIS:HD2  | 1.58                     | 0.83              |
| 1:L:914:VAL:CG1  | 1:L:917:TYR:O    | 2.27                     | 0.83              |
| 1:O:300:LEU:HD13 | 2:O:1501:DTP:H2  | 1.60                     | 0.83              |
| 1:O:463:LEU:HD22 | 1:O:467:PHE:CD2  | 2.12                     | 0.83              |
| 1:G:914:VAL:CG1  | 1:G:917:TYR:O    | 2.27                     | 0.83              |
| 1:N:134:LEU:HD22 | 1:N:164:VAL:HG11 | 1.60                     | 0.83              |
| 1:C:914:VAL:CG1  | 1:C:917:TYR:O    | 2.27                     | 0.83              |
| 1:F:622:LEU:CB   | 1:F:634:ASP:HB2  | 2.09                     | 0.83              |
| 1:H:300:LEU:HD13 | 2:H:1501:DTP:H2  | 1.60                     | 0.83              |
| 1:I:914:VAL:CG1  | 1:I:917:TYR:O    | 2.27                     | 0.83              |
| 1:M:622:LEU:CB   | 1:M:634:ASP:HB2  | 2.09                     | 0.83              |
| 1:A:300:LEU:HD13 | 2:A:1501:DTP:H2  | 1.60                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:622:LEU:CB   | 1:B:634:ASP:HB2  | 2.09                     | 0.83              |
| 1:D:914:VAL:CG1  | 1:D:917:TYR:O    | 2.27                     | 0.83              |
| 1:F:914:VAL:CG1  | 1:F:917:TYR:O    | 2.27                     | 0.83              |
| 1:I:622:LEU:CB   | 1:I:634:ASP:HB2  | 2.09                     | 0.83              |
| 1:P:378:SER:CA   | 1:P:422:ILE:HD12 | 2.09                     | 0.83              |
| 1:P:914:VAL:CG1  | 1:P:917:TYR:O    | 2.27                     | 0.83              |
| 1:A:134:LEU:HD22 | 1:A:164:VAL:HG11 | 1.60                     | 0.82              |
| 1:A:186:CYS:O    | 1:A:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:G:378:SER:CA   | 1:G:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:J:186:CYS:O    | 1:J:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:K:914:VAL:CG1  | 1:K:917:TYR:O    | 2.27                     | 0.82              |
| 1:N:186:CYS:O    | 1:N:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:N:300:LEU:HD13 | 2:N:1501:DTP:H2  | 1.60                     | 0.82              |
| 1:C:389:ILE:HD13 | 1:C:446:HIS:HE2  | 1.42                     | 0.82              |
| 1:C:622:LEU:CB   | 1:C:634:ASP:HB2  | 2.09                     | 0.82              |
| 1:D:442:SER:O    | 1:D:446:HIS:HD2  | 1.57                     | 0.82              |
| 1:E:186:CYS:O    | 1:E:249:ASN:ND2  | 2.13                     | 0.82              |
| 1:E:413:LYS:HD3  | 1:E:422:ILE:O    | 1.79                     | 0.82              |
| 1:F:186:CYS:O    | 1:F:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:H:413:LYS:HD3  | 1:H:422:ILE:O    | 1.79                     | 0.82              |
| 1:H:457:ASP:OD1  | 1:H:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:I:186:CYS:O    | 1:I:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:I:875:LEU:HD11 | 1:I:911:PHE:HD2  | 1.35                     | 0.82              |
| 1:M:413:LYS:HD3  | 1:M:422:ILE:O    | 1.79                     | 0.82              |
| 1:M:457:ASP:OD1  | 1:M:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:N:622:LEU:CB   | 1:N:634:ASP:HB2  | 2.09                     | 0.82              |
| 1:O:413:LYS:HD3  | 1:O:422:ILE:O    | 1.79                     | 0.82              |
| 1:A:249:ASN:HB2  | 1:A:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:A:622:LEU:CB   | 1:A:634:ASP:HB2  | 2.09                     | 0.82              |
| 1:B:413:LYS:HD3  | 1:B:422:ILE:O    | 1.79                     | 0.82              |
| 1:B:457:ASP:OD1  | 1:B:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:G:186:CYS:O    | 1:G:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:G:622:LEU:CB   | 1:G:634:ASP:HB2  | 2.09                     | 0.82              |
| 1:H:622:LEU:CB   | 1:H:634:ASP:HB2  | 2.09                     | 0.82              |
| 1:J:413:LYS:HD3  | 1:J:422:ILE:O    | 1.79                     | 0.82              |
| 1:L:378:SER:CA   | 1:L:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:L:457:ASP:OD1  | 1:L:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:L:622:LEU:CB   | 1:L:634:ASP:HB2  | 2.09                     | 0.82              |
| 1:O:457:ASP:OD1  | 1:O:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:P:186:CYS:O    | 1:P:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:P:622:LEU:CB   | 1:P:634:ASP:HB2  | 2.09                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:249:ASN:HB2  | 1:B:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:C:134:LEU:HD22 | 1:C:164:VAL:HG11 | 1.60                     | 0.82              |
| 1:C:413:LYS:HD3  | 1:C:422:ILE:O    | 1.79                     | 0.82              |
| 1:M:249:ASN:HB2  | 1:M:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:N:249:ASN:HB2  | 1:N:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:A:548:LYS:HZ2  | 1:A:601:GLN:HA   | 1.43                     | 0.82              |
| 1:B:517:THR:O    | 1:B:520:GLN:N    | 2.13                     | 0.82              |
| 1:C:186:CYS:O    | 1:C:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:C:457:ASP:OD1  | 1:C:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:D:505:SER:HG   | 1:D:513:SER:HG   | 1.26                     | 0.82              |
| 1:D:875:LEU:CD1  | 1:D:911:PHE:CD2  | 2.24                     | 0.82              |
| 1:E:249:ASN:HB2  | 1:E:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:K:457:ASP:OD1  | 1:K:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:L:389:ILE:HD13 | 1:L:446:HIS:HE2  | 1.42                     | 0.82              |
| 1:L:413:LYS:HD3  | 1:L:422:ILE:O    | 1.79                     | 0.82              |
| 1:M:517:THR:O    | 1:M:520:GLN:N    | 2.13                     | 0.82              |
| 1:M:914:VAL:CG1  | 1:M:917:TYR:O    | 2.27                     | 0.82              |
| 1:O:622:LEU:CB   | 1:O:634:ASP:HB2  | 2.09                     | 0.82              |
| 1:D:186:CYS:O    | 1:D:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:D:457:ASP:OD1  | 1:D:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:E:389:ILE:HD13 | 1:E:446:HIS:HE2  | 1.42                     | 0.82              |
| 1:F:517:THR:O    | 1:F:520:GLN:N    | 2.13                     | 0.82              |
| 1:H:517:THR:O    | 1:H:520:GLN:N    | 2.13                     | 0.82              |
| 1:I:378:SER:CA   | 1:I:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:I:457:ASP:OD1  | 1:I:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:K:186:CYS:O    | 1:K:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:L:186:CYS:O    | 1:L:249:ASN:ND2  | 2.12                     | 0.82              |
| 1:N:252:ALA:O    | 1:N:254:ASN:N    | 2.13                     | 0.82              |
| 1:O:249:ASN:HB2  | 1:O:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:O:517:THR:O    | 1:O:520:GLN:N    | 2.13                     | 0.82              |
| 1:A:252:ALA:O    | 1:A:254:ASN:N    | 2.13                     | 0.82              |
| 1:A:378:SER:CA   | 1:A:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:B:914:VAL:CG1  | 1:B:917:TYR:O    | 2.27                     | 0.82              |
| 1:D:134:LEU:HD22 | 1:D:164:VAL:HG11 | 1.60                     | 0.82              |
| 1:E:134:LEU:HD22 | 1:E:164:VAL:HG11 | 1.60                     | 0.82              |
| 1:F:457:ASP:OD1  | 1:F:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:H:249:ASN:HB2  | 1:H:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:H:914:VAL:CG1  | 1:H:917:TYR:O    | 2.27                     | 0.82              |
| 1:K:134:LEU:HD22 | 1:K:164:VAL:HG11 | 1.60                     | 0.82              |
| 1:L:134:LEU:HD22 | 1:L:164:VAL:HG11 | 1.60                     | 0.82              |
| 1:N:378:SER:CA   | 1:N:422:ILE:HD12 | 2.09                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:548:LYS:HZ2  | 1:N:601:GLN:HA   | 1.43                     | 0.82              |
| 1:O:378:SER:CA   | 1:O:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:A:312:LEU:HD23 | 1:A:313:PRO:HD2  | 1.62                     | 0.82              |
| 1:B:252:ALA:O    | 1:B:254:ASN:N    | 2.13                     | 0.82              |
| 1:B:633:THR:HG21 | 1:B:643:TYR:HA   | 1.59                     | 0.82              |
| 1:C:378:SER:CA   | 1:C:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:D:252:ALA:O    | 1:D:254:ASN:N    | 2.13                     | 0.82              |
| 1:H:378:SER:CA   | 1:H:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:I:517:THR:O    | 1:I:520:GLN:N    | 2.13                     | 0.82              |
| 1:J:914:VAL:CG1  | 1:J:917:TYR:O    | 2.27                     | 0.82              |
| 1:K:508:TRP:CE3  | 1:K:927:GLN:C    | 2.58                     | 0.82              |
| 1:K:875:LEU:CD1  | 1:K:911:PHE:CD2  | 2.23                     | 0.82              |
| 1:L:517:THR:O    | 1:L:520:GLN:N    | 2.13                     | 0.82              |
| 1:M:252:ALA:O    | 1:M:254:ASN:N    | 2.13                     | 0.82              |
| 1:N:312:LEU:HD23 | 1:N:313:PRO:HD2  | 1.62                     | 0.82              |
| 1:D:508:TRP:CE3  | 1:D:927:GLN:C    | 2.58                     | 0.82              |
| 1:E:914:VAL:CG1  | 1:E:917:TYR:O    | 2.27                     | 0.82              |
| 1:G:517:THR:O    | 1:G:520:GLN:N    | 2.13                     | 0.82              |
| 1:H:492:LEU:HD23 | 1:H:562:LEU:HD23 | 1.62                     | 0.82              |
| 1:K:252:ALA:O    | 1:K:254:ASN:N    | 2.13                     | 0.82              |
| 1:K:517:THR:O    | 1:K:520:GLN:N    | 2.13                     | 0.82              |
| 1:N:507:ALA:O    | 1:N:608:ASN:HB2  | 1.80                     | 0.82              |
| 1:N:914:VAL:CG1  | 1:N:917:TYR:O    | 2.27                     | 0.82              |
| 1:O:492:LEU:HD23 | 1:O:562:LEU:HD23 | 1.62                     | 0.82              |
| 1:O:914:VAL:CG1  | 1:O:917:TYR:O    | 2.27                     | 0.82              |
| 1:P:517:THR:O    | 1:P:520:GLN:N    | 2.13                     | 0.82              |
| 1:A:507:ALA:O    | 1:A:608:ASN:HB2  | 1.80                     | 0.82              |
| 1:A:914:VAL:CG1  | 1:A:917:TYR:O    | 2.27                     | 0.82              |
| 1:B:508:TRP:CE3  | 1:B:927:GLN:C    | 2.58                     | 0.82              |
| 1:C:508:TRP:CE3  | 1:C:927:GLN:C    | 2.58                     | 0.82              |
| 1:C:517:THR:O    | 1:C:520:GLN:N    | 2.13                     | 0.82              |
| 1:D:378:SER:CA   | 1:D:422:ILE:HD12 | 2.09                     | 0.82              |
| 1:D:517:THR:O    | 1:D:520:GLN:N    | 2.13                     | 0.82              |
| 1:E:252:ALA:O    | 1:E:254:ASN:N    | 2.13                     | 0.82              |
| 1:E:457:ASP:OD1  | 1:E:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:H:252:ALA:O    | 1:H:254:ASN:N    | 2.13                     | 0.82              |
| 1:J:134:LEU:HD22 | 1:J:164:VAL:HG11 | 1.60                     | 0.82              |
| 1:J:249:ASN:HB2  | 1:J:252:ALA:HB2  | 1.60                     | 0.82              |
| 1:J:457:ASP:OD1  | 1:J:587:ARG:HB2  | 1.80                     | 0.82              |
| 1:M:633:THR:HG21 | 1:M:643:TYR:HA   | 1.59                     | 0.82              |
| 1:O:507:ALA:O    | 1:O:608:ASN:HB2  | 1.80                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:378:SER:CA   | 1:F:422:ILE:HD12 | 2.09                     | 0.81              |
| 1:I:413:LYS:HD3  | 1:I:422:ILE:O    | 1.79                     | 0.81              |
| 1:J:252:ALA:O    | 1:J:254:ASN:N    | 2.13                     | 0.81              |
| 1:J:389:ILE:HD13 | 1:J:446:HIS:HE2  | 1.42                     | 0.81              |
| 1:K:378:SER:CA   | 1:K:422:ILE:HD12 | 2.09                     | 0.81              |
| 1:L:604:ASN:HD22 | 1:L:929:VAL:H    | 1.28                     | 0.81              |
| 1:M:508:TRP:CE3  | 1:M:927:GLN:C    | 2.58                     | 0.81              |
| 1:O:186:CYS:O    | 1:O:249:ASN:ND2  | 2.12                     | 0.81              |
| 1:O:252:ALA:O    | 1:O:254:ASN:N    | 2.13                     | 0.81              |
| 1:B:186:CYS:O    | 1:B:249:ASN:ND2  | 2.12                     | 0.81              |
| 1:C:604:ASN:HD22 | 1:C:929:VAL:H    | 1.28                     | 0.81              |
| 1:H:186:CYS:O    | 1:H:249:ASN:ND2  | 2.12                     | 0.81              |
| 1:K:413:LYS:HD3  | 1:K:422:ILE:O    | 1.79                     | 0.81              |
| 1:L:508:TRP:CE3  | 1:L:927:GLN:C    | 2.58                     | 0.81              |
| 1:M:186:CYS:O    | 1:M:249:ASN:ND2  | 2.12                     | 0.81              |
| 1:A:508:TRP:CE3  | 1:A:927:GLN:C    | 2.58                     | 0.81              |
| 1:D:413:LYS:HD3  | 1:D:422:ILE:O    | 1.79                     | 0.81              |
| 1:F:413:LYS:HD3  | 1:F:422:ILE:O    | 1.79                     | 0.81              |
| 1:F:508:TRP:CA   | 1:F:606:GLY:CA   | 2.48                     | 0.81              |
| 1:H:507:ALA:O    | 1:H:608:ASN:HB2  | 1.80                     | 0.81              |
| 1:K:507:ALA:O    | 1:K:608:ASN:HB2  | 1.80                     | 0.81              |
| 1:K:622:LEU:CB   | 1:K:634:ASP:HB2  | 2.09                     | 0.81              |
| 1:L:252:ALA:O    | 1:L:254:ASN:N    | 2.13                     | 0.81              |
| 1:L:875:LEU:HD11 | 1:L:911:PHE:HD2  | 1.34                     | 0.81              |
| 1:P:492:LEU:HD23 | 1:P:562:LEU:HD23 | 1.62                     | 0.81              |
| 1:P:508:TRP:CE3  | 1:P:927:GLN:C    | 2.58                     | 0.81              |
| 1:B:134:LEU:HD22 | 1:B:164:VAL:HG11 | 1.60                     | 0.81              |
| 1:G:492:LEU:HD23 | 1:G:562:LEU:HD23 | 1.62                     | 0.81              |
| 1:G:508:TRP:CE3  | 1:G:927:GLN:C    | 2.58                     | 0.81              |
| 1:M:548:LYS:HZ2  | 1:M:601:GLN:HA   | 1.45                     | 0.81              |
| 1:N:508:TRP:CE3  | 1:N:927:GLN:C    | 2.58                     | 0.81              |
| 1:O:312:LEU:HD23 | 1:O:313:PRO:HD2  | 1.62                     | 0.81              |
| 1:A:413:LYS:HD3  | 1:A:422:ILE:O    | 1.79                     | 0.81              |
| 1:A:508:TRP:CA   | 1:A:606:GLY:CA   | 2.48                     | 0.81              |
| 1:C:194:GLU:OE2  | 1:D:216:ASN:ND2  | 2.14                     | 0.81              |
| 1:D:507:ALA:O    | 1:D:608:ASN:HB2  | 1.80                     | 0.81              |
| 1:D:622:LEU:CB   | 1:D:634:ASP:HB2  | 2.09                     | 0.81              |
| 1:G:413:LYS:HD3  | 1:G:422:ILE:O    | 1.79                     | 0.81              |
| 1:H:312:LEU:HD23 | 1:H:313:PRO:HD2  | 1.62                     | 0.81              |
| 1:M:134:LEU:HD22 | 1:M:164:VAL:HG11 | 1.60                     | 0.81              |
| 1:M:312:LEU:HD23 | 1:M:313:PRO:HD2  | 1.62                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:548:LYS:HZ2  | 1:N:601:GLN:CA   | 1.94                     | 0.81              |
| 1:P:413:LYS:HD3  | 1:P:422:ILE:O    | 1.79                     | 0.81              |
| 1:A:457:ASP:OD1  | 1:A:587:ARG:HB2  | 1.79                     | 0.81              |
| 1:A:548:LYS:HZ2  | 1:A:601:GLN:CA   | 1.94                     | 0.81              |
| 1:B:507:ALA:O    | 1:B:608:ASN:HB2  | 1.80                     | 0.81              |
| 1:C:249:ASN:HB2  | 1:C:252:ALA:HB2  | 1.60                     | 0.81              |
| 1:C:252:ALA:O    | 1:C:254:ASN:N    | 2.13                     | 0.81              |
| 1:F:252:ALA:O    | 1:F:254:ASN:N    | 2.13                     | 0.81              |
| 1:H:548:LYS:HZ2  | 1:H:601:GLN:CA   | 1.94                     | 0.81              |
| 1:L:249:ASN:HB2  | 1:L:252:ALA:HB2  | 1.60                     | 0.81              |
| 1:B:312:LEU:HD23 | 1:B:313:PRO:HD2  | 1.62                     | 0.81              |
| 1:B:378:SER:CA   | 1:B:422:ILE:HD12 | 2.09                     | 0.81              |
| 1:E:517:THR:O    | 1:E:520:GLN:N    | 2.13                     | 0.81              |
| 1:I:508:TRP:CA   | 1:I:606:GLY:CA   | 2.48                     | 0.81              |
| 1:J:517:THR:O    | 1:J:520:GLN:N    | 2.13                     | 0.81              |
| 1:M:378:SER:CA   | 1:M:422:ILE:HD12 | 2.09                     | 0.81              |
| 1:M:507:ALA:O    | 1:M:608:ASN:HB2  | 1.80                     | 0.81              |
| 1:N:508:TRP:CA   | 1:N:606:GLY:CA   | 2.48                     | 0.81              |
| 1:E:492:LEU:HD23 | 1:E:562:LEU:HD23 | 1.62                     | 0.81              |
| 1:F:508:TRP:CE3  | 1:F:927:GLN:C    | 2.58                     | 0.81              |
| 1:J:492:LEU:HD23 | 1:J:562:LEU:HD23 | 1.62                     | 0.81              |
| 1:L:440:HIS:O    | 1:L:444:VAL:N    | 2.14                     | 0.81              |
| 1:N:413:LYS:HD3  | 1:N:422:ILE:O    | 1.79                     | 0.81              |
| 1:O:548:LYS:HZ2  | 1:O:601:GLN:CA   | 1.94                     | 0.81              |
| 1:A:440:HIS:O    | 1:A:444:VAL:N    | 2.14                     | 0.81              |
| 1:I:252:ALA:O    | 1:I:254:ASN:N    | 2.13                     | 0.81              |
| 1:J:507:ALA:O    | 1:J:608:ASN:HB2  | 1.80                     | 0.81              |
| 1:N:440:HIS:O    | 1:N:444:VAL:N    | 2.14                     | 0.81              |
| 1:N:457:ASP:OD1  | 1:N:587:ARG:HB2  | 1.80                     | 0.81              |
| 1:N:517:THR:O    | 1:N:520:GLN:N    | 2.13                     | 0.81              |
| 1:A:517:THR:O    | 1:A:520:GLN:N    | 2.13                     | 0.81              |
| 1:C:440:HIS:O    | 1:C:444:VAL:N    | 2.14                     | 0.81              |
| 1:E:354:GLU:OE1  | 1:E:430:LYS:HE3  | 1.81                     | 0.81              |
| 1:E:604:ASN:HD22 | 1:E:929:VAL:H    | 1.28                     | 0.81              |
| 1:G:252:ALA:O    | 1:G:254:ASN:N    | 2.13                     | 0.81              |
| 1:G:548:LYS:HZ2  | 1:G:601:GLN:HA   | 1.45                     | 0.81              |
| 1:I:508:TRP:CE3  | 1:I:927:GLN:C    | 2.58                     | 0.81              |
| 1:J:312:LEU:HD23 | 1:J:313:PRO:HD2  | 1.62                     | 0.81              |
| 1:J:354:GLU:OE1  | 1:J:430:LYS:HE3  | 1.81                     | 0.81              |
| 1:P:252:ALA:O    | 1:P:254:ASN:N    | 2.13                     | 0.81              |
| 1:P:457:ASP:OD1  | 1:P:587:ARG:HB2  | 1.80                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:507:ALA:O    | 1:P:608:ASN:HB2  | 1.80                     | 0.81              |
| 1:E:507:ALA:O    | 1:E:608:ASN:HB2  | 1.80                     | 0.80              |
| 1:G:457:ASP:OD1  | 1:G:587:ARG:HB2  | 1.80                     | 0.80              |
| 1:G:507:ALA:O    | 1:G:608:ASN:HB2  | 1.80                     | 0.80              |
| 1:J:604:ASN:HD22 | 1:J:929:VAL:H    | 1.28                     | 0.80              |
| 1:L:507:ALA:O    | 1:L:608:ASN:HB2  | 1.80                     | 0.80              |
| 1:M:508:TRP:CA   | 1:M:606:GLY:CA   | 2.48                     | 0.80              |
| 1:P:548:LYS:HZ2  | 1:P:601:GLN:HA   | 1.46                     | 0.80              |
| 1:B:508:TRP:CA   | 1:B:606:GLY:CA   | 2.48                     | 0.80              |
| 1:F:492:LEU:HD23 | 1:F:562:LEU:HD23 | 1.62                     | 0.80              |
| 1:C:402:VAL:O    | 1:C:406:HIS:N    | 2.14                     | 0.80              |
| 1:E:312:LEU:HD23 | 1:E:313:PRO:HD2  | 1.62                     | 0.80              |
| 1:A:604:ASN:HD22 | 1:A:929:VAL:H    | 1.28                     | 0.80              |
| 1:H:508:TRP:CE3  | 1:H:927:GLN:C    | 2.58                     | 0.80              |
| 1:N:604:ASN:HD22 | 1:N:929:VAL:H    | 1.28                     | 0.80              |
| 1:O:508:TRP:CE3  | 1:O:927:GLN:C    | 2.58                     | 0.80              |
| 1:B:604:ASN:HD22 | 1:B:929:VAL:H    | 1.28                     | 0.80              |
| 1:F:545:PHE:O    | 1:F:549:ILE:N    | 2.13                     | 0.80              |
| 1:I:354:GLU:OE1  | 1:I:430:LYS:HE3  | 1.81                     | 0.80              |
| 1:I:492:LEU:HD23 | 1:I:562:LEU:HD23 | 1.62                     | 0.80              |
| 1:I:915:TYR:O    | 1:I:916:LYS:HB2  | 1.82                     | 0.80              |
| 1:K:313:PRO:HG3  | 1:K:338:TRP:CE2  | 2.17                     | 0.80              |
| 1:L:402:VAL:O    | 1:L:406:HIS:N    | 2.14                     | 0.80              |
| 1:B:425:ILE:O    | 1:B:429:LEU:N    | 2.15                     | 0.80              |
| 1:C:507:ALA:O    | 1:C:608:ASN:HB2  | 1.80                     | 0.80              |
| 1:C:915:TYR:O    | 1:C:916:LYS:HB2  | 1.82                     | 0.80              |
| 1:D:313:PRO:HG3  | 1:D:338:TRP:CE2  | 2.17                     | 0.80              |
| 1:F:915:TYR:O    | 1:F:916:LYS:HB2  | 1.82                     | 0.80              |
| 1:I:373:SER:HB3  | 1:I:433:LEU:CD1  | 2.12                     | 0.80              |
| 1:M:425:ILE:O    | 1:M:429:LEU:N    | 2.15                     | 0.80              |
| 1:D:312:LEU:HD23 | 1:D:313:PRO:HD2  | 1.62                     | 0.80              |
| 1:E:508:TRP:CE3  | 1:E:927:GLN:C    | 2.58                     | 0.80              |
| 1:E:915:TYR:O    | 1:E:916:LYS:HB2  | 1.82                     | 0.80              |
| 1:F:373:SER:HB3  | 1:F:433:LEU:CD1  | 2.12                     | 0.80              |
| 1:J:313:PRO:HG3  | 1:J:338:TRP:CE2  | 2.17                     | 0.80              |
| 1:K:212:ASP:OD2  | 1:L:209:SER:OG   | 1.98                     | 0.80              |
| 1:K:312:LEU:HD23 | 1:K:313:PRO:HD2  | 1.62                     | 0.80              |
| 1:F:440:HIS:O    | 1:F:444:VAL:N    | 2.14                     | 0.80              |
| 1:G:312:LEU:HD23 | 1:G:313:PRO:HD2  | 1.62                     | 0.80              |
| 1:I:440:HIS:O    | 1:I:444:VAL:N    | 2.14                     | 0.80              |
| 1:J:915:TYR:O    | 1:J:916:LYS:HB2  | 1.82                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:313:PRO:HG3  | 1:L:338:TRP:CE2  | 2.17                     | 0.80              |
| 1:L:915:TYR:O    | 1:L:916:LYS:HB2  | 1.82                     | 0.80              |
| 1:A:545:PHE:O    | 1:A:549:ILE:N    | 2.13                     | 0.80              |
| 1:C:313:PRO:HG3  | 1:C:338:TRP:CE2  | 2.17                     | 0.80              |
| 1:D:915:TYR:O    | 1:D:916:LYS:HB2  | 1.82                     | 0.80              |
| 1:E:313:PRO:HG3  | 1:E:338:TRP:CE2  | 2.17                     | 0.80              |
| 1:E:373:SER:HB3  | 1:E:433:LEU:CD1  | 2.12                     | 0.80              |
| 1:E:508:TRP:HE3  | 1:E:927:GLN:O    | 1.65                     | 0.80              |
| 1:F:209:SER:OG   | 1:G:212:ASP:OD2  | 1.98                     | 0.80              |
| 1:F:312:LEU:HD23 | 1:F:313:PRO:HD2  | 1.62                     | 0.80              |
| 1:F:354:GLU:OE1  | 1:F:430:LYS:HE3  | 1.81                     | 0.80              |
| 1:G:354:GLU:OE1  | 1:G:430:LYS:HE3  | 1.81                     | 0.80              |
| 1:G:373:SER:HB3  | 1:G:433:LEU:CD1  | 2.12                     | 0.80              |
| 1:J:508:TRP:CE3  | 1:J:927:GLN:C    | 2.58                     | 0.80              |
| 1:J:508:TRP:HE3  | 1:J:927:GLN:O    | 1.65                     | 0.80              |
| 1:K:915:TYR:O    | 1:K:916:LYS:HB2  | 1.82                     | 0.80              |
| 1:M:604:ASN:HD22 | 1:M:929:VAL:H    | 1.28                     | 0.80              |
| 1:P:312:LEU:HD23 | 1:P:313:PRO:HD2  | 1.62                     | 0.80              |
| 1:P:354:GLU:OE1  | 1:P:430:LYS:HE3  | 1.81                     | 0.80              |
| 1:P:373:SER:HB3  | 1:P:433:LEU:CD1  | 2.12                     | 0.80              |
| 1:I:545:PHE:O    | 1:I:549:ILE:N    | 2.13                     | 0.80              |
| 1:J:373:SER:HB3  | 1:J:433:LEU:CD1  | 2.12                     | 0.80              |
| 1:A:492:LEU:HD23 | 1:A:562:LEU:HD23 | 1.62                     | 0.79              |
| 1:D:354:GLU:OE1  | 1:D:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:F:507:ALA:O    | 1:F:608:ASN:HB2  | 1.80                     | 0.79              |
| 1:G:915:TYR:O    | 1:G:916:LYS:HB2  | 1.82                     | 0.79              |
| 1:I:507:ALA:O    | 1:I:608:ASN:HB2  | 1.80                     | 0.79              |
| 1:J:622:LEU:CB   | 1:J:634:ASP:HB2  | 2.09                     | 0.79              |
| 1:K:354:GLU:OE1  | 1:K:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:N:545:PHE:O    | 1:N:549:ILE:N    | 2.13                     | 0.79              |
| 1:O:314:ARG:O    | 1:O:315:GLU:CB   | 2.30                     | 0.79              |
| 1:B:915:TYR:O    | 1:B:916:LYS:HB2  | 1.82                     | 0.79              |
| 1:F:548:LYS:HZ2  | 1:F:601:GLN:HA   | 1.46                     | 0.79              |
| 1:H:314:ARG:O    | 1:H:315:GLU:CB   | 2.30                     | 0.79              |
| 1:N:492:LEU:HD23 | 1:N:562:LEU:HD23 | 1.62                     | 0.79              |
| 1:O:373:SER:HB3  | 1:O:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:P:314:ARG:O    | 1:P:315:GLU:CB   | 2.30                     | 0.79              |
| 1:P:915:TYR:O    | 1:P:916:LYS:HB2  | 1.82                     | 0.79              |
| 1:B:402:VAL:O    | 1:B:406:HIS:N    | 2.14                     | 0.79              |
| 1:D:373:SER:HB3  | 1:D:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:D:492:LEU:HD23 | 1:D:562:LEU:HD23 | 1.62                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:314:ARG:O    | 1:G:315:GLU:CB   | 2.30                     | 0.79              |
| 1:I:312:LEU:HD23 | 1:I:313:PRO:HD2  | 1.62                     | 0.79              |
| 1:K:492:LEU:HD23 | 1:K:562:LEU:HD23 | 1.62                     | 0.79              |
| 1:M:402:VAL:O    | 1:M:406:HIS:N    | 2.14                     | 0.79              |
| 1:M:915:TYR:O    | 1:M:916:LYS:HB2  | 1.82                     | 0.79              |
| 1:A:403:ASN:ND2  | 1:H:333:ASP:OD2  | 2.14                     | 0.79              |
| 1:C:314:ARG:O    | 1:C:315:GLU:CB   | 2.30                     | 0.79              |
| 1:E:622:LEU:CB   | 1:E:634:ASP:HB2  | 2.09                     | 0.79              |
| 1:F:313:PRO:HG3  | 1:F:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:G:511:SER:C    | 1:G:513:SER:H    | 1.91                     | 0.79              |
| 1:I:313:PRO:HG3  | 1:I:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:K:314:ARG:O    | 1:K:315:GLU:CB   | 2.30                     | 0.79              |
| 1:K:604:ASN:HD22 | 1:K:929:VAL:H    | 1.28                     | 0.79              |
| 1:L:314:ARG:O    | 1:L:315:GLU:CB   | 2.30                     | 0.79              |
| 1:M:548:LYS:HZ2  | 1:M:601:GLN:CA   | 1.95                     | 0.79              |
| 1:P:443:ILE:HG21 | 1:P:477:ASN:HD22 | 1.48                     | 0.79              |
| 1:B:313:PRO:HG3  | 1:B:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:B:373:SER:HB3  | 1:B:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:D:314:ARG:O    | 1:D:315:GLU:CB   | 2.30                     | 0.79              |
| 1:G:443:ILE:HG21 | 1:G:477:ASN:HD22 | 1.48                     | 0.79              |
| 1:G:548:LYS:HZ2  | 1:G:601:GLN:CA   | 1.95                     | 0.79              |
| 1:H:373:SER:HB3  | 1:H:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:H:443:ILE:HG21 | 1:H:477:ASN:HD22 | 1.48                     | 0.79              |
| 1:M:313:PRO:HG3  | 1:M:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:M:373:SER:HB3  | 1:M:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:M:442:SER:O    | 1:M:446:HIS:HD2  | 1.57                     | 0.79              |
| 1:N:373:SER:HB3  | 1:N:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:O:443:ILE:HG21 | 1:O:477:ASN:HD22 | 1.48                     | 0.79              |
| 1:P:511:SER:C    | 1:P:513:SER:H    | 1.91                     | 0.79              |
| 1:G:389:ILE:HD13 | 1:G:446:HIS:HE2  | 1.42                     | 0.79              |
| 1:H:511:SER:C    | 1:H:513:SER:H    | 1.91                     | 0.79              |
| 1:M:511:SER:C    | 1:M:513:SER:H    | 1.91                     | 0.79              |
| 1:A:314:ARG:O    | 1:A:315:GLU:CB   | 2.30                     | 0.79              |
| 1:A:373:SER:HB3  | 1:A:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:A:443:ILE:HG21 | 1:A:477:ASN:HD22 | 1.48                     | 0.79              |
| 1:B:511:SER:C    | 1:B:513:SER:H    | 1.90                     | 0.79              |
| 1:E:508:TRP:CA   | 1:E:606:GLY:CA   | 2.48                     | 0.79              |
| 1:H:354:GLU:OE1  | 1:H:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:H:508:TRP:HE3  | 1:H:927:GLN:O    | 1.65                     | 0.79              |
| 1:K:373:SER:HB3  | 1:K:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:K:440:HIS:O    | 1:K:444:VAL:N    | 2.14                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:373:SER:HB3  | 1:L:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:N:314:ARG:O    | 1:N:315:GLU:CB   | 2.30                     | 0.79              |
| 1:N:402:VAL:O    | 1:N:406:HIS:N    | 2.14                     | 0.79              |
| 1:N:443:ILE:HG21 | 1:N:477:ASN:HD22 | 1.48                     | 0.79              |
| 1:O:511:SER:C    | 1:O:513:SER:H    | 1.91                     | 0.79              |
| 1:D:440:HIS:O    | 1:D:444:VAL:N    | 2.14                     | 0.79              |
| 1:G:604:ASN:HD22 | 1:G:929:VAL:H    | 1.28                     | 0.79              |
| 1:H:313:PRO:HG3  | 1:H:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:I:314:ARG:O    | 1:I:315:GLU:CB   | 2.30                     | 0.79              |
| 1:L:312:LEU:HD23 | 1:L:313:PRO:HD2  | 1.61                     | 0.79              |
| 1:M:354:GLU:OE1  | 1:M:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:O:354:GLU:OE1  | 1:O:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:P:313:PRO:HG3  | 1:P:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:P:548:LYS:HZ2  | 1:P:601:GLN:CA   | 1.96                     | 0.79              |
| 1:P:604:ASN:HD22 | 1:P:929:VAL:H    | 1.28                     | 0.79              |
| 1:A:313:PRO:HG3  | 1:A:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:A:511:SER:C    | 1:A:513:SER:H    | 1.90                     | 0.79              |
| 1:B:354:GLU:OE1  | 1:B:430:LYS:HE3  | 1.82                     | 0.79              |
| 1:C:312:LEU:HD23 | 1:C:313:PRO:HD2  | 1.62                     | 0.79              |
| 1:D:425:ILE:O    | 1:D:429:LEU:N    | 2.15                     | 0.79              |
| 1:D:604:ASN:HD22 | 1:D:929:VAL:H    | 1.28                     | 0.79              |
| 1:G:545:PHE:O    | 1:G:549:ILE:N    | 2.13                     | 0.79              |
| 1:H:425:ILE:O    | 1:H:429:LEU:N    | 2.15                     | 0.79              |
| 1:I:508:TRP:HE3  | 1:I:927:GLN:O    | 1.65                     | 0.79              |
| 1:J:508:TRP:CA   | 1:J:606:GLY:CA   | 2.48                     | 0.79              |
| 1:K:20:GLU:O     | 1:K:24:VAL:N     | 2.16                     | 0.79              |
| 1:K:425:ILE:O    | 1:K:429:LEU:N    | 2.15                     | 0.79              |
| 1:L:354:GLU:OE1  | 1:L:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:L:492:LEU:HD23 | 1:L:562:LEU:HD23 | 1.62                     | 0.79              |
| 1:L:545:PHE:O    | 1:L:549:ILE:N    | 2.13                     | 0.79              |
| 1:M:492:LEU:HD23 | 1:M:562:LEU:HD23 | 1.62                     | 0.79              |
| 1:N:511:SER:C    | 1:N:513:SER:H    | 1.91                     | 0.79              |
| 1:O:403:ASN:ND2  | 1:P:333:ASP:OD2  | 2.16                     | 0.79              |
| 1:O:425:ILE:O    | 1:O:429:LEU:N    | 2.15                     | 0.79              |
| 1:P:440:HIS:O    | 1:P:444:VAL:N    | 2.14                     | 0.79              |
| 1:A:354:GLU:OE1  | 1:A:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:C:373:SER:HB3  | 1:C:433:LEU:CD1  | 2.12                     | 0.79              |
| 1:E:425:ILE:O    | 1:E:429:LEU:N    | 2.15                     | 0.79              |
| 1:F:314:ARG:O    | 1:F:315:GLU:CB   | 2.30                     | 0.79              |
| 1:G:313:PRO:HG3  | 1:G:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:G:440:HIS:O    | 1:G:444:VAL:N    | 2.14                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:604:ASN:HD22 | 1:H:929:VAL:H    | 1.28                     | 0.79              |
| 1:M:440:HIS:O    | 1:M:444:VAL:N    | 2.14                     | 0.79              |
| 1:N:313:PRO:HG3  | 1:N:338:TRP:CE2  | 2.17                     | 0.79              |
| 1:N:354:GLU:OE1  | 1:N:430:LYS:HE3  | 1.81                     | 0.79              |
| 1:P:402:VAL:O    | 1:P:406:HIS:N    | 2.14                     | 0.79              |
| 1:P:545:PHE:O    | 1:P:549:ILE:N    | 2.13                     | 0.79              |
| 1:A:402:VAL:O    | 1:A:406:HIS:N    | 2.14                     | 0.78              |
| 1:B:492:LEU:HD23 | 1:B:562:LEU:HD23 | 1.62                     | 0.78              |
| 1:C:545:PHE:O    | 1:C:549:ILE:N    | 2.13                     | 0.78              |
| 1:D:20:GLU:O     | 1:D:24:VAL:N     | 2.16                     | 0.78              |
| 1:F:511:SER:C    | 1:F:513:SER:H    | 1.91                     | 0.78              |
| 1:G:402:VAL:O    | 1:G:406:HIS:N    | 2.14                     | 0.78              |
| 1:J:425:ILE:O    | 1:J:429:LEU:N    | 2.15                     | 0.78              |
| 1:O:508:TRP:HE3  | 1:O:927:GLN:O    | 1.66                     | 0.78              |
| 1:C:492:LEU:HD23 | 1:C:562:LEU:HD23 | 1.62                     | 0.78              |
| 1:F:548:LYS:HZ2  | 1:F:601:GLN:CA   | 1.96                     | 0.78              |
| 1:H:20:GLU:O     | 1:H:24:VAL:N     | 2.16                     | 0.78              |
| 1:O:20:GLU:O     | 1:O:24:VAL:N     | 2.16                     | 0.78              |
| 1:O:313:PRO:HG3  | 1:O:338:TRP:CE2  | 2.17                     | 0.78              |
| 1:O:604:ASN:HD22 | 1:O:929:VAL:H    | 1.28                     | 0.78              |
| 1:P:389:ILE:HD13 | 1:P:446:HIS:HE2  | 1.42                     | 0.78              |
| 1:B:440:HIS:O    | 1:B:444:VAL:N    | 2.14                     | 0.78              |
| 1:C:354:GLU:OE1  | 1:C:430:LYS:HE3  | 1.82                     | 0.78              |
| 1:G:20:GLU:O     | 1:G:24:VAL:N     | 2.16                     | 0.78              |
| 1:P:20:GLU:O     | 1:P:24:VAL:N     | 2.16                     | 0.78              |
| 1:N:508:TRP:HE3  | 1:N:927:GLN:O    | 1.65                     | 0.78              |
| 1:D:508:TRP:HE3  | 1:D:927:GLN:O    | 1.65                     | 0.78              |
| 1:I:425:ILE:O    | 1:I:429:LEU:N    | 2.15                     | 0.78              |
| 1:K:508:TRP:HE3  | 1:K:927:GLN:O    | 1.65                     | 0.78              |
| 1:M:403:ASN:ND2  | 1:N:333:ASP:OD2  | 2.17                     | 0.78              |
| 1:A:508:TRP:HE3  | 1:A:927:GLN:O    | 1.65                     | 0.78              |
| 1:B:443:ILE:HG21 | 1:B:477:ASN:HD22 | 1.48                     | 0.78              |
| 1:F:443:ILE:HG21 | 1:F:477:ASN:HD22 | 1.48                     | 0.78              |
| 1:F:508:TRP:HE3  | 1:F:927:GLN:O    | 1.65                     | 0.78              |
| 1:H:915:TYR:O    | 1:H:916:LYS:HB2  | 1.82                     | 0.78              |
| 1:K:402:VAL:O    | 1:K:406:HIS:N    | 2.14                     | 0.78              |
| 1:L:511:SER:C    | 1:L:513:SER:H    | 1.91                     | 0.78              |
| 1:M:443:ILE:HG21 | 1:M:477:ASN:HD22 | 1.48                     | 0.78              |
| 1:D:548:LYS:HZ2  | 1:D:601:GLN:HA   | 1.48                     | 0.78              |
| 1:F:425:ILE:O    | 1:F:429:LEU:N    | 2.15                     | 0.78              |
| 1:G:157:LYS:NZ   | 2:G:1501:DTP:O3B | 2.17                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:157:LYS:NZ   | 2:H:1501:DTP:O3B | 2.17                     | 0.78              |
| 1:K:548:LYS:HZ2  | 1:K:601:GLN:HA   | 1.48                     | 0.78              |
| 1:O:157:LYS:NZ   | 2:O:1501:DTP:O3B | 2.17                     | 0.78              |
| 1:O:915:TYR:O    | 1:O:916:LYS:HB2  | 1.82                     | 0.78              |
| 1:P:157:LYS:NZ   | 2:P:1501:DTP:O3B | 2.17                     | 0.78              |
| 1:D:402:VAL:O    | 1:D:406:HIS:N    | 2.14                     | 0.78              |
| 1:I:604:ASN:HD22 | 1:I:929:VAL:H    | 1.28                     | 0.78              |
| 1:N:425:ILE:O    | 1:N:429:LEU:N    | 2.15                     | 0.78              |
| 1:B:187:ASN:HA   | 1:B:249:ASN:HD21 | 1.49                     | 0.78              |
| 1:B:458:LEU:HD23 | 1:B:459:ILE:H    | 1.49                     | 0.78              |
| 1:C:511:SER:C    | 1:C:513:SER:H    | 1.91                     | 0.78              |
| 1:H:373:SER:OG   | 1:H:433:LEU:HD12 | 1.84                     | 0.78              |
| 1:I:443:ILE:HG21 | 1:I:477:ASN:HD22 | 1.48                     | 0.78              |
| 1:I:511:SER:C    | 1:I:513:SER:H    | 1.91                     | 0.78              |
| 1:L:20:GLU:O     | 1:L:24:VAL:N     | 2.16                     | 0.78              |
| 1:M:314:ARG:O    | 1:M:315:GLU:CB   | 2.30                     | 0.78              |
| 1:M:458:LEU:HD23 | 1:M:459:ILE:H    | 1.49                     | 0.78              |
| 1:O:373:SER:OG   | 1:O:433:LEU:HD12 | 1.84                     | 0.78              |
| 1:P:425:ILE:O    | 1:P:429:LEU:N    | 2.15                     | 0.78              |
| 1:A:425:ILE:O    | 1:A:429:LEU:N    | 2.15                     | 0.78              |
| 1:B:314:ARG:O    | 1:B:315:GLU:CB   | 2.30                     | 0.78              |
| 1:E:548:LYS:HZ2  | 1:E:601:GLN:HA   | 1.49                     | 0.78              |
| 1:G:425:ILE:O    | 1:G:429:LEU:N    | 2.15                     | 0.78              |
| 1:M:187:ASN:HA   | 1:M:249:ASN:HD21 | 1.49                     | 0.78              |
| 1:B:301:LEU:HD21 | 1:B:313:PRO:CG   | 2.14                     | 0.77              |
| 1:C:187:ASN:HA   | 1:C:249:ASN:HD21 | 1.50                     | 0.77              |
| 1:C:333:ASP:OD2  | 1:D:403:ASN:ND2  | 2.17                     | 0.77              |
| 1:F:20:GLU:O     | 1:F:24:VAL:N     | 2.16                     | 0.77              |
| 1:K:511:SER:C    | 1:K:513:SER:H    | 1.91                     | 0.77              |
| 1:M:301:LEU:HD21 | 1:M:313:PRO:CG   | 2.14                     | 0.77              |
| 1:N:915:TYR:O    | 1:N:916:LYS:HB2  | 1.82                     | 0.77              |
| 1:A:301:LEU:HD21 | 1:A:313:PRO:CG   | 2.14                     | 0.77              |
| 1:C:20:GLU:O     | 1:C:24:VAL:N     | 2.16                     | 0.77              |
| 1:C:458:LEU:HD23 | 1:C:459:ILE:H    | 1.49                     | 0.77              |
| 1:D:511:SER:C    | 1:D:513:SER:H    | 1.91                     | 0.77              |
| 1:E:545:PHE:O    | 1:E:549:ILE:N    | 2.13                     | 0.77              |
| 1:F:604:ASN:HD22 | 1:F:929:VAL:H    | 1.28                     | 0.77              |
| 1:L:187:ASN:HA   | 1:L:249:ASN:HD21 | 1.49                     | 0.77              |
| 1:N:20:GLU:O     | 1:N:24:VAL:N     | 2.16                     | 0.77              |
| 1:N:157:LYS:NZ   | 2:N:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:N:301:LEU:HD21 | 1:N:313:PRO:CG   | 2.14                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:157:LYS:NZ   | 2:A:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:A:915:TYR:O    | 1:A:916:LYS:HB2  | 1.82                     | 0.77              |
| 1:E:314:ARG:O    | 1:E:315:GLU:CB   | 2.30                     | 0.77              |
| 1:F:14:ASP:CG    | 1:G:142:ARG:HH12 | 1.92                     | 0.77              |
| 1:H:545:PHE:O    | 1:H:549:ILE:N    | 2.13                     | 0.77              |
| 1:J:314:ARG:O    | 1:J:315:GLU:CB   | 2.30                     | 0.77              |
| 1:L:458:LEU:HD23 | 1:L:459:ILE:H    | 1.49                     | 0.77              |
| 1:L:508:TRP:CA   | 1:L:606:GLY:CA   | 2.48                     | 0.77              |
| 1:A:20:GLU:O     | 1:A:24:VAL:N     | 2.16                     | 0.77              |
| 1:A:458:LEU:HD23 | 1:A:459:ILE:H    | 1.49                     | 0.77              |
| 1:C:313:PRO:CG   | 1:C:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:E:443:ILE:HG21 | 1:E:477:ASN:HD22 | 1.48                     | 0.77              |
| 1:F:122:LYS:HG3  | 1:G:276:SER:CB   | 2.15                     | 0.77              |
| 1:G:373:SER:OG   | 1:G:433:LEU:HD12 | 1.84                     | 0.77              |
| 1:J:915:TYR:CZ   | 1:J:916:LYS:HE3  | 2.20                     | 0.77              |
| 1:O:545:PHE:O    | 1:O:549:ILE:N    | 2.13                     | 0.77              |
| 1:P:373:SER:OG   | 1:P:433:LEU:HD12 | 1.84                     | 0.77              |
| 1:B:548:LYS:HZ2  | 1:B:601:GLN:HA   | 1.49                     | 0.77              |
| 1:F:157:LYS:NZ   | 2:F:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:F:458:LEU:HD23 | 1:F:459:ILE:H    | 1.49                     | 0.77              |
| 1:H:313:PRO:CG   | 1:H:338:TRP:CZ2  | 2.67                     | 0.77              |
| 1:I:20:GLU:O     | 1:I:24:VAL:N     | 2.16                     | 0.77              |
| 1:J:545:PHE:O    | 1:J:549:ILE:N    | 2.13                     | 0.77              |
| 1:M:313:PRO:CG   | 1:M:338:TRP:CZ2  | 2.67                     | 0.77              |
| 1:A:313:PRO:CG   | 1:A:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:B:313:PRO:CG   | 1:B:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:C:548:LYS:HZ2  | 1:C:601:GLN:HA   | 1.49                     | 0.77              |
| 1:E:187:ASN:HA   | 1:E:249:ASN:HD21 | 1.49                     | 0.77              |
| 1:E:915:TYR:CZ   | 1:E:916:LYS:HE3  | 2.20                     | 0.77              |
| 1:G:458:LEU:HD23 | 1:G:459:ILE:H    | 1.49                     | 0.77              |
| 1:I:458:LEU:HD23 | 1:I:459:ILE:H    | 1.49                     | 0.77              |
| 1:J:511:SER:C    | 1:J:513:SER:H    | 1.91                     | 0.77              |
| 1:L:313:PRO:CG   | 1:L:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:L:915:TYR:CZ   | 1:L:916:LYS:HE3  | 2.20                     | 0.77              |
| 1:N:187:ASN:HA   | 1:N:249:ASN:HD21 | 1.49                     | 0.77              |
| 1:N:313:PRO:CG   | 1:N:338:TRP:CZ2  | 2.67                     | 0.77              |
| 1:N:373:SER:OG   | 1:N:433:LEU:HD12 | 1.84                     | 0.77              |
| 1:N:458:LEU:HD23 | 1:N:459:ILE:H    | 1.50                     | 0.77              |
| 1:O:313:PRO:CG   | 1:O:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:P:313:PRO:CG   | 1:P:338:TRP:CZ2  | 2.67                     | 0.77              |
| 1:A:187:ASN:HA   | 1:A:249:ASN:HD21 | 1.49                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:373:SER:OG    | 1:A:433:LEU:HD12 | 1.84                     | 0.77              |
| 1:C:508:TRP:CA    | 1:C:606:GLY:CA   | 2.48                     | 0.77              |
| 1:C:915:TYR:CZ    | 1:C:916:LYS:HE3  | 2.20                     | 0.77              |
| 1:D:915:TYR:CZ    | 1:D:916:LYS:HE3  | 2.20                     | 0.77              |
| 1:E:548:LYS:HZ2   | 1:E:601:GLN:CA   | 1.98                     | 0.77              |
| 1:F:402:VAL:O     | 1:F:406:HIS:N    | 2.14                     | 0.77              |
| 1:G:313:PRO:CG    | 1:G:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:I:157:LYS:NZ    | 2:I:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:J:187:ASN:HA    | 1:J:249:ASN:HD21 | 1.49                     | 0.77              |
| 1:K:915:TYR:CZ    | 1:K:916:LYS:HE3  | 2.20                     | 0.77              |
| 1:L:548:LYS:HZ2   | 1:L:601:GLN:HA   | 1.50                     | 0.77              |
| 1:B:1169:ILE:HD11 | 1:B:1172:CYS:HB2 | 1.67                     | 0.77              |
| 1:C:157:LYS:NZ    | 2:C:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:C:301:LEU:HD21  | 1:C:313:PRO:CG   | 2.14                     | 0.77              |
| 1:E:313:PRO:CG    | 1:E:338:TRP:HZ2  | 1.98                     | 0.77              |
| 1:E:440:HIS:O     | 1:E:444:VAL:N    | 2.14                     | 0.77              |
| 1:F:187:ASN:HA    | 1:F:249:ASN:HD21 | 1.49                     | 0.77              |
| 1:F:301:LEU:HD21  | 1:F:313:PRO:CG   | 2.14                     | 0.77              |
| 1:H:458:LEU:HD23  | 1:H:459:ILE:H    | 1.49                     | 0.77              |
| 1:I:301:LEU:HD21  | 1:I:313:PRO:CG   | 2.14                     | 0.77              |
| 1:J:313:PRO:CG    | 1:J:338:TRP:HZ2  | 1.98                     | 0.77              |
| 1:J:440:HIS:O     | 1:J:444:VAL:N    | 2.14                     | 0.77              |
| 1:J:443:ILE:HG21  | 1:J:477:ASN:HD22 | 1.48                     | 0.77              |
| 1:K:157:LYS:NZ    | 2:K:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:L:157:LYS:NZ    | 2:L:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:O:301:LEU:HD21  | 1:O:313:PRO:CG   | 2.14                     | 0.77              |
| 1:O:440:HIS:O     | 1:O:444:VAL:N    | 2.14                     | 0.77              |
| 1:O:458:LEU:HD23  | 1:O:459:ILE:H    | 1.49                     | 0.77              |
| 1:P:458:LEU:HD23  | 1:P:459:ILE:H    | 1.49                     | 0.77              |
| 1:P:508:TRP:HE3   | 1:P:927:GLN:O    | 1.65                     | 0.77              |
| 1:B:633:THR:CG2   | 1:B:643:TYR:HA   | 2.15                     | 0.77              |
| 1:D:157:LYS:NZ    | 2:D:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:D:313:PRO:CG    | 1:D:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:E:511:SER:C     | 1:E:513:SER:H    | 1.91                     | 0.77              |
| 1:G:508:TRP:HE3   | 1:G:927:GLN:O    | 1.65                     | 0.77              |
| 1:H:301:LEU:HD21  | 1:H:313:PRO:CG   | 2.14                     | 0.77              |
| 1:I:187:ASN:HA    | 1:I:249:ASN:HD21 | 1.49                     | 0.77              |
| 1:K:443:ILE:HG21  | 1:K:477:ASN:HD22 | 1.48                     | 0.77              |
| 1:L:443:ILE:HG21  | 1:L:477:ASN:HD22 | 1.48                     | 0.77              |
| 1:M:915:TYR:CZ    | 1:M:916:LYS:HE3  | 2.20                     | 0.77              |
| 1:N:633:THR:CG2   | 1:N:643:TYR:HA   | 2.15                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:209:SER:OG    | 1:B:212:ASP:OD2  | 2.03                     | 0.77              |
| 1:A:633:THR:CG2   | 1:A:643:TYR:HA   | 2.15                     | 0.77              |
| 1:B:463:LEU:HB3   | 1:B:467:PHE:CD2  | 2.20                     | 0.77              |
| 1:C:1169:ILE:HD11 | 1:C:1172:CYS:HB2 | 1.67                     | 0.77              |
| 1:D:443:ILE:HG21  | 1:D:477:ASN:HD22 | 1.48                     | 0.77              |
| 1:D:1169:ILE:HD11 | 1:D:1172:CYS:HB2 | 1.67                     | 0.77              |
| 1:E:157:LYS:NZ    | 2:E:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:F:633:THR:CG2   | 1:F:643:TYR:HA   | 2.15                     | 0.77              |
| 1:I:403:ASN:ND2   | 1:J:333:ASP:OD2  | 2.17                     | 0.77              |
| 1:I:548:LYS:HZ2   | 1:I:601:GLN:CA   | 1.97                     | 0.77              |
| 1:J:157:LYS:NZ    | 2:J:1501:DTP:O3B | 2.17                     | 0.77              |
| 1:J:402:VAL:O     | 1:J:406:HIS:N    | 2.14                     | 0.77              |
| 1:K:313:PRO:CG    | 1:K:338:TRP:CZ2  | 2.68                     | 0.77              |
| 1:K:313:PRO:CG    | 1:K:338:TRP:HZ2  | 1.98                     | 0.77              |
| 1:K:633:THR:CG2   | 1:K:643:TYR:HA   | 2.15                     | 0.77              |
| 1:K:1169:ILE:HD11 | 1:K:1172:CYS:HB2 | 1.67                     | 0.77              |
| 1:M:1169:ILE:HD11 | 1:M:1172:CYS:HB2 | 1.67                     | 0.77              |
| 1:B:915:TYR:CZ    | 1:B:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:D:313:PRO:CG    | 1:D:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:D:633:THR:CG2   | 1:D:643:TYR:HA   | 2.15                     | 0.76              |
| 1:G:127:ARG:HE    | 1:G:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:G:301:LEU:HD21  | 1:G:313:PRO:CG   | 2.14                     | 0.76              |
| 1:G:633:THR:CG2   | 1:G:643:TYR:HA   | 2.15                     | 0.76              |
| 1:I:548:LYS:HZ2   | 1:I:601:GLN:HA   | 1.48                     | 0.76              |
| 1:I:633:THR:CG2   | 1:I:643:TYR:HA   | 2.15                     | 0.76              |
| 1:L:1169:ILE:HD11 | 1:L:1172:CYS:HB2 | 1.67                     | 0.76              |
| 1:M:463:LEU:HB3   | 1:M:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:M:633:THR:CG2   | 1:M:643:TYR:HA   | 2.15                     | 0.76              |
| 1:P:313:PRO:CG    | 1:P:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:P:633:THR:CG2   | 1:P:643:TYR:HA   | 2.15                     | 0.76              |
| 1:A:1169:ILE:HD11 | 1:A:1172:CYS:HB2 | 1.67                     | 0.76              |
| 1:C:633:THR:CG2   | 1:C:643:TYR:HA   | 2.15                     | 0.76              |
| 1:D:508:TRP:CA    | 1:D:606:GLY:CA   | 2.48                     | 0.76              |
| 1:E:301:LEU:HD21  | 1:E:313:PRO:CG   | 2.14                     | 0.76              |
| 1:E:402:VAL:O     | 1:E:406:HIS:N    | 2.14                     | 0.76              |
| 1:F:915:TYR:CZ    | 1:F:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:G:463:LEU:HB3   | 1:G:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:G:915:TYR:CZ    | 1:G:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:H:127:ARG:HE    | 1:H:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:H:440:HIS:O     | 1:H:444:VAL:N    | 2.14                     | 0.76              |
| 1:H:633:THR:CG2   | 1:H:643:TYR:HA   | 2.15                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:560:ASP:HA    | 1:J:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:L:301:LEU:HD21  | 1:L:313:PRO:CG   | 2.14                     | 0.76              |
| 1:L:633:THR:CG2   | 1:L:643:TYR:HA   | 2.15                     | 0.76              |
| 1:P:301:LEU:HD21  | 1:P:313:PRO:CG   | 2.14                     | 0.76              |
| 1:P:463:LEU:HB3   | 1:P:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:B:157:LYS:NZ    | 2:B:1501:DTP:O3B | 2.17                     | 0.76              |
| 1:B:313:PRO:CG    | 1:B:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:B:548:LYS:HZ2   | 1:B:601:GLN:CA   | 1.98                     | 0.76              |
| 1:C:443:ILE:HG21  | 1:C:477:ASN:HD22 | 1.48                     | 0.76              |
| 1:D:127:ARG:HE    | 1:D:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:E:458:LEU:HD23  | 1:E:459:ILE:H    | 1.49                     | 0.76              |
| 1:E:560:ASP:HA    | 1:E:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:H:915:TYR:CZ    | 1:H:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:I:636:SER:O     | 1:I:637:LEU:C    | 2.29                     | 0.76              |
| 1:J:548:LYS:HZ2   | 1:J:601:GLN:HA   | 1.51                     | 0.76              |
| 1:L:463:LEU:HB3   | 1:L:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:L:548:LYS:HZ2   | 1:L:601:GLN:CA   | 1.98                     | 0.76              |
| 1:M:313:PRO:CG    | 1:M:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:N:127:ARG:HE    | 1:N:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:N:1169:ILE:HD11 | 1:N:1172:CYS:HB2 | 1.67                     | 0.76              |
| 1:O:127:ARG:HE    | 1:O:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:O:633:THR:CG2   | 1:O:643:TYR:HA   | 2.15                     | 0.76              |
| 1:O:915:TYR:CZ    | 1:O:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:P:187:ASN:HA    | 1:P:249:ASN:HD21 | 1.49                     | 0.76              |
| 1:P:508:TRP:CA    | 1:P:606:GLY:CA   | 2.48                     | 0.76              |
| 1:P:915:TYR:CZ    | 1:P:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:A:127:ARG:HE    | 1:A:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:A:915:TYR:CZ    | 1:A:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:C:425:ILE:O     | 1:C:429:LEU:N    | 2.15                     | 0.76              |
| 1:C:463:LEU:HB3   | 1:C:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:D:301:LEU:HD21  | 1:D:313:PRO:CG   | 2.14                     | 0.76              |
| 1:G:313:PRO:CG    | 1:G:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:G:508:TRP:CA    | 1:G:606:GLY:CA   | 2.48                     | 0.76              |
| 1:H:313:PRO:CG    | 1:H:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:J:301:LEU:HD21  | 1:J:313:PRO:CG   | 2.14                     | 0.76              |
| 1:K:301:LEU:HD21  | 1:K:313:PRO:CG   | 2.14                     | 0.76              |
| 1:K:548:LYS:HZ2   | 1:K:601:GLN:CA   | 1.97                     | 0.76              |
| 1:M:157:LYS:NZ    | 2:M:1501:DTP:O3B | 2.17                     | 0.76              |
| 1:M:508:TRP:HE3   | 1:M:927:GLN:O    | 1.65                     | 0.76              |
| 1:N:403:ASN:ND2   | 1:O:333:ASP:OD2  | 2.18                     | 0.76              |
| 1:N:915:TYR:CZ    | 1:N:916:LYS:HE3  | 2.20                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:O:313:PRO:CG    | 1:O:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:O:518:LEU:HD12  | 1:O:518:LEU:H    | 1.51                     | 0.76              |
| 1:P:127:ARG:HE    | 1:P:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:A:463:LEU:HB3   | 1:A:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:C:373:SER:OG    | 1:C:433:LEU:HD12 | 1.84                     | 0.76              |
| 1:C:560:ASP:HA    | 1:C:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:E:313:PRO:CG    | 1:E:338:TRP:CZ2  | 2.68                     | 0.76              |
| 1:E:1169:ILE:HD11 | 1:E:1172:CYS:HB2 | 1.67                     | 0.76              |
| 1:F:122:LYS:HG3   | 1:G:276:SER:HB2  | 1.66                     | 0.76              |
| 1:F:313:PRO:CG    | 1:F:338:TRP:CZ2  | 2.67                     | 0.76              |
| 1:F:373:SER:OG    | 1:F:433:LEU:HD12 | 1.84                     | 0.76              |
| 1:F:636:SER:O     | 1:F:637:LEU:C    | 2.29                     | 0.76              |
| 1:G:187:ASN:HA    | 1:G:249:ASN:HD21 | 1.49                     | 0.76              |
| 1:H:187:ASN:HA    | 1:H:249:ASN:HD21 | 1.49                     | 0.76              |
| 1:H:518:LEU:H     | 1:H:518:LEU:HD12 | 1.51                     | 0.76              |
| 1:I:915:TYR:CZ    | 1:I:916:LYS:HE3  | 2.20                     | 0.76              |
| 1:J:313:PRO:CG    | 1:J:338:TRP:CZ2  | 2.68                     | 0.76              |
| 1:J:1169:ILE:HD11 | 1:J:1172:CYS:HB2 | 1.67                     | 0.76              |
| 1:K:127:ARG:HE    | 1:K:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:K:508:TRP:CA    | 1:K:606:GLY:CA   | 2.48                     | 0.76              |
| 1:N:463:LEU:HB3   | 1:N:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:O:187:ASN:HA    | 1:O:249:ASN:HD21 | 1.49                     | 0.76              |
| 1:B:508:TRP:HE3   | 1:B:927:GLN:O    | 1.65                     | 0.76              |
| 1:D:187:ASN:HA    | 1:D:249:ASN:HD21 | 1.49                     | 0.76              |
| 1:D:548:LYS:HZ2   | 1:D:601:GLN:CA   | 1.97                     | 0.76              |
| 1:I:463:LEU:HB3   | 1:I:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:L:127:ARG:HE    | 1:L:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:B:560:ASP:HA    | 1:B:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:C:127:ARG:HE    | 1:C:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:F:127:ARG:HE    | 1:F:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:F:313:PRO:CG    | 1:F:338:TRP:HZ2  | 1.98                     | 0.76              |
| 1:J:458:LEU:HD23  | 1:J:459:ILE:H    | 1.50                     | 0.76              |
| 1:J:548:LYS:HZ2   | 1:J:601:GLN:CA   | 1.99                     | 0.76              |
| 1:J:633:THR:CG2   | 1:J:643:TYR:HA   | 2.15                     | 0.76              |
| 1:K:276:SER:CB    | 1:L:121:ALA:HB1  | 2.12                     | 0.76              |
| 1:K:458:LEU:HD23  | 1:K:459:ILE:H    | 1.49                     | 0.76              |
| 1:D:458:LEU:HD23  | 1:D:459:ILE:H    | 1.50                     | 0.76              |
| 1:E:633:THR:CG2   | 1:E:643:TYR:HA   | 2.15                     | 0.76              |
| 1:G:518:LEU:HD12  | 1:G:518:LEU:H    | 1.51                     | 0.76              |
| 1:H:560:ASP:HA    | 1:H:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:L:425:ILE:O     | 1:L:429:LEU:N    | 2.15                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:M:560:ASP:HA    | 1:M:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:P:518:LEU:H     | 1:P:518:LEU:HD12 | 1.51                     | 0.76              |
| 1:P:560:ASP:HA    | 1:P:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:A:560:ASP:HA    | 1:A:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:B:20:GLU:O      | 1:B:24:VAL:N     | 2.16                     | 0.76              |
| 1:E:373:SER:OG    | 1:E:433:LEU:HD12 | 1.84                     | 0.76              |
| 1:E:636:SER:O     | 1:E:637:LEU:C    | 2.29                     | 0.76              |
| 1:G:560:ASP:HA    | 1:G:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:H:508:TRP:CA    | 1:H:606:GLY:CA   | 2.48                     | 0.76              |
| 1:I:127:ARG:HE    | 1:I:130:PRO:HG3  | 1.51                     | 0.76              |
| 1:I:313:PRO:CG    | 1:I:338:TRP:CZ2  | 2.68                     | 0.76              |
| 1:J:373:SER:OG    | 1:J:433:LEU:HD12 | 1.84                     | 0.76              |
| 1:J:636:SER:O     | 1:J:637:LEU:C    | 2.29                     | 0.76              |
| 1:K:187:ASN:HA    | 1:K:249:ASN:HD21 | 1.49                     | 0.76              |
| 1:L:373:SER:OG    | 1:L:433:LEU:HD12 | 1.84                     | 0.76              |
| 1:M:20:GLU:O      | 1:M:24:VAL:N     | 2.16                     | 0.76              |
| 1:F:463:LEU:HB3   | 1:F:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:F:545:PHE:HA    | 1:F:548:LYS:HB2  | 1.68                     | 0.76              |
| 1:K:463:LEU:HB3   | 1:K:467:PHE:CD2  | 2.20                     | 0.76              |
| 1:L:560:ASP:HA    | 1:L:592:ASN:HD21 | 1.50                     | 0.76              |
| 1:M:373:SER:OG    | 1:M:433:LEU:HD12 | 1.84                     | 0.76              |
| 1:P:545:PHE:HA    | 1:P:548:LYS:HB2  | 1.68                     | 0.76              |
| 1:D:463:LEU:HB3   | 1:D:467:PHE:CD2  | 2.20                     | 0.75              |
| 1:D:545:PHE:HA    | 1:D:548:LYS:HB2  | 1.68                     | 0.75              |
| 1:D:560:ASP:HA    | 1:D:592:ASN:HD21 | 1.50                     | 0.75              |
| 1:E:20:GLU:O      | 1:E:24:VAL:N     | 2.16                     | 0.75              |
| 1:F:560:ASP:HA    | 1:F:592:ASN:HD21 | 1.50                     | 0.75              |
| 1:G:333:ASP:OD2   | 1:H:403:ASN:ND2  | 2.19                     | 0.75              |
| 1:H:1169:ILE:HD11 | 1:H:1172:CYS:HB2 | 1.67                     | 0.75              |
| 1:I:373:SER:OG    | 1:I:433:LEU:HD12 | 1.84                     | 0.75              |
| 1:M:127:ARG:HE    | 1:M:130:PRO:HG3  | 1.51                     | 0.75              |
| 1:N:146:ASN:HD22  | 1:N:280:THR:HG22 | 1.51                     | 0.75              |
| 1:N:560:ASP:HA    | 1:N:592:ASN:HD21 | 1.50                     | 0.75              |
| 1:O:560:ASP:HA    | 1:O:592:ASN:HD21 | 1.50                     | 0.75              |
| 1:B:127:ARG:HE    | 1:B:130:PRO:HG3  | 1.51                     | 0.75              |
| 1:G:545:PHE:HA    | 1:G:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:I:333:ASP:OD2   | 1:P:403:ASN:ND2  | 2.18                     | 0.75              |
| 1:I:545:PHE:HA    | 1:I:548:LYS:HB2  | 1.68                     | 0.75              |
| 1:N:518:LEU:H     | 1:N:518:LEU:HD12 | 1.51                     | 0.75              |
| 1:A:146:ASN:HD22  | 1:A:280:THR:HG22 | 1.51                     | 0.75              |
| 1:B:373:SER:OG    | 1:B:433:LEU:HD12 | 1.84                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:545:PHE:HA    | 1:E:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:I:560:ASP:HA    | 1:I:592:ASN:HD21 | 1.50                     | 0.75              |
| 1:J:127:ARG:HE    | 1:J:130:PRO:HG3  | 1.51                     | 0.75              |
| 1:K:545:PHE:HA    | 1:K:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:O:402:VAL:O     | 1:O:406:HIS:N    | 2.14                     | 0.75              |
| 1:O:1169:ILE:HD11 | 1:O:1172:CYS:HB2 | 1.67                     | 0.75              |
| 1:C:548:LYS:HZ2   | 1:C:601:GLN:CA   | 1.98                     | 0.75              |
| 1:I:402:VAL:O     | 1:I:406:HIS:N    | 2.14                     | 0.75              |
| 1:J:545:PHE:HA    | 1:J:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:K:373:SER:OG    | 1:K:433:LEU:HD12 | 1.84                     | 0.75              |
| 1:L:545:PHE:HA    | 1:L:548:LYS:HB2  | 1.68                     | 0.75              |
| 1:O:146:ASN:HD22  | 1:O:280:THR:HG22 | 1.51                     | 0.75              |
| 1:O:508:TRP:CA    | 1:O:606:GLY:CA   | 2.48                     | 0.75              |
| 1:C:548:LYS:NZ    | 1:C:601:GLN:HA   | 2.01                     | 0.75              |
| 1:H:146:ASN:HD22  | 1:H:280:THR:HG22 | 1.51                     | 0.75              |
| 1:H:463:LEU:HB3   | 1:H:467:PHE:CD2  | 2.20                     | 0.75              |
| 1:J:20:GLU:O      | 1:J:24:VAL:N     | 2.16                     | 0.75              |
| 1:K:560:ASP:HA    | 1:K:592:ASN:HD21 | 1.50                     | 0.75              |
| 1:N:313:PRO:CG    | 1:N:338:TRP:HZ2  | 1.98                     | 0.75              |
| 1:O:463:LEU:HB3   | 1:O:467:PHE:CD2  | 2.20                     | 0.75              |
| 1:A:518:LEU:H     | 1:A:518:LEU:HD12 | 1.51                     | 0.75              |
| 1:B:146:ASN:HD22  | 1:B:280:THR:HG22 | 1.51                     | 0.75              |
| 1:D:548:LYS:NZ    | 1:D:601:GLN:HA   | 2.01                     | 0.75              |
| 1:F:1169:ILE:HD11 | 1:F:1172:CYS:HB2 | 1.67                     | 0.75              |
| 1:H:402:VAL:O     | 1:H:406:HIS:N    | 2.14                     | 0.75              |
| 1:H:545:PHE:HA    | 1:H:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:H:636:SER:O     | 1:H:637:LEU:C    | 2.29                     | 0.75              |
| 1:L:636:SER:O     | 1:L:637:LEU:C    | 2.29                     | 0.75              |
| 1:M:146:ASN:HD22  | 1:M:280:THR:HG22 | 1.51                     | 0.75              |
| 1:M:545:PHE:HA    | 1:M:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:O:545:PHE:HA    | 1:O:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:A:313:PRO:CG    | 1:A:338:TRP:HZ2  | 1.98                     | 0.75              |
| 1:B:545:PHE:HA    | 1:B:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:C:545:PHE:HA    | 1:C:548:LYS:HB2  | 1.69                     | 0.75              |
| 1:D:373:SER:OG    | 1:D:433:LEU:HD12 | 1.84                     | 0.75              |
| 1:E:463:LEU:HB3   | 1:E:467:PHE:CD2  | 2.20                     | 0.75              |
| 1:I:1169:ILE:HD11 | 1:I:1172:CYS:HB2 | 1.67                     | 0.75              |
| 1:K:636:SER:O     | 1:K:637:LEU:C    | 2.29                     | 0.75              |
| 1:O:636:SER:O     | 1:O:637:LEU:C    | 2.29                     | 0.75              |
| 1:J:463:LEU:HB3   | 1:J:467:PHE:CD2  | 2.20                     | 0.75              |
| 1:L:508:TRP:HE3   | 1:L:927:GLN:O    | 1.65                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:548:LYS:NZ   | 1:B:601:GLN:HA   | 2.01                     | 0.75              |
| 1:D:505:SER:OG   | 1:D:513:SER:OG   | 2.05                     | 0.75              |
| 1:D:548:LYS:HA   | 1:D:602:ILE:O    | 1.87                     | 0.75              |
| 1:E:127:ARG:HE   | 1:E:130:PRO:HG3  | 1.51                     | 0.75              |
| 1:F:518:LEU:H    | 1:F:518:LEU:HD12 | 1.51                     | 0.75              |
| 1:K:403:ASN:ND2  | 1:L:333:ASP:OD2  | 2.20                     | 0.75              |
| 1:K:548:LYS:HA   | 1:K:602:ILE:O    | 1.87                     | 0.75              |
| 1:K:548:LYS:NZ   | 1:K:601:GLN:HA   | 2.01                     | 0.75              |
| 1:P:636:SER:O    | 1:P:637:LEU:C    | 2.29                     | 0.75              |
| 1:D:636:SER:O    | 1:D:637:LEU:C    | 2.29                     | 0.74              |
| 1:G:636:SER:O    | 1:G:637:LEU:C    | 2.29                     | 0.74              |
| 1:L:313:PRO:CG   | 1:L:338:TRP:HZ2  | 1.98                     | 0.74              |
| 1:M:548:LYS:NZ   | 1:M:601:GLN:HA   | 2.01                     | 0.74              |
| 1:A:545:PHE:HA   | 1:A:548:LYS:HB2  | 1.68                     | 0.74              |
| 1:A:636:SER:O    | 1:A:637:LEU:C    | 2.29                     | 0.74              |
| 1:C:636:SER:O    | 1:C:637:LEU:C    | 2.29                     | 0.74              |
| 1:E:548:LYS:NZ   | 1:E:601:GLN:HA   | 2.01                     | 0.74              |
| 1:G:383:THR:HG23 | 1:G:419:THR:C    | 2.13                     | 0.74              |
| 1:I:902:ILE:HD13 | 1:I:930:HIS:HE1  | 1.52                     | 0.74              |
| 1:J:902:ILE:HD13 | 1:J:930:HIS:HE1  | 1.53                     | 0.74              |
| 1:L:548:LYS:NZ   | 1:L:601:GLN:HA   | 2.01                     | 0.74              |
| 1:N:636:SER:O    | 1:N:637:LEU:C    | 2.29                     | 0.74              |
| 1:O:548:LYS:NZ   | 1:O:601:GLN:HA   | 2.01                     | 0.74              |
| 1:P:146:ASN:HD22 | 1:P:280:THR:HG22 | 1.51                     | 0.74              |
| 1:P:383:THR:HG23 | 1:P:419:THR:C    | 2.12                     | 0.74              |
| 1:C:313:PRO:CG   | 1:C:338:TRP:HZ2  | 1.98                     | 0.74              |
| 1:E:119:VAL:HG23 | 1:E:120:PHE:H    | 1.53                     | 0.74              |
| 1:E:902:ILE:HD13 | 1:E:930:HIS:HE1  | 1.53                     | 0.74              |
| 1:G:146:ASN:HD22 | 1:G:280:THR:HG22 | 1.51                     | 0.74              |
| 1:G:492:LEU:HD23 | 1:G:562:LEU:CD2  | 2.17                     | 0.74              |
| 1:H:548:LYS:NZ   | 1:H:601:GLN:HA   | 2.01                     | 0.74              |
| 1:J:548:LYS:NZ   | 1:J:601:GLN:HA   | 2.01                     | 0.74              |
| 1:M:636:SER:O    | 1:M:637:LEU:C    | 2.29                     | 0.74              |
| 1:B:636:SER:O    | 1:B:637:LEU:C    | 2.29                     | 0.74              |
| 1:C:508:TRP:HE3  | 1:C:927:GLN:O    | 1.65                     | 0.74              |
| 1:F:902:ILE:HD13 | 1:F:930:HIS:HE1  | 1.53                     | 0.74              |
| 1:H:383:THR:HG23 | 1:H:419:THR:C    | 2.12                     | 0.74              |
| 1:J:119:VAL:HG23 | 1:J:120:PHE:H    | 1.53                     | 0.74              |
| 1:K:383:THR:HG23 | 1:K:419:THR:C    | 2.12                     | 0.74              |
| 1:L:146:ASN:HD22 | 1:L:280:THR:HG22 | 1.51                     | 0.74              |
| 1:N:545:PHE:HA   | 1:N:548:LYS:HB2  | 1.68                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:P:492:LEU:HD23  | 1:P:562:LEU:CD2  | 2.17                     | 0.74              |
| 1:D:333:ASP:OD2   | 1:E:403:ASN:ND2  | 2.21                     | 0.74              |
| 1:F:207:TRP:CD1   | 1:F:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:I:207:TRP:CD1   | 1:I:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:J:383:THR:HG23  | 1:J:419:THR:C    | 2.13                     | 0.74              |
| 1:L:383:THR:HG23  | 1:L:419:THR:C    | 2.12                     | 0.74              |
| 1:O:383:THR:HG23  | 1:O:419:THR:C    | 2.12                     | 0.74              |
| 1:B:517:THR:O     | 1:B:518:LEU:C    | 2.30                     | 0.74              |
| 1:C:492:LEU:HD23  | 1:C:562:LEU:CD2  | 2.17                     | 0.74              |
| 1:E:383:THR:HG23  | 1:E:419:THR:C    | 2.12                     | 0.74              |
| 1:F:548:LYS:NZ    | 1:F:601:GLN:HA   | 2.01                     | 0.74              |
| 1:G:207:TRP:CD1   | 1:G:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:G:1169:ILE:HD11 | 1:G:1172:CYS:HB2 | 1.67                     | 0.74              |
| 1:I:518:LEU:H     | 1:I:518:LEU:HD12 | 1.51                     | 0.74              |
| 1:J:518:LEU:HD12  | 1:J:518:LEU:H    | 1.51                     | 0.74              |
| 1:M:517:THR:O     | 1:M:518:LEU:C    | 2.30                     | 0.74              |
| 1:M:548:LYS:HA    | 1:M:602:ILE:O    | 1.87                     | 0.74              |
| 1:P:1169:ILE:HD11 | 1:P:1172:CYS:HB2 | 1.67                     | 0.74              |
| 1:B:548:LYS:HA    | 1:B:602:ILE:O    | 1.87                     | 0.74              |
| 1:D:146:ASN:HD22  | 1:D:280:THR:HG22 | 1.51                     | 0.74              |
| 1:D:383:THR:HG23  | 1:D:419:THR:C    | 2.12                     | 0.74              |
| 1:F:548:LYS:HA    | 1:F:602:ILE:O    | 1.87                     | 0.74              |
| 1:H:207:TRP:CD1   | 1:H:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:I:383:THR:HG23  | 1:I:419:THR:C    | 2.12                     | 0.74              |
| 1:L:492:LEU:HD23  | 1:L:562:LEU:CD2  | 2.17                     | 0.74              |
| 1:M:207:TRP:CD1   | 1:M:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:O:207:TRP:CD1   | 1:O:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:O:492:LEU:HD23  | 1:O:562:LEU:CD2  | 2.17                     | 0.74              |
| 1:P:207:TRP:CD1   | 1:P:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:P:902:ILE:HD13  | 1:P:930:HIS:HE1  | 1.53                     | 0.74              |
| 1:A:902:ILE:HD13  | 1:A:930:HIS:HE1  | 1.52                     | 0.74              |
| 1:B:207:TRP:CD1   | 1:B:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:C:146:ASN:HD22  | 1:C:280:THR:HG22 | 1.51                     | 0.74              |
| 1:C:548:LYS:HA    | 1:C:602:ILE:O    | 1.87                     | 0.74              |
| 1:E:517:THR:HG23  | 1:E:518:LEU:HD12 | 1.70                     | 0.74              |
| 1:F:383:THR:HG23  | 1:F:419:THR:C    | 2.12                     | 0.74              |
| 1:G:119:VAL:HG23  | 1:G:120:PHE:H    | 1.53                     | 0.74              |
| 1:G:902:ILE:HD13  | 1:G:930:HIS:HE1  | 1.53                     | 0.74              |
| 1:H:492:LEU:HD23  | 1:H:562:LEU:CD2  | 2.17                     | 0.74              |
| 1:H:517:THR:HG23  | 1:H:518:LEU:HD12 | 1.70                     | 0.74              |
| 1:I:548:LYS:NZ    | 1:I:601:GLN:HA   | 2.01                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:517:THR:HG23 | 1:J:518:LEU:HD12 | 1.70                     | 0.74              |
| 1:J:548:LYS:HA   | 1:J:602:ILE:O    | 1.87                     | 0.74              |
| 1:K:146:ASN:HD22 | 1:K:280:THR:HG22 | 1.51                     | 0.74              |
| 1:M:518:LEU:H    | 1:M:518:LEU:HD12 | 1.51                     | 0.74              |
| 1:N:902:ILE:HD13 | 1:N:930:HIS:HE1  | 1.53                     | 0.74              |
| 1:O:517:THR:HG23 | 1:O:518:LEU:HD12 | 1.70                     | 0.74              |
| 1:O:902:ILE:HD13 | 1:O:930:HIS:HE1  | 1.52                     | 0.74              |
| 1:A:383:THR:HG23 | 1:A:419:THR:C    | 2.12                     | 0.74              |
| 1:B:518:LEU:HD12 | 1:B:518:LEU:H    | 1.51                     | 0.74              |
| 1:D:517:THR:O    | 1:D:518:LEU:C    | 2.30                     | 0.74              |
| 1:D:902:ILE:HD13 | 1:D:930:HIS:HE1  | 1.52                     | 0.74              |
| 1:H:119:VAL:HG23 | 1:H:120:PHE:H    | 1.52                     | 0.74              |
| 1:I:517:THR:HG23 | 1:I:518:LEU:HD12 | 1.70                     | 0.74              |
| 1:J:207:TRP:CD1  | 1:J:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:K:902:ILE:HD13 | 1:K:930:HIS:HE1  | 1.52                     | 0.74              |
| 1:N:517:THR:HG23 | 1:N:518:LEU:HD12 | 1.70                     | 0.74              |
| 1:P:119:VAL:HG23 | 1:P:120:PHE:H    | 1.53                     | 0.74              |
| 1:A:517:THR:HG23 | 1:A:518:LEU:HD12 | 1.70                     | 0.74              |
| 1:B:492:LEU:HD23 | 1:B:562:LEU:CD2  | 2.17                     | 0.74              |
| 1:C:383:THR:HG23 | 1:C:419:THR:C    | 2.12                     | 0.74              |
| 1:E:207:TRP:CD1  | 1:E:227:GLU:OE2  | 2.41                     | 0.74              |
| 1:E:518:LEU:HD12 | 1:E:518:LEU:H    | 1.51                     | 0.74              |
| 1:F:146:ASN:HD22 | 1:F:280:THR:HG22 | 1.51                     | 0.74              |
| 1:H:902:ILE:HD13 | 1:H:930:HIS:HE1  | 1.52                     | 0.74              |
| 1:K:517:THR:O    | 1:K:518:LEU:C    | 2.30                     | 0.74              |
| 1:L:39:ILE:HD11  | 1:L:76:PHE:HB2   | 1.70                     | 0.74              |
| 1:A:119:VAL:HG23 | 1:A:120:PHE:H    | 1.52                     | 0.73              |
| 1:A:517:THR:O    | 1:A:518:LEU:C    | 2.30                     | 0.73              |
| 1:A:548:LYS:NZ   | 1:A:601:GLN:HA   | 2.01                     | 0.73              |
| 1:B:119:VAL:HG23 | 1:B:120:PHE:H    | 1.53                     | 0.73              |
| 1:C:39:ILE:HD11  | 1:C:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:F:39:ILE:HD11  | 1:F:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:F:517:THR:HG23 | 1:F:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:I:548:LYS:HA   | 1:I:602:ILE:O    | 1.87                     | 0.73              |
| 1:J:39:ILE:HD11  | 1:J:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:L:119:VAL:HG23 | 1:L:120:PHE:H    | 1.53                     | 0.73              |
| 1:M:119:VAL:HG23 | 1:M:120:PHE:H    | 1.53                     | 0.73              |
| 1:M:492:LEU:HD23 | 1:M:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:M:902:ILE:HD13 | 1:M:930:HIS:HE1  | 1.52                     | 0.73              |
| 1:N:119:VAL:HG23 | 1:N:120:PHE:H    | 1.53                     | 0.73              |
| 1:O:119:VAL:HG23 | 1:O:120:PHE:H    | 1.53                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:492:LEU:HD23 | 1:A:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:C:207:TRP:CD1  | 1:C:227:GLU:OE2  | 2.41                     | 0.73              |
| 1:E:517:THR:O    | 1:E:518:LEU:C    | 2.30                     | 0.73              |
| 1:E:548:LYS:HA   | 1:E:602:ILE:O    | 1.87                     | 0.73              |
| 1:G:548:LYS:NZ   | 1:G:601:GLN:HA   | 2.01                     | 0.73              |
| 1:I:39:ILE:HD11  | 1:I:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:J:517:THR:O    | 1:J:518:LEU:C    | 2.30                     | 0.73              |
| 1:K:518:LEU:H    | 1:K:518:LEU:HD12 | 1.51                     | 0.73              |
| 1:L:207:TRP:CD1  | 1:L:227:GLU:OE2  | 2.41                     | 0.73              |
| 1:N:383:THR:HG23 | 1:N:419:THR:C    | 2.13                     | 0.73              |
| 1:N:517:THR:O    | 1:N:518:LEU:C    | 2.30                     | 0.73              |
| 1:P:548:LYS:NZ   | 1:P:601:GLN:HA   | 2.01                     | 0.73              |
| 1:B:902:ILE:HD13 | 1:B:930:HIS:HE1  | 1.53                     | 0.73              |
| 1:D:39:ILE:HD11  | 1:D:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:D:517:THR:HG23 | 1:D:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:I:146:ASN:HD22 | 1:I:280:THR:HG22 | 1.51                     | 0.73              |
| 1:I:508:TRP:HA   | 1:I:606:GLY:C    | 2.14                     | 0.73              |
| 1:K:207:TRP:CD1  | 1:K:227:GLU:OE2  | 2.41                     | 0.73              |
| 1:N:492:LEU:HD23 | 1:N:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:B:545:PHE:O    | 1:B:549:ILE:N    | 2.13                     | 0.73              |
| 1:C:119:VAL:HG23 | 1:C:120:PHE:H    | 1.52                     | 0.73              |
| 1:D:207:TRP:CD1  | 1:D:227:GLU:OE2  | 2.41                     | 0.73              |
| 1:E:39:ILE:HD11  | 1:E:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:E:492:LEU:HD23 | 1:E:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:F:53:ASP:OD1   | 1:F:54:ALA:N     | 2.22                     | 0.73              |
| 1:F:119:VAL:HG23 | 1:F:120:PHE:H    | 1.52                     | 0.73              |
| 1:G:508:TRP:HA   | 1:G:606:GLY:C    | 2.13                     | 0.73              |
| 1:G:517:THR:HG23 | 1:G:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:I:53:ASP:OD1   | 1:I:54:ALA:N     | 2.22                     | 0.73              |
| 1:I:492:LEU:HD23 | 1:I:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:K:119:VAL:HG23 | 1:K:120:PHE:H    | 1.52                     | 0.73              |
| 1:K:517:THR:HG23 | 1:K:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:L:902:ILE:HD13 | 1:L:930:HIS:HE1  | 1.52                     | 0.73              |
| 1:M:383:THR:HG23 | 1:M:419:THR:C    | 2.12                     | 0.73              |
| 1:N:508:TRP:HA   | 1:N:606:GLY:C    | 2.13                     | 0.73              |
| 1:N:548:LYS:NZ   | 1:N:601:GLN:HA   | 2.01                     | 0.73              |
| 1:P:508:TRP:HA   | 1:P:606:GLY:C    | 2.13                     | 0.73              |
| 1:P:517:THR:HG23 | 1:P:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:A:508:TRP:HA   | 1:A:606:GLY:C    | 2.13                     | 0.73              |
| 1:B:383:THR:HG23 | 1:B:419:THR:C    | 2.12                     | 0.73              |
| 1:C:902:ILE:HD13 | 1:C:930:HIS:HE1  | 1.53                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:492:LEU:HD23 | 1:D:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:E:53:ASP:OD1   | 1:E:54:ALA:N     | 2.22                     | 0.73              |
| 1:F:508:TRP:HA   | 1:F:606:GLY:C    | 2.13                     | 0.73              |
| 1:J:492:LEU:HD23 | 1:J:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:K:492:LEU:HD23 | 1:K:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:M:517:THR:HG23 | 1:M:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:N:207:TRP:CD1  | 1:N:227:GLU:OE2  | 2.41                     | 0.73              |
| 1:O:508:TRP:HA   | 1:O:606:GLY:C    | 2.13                     | 0.73              |
| 1:D:518:LEU:HD12 | 1:D:518:LEU:H    | 1.51                     | 0.73              |
| 1:E:146:ASN:HD22 | 1:E:280:THR:HG22 | 1.51                     | 0.73              |
| 1:G:383:THR:H    | 1:G:419:THR:HA   | 1.54                     | 0.73              |
| 1:H:508:TRP:HA   | 1:H:606:GLY:C    | 2.13                     | 0.73              |
| 1:K:39:ILE:HD11  | 1:K:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:K:521:LEU:HA   | 1:K:524:TYR:CD2  | 2.23                     | 0.73              |
| 1:L:548:LYS:HA   | 1:L:602:ILE:O    | 1.87                     | 0.73              |
| 1:P:383:THR:H    | 1:P:419:THR:HA   | 1.54                     | 0.73              |
| 1:A:207:TRP:CD1  | 1:A:227:GLU:OE2  | 2.41                     | 0.73              |
| 1:B:517:THR:HG23 | 1:B:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:C:517:THR:HG23 | 1:C:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:C:518:LEU:H    | 1:C:518:LEU:HD12 | 1.51                     | 0.73              |
| 1:D:119:VAL:HG23 | 1:D:120:PHE:H    | 1.53                     | 0.73              |
| 1:F:492:LEU:HD23 | 1:F:562:LEU:CD2  | 2.17                     | 0.73              |
| 1:H:548:LYS:HA   | 1:H:602:ILE:O    | 1.87                     | 0.73              |
| 1:J:53:ASP:OD1   | 1:J:54:ALA:N     | 2.22                     | 0.73              |
| 1:P:53:ASP:OD1   | 1:P:54:ALA:N     | 2.22                     | 0.73              |
| 1:D:521:LEU:HA   | 1:D:524:TYR:CD2  | 2.23                     | 0.73              |
| 1:E:508:TRP:HA   | 1:E:606:GLY:C    | 2.13                     | 0.73              |
| 1:G:53:ASP:OD1   | 1:G:54:ALA:N     | 2.22                     | 0.73              |
| 1:J:146:ASN:HD22 | 1:J:280:THR:HG22 | 1.51                     | 0.73              |
| 1:L:517:THR:HG23 | 1:L:518:LEU:HD12 | 1.70                     | 0.73              |
| 1:M:545:PHE:O    | 1:M:549:ILE:N    | 2.13                     | 0.73              |
| 1:N:53:ASP:OD1   | 1:N:54:ALA:N     | 2.22                     | 0.73              |
| 1:O:548:LYS:HA   | 1:O:602:ILE:O    | 1.87                     | 0.73              |
| 1:C:517:THR:O    | 1:C:518:LEU:C    | 2.30                     | 0.73              |
| 1:G:39:ILE:HD11  | 1:G:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:I:119:VAL:HG23 | 1:I:120:PHE:H    | 1.53                     | 0.73              |
| 1:O:53:ASP:OD1   | 1:O:54:ALA:N     | 2.22                     | 0.73              |
| 1:P:39:ILE:HD11  | 1:P:76:PHE:HB2   | 1.70                     | 0.73              |
| 1:P:548:LYS:HA   | 1:P:602:ILE:O    | 1.87                     | 0.73              |
| 1:A:14:ASP:OD2   | 1:B:142:ARG:NH1  | 2.21                     | 0.73              |
| 1:A:53:ASP:OD1   | 1:A:54:ALA:N     | 2.22                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:548:LYS:HA   | 1:A:602:ILE:O   | 1.87                     | 0.73              |
| 1:C:521:LEU:HA   | 1:C:524:TYR:CD2 | 2.23                     | 0.73              |
| 1:H:53:ASP:OD1   | 1:H:54:ALA:N    | 2.22                     | 0.73              |
| 1:J:508:TRP:HA   | 1:J:606:GLY:C   | 2.13                     | 0.73              |
| 1:L:518:LEU:HD12 | 1:L:518:LEU:H   | 1.51                     | 0.73              |
| 1:B:508:TRP:HA   | 1:B:606:GLY:C   | 2.13                     | 0.72              |
| 1:D:508:TRP:HA   | 1:D:606:GLY:C   | 2.13                     | 0.72              |
| 1:D:545:PHE:O    | 1:D:549:ILE:N   | 2.13                     | 0.72              |
| 1:G:548:LYS:HA   | 1:G:602:ILE:O   | 1.87                     | 0.72              |
| 1:K:508:TRP:HA   | 1:K:606:GLY:C   | 2.14                     | 0.72              |
| 1:K:545:PHE:O    | 1:K:549:ILE:N   | 2.13                     | 0.72              |
| 1:L:403:ASN:ND2  | 1:M:333:ASP:OD2 | 2.21                     | 0.72              |
| 1:M:508:TRP:HA   | 1:M:606:GLY:C   | 2.14                     | 0.72              |
| 1:B:383:THR:H    | 1:B:419:THR:HA  | 1.54                     | 0.72              |
| 1:D:53:ASP:OD1   | 1:D:54:ALA:N    | 2.22                     | 0.72              |
| 1:H:502:ARG:NH2  | 1:H:519:GLN:OE1 | 2.22                     | 0.72              |
| 1:L:521:LEU:HA   | 1:L:524:TYR:CD2 | 2.23                     | 0.72              |
| 1:N:383:THR:H    | 1:N:419:THR:HA  | 1.54                     | 0.72              |
| 1:O:502:ARG:NH2  | 1:O:519:GLN:OE1 | 2.22                     | 0.72              |
| 1:P:521:LEU:HA   | 1:P:524:TYR:CD2 | 2.23                     | 0.72              |
| 1:A:458:LEU:HG   | 1:A:587:ARG:NH2 | 2.05                     | 0.72              |
| 1:A:521:LEU:HA   | 1:A:524:TYR:CD2 | 2.23                     | 0.72              |
| 1:F:517:THR:O    | 1:F:518:LEU:C   | 2.30                     | 0.72              |
| 1:G:521:LEU:HA   | 1:G:524:TYR:CD2 | 2.23                     | 0.72              |
| 1:H:39:ILE:HD11  | 1:H:76:PHE:HB2  | 1.70                     | 0.72              |
| 1:I:517:THR:O    | 1:I:518:LEU:C   | 2.30                     | 0.72              |
| 1:K:53:ASP:OD1   | 1:K:54:ALA:N    | 2.22                     | 0.72              |
| 1:L:517:THR:O    | 1:L:518:LEU:C   | 2.30                     | 0.72              |
| 1:M:383:THR:H    | 1:M:419:THR:HA  | 1.54                     | 0.72              |
| 1:N:458:LEU:HG   | 1:N:587:ARG:NH2 | 2.05                     | 0.72              |
| 1:N:548:LYS:HA   | 1:N:602:ILE:O   | 1.87                     | 0.72              |
| 1:A:39:ILE:HD11  | 1:A:76:PHE:HB2  | 1.70                     | 0.72              |
| 1:B:39:ILE:HD11  | 1:B:76:PHE:HB2  | 1.70                     | 0.72              |
| 1:B:521:LEU:HA   | 1:B:524:TYR:CD2 | 2.23                     | 0.72              |
| 1:C:508:TRP:HA   | 1:C:606:GLY:C   | 2.13                     | 0.72              |
| 1:H:521:LEU:HA   | 1:H:524:TYR:CD2 | 2.23                     | 0.72              |
| 1:I:502:ARG:NH2  | 1:I:519:GLN:OE1 | 2.22                     | 0.72              |
| 1:J:521:LEU:HA   | 1:J:524:TYR:CD2 | 2.23                     | 0.72              |
| 1:L:508:TRP:HA   | 1:L:606:GLY:C   | 2.13                     | 0.72              |
| 1:M:39:ILE:HD11  | 1:M:76:PHE:HB2  | 1.70                     | 0.72              |
| 1:M:53:ASP:OD1   | 1:M:54:ALA:N    | 2.22                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:39:ILE:HD11 | 1:N:76:PHE:HB2   | 1.70                     | 0.72              |
| 1:A:383:THR:H   | 1:A:419:THR:HA   | 1.54                     | 0.72              |
| 1:B:53:ASP:OD1  | 1:B:54:ALA:N     | 2.22                     | 0.72              |
| 1:D:383:THR:H   | 1:D:419:THR:HA   | 1.54                     | 0.72              |
| 1:E:502:ARG:NH2 | 1:E:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:F:502:ARG:NH2 | 1:F:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:F:544:ASP:OD1 | 1:F:545:PHE:N    | 2.23                     | 0.72              |
| 1:I:544:ASP:OD1 | 1:I:545:PHE:N    | 2.23                     | 0.72              |
| 1:J:502:ARG:NH2 | 1:J:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:M:521:LEU:HA  | 1:M:524:TYR:CD2  | 2.23                     | 0.72              |
| 1:O:521:LEU:HA  | 1:O:524:TYR:CD2  | 2.23                     | 0.72              |
| 1:E:521:LEU:HA  | 1:E:524:TYR:CD2  | 2.23                     | 0.72              |
| 1:H:383:THR:H   | 1:H:419:THR:HA   | 1.54                     | 0.72              |
| 1:N:521:LEU:HA  | 1:N:524:TYR:CD2  | 2.23                     | 0.72              |
| 1:O:39:ILE:HD11 | 1:O:76:PHE:HB2   | 1.70                     | 0.72              |
| 1:B:513:SER:HB3 | 1:B:514:ILE:HD12 | 1.72                     | 0.72              |
| 1:C:458:LEU:HG  | 1:C:587:ARG:NH2  | 2.05                     | 0.72              |
| 1:C:502:ARG:NH2 | 1:C:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:C:544:ASP:OD1 | 1:C:545:PHE:N    | 2.23                     | 0.72              |
| 1:D:544:ASP:OD1 | 1:D:545:PHE:N    | 2.23                     | 0.72              |
| 1:E:383:THR:H   | 1:E:419:THR:HA   | 1.54                     | 0.72              |
| 1:F:521:LEU:HA  | 1:F:524:TYR:CD2  | 2.23                     | 0.72              |
| 1:H:517:THR:O   | 1:H:518:LEU:C    | 2.30                     | 0.72              |
| 1:K:383:THR:H   | 1:K:419:THR:HA   | 1.54                     | 0.72              |
| 1:K:544:ASP:OD1 | 1:K:545:PHE:N    | 2.23                     | 0.72              |
| 1:L:458:LEU:HG  | 1:L:587:ARG:NH2  | 2.05                     | 0.72              |
| 1:L:544:ASP:OD1 | 1:L:545:PHE:N    | 2.23                     | 0.72              |
| 1:O:383:THR:H   | 1:O:419:THR:HA   | 1.54                     | 0.72              |
| 1:O:517:THR:O   | 1:O:518:LEU:C    | 2.30                     | 0.72              |
| 1:P:502:ARG:NH2 | 1:P:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:G:502:ARG:NH2 | 1:G:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:J:383:THR:H   | 1:J:419:THR:HA   | 1.54                     | 0.72              |
| 1:K:502:ARG:NH2 | 1:K:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:M:513:SER:HB3 | 1:M:514:ILE:HD12 | 1.72                     | 0.72              |
| 1:N:513:SER:HB3 | 1:N:514:ILE:HD12 | 1.72                     | 0.72              |
| 1:O:544:ASP:OD1 | 1:O:545:PHE:N    | 2.23                     | 0.72              |
| 1:C:53:ASP:OD1  | 1:C:54:ALA:N     | 2.22                     | 0.72              |
| 1:D:121:ALA:CB  | 1:E:276:SER:HB3  | 2.08                     | 0.72              |
| 1:D:502:ARG:NH2 | 1:D:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:G:547:PRO:CB  | 1:G:603:ILE:HG13 | 2.20                     | 0.72              |
| 1:H:544:ASP:OD1 | 1:H:545:PHE:N    | 2.23                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:521:LEU:HA  | 1:I:524:TYR:CD2  | 2.23                     | 0.72              |
| 1:L:53:ASP:OD1  | 1:L:54:ALA:N     | 2.22                     | 0.72              |
| 1:L:502:ARG:NH2 | 1:L:519:GLN:OE1  | 2.22                     | 0.72              |
| 1:A:513:SER:HB3 | 1:A:514:ILE:HD12 | 1.72                     | 0.71              |
| 1:B:544:ASP:OD1 | 1:B:545:PHE:N    | 2.23                     | 0.71              |
| 1:C:383:THR:H   | 1:C:419:THR:HA   | 1.54                     | 0.71              |
| 1:D:458:LEU:HG  | 1:D:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:G:458:LEU:HG  | 1:G:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:I:121:ALA:HB1 | 1:P:276:SER:CB   | 2.12                     | 0.71              |
| 1:J:207:TRP:NE1 | 1:J:227:GLU:OE1  | 2.23                     | 0.71              |
| 1:P:547:PRO:CB  | 1:P:603:ILE:HG13 | 2.20                     | 0.71              |
| 1:E:207:TRP:NE1 | 1:E:227:GLU:OE1  | 2.23                     | 0.71              |
| 1:M:544:ASP:OD1 | 1:M:545:PHE:N    | 2.23                     | 0.71              |
| 1:P:458:LEU:HG  | 1:P:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:A:502:ARG:NH2 | 1:A:519:GLN:OE1  | 2.22                     | 0.71              |
| 1:F:458:LEU:HG  | 1:F:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:K:458:LEU:HG  | 1:K:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:M:502:ARG:NH2 | 1:M:519:GLN:OE1  | 2.22                     | 0.71              |
| 1:O:458:LEU:HG  | 1:O:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:B:502:ARG:NH2 | 1:B:519:GLN:OE1  | 2.22                     | 0.71              |
| 1:L:383:THR:H   | 1:L:419:THR:HA   | 1.54                     | 0.71              |
| 1:N:547:PRO:CB  | 1:N:603:ILE:HG13 | 2.20                     | 0.71              |
| 1:D:1149:LEU:H  | 1:D:1196:ALA:HB2 | 1.56                     | 0.71              |
| 1:F:248:GLN:OE1 | 1:F:268:PHE:CZ   | 2.44                     | 0.71              |
| 1:H:458:LEU:HG  | 1:H:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:I:458:LEU:HG  | 1:I:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:K:1149:LEU:H  | 1:K:1196:ALA:HB2 | 1.56                     | 0.71              |
| 1:M:458:LEU:HG  | 1:M:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:N:502:ARG:NH2 | 1:N:519:GLN:OE1  | 2.22                     | 0.71              |
| 1:B:458:LEU:HG  | 1:B:587:ARG:NH2  | 2.05                     | 0.71              |
| 1:G:544:ASP:OD1 | 1:G:545:PHE:N    | 2.23                     | 0.71              |
| 1:I:248:GLN:OE1 | 1:I:268:PHE:CZ   | 2.43                     | 0.71              |
| 1:L:207:TRP:HD1 | 1:L:227:GLU:OE2  | 1.74                     | 0.71              |
| 1:L:284:SER:OG  | 1:L:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:O:284:SER:OG  | 1:O:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:B:314:ARG:C   | 1:B:315:GLU:HG3  | 2.15                     | 0.71              |
| 1:C:207:TRP:HD1 | 1:C:227:GLU:OE2  | 1.74                     | 0.71              |
| 1:C:1149:LEU:H  | 1:C:1196:ALA:HB2 | 1.56                     | 0.71              |
| 1:D:513:SER:HB3 | 1:D:514:ILE:HD12 | 1.72                     | 0.71              |
| 1:G:248:GLN:OE1 | 1:G:268:PHE:CZ   | 2.43                     | 0.71              |
| 1:H:284:SER:OG  | 1:H:286:ASP:OD1  | 2.09                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:207:TRP:NE1  | 1:K:227:GLU:OE1  | 2.23                     | 0.71              |
| 1:C:284:SER:OG   | 1:C:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:D:207:TRP:NE1  | 1:D:227:GLU:OE1  | 2.23                     | 0.71              |
| 1:E:121:ALA:CB   | 1:F:276:SER:HB3  | 2.05                     | 0.71              |
| 1:E:284:SER:OG   | 1:E:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:G:517:THR:O    | 1:G:518:LEU:C    | 2.30                     | 0.71              |
| 1:J:544:ASP:OD1  | 1:J:545:PHE:N    | 2.23                     | 0.71              |
| 1:L:1149:LEU:H   | 1:L:1196:ALA:HB2 | 1.56                     | 0.71              |
| 1:M:101:MET:SD   | 1:M:104:ARG:NH2  | 2.64                     | 0.71              |
| 1:M:314:ARG:C    | 1:M:315:GLU:HG3  | 2.15                     | 0.71              |
| 1:P:248:GLN:OE1  | 1:P:268:PHE:CZ   | 2.44                     | 0.71              |
| 1:P:463:LEU:HD22 | 1:P:467:PHE:HE2  | 1.55                     | 0.71              |
| 1:P:517:THR:O    | 1:P:518:LEU:C    | 2.30                     | 0.71              |
| 1:P:544:ASP:OD1  | 1:P:545:PHE:N    | 2.23                     | 0.71              |
| 1:A:314:ARG:C    | 1:A:315:GLU:HG3  | 2.16                     | 0.71              |
| 1:B:101:MET:SD   | 1:B:104:ARG:NH2  | 2.64                     | 0.71              |
| 1:E:547:PRO:CB   | 1:E:603:ILE:HG13 | 2.20                     | 0.71              |
| 1:F:383:THR:H    | 1:F:419:THR:HA   | 1.54                     | 0.71              |
| 1:G:389:ILE:CD1  | 1:G:446:HIS:CE1  | 2.70                     | 0.71              |
| 1:H:547:PRO:CB   | 1:H:603:ILE:HG13 | 2.20                     | 0.71              |
| 1:I:383:THR:H    | 1:I:419:THR:HA   | 1.54                     | 0.71              |
| 1:J:284:SER:OG   | 1:J:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:L:207:TRP:NE1  | 1:L:227:GLU:OE1  | 2.23                     | 0.71              |
| 1:N:314:ARG:C    | 1:N:315:GLU:HG3  | 2.16                     | 0.71              |
| 1:P:389:ILE:CD1  | 1:P:446:HIS:CE1  | 2.70                     | 0.71              |
| 1:P:1149:LEU:H   | 1:P:1196:ALA:HB2 | 1.56                     | 0.71              |
| 1:C:207:TRP:NE1  | 1:C:227:GLU:OE1  | 2.23                     | 0.71              |
| 1:C:314:ARG:C    | 1:C:315:GLU:HG3  | 2.16                     | 0.71              |
| 1:E:544:ASP:OD1  | 1:E:545:PHE:N    | 2.23                     | 0.71              |
| 1:G:284:SER:OG   | 1:G:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:G:463:LEU:HD22 | 1:G:467:PHE:HE2  | 1.55                     | 0.71              |
| 1:G:1149:LEU:H   | 1:G:1196:ALA:HB2 | 1.56                     | 0.71              |
| 1:H:513:SER:HB3  | 1:H:514:ILE:HD12 | 1.72                     | 0.71              |
| 1:I:284:SER:OG   | 1:I:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:J:101:MET:SD   | 1:J:104:ARG:NH2  | 2.64                     | 0.71              |
| 1:J:248:GLN:OE1  | 1:J:268:PHE:CZ   | 2.43                     | 0.71              |
| 1:J:276:SER:HB3  | 1:K:121:ALA:CB   | 2.09                     | 0.71              |
| 1:J:547:PRO:CB   | 1:J:603:ILE:HG13 | 2.20                     | 0.71              |
| 1:K:513:SER:HB3  | 1:K:514:ILE:HD12 | 1.72                     | 0.71              |
| 1:N:544:ASP:OD1  | 1:N:545:PHE:N    | 2.23                     | 0.71              |
| 1:O:547:PRO:CB   | 1:O:603:ILE:HG13 | 2.20                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:284:SER:OG   | 1:P:286:ASP:OD1  | 2.09                     | 0.71              |
| 1:P:513:SER:HB3  | 1:P:514:ILE:HD12 | 1.72                     | 0.71              |
| 1:C:14:ASP:CG    | 1:D:142:ARG:HH22 | 1.98                     | 0.70              |
| 1:D:14:ASP:OD2   | 1:E:142:ARG:NH1  | 2.24                     | 0.70              |
| 1:E:101:MET:SD   | 1:E:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:F:207:TRP:HD1  | 1:F:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:F:463:LEU:HD22 | 1:F:467:PHE:HE2  | 1.55                     | 0.70              |
| 1:I:389:ILE:CD1  | 1:I:446:HIS:CE1  | 2.70                     | 0.70              |
| 1:I:463:LEU:HD22 | 1:I:467:PHE:HE2  | 1.55                     | 0.70              |
| 1:M:207:TRP:NE1  | 1:M:227:GLU:OE1  | 2.23                     | 0.70              |
| 1:O:513:SER:HB3  | 1:O:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:A:544:ASP:OD1  | 1:A:545:PHE:N    | 2.23                     | 0.70              |
| 1:B:207:TRP:NE1  | 1:B:227:GLU:OE1  | 2.23                     | 0.70              |
| 1:D:248:GLN:OE1  | 1:D:268:PHE:CZ   | 2.43                     | 0.70              |
| 1:E:248:GLN:OE1  | 1:E:268:PHE:CZ   | 2.44                     | 0.70              |
| 1:E:314:ARG:C    | 1:E:315:GLU:HG3  | 2.15                     | 0.70              |
| 1:E:1149:LEU:H   | 1:E:1196:ALA:HB2 | 1.56                     | 0.70              |
| 1:F:284:SER:OG   | 1:F:286:ASP:OD1  | 2.09                     | 0.70              |
| 1:G:101:MET:SD   | 1:G:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:G:513:SER:HB3  | 1:G:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:I:207:TRP:HD1  | 1:I:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:K:248:GLN:OE1  | 1:K:268:PHE:CZ   | 2.44                     | 0.70              |
| 1:K:284:SER:OG   | 1:K:286:ASP:OD1  | 2.09                     | 0.70              |
| 1:L:101:MET:SD   | 1:L:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:P:101:MET:SD   | 1:P:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:D:284:SER:OG   | 1:D:286:ASP:OD1  | 2.09                     | 0.70              |
| 1:D:547:PRO:CB   | 1:D:603:ILE:HG13 | 2.20                     | 0.70              |
| 1:G:314:ARG:C    | 1:G:315:GLU:HG3  | 2.15                     | 0.70              |
| 1:J:314:ARG:C    | 1:J:315:GLU:HG3  | 2.16                     | 0.70              |
| 1:K:547:PRO:CB   | 1:K:603:ILE:HG13 | 2.20                     | 0.70              |
| 1:L:314:ARG:C    | 1:L:315:GLU:HG3  | 2.16                     | 0.70              |
| 1:B:547:PRO:CB   | 1:B:603:ILE:HG13 | 2.20                     | 0.70              |
| 1:C:101:MET:SD   | 1:C:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:C:547:PRO:CB   | 1:C:603:ILE:HG13 | 2.20                     | 0.70              |
| 1:F:101:MET:SD   | 1:F:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:F:389:ILE:CD1  | 1:F:446:HIS:CE1  | 2.70                     | 0.70              |
| 1:H:101:MET:SD   | 1:H:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:H:248:GLN:OE1  | 1:H:268:PHE:CZ   | 2.43                     | 0.70              |
| 1:H:314:ARG:C    | 1:H:315:GLU:HG3  | 2.15                     | 0.70              |
| 1:I:101:MET:SD   | 1:I:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:J:207:TRP:HD1  | 1:J:227:GLU:OE2  | 1.74                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:1149:LEU:H  | 1:J:1196:ALA:HB2 | 1.56                     | 0.70              |
| 1:M:1149:LEU:H  | 1:M:1196:ALA:HB2 | 1.56                     | 0.70              |
| 1:O:101:MET:SD  | 1:O:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:O:314:ARG:C   | 1:O:315:GLU:HG3  | 2.16                     | 0.70              |
| 1:P:314:ARG:C   | 1:P:315:GLU:HG3  | 2.16                     | 0.70              |
| 1:A:317:LEU:C   | 1:A:318:THR:HG1  | 1.95                     | 0.70              |
| 1:B:207:TRP:HD1 | 1:B:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:I:313:PRO:CG  | 1:I:338:TRP:HZ2  | 1.98                     | 0.70              |
| 1:L:547:PRO:CB  | 1:L:603:ILE:HG13 | 2.20                     | 0.70              |
| 1:M:207:TRP:HD1 | 1:M:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:M:547:PRO:CB  | 1:M:603:ILE:HG13 | 2.20                     | 0.70              |
| 1:B:1149:LEU:H  | 1:B:1196:ALA:HB2 | 1.56                     | 0.70              |
| 1:D:207:TRP:HD1 | 1:D:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:E:207:TRP:HD1 | 1:E:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:N:317:LEU:C   | 1:N:318:THR:HG1  | 1.94                     | 0.70              |
| 1:K:207:TRP:HD1 | 1:K:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:N:1149:LEU:H  | 1:N:1196:ALA:HB2 | 1.56                     | 0.70              |
| 1:O:248:GLN:OE1 | 1:O:268:PHE:CZ   | 2.44                     | 0.70              |
| 1:A:1149:LEU:H  | 1:A:1196:ALA:HB2 | 1.56                     | 0.70              |
| 1:D:101:MET:SD  | 1:D:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:J:458:LEU:HG  | 1:J:587:ARG:NH2  | 2.05                     | 0.70              |
| 1:K:101:MET:SD  | 1:K:104:ARG:NH2  | 2.64                     | 0.70              |
| 1:N:248:GLN:OE1 | 1:N:268:PHE:CZ   | 2.43                     | 0.70              |
| 1:O:207:TRP:HD1 | 1:O:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:A:248:GLN:OE1 | 1:A:268:PHE:CZ   | 2.43                     | 0.70              |
| 1:B:284:SER:OG  | 1:B:286:ASP:OD1  | 2.09                     | 0.70              |
| 1:D:317:LEU:C   | 1:D:318:THR:HG1  | 1.95                     | 0.70              |
| 1:E:513:SER:HB3 | 1:E:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:H:1149:LEU:H  | 1:H:1196:ALA:HB2 | 1.56                     | 0.70              |
| 1:I:314:ARG:C   | 1:I:315:GLU:HG3  | 2.15                     | 0.70              |
| 1:N:207:TRP:HD1 | 1:N:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:A:207:TRP:HD1 | 1:A:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:C:513:SER:HB3 | 1:C:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:E:458:LEU:HG  | 1:E:587:ARG:NH2  | 2.05                     | 0.70              |
| 1:F:513:SER:HB3 | 1:F:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:H:207:TRP:HD1 | 1:H:227:GLU:OE2  | 1.74                     | 0.70              |
| 1:I:513:SER:HB3 | 1:I:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:J:513:SER:HB3 | 1:J:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:L:513:SER:HB3 | 1:L:514:ILE:HD12 | 1.72                     | 0.70              |
| 1:M:284:SER:OG  | 1:M:286:ASP:OD1  | 2.09                     | 0.70              |
| 1:N:284:SER:OG  | 1:N:286:ASP:OD1  | 2.09                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:389:ILE:CD1  | 1:O:446:HIS:CE1  | 2.70                     | 0.70              |
| 1:D:314:ARG:C    | 1:D:315:GLU:HG3  | 2.15                     | 0.69              |
| 1:K:222:HIS:CD2  | 1:L:198:LYS:NZ   | 2.59                     | 0.69              |
| 1:O:1149:LEU:H   | 1:O:1196:ALA:HB2 | 1.56                     | 0.69              |
| 1:P:317:LEU:HD21 | 1:P:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:B:317:LEU:HD21 | 1:B:341:TRP:CZ2  | 2.28                     | 0.69              |
| 1:C:545:PHE:HZ   | 1:C:565:ALA:HA   | 1.57                     | 0.69              |
| 1:G:317:LEU:HD21 | 1:G:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:K:314:ARG:C    | 1:K:315:GLU:HG3  | 2.16                     | 0.69              |
| 1:L:545:PHE:HZ   | 1:L:565:ALA:HA   | 1.57                     | 0.69              |
| 1:M:317:LEU:HD21 | 1:M:341:TRP:CZ2  | 2.28                     | 0.69              |
| 1:A:284:SER:OG   | 1:A:286:ASP:OD1  | 2.09                     | 0.69              |
| 1:F:314:ARG:C    | 1:F:315:GLU:HG3  | 2.15                     | 0.69              |
| 1:H:389:ILE:CD1  | 1:H:446:HIS:CE1  | 2.70                     | 0.69              |
| 1:I:1149:LEU:H   | 1:I:1196:ALA:HB2 | 1.56                     | 0.69              |
| 1:N:101:MET:SD   | 1:N:104:ARG:NH2  | 2.64                     | 0.69              |
| 1:N:207:TRP:NE1  | 1:N:227:GLU:OE1  | 2.23                     | 0.69              |
| 1:A:101:MET:SD   | 1:A:104:ARG:NH2  | 2.64                     | 0.69              |
| 1:A:207:TRP:NE1  | 1:A:227:GLU:OE1  | 2.23                     | 0.69              |
| 1:B:476:LYS:HA   | 1:B:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:B:505:SER:OG   | 1:B:513:SER:OG   | 2.05                     | 0.69              |
| 1:D:279:THR:HG23 | 1:D:280:THR:HG23 | 1.74                     | 0.69              |
| 1:E:279:THR:HG23 | 1:E:280:THR:HG23 | 1.74                     | 0.69              |
| 1:F:547:PRO:CB   | 1:F:603:ILE:HG13 | 2.20                     | 0.69              |
| 1:H:317:LEU:HD21 | 1:H:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:K:279:THR:HG23 | 1:K:280:THR:HG23 | 1.74                     | 0.69              |
| 1:M:476:LYS:HA   | 1:M:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:M:505:SER:OG   | 1:M:513:SER:OG   | 2.05                     | 0.69              |
| 1:A:476:LYS:HA   | 1:A:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:C:476:LYS:HA   | 1:C:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:F:1149:LEU:H   | 1:F:1196:ALA:HB2 | 1.56                     | 0.69              |
| 1:G:301:LEU:CD2  | 1:G:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:J:317:LEU:HD21 | 1:J:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:K:463:LEU:HD22 | 1:K:467:PHE:HE2  | 1.54                     | 0.69              |
| 1:N:476:LYS:HA   | 1:N:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:O:317:LEU:HD21 | 1:O:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:E:317:LEU:HD21 | 1:E:341:TRP:CZ2  | 2.28                     | 0.69              |
| 1:F:301:LEU:CD2  | 1:F:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:L:301:LEU:CD2  | 1:L:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:P:301:LEU:CD2  | 1:P:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:D:916:LYS:CE   | 1:E:1177:TYR:HE2 | 2.06                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:476:LYS:HA   | 1:H:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:I:279:THR:HG23 | 1:I:280:THR:HG23 | 1.74                     | 0.69              |
| 1:I:617:HIS:HE1  | 1:I:663:GLN:HB3  | 1.58                     | 0.69              |
| 1:J:279:THR:HG23 | 1:J:280:THR:HG23 | 1.74                     | 0.69              |
| 1:J:463:LEU:HD22 | 1:J:467:PHE:HE2  | 1.55                     | 0.69              |
| 1:N:317:LEU:HD21 | 1:N:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:A:279:THR:HG23 | 1:A:280:THR:HG23 | 1.74                     | 0.69              |
| 1:A:317:LEU:HD21 | 1:A:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:A:918:ILE:O    | 1:A:919:VAL:HG13 | 1.93                     | 0.69              |
| 1:B:248:GLN:OE1  | 1:B:268:PHE:CZ   | 2.43                     | 0.69              |
| 1:B:504:ASP:CB   | 1:B:509:ASN:O    | 2.41                     | 0.69              |
| 1:C:317:LEU:HD21 | 1:C:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:D:463:LEU:HD22 | 1:D:467:PHE:HE2  | 1.55                     | 0.69              |
| 1:E:617:HIS:HE1  | 1:E:663:GLN:HB3  | 1.58                     | 0.69              |
| 1:F:279:THR:HG23 | 1:F:280:THR:HG23 | 1.74                     | 0.69              |
| 1:F:617:HIS:HE1  | 1:F:663:GLN:HB3  | 1.58                     | 0.69              |
| 1:G:918:ILE:O    | 1:G:919:VAL:HG13 | 1.93                     | 0.69              |
| 1:I:301:LEU:CD2  | 1:I:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:J:617:HIS:HE1  | 1:J:663:GLN:HB3  | 1.58                     | 0.69              |
| 1:L:248:GLN:OE1  | 1:L:268:PHE:CZ   | 2.43                     | 0.69              |
| 1:L:279:THR:HG23 | 1:L:280:THR:HG23 | 1.74                     | 0.69              |
| 1:L:317:LEU:HD21 | 1:L:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:L:476:LYS:HA   | 1:L:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:M:248:GLN:OE1  | 1:M:268:PHE:CZ   | 2.44                     | 0.69              |
| 1:M:313:PRO:HG3  | 1:M:338:TRP:CZ2  | 2.28                     | 0.69              |
| 1:M:504:ASP:CB   | 1:M:509:ASN:O    | 2.41                     | 0.69              |
| 1:N:279:THR:HG23 | 1:N:280:THR:HG23 | 1.74                     | 0.69              |
| 1:N:918:ILE:O    | 1:N:919:VAL:HG13 | 1.93                     | 0.69              |
| 1:O:476:LYS:HA   | 1:O:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:B:313:PRO:HG3  | 1:B:338:TRP:CZ2  | 2.28                     | 0.69              |
| 1:D:317:LEU:HD21 | 1:D:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:E:476:LYS:HA   | 1:E:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:H:301:LEU:CD2  | 1:H:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:I:547:PRO:CB   | 1:I:603:ILE:HG13 | 2.20                     | 0.69              |
| 1:J:389:ILE:CD1  | 1:J:446:HIS:CE1  | 2.70                     | 0.69              |
| 1:J:476:LYS:HA   | 1:J:483:ARG:HH12 | 1.58                     | 0.69              |
| 1:J:545:PHE:HZ   | 1:J:565:ALA:HA   | 1.57                     | 0.69              |
| 1:K:130:PRO:HA   | 1:K:290:MET:HE1  | 1.75                     | 0.69              |
| 1:K:317:LEU:HD21 | 1:K:341:TRP:CZ2  | 2.27                     | 0.69              |
| 1:P:504:ASP:CB   | 1:P:509:ASN:O    | 2.41                     | 0.69              |
| 1:P:918:ILE:O    | 1:P:919:VAL:HG13 | 1.93                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:130:PRO:HA   | 1:C:290:MET:HE1  | 1.75                     | 0.69              |
| 1:C:301:LEU:CD2  | 1:C:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:D:130:PRO:HA   | 1:D:290:MET:HE1  | 1.75                     | 0.69              |
| 1:E:545:PHE:HZ   | 1:E:565:ALA:HA   | 1.57                     | 0.69              |
| 1:G:504:ASP:CB   | 1:G:509:ASN:O    | 2.41                     | 0.69              |
| 1:H:317:LEU:C    | 1:H:318:THR:HG1  | 1.95                     | 0.69              |
| 1:K:216:ASN:ND2  | 1:L:194:GLU:OE2  | 2.26                     | 0.69              |
| 1:M:918:ILE:O    | 1:M:919:VAL:HG13 | 1.93                     | 0.69              |
| 1:O:301:LEU:CD2  | 1:O:313:PRO:HG2  | 2.22                     | 0.69              |
| 1:B:617:HIS:HE1  | 1:B:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:B:918:ILE:O    | 1:B:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:C:248:GLN:OE1  | 1:C:268:PHE:CZ   | 2.43                     | 0.68              |
| 1:C:918:ILE:O    | 1:C:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:E:313:PRO:HG3  | 1:E:338:TRP:CZ2  | 2.28                     | 0.68              |
| 1:E:389:ILE:CD1  | 1:E:446:HIS:CE1  | 2.70                     | 0.68              |
| 1:F:122:LYS:HG3  | 1:G:276:SER:OG   | 1.93                     | 0.68              |
| 1:H:918:ILE:O    | 1:H:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:J:313:PRO:HG3  | 1:J:338:TRP:CZ2  | 2.28                     | 0.68              |
| 1:O:918:ILE:O    | 1:O:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:A:617:HIS:HE1  | 1:A:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:B:301:LEU:CD2  | 1:B:313:PRO:HG2  | 2.22                     | 0.68              |
| 1:E:523:PHE:HD1  | 1:E:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:F:317:LEU:HD21 | 1:F:341:TRP:CZ2  | 2.27                     | 0.68              |
| 1:F:383:THR:HG22 | 1:F:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:F:504:ASP:CB   | 1:F:509:ASN:O    | 2.41                     | 0.68              |
| 1:G:207:TRP:HD1  | 1:G:227:GLU:OE2  | 1.74                     | 0.68              |
| 1:G:382:PRO:CA   | 1:G:419:THR:HG22 | 2.24                     | 0.68              |
| 1:G:383:THR:HG22 | 1:G:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:H:313:PRO:HG3  | 1:H:338:TRP:CZ2  | 2.28                     | 0.68              |
| 1:H:463:LEU:HD22 | 1:H:467:PHE:HE2  | 1.55                     | 0.68              |
| 1:I:383:THR:HG22 | 1:I:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:J:523:PHE:HD1  | 1:J:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:L:130:PRO:HA   | 1:L:290:MET:HE1  | 1.76                     | 0.68              |
| 1:L:918:ILE:O    | 1:L:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:M:617:HIS:HE1  | 1:M:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:N:617:HIS:HE1  | 1:N:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:P:382:PRO:CA   | 1:P:419:THR:HG22 | 2.23                     | 0.68              |
| 1:A:504:ASP:CB   | 1:A:509:ASN:O    | 2.41                     | 0.68              |
| 1:C:279:THR:HG23 | 1:C:280:THR:HG23 | 1.74                     | 0.68              |
| 1:D:504:ASP:CB   | 1:D:509:ASN:O    | 2.41                     | 0.68              |
| 1:I:194:GLU:OE2  | 1:P:216:ASN:ND2  | 2.26                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:317:LEU:HD21 | 1:I:341:TRP:CZ2  | 2.27                     | 0.68              |
| 1:M:301:LEU:CD2  | 1:M:313:PRO:HG2  | 2.22                     | 0.68              |
| 1:N:383:THR:HG22 | 1:N:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:O:317:LEU:C    | 1:O:318:THR:HG1  | 1.95                     | 0.68              |
| 1:P:207:TRP:HD1  | 1:P:227:GLU:OE2  | 1.74                     | 0.68              |
| 1:P:383:THR:HG22 | 1:P:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:A:383:THR:HG22 | 1:A:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:B:130:PRO:HA   | 1:B:290:MET:HE1  | 1.76                     | 0.68              |
| 1:B:383:THR:HG22 | 1:B:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:D:476:LYS:HA   | 1:D:483:ARG:HH12 | 1.58                     | 0.68              |
| 1:D:523:PHE:HD1  | 1:D:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:E:382:PRO:CA   | 1:E:419:THR:HG22 | 2.23                     | 0.68              |
| 1:G:476:LYS:HA   | 1:G:483:ARG:HH12 | 1.58                     | 0.68              |
| 1:H:279:THR:HG23 | 1:H:280:THR:HG23 | 1.74                     | 0.68              |
| 1:I:504:ASP:CB   | 1:I:509:ASN:O    | 2.41                     | 0.68              |
| 1:K:476:LYS:HA   | 1:K:483:ARG:HH12 | 1.58                     | 0.68              |
| 1:K:504:ASP:CB   | 1:K:509:ASN:O    | 2.41                     | 0.68              |
| 1:K:523:PHE:HD1  | 1:K:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:M:130:PRO:HA   | 1:M:290:MET:HE1  | 1.75                     | 0.68              |
| 1:O:313:PRO:HG3  | 1:O:338:TRP:CZ2  | 2.28                     | 0.68              |
| 1:O:463:LEU:HD22 | 1:O:467:PHE:HE2  | 1.55                     | 0.68              |
| 1:A:301:LEU:CD2  | 1:A:313:PRO:HG2  | 2.22                     | 0.68              |
| 1:A:523:PHE:HD1  | 1:A:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:A:547:PRO:CB   | 1:A:603:ILE:HG13 | 2.20                     | 0.68              |
| 1:E:130:PRO:HA   | 1:E:290:MET:HE1  | 1.75                     | 0.68              |
| 1:F:545:PHE:HZ   | 1:F:565:ALA:HA   | 1.57                     | 0.68              |
| 1:H:207:TRP:NE1  | 1:H:227:GLU:OE1  | 2.23                     | 0.68              |
| 1:I:14:ASP:OD2   | 1:P:142:ARG:NH1  | 2.27                     | 0.68              |
| 1:I:313:PRO:HG3  | 1:I:338:TRP:CZ2  | 2.28                     | 0.68              |
| 1:I:545:PHE:HZ   | 1:I:565:ALA:HA   | 1.57                     | 0.68              |
| 1:J:130:PRO:HA   | 1:J:290:MET:HE1  | 1.76                     | 0.68              |
| 1:J:382:PRO:CA   | 1:J:419:THR:HG22 | 2.24                     | 0.68              |
| 1:M:383:THR:HG22 | 1:M:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:N:301:LEU:CD2  | 1:N:313:PRO:HG2  | 2.22                     | 0.68              |
| 1:N:504:ASP:CB   | 1:N:509:ASN:O    | 2.41                     | 0.68              |
| 1:O:383:THR:HG22 | 1:O:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:P:476:LYS:HA   | 1:P:483:ARG:HH12 | 1.58                     | 0.68              |
| 1:B:523:PHE:HD1  | 1:B:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:C:504:ASP:CB   | 1:C:509:ASN:O    | 2.41                     | 0.68              |
| 1:C:617:HIS:HE1  | 1:C:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:I:523:PHE:HD1  | 1:I:527:TYR:HE2  | 1.42                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:523:PHE:HD1  | 1:M:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:N:523:PHE:HD1  | 1:N:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:E:918:ILE:O    | 1:E:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:F:523:PHE:HD1  | 1:F:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:F:918:ILE:O    | 1:F:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:H:383:THR:HG22 | 1:H:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:L:504:ASP:CB   | 1:L:509:ASN:O    | 2.41                     | 0.68              |
| 1:O:279:THR:HG23 | 1:O:280:THR:HG23 | 1.74                     | 0.68              |
| 1:O:617:HIS:HE1  | 1:O:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:E:383:THR:HG22 | 1:E:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:F:313:PRO:HG3  | 1:F:338:TRP:CZ2  | 2.28                     | 0.68              |
| 1:G:207:TRP:NE1  | 1:G:227:GLU:OE1  | 2.23                     | 0.68              |
| 1:G:617:HIS:HE1  | 1:G:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:J:918:ILE:O    | 1:J:919:VAL:HG13 | 1.93                     | 0.68              |
| 1:O:207:TRP:NE1  | 1:O:227:GLU:OE1  | 2.23                     | 0.68              |
| 1:O:523:PHE:HD1  | 1:O:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:P:207:TRP:NE1  | 1:P:227:GLU:OE1  | 2.23                     | 0.68              |
| 1:P:523:PHE:HD1  | 1:P:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:P:617:HIS:HE1  | 1:P:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:A:130:PRO:HA   | 1:A:290:MET:HE1  | 1.75                     | 0.68              |
| 1:D:617:HIS:HE1  | 1:D:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:E:301:LEU:CD2  | 1:E:313:PRO:HG2  | 2.22                     | 0.68              |
| 1:E:463:LEU:HD22 | 1:E:467:PHE:HE2  | 1.55                     | 0.68              |
| 1:F:517:THR:HG23 | 1:F:518:LEU:N    | 2.09                     | 0.68              |
| 1:H:523:PHE:HD1  | 1:H:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:H:617:HIS:HE1  | 1:H:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:I:517:THR:HG23 | 1:I:518:LEU:N    | 2.09                     | 0.68              |
| 1:N:130:PRO:HA   | 1:N:290:MET:HE1  | 1.75                     | 0.68              |
| 1:N:463:LEU:HD22 | 1:N:467:PHE:HE2  | 1.55                     | 0.68              |
| 1:A:463:LEU:HD22 | 1:A:467:PHE:HE2  | 1.55                     | 0.68              |
| 1:D:517:THR:HG23 | 1:D:518:LEU:N    | 2.09                     | 0.68              |
| 1:G:279:THR:HG23 | 1:G:280:THR:HG23 | 1.74                     | 0.68              |
| 1:G:523:PHE:HD1  | 1:G:527:TYR:HE2  | 1.42                     | 0.68              |
| 1:J:383:THR:HG22 | 1:J:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:K:617:HIS:HE1  | 1:K:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:L:383:THR:HG22 | 1:L:420:ILE:HG23 | 1.76                     | 0.68              |
| 1:L:617:HIS:HE1  | 1:L:663:GLN:HB3  | 1.58                     | 0.68              |
| 1:N:517:THR:HG23 | 1:N:518:LEU:N    | 2.09                     | 0.68              |
| 1:P:279:THR:HG23 | 1:P:280:THR:HG23 | 1.74                     | 0.67              |
| 1:A:517:THR:HG23 | 1:A:518:LEU:N    | 2.09                     | 0.67              |
| 1:C:383:THR:HG22 | 1:C:420:ILE:HG23 | 1.76                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:476:LYS:HA   | 1:F:483:ARG:HH12 | 1.58                     | 0.67              |
| 1:H:130:PRO:HA   | 1:H:290:MET:HE1  | 1.75                     | 0.67              |
| 1:H:398:VAL:HG23 | 1:H:399:MET:H    | 1.60                     | 0.67              |
| 1:I:918:ILE:O    | 1:I:919:VAL:HG13 | 1.93                     | 0.67              |
| 1:J:301:LEU:CD2  | 1:J:313:PRO:HG2  | 2.22                     | 0.67              |
| 1:K:517:THR:HG23 | 1:K:518:LEU:N    | 2.09                     | 0.67              |
| 1:L:382:PRO:CA   | 1:L:419:THR:HG22 | 2.24                     | 0.67              |
| 1:N:389:ILE:CD1  | 1:N:446:HIS:CE1  | 2.70                     | 0.67              |
| 1:O:504:ASP:CB   | 1:O:509:ASN:O    | 2.41                     | 0.67              |
| 1:P:517:THR:HG23 | 1:P:518:LEU:N    | 2.09                     | 0.67              |
| 1:B:517:THR:HG23 | 1:B:518:LEU:N    | 2.09                     | 0.67              |
| 1:C:517:THR:HG23 | 1:C:518:LEU:N    | 2.09                     | 0.67              |
| 1:D:313:PRO:HG3  | 1:D:338:TRP:CZ2  | 2.28                     | 0.67              |
| 1:F:130:PRO:HA   | 1:F:290:MET:HE1  | 1.75                     | 0.67              |
| 1:G:517:THR:HG23 | 1:G:518:LEU:N    | 2.09                     | 0.67              |
| 1:H:504:ASP:CB   | 1:H:509:ASN:O    | 2.41                     | 0.67              |
| 1:H:517:THR:HG23 | 1:H:518:LEU:N    | 2.09                     | 0.67              |
| 1:I:476:LYS:HA   | 1:I:483:ARG:HH12 | 1.58                     | 0.67              |
| 1:L:517:THR:HG23 | 1:L:518:LEU:N    | 2.09                     | 0.67              |
| 1:N:398:VAL:HG23 | 1:N:399:MET:H    | 1.60                     | 0.67              |
| 1:O:130:PRO:HA   | 1:O:290:MET:HE1  | 1.75                     | 0.67              |
| 1:O:398:VAL:HG23 | 1:O:399:MET:H    | 1.60                     | 0.67              |
| 1:A:398:VAL:HG23 | 1:A:399:MET:H    | 1.60                     | 0.67              |
| 1:A:545:PHE:HZ   | 1:A:565:ALA:HA   | 1.57                     | 0.67              |
| 1:D:383:THR:HG22 | 1:D:420:ILE:HG23 | 1.76                     | 0.67              |
| 1:D:405:LEU:HG   | 1:D:411:VAL:HG23 | 1.77                     | 0.67              |
| 1:G:398:VAL:HG23 | 1:G:399:MET:H    | 1.60                     | 0.67              |
| 1:K:313:PRO:HG3  | 1:K:338:TRP:CZ2  | 2.28                     | 0.67              |
| 1:K:383:THR:HG22 | 1:K:420:ILE:HG23 | 1.76                     | 0.67              |
| 1:L:523:PHE:HD1  | 1:L:527:TYR:HE2  | 1.42                     | 0.67              |
| 1:M:517:THR:HG23 | 1:M:518:LEU:N    | 2.09                     | 0.67              |
| 1:B:279:THR:HG23 | 1:B:280:THR:HG23 | 1.74                     | 0.67              |
| 1:B:398:VAL:HG23 | 1:B:399:MET:H    | 1.60                     | 0.67              |
| 1:C:313:PRO:HG3  | 1:C:338:TRP:CZ2  | 2.28                     | 0.67              |
| 1:C:523:PHE:HD1  | 1:C:527:TYR:HE2  | 1.42                     | 0.67              |
| 1:G:517:THR:HA   | 1:G:520:GLN:CD   | 2.19                     | 0.67              |
| 1:I:207:TRP:NE1  | 1:I:227:GLU:OE1  | 2.23                     | 0.67              |
| 1:L:398:VAL:HG23 | 1:L:399:MET:H    | 1.60                     | 0.67              |
| 1:M:398:VAL:HG23 | 1:M:399:MET:H    | 1.60                     | 0.67              |
| 1:P:130:PRO:HA   | 1:P:290:MET:HE1  | 1.75                     | 0.67              |
| 1:I:130:PRO:HA   | 1:I:290:MET:HE1  | 1.75                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:398:VAL:HG23 | 1:I:399:MET:H    | 1.60                     | 0.67              |
| 1:J:517:THR:HG23 | 1:J:518:LEU:N    | 2.09                     | 0.67              |
| 1:K:276:SER:HB3  | 1:L:121:ALA:CB   | 2.14                     | 0.67              |
| 1:K:405:LEU:HG   | 1:K:411:VAL:HG23 | 1.77                     | 0.67              |
| 1:O:142:ARG:NH1  | 1:P:14:ASP:OD2   | 2.28                     | 0.67              |
| 1:O:382:PRO:CA   | 1:O:419:THR:HG22 | 2.23                     | 0.67              |
| 1:P:398:VAL:HG23 | 1:P:399:MET:H    | 1.60                     | 0.67              |
| 1:P:517:THR:HA   | 1:P:520:GLN:CD   | 2.20                     | 0.67              |
| 1:A:389:ILE:CD1  | 1:A:446:HIS:CE1  | 2.70                     | 0.67              |
| 1:B:545:PHE:HZ   | 1:B:565:ALA:HA   | 1.57                     | 0.67              |
| 1:C:382:PRO:CA   | 1:C:419:THR:HG22 | 2.24                     | 0.67              |
| 1:C:398:VAL:HG23 | 1:C:399:MET:H    | 1.60                     | 0.67              |
| 1:E:517:THR:HG23 | 1:E:518:LEU:N    | 2.09                     | 0.67              |
| 1:G:130:PRO:HA   | 1:G:290:MET:HE1  | 1.76                     | 0.67              |
| 1:K:142:ARG:NH1  | 1:L:14:ASP:OD2   | 2.27                     | 0.67              |
| 1:M:279:THR:HG23 | 1:M:280:THR:HG23 | 1.74                     | 0.67              |
| 1:M:545:PHE:HZ   | 1:M:565:ALA:HA   | 1.58                     | 0.67              |
| 1:N:545:PHE:HZ   | 1:N:565:ALA:HA   | 1.57                     | 0.67              |
| 1:A:11:GLN:HE21  | 1:A:70:GLU:HB3   | 1.60                     | 0.67              |
| 1:A:382:PRO:CA   | 1:A:419:THR:HG22 | 2.23                     | 0.67              |
| 1:B:382:PRO:CA   | 1:B:419:THR:HG22 | 2.23                     | 0.67              |
| 1:F:207:TRP:NE1  | 1:F:227:GLU:OE1  | 2.23                     | 0.67              |
| 1:H:11:GLN:HE21  | 1:H:70:GLU:HB3   | 1.60                     | 0.67              |
| 1:H:382:PRO:CA   | 1:H:419:THR:HG22 | 2.23                     | 0.67              |
| 1:H:517:THR:HA   | 1:H:520:GLN:CD   | 2.19                     | 0.67              |
| 1:I:517:THR:HA   | 1:I:520:GLN:CD   | 2.19                     | 0.67              |
| 1:K:918:ILE:O    | 1:K:919:VAL:HG13 | 1.93                     | 0.67              |
| 1:L:313:PRO:HG3  | 1:L:338:TRP:CZ2  | 2.28                     | 0.67              |
| 1:L:405:LEU:HG   | 1:L:411:VAL:HG23 | 1.77                     | 0.67              |
| 1:M:11:GLN:HE21  | 1:M:70:GLU:HB3   | 1.60                     | 0.67              |
| 1:N:517:THR:HA   | 1:N:520:GLN:CD   | 2.19                     | 0.67              |
| 1:O:517:THR:HG23 | 1:O:518:LEU:N    | 2.09                     | 0.67              |
| 1:B:11:GLN:HE21  | 1:B:70:GLU:HB3   | 1.60                     | 0.67              |
| 1:D:918:ILE:O    | 1:D:919:VAL:HG13 | 1.93                     | 0.67              |
| 1:E:398:VAL:HG23 | 1:E:399:MET:H    | 1.60                     | 0.67              |
| 1:F:517:THR:HA   | 1:F:520:GLN:CD   | 2.20                     | 0.67              |
| 1:J:398:VAL:HG23 | 1:J:399:MET:H    | 1.60                     | 0.67              |
| 1:L:11:GLN:HE21  | 1:L:70:GLU:HB3   | 1.60                     | 0.67              |
| 1:N:11:GLN:HE21  | 1:N:70:GLU:HB3   | 1.60                     | 0.67              |
| 1:O:11:GLN:HE21  | 1:O:70:GLU:HB3   | 1.60                     | 0.67              |
| 1:O:517:THR:HA   | 1:O:520:GLN:CD   | 2.19                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:11:GLN:HE21  | 1:P:70:GLU:HB3    | 1.60                     | 0.67              |
| 1:P:313:PRO:HG3  | 1:P:338:TRP:CZ2   | 2.28                     | 0.67              |
| 1:C:317:LEU:CD2  | 1:C:341:TRP:CZ2   | 2.78                     | 0.67              |
| 1:K:398:VAL:HG23 | 1:K:399:MET:H     | 1.60                     | 0.67              |
| 1:M:382:PRO:CA   | 1:M:419:THR:HG22  | 2.24                     | 0.67              |
| 1:N:382:PRO:CA   | 1:N:419:THR:HG22  | 2.24                     | 0.67              |
| 1:O:545:PHE:HZ   | 1:O:565:ALA:HA    | 1.57                     | 0.67              |
| 1:P:598:GLN:HG2  | 1:P:1228:ILE:HG23 | 1.77                     | 0.67              |
| 1:C:11:GLN:HE21  | 1:C:70:GLU:HB3    | 1.60                     | 0.66              |
| 1:F:398:VAL:HG23 | 1:F:399:MET:H     | 1.60                     | 0.66              |
| 1:F:598:GLN:HG2  | 1:F:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:G:11:GLN:HE21  | 1:G:70:GLU:HB3    | 1.60                     | 0.66              |
| 1:G:313:PRO:HG3  | 1:G:338:TRP:CZ2   | 2.28                     | 0.66              |
| 1:H:598:GLN:HG2  | 1:H:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:I:317:LEU:CD2  | 1:I:341:TRP:CZ2   | 2.79                     | 0.66              |
| 1:I:382:PRO:CA   | 1:I:419:THR:HG22  | 2.23                     | 0.66              |
| 1:J:317:LEU:CD2  | 1:J:341:TRP:CZ2   | 2.78                     | 0.66              |
| 1:J:598:GLN:HG2  | 1:J:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:L:317:LEU:CD2  | 1:L:341:TRP:CZ2   | 2.79                     | 0.66              |
| 1:M:517:THR:HA   | 1:M:520:GLN:CD    | 2.20                     | 0.66              |
| 1:M:520:GLN:HB3  | 1:M:524:TYR:OH    | 1.95                     | 0.66              |
| 1:O:598:GLN:HG2  | 1:O:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:A:313:PRO:HG3  | 1:A:338:TRP:CZ2   | 2.28                     | 0.66              |
| 1:A:517:THR:HA   | 1:A:520:GLN:CD    | 2.20                     | 0.66              |
| 1:B:520:GLN:HB3  | 1:B:524:TYR:OH    | 1.95                     | 0.66              |
| 1:C:405:LEU:HG   | 1:C:411:VAL:HG23  | 1.77                     | 0.66              |
| 1:D:398:VAL:HG23 | 1:D:399:MET:H     | 1.60                     | 0.66              |
| 1:E:317:LEU:CD2  | 1:E:341:TRP:CZ2   | 2.79                     | 0.66              |
| 1:E:598:GLN:HG2  | 1:E:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:F:317:LEU:CD2  | 1:F:341:TRP:CZ2   | 2.79                     | 0.66              |
| 1:G:598:GLN:HG2  | 1:G:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:H:545:PHE:HZ   | 1:H:565:ALA:HA    | 1.57                     | 0.66              |
| 1:I:598:GLN:HG2  | 1:I:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:K:11:GLN:HE21  | 1:K:70:GLU:HB3    | 1.60                     | 0.66              |
| 1:L:914:VAL:CG2  | 1:L:917:TYR:O     | 2.44                     | 0.66              |
| 1:M:637:LEU:O    | 1:M:638:GLU:CB    | 2.43                     | 0.66              |
| 1:B:121:ALA:CB   | 1:C:276:SER:CB    | 2.61                     | 0.66              |
| 1:C:914:VAL:CG2  | 1:C:917:TYR:O     | 2.44                     | 0.66              |
| 1:D:11:GLN:HE21  | 1:D:70:GLU:HB3    | 1.60                     | 0.66              |
| 1:D:520:GLN:HB3  | 1:D:524:TYR:OH    | 1.96                     | 0.66              |
| 1:E:914:VAL:CG2  | 1:E:917:TYR:O     | 2.44                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:122:LYS:CG   | 1:G:276:SER:OG    | 2.43                     | 0.66              |
| 1:J:914:VAL:CG2  | 1:J:917:TYR:O     | 2.44                     | 0.66              |
| 1:J:1177:TYR:HE2 | 1:K:916:LYS:CE    | 2.08                     | 0.66              |
| 1:L:463:LEU:HD22 | 1:L:467:PHE:HE2   | 1.55                     | 0.66              |
| 1:N:313:PRO:HG3  | 1:N:338:TRP:CZ2   | 2.28                     | 0.66              |
| 1:A:520:GLN:HB3  | 1:A:524:TYR:OH    | 1.95                     | 0.66              |
| 1:B:517:THR:HA   | 1:B:520:GLN:CD    | 2.20                     | 0.66              |
| 1:K:520:GLN:HB3  | 1:K:524:TYR:OH    | 1.96                     | 0.66              |
| 1:L:517:THR:HA   | 1:L:520:GLN:CD    | 2.19                     | 0.66              |
| 1:N:598:GLN:HG2  | 1:N:1228:ILE:HG23 | 1.77                     | 0.66              |
| 1:B:463:LEU:HD22 | 1:B:467:PHE:HE2   | 1.55                     | 0.66              |
| 1:F:382:PRO:CA   | 1:F:419:THR:HG22  | 2.24                     | 0.66              |
| 1:N:520:GLN:HB3  | 1:N:524:TYR:OH    | 1.95                     | 0.66              |
| 1:D:266:THR:HG21 | 1:D:271:VAL:HB    | 1.78                     | 0.66              |
| 1:H:1214:LEU:HB3 | 1:H:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:I:464:ASP:O    | 1:I:468:TYR:CE2   | 2.49                     | 0.66              |
| 1:K:266:THR:HG21 | 1:K:271:VAL:HB    | 1.78                     | 0.66              |
| 1:K:389:ILE:CD1  | 1:K:446:HIS:CE1   | 2.70                     | 0.66              |
| 1:O:1214:LEU:HB3 | 1:O:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:A:598:GLN:HG2  | 1:A:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:B:317:LEU:CD2  | 1:B:341:TRP:CZ2   | 2.79                     | 0.66              |
| 1:D:916:LYS:HE2  | 1:E:1177:TYR:HE2  | 1.60                     | 0.66              |
| 1:F:198:LYS:HZ1  | 1:G:222:HIS:CG    | 2.14                     | 0.66              |
| 1:G:464:ASP:O    | 1:G:468:TYR:CE2   | 2.49                     | 0.66              |
| 1:G:1214:LEU:HB3 | 1:G:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:J:517:THR:HA   | 1:J:520:GLN:CD    | 2.20                     | 0.66              |
| 1:O:413:LYS:O    | 1:O:421:SER:HB3   | 1.95                     | 0.66              |
| 1:C:266:THR:HG21 | 1:C:271:VAL:HB    | 1.78                     | 0.66              |
| 1:F:464:ASP:O    | 1:F:468:TYR:CE2   | 2.49                     | 0.66              |
| 1:G:499:GLN:NE2  | 1:G:516:ASN:HB3   | 2.11                     | 0.66              |
| 1:H:405:LEU:HG   | 1:H:411:VAL:HG23  | 1.77                     | 0.66              |
| 1:H:413:LYS:O    | 1:H:421:SER:HB3   | 1.96                     | 0.66              |
| 1:I:914:VAL:CG2  | 1:I:917:TYR:O     | 2.44                     | 0.66              |
| 1:J:266:THR:HG21 | 1:J:271:VAL:HB    | 1.78                     | 0.66              |
| 1:J:464:ASP:O    | 1:J:468:TYR:CE2   | 2.49                     | 0.66              |
| 1:J:1214:LEU:HB3 | 1:J:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:K:492:LEU:HD11 | 1:K:561:LEU:HD21  | 1.78                     | 0.66              |
| 1:L:216:ASN:ND2  | 1:M:194:GLU:OE2   | 2.29                     | 0.66              |
| 1:L:266:THR:HG21 | 1:L:271:VAL:HB    | 1.78                     | 0.66              |
| 1:L:313:PRO:CG   | 1:L:338:TRP:HE1   | 2.07                     | 0.66              |
| 1:M:317:LEU:CD2  | 1:M:341:TRP:CZ2   | 2.79                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:464:ASP:O    | 1:P:468:TYR:CE2   | 2.49                     | 0.66              |
| 1:A:914:VAL:CG2  | 1:A:917:TYR:O     | 2.44                     | 0.66              |
| 1:D:317:LEU:CD2  | 1:D:341:TRP:CZ2   | 2.79                     | 0.66              |
| 1:D:389:ILE:CD1  | 1:D:446:HIS:CE1   | 2.70                     | 0.66              |
| 1:D:492:LEU:HD11 | 1:D:561:LEU:HD21  | 1.78                     | 0.66              |
| 1:D:517:THR:HA   | 1:D:520:GLN:CD    | 2.20                     | 0.66              |
| 1:D:598:GLN:HG2  | 1:D:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:D:637:LEU:O    | 1:D:638:GLU:CB    | 2.43                     | 0.66              |
| 1:E:464:ASP:O    | 1:E:468:TYR:CE2   | 2.49                     | 0.66              |
| 1:E:517:THR:HA   | 1:E:520:GLN:CD    | 2.20                     | 0.66              |
| 1:E:637:LEU:O    | 1:E:638:GLU:CB    | 2.43                     | 0.66              |
| 1:E:1214:LEU:HB3 | 1:E:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:F:914:VAL:CG2  | 1:F:917:TYR:O     | 2.44                     | 0.66              |
| 1:I:1214:LEU:HB3 | 1:I:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:K:317:LEU:CD2  | 1:K:341:TRP:CZ2   | 2.79                     | 0.66              |
| 1:K:598:GLN:HG2  | 1:K:1228:ILE:HG23 | 1.78                     | 0.66              |
| 1:N:914:VAL:CG2  | 1:N:917:TYR:O     | 2.44                     | 0.66              |
| 1:O:405:LEU:HG   | 1:O:411:VAL:HG23  | 1.77                     | 0.66              |
| 1:P:405:LEU:HG   | 1:P:411:VAL:HG23  | 1.77                     | 0.66              |
| 1:P:492:LEU:HD11 | 1:P:561:LEU:HD21  | 1.78                     | 0.66              |
| 1:P:499:GLN:NE2  | 1:P:516:ASN:HB3   | 2.11                     | 0.66              |
| 1:P:1214:LEU:HB3 | 1:P:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:A:413:LYS:O    | 1:A:421:SER:HB3   | 1.96                     | 0.66              |
| 1:A:1214:LEU:HB3 | 1:A:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:B:413:LYS:O    | 1:B:421:SER:HB3   | 1.96                     | 0.66              |
| 1:C:413:LYS:O    | 1:C:421:SER:HB3   | 1.96                     | 0.66              |
| 1:C:517:THR:HA   | 1:C:520:GLN:CD    | 2.20                     | 0.66              |
| 1:D:914:VAL:CG2  | 1:D:917:TYR:O     | 2.44                     | 0.66              |
| 1:E:266:THR:HG21 | 1:E:271:VAL:HB    | 1.78                     | 0.66              |
| 1:E:413:LYS:O    | 1:E:421:SER:HB3   | 1.96                     | 0.66              |
| 1:E:504:ASP:CB   | 1:E:509:ASN:O     | 2.41                     | 0.66              |
| 1:F:11:GLN:HE21  | 1:F:70:GLU:HB3    | 1.60                     | 0.66              |
| 1:F:492:LEU:HD11 | 1:F:561:LEU:HD21  | 1.78                     | 0.66              |
| 1:F:1214:LEU:HB3 | 1:F:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:G:317:LEU:C    | 1:G:318:THR:HG1   | 1.95                     | 0.66              |
| 1:G:405:LEU:HG   | 1:G:411:VAL:HG23  | 1.77                     | 0.66              |
| 1:G:508:TRP:C    | 1:G:606:GLY:CA    | 2.69                     | 0.66              |
| 1:G:520:GLN:HB3  | 1:G:524:TYR:OH    | 1.96                     | 0.66              |
| 1:J:142:ARG:NH1  | 1:K:14:ASP:OD2    | 2.29                     | 0.66              |
| 1:J:504:ASP:CB   | 1:J:509:ASN:O     | 2.41                     | 0.66              |
| 1:J:637:LEU:O    | 1:J:638:GLU:CB    | 2.43                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:517:THR:HA   | 1:K:520:GLN:CD    | 2.20                     | 0.66              |
| 1:K:637:LEU:O    | 1:K:638:GLU:CB    | 2.43                     | 0.66              |
| 1:K:914:VAL:CG2  | 1:K:917:TYR:O     | 2.44                     | 0.66              |
| 1:M:413:LYS:O    | 1:M:421:SER:HB3   | 1.96                     | 0.66              |
| 1:M:463:LEU:HD22 | 1:M:467:PHE:HE2   | 1.55                     | 0.66              |
| 1:N:1214:LEU:HB3 | 1:N:1223:GLN:HA   | 1.78                     | 0.66              |
| 1:O:499:GLN:NE2  | 1:O:516:ASN:HB3   | 2.11                     | 0.66              |
| 1:P:317:LEU:CD2  | 1:P:341:TRP:CZ2   | 2.78                     | 0.66              |
| 1:P:508:TRP:C    | 1:P:606:GLY:CA    | 2.69                     | 0.66              |
| 1:P:520:GLN:HB3  | 1:P:524:TYR:OH    | 1.96                     | 0.66              |
| 1:A:405:LEU:HG   | 1:A:411:VAL:HG23  | 1.77                     | 0.65              |
| 1:B:598:GLN:HG2  | 1:B:1228:ILE:HG23 | 1.78                     | 0.65              |
| 1:C:313:PRO:CG   | 1:C:338:TRP:HE1   | 2.07                     | 0.65              |
| 1:D:301:LEU:CD2  | 1:D:313:PRO:HG2   | 2.22                     | 0.65              |
| 1:G:317:LEU:CD2  | 1:G:341:TRP:CZ2   | 2.79                     | 0.65              |
| 1:G:492:LEU:HD11 | 1:G:561:LEU:HD21  | 1.78                     | 0.65              |
| 1:G:914:VAL:CG2  | 1:G:917:TYR:O     | 2.44                     | 0.65              |
| 1:H:451:LYS:HD3  | 1:H:486:LEU:CD2   | 2.26                     | 0.65              |
| 1:H:508:TRP:C    | 1:H:606:GLY:CA    | 2.70                     | 0.65              |
| 1:I:508:TRP:C    | 1:I:606:GLY:CA    | 2.69                     | 0.65              |
| 1:J:413:LYS:O    | 1:J:421:SER:HB3   | 1.96                     | 0.65              |
| 1:J:499:GLN:NE2  | 1:J:516:ASN:HB3   | 2.11                     | 0.65              |
| 1:M:598:GLN:HG2  | 1:M:1228:ILE:HG23 | 1.78                     | 0.65              |
| 1:N:492:LEU:HD11 | 1:N:561:LEU:HD21  | 1.78                     | 0.65              |
| 1:O:508:TRP:C    | 1:O:606:GLY:CA    | 2.69                     | 0.65              |
| 1:O:520:GLN:HB3  | 1:O:524:TYR:OH    | 1.96                     | 0.65              |
| 1:E:499:GLN:NE2  | 1:E:516:ASN:HB3   | 2.11                     | 0.65              |
| 1:F:413:LYS:O    | 1:F:421:SER:HB3   | 1.95                     | 0.65              |
| 1:F:508:TRP:C    | 1:F:606:GLY:CA    | 2.69                     | 0.65              |
| 1:F:520:GLN:HB3  | 1:F:524:TYR:OH    | 1.95                     | 0.65              |
| 1:H:499:GLN:NE2  | 1:H:516:ASN:HB3   | 2.11                     | 0.65              |
| 1:H:520:GLN:HB3  | 1:H:524:TYR:OH    | 1.95                     | 0.65              |
| 1:H:914:VAL:CG2  | 1:H:917:TYR:O     | 2.44                     | 0.65              |
| 1:I:492:LEU:HD11 | 1:I:561:LEU:HD21  | 1.78                     | 0.65              |
| 1:J:517:THR:HG23 | 1:J:518:LEU:H     | 1.62                     | 0.65              |
| 1:K:464:ASP:O    | 1:K:468:TYR:CE2   | 2.49                     | 0.65              |
| 1:L:598:GLN:HG2  | 1:L:1228:ILE:HG23 | 1.78                     | 0.65              |
| 1:M:389:ILE:CD1  | 1:M:446:HIS:CE1   | 2.70                     | 0.65              |
| 1:O:451:LYS:HD3  | 1:O:486:LEU:CD2   | 2.26                     | 0.65              |
| 1:O:464:ASP:O    | 1:O:468:TYR:CE2   | 2.49                     | 0.65              |
| 1:O:517:THR:HG23 | 1:O:518:LEU:H     | 1.62                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:317:LEU:C    | 1:P:318:THR:HG1   | 1.95                     | 0.65              |
| 1:P:914:VAL:CG2  | 1:P:917:TYR:O     | 2.44                     | 0.65              |
| 1:A:492:LEU:HD11 | 1:A:561:LEU:HD21  | 1.78                     | 0.65              |
| 1:A:508:TRP:C    | 1:A:606:GLY:CA    | 2.69                     | 0.65              |
| 1:B:266:THR:HG21 | 1:B:271:VAL:HB    | 1.78                     | 0.65              |
| 1:C:315:GLU:O    | 1:C:316:VAL:HG22  | 1.97                     | 0.65              |
| 1:E:11:GLN:HE21  | 1:E:70:GLU:HB3    | 1.60                     | 0.65              |
| 1:E:517:THR:HG23 | 1:E:518:LEU:H     | 1.62                     | 0.65              |
| 1:F:266:THR:HG21 | 1:F:271:VAL:HB    | 1.78                     | 0.65              |
| 1:H:464:ASP:O    | 1:H:468:TYR:CE2   | 2.49                     | 0.65              |
| 1:H:517:THR:HG23 | 1:H:518:LEU:H     | 1.62                     | 0.65              |
| 1:K:301:LEU:CD2  | 1:K:313:PRO:HG2   | 2.22                     | 0.65              |
| 1:L:389:ILE:CD1  | 1:L:446:HIS:CE1   | 2.70                     | 0.65              |
| 1:L:413:LYS:O    | 1:L:421:SER:HB3   | 1.96                     | 0.65              |
| 1:M:266:THR:HG21 | 1:M:271:VAL:HB    | 1.78                     | 0.65              |
| 1:N:266:THR:HG21 | 1:N:271:VAL:HB    | 1.78                     | 0.65              |
| 1:N:405:LEU:HG   | 1:N:411:VAL:HG23  | 1.77                     | 0.65              |
| 1:N:413:LYS:O    | 1:N:421:SER:HB3   | 1.96                     | 0.65              |
| 1:N:508:TRP:C    | 1:N:606:GLY:CA    | 2.69                     | 0.65              |
| 1:O:914:VAL:CG2  | 1:O:917:TYR:O     | 2.44                     | 0.65              |
| 1:A:266:THR:HG21 | 1:A:271:VAL:HB    | 1.78                     | 0.65              |
| 1:C:463:LEU:HD22 | 1:C:467:PHE:HE2   | 1.55                     | 0.65              |
| 1:C:598:GLN:HG2  | 1:C:1228:ILE:HG23 | 1.78                     | 0.65              |
| 1:D:315:GLU:O    | 1:D:316:VAL:HG22  | 1.97                     | 0.65              |
| 1:D:464:ASP:O    | 1:D:468:TYR:CE2   | 2.49                     | 0.65              |
| 1:D:499:GLN:NE2  | 1:D:516:ASN:HB3   | 2.11                     | 0.65              |
| 1:D:517:THR:HG23 | 1:D:518:LEU:H     | 1.62                     | 0.65              |
| 1:D:1214:LEU:HB3 | 1:D:1223:GLN:HA   | 1.78                     | 0.65              |
| 2:F:1501:DTP:O2A | 2:F:1501:DTP:H8   | 1.96                     | 0.65              |
| 1:G:315:GLU:O    | 1:G:316:VAL:HG22  | 1.97                     | 0.65              |
| 1:H:252:ALA:O    | 1:H:255:ALA:N     | 2.25                     | 0.65              |
| 1:I:520:GLN:HB3  | 1:I:524:TYR:OH    | 1.96                     | 0.65              |
| 2:I:1501:DTP:O1A | 2:I:1501:DTP:H8   | 1.97                     | 0.65              |
| 1:K:315:GLU:O    | 1:K:316:VAL:HG22  | 1.97                     | 0.65              |
| 1:K:499:GLN:NE2  | 1:K:516:ASN:HB3   | 2.11                     | 0.65              |
| 1:K:1214:LEU:HB3 | 1:K:1223:GLN:HA   | 1.78                     | 0.65              |
| 1:L:315:GLU:O    | 1:L:316:VAL:HG22  | 1.97                     | 0.65              |
| 1:L:520:GLN:HB3  | 1:L:524:TYR:OH    | 1.95                     | 0.65              |
| 1:M:373:SER:OG   | 1:M:433:LEU:HB2   | 1.97                     | 0.65              |
| 1:B:373:SER:OG   | 1:B:433:LEU:HB2   | 1.97                     | 0.65              |
| 1:B:389:ILE:CD1  | 1:B:446:HIS:CE1   | 2.70                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:405:LEU:HG   | 1:B:411:VAL:HG23 | 1.77                     | 0.65              |
| 1:C:520:GLN:HB3  | 1:C:524:TYR:OH   | 1.95                     | 0.65              |
| 1:I:266:THR:HG21 | 1:I:271:VAL:HB   | 1.78                     | 0.65              |
| 1:I:405:LEU:HG   | 1:I:411:VAL:HG23 | 1.77                     | 0.65              |
| 1:I:413:LYS:O    | 1:I:421:SER:HB3  | 1.96                     | 0.65              |
| 1:K:517:THR:HG23 | 1:K:518:LEU:H    | 1.62                     | 0.65              |
| 2:K:1501:DTP:O1A | 2:K:1501:DTP:H8  | 1.97                     | 0.65              |
| 1:M:405:LEU:HG   | 1:M:411:VAL:HG23 | 1.77                     | 0.65              |
| 1:O:252:ALA:O    | 1:O:255:ALA:N    | 2.25                     | 0.65              |
| 1:A:315:GLU:O    | 1:A:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:A:373:SER:OG   | 1:A:433:LEU:HB2  | 1.97                     | 0.65              |
| 1:A:464:ASP:O    | 1:A:468:TYR:CE2  | 2.49                     | 0.65              |
| 1:A:499:GLN:NE2  | 1:A:516:ASN:HB3  | 2.11                     | 0.65              |
| 1:B:464:ASP:O    | 1:B:468:TYR:CE2  | 2.49                     | 0.65              |
| 1:B:538:LEU:HG   | 1:B:571:GLU:OE2  | 1.97                     | 0.65              |
| 1:C:464:ASP:O    | 1:C:468:TYR:CE2  | 2.49                     | 0.65              |
| 1:E:315:GLU:O    | 1:E:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:E:508:TRP:C    | 1:E:606:GLY:CA   | 2.69                     | 0.65              |
| 1:F:378:SER:N    | 1:F:422:ILE:HD11 | 2.10                     | 0.65              |
| 1:G:413:LYS:O    | 1:G:421:SER:HB3  | 1.96                     | 0.65              |
| 1:G:538:LEU:HG   | 1:G:571:GLU:OE2  | 1.97                     | 0.65              |
| 1:H:914:VAL:HG22 | 1:H:917:TYR:O    | 1.97                     | 0.65              |
| 1:I:11:GLN:HE21  | 1:I:70:GLU:HB3   | 1.60                     | 0.65              |
| 1:I:482:GLU:O    | 1:I:485:THR:OG1  | 2.15                     | 0.65              |
| 1:J:11:GLN:HE21  | 1:J:70:GLU:HB3   | 1.60                     | 0.65              |
| 1:J:313:PRO:CG   | 1:J:338:TRP:HE1  | 2.07                     | 0.65              |
| 1:L:464:ASP:O    | 1:L:468:TYR:CE2  | 2.49                     | 0.65              |
| 1:M:315:GLU:O    | 1:M:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:M:538:LEU:HG   | 1:M:571:GLU:OE2  | 1.97                     | 0.65              |
| 1:N:315:GLU:O    | 1:N:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:N:499:GLN:NE2  | 1:N:516:ASN:HB3  | 2.11                     | 0.65              |
| 1:O:914:VAL:HG22 | 1:O:917:TYR:O    | 1.97                     | 0.65              |
| 1:P:315:GLU:O    | 1:P:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:P:413:LYS:O    | 1:P:421:SER:HB3  | 1.96                     | 0.65              |
| 1:B:315:GLU:O    | 1:B:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:B:482:GLU:O    | 1:B:485:THR:OG1  | 2.15                     | 0.65              |
| 1:B:492:LEU:HD11 | 1:B:561:LEU:HD21 | 1.78                     | 0.65              |
| 1:C:389:ILE:CD1  | 1:C:446:HIS:CE1  | 2.70                     | 0.65              |
| 2:D:1501:DTP:H8  | 2:D:1501:DTP:O2A | 1.97                     | 0.65              |
| 1:E:405:LEU:HG   | 1:E:411:VAL:HG23 | 1.77                     | 0.65              |
| 1:F:405:LEU:HG   | 1:F:411:VAL:HG23 | 1.77                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:482:GLU:O    | 1:F:485:THR:OG1  | 2.15                     | 0.65              |
| 1:F:517:THR:HG23 | 1:F:518:LEU:H    | 1.62                     | 0.65              |
| 1:G:266:THR:HG21 | 1:G:271:VAL:HB   | 1.78                     | 0.65              |
| 1:G:482:GLU:O    | 1:G:485:THR:OG1  | 2.15                     | 0.65              |
| 1:I:517:THR:HG23 | 1:I:518:LEU:H    | 1.62                     | 0.65              |
| 1:J:508:TRP:C    | 1:J:606:GLY:CA   | 2.69                     | 0.65              |
| 1:J:1177:TYR:HE2 | 1:K:916:LYS:HE2  | 1.61                     | 0.65              |
| 1:K:545:PHE:HZ   | 1:K:565:ALA:HA   | 1.57                     | 0.65              |
| 1:L:517:THR:HG23 | 1:L:518:LEU:H    | 1.62                     | 0.65              |
| 1:M:464:ASP:O    | 1:M:468:TYR:CE2  | 2.49                     | 0.65              |
| 1:M:1214:LEU:HB3 | 1:M:1223:GLN:HA  | 1.78                     | 0.65              |
| 1:N:373:SER:OG   | 1:N:433:LEU:HB2  | 1.97                     | 0.65              |
| 1:O:317:LEU:CD2  | 1:O:341:TRP:CZ2  | 2.79                     | 0.65              |
| 1:P:538:LEU:HG   | 1:P:571:GLU:OE2  | 1.97                     | 0.65              |
| 1:A:317:LEU:CD2  | 1:A:341:TRP:CZ2  | 2.79                     | 0.65              |
| 1:C:482:GLU:O    | 1:C:485:THR:OG1  | 2.15                     | 0.65              |
| 1:C:517:THR:HG23 | 1:C:518:LEU:H    | 1.62                     | 0.65              |
| 1:C:538:LEU:HG   | 1:C:571:GLU:OE2  | 1.97                     | 0.65              |
| 1:E:313:PRO:CG   | 1:E:338:TRP:HE1  | 2.07                     | 0.65              |
| 1:G:373:SER:OG   | 1:G:433:LEU:HB2  | 1.97                     | 0.65              |
| 1:G:378:SER:N    | 1:G:422:ILE:HD11 | 2.10                     | 0.65              |
| 1:H:317:LEU:CD2  | 1:H:341:TRP:CZ2  | 2.79                     | 0.65              |
| 1:H:492:LEU:HD11 | 1:H:561:LEU:HD21 | 1.78                     | 0.65              |
| 1:I:315:GLU:O    | 1:I:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:I:447:TYR:OH   | 1:I:486:LEU:HD23 | 1.97                     | 0.65              |
| 1:J:315:GLU:O    | 1:J:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:J:405:LEU:HG   | 1:J:411:VAL:HG23 | 1.77                     | 0.65              |
| 1:L:378:SER:N    | 1:L:422:ILE:HD11 | 2.10                     | 0.65              |
| 1:L:499:GLN:NE2  | 1:L:516:ASN:HB3  | 2.11                     | 0.65              |
| 1:L:538:LEU:HG   | 1:L:571:GLU:OE2  | 1.97                     | 0.65              |
| 1:M:482:GLU:O    | 1:M:485:THR:OG1  | 2.15                     | 0.65              |
| 1:N:464:ASP:O    | 1:N:468:TYR:CE2  | 2.49                     | 0.65              |
| 1:O:266:THR:HG21 | 1:O:271:VAL:HB   | 1.78                     | 0.65              |
| 1:P:266:THR:HG21 | 1:P:271:VAL:HB   | 1.78                     | 0.65              |
| 1:P:482:GLU:O    | 1:P:485:THR:OG1  | 2.15                     | 0.65              |
| 1:B:914:VAL:CG2  | 1:B:917:TYR:O    | 2.44                     | 0.65              |
| 1:B:914:VAL:HG22 | 1:B:917:TYR:O    | 1.97                     | 0.65              |
| 1:B:1214:LEU:HB3 | 1:B:1223:GLN:HA  | 1.78                     | 0.65              |
| 2:B:1501:DTP:H8  | 2:B:1501:DTP:O2A | 1.97                     | 0.65              |
| 1:F:315:GLU:O    | 1:F:316:VAL:HG22 | 1.97                     | 0.65              |
| 1:F:637:LEU:O    | 1:F:638:GLU:CB   | 2.43                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:266:THR:HG21 | 1:H:271:VAL:HB   | 1.78                     | 0.65              |
| 1:M:492:LEU:HD11 | 1:M:561:LEU:HD21 | 1.78                     | 0.65              |
| 1:M:508:TRP:C    | 1:M:606:GLY:CA   | 2.69                     | 0.65              |
| 1:M:914:VAL:CG2  | 1:M:917:TYR:O    | 2.44                     | 0.65              |
| 1:M:914:VAL:HG22 | 1:M:917:TYR:O    | 1.97                     | 0.65              |
| 2:M:1501:DTP:O1A | 2:M:1501:DTP:H8  | 1.97                     | 0.65              |
| 1:N:317:LEU:CD2  | 1:N:341:TRP:CZ2  | 2.79                     | 0.65              |
| 2:N:1501:DTP:O1A | 2:N:1501:DTP:H8  | 1.97                     | 0.65              |
| 1:P:378:SER:N    | 1:P:422:ILE:HD11 | 2.10                     | 0.65              |
| 1:B:508:TRP:C    | 1:B:606:GLY:CA   | 2.69                     | 0.65              |
| 1:C:447:TYR:OH   | 1:C:486:LEU:HD23 | 1.97                     | 0.65              |
| 1:C:1214:LEU:HB3 | 1:C:1223:GLN:HA  | 1.78                     | 0.65              |
| 1:D:383:THR:HG23 | 1:D:419:THR:CA   | 2.27                     | 0.65              |
| 1:D:545:PHE:HZ   | 1:D:565:ALA:HA   | 1.57                     | 0.65              |
| 1:E:482:GLU:O    | 1:E:485:THR:OG1  | 2.15                     | 0.65              |
| 1:G:451:LYS:HD3  | 1:G:486:LEU:CD2  | 2.26                     | 0.65              |
| 1:I:373:SER:OG   | 1:I:433:LEU:HB2  | 1.97                     | 0.65              |
| 1:J:482:GLU:O    | 1:J:485:THR:OG1  | 2.15                     | 0.65              |
| 1:L:383:THR:HG23 | 1:L:419:THR:CA   | 2.27                     | 0.65              |
| 1:L:1214:LEU:HB3 | 1:L:1223:GLN:HA  | 1.78                     | 0.65              |
| 1:N:447:TYR:OH   | 1:N:486:LEU:HD23 | 1.97                     | 0.65              |
| 1:O:538:LEU:HG   | 1:O:571:GLU:OE2  | 1.97                     | 0.65              |
| 1:P:373:SER:OG   | 1:P:433:LEU:HB2  | 1.97                     | 0.65              |
| 1:A:447:TYR:OH   | 1:A:486:LEU:HD23 | 1.97                     | 0.64              |
| 1:A:482:GLU:O    | 1:A:485:THR:OG1  | 2.15                     | 0.64              |
| 2:A:1501:DTP:H8  | 2:A:1501:DTP:O2A | 1.97                     | 0.64              |
| 1:B:499:GLN:NE2  | 1:B:516:ASN:HB3  | 2.11                     | 0.64              |
| 1:E:378:SER:N    | 1:E:422:ILE:HD11 | 2.10                     | 0.64              |
| 1:E:447:TYR:OH   | 1:E:486:LEU:HD23 | 1.97                     | 0.64              |
| 1:F:373:SER:OG   | 1:F:433:LEU:HB2  | 1.97                     | 0.64              |
| 1:H:378:SER:N    | 1:H:422:ILE:HD11 | 2.10                     | 0.64              |
| 1:H:538:LEU:HG   | 1:H:571:GLU:OE2  | 1.97                     | 0.64              |
| 1:J:447:TYR:OH   | 1:J:486:LEU:HD23 | 1.97                     | 0.64              |
| 1:K:383:THR:HG23 | 1:K:419:THR:CA   | 2.27                     | 0.64              |
| 1:K:413:LYS:O    | 1:K:421:SER:HB3  | 1.95                     | 0.64              |
| 1:M:499:GLN:NE2  | 1:M:516:ASN:HB3  | 2.11                     | 0.64              |
| 1:O:492:LEU:HD11 | 1:O:561:LEU:HD21 | 1.78                     | 0.64              |
| 1:P:451:LYS:HD3  | 1:P:486:LEU:CD2  | 2.26                     | 0.64              |
| 1:A:378:SER:N    | 1:A:422:ILE:HD11 | 2.10                     | 0.64              |
| 1:A:538:LEU:HG   | 1:A:571:GLU:OE2  | 1.97                     | 0.64              |
| 2:C:1501:DTP:O2A | 2:C:1501:DTP:H8  | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:378:SER:N    | 1:D:422:ILE:HD11  | 2.10                     | 0.64              |
| 1:E:53:ASP:O     | 1:E:57:GLY:N      | 2.27                     | 0.64              |
| 1:E:373:SER:OG   | 1:E:433:LEU:HB2   | 1.97                     | 0.64              |
| 1:E:520:GLN:HB3  | 1:E:524:TYR:OH    | 1.95                     | 0.64              |
| 1:F:447:TYR:OH   | 1:F:486:LEU:HD23  | 1.97                     | 0.64              |
| 1:F:547:PRO:HB2  | 1:F:603:ILE:HA    | 1.80                     | 0.64              |
| 1:G:547:PRO:HB2  | 1:G:603:ILE:HA    | 1.80                     | 0.64              |
| 1:H:373:SER:OG   | 1:H:433:LEU:HB2   | 1.97                     | 0.64              |
| 1:I:378:SER:N    | 1:I:422:ILE:HD11  | 2.10                     | 0.64              |
| 1:I:499:GLN:NE2  | 1:I:516:ASN:HB3   | 2.11                     | 0.64              |
| 1:J:492:LEU:HD11 | 1:J:561:LEU:HD21  | 1.78                     | 0.64              |
| 1:J:520:GLN:HB3  | 1:J:524:TYR:OH    | 1.96                     | 0.64              |
| 1:L:482:GLU:O    | 1:L:485:THR:OG1   | 2.15                     | 0.64              |
| 1:M:313:PRO:CG   | 1:M:338:TRP:HE1   | 2.07                     | 0.64              |
| 1:P:517:THR:HG23 | 1:P:518:LEU:H     | 1.62                     | 0.64              |
| 1:P:545:PHE:HZ   | 1:P:565:ALA:HA    | 1.57                     | 0.64              |
| 1:A:989:SER:HB2  | 1:A:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:C:373:SER:OG   | 1:C:433:LEU:HB2   | 1.97                     | 0.64              |
| 1:C:383:THR:HG23 | 1:C:419:THR:CA    | 2.27                     | 0.64              |
| 2:E:1501:DTP:H8  | 2:E:1501:DTP:O2A  | 1.96                     | 0.64              |
| 1:F:499:GLN:NE2  | 1:F:516:ASN:HB3   | 2.11                     | 0.64              |
| 1:F:635:VAL:HB   | 1:F:641:ASP:OD1   | 1.98                     | 0.64              |
| 1:I:547:PRO:HB2  | 1:I:603:ILE:HA    | 1.80                     | 0.64              |
| 1:I:637:LEU:O    | 1:I:638:GLU:CB    | 2.43                     | 0.64              |
| 1:J:373:SER:OG   | 1:J:433:LEU:HB2   | 1.97                     | 0.64              |
| 1:J:378:SER:N    | 1:J:422:ILE:HD11  | 2.10                     | 0.64              |
| 1:J:383:THR:HG23 | 1:J:419:THR:CA    | 2.27                     | 0.64              |
| 1:K:382:PRO:CA   | 1:K:419:THR:HG22  | 2.23                     | 0.64              |
| 1:L:373:SER:OG   | 1:L:433:LEU:HB2   | 1.97                     | 0.64              |
| 1:L:492:LEU:HD11 | 1:L:561:LEU:HD21  | 1.78                     | 0.64              |
| 1:N:482:GLU:O    | 1:N:485:THR:OG1   | 2.15                     | 0.64              |
| 1:O:373:SER:OG   | 1:O:433:LEU:HB2   | 1.97                     | 0.64              |
| 1:P:313:PRO:CG   | 1:P:338:TRP:HE1   | 2.07                     | 0.64              |
| 1:P:547:PRO:HB2  | 1:P:603:ILE:HA    | 1.80                     | 0.64              |
| 1:B:313:PRO:CG   | 1:B:338:TRP:HE1   | 2.08                     | 0.64              |
| 1:E:383:THR:HG23 | 1:E:419:THR:CA    | 2.27                     | 0.64              |
| 1:G:383:THR:HG23 | 1:G:419:THR:CA    | 2.27                     | 0.64              |
| 1:G:517:THR:HG23 | 1:G:518:LEU:H     | 1.62                     | 0.64              |
| 1:H:547:PRO:HB2  | 1:H:603:ILE:HA    | 1.80                     | 0.64              |
| 1:I:635:VAL:HB   | 1:I:641:ASP:OD1   | 1.98                     | 0.64              |
| 1:J:635:VAL:HB   | 1:J:641:ASP:OD1   | 1.98                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:378:SER:N    | 1:K:422:ILE:HD11  | 2.11                     | 0.64              |
| 1:L:447:TYR:OH   | 1:L:486:LEU:HD23  | 1.97                     | 0.64              |
| 1:N:538:LEU:HG   | 1:N:571:GLU:OE2   | 1.97                     | 0.64              |
| 1:N:989:SER:HB2  | 1:N:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:O:378:SER:N    | 1:O:422:ILE:HD11  | 2.10                     | 0.64              |
| 1:O:547:PRO:HB2  | 1:O:603:ILE:HA    | 1.80                     | 0.64              |
| 1:P:383:THR:HG23 | 1:P:419:THR:CA    | 2.27                     | 0.64              |
| 1:P:447:TYR:OH   | 1:P:486:LEU:HD23  | 1.97                     | 0.64              |
| 1:A:53:ASP:O     | 1:A:57:GLY:N      | 2.27                     | 0.64              |
| 1:C:248:GLN:CD   | 1:C:268:PHE:CE2   | 2.74                     | 0.64              |
| 1:C:499:GLN:NE2  | 1:C:516:ASN:HB3   | 2.11                     | 0.64              |
| 1:D:413:LYS:O    | 1:D:421:SER:HB3   | 1.96                     | 0.64              |
| 1:D:538:LEU:HG   | 1:D:571:GLU:OE2   | 1.97                     | 0.64              |
| 1:E:104:ARG:HA   | 1:E:107:ILE:HG22  | 1.80                     | 0.64              |
| 1:E:492:LEU:HD11 | 1:E:561:LEU:HD21  | 1.78                     | 0.64              |
| 1:E:635:VAL:HB   | 1:E:641:ASP:OD1   | 1.98                     | 0.64              |
| 1:F:914:VAL:HG22 | 1:F:917:TYR:O     | 1.97                     | 0.64              |
| 1:G:447:TYR:OH   | 1:G:486:LEU:HD23  | 1.97                     | 0.64              |
| 1:G:545:PHE:HZ   | 1:G:565:ALA:HA    | 1.58                     | 0.64              |
| 1:H:482:GLU:O    | 1:H:485:THR:OG1   | 2.15                     | 0.64              |
| 1:H:989:SER:HB2  | 1:H:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:I:538:LEU:HG   | 1:I:571:GLU:OE2   | 1.97                     | 0.64              |
| 2:J:1501:DTP:O1A | 2:J:1501:DTP:H8   | 1.97                     | 0.64              |
| 1:K:464:ASP:O    | 1:K:468:TYR:HE2   | 1.81                     | 0.64              |
| 1:K:508:TRP:C    | 1:K:606:GLY:CA    | 2.69                     | 0.64              |
| 1:L:464:ASP:O    | 1:L:468:TYR:HE2   | 1.81                     | 0.64              |
| 1:L:508:TRP:C    | 1:L:606:GLY:CA    | 2.69                     | 0.64              |
| 2:L:1501:DTP:H8  | 2:L:1501:DTP:O1A  | 1.97                     | 0.64              |
| 1:M:989:SER:HB2  | 1:M:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:N:378:SER:N    | 1:N:422:ILE:HD11  | 2.10                     | 0.64              |
| 1:O:482:GLU:O    | 1:O:485:THR:OG1   | 2.15                     | 0.64              |
| 1:O:989:SER:HB2  | 1:O:1027:ASN:HD22 | 1.63                     | 0.64              |
| 2:O:1501:DTP:O1A | 2:O:1501:DTP:H8   | 1.96                     | 0.64              |
| 1:A:547:PRO:HB2  | 1:A:603:ILE:HA    | 1.80                     | 0.64              |
| 1:B:464:ASP:O    | 1:B:468:TYR:HE2   | 1.81                     | 0.64              |
| 1:B:989:SER:HB2  | 1:B:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:C:464:ASP:O    | 1:C:468:TYR:HE2   | 1.81                     | 0.64              |
| 1:D:464:ASP:O    | 1:D:468:TYR:HE2   | 1.81                     | 0.64              |
| 1:D:508:TRP:C    | 1:D:606:GLY:CA    | 2.69                     | 0.64              |
| 1:G:313:PRO:CG   | 1:G:338:TRP:HE1   | 2.08                     | 0.64              |
| 1:I:104:ARG:HA   | 1:I:107:ILE:HG22  | 1.80                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:914:VAL:HG22 | 1:I:917:TYR:O    | 1.97                     | 0.64              |
| 1:J:548:LYS:HZ2  | 1:J:601:GLN:N    | 1.96                     | 0.64              |
| 1:K:104:ARG:HA   | 1:K:107:ILE:HG22 | 1.80                     | 0.64              |
| 1:K:538:LEU:HG   | 1:K:571:GLU:OE2  | 1.97                     | 0.64              |
| 1:M:464:ASP:O    | 1:M:468:TYR:HE2  | 1.81                     | 0.64              |
| 1:N:53:ASP:O     | 1:N:57:GLY:N     | 2.27                     | 0.64              |
| 1:B:447:TYR:OH   | 1:B:486:LEU:HD23 | 1.97                     | 0.64              |
| 1:D:373:SER:OG   | 1:D:433:LEU:HB2  | 1.97                     | 0.64              |
| 1:D:382:PRO:CA   | 1:D:419:THR:HG22 | 2.24                     | 0.64              |
| 1:F:383:THR:HG23 | 1:F:419:THR:CA   | 2.27                     | 0.64              |
| 1:H:383:THR:HG23 | 1:H:419:THR:CA   | 2.27                     | 0.64              |
| 1:H:447:TYR:OH   | 1:H:486:LEU:HD23 | 1.97                     | 0.64              |
| 2:H:1501:DTP:H8  | 2:H:1501:DTP:O2A | 1.96                     | 0.64              |
| 1:J:104:ARG:HA   | 1:J:107:ILE:HG22 | 1.80                     | 0.64              |
| 1:K:165:CYS:SG   | 1:K:178:ILE:HD13 | 2.38                     | 0.64              |
| 1:L:104:ARG:HA   | 1:L:107:ILE:HG22 | 1.80                     | 0.64              |
| 1:L:208:THR:OG1  | 1:L:210:ARG:NH1  | 2.31                     | 0.64              |
| 1:N:165:CYS:SG   | 1:N:178:ILE:HD13 | 2.38                     | 0.64              |
| 1:N:547:PRO:HB2  | 1:N:603:ILE:HA   | 1.80                     | 0.64              |
| 1:A:121:ALA:HB1  | 1:B:276:SER:CB   | 2.20                     | 0.64              |
| 1:A:165:CYS:SG   | 1:A:178:ILE:HD13 | 2.38                     | 0.64              |
| 1:A:333:ASP:OD2  | 1:B:403:ASN:ND2  | 2.31                     | 0.64              |
| 1:C:208:THR:OG1  | 1:C:210:ARG:NH1  | 2.31                     | 0.64              |
| 1:C:492:LEU:HD11 | 1:C:561:LEU:HD21 | 1.78                     | 0.64              |
| 1:C:508:TRP:C    | 1:C:606:GLY:CA   | 2.70                     | 0.64              |
| 1:C:587:ARG:HG3  | 1:C:588:VAL:H    | 1.63                     | 0.64              |
| 1:D:104:ARG:HA   | 1:D:107:ILE:HG22 | 1.80                     | 0.64              |
| 1:D:165:CYS:SG   | 1:D:178:ILE:HD13 | 2.38                     | 0.64              |
| 1:D:208:THR:OG1  | 1:D:210:ARG:NH1  | 2.31                     | 0.64              |
| 1:D:635:VAL:HB   | 1:D:641:ASP:OD1  | 1.98                     | 0.64              |
| 1:E:464:ASP:O    | 1:E:468:TYR:HE2  | 1.81                     | 0.64              |
| 1:E:538:LEU:HG   | 1:E:571:GLU:OE2  | 1.97                     | 0.64              |
| 1:E:547:PRO:HB2  | 1:E:603:ILE:HA   | 1.80                     | 0.64              |
| 1:E:548:LYS:HZ2  | 1:E:601:GLN:N    | 1.96                     | 0.64              |
| 1:F:104:ARG:HA   | 1:F:107:ILE:HG22 | 1.80                     | 0.64              |
| 1:F:451:LYS:HD3  | 1:F:486:LEU:CD2  | 2.26                     | 0.64              |
| 1:F:538:LEU:HG   | 1:F:571:GLU:OE2  | 1.97                     | 0.64              |
| 1:G:548:LYS:NZ   | 1:G:601:GLN:CA   | 2.61                     | 0.64              |
| 1:G:914:VAL:HG22 | 1:G:917:TYR:O    | 1.97                     | 0.64              |
| 1:H:165:CYS:SG   | 1:H:178:ILE:HD13 | 2.38                     | 0.64              |
| 1:H:386:LEU:CD1  | 1:H:420:ILE:HD13 | 2.28                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:464:ASP:O    | 1:J:468:TYR:HE2   | 1.81                     | 0.64              |
| 1:J:989:SER:HB2  | 1:J:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:K:208:THR:OG1  | 1:K:210:ARG:NH1   | 2.31                     | 0.64              |
| 1:K:373:SER:OG   | 1:K:433:LEU:HB2   | 1.97                     | 0.64              |
| 1:K:447:TYR:OH   | 1:K:486:LEU:HD23  | 1.97                     | 0.64              |
| 1:K:635:VAL:HB   | 1:K:641:ASP:OD1   | 1.98                     | 0.64              |
| 1:L:635:VAL:HB   | 1:L:641:ASP:OD1   | 1.98                     | 0.64              |
| 1:M:517:THR:HG23 | 1:M:518:LEU:H     | 1.62                     | 0.64              |
| 1:N:464:ASP:O    | 1:N:468:TYR:HE2   | 1.81                     | 0.64              |
| 1:O:165:CYS:SG   | 1:O:178:ILE:HD13  | 2.38                     | 0.64              |
| 1:O:208:THR:OG1  | 1:O:210:ARG:NH1   | 2.31                     | 0.64              |
| 1:O:383:THR:HG23 | 1:O:419:THR:CA    | 2.27                     | 0.64              |
| 1:O:386:LEU:CD1  | 1:O:420:ILE:HD13  | 2.28                     | 0.64              |
| 1:O:447:TYR:OH   | 1:O:486:LEU:HD23  | 1.97                     | 0.64              |
| 1:O:635:VAL:HB   | 1:O:641:ASP:OD1   | 1.98                     | 0.64              |
| 1:B:383:THR:HG23 | 1:B:419:THR:CA    | 2.27                     | 0.64              |
| 1:B:517:THR:HG23 | 1:B:518:LEU:H     | 1.62                     | 0.64              |
| 1:C:104:ARG:HA   | 1:C:107:ILE:HG22  | 1.80                     | 0.64              |
| 1:C:437:TYR:O    | 1:C:441:ARG:NH1   | 2.31                     | 0.64              |
| 1:C:989:SER:HB2  | 1:C:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:D:482:GLU:O    | 1:D:485:THR:OG1   | 2.15                     | 0.64              |
| 1:E:208:THR:OG1  | 1:E:210:ARG:NH1   | 2.31                     | 0.64              |
| 1:E:989:SER:HB2  | 1:E:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:F:14:ASP:CG    | 1:G:142:ARG:HH22  | 2.06                     | 0.64              |
| 1:G:104:ARG:HA   | 1:G:107:ILE:HG22  | 1.80                     | 0.64              |
| 1:H:208:THR:OG1  | 1:H:210:ARG:NH1   | 2.31                     | 0.64              |
| 1:H:635:VAL:HB   | 1:H:641:ASP:OD1   | 1.98                     | 0.64              |
| 1:J:437:TYR:O    | 1:J:441:ARG:NH1   | 2.31                     | 0.64              |
| 1:J:538:LEU:HG   | 1:J:571:GLU:OE2   | 1.97                     | 0.64              |
| 1:J:547:PRO:HB2  | 1:J:603:ILE:HA    | 1.80                     | 0.64              |
| 1:K:989:SER:HB2  | 1:K:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:M:383:THR:HG23 | 1:M:419:THR:CA    | 2.27                     | 0.64              |
| 1:M:447:TYR:OH   | 1:M:486:LEU:HD23  | 1.97                     | 0.64              |
| 1:O:499:GLN:HB2  | 1:O:520:GLN:HE22  | 1.63                     | 0.64              |
| 1:P:548:LYS:NZ   | 1:P:601:GLN:CA    | 2.61                     | 0.64              |
| 1:P:914:VAL:HG22 | 1:P:917:TYR:O     | 1.97                     | 0.64              |
| 1:P:989:SER:HB2  | 1:P:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:A:386:LEU:CD1  | 1:A:420:ILE:HD13  | 2.28                     | 0.64              |
| 1:B:248:GLN:CD   | 1:B:268:PHE:CE2   | 2.74                     | 0.64              |
| 1:B:437:TYR:O    | 1:B:441:ARG:NH1   | 2.31                     | 0.64              |
| 1:D:447:TYR:OH   | 1:D:486:LEU:HD23  | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:914:VAL:HG22 | 1:D:917:TYR:O     | 1.97                     | 0.64              |
| 1:D:989:SER:HB2  | 1:D:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:E:165:CYS:SG   | 1:E:178:ILE:HD13  | 2.38                     | 0.64              |
| 1:E:437:TYR:O    | 1:E:441:ARG:NH1   | 2.31                     | 0.64              |
| 1:F:208:THR:OG1  | 1:F:210:ARG:NH1   | 2.31                     | 0.64              |
| 1:G:989:SER:HB2  | 1:G:1027:ASN:HD22 | 1.63                     | 0.64              |
| 1:H:104:ARG:HA   | 1:H:107:ILE:HG22  | 1.80                     | 0.64              |
| 1:H:315:GLU:O    | 1:H:316:VAL:HG22  | 1.97                     | 0.64              |
| 1:I:383:THR:HG23 | 1:I:419:THR:CA    | 2.27                     | 0.64              |
| 1:I:548:LYS:HZ2  | 1:I:601:GLN:N     | 1.96                     | 0.64              |
| 1:J:208:THR:OG1  | 1:J:210:ARG:NH1   | 2.31                     | 0.64              |
| 1:L:248:GLN:CD   | 1:L:268:PHE:CE2   | 2.74                     | 0.64              |
| 1:N:386:LEU:CD1  | 1:N:420:ILE:HD13  | 2.28                     | 0.64              |
| 1:O:315:GLU:O    | 1:O:316:VAL:HG22  | 1.97                     | 0.64              |
| 1:P:104:ARG:HA   | 1:P:107:ILE:HG22  | 1.80                     | 0.64              |
| 1:A:475:LEU:HD23 | 1:A:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:A:517:THR:HG23 | 1:A:518:LEU:H     | 1.62                     | 0.63              |
| 1:B:208:THR:OG1  | 1:B:210:ARG:NH1   | 2.31                     | 0.63              |
| 1:D:603:ILE:HD11 | 1:D:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:H:499:GLN:HB2  | 1:H:520:GLN:HE22  | 1.64                     | 0.63              |
| 1:J:165:CYS:SG   | 1:J:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:K:437:TYR:O    | 1:K:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:K:482:GLU:O    | 1:K:485:THR:OG1   | 2.15                     | 0.63              |
| 1:K:603:ILE:HD11 | 1:K:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:L:587:ARG:HG3  | 1:L:588:VAL:H     | 1.63                     | 0.63              |
| 1:M:165:CYS:SG   | 1:M:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:M:437:TYR:O    | 1:M:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:O:104:ARG:HA   | 1:O:107:ILE:HG22  | 1.80                     | 0.63              |
| 1:A:208:THR:OG1  | 1:A:210:ARG:NH1   | 2.31                     | 0.63              |
| 1:A:635:VAL:HB   | 1:A:641:ASP:OD1   | 1.98                     | 0.63              |
| 1:A:914:VAL:HG22 | 1:A:917:TYR:O     | 1.97                     | 0.63              |
| 1:B:165:CYS:SG   | 1:B:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:B:603:ILE:HD11 | 1:B:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:D:248:GLN:CD   | 1:D:268:PHE:CE2   | 2.74                     | 0.63              |
| 1:D:437:TYR:O    | 1:D:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:F:165:CYS:SG   | 1:F:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:I:208:THR:OG1  | 1:I:210:ARG:NH1   | 2.31                     | 0.63              |
| 1:J:386:LEU:CD1  | 1:J:420:ILE:HD13  | 2.28                     | 0.63              |
| 1:K:914:VAL:HG22 | 1:K:917:TYR:O     | 1.97                     | 0.63              |
| 1:L:165:CYS:SG   | 1:L:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:L:437:TYR:O    | 1:L:441:ARG:NH1   | 2.31                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:208:THR:OG1  | 1:M:210:ARG:NH1   | 2.31                     | 0.63              |
| 1:M:248:GLN:CD   | 1:M:268:PHE:CE2   | 2.74                     | 0.63              |
| 1:M:603:ILE:HD11 | 1:M:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:N:517:THR:HG23 | 1:N:518:LEU:H     | 1.62                     | 0.63              |
| 1:A:548:LYS:NZ   | 1:A:601:GLN:CA    | 2.61                     | 0.63              |
| 1:C:165:CYS:SG   | 1:C:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:E:386:LEU:CD1  | 1:E:420:ILE:HD13  | 2.28                     | 0.63              |
| 1:G:208:THR:OG1  | 1:G:210:ARG:NH1   | 2.31                     | 0.63              |
| 1:G:386:LEU:CD1  | 1:G:420:ILE:HD13  | 2.28                     | 0.63              |
| 1:H:552:ASN:HB3  | 1:H:1226:TYR:HE1  | 1.64                     | 0.63              |
| 1:H:603:ILE:HD11 | 1:H:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:J:411:VAL:O    | 1:J:423:PRO:HB3   | 1.99                     | 0.63              |
| 1:K:248:GLN:CD   | 1:K:268:PHE:CE2   | 2.74                     | 0.63              |
| 1:L:552:ASN:HB3  | 1:L:1226:TYR:HE1  | 1.64                     | 0.63              |
| 1:L:989:SER:HB2  | 1:L:1027:ASN:HD22 | 1.63                     | 0.63              |
| 1:N:104:ARG:HA   | 1:N:107:ILE:HG22  | 1.80                     | 0.63              |
| 1:N:208:THR:OG1  | 1:N:210:ARG:NH1   | 2.31                     | 0.63              |
| 1:N:383:THR:HG23 | 1:N:419:THR:CA    | 2.27                     | 0.63              |
| 1:N:475:LEU:HD23 | 1:N:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:O:603:ILE:HD11 | 1:O:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:P:208:THR:OG1  | 1:P:210:ARG:NH1   | 2.31                     | 0.63              |
| 1:A:383:THR:HG23 | 1:A:419:THR:CA    | 2.27                     | 0.63              |
| 1:A:587:ARG:HG3  | 1:A:588:VAL:H     | 1.63                     | 0.63              |
| 1:B:104:ARG:HA   | 1:B:107:ILE:HG22  | 1.80                     | 0.63              |
| 1:B:317:LEU:C    | 1:B:318:THR:HG1   | 1.95                     | 0.63              |
| 1:B:378:SER:N    | 1:B:422:ILE:HD11  | 2.10                     | 0.63              |
| 1:C:552:ASN:HB3  | 1:C:1226:TYR:HE1  | 1.64                     | 0.63              |
| 1:C:635:VAL:HB   | 1:C:641:ASP:OD1   | 1.98                     | 0.63              |
| 1:E:411:VAL:O    | 1:E:423:PRO:HB3   | 1.99                     | 0.63              |
| 1:F:41:SER:HB3   | 1:F:44:GLU:HG2    | 1.81                     | 0.63              |
| 1:F:548:LYS:HZ2  | 1:F:601:GLN:N     | 1.96                     | 0.63              |
| 1:G:548:LYS:HZ2  | 1:G:601:GLN:N     | 1.96                     | 0.63              |
| 1:I:437:TYR:O    | 1:I:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:I:451:LYS:HD3  | 1:I:486:LEU:CD2   | 2.26                     | 0.63              |
| 1:K:548:LYS:HZ2  | 1:K:601:GLN:N     | 1.96                     | 0.63              |
| 1:M:104:ARG:HA   | 1:M:107:ILE:HG22  | 1.80                     | 0.63              |
| 1:M:378:SER:N    | 1:M:422:ILE:HD11  | 2.10                     | 0.63              |
| 1:M:547:PRO:HB2  | 1:M:603:ILE:HA    | 1.80                     | 0.63              |
| 1:N:914:VAL:HG22 | 1:N:917:TYR:O     | 1.97                     | 0.63              |
| 1:O:552:ASN:HB3  | 1:O:1226:TYR:HE1  | 1.64                     | 0.63              |
| 1:P:386:LEU:CD1  | 1:P:420:ILE:HD13  | 2.28                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:547:PRO:HB2  | 1:B:603:ILE:HA    | 1.80                     | 0.63              |
| 1:C:41:SER:HB3   | 1:C:44:GLU:HG2    | 1.81                     | 0.63              |
| 1:D:548:LYS:HZ2  | 1:D:601:GLN:N     | 1.96                     | 0.63              |
| 1:F:437:TYR:O    | 1:F:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:F:603:ILE:HD11 | 1:F:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:F:989:SER:HB2  | 1:F:1027:ASN:HD22 | 1.63                     | 0.63              |
| 1:G:552:ASN:HB3  | 1:G:1226:TYR:HE1  | 1.63                     | 0.63              |
| 2:G:1501:DTP:H8  | 2:G:1501:DTP:O2A  | 1.97                     | 0.63              |
| 1:I:41:SER:HB3   | 1:I:44:GLU:HG2    | 1.81                     | 0.63              |
| 1:I:165:CYS:SG   | 1:I:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:I:475:LEU:HD23 | 1:I:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:I:603:ILE:HD11 | 1:I:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:J:914:VAL:HG22 | 1:J:917:TYR:O     | 1.97                     | 0.63              |
| 1:L:41:SER:HB3   | 1:L:44:GLU:HG2    | 1.81                     | 0.63              |
| 1:N:548:LYS:NZ   | 1:N:601:GLN:CA    | 2.61                     | 0.63              |
| 1:N:635:VAL:HB   | 1:N:641:ASP:OD1   | 1.98                     | 0.63              |
| 1:P:552:ASN:HB3  | 1:P:1226:TYR:HE1  | 1.64                     | 0.63              |
| 1:A:104:ARG:HA   | 1:A:107:ILE:HG22  | 1.80                     | 0.63              |
| 1:A:248:GLN:CD   | 1:A:268:PHE:CE2   | 2.74                     | 0.63              |
| 1:B:386:LEU:CD1  | 1:B:420:ILE:HD13  | 2.28                     | 0.63              |
| 1:B:475:LEU:HD23 | 1:B:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:D:386:LEU:CD1  | 1:D:420:ILE:HD13  | 2.28                     | 0.63              |
| 1:D:411:VAL:O    | 1:D:423:PRO:HB3   | 1.99                     | 0.63              |
| 1:F:475:LEU:HD23 | 1:F:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:F:499:GLN:HB2  | 1:F:520:GLN:HE22  | 1.63                     | 0.63              |
| 1:G:635:VAL:HB   | 1:G:641:ASP:OD1   | 1.98                     | 0.63              |
| 1:H:437:TYR:O    | 1:H:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:I:198:LYS:NZ   | 1:P:222:HIS:CG    | 2.66                     | 0.63              |
| 1:I:499:GLN:HB2  | 1:I:520:GLN:HE22  | 1.63                     | 0.63              |
| 1:K:411:VAL:O    | 1:K:423:PRO:HB3   | 1.99                     | 0.63              |
| 1:K:547:PRO:HB2  | 1:K:603:ILE:HA    | 1.80                     | 0.63              |
| 1:L:411:VAL:O    | 1:L:423:PRO:HB3   | 1.99                     | 0.63              |
| 1:L:547:PRO:HB2  | 1:L:603:ILE:HA    | 1.80                     | 0.63              |
| 1:L:548:LYS:HZ2  | 1:L:601:GLN:N     | 1.96                     | 0.63              |
| 1:L:914:VAL:HG22 | 1:L:917:TYR:O     | 1.97                     | 0.63              |
| 1:M:386:LEU:CD1  | 1:M:420:ILE:HD13  | 2.28                     | 0.63              |
| 1:M:587:ARG:HG3  | 1:M:588:VAL:H     | 1.63                     | 0.63              |
| 1:N:587:ARG:HG3  | 1:N:588:VAL:H     | 1.63                     | 0.63              |
| 1:O:437:TYR:O    | 1:O:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:P:548:LYS:HZ2  | 1:P:601:GLN:N     | 1.96                     | 0.63              |
| 1:P:635:VAL:HB   | 1:P:641:ASP:OD1   | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:437:TYR:O    | 1:A:441:ARG:NH1   | 2.31                     | 0.63              |
| 1:B:587:ARG:HG3  | 1:B:588:VAL:H     | 1.63                     | 0.63              |
| 1:C:371:ARG:HG3  | 1:C:390:TRP:CD1   | 2.34                     | 0.63              |
| 1:C:548:LYS:HZ2  | 1:C:601:GLN:N     | 1.96                     | 0.63              |
| 1:D:547:PRO:HB2  | 1:D:603:ILE:HA    | 1.80                     | 0.63              |
| 1:E:378:SER:H    | 1:E:422:ILE:HD13  | 1.61                     | 0.63              |
| 1:E:499:GLN:HB2  | 1:E:520:GLN:HE22  | 1.63                     | 0.63              |
| 1:E:914:VAL:HG22 | 1:E:917:TYR:O     | 1.97                     | 0.63              |
| 1:G:411:VAL:O    | 1:G:423:PRO:HB3   | 1.99                     | 0.63              |
| 1:J:41:SER:HB3   | 1:J:44:GLU:HG2    | 1.81                     | 0.63              |
| 1:J:499:GLN:HB2  | 1:J:520:GLN:HE22  | 1.63                     | 0.63              |
| 1:K:386:LEU:CD1  | 1:K:420:ILE:HD13  | 2.28                     | 0.63              |
| 1:L:371:ARG:HG3  | 1:L:390:TRP:CD1   | 2.34                     | 0.63              |
| 1:M:475:LEU:HD23 | 1:M:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:P:411:VAL:O    | 1:P:423:PRO:HB3   | 1.99                     | 0.63              |
| 2:P:1501:DTP:O1A | 2:P:1501:DTP:H8   | 1.97                     | 0.63              |
| 1:A:252:ALA:O    | 1:A:255:ALA:N     | 2.25                     | 0.63              |
| 1:C:411:VAL:O    | 1:C:423:PRO:HB3   | 1.99                     | 0.63              |
| 1:E:475:LEU:HD23 | 1:E:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:G:165:CYS:SG   | 1:G:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:I:989:SER:HB2  | 1:I:1027:ASN:HD22 | 1.63                     | 0.63              |
| 1:K:371:ARG:HG3  | 1:K:390:TRP:CD1   | 2.34                     | 0.63              |
| 1:L:458:LEU:CB   | 1:L:587:ARG:HH21  | 2.12                     | 0.63              |
| 1:M:317:LEU:C    | 1:M:318:THR:HG1   | 1.95                     | 0.63              |
| 1:N:41:SER:HB3   | 1:N:44:GLU:HG2    | 1.81                     | 0.63              |
| 1:P:165:CYS:SG   | 1:P:178:ILE:HD13  | 2.38                     | 0.63              |
| 1:A:41:SER:HB3   | 1:A:44:GLU:HG2    | 1.81                     | 0.63              |
| 1:A:458:LEU:CB   | 1:A:587:ARG:HH21  | 2.12                     | 0.63              |
| 1:A:603:ILE:HD11 | 1:A:635:VAL:CG1   | 2.29                     | 0.63              |
| 1:C:914:VAL:HG22 | 1:C:917:TYR:O     | 1.97                     | 0.63              |
| 1:D:371:ARG:HG3  | 1:D:390:TRP:CD1   | 2.34                     | 0.63              |
| 1:D:499:GLN:HB2  | 1:D:520:GLN:HE22  | 1.63                     | 0.63              |
| 1:E:913:PRO:O    | 1:E:914:VAL:HG12  | 1.99                     | 0.63              |
| 1:G:475:LEU:HD23 | 1:G:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:G:637:LEU:O    | 1:G:638:GLU:CB    | 2.43                     | 0.63              |
| 1:H:475:LEU:HD23 | 1:H:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:J:475:LEU:HD23 | 1:J:478:ILE:HD12  | 1.80                     | 0.63              |
| 1:J:913:PRO:O    | 1:J:914:VAL:HG12  | 1.99                     | 0.63              |
| 1:K:499:GLN:HB2  | 1:K:520:GLN:HE22  | 1.63                     | 0.63              |
| 1:N:216:ASN:ND2  | 1:O:194:GLU:OE2   | 2.32                     | 0.63              |
| 1:N:248:GLN:CD   | 1:N:268:PHE:CE2   | 2.74                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:252:ALA:O    | 1:N:255:ALA:N    | 2.25                     | 0.63              |
| 1:N:437:TYR:O    | 1:N:441:ARG:NH1  | 2.31                     | 0.63              |
| 1:N:458:LEU:CB   | 1:N:587:ARG:HH21 | 2.12                     | 0.63              |
| 1:O:915:TYR:O    | 1:O:916:LYS:CB   | 2.47                     | 0.63              |
| 1:A:371:ARG:HG3  | 1:A:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:A:913:PRO:O    | 1:A:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:B:838:ARG:HB2  | 1:B:847:VAL:HB   | 1.81                     | 0.62              |
| 1:C:499:GLN:HB2  | 1:C:520:GLN:HE22 | 1.64                     | 0.62              |
| 1:C:547:PRO:HB2  | 1:C:603:ILE:HA   | 1.80                     | 0.62              |
| 1:D:41:SER:HB3   | 1:D:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:E:41:SER:HB3   | 1:E:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:F:53:ASP:O     | 1:F:57:GLY:N     | 2.27                     | 0.62              |
| 1:F:371:ARG:HG3  | 1:F:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:F:386:LEU:CD1  | 1:F:420:ILE:HD13 | 2.28                     | 0.62              |
| 1:F:548:LYS:NZ   | 1:F:601:GLN:CA   | 2.61                     | 0.62              |
| 1:G:41:SER:HB3   | 1:G:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:G:437:TYR:O    | 1:G:441:ARG:NH1  | 2.31                     | 0.62              |
| 1:H:41:SER:HB3   | 1:H:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:H:838:ARG:HB2  | 1:H:847:VAL:HB   | 1.81                     | 0.62              |
| 1:H:915:TYR:O    | 1:H:916:LYS:CB   | 2.47                     | 0.62              |
| 1:I:552:ASN:HB3  | 1:I:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:J:371:ARG:HG3  | 1:J:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:L:499:GLN:HB2  | 1:L:520:GLN:HE22 | 1.63                     | 0.62              |
| 1:N:371:ARG:HG3  | 1:N:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:N:603:ILE:HD11 | 1:N:635:VAL:CG1  | 2.29                     | 0.62              |
| 1:N:913:PRO:O    | 1:N:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:O:475:LEU:HD23 | 1:O:478:ILE:HD12 | 1.80                     | 0.62              |
| 1:O:838:ARG:HB2  | 1:O:847:VAL:HB   | 1.81                     | 0.62              |
| 1:P:41:SER:HB3   | 1:P:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:P:371:ARG:HG3  | 1:P:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:P:475:LEU:HD23 | 1:P:478:ILE:HD12 | 1.80                     | 0.62              |
| 1:P:499:GLN:HB2  | 1:P:520:GLN:HE22 | 1.63                     | 0.62              |
| 1:A:411:VAL:O    | 1:A:423:PRO:HB3  | 1.99                     | 0.62              |
| 1:B:41:SER:HB3   | 1:B:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:C:458:LEU:CB   | 1:C:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:D:194:GLU:OE2  | 1:E:216:ASN:ND2  | 2.33                     | 0.62              |
| 1:E:371:ARG:HG3  | 1:E:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:F:464:ASP:O    | 1:F:468:TYR:HE2  | 1.81                     | 0.62              |
| 1:G:248:GLN:CD   | 1:G:268:PHE:CE2  | 2.74                     | 0.62              |
| 1:G:371:ARG:HG3  | 1:G:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:G:458:LEU:CB   | 1:G:587:ARG:HH21 | 2.12                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:499:GLN:HB2  | 1:G:520:GLN:HE22 | 1.63                     | 0.62              |
| 1:I:371:ARG:HG3  | 1:I:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:J:518:LEU:HD22 | 1:J:643:TYR:CE1  | 2.22                     | 0.62              |
| 1:K:913:PRO:O    | 1:K:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:M:552:ASN:HB3  | 1:M:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:M:838:ARG:HB2  | 1:M:847:VAL:HB   | 1.81                     | 0.62              |
| 1:N:411:VAL:O    | 1:N:423:PRO:HB3  | 1.99                     | 0.62              |
| 1:P:248:GLN:CD   | 1:P:268:PHE:CE2  | 2.74                     | 0.62              |
| 1:P:437:TYR:O    | 1:P:441:ARG:NH1  | 2.31                     | 0.62              |
| 1:P:458:LEU:CB   | 1:P:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:P:637:LEU:O    | 1:P:638:GLU:CB   | 2.43                     | 0.62              |
| 1:A:499:GLN:HB2  | 1:A:520:GLN:HE22 | 1.63                     | 0.62              |
| 1:A:548:LYS:HG2  | 1:A:601:GLN:HA   | 1.81                     | 0.62              |
| 1:B:38:SER:HB3   | 1:B:72:MET:HE1   | 1.81                     | 0.62              |
| 1:B:499:GLN:HB2  | 1:B:520:GLN:HE22 | 1.63                     | 0.62              |
| 1:B:548:LYS:HG2  | 1:B:601:GLN:HA   | 1.81                     | 0.62              |
| 1:D:913:PRO:O    | 1:D:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:F:312:LEU:CD2  | 1:F:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:I:411:VAL:O    | 1:I:423:PRO:HB3  | 1.99                     | 0.62              |
| 1:K:41:SER:HB3   | 1:K:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:M:41:SER:HB3   | 1:M:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:M:499:GLN:HB2  | 1:M:520:GLN:HE22 | 1.63                     | 0.62              |
| 1:N:548:LYS:HG2  | 1:N:601:GLN:HA   | 1.81                     | 0.62              |
| 1:O:41:SER:HB3   | 1:O:44:GLU:HG2   | 1.81                     | 0.62              |
| 1:A:915:TYR:O    | 1:A:916:LYS:CB   | 2.47                     | 0.62              |
| 1:C:603:ILE:HD11 | 1:C:635:VAL:CG1  | 2.29                     | 0.62              |
| 1:E:451:LYS:HD3  | 1:E:486:LEU:CD2  | 2.26                     | 0.62              |
| 1:E:552:ASN:HB3  | 1:E:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:F:411:VAL:O    | 1:F:423:PRO:HB3  | 1.99                     | 0.62              |
| 1:F:552:ASN:HB3  | 1:F:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:I:53:ASP:O     | 1:I:57:GLY:N     | 2.27                     | 0.62              |
| 1:J:552:ASN:HB3  | 1:J:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:L:312:LEU:CD2  | 1:L:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:M:38:SER:HB3   | 1:M:72:MET:HE1   | 1.81                     | 0.62              |
| 1:M:548:LYS:HG2  | 1:M:601:GLN:HA   | 1.81                     | 0.62              |
| 1:N:915:TYR:O    | 1:N:916:LYS:CB   | 2.47                     | 0.62              |
| 1:O:411:VAL:O    | 1:O:423:PRO:HB3  | 1.99                     | 0.62              |
| 1:B:552:ASN:HB3  | 1:B:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:D:552:ASN:HB3  | 1:D:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:G:603:ILE:HD11 | 1:G:635:VAL:CG1  | 2.29                     | 0.62              |
| 1:H:548:LYS:HZ2  | 1:H:601:GLN:N    | 1.97                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:312:LEU:CD2  | 1:I:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:I:386:LEU:CD1  | 1:I:420:ILE:HD13 | 2.28                     | 0.62              |
| 1:K:378:SER:H    | 1:K:422:ILE:HD13 | 1.62                     | 0.62              |
| 1:M:635:VAL:HB   | 1:M:641:ASP:OD1  | 1.98                     | 0.62              |
| 1:N:313:PRO:CG   | 1:N:338:TRP:HE1  | 2.07                     | 0.62              |
| 1:O:548:LYS:HZ2  | 1:O:601:GLN:N    | 1.97                     | 0.62              |
| 1:O:587:ARG:HG3  | 1:O:588:VAL:H    | 1.63                     | 0.62              |
| 1:P:603:ILE:HD11 | 1:P:635:VAL:CG1  | 2.29                     | 0.62              |
| 1:A:552:ASN:HB3  | 1:A:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:B:411:VAL:O    | 1:B:423:PRO:HB3  | 1.99                     | 0.62              |
| 1:B:548:LYS:HZ2  | 1:B:601:GLN:N    | 1.96                     | 0.62              |
| 1:B:635:VAL:HB   | 1:B:641:ASP:OD1  | 1.98                     | 0.62              |
| 1:C:244:LEU:HD21 | 1:C:256:PHE:HD2  | 1.64                     | 0.62              |
| 1:D:312:LEU:CD2  | 1:D:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:F:913:PRO:O    | 1:F:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:G:312:LEU:CD2  | 1:G:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:H:371:ARG:HG3  | 1:H:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:H:411:VAL:O    | 1:H:423:PRO:HB3  | 1.99                     | 0.62              |
| 1:I:216:ASN:ND2  | 1:J:194:GLU:OE2  | 2.33                     | 0.62              |
| 1:I:464:ASP:O    | 1:I:468:TYR:HE2  | 1.81                     | 0.62              |
| 1:I:548:LYS:NZ   | 1:I:601:GLN:CA   | 2.61                     | 0.62              |
| 1:J:451:LYS:HD3  | 1:J:486:LEU:CD2  | 2.26                     | 0.62              |
| 1:K:276:SER:OG   | 1:L:122:LYS:HG3  | 2.00                     | 0.62              |
| 1:L:603:ILE:HD11 | 1:L:635:VAL:CG1  | 2.29                     | 0.62              |
| 1:N:499:GLN:HB2  | 1:N:520:GLN:HE22 | 1.64                     | 0.62              |
| 1:A:38:SER:HB3   | 1:A:72:MET:HE1   | 1.81                     | 0.62              |
| 1:B:371:ARG:HG3  | 1:B:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:B:538:LEU:HG   | 1:B:571:GLU:HG2  | 1.82                     | 0.62              |
| 1:D:458:LEU:CB   | 1:D:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:E:587:ARG:HG3  | 1:E:588:VAL:H    | 1.63                     | 0.62              |
| 1:E:603:ILE:HD11 | 1:E:635:VAL:CG1  | 2.29                     | 0.62              |
| 1:H:587:ARG:HG3  | 1:H:588:VAL:H    | 1.63                     | 0.62              |
| 1:I:313:PRO:HA   | 1:I:338:TRP:HH2  | 1.63                     | 0.62              |
| 1:I:913:PRO:O    | 1:I:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:J:458:LEU:CB   | 1:J:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:J:587:ARG:HG3  | 1:J:588:VAL:H    | 1.63                     | 0.62              |
| 1:J:603:ILE:HD11 | 1:J:635:VAL:CG1  | 2.29                     | 0.62              |
| 1:K:312:LEU:CD2  | 1:K:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:L:386:LEU:CD1  | 1:L:420:ILE:HD13 | 2.28                     | 0.62              |
| 1:M:244:LEU:HD21 | 1:M:256:PHE:HD2  | 1.64                     | 0.62              |
| 1:M:411:VAL:O    | 1:M:423:PRO:HB3  | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:538:LEU:HG   | 1:M:571:GLU:HG2  | 1.82                     | 0.62              |
| 1:O:244:LEU:HD21 | 1:O:256:PHE:HD2  | 1.64                     | 0.62              |
| 1:P:312:LEU:CD2  | 1:P:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:P:913:PRO:O    | 1:P:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:A:313:PRO:CG   | 1:A:338:TRP:HE1  | 2.07                     | 0.62              |
| 1:A:538:LEU:HG   | 1:A:571:GLU:HG2  | 1.82                     | 0.62              |
| 1:A:916:LYS:HE2  | 1:B:1177:TYR:HE2 | 1.63                     | 0.62              |
| 1:B:244:LEU:HD21 | 1:B:256:PHE:HD2  | 1.64                     | 0.62              |
| 1:B:312:LEU:CD2  | 1:B:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:B:458:LEU:CB   | 1:B:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:C:475:LEU:HD23 | 1:C:478:ILE:HD12 | 1.80                     | 0.62              |
| 1:C:538:LEU:HG   | 1:C:571:GLU:HG2  | 1.82                     | 0.62              |
| 1:D:451:LYS:HD3  | 1:D:486:LEU:CD2  | 2.26                     | 0.62              |
| 1:D:475:LEU:HD23 | 1:D:478:ILE:HD12 | 1.80                     | 0.62              |
| 1:E:458:LEU:CB   | 1:E:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:E:548:LYS:HG2  | 1:E:601:GLN:HA   | 1.81                     | 0.62              |
| 1:F:198:LYS:NZ   | 1:G:222:HIS:CG   | 2.68                     | 0.62              |
| 1:K:475:LEU:HD23 | 1:K:478:ILE:HD12 | 1.80                     | 0.62              |
| 1:K:552:ASN:HB3  | 1:K:1226:TYR:HE1 | 1.64                     | 0.62              |
| 1:M:371:ARG:HG3  | 1:M:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:M:458:LEU:CB   | 1:M:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:N:538:LEU:HG   | 1:N:571:GLU:HG2  | 1.82                     | 0.62              |
| 1:N:552:ASN:HB3  | 1:N:1226:TYR:HE1 | 1.63                     | 0.62              |
| 1:O:53:ASP:O     | 1:O:57:GLY:N     | 2.27                     | 0.62              |
| 1:O:371:ARG:HG3  | 1:O:390:TRP:CD1  | 2.34                     | 0.62              |
| 1:O:458:LEU:CB   | 1:O:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:P:587:ARG:HG3  | 1:P:588:VAL:H    | 1.63                     | 0.62              |
| 1:C:38:SER:HB3   | 1:C:72:MET:HE1   | 1.81                     | 0.62              |
| 1:D:378:SER:H    | 1:D:422:ILE:HD13 | 1.62                     | 0.62              |
| 1:E:248:GLN:CD   | 1:E:268:PHE:CE2  | 2.74                     | 0.62              |
| 1:G:587:ARG:HG3  | 1:G:588:VAL:H    | 1.63                     | 0.62              |
| 1:G:913:PRO:O    | 1:G:914:VAL:HG12 | 1.99                     | 0.62              |
| 1:H:53:ASP:O     | 1:H:57:GLY:N     | 2.27                     | 0.62              |
| 1:H:244:LEU:HD21 | 1:H:256:PHE:HD2  | 1.64                     | 0.62              |
| 1:H:248:GLN:CD   | 1:H:268:PHE:CE2  | 2.74                     | 0.62              |
| 1:I:248:GLN:CD   | 1:I:268:PHE:CE2  | 2.74                     | 0.62              |
| 1:I:458:LEU:CB   | 1:I:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:I:548:LYS:HG2  | 1:I:601:GLN:HA   | 1.81                     | 0.62              |
| 1:J:548:LYS:HG2  | 1:J:601:GLN:HA   | 1.81                     | 0.62              |
| 1:K:458:LEU:CB   | 1:K:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:K:587:ARG:HG3  | 1:K:588:VAL:H    | 1.63                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:38:SER:HB3   | 1:N:72:MET:HE1   | 1.81                     | 0.62              |
| 1:N:312:LEU:CD2  | 1:N:313:PRO:HD2  | 2.30                     | 0.62              |
| 1:O:378:SER:H    | 1:O:422:ILE:HD13 | 1.61                     | 0.62              |
| 1:P:518:LEU:H    | 1:P:518:LEU:CD1  | 2.13                     | 0.62              |
| 1:A:835:SER:OG   | 1:A:850:GLN:NE2  | 2.33                     | 0.62              |
| 1:B:915:TYR:O    | 1:B:916:LYS:CB   | 2.47                     | 0.62              |
| 1:C:386:LEU:CD1  | 1:C:420:ILE:HD13 | 2.28                     | 0.62              |
| 1:C:548:LYS:HG2  | 1:C:601:GLN:HA   | 1.81                     | 0.62              |
| 1:D:244:LEU:HD21 | 1:D:256:PHE:HD2  | 1.64                     | 0.62              |
| 1:D:587:ARG:HG3  | 1:D:588:VAL:H    | 1.63                     | 0.62              |
| 1:F:313:PRO:HA   | 1:F:338:TRP:HH2  | 1.63                     | 0.62              |
| 1:G:518:LEU:H    | 1:G:518:LEU:CD1  | 2.13                     | 0.62              |
| 1:H:458:LEU:CB   | 1:H:587:ARG:HH21 | 2.12                     | 0.62              |
| 1:H:548:LYS:HG2  | 1:H:601:GLN:HA   | 1.81                     | 0.62              |
| 1:N:835:SER:OG   | 1:N:850:GLN:NE2  | 2.33                     | 0.62              |
| 1:O:518:LEU:H    | 1:O:518:LEU:CD1  | 2.13                     | 0.62              |
| 1:A:312:LEU:CD2  | 1:A:313:PRO:HD2  | 2.30                     | 0.61              |
| 1:C:451:LYS:HD3  | 1:C:486:LEU:CD2  | 2.26                     | 0.61              |
| 1:F:458:LEU:CB   | 1:F:587:ARG:HH21 | 2.12                     | 0.61              |
| 1:F:587:ARG:HG3  | 1:F:588:VAL:H    | 1.63                     | 0.61              |
| 1:H:38:SER:HB3   | 1:H:72:MET:HE1   | 1.81                     | 0.61              |
| 1:H:518:LEU:H    | 1:H:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:I:587:ARG:HG3  | 1:I:588:VAL:H    | 1.63                     | 0.61              |
| 1:J:248:GLN:CD   | 1:J:268:PHE:CE2  | 2.74                     | 0.61              |
| 1:J:317:LEU:C    | 1:J:318:THR:HG1  | 1.94                     | 0.61              |
| 1:K:451:LYS:HD3  | 1:K:486:LEU:CD2  | 2.26                     | 0.61              |
| 1:L:244:LEU:HD21 | 1:L:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:L:538:LEU:HG   | 1:L:571:GLU:HG2  | 1.82                     | 0.61              |
| 1:M:548:LYS:HZ2  | 1:M:601:GLN:N    | 1.96                     | 0.61              |
| 1:M:913:PRO:O    | 1:M:914:VAL:HG12 | 1.99                     | 0.61              |
| 1:M:915:TYR:O    | 1:M:916:LYS:CB   | 2.47                     | 0.61              |
| 1:O:38:SER:HB3   | 1:O:72:MET:HE1   | 1.81                     | 0.61              |
| 1:O:248:GLN:CD   | 1:O:268:PHE:CE2  | 2.74                     | 0.61              |
| 1:P:244:LEU:HD21 | 1:P:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:B:835:SER:OG   | 1:B:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:C:378:SER:N    | 1:C:422:ILE:HD11 | 2.10                     | 0.61              |
| 1:D:518:LEU:H    | 1:D:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:D:838:ARG:HB2  | 1:D:847:VAL:HB   | 1.81                     | 0.61              |
| 1:E:38:SER:HB3   | 1:E:72:MET:HE1   | 1.81                     | 0.61              |
| 1:F:333:ASP:OD2  | 1:G:403:ASN:ND2  | 2.33                     | 0.61              |
| 1:F:548:LYS:HG2  | 1:F:601:GLN:HA   | 1.81                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:913:PRO:O    | 1:H:914:VAL:HG12 | 1.99                     | 0.61              |
| 1:J:38:SER:HB3   | 1:J:72:MET:HE1   | 1.81                     | 0.61              |
| 1:J:312:LEU:CD2  | 1:J:313:PRO:HD2  | 2.30                     | 0.61              |
| 1:K:244:LEU:HD21 | 1:K:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:K:518:LEU:H    | 1:K:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:M:216:ASN:ND2  | 1:N:194:GLU:OE2  | 2.33                     | 0.61              |
| 1:M:835:SER:OG   | 1:M:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:O:548:LYS:HG2  | 1:O:601:GLN:HA   | 1.81                     | 0.61              |
| 1:B:913:PRO:O    | 1:B:914:VAL:HG12 | 1.99                     | 0.61              |
| 1:C:397:ASP:O    | 1:C:401:VAL:N    | 2.28                     | 0.61              |
| 1:C:838:ARG:HB2  | 1:C:847:VAL:HB   | 1.81                     | 0.61              |
| 1:F:244:LEU:HD21 | 1:F:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:G:244:LEU:HD21 | 1:G:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:L:38:SER:HB3   | 1:L:72:MET:HE1   | 1.81                     | 0.61              |
| 1:L:518:LEU:H    | 1:L:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:L:548:LYS:HG2  | 1:L:601:GLN:HA   | 1.81                     | 0.61              |
| 1:N:244:LEU:HD21 | 1:N:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:P:53:ASP:O     | 1:P:57:GLY:N     | 2.27                     | 0.61              |
| 1:A:244:LEU:HD21 | 1:A:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:A:464:ASP:O    | 1:A:468:TYR:HE2  | 1.81                     | 0.61              |
| 1:A:548:LYS:HZ2  | 1:A:601:GLN:N    | 1.97                     | 0.61              |
| 1:A:838:ARG:HB2  | 1:A:847:VAL:HB   | 1.81                     | 0.61              |
| 1:D:130:PRO:HA   | 1:D:290:MET:CE   | 2.31                     | 0.61              |
| 1:D:557:LYS:HZ2  | 1:D:1223:GLN:HG3 | 1.64                     | 0.61              |
| 1:E:130:PRO:HA   | 1:E:290:MET:CE   | 2.31                     | 0.61              |
| 1:E:312:LEU:CD2  | 1:E:313:PRO:HD2  | 2.30                     | 0.61              |
| 1:F:838:ARG:HB2  | 1:F:847:VAL:HB   | 1.81                     | 0.61              |
| 1:G:464:ASP:O    | 1:G:468:TYR:HE2  | 1.81                     | 0.61              |
| 1:J:244:LEU:HD21 | 1:J:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:K:276:SER:CB   | 1:L:122:LYS:HG3  | 2.30                     | 0.61              |
| 1:K:838:ARG:HB2  | 1:K:847:VAL:HB   | 1.81                     | 0.61              |
| 1:O:913:PRO:O    | 1:O:914:VAL:HG12 | 1.99                     | 0.61              |
| 1:B:88:LEU:O     | 1:B:91:PRO:HD2   | 2.01                     | 0.61              |
| 1:C:88:LEU:O     | 1:C:91:PRO:HD2   | 2.01                     | 0.61              |
| 1:C:130:PRO:HA   | 1:C:290:MET:CE   | 2.31                     | 0.61              |
| 1:C:518:LEU:H    | 1:C:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:C:913:PRO:O    | 1:C:914:VAL:HG12 | 1.99                     | 0.61              |
| 1:E:244:LEU:HD21 | 1:E:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:F:248:GLN:CD   | 1:F:268:PHE:CE2  | 2.74                     | 0.61              |
| 1:G:53:ASP:O     | 1:G:57:GLY:N     | 2.27                     | 0.61              |
| 1:G:194:GLU:OE2  | 1:H:216:ASN:ND2  | 2.33                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:378:SER:H    | 1:H:422:ILE:HD13 | 1.62                     | 0.61              |
| 1:I:244:LEU:HD21 | 1:I:256:PHE:HD2  | 1.64                     | 0.61              |
| 1:I:838:ARG:HB2  | 1:I:847:VAL:HB   | 1.81                     | 0.61              |
| 1:J:130:PRO:HA   | 1:J:290:MET:CE   | 2.31                     | 0.61              |
| 1:K:130:PRO:HA   | 1:K:290:MET:CE   | 2.31                     | 0.61              |
| 1:L:475:LEU:HD23 | 1:L:478:ILE:HD12 | 1.80                     | 0.61              |
| 1:L:590:PHE:HD2  | 1:L:1263:MET:HA  | 1.66                     | 0.61              |
| 1:M:88:LEU:O     | 1:M:91:PRO:HD2   | 2.01                     | 0.61              |
| 1:N:548:LYS:HZ2  | 1:N:601:GLN:N    | 1.97                     | 0.61              |
| 1:O:312:LEU:CD2  | 1:O:313:PRO:HD2  | 2.30                     | 0.61              |
| 1:B:252:ALA:O    | 1:B:255:ALA:N    | 2.25                     | 0.61              |
| 1:C:590:PHE:HD2  | 1:C:1263:MET:HA  | 1.66                     | 0.61              |
| 1:F:518:LEU:H    | 1:F:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:H:538:LEU:HG   | 1:H:571:GLU:HG2  | 1.82                     | 0.61              |
| 1:H:548:LYS:NZ   | 1:H:601:GLN:CA   | 2.61                     | 0.61              |
| 1:I:38:SER:HB3   | 1:I:72:MET:HE1   | 1.81                     | 0.61              |
| 1:I:198:LYS:HZ1  | 1:P:222:HIS:CG   | 2.18                     | 0.61              |
| 1:K:835:SER:OG   | 1:K:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:L:913:PRO:O    | 1:L:914:VAL:HG12 | 1.99                     | 0.61              |
| 1:N:838:ARG:HB2  | 1:N:847:VAL:HB   | 1.81                     | 0.61              |
| 1:O:835:SER:OG   | 1:O:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:P:464:ASP:O    | 1:P:468:TYR:HE2  | 1.81                     | 0.61              |
| 1:A:590:PHE:HD2  | 1:A:1263:MET:HA  | 1.66                     | 0.61              |
| 1:B:130:PRO:HA   | 1:B:290:MET:CE   | 2.31                     | 0.61              |
| 1:B:590:PHE:HD2  | 1:B:1263:MET:HA  | 1.66                     | 0.61              |
| 1:D:548:LYS:HG2  | 1:D:601:GLN:HA   | 1.81                     | 0.61              |
| 1:D:835:SER:OG   | 1:D:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:E:252:ALA:O    | 1:E:255:ALA:N    | 2.25                     | 0.61              |
| 1:F:378:SER:H    | 1:F:422:ILE:HD13 | 1.62                     | 0.61              |
| 1:H:88:LEU:O     | 1:H:91:PRO:HD2   | 2.01                     | 0.61              |
| 1:H:312:LEU:CD2  | 1:H:313:PRO:HD2  | 2.30                     | 0.61              |
| 1:H:464:ASP:O    | 1:H:468:TYR:HE2  | 1.81                     | 0.61              |
| 1:K:548:LYS:HG2  | 1:K:601:GLN:HA   | 1.81                     | 0.61              |
| 1:K:590:PHE:HD2  | 1:K:1263:MET:HA  | 1.66                     | 0.61              |
| 1:L:88:LEU:O     | 1:L:91:PRO:HD2   | 2.01                     | 0.61              |
| 1:L:130:PRO:HA   | 1:L:290:MET:CE   | 2.31                     | 0.61              |
| 1:L:631:LEU:HD23 | 1:L:646:ARG:HH21 | 1.66                     | 0.61              |
| 1:M:130:PRO:HA   | 1:M:290:MET:CE   | 2.31                     | 0.61              |
| 1:M:590:PHE:HD2  | 1:M:1263:MET:HA  | 1.66                     | 0.61              |
| 1:N:590:PHE:HD2  | 1:N:1263:MET:HA  | 1.66                     | 0.61              |
| 1:O:538:LEU:HG   | 1:O:571:GLU:HG2  | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:915:TYR:O    | 1:C:916:LYS:CB   | 2.47                     | 0.61              |
| 1:D:590:PHE:HD2  | 1:D:1263:MET:HA  | 1.66                     | 0.61              |
| 1:F:130:PRO:HA   | 1:F:290:MET:CE   | 2.31                     | 0.61              |
| 1:H:835:SER:OG   | 1:H:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:I:130:PRO:HA   | 1:I:290:MET:CE   | 2.31                     | 0.61              |
| 1:I:518:LEU:H    | 1:I:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:K:538:LEU:HG   | 1:K:571:GLU:HG2  | 1.82                     | 0.61              |
| 1:M:252:ALA:O    | 1:M:255:ALA:N    | 2.25                     | 0.61              |
| 1:O:88:LEU:O     | 1:O:91:PRO:HD2   | 2.01                     | 0.61              |
| 1:A:130:PRO:HA   | 1:A:290:MET:CE   | 2.31                     | 0.61              |
| 1:B:631:LEU:HD23 | 1:B:646:ARG:HH21 | 1.66                     | 0.61              |
| 1:C:378:SER:H    | 1:C:422:ILE:HD13 | 1.61                     | 0.61              |
| 1:C:631:LEU:HD23 | 1:C:646:ARG:HH21 | 1.66                     | 0.61              |
| 1:C:919:VAL:HG12 | 1:C:933:THR:HG22 | 1.83                     | 0.61              |
| 1:D:538:LEU:HG   | 1:D:571:GLU:HG2  | 1.82                     | 0.61              |
| 1:E:548:LYS:NZ   | 1:E:601:GLN:CA   | 2.61                     | 0.61              |
| 1:H:631:LEU:HD23 | 1:H:646:ARG:HH21 | 1.66                     | 0.61              |
| 1:I:357:LEU:HD21 | 1:I:427:LEU:HD22 | 1.83                     | 0.61              |
| 1:K:313:PRO:CG   | 1:K:338:TRP:HE1  | 2.08                     | 0.61              |
| 1:L:378:SER:H    | 1:L:422:ILE:HD13 | 1.62                     | 0.61              |
| 1:L:451:LYS:HD3  | 1:L:486:LEU:CD2  | 2.26                     | 0.61              |
| 1:L:838:ARG:HB2  | 1:L:847:VAL:HB   | 1.81                     | 0.61              |
| 1:L:915:TYR:O    | 1:L:916:LYS:CB   | 2.47                     | 0.61              |
| 1:M:631:LEU:HD23 | 1:M:646:ARG:HH21 | 1.66                     | 0.61              |
| 1:O:464:ASP:O    | 1:O:468:TYR:HE2  | 1.81                     | 0.61              |
| 1:O:548:LYS:NZ   | 1:O:601:GLN:CA   | 2.61                     | 0.61              |
| 1:O:631:LEU:HD23 | 1:O:646:ARG:HH21 | 1.66                     | 0.61              |
| 1:P:548:LYS:HG2  | 1:P:601:GLN:HA   | 1.81                     | 0.61              |
| 1:E:835:SER:OG   | 1:E:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:F:38:SER:HB3   | 1:F:72:MET:HE1   | 1.81                     | 0.61              |
| 1:F:357:LEU:HD21 | 1:F:427:LEU:HD22 | 1.83                     | 0.61              |
| 1:G:38:SER:HB3   | 1:G:72:MET:HE1   | 1.81                     | 0.61              |
| 1:G:548:LYS:HG2  | 1:G:601:GLN:HA   | 1.81                     | 0.61              |
| 1:J:835:SER:OG   | 1:J:850:GLN:NE2  | 2.33                     | 0.61              |
| 1:L:252:ALA:O    | 1:L:255:ALA:N    | 2.25                     | 0.61              |
| 1:N:130:PRO:HA   | 1:N:290:MET:CE   | 2.31                     | 0.61              |
| 1:N:518:LEU:H    | 1:N:518:LEU:CD1  | 2.13                     | 0.61              |
| 1:P:38:SER:HB3   | 1:P:72:MET:HE1   | 1.81                     | 0.61              |
| 1:B:919:VAL:HG12 | 1:B:933:THR:HG22 | 1.83                     | 0.60              |
| 1:C:835:SER:OG   | 1:C:850:GLN:NE2  | 2.33                     | 0.60              |
| 1:D:252:ALA:O    | 1:D:255:ALA:N    | 2.25                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:313:PRO:CG   | 1:D:338:TRP:HE1  | 2.07                     | 0.60              |
| 1:E:590:PHE:HD2  | 1:E:1263:MET:HA  | 1.66                     | 0.60              |
| 1:G:88:LEU:O     | 1:G:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:H:412:GLU:O    | 1:H:421:SER:O    | 2.19                     | 0.60              |
| 1:J:590:PHE:HD2  | 1:J:1263:MET:HA  | 1.66                     | 0.60              |
| 1:K:357:LEU:HD21 | 1:K:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:K:631:LEU:HD23 | 1:K:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:L:919:VAL:HG12 | 1:L:933:THR:HG22 | 1.83                     | 0.60              |
| 1:O:412:GLU:O    | 1:O:421:SER:O    | 2.19                     | 0.60              |
| 1:P:88:LEU:O     | 1:P:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:P:313:PRO:HA   | 1:P:338:TRP:HH2  | 1.63                     | 0.60              |
| 1:P:557:LYS:HZ2  | 1:P:1223:GLN:HG3 | 1.65                     | 0.60              |
| 1:A:412:GLU:O    | 1:A:421:SER:O    | 2.19                     | 0.60              |
| 1:A:631:LEU:HD23 | 1:A:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:B:412:GLU:O    | 1:B:421:SER:O    | 2.19                     | 0.60              |
| 1:D:631:LEU:HD23 | 1:D:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:E:838:ARG:HB2  | 1:E:847:VAL:HB   | 1.81                     | 0.60              |
| 1:F:252:ALA:O    | 1:F:255:ALA:N    | 2.25                     | 0.60              |
| 1:F:590:PHE:HD2  | 1:F:1263:MET:HA  | 1.66                     | 0.60              |
| 1:F:631:LEU:HD23 | 1:F:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:G:557:LYS:HZ2  | 1:G:1223:GLN:HG3 | 1.66                     | 0.60              |
| 1:H:130:PRO:HA   | 1:H:290:MET:CE   | 2.31                     | 0.60              |
| 1:H:637:LEU:O    | 1:H:638:GLU:CB   | 2.43                     | 0.60              |
| 1:J:548:LYS:NZ   | 1:J:601:GLN:CA   | 2.61                     | 0.60              |
| 1:M:412:GLU:O    | 1:M:421:SER:O    | 2.19                     | 0.60              |
| 1:N:412:GLU:O    | 1:N:421:SER:O    | 2.19                     | 0.60              |
| 1:O:357:LEU:HD21 | 1:O:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:O:590:PHE:HD2  | 1:O:1263:MET:HA  | 1.66                     | 0.60              |
| 1:B:451:LYS:HD3  | 1:B:486:LEU:CD2  | 2.26                     | 0.60              |
| 1:D:38:SER:HB3   | 1:D:72:MET:HE1   | 1.81                     | 0.60              |
| 1:E:357:LEU:HD21 | 1:E:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:G:488:ARG:HG2  | 1:G:491:PHE:CD2  | 2.36                     | 0.60              |
| 1:G:590:PHE:HD2  | 1:G:1263:MET:HA  | 1.66                     | 0.60              |
| 1:H:357:LEU:HD21 | 1:H:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:H:590:PHE:HD2  | 1:H:1263:MET:HA  | 1.66                     | 0.60              |
| 1:H:663:GLN:HB2  | 1:H:680:LEU:HD12 | 1.83                     | 0.60              |
| 1:H:712:LEU:HD13 | 1:H:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:K:252:ALA:O    | 1:K:255:ALA:N    | 2.25                     | 0.60              |
| 1:L:357:LEU:HD21 | 1:L:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:L:835:SER:OG   | 1:L:850:GLN:NE2  | 2.33                     | 0.60              |
| 1:O:663:GLN:HB2  | 1:O:680:LEU:HD12 | 1.83                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:712:LEU:HD13 | 1:O:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:A:518:LEU:H    | 1:A:518:LEU:CD1  | 2.13                     | 0.60              |
| 1:A:663:GLN:HB2  | 1:A:680:LEU:HD12 | 1.83                     | 0.60              |
| 1:C:412:GLU:O    | 1:C:421:SER:O    | 2.19                     | 0.60              |
| 1:D:357:LEU:HD21 | 1:D:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:D:412:GLU:O    | 1:D:421:SER:O    | 2.19                     | 0.60              |
| 1:D:915:TYR:O    | 1:D:916:LYS:CB   | 2.47                     | 0.60              |
| 1:G:313:PRO:HA   | 1:G:338:TRP:HH2  | 1.63                     | 0.60              |
| 1:G:412:GLU:O    | 1:G:421:SER:O    | 2.19                     | 0.60              |
| 1:G:538:LEU:HG   | 1:G:571:GLU:HG2  | 1.82                     | 0.60              |
| 1:G:838:ARG:HB2  | 1:G:847:VAL:HB   | 1.81                     | 0.60              |
| 1:H:488:ARG:HG2  | 1:H:491:PHE:CD2  | 2.37                     | 0.60              |
| 1:J:252:ALA:O    | 1:J:255:ALA:N    | 2.25                     | 0.60              |
| 1:J:357:LEU:HD21 | 1:J:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:J:838:ARG:HB2  | 1:J:847:VAL:HB   | 1.81                     | 0.60              |
| 1:K:53:ASP:O     | 1:K:57:GLY:N     | 2.27                     | 0.60              |
| 1:L:412:GLU:O    | 1:L:421:SER:O    | 2.20                     | 0.60              |
| 1:M:919:VAL:HG12 | 1:M:933:THR:HG22 | 1.84                     | 0.60              |
| 1:O:130:PRO:HA   | 1:O:290:MET:CE   | 2.31                     | 0.60              |
| 1:O:637:LEU:O    | 1:O:638:GLU:CB   | 2.43                     | 0.60              |
| 1:P:412:GLU:O    | 1:P:421:SER:O    | 2.19                     | 0.60              |
| 1:P:488:ARG:HG2  | 1:P:491:PHE:CD2  | 2.37                     | 0.60              |
| 1:P:590:PHE:HD2  | 1:P:1263:MET:HA  | 1.66                     | 0.60              |
| 1:P:835:SER:OG   | 1:P:850:GLN:NE2  | 2.33                     | 0.60              |
| 1:P:838:ARG:HB2  | 1:P:847:VAL:HB   | 1.81                     | 0.60              |
| 1:B:518:LEU:H    | 1:B:518:LEU:CD1  | 2.13                     | 0.60              |
| 1:C:97:ARG:NH2   | 1:L:97:ARG:NH2   | 2.49                     | 0.60              |
| 1:C:357:LEU:HD21 | 1:C:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:D:548:LYS:NZ   | 1:D:601:GLN:CA   | 2.61                     | 0.60              |
| 1:D:916:LYS:CE   | 1:E:1177:TYR:CE2 | 2.85                     | 0.60              |
| 1:D:919:VAL:HG12 | 1:D:933:THR:HG22 | 1.83                     | 0.60              |
| 1:E:915:TYR:O    | 1:E:916:LYS:CB   | 2.47                     | 0.60              |
| 1:F:915:TYR:O    | 1:F:916:LYS:CB   | 2.47                     | 0.60              |
| 1:G:835:SER:OG   | 1:G:850:GLN:NE2  | 2.33                     | 0.60              |
| 1:J:53:ASP:O     | 1:J:57:GLY:N     | 2.27                     | 0.60              |
| 1:K:38:SER:HB3   | 1:K:72:MET:HE1   | 1.81                     | 0.60              |
| 1:K:412:GLU:O    | 1:K:421:SER:O    | 2.19                     | 0.60              |
| 1:K:919:VAL:HG12 | 1:K:933:THR:HG22 | 1.83                     | 0.60              |
| 1:M:451:LYS:HD3  | 1:M:486:LEU:CD2  | 2.26                     | 0.60              |
| 1:N:631:LEU:HD23 | 1:N:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:O:488:ARG:HG2  | 1:O:491:PHE:CD2  | 2.37                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:130:PRO:HA   | 1:P:290:MET:CE   | 2.31                     | 0.60              |
| 1:P:663:GLN:HB2  | 1:P:680:LEU:HD12 | 1.83                     | 0.60              |
| 1:A:488:ARG:HG2  | 1:A:491:PHE:CD2  | 2.36                     | 0.60              |
| 1:C:53:ASP:O     | 1:C:57:GLY:N     | 2.27                     | 0.60              |
| 1:C:488:ARG:HG2  | 1:C:491:PHE:CD2  | 2.36                     | 0.60              |
| 1:D:53:ASP:O     | 1:D:57:GLY:N     | 2.27                     | 0.60              |
| 1:F:397:ASP:O    | 1:F:401:VAL:N    | 2.28                     | 0.60              |
| 1:F:835:SER:OG   | 1:F:850:GLN:NE2  | 2.33                     | 0.60              |
| 1:G:130:PRO:HA   | 1:G:290:MET:CE   | 2.31                     | 0.60              |
| 1:G:186:CYS:O    | 1:G:187:ASN:ND2  | 2.35                     | 0.60              |
| 1:G:712:LEU:HD13 | 1:G:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:I:538:LEU:HG   | 1:I:571:GLU:HG2  | 1.82                     | 0.60              |
| 1:I:590:PHE:HD2  | 1:I:1263:MET:HA  | 1.66                     | 0.60              |
| 1:I:631:LEU:HD23 | 1:I:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:I:835:SER:OG   | 1:I:850:GLN:NE2  | 2.33                     | 0.60              |
| 1:J:631:LEU:HD23 | 1:J:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:K:915:TYR:O    | 1:K:916:LYS:CB   | 2.47                     | 0.60              |
| 1:L:397:ASP:O    | 1:L:401:VAL:N    | 2.28                     | 0.60              |
| 1:M:518:LEU:H    | 1:M:518:LEU:CD1  | 2.13                     | 0.60              |
| 1:N:663:GLN:HB2  | 1:N:680:LEU:HD12 | 1.83                     | 0.60              |
| 1:P:538:LEU:HG   | 1:P:571:GLU:HG2  | 1.82                     | 0.60              |
| 1:C:121:ALA:HB1  | 1:D:276:SER:CB   | 2.22                     | 0.60              |
| 1:C:252:ALA:O    | 1:C:255:ALA:N    | 2.25                     | 0.60              |
| 1:C:712:LEU:HD13 | 1:C:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:E:518:LEU:H    | 1:E:518:LEU:CD1  | 2.13                     | 0.60              |
| 1:E:538:LEU:HG   | 1:E:571:GLU:HG2  | 1.82                     | 0.60              |
| 1:E:631:LEU:HD23 | 1:E:646:ARG:HH21 | 1.66                     | 0.60              |
| 1:F:88:LEU:O     | 1:F:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:G:357:LEU:HD21 | 1:G:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:G:663:GLN:HB2  | 1:G:680:LEU:HD12 | 1.83                     | 0.60              |
| 1:I:252:ALA:O    | 1:I:255:ALA:N    | 2.25                     | 0.60              |
| 1:J:538:LEU:HG   | 1:J:571:GLU:HG2  | 1.82                     | 0.60              |
| 1:N:488:ARG:HG2  | 1:N:491:PHE:CD2  | 2.37                     | 0.60              |
| 1:P:186:CYS:O    | 1:P:187:ASN:ND2  | 2.35                     | 0.60              |
| 1:B:357:LEU:HD21 | 1:B:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:B:712:LEU:HD13 | 1:B:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:C:548:LYS:NZ   | 1:C:601:GLN:CA   | 2.61                     | 0.60              |
| 1:D:712:LEU:HD13 | 1:D:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:E:88:LEU:O     | 1:E:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:E:188:SER:N    | 1:E:251:APK:O2P  | 2.31                     | 0.60              |
| 1:E:198:LYS:NZ   | 1:F:222:HIS:CG   | 2.70                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:412:GLU:O    | 1:E:421:SER:O    | 2.19                     | 0.60              |
| 1:I:88:LEU:O     | 1:I:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:J:412:GLU:O    | 1:J:421:SER:O    | 2.19                     | 0.60              |
| 1:J:518:LEU:H    | 1:J:518:LEU:CD1  | 2.13                     | 0.60              |
| 1:J:915:TYR:O    | 1:J:916:LYS:CB   | 2.47                     | 0.60              |
| 1:M:357:LEU:HD21 | 1:M:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:M:663:GLN:HB2  | 1:M:680:LEU:HD12 | 1.83                     | 0.60              |
| 1:N:186:CYS:O    | 1:N:187:ASN:ND2  | 2.35                     | 0.60              |
| 1:N:518:LEU:HA   | 1:N:521:LEU:HB3  | 1.84                     | 0.60              |
| 1:N:712:LEU:HD13 | 1:N:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:P:357:LEU:HD21 | 1:P:427:LEU:HD22 | 1.83                     | 0.60              |
| 1:P:712:LEU:HD13 | 1:P:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:A:88:LEU:O     | 1:A:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:A:186:CYS:O    | 1:A:187:ASN:ND2  | 2.35                     | 0.60              |
| 1:A:397:ASP:O    | 1:A:401:VAL:N    | 2.28                     | 0.60              |
| 1:A:518:LEU:HA   | 1:A:521:LEU:HB3  | 1.84                     | 0.60              |
| 1:B:663:GLN:HB2  | 1:B:680:LEU:HD12 | 1.83                     | 0.60              |
| 1:D:88:LEU:O     | 1:D:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:F:538:LEU:HG   | 1:F:571:GLU:HG2  | 1.82                     | 0.60              |
| 1:I:186:CYS:O    | 1:I:187:ASN:ND2  | 2.35                     | 0.60              |
| 1:I:412:GLU:O    | 1:I:421:SER:O    | 2.19                     | 0.60              |
| 1:I:915:TYR:O    | 1:I:916:LYS:CB   | 2.47                     | 0.60              |
| 1:N:88:LEU:O     | 1:N:91:PRO:HD2   | 2.01                     | 0.60              |
| 1:O:313:PRO:HA   | 1:O:338:TRP:HH2  | 1.63                     | 0.60              |
| 1:P:518:LEU:HA   | 1:P:521:LEU:HB3  | 1.84                     | 0.60              |
| 1:A:216:ASN:ND2  | 1:H:194:GLU:OE2  | 2.35                     | 0.60              |
| 1:A:378:SER:HA   | 1:A:422:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:712:LEU:HD13 | 1:A:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:A:919:VAL:HG12 | 1:A:933:THR:HG22 | 1.83                     | 0.60              |
| 1:F:186:CYS:O    | 1:F:187:ASN:ND2  | 2.35                     | 0.60              |
| 1:F:412:GLU:O    | 1:F:421:SER:O    | 2.19                     | 0.60              |
| 1:I:313:PRO:CG   | 1:I:338:TRP:HE1  | 2.07                     | 0.60              |
| 1:J:769:ARG:HH12 | 1:J:771:PHE:HB2  | 1.67                     | 0.60              |
| 1:K:519:GLN:HG2  | 1:K:523:PHE:CE2  | 2.37                     | 0.60              |
| 1:K:548:LYS:NZ   | 1:K:601:GLN:CA   | 2.61                     | 0.60              |
| 1:K:712:LEU:HD13 | 1:K:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:L:712:LEU:HD13 | 1:L:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:M:712:LEU:HD13 | 1:M:738:ASN:HD22 | 1.67                     | 0.60              |
| 1:B:519:GLN:HG2  | 1:B:523:PHE:CE2  | 2.37                     | 0.59              |
| 1:D:663:GLN:HB2  | 1:D:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:D:769:ARG:HH12 | 1:D:771:PHE:HB2  | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:663:GLN:HB2  | 1:E:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:E:769:ARG:HH12 | 1:E:771:PHE:HB2  | 1.67                     | 0.59              |
| 1:F:316:VAL:HG23 | 1:F:316:VAL:O    | 2.02                     | 0.59              |
| 1:G:518:LEU:HA   | 1:G:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:I:511:SER:HA   | 1:I:514:ILE:N    | 2.17                     | 0.59              |
| 1:I:769:ARG:HH12 | 1:I:771:PHE:HB2  | 1.67                     | 0.59              |
| 1:J:188:SER:N    | 1:J:251:APK:O2P  | 2.31                     | 0.59              |
| 1:K:88:LEU:O     | 1:K:91:PRO:HD2   | 2.01                     | 0.59              |
| 1:K:663:GLN:HB2  | 1:K:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:L:53:ASP:O     | 1:L:57:GLY:N     | 2.27                     | 0.59              |
| 1:M:519:GLN:HG2  | 1:M:523:PHE:CE2  | 2.37                     | 0.59              |
| 1:N:378:SER:HA   | 1:N:422:ILE:HD12 | 1.84                     | 0.59              |
| 1:B:488:ARG:HG2  | 1:B:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:D:519:GLN:HG2  | 1:D:523:PHE:CE2  | 2.37                     | 0.59              |
| 1:F:511:SER:HA   | 1:F:514:ILE:N    | 2.17                     | 0.59              |
| 1:H:313:PRO:HA   | 1:H:338:TRP:HH2  | 1.63                     | 0.59              |
| 1:I:316:VAL:HG23 | 1:I:316:VAL:O    | 2.02                     | 0.59              |
| 1:I:488:ARG:HG2  | 1:I:491:PHE:CD2  | 2.36                     | 0.59              |
| 1:J:88:LEU:O     | 1:J:91:PRO:HD2   | 2.01                     | 0.59              |
| 1:J:663:GLN:HB2  | 1:J:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:J:919:VAL:HG12 | 1:J:933:THR:HG22 | 1.83                     | 0.59              |
| 1:K:222:HIS:CG   | 1:L:198:LYS:HZ2  | 2.19                     | 0.59              |
| 1:K:365:TYR:O    | 1:K:368:MET:N    | 2.21                     | 0.59              |
| 1:K:769:ARG:HH12 | 1:K:771:PHE:HB2  | 1.67                     | 0.59              |
| 1:L:488:ARG:HG2  | 1:L:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:M:511:SER:HA   | 1:M:514:ILE:N    | 2.17                     | 0.59              |
| 1:N:365:TYR:O    | 1:N:368:MET:N    | 2.21                     | 0.59              |
| 1:N:919:VAL:HG12 | 1:N:933:THR:HG22 | 1.83                     | 0.59              |
| 1:A:357:LEU:HD21 | 1:A:427:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:916:LYS:CE   | 1:B:1177:TYR:HE2 | 2.15                     | 0.59              |
| 1:B:511:SER:HA   | 1:B:514:ILE:N    | 2.17                     | 0.59              |
| 1:E:519:GLN:HG2  | 1:E:523:PHE:CE2  | 2.37                     | 0.59              |
| 1:E:919:VAL:HG12 | 1:E:933:THR:HG22 | 1.83                     | 0.59              |
| 1:F:313:PRO:CG   | 1:F:338:TRP:HE1  | 2.07                     | 0.59              |
| 1:H:511:SER:HA   | 1:H:514:ILE:N    | 2.17                     | 0.59              |
| 1:I:142:ARG:NH1  | 1:J:14:ASP:OD2   | 2.35                     | 0.59              |
| 1:I:365:TYR:O    | 1:I:368:MET:N    | 2.21                     | 0.59              |
| 1:I:517:THR:O    | 1:I:519:GLN:N    | 2.35                     | 0.59              |
| 1:J:488:ARG:HG2  | 1:J:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:J:511:SER:HA   | 1:J:514:ILE:N    | 2.18                     | 0.59              |
| 1:J:517:THR:O    | 1:J:519:GLN:N    | 2.35                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:488:ARG:HG2  | 1:M:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:M:518:LEU:HA   | 1:M:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:N:519:GLN:HG2  | 1:N:523:PHE:CE2  | 2.37                     | 0.59              |
| 1:O:511:SER:HA   | 1:O:514:ILE:N    | 2.17                     | 0.59              |
| 1:A:519:GLN:HG2  | 1:A:523:PHE:CE2  | 2.37                     | 0.59              |
| 1:B:518:LEU:HA   | 1:B:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:C:518:LEU:HA   | 1:C:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:D:488:ARG:HG2  | 1:D:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:E:186:CYS:O    | 1:E:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:E:488:ARG:HG2  | 1:E:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:E:511:SER:HA   | 1:E:514:ILE:N    | 2.18                     | 0.59              |
| 1:E:517:THR:O    | 1:E:519:GLN:N    | 2.35                     | 0.59              |
| 1:E:712:LEU:HD13 | 1:E:738:ASN:HD22 | 1.67                     | 0.59              |
| 1:F:769:ARG:HH12 | 1:F:771:PHE:HB2  | 1.67                     | 0.59              |
| 1:J:519:GLN:HG2  | 1:J:523:PHE:CE2  | 2.37                     | 0.59              |
| 1:L:663:GLN:HB2  | 1:L:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:N:142:ARG:NH1  | 1:O:14:ASP:OD2   | 2.33                     | 0.59              |
| 1:N:397:ASP:O    | 1:N:401:VAL:N    | 2.28                     | 0.59              |
| 1:C:769:ARG:HH12 | 1:C:771:PHE:HB2  | 1.67                     | 0.59              |
| 1:D:365:TYR:O    | 1:D:368:MET:N    | 2.21                     | 0.59              |
| 1:D:511:SER:HA   | 1:D:514:ILE:N    | 2.18                     | 0.59              |
| 1:F:663:GLN:HB2  | 1:F:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:I:397:ASP:O    | 1:I:401:VAL:N    | 2.28                     | 0.59              |
| 1:J:216:ASN:ND2  | 1:K:194:GLU:OE2  | 2.36                     | 0.59              |
| 1:J:712:LEU:HD13 | 1:J:738:ASN:HD22 | 1.67                     | 0.59              |
| 1:K:276:SER:HB2  | 1:L:122:LYS:HG3  | 1.84                     | 0.59              |
| 1:K:488:ARG:HG2  | 1:K:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:K:511:SER:HA   | 1:K:514:ILE:N    | 2.18                     | 0.59              |
| 1:L:186:CYS:O    | 1:L:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:M:142:ARG:NH1  | 1:N:14:ASP:OD2   | 2.34                     | 0.59              |
| 1:N:357:LEU:HD21 | 1:N:427:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:365:TYR:O    | 1:A:368:MET:N    | 2.21                     | 0.59              |
| 1:B:188:SER:N    | 1:B:251:APK:O2P  | 2.31                     | 0.59              |
| 1:C:312:LEU:CD2  | 1:C:313:PRO:HD2  | 2.30                     | 0.59              |
| 1:C:517:THR:O    | 1:C:519:GLN:N    | 2.35                     | 0.59              |
| 1:E:316:VAL:O    | 1:E:316:VAL:HG23 | 2.02                     | 0.59              |
| 1:H:378:SER:HA   | 1:H:422:ILE:HD12 | 1.84                     | 0.59              |
| 1:I:663:GLN:HB2  | 1:I:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:J:186:CYS:O    | 1:J:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:J:316:VAL:O    | 1:J:316:VAL:HG23 | 2.02                     | 0.59              |
| 1:K:518:LEU:HA   | 1:K:521:LEU:HB3  | 1.84                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:518:LEU:HA   | 1:L:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:M:186:CYS:O    | 1:M:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:M:188:SER:N    | 1:M:251:APK:O2P  | 2.31                     | 0.59              |
| 1:N:24:VAL:HA    | 1:N:58:THR:HG21  | 1.85                     | 0.59              |
| 1:B:24:VAL:HA    | 1:B:58:THR:HG21  | 1.85                     | 0.59              |
| 1:B:186:CYS:O    | 1:B:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:B:499:GLN:HB2  | 1:B:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:C:186:CYS:O    | 1:C:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:C:365:TYR:O    | 1:C:368:MET:N    | 2.21                     | 0.59              |
| 1:C:663:GLN:HB2  | 1:C:680:LEU:HD12 | 1.83                     | 0.59              |
| 1:D:517:THR:O    | 1:D:519:GLN:N    | 2.35                     | 0.59              |
| 1:E:442:SER:O    | 1:E:446:HIS:CG   | 2.55                     | 0.59              |
| 1:F:314:ARG:O    | 1:F:315:GLU:HB2  | 2.03                     | 0.59              |
| 1:F:517:THR:O    | 1:F:519:GLN:N    | 2.35                     | 0.59              |
| 1:F:712:LEU:HD13 | 1:F:738:ASN:HD22 | 1.67                     | 0.59              |
| 1:G:316:VAL:HG23 | 1:G:316:VAL:O    | 2.02                     | 0.59              |
| 1:G:915:TYR:O    | 1:G:916:LYS:CB   | 2.47                     | 0.59              |
| 1:L:769:ARG:HH12 | 1:L:771:PHE:HB2  | 1.67                     | 0.59              |
| 1:M:378:SER:HA   | 1:M:422:ILE:HD12 | 1.84                     | 0.59              |
| 1:M:499:GLN:HB2  | 1:M:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:O:499:GLN:HB2  | 1:O:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:A:24:VAL:HA    | 1:A:58:THR:HG21  | 1.85                     | 0.59              |
| 1:B:378:SER:HA   | 1:B:422:ILE:HD12 | 1.84                     | 0.59              |
| 1:C:511:SER:HA   | 1:C:514:ILE:N    | 2.17                     | 0.59              |
| 1:D:518:LEU:HA   | 1:D:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:E:499:GLN:HB2  | 1:E:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:E:518:LEU:HA   | 1:E:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:F:444:VAL:HG22 | 1:F:478:ILE:HG12 | 1.85                     | 0.59              |
| 1:F:488:ARG:HG2  | 1:F:491:PHE:CD2  | 2.37                     | 0.59              |
| 1:F:504:ASP:OD2  | 1:F:509:ASN:O    | 2.21                     | 0.59              |
| 1:F:919:VAL:HG12 | 1:F:933:THR:HG22 | 1.83                     | 0.59              |
| 1:H:442:SER:O    | 1:H:446:HIS:CG   | 2.55                     | 0.59              |
| 1:H:517:THR:O    | 1:H:519:GLN:N    | 2.35                     | 0.59              |
| 1:I:314:ARG:O    | 1:I:315:GLU:HB2  | 2.03                     | 0.59              |
| 1:I:444:VAL:HG22 | 1:I:478:ILE:HG12 | 1.85                     | 0.59              |
| 1:I:504:ASP:OD2  | 1:I:509:ASN:O    | 2.21                     | 0.59              |
| 1:J:518:LEU:HA   | 1:J:521:LEU:HB3  | 1.84                     | 0.59              |
| 1:K:517:THR:O    | 1:K:519:GLN:N    | 2.35                     | 0.59              |
| 1:L:442:SER:O    | 1:L:446:HIS:CG   | 2.55                     | 0.59              |
| 1:L:511:SER:HA   | 1:L:514:ILE:N    | 2.17                     | 0.59              |
| 1:M:24:VAL:HA    | 1:M:58:THR:HG21  | 1.85                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:312:LEU:CD2  | 1:M:313:PRO:HD2  | 2.30                     | 0.59              |
| 1:O:378:SER:HA   | 1:O:422:ILE:HD12 | 1.84                     | 0.59              |
| 1:P:316:VAL:HG23 | 1:P:316:VAL:O    | 2.02                     | 0.59              |
| 1:P:915:TYR:O    | 1:P:916:LYS:CB   | 2.47                     | 0.59              |
| 1:A:188:SER:N    | 1:A:251:APK:O2P  | 2.31                     | 0.59              |
| 1:A:637:LEU:O    | 1:A:638:GLU:CB   | 2.43                     | 0.59              |
| 1:C:24:VAL:HA    | 1:C:58:THR:HG21  | 1.85                     | 0.59              |
| 1:F:371:ARG:HB3  | 1:F:389:ILE:HG21 | 1.85                     | 0.59              |
| 1:G:252:ALA:O    | 1:G:255:ALA:N    | 2.25                     | 0.59              |
| 1:G:371:ARG:HB3  | 1:G:389:ILE:HG21 | 1.85                     | 0.59              |
| 1:G:444:VAL:HG22 | 1:G:478:ILE:HG12 | 1.85                     | 0.59              |
| 1:G:631:LEU:HD23 | 1:G:646:ARG:HH21 | 1.66                     | 0.59              |
| 1:H:313:PRO:CG   | 1:H:338:TRP:HE1  | 2.07                     | 0.59              |
| 1:H:499:GLN:HB2  | 1:H:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:H:504:ASP:OD2  | 1:H:509:ASN:O    | 2.21                     | 0.59              |
| 1:H:919:VAL:HG12 | 1:H:933:THR:HG22 | 1.83                     | 0.59              |
| 1:I:371:ARG:HB3  | 1:I:389:ILE:HG21 | 1.85                     | 0.59              |
| 1:I:499:GLN:HB2  | 1:I:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:J:442:SER:O    | 1:J:446:HIS:CG   | 2.55                     | 0.59              |
| 1:J:499:GLN:HB2  | 1:J:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:L:517:THR:O    | 1:L:519:GLN:N    | 2.35                     | 0.59              |
| 1:M:11:GLN:NE2   | 1:M:70:GLU:OE1   | 2.36                     | 0.59              |
| 1:O:24:VAL:HA    | 1:O:58:THR:HG21  | 1.85                     | 0.59              |
| 1:O:313:PRO:CG   | 1:O:338:TRP:HE1  | 2.07                     | 0.59              |
| 1:O:442:SER:O    | 1:O:446:HIS:CG   | 2.55                     | 0.59              |
| 1:O:919:VAL:HG12 | 1:O:933:THR:HG22 | 1.83                     | 0.59              |
| 1:O:1177:TYR:HE2 | 1:P:916:LYS:CE   | 2.16                     | 0.59              |
| 1:P:371:ARG:HB3  | 1:P:389:ILE:HG21 | 1.85                     | 0.59              |
| 1:P:444:VAL:HG22 | 1:P:478:ILE:HG12 | 1.85                     | 0.59              |
| 1:P:504:ASP:OD2  | 1:P:509:ASN:O    | 2.21                     | 0.59              |
| 1:A:451:LYS:HD3  | 1:A:486:LEU:CD2  | 2.26                     | 0.59              |
| 1:B:11:GLN:NE2   | 1:B:70:GLU:OE1   | 2.36                     | 0.59              |
| 1:B:53:ASP:O     | 1:B:57:GLY:N     | 2.27                     | 0.59              |
| 1:C:442:SER:O    | 1:C:446:HIS:CG   | 2.55                     | 0.59              |
| 1:D:186:CYS:O    | 1:D:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:D:819:PHE:HD1  | 1:D:830:LEU:HD13 | 1.68                     | 0.59              |
| 1:E:444:VAL:HG22 | 1:E:478:ILE:HG12 | 1.85                     | 0.59              |
| 1:E:819:PHE:HD1  | 1:E:830:LEU:HD13 | 1.68                     | 0.59              |
| 1:F:11:GLN:NE2   | 1:F:70:GLU:OE1   | 2.36                     | 0.59              |
| 1:G:499:GLN:HB2  | 1:G:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:G:504:ASP:OD2  | 1:G:509:ASN:O    | 2.21                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:24:VAL:HA    | 1:H:58:THR:HG21  | 1.85                     | 0.59              |
| 1:H:186:CYS:O    | 1:H:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:I:919:VAL:HG12 | 1:I:933:THR:HG22 | 1.83                     | 0.59              |
| 1:J:444:VAL:HG22 | 1:J:478:ILE:HG12 | 1.85                     | 0.59              |
| 1:J:633:THR:HG21 | 1:J:643:TYR:CA   | 2.33                     | 0.59              |
| 1:J:819:PHE:HD1  | 1:J:830:LEU:HD13 | 1.68                     | 0.59              |
| 1:K:186:CYS:O    | 1:K:187:ASN:ND2  | 2.35                     | 0.59              |
| 1:K:819:PHE:HD1  | 1:K:830:LEU:HD13 | 1.68                     | 0.59              |
| 1:K:1055:GLU:HG3 | 1:K:1056:GLU:H   | 1.68                     | 0.59              |
| 1:M:53:ASP:O     | 1:M:57:GLY:N     | 2.27                     | 0.59              |
| 1:O:504:ASP:OD2  | 1:O:509:ASN:O    | 2.21                     | 0.59              |
| 1:P:11:GLN:NE2   | 1:P:70:GLU:OE1   | 2.36                     | 0.59              |
| 1:P:499:GLN:HB2  | 1:P:520:GLN:NE2  | 2.18                     | 0.59              |
| 1:P:769:ARG:HH12 | 1:P:771:PHE:HB2  | 1.67                     | 0.59              |
| 1:A:371:ARG:HB3  | 1:A:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:A:499:GLN:HB2  | 1:A:520:GLN:NE2  | 2.18                     | 0.58              |
| 1:A:511:SER:HA   | 1:A:514:ILE:N    | 2.17                     | 0.58              |
| 1:D:24:VAL:HA    | 1:D:58:THR:HG21  | 1.85                     | 0.58              |
| 1:D:444:VAL:HG22 | 1:D:478:ILE:HG12 | 1.85                     | 0.58              |
| 1:E:314:ARG:O    | 1:E:315:GLU:HB2  | 2.03                     | 0.58              |
| 1:E:557:LYS:HZ2  | 1:E:1223:GLN:HG3 | 1.68                     | 0.58              |
| 1:F:365:TYR:O    | 1:F:368:MET:N    | 2.21                     | 0.58              |
| 1:F:499:GLN:HB2  | 1:F:520:GLN:NE2  | 2.18                     | 0.58              |
| 1:F:519:GLN:HG2  | 1:F:523:PHE:CE2  | 2.37                     | 0.58              |
| 1:G:11:GLN:NE2   | 1:G:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:G:769:ARG:HH12 | 1:G:771:PHE:HB2  | 1.67                     | 0.58              |
| 1:H:518:LEU:HA   | 1:H:521:LEU:HB3  | 1.84                     | 0.58              |
| 1:I:712:LEU:HD13 | 1:I:738:ASN:HD22 | 1.67                     | 0.58              |
| 1:J:314:ARG:O    | 1:J:315:GLU:HB2  | 2.03                     | 0.58              |
| 1:J:504:ASP:OD2  | 1:J:509:ASN:O    | 2.21                     | 0.58              |
| 1:K:444:VAL:HG22 | 1:K:478:ILE:HG12 | 1.85                     | 0.58              |
| 1:K:499:GLN:HB2  | 1:K:520:GLN:NE2  | 2.18                     | 0.58              |
| 1:L:548:LYS:NZ   | 1:L:601:GLN:CA   | 2.61                     | 0.58              |
| 1:M:769:ARG:HH12 | 1:M:771:PHE:HB2  | 1.67                     | 0.58              |
| 1:M:819:PHE:HD1  | 1:M:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:N:11:GLN:NE2   | 1:N:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:N:188:SER:N    | 1:N:251:APK:O2P  | 2.31                     | 0.58              |
| 1:N:637:LEU:O    | 1:N:638:GLU:CB   | 2.43                     | 0.58              |
| 1:O:11:GLN:NE2   | 1:O:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:O:186:CYS:O    | 1:O:187:ASN:ND2  | 2.35                     | 0.58              |
| 1:O:519:GLN:HG2  | 1:O:523:PHE:CE2  | 2.37                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:314:ARG:O    | 1:P:315:GLU:HB2  | 2.03                     | 0.58              |
| 1:P:919:VAL:HG12 | 1:P:933:THR:HG22 | 1.83                     | 0.58              |
| 1:A:11:GLN:NE2   | 1:A:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:A:819:PHE:HD1  | 1:A:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:B:365:TYR:O    | 1:B:368:MET:N    | 2.21                     | 0.58              |
| 1:B:517:THR:O    | 1:B:519:GLN:N    | 2.35                     | 0.58              |
| 1:B:819:PHE:HD1  | 1:B:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:C:343:HIS:O    | 1:C:344:VAL:C    | 2.46                     | 0.58              |
| 1:C:819:PHE:HD1  | 1:C:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:D:499:GLN:HB2  | 1:D:520:GLN:NE2  | 2.18                     | 0.58              |
| 1:D:1055:GLU:HG3 | 1:D:1056:GLU:H   | 1.68                     | 0.58              |
| 1:E:504:ASP:OD2  | 1:E:509:ASN:O    | 2.21                     | 0.58              |
| 1:G:314:ARG:O    | 1:G:315:GLU:HB2  | 2.03                     | 0.58              |
| 1:H:11:GLN:NE2   | 1:H:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:I:11:GLN:NE2   | 1:I:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:L:24:VAL:HA    | 1:L:58:THR:HG21  | 1.85                     | 0.58              |
| 1:L:519:GLN:HG2  | 1:L:523:PHE:CE2  | 2.37                     | 0.58              |
| 1:L:819:PHE:HD1  | 1:L:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:M:365:TYR:O    | 1:M:368:MET:N    | 2.21                     | 0.58              |
| 1:M:517:THR:O    | 1:M:519:GLN:N    | 2.35                     | 0.58              |
| 1:N:371:ARG:HB3  | 1:N:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:N:819:PHE:HD1  | 1:N:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:P:252:ALA:O    | 1:P:255:ALA:N    | 2.25                     | 0.58              |
| 1:P:631:LEU:HD23 | 1:P:646:ARG:HH21 | 1.66                     | 0.58              |
| 1:B:343:HIS:O    | 1:B:344:VAL:C    | 2.46                     | 0.58              |
| 1:B:769:ARG:HH12 | 1:B:771:PHE:HB2  | 1.67                     | 0.58              |
| 1:C:519:GLN:HG2  | 1:C:523:PHE:CE2  | 2.37                     | 0.58              |
| 1:E:371:ARG:HB3  | 1:E:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:E:633:THR:HG21 | 1:E:643:TYR:CA   | 2.33                     | 0.58              |
| 1:F:458:LEU:HA   | 1:F:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:G:919:VAL:HG12 | 1:G:933:THR:HG22 | 1.83                     | 0.58              |
| 1:H:519:GLN:HG2  | 1:H:523:PHE:CE2  | 2.37                     | 0.58              |
| 1:J:371:ARG:HB3  | 1:J:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:K:24:VAL:HA    | 1:K:58:THR:HG21  | 1.85                     | 0.58              |
| 1:L:499:GLN:HB2  | 1:L:520:GLN:NE2  | 2.18                     | 0.58              |
| 1:N:499:GLN:HB2  | 1:N:520:GLN:NE2  | 2.18                     | 0.58              |
| 1:N:511:SER:HA   | 1:N:514:ILE:N    | 2.17                     | 0.58              |
| 1:O:371:ARG:HB3  | 1:O:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:P:819:PHE:HD1  | 1:P:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:P:1055:GLU:HG3 | 1:P:1056:GLU:H   | 1.68                     | 0.58              |
| 1:A:517:THR:O    | 1:A:519:GLN:N    | 2.35                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:194:GLU:O    | 1:C:197:GLN:N    | 2.37                     | 0.58              |
| 1:C:313:PRO:HA   | 1:C:338:TRP:HH2  | 1.63                     | 0.58              |
| 1:C:316:VAL:HG23 | 1:C:316:VAL:O    | 2.02                     | 0.58              |
| 1:C:499:GLN:HB2  | 1:C:520:GLN:NE2  | 2.18                     | 0.58              |
| 1:C:637:LEU:O    | 1:C:638:GLU:CB   | 2.43                     | 0.58              |
| 1:E:198:LYS:HZ1  | 1:F:222:HIS:CG   | 2.22                     | 0.58              |
| 1:E:336:ALA:HA   | 1:E:340:ASN:HB3  | 1.85                     | 0.58              |
| 1:F:111:ASP:HB3  | 1:G:144:ALA:HB3  | 1.85                     | 0.58              |
| 1:G:14:ASP:OD2   | 1:H:142:ARG:NH1  | 2.36                     | 0.58              |
| 1:G:194:GLU:O    | 1:G:197:GLN:N    | 2.37                     | 0.58              |
| 1:G:458:LEU:HA   | 1:G:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:G:511:SER:HA   | 1:G:514:ILE:N    | 2.18                     | 0.58              |
| 1:G:819:PHE:HD1  | 1:G:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:G:1055:GLU:HG3 | 1:G:1056:GLU:H   | 1.68                     | 0.58              |
| 1:H:371:ARG:HB3  | 1:H:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:H:444:VAL:HG22 | 1:H:478:ILE:HG12 | 1.85                     | 0.58              |
| 1:I:194:GLU:O    | 1:I:197:GLN:N    | 2.37                     | 0.58              |
| 1:I:519:GLN:HG2  | 1:I:523:PHE:CE2  | 2.37                     | 0.58              |
| 1:J:336:ALA:HA   | 1:J:340:ASN:HB3  | 1.85                     | 0.58              |
| 1:L:343:HIS:O    | 1:L:344:VAL:C    | 2.46                     | 0.58              |
| 1:L:1055:GLU:HG3 | 1:L:1056:GLU:H   | 1.68                     | 0.58              |
| 1:M:343:HIS:O    | 1:M:344:VAL:C    | 2.46                     | 0.58              |
| 1:N:194:GLU:O    | 1:N:197:GLN:N    | 2.37                     | 0.58              |
| 1:N:451:LYS:HD3  | 1:N:486:LEU:CD2  | 2.26                     | 0.58              |
| 1:N:517:THR:O    | 1:N:519:GLN:N    | 2.35                     | 0.58              |
| 1:O:444:VAL:HG22 | 1:O:478:ILE:HG12 | 1.85                     | 0.58              |
| 1:O:517:THR:O    | 1:O:519:GLN:N    | 2.35                     | 0.58              |
| 1:O:518:LEU:HA   | 1:O:521:LEU:HB3  | 1.84                     | 0.58              |
| 1:O:1055:GLU:HG3 | 1:O:1056:GLU:H   | 1.68                     | 0.58              |
| 1:P:458:LEU:HA   | 1:P:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:P:511:SER:HA   | 1:P:514:ILE:N    | 2.17                     | 0.58              |
| 1:A:194:GLU:O    | 1:A:197:GLN:N    | 2.37                     | 0.58              |
| 1:A:458:LEU:HA   | 1:A:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:B:121:ALA:HB1  | 1:C:276:SER:HB2  | 1.79                     | 0.58              |
| 1:D:319:THR:O    | 1:D:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:E:209:SER:HG   | 1:F:212:ASP:CG   | 1.92                     | 0.58              |
| 1:E:882:LEU:HG   | 1:E:883:ILE:HG13 | 1.86                     | 0.58              |
| 1:F:194:GLU:O    | 1:F:197:GLN:N    | 2.37                     | 0.58              |
| 1:F:1055:GLU:HG3 | 1:F:1056:GLU:H   | 1.68                     | 0.58              |
| 1:H:314:ARG:O    | 1:H:315:GLU:HB2  | 2.03                     | 0.58              |
| 1:H:1055:GLU:HG3 | 1:H:1056:GLU:H   | 1.68                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:458:LEU:HA   | 1:I:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:K:314:ARG:O    | 1:K:315:GLU:HB2  | 2.03                     | 0.58              |
| 1:K:319:THR:O    | 1:K:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:K:371:ARG:HB3  | 1:K:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:N:504:ASP:OD2  | 1:N:509:ASN:O    | 2.21                     | 0.58              |
| 1:P:194:GLU:O    | 1:P:197:GLN:N    | 2.37                     | 0.58              |
| 1:P:519:GLN:HG2  | 1:P:523:PHE:CE2  | 2.37                     | 0.58              |
| 1:A:1055:GLU:HG3 | 1:A:1056:GLU:H   | 1.68                     | 0.58              |
| 1:B:319:THR:O    | 1:B:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:B:637:LEU:O    | 1:B:638:GLU:CB   | 2.43                     | 0.58              |
| 1:F:518:LEU:HA   | 1:F:521:LEU:HB3  | 1.84                     | 0.58              |
| 1:G:24:VAL:HA    | 1:G:58:THR:HG21  | 1.85                     | 0.58              |
| 1:G:319:THR:O    | 1:G:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:I:1055:GLU:HG3 | 1:I:1056:GLU:H   | 1.68                     | 0.58              |
| 1:J:882:LEU:HG   | 1:J:883:ILE:HG13 | 1.86                     | 0.58              |
| 1:J:1055:GLU:HG3 | 1:J:1056:GLU:H   | 1.68                     | 0.58              |
| 1:L:194:GLU:O    | 1:L:197:GLN:N    | 2.37                     | 0.58              |
| 1:L:313:PRO:HA   | 1:L:338:TRP:HH2  | 1.63                     | 0.58              |
| 1:L:371:ARG:HB3  | 1:L:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:L:444:VAL:HG22 | 1:L:478:ILE:HG12 | 1.85                     | 0.58              |
| 1:M:319:THR:O    | 1:M:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:M:371:ARG:HB3  | 1:M:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:M:1055:GLU:HG3 | 1:M:1056:GLU:H   | 1.68                     | 0.58              |
| 1:N:458:LEU:HA   | 1:N:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:N:1055:GLU:HG3 | 1:N:1056:GLU:H   | 1.68                     | 0.58              |
| 1:O:319:THR:O    | 1:O:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:P:24:VAL:HA    | 1:P:58:THR:HG21  | 1.85                     | 0.58              |
| 1:P:319:THR:O    | 1:P:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:A:492:LEU:HD21 | 1:A:562:LEU:HD23 | 1.86                     | 0.58              |
| 1:A:504:ASP:OD2  | 1:A:509:ASN:O    | 2.21                     | 0.58              |
| 1:B:371:ARG:HB3  | 1:B:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:B:548:LYS:HZ2  | 1:B:601:GLN:H    | 1.52                     | 0.58              |
| 1:B:1055:GLU:HG3 | 1:B:1056:GLU:H   | 1.68                     | 0.58              |
| 1:C:882:LEU:HG   | 1:C:883:ILE:HG13 | 1.86                     | 0.58              |
| 1:D:194:GLU:O    | 1:D:197:GLN:N    | 2.37                     | 0.58              |
| 1:D:314:ARG:O    | 1:D:315:GLU:HB2  | 2.03                     | 0.58              |
| 1:D:343:HIS:O    | 1:D:344:VAL:C    | 2.46                     | 0.58              |
| 1:D:371:ARG:HB3  | 1:D:389:ILE:HG21 | 1.85                     | 0.58              |
| 1:E:24:VAL:HA    | 1:E:58:THR:HG21  | 1.85                     | 0.58              |
| 1:G:336:ALA:HA   | 1:G:340:ASN:HB3  | 1.85                     | 0.58              |
| 1:G:519:GLN:HG2  | 1:G:523:PHE:CE2  | 2.37                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:563:ARG:HD3  | 1:G:566:LEU:HD12 | 1.86                     | 0.58              |
| 1:H:319:THR:O    | 1:H:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:I:819:PHE:HD1  | 1:I:830:LEU:HD13 | 1.68                     | 0.58              |
| 1:J:24:VAL:HA    | 1:J:58:THR:HG21  | 1.85                     | 0.58              |
| 1:K:343:HIS:O    | 1:K:344:VAL:C    | 2.46                     | 0.58              |
| 1:L:11:GLN:NE2   | 1:L:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:L:882:LEU:HG   | 1:L:883:ILE:HG13 | 1.86                     | 0.58              |
| 1:N:492:LEU:HD21 | 1:N:562:LEU:HD23 | 1.86                     | 0.58              |
| 1:P:553:LEU:HB3  | 1:P:556:SER:OG   | 2.04                     | 0.58              |
| 1:P:563:ARG:HD3  | 1:P:566:LEU:HD12 | 1.86                     | 0.58              |
| 1:A:343:HIS:O    | 1:A:344:VAL:C    | 2.46                     | 0.58              |
| 1:B:548:LYS:NZ   | 1:B:601:GLN:CA   | 2.61                     | 0.58              |
| 1:C:11:GLN:NE2   | 1:C:70:GLU:OE1   | 2.36                     | 0.58              |
| 1:C:1055:GLU:HG3 | 1:C:1056:GLU:H   | 1.68                     | 0.58              |
| 1:D:397:ASP:O    | 1:D:401:VAL:N    | 2.28                     | 0.58              |
| 1:D:458:LEU:HA   | 1:D:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:E:1055:GLU:HG3 | 1:E:1056:GLU:H   | 1.68                     | 0.58              |
| 1:G:553:LEU:HB3  | 1:G:556:SER:OG   | 2.04                     | 0.58              |
| 1:I:492:LEU:HD21 | 1:I:562:LEU:HD23 | 1.85                     | 0.58              |
| 1:I:518:LEU:HA   | 1:I:521:LEU:HB3  | 1.84                     | 0.58              |
| 1:J:194:GLU:O    | 1:J:197:GLN:N    | 2.37                     | 0.58              |
| 1:J:319:THR:O    | 1:J:320:ASN:ND2  | 2.37                     | 0.58              |
| 1:K:194:GLU:O    | 1:K:197:GLN:N    | 2.37                     | 0.58              |
| 1:M:194:GLU:O    | 1:M:197:GLN:N    | 2.37                     | 0.58              |
| 1:M:458:LEU:HA   | 1:M:587:ARG:NH2  | 2.19                     | 0.58              |
| 1:P:517:THR:O    | 1:P:519:GLN:N    | 2.35                     | 0.58              |
| 1:B:194:GLU:O    | 1:B:197:GLN:N    | 2.37                     | 0.58              |
| 1:B:444:VAL:HG22 | 1:B:478:ILE:HG12 | 1.85                     | 0.58              |
| 1:B:553:LEU:HB3  | 1:B:556:SER:OG   | 2.04                     | 0.58              |
| 1:B:882:LEU:HG   | 1:B:883:ILE:HG13 | 1.86                     | 0.58              |
| 1:C:799:ASN:C    | 1:C:800:THR:HG23 | 2.29                     | 0.58              |
| 1:D:316:VAL:HG23 | 1:D:316:VAL:O    | 2.02                     | 0.58              |
| 1:D:799:ASN:C    | 1:D:800:THR:HG23 | 2.29                     | 0.58              |
| 1:E:194:GLU:O    | 1:E:197:GLN:N    | 2.37                     | 0.58              |
| 1:F:492:LEU:HD21 | 1:F:562:LEU:HD23 | 1.86                     | 0.58              |
| 1:G:517:THR:O    | 1:G:519:GLN:N    | 2.35                     | 0.58              |
| 1:H:316:VAL:HG23 | 1:H:316:VAL:O    | 2.02                     | 0.58              |
| 1:H:553:LEU:HB3  | 1:H:556:SER:OG   | 2.04                     | 0.58              |
| 1:H:799:ASN:C    | 1:H:800:THR:HG23 | 2.29                     | 0.58              |
| 1:K:316:VAL:HG23 | 1:K:316:VAL:O    | 2.03                     | 0.58              |
| 1:K:458:LEU:HA   | 1:K:587:ARG:NH2  | 2.19                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:799:ASN:C     | 1:K:800:THR:HG23  | 2.29                     | 0.58              |
| 1:L:365:TYR:O     | 1:L:368:MET:N     | 2.21                     | 0.58              |
| 1:L:458:LEU:HA    | 1:L:587:ARG:NH2   | 2.19                     | 0.58              |
| 1:L:799:ASN:C     | 1:L:800:THR:HG23  | 2.29                     | 0.58              |
| 1:M:444:VAL:HG22  | 1:M:478:ILE:HG12  | 1.85                     | 0.58              |
| 1:M:553:LEU:HB3   | 1:M:556:SER:OG    | 2.04                     | 0.58              |
| 1:M:882:LEU:HG    | 1:M:883:ILE:HG13  | 1.86                     | 0.58              |
| 1:N:316:VAL:HG23  | 1:N:316:VAL:O     | 2.02                     | 0.58              |
| 1:N:343:HIS:O     | 1:N:344:VAL:C     | 2.46                     | 0.58              |
| 1:O:194:GLU:O     | 1:O:197:GLN:N     | 2.37                     | 0.58              |
| 1:P:336:ALA:HA    | 1:P:340:ASN:HB3   | 1.85                     | 0.58              |
| 1:A:553:LEU:HB3   | 1:A:556:SER:OG    | 2.04                     | 0.58              |
| 1:B:458:LEU:HA    | 1:B:587:ARG:NH2   | 2.19                     | 0.58              |
| 1:B:799:ASN:C     | 1:B:800:THR:HG23  | 2.29                     | 0.58              |
| 1:C:444:VAL:HG22  | 1:C:478:ILE:HG12  | 1.85                     | 0.58              |
| 1:C:458:LEU:HA    | 1:C:587:ARG:NH2   | 2.19                     | 0.58              |
| 1:C:499:GLN:HA    | 1:C:502:ARG:HD2   | 1.86                     | 0.58              |
| 1:C:548:LYS:HZ2   | 1:C:601:GLN:H     | 1.52                     | 0.58              |
| 1:E:319:THR:O     | 1:E:320:ASN:ND2   | 2.37                     | 0.58              |
| 1:E:508:TRP:CZ3   | 1:E:927:GLN:C     | 2.82                     | 0.58              |
| 1:F:819:PHE:HD1   | 1:F:830:LEU:HD13  | 1.68                     | 0.58              |
| 1:H:188:SER:N     | 1:H:251:APK:O2P   | 2.31                     | 0.58              |
| 1:H:194:GLU:O     | 1:H:197:GLN:N     | 2.37                     | 0.58              |
| 1:H:819:PHE:HD1   | 1:H:830:LEU:HD13  | 1.68                     | 0.58              |
| 1:I:343:HIS:O     | 1:I:344:VAL:C     | 2.46                     | 0.58              |
| 1:I:882:LEU:HG    | 1:I:883:ILE:HG13  | 1.86                     | 0.58              |
| 1:I:1031:ILE:HD11 | 1:I:1068:ILE:HD13 | 1.86                     | 0.58              |
| 1:L:314:ARG:O     | 1:L:315:GLU:HB2   | 2.03                     | 0.58              |
| 1:L:316:VAL:HG23  | 1:L:316:VAL:O     | 2.03                     | 0.58              |
| 1:M:508:TRP:CZ3   | 1:M:927:GLN:C     | 2.82                     | 0.58              |
| 1:M:799:ASN:C     | 1:M:800:THR:HG23  | 2.29                     | 0.58              |
| 1:N:319:THR:O     | 1:N:320:ASN:ND2   | 2.37                     | 0.58              |
| 1:N:508:TRP:CZ3   | 1:N:927:GLN:C     | 2.82                     | 0.58              |
| 1:N:553:LEU:HB3   | 1:N:556:SER:OG    | 2.04                     | 0.58              |
| 1:O:316:VAL:HG23  | 1:O:316:VAL:O     | 2.02                     | 0.58              |
| 1:O:492:LEU:HD21  | 1:O:562:LEU:HD23  | 1.86                     | 0.58              |
| 1:O:553:LEU:HB3   | 1:O:556:SER:OG    | 2.04                     | 0.58              |
| 1:O:799:ASN:C     | 1:O:800:THR:HG23  | 2.29                     | 0.58              |
| 1:P:378:SER:HA    | 1:P:422:ILE:HD12  | 1.84                     | 0.58              |
| 1:A:319:THR:O     | 1:A:320:ASN:ND2   | 2.37                     | 0.57              |
| 1:B:336:ALA:HA    | 1:B:340:ASN:HB3   | 1.85                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:508:TRP:CZ3   | 1:B:927:GLN:C     | 2.82                     | 0.57              |
| 1:C:371:ARG:HB3   | 1:C:389:ILE:HG21  | 1.85                     | 0.57              |
| 1:D:553:LEU:HB3   | 1:D:556:SER:OG    | 2.04                     | 0.57              |
| 1:D:882:LEU:HG    | 1:D:883:ILE:HG13  | 1.86                     | 0.57              |
| 1:E:458:LEU:HA    | 1:E:587:ARG:NH2   | 2.19                     | 0.57              |
| 1:E:799:ASN:C     | 1:E:800:THR:HG23  | 2.29                     | 0.57              |
| 1:F:114:TYR:O     | 1:F:117:ASN:N     | 2.36                     | 0.57              |
| 1:F:799:ASN:C     | 1:F:800:THR:HG23  | 2.29                     | 0.57              |
| 1:F:1031:ILE:HD11 | 1:F:1068:ILE:HD13 | 1.86                     | 0.57              |
| 1:G:378:SER:HA    | 1:G:422:ILE:HD12  | 1.84                     | 0.57              |
| 1:G:799:ASN:C     | 1:G:800:THR:HG23  | 2.29                     | 0.57              |
| 1:I:600:ARG:NE    | 1:I:1229:GLU:OE1  | 2.37                     | 0.57              |
| 1:I:799:ASN:C     | 1:I:800:THR:HG23  | 2.29                     | 0.57              |
| 1:J:458:LEU:HA    | 1:J:587:ARG:NH2   | 2.19                     | 0.57              |
| 1:K:553:LEU:HB3   | 1:K:556:SER:OG    | 2.04                     | 0.57              |
| 1:K:882:LEU:HG    | 1:K:883:ILE:HG13  | 1.86                     | 0.57              |
| 1:L:369:PHE:O     | 1:L:372:LEU:N     | 2.37                     | 0.57              |
| 1:L:548:LYS:HZ2   | 1:L:601:GLN:H     | 1.52                     | 0.57              |
| 1:M:336:ALA:HA    | 1:M:340:ASN:HB3   | 1.85                     | 0.57              |
| 1:M:378:SER:H     | 1:M:422:ILE:HD13  | 1.62                     | 0.57              |
| 1:M:548:LYS:NZ    | 1:M:601:GLN:CA    | 2.61                     | 0.57              |
| 1:N:336:ALA:HA    | 1:N:340:ASN:HB3   | 1.85                     | 0.57              |
| 1:O:769:ARG:HH12  | 1:O:771:PHE:HB2   | 1.67                     | 0.57              |
| 1:A:316:VAL:HG23  | 1:A:316:VAL:O     | 2.02                     | 0.57              |
| 1:A:369:PHE:O     | 1:A:372:LEU:N     | 2.37                     | 0.57              |
| 1:A:444:VAL:HG22  | 1:A:478:ILE:HG12  | 1.85                     | 0.57              |
| 1:A:508:TRP:CZ3   | 1:A:927:GLN:C     | 2.82                     | 0.57              |
| 1:A:633:THR:HG21  | 1:A:643:TYR:CA    | 2.33                     | 0.57              |
| 1:B:369:PHE:O     | 1:B:372:LEU:N     | 2.37                     | 0.57              |
| 1:B:499:GLN:HA    | 1:B:502:ARG:HD2   | 1.86                     | 0.57              |
| 1:B:504:ASP:OD2   | 1:B:509:ASN:O     | 2.21                     | 0.57              |
| 1:C:314:ARG:O     | 1:C:315:GLU:HB2   | 2.03                     | 0.57              |
| 1:C:336:ALA:HA    | 1:C:340:ASN:HB3   | 1.85                     | 0.57              |
| 1:C:553:LEU:HB3   | 1:C:556:SER:OG    | 2.04                     | 0.57              |
| 1:D:11:GLN:NE2    | 1:D:70:GLU:OE1    | 2.36                     | 0.57              |
| 1:F:553:LEU:HB3   | 1:F:556:SER:OG    | 2.04                     | 0.57              |
| 1:F:600:ARG:NE    | 1:F:1229:GLU:OE1  | 2.37                     | 0.57              |
| 1:F:882:LEU:HG    | 1:F:883:ILE:HG13  | 1.86                     | 0.57              |
| 1:G:492:LEU:HD21  | 1:G:562:LEU:HD23  | 1.85                     | 0.57              |
| 1:H:492:LEU:HD21  | 1:H:562:LEU:HD23  | 1.86                     | 0.57              |
| 1:H:769:ARG:HH12  | 1:H:771:PHE:HB2   | 1.67                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:553:LEU:HB3   | 1:I:556:SER:OG    | 2.04                     | 0.57              |
| 1:J:508:TRP:CZ3   | 1:J:927:GLN:C     | 2.82                     | 0.57              |
| 1:J:799:ASN:C     | 1:J:800:THR:HG23  | 2.29                     | 0.57              |
| 1:K:11:GLN:NE2    | 1:K:70:GLU:OE1    | 2.36                     | 0.57              |
| 1:K:499:GLN:HA    | 1:K:502:ARG:HD2   | 1.86                     | 0.57              |
| 1:K:504:ASP:OD2   | 1:K:509:ASN:O     | 2.21                     | 0.57              |
| 1:K:1031:ILE:HD11 | 1:K:1068:ILE:HD13 | 1.86                     | 0.57              |
| 1:M:369:PHE:O     | 1:M:372:LEU:N     | 2.37                     | 0.57              |
| 1:M:499:GLN:HA    | 1:M:502:ARG:HD2   | 1.86                     | 0.57              |
| 1:M:504:ASP:OD2   | 1:M:509:ASN:O     | 2.21                     | 0.57              |
| 1:N:369:PHE:O     | 1:N:372:LEU:N     | 2.37                     | 0.57              |
| 1:N:444:VAL:HG22  | 1:N:478:ILE:HG12  | 1.85                     | 0.57              |
| 1:O:819:PHE:HD1   | 1:O:830:LEU:HD13  | 1.68                     | 0.57              |
| 1:P:365:TYR:O     | 1:P:368:MET:N     | 2.21                     | 0.57              |
| 1:P:492:LEU:HD21  | 1:P:562:LEU:HD23  | 1.85                     | 0.57              |
| 1:P:799:ASN:C     | 1:P:800:THR:HG23  | 2.29                     | 0.57              |
| 1:A:336:ALA:HA    | 1:A:340:ASN:HB3   | 1.85                     | 0.57              |
| 1:C:369:PHE:O     | 1:C:372:LEU:N     | 2.38                     | 0.57              |
| 1:D:369:PHE:O     | 1:D:372:LEU:N     | 2.38                     | 0.57              |
| 1:D:504:ASP:OD2   | 1:D:509:ASN:O     | 2.21                     | 0.57              |
| 1:D:1031:ILE:HD11 | 1:D:1068:ILE:HD13 | 1.86                     | 0.57              |
| 1:E:11:GLN:NE2    | 1:E:70:GLU:OE1    | 2.36                     | 0.57              |
| 1:F:603:ILE:HD11  | 1:F:635:VAL:HG13  | 1.87                     | 0.57              |
| 1:H:458:LEU:HA    | 1:H:587:ARG:NH2   | 2.19                     | 0.57              |
| 1:I:319:THR:O     | 1:I:320:ASN:ND2   | 2.37                     | 0.57              |
| 1:I:603:ILE:HD11  | 1:I:635:VAL:HG13  | 1.87                     | 0.57              |
| 1:K:369:PHE:O     | 1:K:372:LEU:N     | 2.38                     | 0.57              |
| 1:K:397:ASP:O     | 1:K:401:VAL:N     | 2.28                     | 0.57              |
| 1:L:114:TYR:O     | 1:L:117:ASN:N     | 2.36                     | 0.57              |
| 1:L:319:THR:O     | 1:L:320:ASN:ND2   | 2.37                     | 0.57              |
| 1:L:499:GLN:HA    | 1:L:502:ARG:HD2   | 1.86                     | 0.57              |
| 1:N:633:THR:HG21  | 1:N:643:TYR:CA    | 2.33                     | 0.57              |
| 1:A:142:ARG:NH1   | 1:H:14:ASP:OD2    | 2.35                     | 0.57              |
| 1:C:319:THR:O     | 1:C:320:ASN:ND2   | 2.37                     | 0.57              |
| 1:D:499:GLN:HA    | 1:D:502:ARG:HD2   | 1.86                     | 0.57              |
| 1:D:508:TRP:CZ3   | 1:D:927:GLN:C     | 2.82                     | 0.57              |
| 1:F:557:LYS:HZ2   | 1:F:1223:GLN:HG3  | 1.69                     | 0.57              |
| 1:G:365:TYR:O     | 1:G:368:MET:N     | 2.21                     | 0.57              |
| 1:I:24:VAL:HA     | 1:I:58:THR:HG21   | 1.85                     | 0.57              |
| 1:J:369:PHE:O     | 1:J:372:LEU:N     | 2.37                     | 0.57              |
| 1:K:548:LYS:HZ2   | 1:K:601:GLN:H     | 1.53                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:378:SER:HA   | 1:L:422:ILE:HD12 | 1.84                     | 0.57              |
| 1:L:504:ASP:OD2  | 1:L:509:ASN:O    | 2.21                     | 0.57              |
| 1:O:188:SER:N    | 1:O:251:APK:O2P  | 2.31                     | 0.57              |
| 1:O:603:ILE:HD11 | 1:O:635:VAL:HG13 | 1.87                     | 0.57              |
| 1:A:518:LEU:HD22 | 1:A:643:TYR:CE1  | 2.22                     | 0.57              |
| 1:B:378:SER:H    | 1:B:422:ILE:HD13 | 1.62                     | 0.57              |
| 1:B:951:VAL:HA   | 1:B:987:VAL:HG11 | 1.87                     | 0.57              |
| 1:C:378:SER:HA   | 1:C:422:ILE:HD12 | 1.84                     | 0.57              |
| 1:C:504:ASP:OD2  | 1:C:509:ASN:O    | 2.21                     | 0.57              |
| 1:E:369:PHE:O    | 1:E:372:LEU:N    | 2.37                     | 0.57              |
| 1:H:603:ILE:HD11 | 1:H:635:VAL:HG13 | 1.87                     | 0.57              |
| 1:I:563:ARG:HD3  | 1:I:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:J:11:GLN:NE2   | 1:J:70:GLU:OE1   | 2.36                     | 0.57              |
| 1:L:508:TRP:CZ3  | 1:L:927:GLN:C    | 2.82                     | 0.57              |
| 1:L:553:LEU:HB3  | 1:L:556:SER:OG   | 2.04                     | 0.57              |
| 1:M:316:VAL:O    | 1:M:316:VAL:HG23 | 2.02                     | 0.57              |
| 1:M:518:LEU:HD22 | 1:M:643:TYR:CE1  | 2.22                     | 0.57              |
| 1:B:423:PRO:O    | 1:B:424:SER:HB3  | 2.05                     | 0.57              |
| 1:B:518:LEU:HD22 | 1:B:643:TYR:CE1  | 2.22                     | 0.57              |
| 1:C:423:PRO:O    | 1:C:424:SER:HB3  | 2.05                     | 0.57              |
| 1:C:508:TRP:CZ3  | 1:C:927:GLN:C    | 2.82                     | 0.57              |
| 1:E:557:LYS:CE   | 1:E:1224:LEU:O   | 2.51                     | 0.57              |
| 1:F:24:VAL:HA    | 1:F:58:THR:HG21  | 1.85                     | 0.57              |
| 1:F:563:ARG:HD3  | 1:F:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:H:369:PHE:O    | 1:H:372:LEU:N    | 2.38                     | 0.57              |
| 1:M:314:ARG:O    | 1:M:315:GLU:HB2  | 2.03                     | 0.57              |
| 1:M:951:VAL:HA   | 1:M:987:VAL:HG11 | 1.87                     | 0.57              |
| 1:N:472:GLY:HA2  | 1:N:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:N:518:LEU:HD22 | 1:N:643:TYR:CE1  | 2.22                     | 0.57              |
| 1:N:563:ARG:HD3  | 1:N:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:O:458:LEU:HA   | 1:O:587:ARG:NH2  | 2.19                     | 0.57              |
| 1:O:1177:TYR:HE2 | 1:P:916:LYS:HE2  | 1.70                     | 0.57              |
| 1:P:301:LEU:HD23 | 1:P:313:PRO:CD   | 2.35                     | 0.57              |
| 1:P:633:THR:HG21 | 1:P:643:TYR:CA   | 2.33                     | 0.57              |
| 1:A:472:GLY:HA2  | 1:A:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:A:563:ARG:HD3  | 1:A:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:882:LEU:HG   | 1:A:883:ILE:HG13 | 1.86                     | 0.57              |
| 1:F:319:THR:O    | 1:F:320:ASN:ND2  | 2.37                     | 0.57              |
| 1:G:124:ASN:H    | 1:G:303:LYS:HZ3  | 1.52                     | 0.57              |
| 1:G:301:LEU:HD23 | 1:G:313:PRO:CD   | 2.35                     | 0.57              |
| 1:G:442:SER:O    | 1:G:446:HIS:CG   | 2.55                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:505:SER:OG   | 1:G:513:SER:OG   | 2.05                     | 0.57              |
| 1:H:449:ILE:HB   | 1:H:450:PRO:HD3  | 1.86                     | 0.57              |
| 1:H:563:ARG:HD3  | 1:H:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:J:378:SER:H    | 1:J:422:ILE:HD13 | 1.62                     | 0.57              |
| 1:K:508:TRP:CZ3  | 1:K:927:GLN:C    | 2.82                     | 0.57              |
| 1:L:336:ALA:HA   | 1:L:340:ASN:HB3  | 1.85                     | 0.57              |
| 1:L:423:PRO:O    | 1:L:424:SER:HB3  | 2.05                     | 0.57              |
| 1:L:472:GLY:HA2  | 1:L:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:M:423:PRO:O    | 1:M:424:SER:HB3  | 2.05                     | 0.57              |
| 1:O:369:PHE:O    | 1:O:372:LEU:N    | 2.38                     | 0.57              |
| 1:O:508:TRP:CZ3  | 1:O:927:GLN:C    | 2.82                     | 0.57              |
| 1:P:505:SER:OG   | 1:P:513:SER:OG   | 2.05                     | 0.57              |
| 1:P:882:LEU:HG   | 1:P:883:ILE:HG13 | 1.86                     | 0.57              |
| 1:A:449:ILE:HB   | 1:A:450:PRO:HD3  | 1.87                     | 0.57              |
| 1:B:316:VAL:O    | 1:B:316:VAL:HG23 | 2.02                     | 0.57              |
| 1:B:472:GLY:HA2  | 1:B:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:B:603:ILE:HD11 | 1:B:635:VAL:HG13 | 1.87                     | 0.57              |
| 1:D:423:PRO:O    | 1:D:424:SER:HB3  | 2.05                     | 0.57              |
| 1:F:115:ASN:HB3  | 1:G:257:ASN:OD1  | 2.04                     | 0.57              |
| 1:G:371:ARG:HD3  | 1:G:435:ASN:HD21 | 1.70                     | 0.57              |
| 1:G:499:GLN:HA   | 1:G:502:ARG:HD2  | 1.86                     | 0.57              |
| 1:G:600:ARG:NE   | 1:G:1229:GLU:OE1 | 2.37                     | 0.57              |
| 1:G:633:THR:HG21 | 1:G:643:TYR:CA   | 2.33                     | 0.57              |
| 1:G:882:LEU:HG   | 1:G:883:ILE:HG13 | 1.86                     | 0.57              |
| 1:H:301:LEU:HD23 | 1:H:313:PRO:CD   | 2.35                     | 0.57              |
| 1:H:508:TRP:CZ3  | 1:H:927:GLN:C    | 2.82                     | 0.57              |
| 1:I:114:TYR:O    | 1:I:117:ASN:N    | 2.36                     | 0.57              |
| 1:J:423:PRO:O    | 1:J:424:SER:HB3  | 2.05                     | 0.57              |
| 1:J:557:LYS:CE   | 1:J:1224:LEU:O   | 2.51                     | 0.57              |
| 1:K:423:PRO:O    | 1:K:424:SER:HB3  | 2.05                     | 0.57              |
| 1:K:472:GLY:HA2  | 1:K:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:K:603:ILE:HD11 | 1:K:635:VAL:HG13 | 1.87                     | 0.57              |
| 1:M:472:GLY:HA2  | 1:M:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:M:603:ILE:HD11 | 1:M:635:VAL:HG13 | 1.87                     | 0.57              |
| 1:N:449:ILE:HB   | 1:N:450:PRO:HD3  | 1.87                     | 0.57              |
| 1:O:301:LEU:HD23 | 1:O:313:PRO:CD   | 2.35                     | 0.57              |
| 1:O:449:ILE:HB   | 1:O:450:PRO:HD3  | 1.86                     | 0.57              |
| 1:O:472:GLY:HA2  | 1:O:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:P:371:ARG:HD3  | 1:P:435:ASN:HD21 | 1.70                     | 0.57              |
| 1:P:442:SER:O    | 1:P:446:HIS:CG   | 2.55                     | 0.57              |
| 1:P:600:ARG:NE   | 1:P:1229:GLU:OE1 | 2.37                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:314:ARG:O    | 1:B:315:GLU:HB2  | 2.03                     | 0.57              |
| 1:C:472:GLY:HA2  | 1:C:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:D:472:GLY:HA2  | 1:D:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:D:603:ILE:HD11 | 1:D:635:VAL:HG13 | 1.87                     | 0.57              |
| 1:E:600:ARG:NE   | 1:E:1229:GLU:OE1 | 2.37                     | 0.57              |
| 1:F:508:TRP:CZ3  | 1:F:927:GLN:C    | 2.82                     | 0.57              |
| 1:G:508:TRP:CZ3  | 1:G:927:GLN:C    | 2.82                     | 0.57              |
| 1:H:336:ALA:O    | 1:H:338:TRP:N    | 2.38                     | 0.57              |
| 1:H:371:ARG:HD3  | 1:H:435:ASN:HD21 | 1.70                     | 0.57              |
| 1:H:472:GLY:HA2  | 1:H:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:I:124:ASN:H    | 1:I:303:LYS:NZ   | 2.03                     | 0.57              |
| 1:I:301:LEU:HD23 | 1:I:313:PRO:CD   | 2.35                     | 0.57              |
| 1:I:336:ALA:HA   | 1:I:340:ASN:HB3  | 1.85                     | 0.57              |
| 1:I:557:LYS:HZ2  | 1:I:1223:GLN:HG3 | 1.69                     | 0.57              |
| 1:J:343:HIS:O    | 1:J:344:VAL:C    | 2.46                     | 0.57              |
| 1:N:371:ARG:HD3  | 1:N:435:ASN:HD21 | 1.70                     | 0.57              |
| 1:N:769:ARG:HH12 | 1:N:771:PHE:HB2  | 1.67                     | 0.57              |
| 1:N:882:LEU:HG   | 1:N:883:ILE:HG13 | 1.86                     | 0.57              |
| 1:O:124:ASN:H    | 1:O:303:LYS:HZ3  | 1.53                     | 0.57              |
| 1:O:336:ALA:O    | 1:O:338:TRP:N    | 2.38                     | 0.57              |
| 1:O:371:ARG:HD3  | 1:O:435:ASN:HD21 | 1.70                     | 0.57              |
| 1:O:882:LEU:HG   | 1:O:883:ILE:HG13 | 1.86                     | 0.57              |
| 1:P:124:ASN:H    | 1:P:303:LYS:NZ   | 2.03                     | 0.57              |
| 1:P:499:GLN:HA   | 1:P:502:ARG:HD2  | 1.86                     | 0.57              |
| 1:P:508:TRP:CZ3  | 1:P:927:GLN:C    | 2.82                     | 0.57              |
| 1:A:799:ASN:C    | 1:A:800:THR:HG23 | 2.29                     | 0.57              |
| 1:B:347:ASP:OD1  | 1:B:348:LYS:N    | 2.37                     | 0.57              |
| 1:B:563:ARG:HD3  | 1:B:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:D:155:SER:HA   | 1:D:321:PRO:HD2  | 1.87                     | 0.57              |
| 1:E:423:PRO:O    | 1:E:424:SER:HB3  | 2.05                     | 0.57              |
| 1:E:449:ILE:HB   | 1:E:450:PRO:HD3  | 1.86                     | 0.57              |
| 1:E:472:GLY:HA2  | 1:E:475:LEU:HD12 | 1.87                     | 0.57              |
| 1:F:124:ASN:H    | 1:F:303:LYS:NZ   | 2.03                     | 0.57              |
| 1:F:198:LYS:NZ   | 1:G:222:HIS:CD2  | 2.73                     | 0.57              |
| 1:F:301:LEU:HD23 | 1:F:313:PRO:CD   | 2.35                     | 0.57              |
| 1:F:371:ARG:HD3  | 1:F:435:ASN:HD21 | 1.70                     | 0.57              |
| 1:G:124:ASN:H    | 1:G:303:LYS:NZ   | 2.03                     | 0.57              |
| 1:G:458:LEU:CD2  | 1:G:459:ILE:H    | 2.18                     | 0.57              |
| 1:H:336:ALA:HA   | 1:H:340:ASN:HB3  | 1.85                     | 0.57              |
| 1:H:423:PRO:O    | 1:H:424:SER:HB3  | 2.05                     | 0.57              |
| 1:H:458:LEU:CD2  | 1:H:459:ILE:H    | 2.18                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:155:SER:HA    | 1:K:321:PRO:HD2  | 1.87                     | 0.57              |
| 1:K:951:VAL:HA    | 1:K:987:VAL:HG11 | 1.87                     | 0.57              |
| 1:M:347:ASP:OD1   | 1:M:348:LYS:N    | 2.37                     | 0.57              |
| 1:M:563:ARG:HD3   | 1:M:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:N:799:ASN:C     | 1:N:800:THR:HG23 | 2.29                     | 0.57              |
| 1:O:458:LEU:CD2   | 1:O:459:ILE:H    | 2.18                     | 0.57              |
| 1:O:563:ARG:HD3   | 1:O:566:LEU:HD12 | 1.86                     | 0.57              |
| 1:O:951:VAL:HA    | 1:O:987:VAL:HG11 | 1.87                     | 0.57              |
| 1:A:371:ARG:HD3   | 1:A:435:ASN:HD21 | 1.70                     | 0.56              |
| 1:A:769:ARG:HH12  | 1:A:771:PHE:HB2  | 1.67                     | 0.56              |
| 1:B:511:SER:C     | 1:B:513:SER:N    | 2.60                     | 0.56              |
| 1:B:633:THR:HG21  | 1:B:643:TYR:CA   | 2.33                     | 0.56              |
| 1:C:557:LYS:CE    | 1:C:1224:LEU:O   | 2.50                     | 0.56              |
| 1:D:124:ASN:H     | 1:D:303:LYS:NZ   | 2.03                     | 0.56              |
| 1:D:951:VAL:HA    | 1:D:987:VAL:HG11 | 1.87                     | 0.56              |
| 1:E:124:ASN:H     | 1:E:303:LYS:NZ   | 2.03                     | 0.56              |
| 1:E:343:HIS:O     | 1:E:344:VAL:C    | 2.46                     | 0.56              |
| 1:E:499:GLN:HA    | 1:E:502:ARG:HD2  | 1.86                     | 0.56              |
| 1:F:336:ALA:O     | 1:F:338:TRP:N    | 2.38                     | 0.56              |
| 1:H:882:LEU:HG    | 1:H:883:ILE:HG13 | 1.86                     | 0.56              |
| 1:H:951:VAL:HA    | 1:H:987:VAL:HG11 | 1.87                     | 0.56              |
| 1:H:1058:ILE:HG13 | 1:H:1059:ASP:H   | 1.70                     | 0.56              |
| 1:I:508:TRP:CZ3   | 1:I:927:GLN:C    | 2.82                     | 0.56              |
| 1:J:124:ASN:H     | 1:J:303:LYS:NZ   | 2.03                     | 0.56              |
| 1:J:449:ILE:HB    | 1:J:450:PRO:HD3  | 1.87                     | 0.56              |
| 1:J:600:ARG:NE    | 1:J:1229:GLU:OE1 | 2.37                     | 0.56              |
| 1:K:124:ASN:H     | 1:K:303:LYS:NZ   | 2.03                     | 0.56              |
| 1:L:557:LYS:CE    | 1:L:1224:LEU:O   | 2.50                     | 0.56              |
| 1:M:301:LEU:HD23  | 1:M:313:PRO:CD   | 2.35                     | 0.56              |
| 1:M:1058:ILE:HG13 | 1:M:1059:ASP:H   | 1.70                     | 0.56              |
| 1:N:301:LEU:HD23  | 1:N:313:PRO:CD   | 2.35                     | 0.56              |
| 1:N:1058:ILE:HG13 | 1:N:1059:ASP:H   | 1.70                     | 0.56              |
| 1:O:336:ALA:HA    | 1:O:340:ASN:HB3  | 1.85                     | 0.56              |
| 1:O:423:PRO:O     | 1:O:424:SER:HB3  | 2.05                     | 0.56              |
| 1:O:1058:ILE:HG13 | 1:O:1059:ASP:H   | 1.70                     | 0.56              |
| 1:P:458:LEU:CD2   | 1:P:459:ILE:H    | 2.18                     | 0.56              |
| 1:A:301:LEU:HD23  | 1:A:313:PRO:CD   | 2.35                     | 0.56              |
| 1:B:301:LEU:HD23  | 1:B:313:PRO:CD   | 2.35                     | 0.56              |
| 1:B:336:ALA:O     | 1:B:338:TRP:N    | 2.38                     | 0.56              |
| 1:F:336:ALA:HA    | 1:F:340:ASN:HB3  | 1.85                     | 0.56              |
| 1:F:343:HIS:O     | 1:F:344:VAL:C    | 2.46                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:518:LEU:HD12  | 1:F:518:LEU:N     | 2.20                     | 0.56              |
| 1:G:343:HIS:O     | 1:G:344:VAL:C     | 2.46                     | 0.56              |
| 1:G:1058:ILE:HG13 | 1:G:1059:ASP:H    | 1.70                     | 0.56              |
| 1:H:124:ASN:H     | 1:H:303:LYS:HZ3   | 1.54                     | 0.56              |
| 1:I:336:ALA:O     | 1:I:338:TRP:N     | 2.38                     | 0.56              |
| 1:I:371:ARG:HD3   | 1:I:435:ASN:HD21  | 1.70                     | 0.56              |
| 1:J:155:SER:HA    | 1:J:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:J:472:GLY:HA2   | 1:J:475:LEU:HD12  | 1.87                     | 0.56              |
| 1:M:336:ALA:O     | 1:M:338:TRP:N     | 2.38                     | 0.56              |
| 1:M:633:THR:HG21  | 1:M:643:TYR:CA    | 2.33                     | 0.56              |
| 1:A:124:ASN:H     | 1:A:303:LYS:HZ3   | 1.54                     | 0.56              |
| 1:A:423:PRO:O     | 1:A:424:SER:HB3   | 2.05                     | 0.56              |
| 1:A:458:LEU:CD2   | 1:A:459:ILE:H     | 2.18                     | 0.56              |
| 1:A:499:GLN:HA    | 1:A:502:ARG:HD2   | 1.86                     | 0.56              |
| 1:A:603:ILE:HD11  | 1:A:635:VAL:HG13  | 1.87                     | 0.56              |
| 1:A:1058:ILE:HG13 | 1:A:1059:ASP:H    | 1.70                     | 0.56              |
| 1:B:1058:ILE:HG13 | 1:B:1059:ASP:H    | 1.70                     | 0.56              |
| 1:C:124:ASN:H     | 1:C:303:LYS:NZ    | 2.03                     | 0.56              |
| 1:C:301:LEU:HD23  | 1:C:313:PRO:CD    | 2.35                     | 0.56              |
| 1:C:633:THR:HG21  | 1:C:643:TYR:CA    | 2.33                     | 0.56              |
| 1:D:188:SER:N     | 1:D:251:APK:O2P   | 2.31                     | 0.56              |
| 1:D:301:LEU:HD23  | 1:D:313:PRO:CD    | 2.35                     | 0.56              |
| 1:D:336:ALA:HA    | 1:D:340:ASN:HB3   | 1.85                     | 0.56              |
| 1:D:449:ILE:HB    | 1:D:450:PRO:HD3   | 1.86                     | 0.56              |
| 1:D:486:LEU:O     | 1:D:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:E:155:SER:HA    | 1:E:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:E:241:LEU:HD12  | 1:E:241:LEU:O     | 2.06                     | 0.56              |
| 1:E:486:LEU:O     | 1:E:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:F:115:ASN:O     | 1:G:257:ASN:ND2   | 2.38                     | 0.56              |
| 1:F:378:SER:HA    | 1:F:422:ILE:HD12  | 1.84                     | 0.56              |
| 1:F:472:GLY:HA2   | 1:F:475:LEU:HD12  | 1.87                     | 0.56              |
| 1:G:155:SER:HA    | 1:G:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:G:449:ILE:HB    | 1:G:450:PRO:HD3   | 1.86                     | 0.56              |
| 1:G:520:GLN:HA    | 1:G:523:PHE:HD2   | 1.71                     | 0.56              |
| 1:H:343:HIS:O     | 1:H:344:VAL:C     | 2.46                     | 0.56              |
| 1:H:397:ASP:O     | 1:H:401:VAL:N     | 2.28                     | 0.56              |
| 1:H:486:LEU:O     | 1:H:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:H:1031:ILE:HD11 | 1:H:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:I:369:PHE:O     | 1:I:372:LEU:N     | 2.38                     | 0.56              |
| 1:J:241:LEU:HD12  | 1:J:241:LEU:O     | 2.06                     | 0.56              |
| 1:J:301:LEU:HD23  | 1:J:313:PRO:CD    | 2.35                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:486:LEU:O     | 1:J:488:ARG:HG3  | 2.06                     | 0.56              |
| 1:J:499:GLN:HA    | 1:J:502:ARG:HD2  | 1.86                     | 0.56              |
| 1:J:518:LEU:HD12  | 1:J:518:LEU:N    | 2.20                     | 0.56              |
| 1:J:553:LEU:HB3   | 1:J:556:SER:OG   | 2.04                     | 0.56              |
| 1:K:301:LEU:HD23  | 1:K:313:PRO:CD   | 2.35                     | 0.56              |
| 1:K:336:ALA:O     | 1:K:338:TRP:N    | 2.38                     | 0.56              |
| 1:K:449:ILE:HB    | 1:K:450:PRO:HD3  | 1.86                     | 0.56              |
| 1:K:600:ARG:NE    | 1:K:1229:GLU:OE1 | 2.37                     | 0.56              |
| 1:L:124:ASN:H     | 1:L:303:LYS:NZ   | 2.03                     | 0.56              |
| 1:L:1058:ILE:HG13 | 1:L:1059:ASP:H   | 1.70                     | 0.56              |
| 1:M:449:ILE:HB    | 1:M:450:PRO:HD3  | 1.86                     | 0.56              |
| 1:M:554:ILE:C     | 1:M:556:SER:H    | 2.13                     | 0.56              |
| 1:N:155:SER:HA    | 1:N:321:PRO:HD2  | 1.87                     | 0.56              |
| 1:N:314:ARG:O     | 1:N:315:GLU:HB2  | 2.03                     | 0.56              |
| 1:N:458:LEU:CD2   | 1:N:459:ILE:H    | 2.18                     | 0.56              |
| 1:N:486:LEU:O     | 1:N:488:ARG:HG3  | 2.05                     | 0.56              |
| 1:N:499:GLN:HA    | 1:N:502:ARG:HD2  | 1.86                     | 0.56              |
| 1:O:343:HIS:O     | 1:O:344:VAL:C    | 2.46                     | 0.56              |
| 1:O:486:LEU:O     | 1:O:488:ARG:HG3  | 2.05                     | 0.56              |
| 1:P:449:ILE:HB    | 1:P:450:PRO:HD3  | 1.87                     | 0.56              |
| 1:P:1058:ILE:HG13 | 1:P:1059:ASP:H   | 1.70                     | 0.56              |
| 1:A:155:SER:HA    | 1:A:321:PRO:HD2  | 1.87                     | 0.56              |
| 1:A:336:ALA:O     | 1:A:338:TRP:N    | 2.38                     | 0.56              |
| 1:B:442:SER:O     | 1:B:446:HIS:CG   | 2.55                     | 0.56              |
| 1:B:449:ILE:HB    | 1:B:450:PRO:HD3  | 1.87                     | 0.56              |
| 1:B:520:GLN:HA    | 1:B:523:PHE:HD2  | 1.71                     | 0.56              |
| 1:B:554:ILE:C     | 1:B:556:SER:H    | 2.13                     | 0.56              |
| 1:C:1058:ILE:HG13 | 1:C:1059:ASP:H   | 1.70                     | 0.56              |
| 1:D:336:ALA:O     | 1:D:338:TRP:N    | 2.38                     | 0.56              |
| 1:D:563:ARG:HD3   | 1:D:566:LEU:HD12 | 1.86                     | 0.56              |
| 1:E:301:LEU:HD23  | 1:E:313:PRO:CD   | 2.35                     | 0.56              |
| 1:E:518:LEU:HD12  | 1:E:518:LEU:N    | 2.20                     | 0.56              |
| 1:E:553:LEU:HB3   | 1:E:556:SER:OG   | 2.04                     | 0.56              |
| 1:E:563:ARG:HD3   | 1:E:566:LEU:HD12 | 1.86                     | 0.56              |
| 1:F:520:GLN:HA    | 1:F:523:PHE:HD2  | 1.71                     | 0.56              |
| 1:G:369:PHE:O     | 1:G:372:LEU:N    | 2.37                     | 0.56              |
| 1:H:600:ARG:NE    | 1:H:1229:GLU:OE1 | 2.37                     | 0.56              |
| 1:I:458:LEU:CD2   | 1:I:459:ILE:H    | 2.18                     | 0.56              |
| 1:I:520:GLN:HA    | 1:I:523:PHE:HD2  | 1.71                     | 0.56              |
| 1:J:548:LYS:HZ2   | 1:J:601:GLN:H    | 1.51                     | 0.56              |
| 1:K:188:SER:N     | 1:K:251:APK:O2P  | 2.31                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:336:ALA:HA    | 1:K:340:ASN:HB3   | 1.85                     | 0.56              |
| 1:K:486:LEU:O     | 1:K:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:K:563:ARG:HD3   | 1:K:566:LEU:HD12  | 1.86                     | 0.56              |
| 1:L:301:LEU:HD23  | 1:L:313:PRO:CD    | 2.35                     | 0.56              |
| 1:N:124:ASN:H     | 1:N:303:LYS:NZ    | 2.03                     | 0.56              |
| 1:N:423:PRO:O     | 1:N:424:SER:HB3   | 2.05                     | 0.56              |
| 1:O:124:ASN:H     | 1:O:303:LYS:NZ    | 2.03                     | 0.56              |
| 1:O:1031:ILE:HD11 | 1:O:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:P:155:SER:HA    | 1:P:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:P:343:HIS:O     | 1:P:344:VAL:C     | 2.46                     | 0.56              |
| 1:P:369:PHE:O     | 1:P:372:LEU:N     | 2.38                     | 0.56              |
| 1:P:378:SER:H     | 1:P:422:ILE:HD13  | 1.61                     | 0.56              |
| 1:P:472:GLY:HA2   | 1:P:475:LEU:HD12  | 1.87                     | 0.56              |
| 1:A:124:ASN:H     | 1:A:303:LYS:NZ    | 2.03                     | 0.56              |
| 1:B:371:ARG:HD3   | 1:B:435:ASN:HD21  | 1.70                     | 0.56              |
| 1:C:347:ASP:OD1   | 1:C:348:LYS:N     | 2.37                     | 0.56              |
| 1:C:492:LEU:HD21  | 1:C:562:LEU:HD23  | 1.86                     | 0.56              |
| 1:D:241:LEU:HD12  | 1:D:241:LEU:O     | 2.05                     | 0.56              |
| 1:D:600:ARG:NE    | 1:D:1229:GLU:OE1  | 2.37                     | 0.56              |
| 1:E:520:GLN:HA    | 1:E:523:PHE:HD2   | 1.71                     | 0.56              |
| 1:F:241:LEU:O     | 1:F:241:LEU:HD12  | 2.06                     | 0.56              |
| 1:F:458:LEU:CD2   | 1:F:459:ILE:H     | 2.18                     | 0.56              |
| 1:F:486:LEU:O     | 1:F:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:F:499:GLN:HA    | 1:F:502:ARG:HD2   | 1.86                     | 0.56              |
| 1:G:368:MET:HE1   | 1:G:401:VAL:HG21  | 1.88                     | 0.56              |
| 1:G:472:GLY:HA2   | 1:G:475:LEU:HD12  | 1.87                     | 0.56              |
| 1:H:350:THR:HA    | 1:H:353:ILE:HG22  | 1.88                     | 0.56              |
| 1:H:633:THR:HG21  | 1:H:643:TYR:CA    | 2.33                     | 0.56              |
| 1:I:423:PRO:O     | 1:I:424:SER:HB3   | 2.05                     | 0.56              |
| 1:I:449:ILE:HB    | 1:I:450:PRO:HD3   | 1.86                     | 0.56              |
| 1:I:472:GLY:HA2   | 1:I:475:LEU:HD12  | 1.87                     | 0.56              |
| 1:J:1031:ILE:HD11 | 1:J:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:K:241:LEU:HD12  | 1:K:241:LEU:O     | 2.06                     | 0.56              |
| 1:L:492:LEU:HD21  | 1:L:562:LEU:HD23  | 1.86                     | 0.56              |
| 1:L:554:ILE:C     | 1:L:556:SER:H     | 2.13                     | 0.56              |
| 1:L:563:ARG:HD3   | 1:L:566:LEU:HD12  | 1.86                     | 0.56              |
| 1:M:371:ARG:HD3   | 1:M:435:ASN:HD21  | 1.70                     | 0.56              |
| 1:M:442:SER:O     | 1:M:446:HIS:CG    | 2.55                     | 0.56              |
| 1:M:520:GLN:HA    | 1:M:523:PHE:HD2   | 1.71                     | 0.56              |
| 1:N:603:ILE:HD11  | 1:N:635:VAL:HG13  | 1.87                     | 0.56              |
| 1:O:350:THR:HA    | 1:O:353:ILE:HG22  | 1.88                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:336:ALA:O     | 1:P:338:TRP:N     | 2.38                     | 0.56              |
| 1:P:350:THR:HA    | 1:P:353:ILE:HG22  | 1.88                     | 0.56              |
| 1:P:368:MET:HE1   | 1:P:401:VAL:HG21  | 1.88                     | 0.56              |
| 1:P:486:LEU:O     | 1:P:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:P:520:GLN:HA    | 1:P:523:PHE:HD2   | 1.71                     | 0.56              |
| 1:A:314:ARG:O     | 1:A:315:GLU:HB2   | 2.03                     | 0.56              |
| 1:A:486:LEU:O     | 1:A:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:C:563:ARG:HD3   | 1:C:566:LEU:HD12  | 1.86                     | 0.56              |
| 1:C:984:LEU:HD12  | 1:C:1022:ALA:HB2  | 1.88                     | 0.56              |
| 1:F:369:PHE:O     | 1:F:372:LEU:N     | 2.38                     | 0.56              |
| 1:F:946:ARG:HG3   | 1:F:947:GLU:H     | 1.71                     | 0.56              |
| 1:G:336:ALA:O     | 1:G:338:TRP:N     | 2.38                     | 0.56              |
| 1:G:350:THR:HA    | 1:G:353:ILE:HG22  | 1.88                     | 0.56              |
| 1:G:378:SER:H     | 1:G:422:ILE:HD13  | 1.61                     | 0.56              |
| 1:G:486:LEU:O     | 1:G:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:H:124:ASN:H     | 1:H:303:LYS:NZ    | 2.03                     | 0.56              |
| 1:J:520:GLN:HA    | 1:J:523:PHE:HD2   | 1.71                     | 0.56              |
| 1:J:563:ARG:HD3   | 1:J:566:LEU:HD12  | 1.86                     | 0.56              |
| 1:K:557:LYS:HZ2   | 1:K:1223:GLN:HG3  | 1.70                     | 0.56              |
| 1:L:241:LEU:HD12  | 1:L:241:LEU:O     | 2.06                     | 0.56              |
| 1:M:124:ASN:H     | 1:M:303:LYS:NZ    | 2.03                     | 0.56              |
| 1:M:1031:ILE:HD11 | 1:M:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:N:336:ALA:O     | 1:N:338:TRP:N     | 2.38                     | 0.56              |
| 1:O:518:LEU:HD12  | 1:O:518:LEU:N     | 2.20                     | 0.56              |
| 1:O:600:ARG:NE    | 1:O:1229:GLU:OE1  | 2.37                     | 0.56              |
| 1:O:633:THR:HG21  | 1:O:643:TYR:CA    | 2.33                     | 0.56              |
| 1:A:350:THR:HA    | 1:A:353:ILE:HG22  | 1.88                     | 0.56              |
| 1:A:368:MET:HE1   | 1:A:401:VAL:HG21  | 1.88                     | 0.56              |
| 1:A:554:ILE:C     | 1:A:556:SER:H     | 2.13                     | 0.56              |
| 1:A:1031:ILE:HD11 | 1:A:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:B:124:ASN:H     | 1:B:303:LYS:NZ    | 2.03                     | 0.56              |
| 1:B:984:LEU:HD12  | 1:B:1022:ALA:HB2  | 1.88                     | 0.56              |
| 1:B:1031:ILE:HD11 | 1:B:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:C:155:SER:HA    | 1:C:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:C:336:ALA:O     | 1:C:338:TRP:N     | 2.38                     | 0.56              |
| 1:C:511:SER:C     | 1:C:513:SER:N     | 2.61                     | 0.56              |
| 1:C:554:ILE:C     | 1:C:556:SER:H     | 2.13                     | 0.56              |
| 1:D:378:SER:HA    | 1:D:422:ILE:HD12  | 1.84                     | 0.56              |
| 1:D:492:LEU:HD21  | 1:D:562:LEU:HD23  | 1.86                     | 0.56              |
| 1:E:1031:ILE:HD11 | 1:E:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:H:518:LEU:HD12  | 1:H:518:LEU:N     | 2.20                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:557:LYS:CE    | 1:H:1224:LEU:O    | 2.50                     | 0.56              |
| 1:I:241:LEU:HD12  | 1:I:241:LEU:O     | 2.06                     | 0.56              |
| 1:I:486:LEU:O     | 1:I:488:ARG:HG3   | 2.06                     | 0.56              |
| 1:K:946:ARG:HG3   | 1:K:947:GLU:H     | 1.71                     | 0.56              |
| 1:L:155:SER:HA    | 1:L:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:L:347:ASP:OD1   | 1:L:348:LYS:N     | 2.37                     | 0.56              |
| 1:L:633:THR:HG21  | 1:L:643:TYR:CA    | 2.33                     | 0.56              |
| 1:N:368:MET:HE1   | 1:N:401:VAL:HG21  | 1.88                     | 0.56              |
| 1:N:554:ILE:C     | 1:N:556:SER:H     | 2.13                     | 0.56              |
| 1:O:314:ARG:O     | 1:O:315:GLU:HB2   | 2.03                     | 0.56              |
| 1:O:397:ASP:O     | 1:O:401:VAL:N     | 2.28                     | 0.56              |
| 1:O:520:GLN:HA    | 1:O:523:PHE:HD2   | 1.71                     | 0.56              |
| 1:P:603:ILE:HD11  | 1:P:635:VAL:HG13  | 1.87                     | 0.56              |
| 1:P:1031:ILE:HD11 | 1:P:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:A:23:PHE:CD1    | 1:A:88:LEU:HD21   | 2.41                     | 0.56              |
| 1:B:557:LYS:CE    | 1:B:1224:LEU:O    | 2.50                     | 0.56              |
| 1:E:371:ARG:HD3   | 1:E:435:ASN:HD21  | 1.70                     | 0.56              |
| 1:F:350:THR:HA    | 1:F:353:ILE:HG22  | 1.88                     | 0.56              |
| 1:G:603:ILE:HD11  | 1:G:635:VAL:HG13  | 1.87                     | 0.56              |
| 1:H:155:SER:HA    | 1:H:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:H:520:GLN:HA    | 1:H:523:PHE:HD2   | 1.71                     | 0.56              |
| 1:I:499:GLN:HA    | 1:I:502:ARG:HD2   | 1.86                     | 0.56              |
| 1:J:23:PHE:CD1    | 1:J:88:LEU:HD21   | 2.41                     | 0.56              |
| 1:J:383:THR:N     | 1:J:419:THR:HA    | 2.21                     | 0.56              |
| 1:J:1058:ILE:HG13 | 1:J:1059:ASP:H    | 1.70                     | 0.56              |
| 1:K:492:LEU:HD21  | 1:K:562:LEU:HD23  | 1.86                     | 0.56              |
| 1:K:633:THR:HG21  | 1:K:643:TYR:CA    | 2.33                     | 0.56              |
| 1:L:984:LEU:HD12  | 1:L:1022:ALA:HB2  | 1.88                     | 0.56              |
| 1:M:548:LYS:HZ2   | 1:M:601:GLN:H     | 1.54                     | 0.56              |
| 1:M:946:ARG:HG3   | 1:M:947:GLU:H     | 1.71                     | 0.56              |
| 1:N:23:PHE:CD1    | 1:N:88:LEU:HD21   | 2.41                     | 0.56              |
| 1:N:350:THR:HA    | 1:N:353:ILE:HG22  | 1.88                     | 0.56              |
| 1:O:946:ARG:HG3   | 1:O:947:GLU:H     | 1.71                     | 0.56              |
| 1:B:23:PHE:CD1    | 1:B:88:LEU:HD21   | 2.41                     | 0.56              |
| 1:B:946:ARG:HG3   | 1:B:947:GLU:H     | 1.71                     | 0.56              |
| 1:C:241:LEU:HD12  | 1:C:241:LEU:O     | 2.06                     | 0.56              |
| 1:C:951:VAL:HA    | 1:C:987:VAL:HG11  | 1.87                     | 0.56              |
| 1:D:548:LYS:HZ2   | 1:D:601:GLN:H     | 1.53                     | 0.56              |
| 1:D:946:ARG:HG3   | 1:D:947:GLU:H     | 1.71                     | 0.56              |
| 1:E:23:PHE:CD1    | 1:E:88:LEU:HD21   | 2.41                     | 0.56              |
| 1:E:383:THR:N     | 1:E:419:THR:HA    | 2.21                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:449:ILE:HB    | 1:F:450:PRO:HD3   | 1.87                     | 0.56              |
| 1:G:1031:ILE:HD11 | 1:G:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:H:241:LEU:HD12  | 1:H:241:LEU:O     | 2.06                     | 0.56              |
| 1:H:499:GLN:HA    | 1:H:502:ARG:HD2   | 1.86                     | 0.56              |
| 1:H:946:ARG:HG3   | 1:H:947:GLU:H     | 1.71                     | 0.56              |
| 1:I:350:THR:HA    | 1:I:353:ILE:HG22  | 1.88                     | 0.56              |
| 1:I:378:SER:HA    | 1:I:422:ILE:HD12  | 1.84                     | 0.56              |
| 1:I:946:ARG:HG3   | 1:I:947:GLU:H     | 1.71                     | 0.56              |
| 1:M:458:LEU:CG    | 1:M:587:ARG:HH21  | 2.19                     | 0.56              |
| 1:M:984:LEU:HD12  | 1:M:1022:ALA:HB2  | 1.88                     | 0.56              |
| 1:N:951:VAL:HA    | 1:N:987:VAL:HG11  | 1.87                     | 0.56              |
| 1:O:410:LEU:HD22  | 1:O:413:LYS:HA    | 1.88                     | 0.56              |
| 1:O:499:GLN:HA    | 1:O:502:ARG:HD2   | 1.86                     | 0.56              |
| 1:A:458:LEU:CG    | 1:A:587:ARG:HH21  | 2.19                     | 0.56              |
| 1:B:458:LEU:CD2   | 1:B:459:ILE:H     | 2.18                     | 0.56              |
| 1:B:492:LEU:HD21  | 1:B:562:LEU:HD23  | 1.86                     | 0.56              |
| 1:C:516:ASN:O     | 1:C:517:THR:HG22  | 2.06                     | 0.56              |
| 1:E:1058:ILE:HG13 | 1:E:1059:ASP:H    | 1.70                     | 0.56              |
| 1:F:410:LEU:HD22  | 1:F:413:LYS:HA    | 1.88                     | 0.56              |
| 1:F:423:PRO:O     | 1:F:424:SER:HB3   | 2.05                     | 0.56              |
| 1:G:114:TYR:O     | 1:G:117:ASN:N     | 2.36                     | 0.56              |
| 1:H:410:LEU:HD22  | 1:H:413:LYS:HA    | 1.88                     | 0.56              |
| 1:I:155:SER:HA    | 1:I:321:PRO:HD2   | 1.87                     | 0.56              |
| 1:J:371:ARG:HD3   | 1:J:435:ASN:HD21  | 1.70                     | 0.56              |
| 1:J:492:LEU:HD21  | 1:J:562:LEU:HD23  | 1.86                     | 0.56              |
| 1:K:984:LEU:HD12  | 1:K:1022:ALA:HB2  | 1.88                     | 0.56              |
| 1:L:516:ASN:O     | 1:L:517:THR:HG22  | 2.06                     | 0.56              |
| 1:M:458:LEU:CD2   | 1:M:459:ILE:H     | 2.18                     | 0.56              |
| 1:M:557:LYS:CE    | 1:M:1224:LEU:O    | 2.51                     | 0.56              |
| 1:N:458:LEU:CG    | 1:N:587:ARG:HH21  | 2.19                     | 0.56              |
| 1:N:1031:ILE:HD11 | 1:N:1068:ILE:HD13 | 1.86                     | 0.56              |
| 1:O:241:LEU:HD12  | 1:O:241:LEU:O     | 2.06                     | 0.56              |
| 1:A:951:VAL:HA    | 1:A:987:VAL:HG11  | 1.87                     | 0.55              |
| 1:B:458:LEU:CG    | 1:B:587:ARG:HH21  | 2.20                     | 0.55              |
| 1:C:486:LEU:O     | 1:C:488:ARG:HG3   | 2.06                     | 0.55              |
| 1:C:946:ARG:HG3   | 1:C:947:GLU:H     | 1.71                     | 0.55              |
| 1:C:1031:ILE:HD11 | 1:C:1068:ILE:HD13 | 1.86                     | 0.55              |
| 1:D:442:SER:O     | 1:D:446:HIS:CG    | 2.55                     | 0.55              |
| 1:D:516:ASN:O     | 1:D:517:THR:HG22  | 2.06                     | 0.55              |
| 1:D:633:THR:HG21  | 1:D:643:TYR:CA    | 2.33                     | 0.55              |
| 1:D:984:LEU:HD12  | 1:D:1022:ALA:HB2  | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:336:ALA:O     | 1:E:338:TRP:N    | 2.38                     | 0.55              |
| 1:E:548:LYS:HZ2   | 1:E:601:GLN:H    | 1.52                     | 0.55              |
| 1:E:603:ILE:HD11  | 1:E:635:VAL:HG13 | 1.87                     | 0.55              |
| 1:F:347:ASP:OD1   | 1:F:348:LYS:N    | 2.37                     | 0.55              |
| 1:F:951:VAL:HA    | 1:F:987:VAL:HG11 | 1.87                     | 0.55              |
| 1:F:1058:ILE:HG13 | 1:F:1059:ASP:H   | 1.70                     | 0.55              |
| 1:H:383:THR:N     | 1:H:419:THR:HA   | 2.21                     | 0.55              |
| 1:H:458:LEU:CG    | 1:H:587:ARG:HH21 | 2.19                     | 0.55              |
| 1:H:518:LEU:HD22  | 1:H:643:TYR:CE1  | 2.22                     | 0.55              |
| 1:H:554:ILE:C     | 1:H:556:SER:H    | 2.13                     | 0.55              |
| 1:I:410:LEU:HD22  | 1:I:413:LYS:HA   | 1.88                     | 0.55              |
| 1:I:951:VAL:HA    | 1:I:987:VAL:HG11 | 1.87                     | 0.55              |
| 1:J:336:ALA:O     | 1:J:338:TRP:N    | 2.38                     | 0.55              |
| 1:K:378:SER:HA    | 1:K:422:ILE:HD12 | 1.84                     | 0.55              |
| 1:K:442:SER:O     | 1:K:446:HIS:CG   | 2.55                     | 0.55              |
| 1:K:516:ASN:O     | 1:K:517:THR:HG22 | 2.06                     | 0.55              |
| 1:K:554:ILE:C     | 1:K:556:SER:H    | 2.13                     | 0.55              |
| 1:L:486:LEU:O     | 1:L:488:ARG:HG3  | 2.06                     | 0.55              |
| 1:M:23:PHE:CD1    | 1:M:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:M:492:LEU:HD21  | 1:M:562:LEU:HD23 | 1.86                     | 0.55              |
| 1:O:23:PHE:CD1    | 1:O:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:O:458:LEU:CG    | 1:O:587:ARG:HH21 | 2.19                     | 0.55              |
| 1:O:518:LEU:HD22  | 1:O:643:TYR:CE1  | 2.22                     | 0.55              |
| 1:O:554:ILE:C     | 1:O:556:SER:H    | 2.13                     | 0.55              |
| 1:O:557:LYS:CE    | 1:O:1224:LEU:O   | 2.50                     | 0.55              |
| 1:P:114:TYR:O     | 1:P:117:ASN:N    | 2.36                     | 0.55              |
| 1:C:458:LEU:CG    | 1:C:587:ARG:HH21 | 2.19                     | 0.55              |
| 1:C:603:ILE:HD11  | 1:C:635:VAL:HG13 | 1.87                     | 0.55              |
| 1:D:520:GLN:HA    | 1:D:523:PHE:HD2  | 1.71                     | 0.55              |
| 1:D:1058:ILE:HG13 | 1:D:1059:ASP:H   | 1.70                     | 0.55              |
| 1:E:378:SER:HA    | 1:E:422:ILE:HD12 | 1.84                     | 0.55              |
| 1:E:458:LEU:CD2   | 1:E:459:ILE:H    | 2.18                     | 0.55              |
| 1:F:155:SER:HA    | 1:F:321:PRO:HD2  | 1.87                     | 0.55              |
| 1:G:188:SER:N     | 1:G:251:APK:O2P  | 2.31                     | 0.55              |
| 1:H:23:PHE:CD1    | 1:H:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:J:458:LEU:CD2   | 1:J:459:ILE:H    | 2.18                     | 0.55              |
| 1:K:520:GLN:HA    | 1:K:523:PHE:HD2  | 1.71                     | 0.55              |
| 1:K:1058:ILE:HG13 | 1:K:1059:ASP:H   | 1.70                     | 0.55              |
| 1:L:336:ALA:O     | 1:L:338:TRP:N    | 2.38                     | 0.55              |
| 1:L:458:LEU:CG    | 1:L:587:ARG:HH21 | 2.19                     | 0.55              |
| 1:L:511:SER:C     | 1:L:513:SER:N    | 2.60                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:951:VAL:HA    | 1:L:987:VAL:HG11  | 1.87                     | 0.55              |
| 1:L:1031:ILE:HD11 | 1:L:1068:ILE:HD13 | 1.86                     | 0.55              |
| 1:N:520:GLN:HA    | 1:N:523:PHE:HD2   | 1.71                     | 0.55              |
| 1:O:155:SER:HA    | 1:O:321:PRO:HD2   | 1.87                     | 0.55              |
| 1:A:241:LEU:HD12  | 1:A:241:LEU:O     | 2.06                     | 0.55              |
| 1:A:410:LEU:HD22  | 1:A:413:LYS:HA    | 1.88                     | 0.55              |
| 1:A:520:GLN:HA    | 1:A:523:PHE:HD2   | 1.71                     | 0.55              |
| 1:A:984:LEU:HD12  | 1:A:1022:ALA:HB2  | 1.88                     | 0.55              |
| 1:B:155:SER:HA    | 1:B:321:PRO:HD2   | 1.87                     | 0.55              |
| 1:C:449:ILE:HB    | 1:C:450:PRO:HD3   | 1.87                     | 0.55              |
| 1:C:518:LEU:HD22  | 1:C:643:TYR:CE1   | 2.22                     | 0.55              |
| 1:C:520:GLN:HA    | 1:C:523:PHE:HD2   | 1.71                     | 0.55              |
| 1:D:554:ILE:C     | 1:D:556:SER:H     | 2.13                     | 0.55              |
| 1:D:563:ARG:NH1   | 1:D:591:THR:O     | 2.40                     | 0.55              |
| 1:E:492:LEU:HD21  | 1:E:562:LEU:HD23  | 1.86                     | 0.55              |
| 1:F:194:GLU:OE2   | 1:G:216:ASN:ND2   | 2.40                     | 0.55              |
| 1:H:563:ARG:NH1   | 1:H:591:THR:O     | 2.40                     | 0.55              |
| 1:I:23:PHE:CD1    | 1:I:88:LEU:HD21   | 2.41                     | 0.55              |
| 1:I:1058:ILE:HG13 | 1:I:1059:ASP:H    | 1.70                     | 0.55              |
| 1:J:557:LYS:HZ2   | 1:J:1223:GLN:HG3  | 1.71                     | 0.55              |
| 1:J:603:ILE:HD11  | 1:J:635:VAL:HG13  | 1.87                     | 0.55              |
| 1:L:600:ARG:NE    | 1:L:1229:GLU:OE1  | 2.37                     | 0.55              |
| 1:L:603:ILE:HD11  | 1:L:635:VAL:HG13  | 1.87                     | 0.55              |
| 1:N:241:LEU:O     | 1:N:241:LEU:HD12  | 2.06                     | 0.55              |
| 1:N:410:LEU:HD22  | 1:N:413:LYS:HA    | 1.88                     | 0.55              |
| 1:O:383:THR:N     | 1:O:419:THR:HA    | 2.21                     | 0.55              |
| 1:P:188:SER:N     | 1:P:251:APK:O2P   | 2.31                     | 0.55              |
| 1:P:241:LEU:HD12  | 1:P:241:LEU:O     | 2.06                     | 0.55              |
| 1:A:557:LYS:CE    | 1:A:1224:LEU:O    | 2.50                     | 0.55              |
| 1:B:447:TYR:O     | 1:B:450:PRO:HD2   | 2.07                     | 0.55              |
| 1:B:486:LEU:O     | 1:B:488:ARG:HG3   | 2.06                     | 0.55              |
| 1:C:447:TYR:O     | 1:C:450:PRO:HD2   | 2.07                     | 0.55              |
| 1:C:563:ARG:NH1   | 1:C:591:THR:O     | 2.40                     | 0.55              |
| 1:F:23:PHE:CD1    | 1:F:88:LEU:HD21   | 2.41                     | 0.55              |
| 1:G:241:LEU:HD12  | 1:G:241:LEU:O     | 2.06                     | 0.55              |
| 1:G:317:LEU:CD2   | 1:G:341:TRP:CH2   | 2.90                     | 0.55              |
| 1:G:383:THR:N     | 1:G:419:THR:HA    | 2.21                     | 0.55              |
| 1:H:317:LEU:CD2   | 1:H:341:TRP:CH2   | 2.90                     | 0.55              |
| 1:K:313:PRO:HA    | 1:K:338:TRP:HH2   | 1.63                     | 0.55              |
| 1:K:563:ARG:NH1   | 1:K:591:THR:O     | 2.40                     | 0.55              |
| 1:L:447:TYR:O     | 1:L:450:PRO:HD2   | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:520:GLN:HA   | 1:L:523:PHE:HD2  | 1.71                     | 0.55              |
| 1:M:155:SER:HA   | 1:M:321:PRO:HD2  | 1.87                     | 0.55              |
| 1:M:486:LEU:O    | 1:M:488:ARG:HG3  | 2.06                     | 0.55              |
| 1:N:600:ARG:NE   | 1:N:1229:GLU:OE1 | 2.37                     | 0.55              |
| 1:N:984:LEU:HD12 | 1:N:1022:ALA:HB2 | 1.88                     | 0.55              |
| 1:O:317:LEU:CD2  | 1:O:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:O:368:MET:HE1  | 1:O:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:O:563:ARG:NH1  | 1:O:591:THR:O    | 2.40                     | 0.55              |
| 1:P:317:LEU:CD2  | 1:P:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:P:383:THR:N    | 1:P:419:THR:HA   | 2.21                     | 0.55              |
| 1:A:114:TYR:O    | 1:A:117:ASN:N    | 2.36                     | 0.55              |
| 1:A:301:LEU:HD23 | 1:A:313:PRO:HD2  | 1.89                     | 0.55              |
| 1:A:383:THR:N    | 1:A:419:THR:HA   | 2.21                     | 0.55              |
| 1:B:241:LEU:HD12 | 1:B:241:LEU:O    | 2.06                     | 0.55              |
| 1:C:541:ALA:O    | 1:C:544:ASP:N    | 2.30                     | 0.55              |
| 1:D:313:PRO:HA   | 1:D:338:TRP:HH2  | 1.63                     | 0.55              |
| 1:D:347:ASP:OD1  | 1:D:348:LYS:N    | 2.37                     | 0.55              |
| 1:D:371:ARG:HD3  | 1:D:435:ASN:HD21 | 1.70                     | 0.55              |
| 1:F:317:LEU:CD2  | 1:F:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:F:554:ILE:C    | 1:F:556:SER:H    | 2.13                     | 0.55              |
| 1:G:458:LEU:CG   | 1:G:587:ARG:HH21 | 2.19                     | 0.55              |
| 1:H:114:TYR:O    | 1:H:117:ASN:N    | 2.36                     | 0.55              |
| 1:I:347:ASP:OD1  | 1:I:348:LYS:N    | 2.37                     | 0.55              |
| 1:I:510:ALA:O    | 1:I:511:SER:HB2  | 2.07                     | 0.55              |
| 1:J:378:SER:HA   | 1:J:422:ILE:HD12 | 1.84                     | 0.55              |
| 1:K:23:PHE:CD1   | 1:K:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:L:563:ARG:NH1  | 1:L:591:THR:O    | 2.40                     | 0.55              |
| 1:L:946:ARG:HG3  | 1:L:947:GLU:H    | 1.71                     | 0.55              |
| 1:M:301:LEU:HD23 | 1:M:313:PRO:HD2  | 1.89                     | 0.55              |
| 1:M:447:TYR:O    | 1:M:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:N:114:TYR:O    | 1:N:117:ASN:N    | 2.36                     | 0.55              |
| 1:P:554:ILE:C    | 1:P:556:SER:H    | 2.13                     | 0.55              |
| 1:P:563:ARG:NH1  | 1:P:591:THR:O    | 2.40                     | 0.55              |
| 1:A:447:TYR:O    | 1:A:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:A:563:ARG:NH1  | 1:A:591:THR:O    | 2.40                     | 0.55              |
| 1:A:600:ARG:NE   | 1:A:1229:GLU:OE1 | 2.37                     | 0.55              |
| 1:B:301:LEU:HD23 | 1:B:313:PRO:HD2  | 1.89                     | 0.55              |
| 1:C:458:LEU:CD2  | 1:C:459:ILE:H    | 2.18                     | 0.55              |
| 1:D:557:LYS:CE   | 1:D:1224:LEU:O   | 2.50                     | 0.55              |
| 1:E:554:ILE:C    | 1:E:556:SER:H    | 2.13                     | 0.55              |
| 1:E:984:LEU:HD12 | 1:E:1022:ALA:HB2 | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:516:ASN:O    | 1:F:517:THR:HG22 | 2.06                     | 0.55              |
| 1:G:511:SER:C    | 1:G:513:SER:N    | 2.61                     | 0.55              |
| 1:G:554:ILE:C    | 1:G:556:SER:H    | 2.13                     | 0.55              |
| 1:G:563:ARG:NH1  | 1:G:591:THR:O    | 2.40                     | 0.55              |
| 1:I:317:LEU:CD2  | 1:I:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:J:124:ASN:H    | 1:J:303:LYS:HZ3  | 1.53                     | 0.55              |
| 1:J:510:ALA:O    | 1:J:511:SER:HB2  | 2.07                     | 0.55              |
| 1:J:984:LEU:HD12 | 1:J:1022:ALA:HB2 | 1.88                     | 0.55              |
| 1:K:347:ASP:OD1  | 1:K:348:LYS:N    | 2.37                     | 0.55              |
| 1:K:371:ARG:HD3  | 1:K:435:ASN:HD21 | 1.70                     | 0.55              |
| 1:L:371:ARG:HD3  | 1:L:435:ASN:HD21 | 1.70                     | 0.55              |
| 1:L:458:LEU:CD2  | 1:L:459:ILE:H    | 2.18                     | 0.55              |
| 1:M:241:LEU:HD12 | 1:M:241:LEU:O    | 2.06                     | 0.55              |
| 1:N:301:LEU:HD23 | 1:N:313:PRO:HD2  | 1.89                     | 0.55              |
| 1:N:317:LEU:CD2  | 1:N:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:N:563:ARG:NH1  | 1:N:591:THR:O    | 2.40                     | 0.55              |
| 1:O:114:TYR:O    | 1:O:117:ASN:N    | 2.36                     | 0.55              |
| 1:P:458:LEU:CG   | 1:P:587:ARG:HH21 | 2.19                     | 0.55              |
| 1:P:518:LEU:HD12 | 1:P:518:LEU:N    | 2.20                     | 0.55              |
| 1:P:946:ARG:HG3  | 1:P:947:GLU:H    | 1.71                     | 0.55              |
| 1:A:317:LEU:CD2  | 1:A:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:A:412:GLU:OE1  | 1:A:414:GLN:N    | 2.40                     | 0.55              |
| 1:B:350:THR:HA   | 1:B:353:ILE:HG22 | 1.88                     | 0.55              |
| 1:B:412:GLU:OE1  | 1:B:414:GLN:N    | 2.40                     | 0.55              |
| 1:C:371:ARG:HD3  | 1:C:435:ASN:HD21 | 1.70                     | 0.55              |
| 1:E:124:ASN:H    | 1:E:303:LYS:HZ3  | 1.53                     | 0.55              |
| 1:E:350:THR:HA   | 1:E:353:ILE:HG22 | 1.88                     | 0.55              |
| 1:E:510:ALA:O    | 1:E:511:SER:HB2  | 2.07                     | 0.55              |
| 1:F:317:LEU:HD22 | 1:F:341:TRP:CH2  | 2.42                     | 0.55              |
| 1:F:412:GLU:OE1  | 1:F:414:GLN:N    | 2.40                     | 0.55              |
| 1:G:518:LEU:HD12 | 1:G:518:LEU:N    | 2.20                     | 0.55              |
| 1:G:946:ARG:HG3  | 1:G:947:GLU:H    | 1.71                     | 0.55              |
| 1:H:368:MET:HE1  | 1:H:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:I:317:LEU:HD22 | 1:I:341:TRP:CH2  | 2.42                     | 0.55              |
| 1:I:516:ASN:O    | 1:I:517:THR:HG22 | 2.06                     | 0.55              |
| 1:J:346:CYS:O    | 1:J:350:THR:N    | 2.25                     | 0.55              |
| 1:J:347:ASP:OD1  | 1:J:348:LYS:N    | 2.37                     | 0.55              |
| 1:J:412:GLU:OE1  | 1:J:414:GLN:N    | 2.40                     | 0.55              |
| 1:J:516:ASN:O    | 1:J:517:THR:HG22 | 2.06                     | 0.55              |
| 1:J:563:ARG:NH1  | 1:J:591:THR:O    | 2.40                     | 0.55              |
| 1:K:518:LEU:HD12 | 1:K:518:LEU:N    | 2.20                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:410:LEU:HD22 | 1:M:413:LYS:HA   | 1.88                     | 0.55              |
| 1:M:412:GLU:OE1  | 1:M:414:GLN:N    | 2.40                     | 0.55              |
| 1:N:383:THR:N    | 1:N:419:THR:HA   | 2.21                     | 0.55              |
| 1:N:412:GLU:OE1  | 1:N:414:GLN:N    | 2.40                     | 0.55              |
| 1:N:557:LYS:CE   | 1:N:1224:LEU:O   | 2.51                     | 0.55              |
| 1:O:487:PHE:CD2  | 1:O:489:MET:HG3  | 2.42                     | 0.55              |
| 1:P:511:SER:C    | 1:P:513:SER:N    | 2.60                     | 0.55              |
| 1:B:410:LEU:HD22 | 1:B:413:LYS:HA   | 1.88                     | 0.55              |
| 1:B:487:PHE:CD2  | 1:B:489:MET:HG3  | 2.42                     | 0.55              |
| 1:B:563:ARG:NH1  | 1:B:591:THR:O    | 2.40                     | 0.55              |
| 1:C:301:LEU:HD23 | 1:C:313:PRO:HD2  | 1.89                     | 0.55              |
| 1:D:23:PHE:CD1   | 1:D:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:D:458:LEU:CG   | 1:D:587:ARG:HH21 | 2.20                     | 0.55              |
| 1:D:458:LEU:CD2  | 1:D:459:ILE:H    | 2.18                     | 0.55              |
| 1:E:347:ASP:OD1  | 1:E:348:LYS:N    | 2.37                     | 0.55              |
| 1:E:412:GLU:OE1  | 1:E:414:GLN:N    | 2.40                     | 0.55              |
| 1:E:516:ASN:O    | 1:E:517:THR:HG22 | 2.06                     | 0.55              |
| 1:E:563:ARG:NH1  | 1:E:591:THR:O    | 2.40                     | 0.55              |
| 1:F:510:ALA:O    | 1:F:511:SER:HB2  | 2.07                     | 0.55              |
| 1:F:984:LEU:HD12 | 1:F:1022:ALA:HB2 | 1.88                     | 0.55              |
| 1:H:487:PHE:CD2  | 1:H:489:MET:HG3  | 2.42                     | 0.55              |
| 1:I:412:GLU:OE1  | 1:I:414:GLN:N    | 2.40                     | 0.55              |
| 1:I:554:ILE:C    | 1:I:556:SER:H    | 2.13                     | 0.55              |
| 1:J:350:THR:HA   | 1:J:353:ILE:HG22 | 1.88                     | 0.55              |
| 1:K:368:MET:HE1  | 1:K:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:K:447:TYR:O    | 1:K:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:K:458:LEU:CG   | 1:K:587:ARG:HH21 | 2.20                     | 0.55              |
| 1:L:767:GLY:HA2  | 1:L:783:THR:HG22 | 1.89                     | 0.55              |
| 1:M:350:THR:HA   | 1:M:353:ILE:HG22 | 1.88                     | 0.55              |
| 1:M:487:PHE:CD2  | 1:M:489:MET:HG3  | 2.42                     | 0.55              |
| 1:M:563:ARG:NH1  | 1:M:591:THR:O    | 2.40                     | 0.55              |
| 1:N:447:TYR:O    | 1:N:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:P:23:PHE:CD1   | 1:P:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:B:541:ALA:O    | 1:B:544:ASP:N    | 2.30                     | 0.55              |
| 1:B:600:ARG:NE   | 1:B:1229:GLU:OE1 | 2.37                     | 0.55              |
| 1:C:23:PHE:CD1   | 1:C:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:C:350:THR:HA   | 1:C:353:ILE:HG22 | 1.88                     | 0.55              |
| 1:C:412:GLU:OE1  | 1:C:414:GLN:N    | 2.40                     | 0.55              |
| 1:C:600:ARG:NE   | 1:C:1229:GLU:OE1 | 2.37                     | 0.55              |
| 1:D:368:MET:HE1  | 1:D:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:E:317:LEU:CD2  | 1:E:341:TRP:CH2  | 2.90                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:397:ASP:O    | 1:E:401:VAL:N    | 2.28                     | 0.55              |
| 1:E:447:TYR:O    | 1:E:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:F:97:ARG:NH2   | 1:O:97:ARG:NH2   | 2.55                     | 0.55              |
| 1:F:538:LEU:CD1  | 1:F:571:GLU:HG2  | 2.37                     | 0.55              |
| 1:G:23:PHE:CD1   | 1:G:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:G:447:TYR:O    | 1:G:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:H:301:LEU:HD23 | 1:H:313:PRO:HD2  | 1.89                     | 0.55              |
| 1:H:412:GLU:OE1  | 1:H:414:GLN:N    | 2.40                     | 0.55              |
| 1:H:447:TYR:O    | 1:H:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:I:984:LEU:HD12 | 1:I:1022:ALA:HB2 | 1.88                     | 0.55              |
| 1:J:317:LEU:CD2  | 1:J:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:J:365:TYR:O    | 1:J:368:MET:N    | 2.21                     | 0.55              |
| 1:J:368:MET:HE1  | 1:J:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:K:353:ILE:HD11 | 1:K:427:LEU:HA   | 1.89                     | 0.55              |
| 1:K:410:LEU:HD22 | 1:K:413:LYS:HA   | 1.88                     | 0.55              |
| 1:K:458:LEU:CD2  | 1:K:459:ILE:H    | 2.18                     | 0.55              |
| 1:K:557:LYS:CE   | 1:K:1224:LEU:O   | 2.50                     | 0.55              |
| 1:L:23:PHE:CD1   | 1:L:88:LEU:HD21  | 2.41                     | 0.55              |
| 1:L:449:ILE:HB   | 1:L:450:PRO:HD3  | 1.87                     | 0.55              |
| 1:M:317:LEU:CD2  | 1:M:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:M:541:ALA:O    | 1:M:544:ASP:N    | 2.30                     | 0.55              |
| 1:M:600:ARG:NE   | 1:M:1229:GLU:OE1 | 2.37                     | 0.55              |
| 1:O:447:TYR:O    | 1:O:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:O:767:GLY:HA2  | 1:O:783:THR:HG22 | 1.89                     | 0.55              |
| 1:P:447:TYR:O    | 1:P:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:B:317:LEU:CD2  | 1:B:341:TRP:CH2  | 2.90                     | 0.55              |
| 1:B:368:MET:HE1  | 1:B:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:B:516:ASN:O    | 1:B:517:THR:HG22 | 2.06                     | 0.55              |
| 1:B:767:GLY:HA2  | 1:B:783:THR:HG22 | 1.89                     | 0.55              |
| 1:C:368:MET:HE1  | 1:C:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:C:487:PHE:CD2  | 1:C:489:MET:HG3  | 2.42                     | 0.55              |
| 1:C:767:GLY:HA2  | 1:C:783:THR:HG22 | 1.90                     | 0.55              |
| 1:D:353:ILE:HD11 | 1:D:427:LEU:HA   | 1.89                     | 0.55              |
| 1:D:447:TYR:O    | 1:D:450:PRO:HD2  | 2.07                     | 0.55              |
| 1:D:487:PHE:CD2  | 1:D:489:MET:HG3  | 2.42                     | 0.55              |
| 1:D:518:LEU:HD12 | 1:D:518:LEU:N    | 2.20                     | 0.55              |
| 1:E:353:ILE:HD11 | 1:E:427:LEU:HA   | 1.89                     | 0.55              |
| 1:E:368:MET:HE1  | 1:E:401:VAL:HG21 | 1.88                     | 0.55              |
| 1:E:951:VAL:HA   | 1:E:987:VAL:HG11 | 1.87                     | 0.55              |
| 1:H:767:GLY:HA2  | 1:H:783:THR:HG22 | 1.89                     | 0.55              |
| 1:I:442:SER:O    | 1:I:446:HIS:CG   | 2.55                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:353:ILE:HD11 | 1:J:427:LEU:HA   | 1.89                     | 0.55              |
| 1:J:554:ILE:C    | 1:J:556:SER:H    | 2.13                     | 0.55              |
| 1:J:951:VAL:HA   | 1:J:987:VAL:HG11 | 1.87                     | 0.55              |
| 1:L:317:LEU:HD22 | 1:L:341:TRP:CH2  | 2.42                     | 0.55              |
| 1:L:350:THR:HA   | 1:L:353:ILE:HG22 | 1.88                     | 0.55              |
| 1:L:487:PHE:CD2  | 1:L:489:MET:HG3  | 2.42                     | 0.55              |
| 1:N:353:ILE:HD11 | 1:N:427:LEU:HA   | 1.89                     | 0.55              |
| 1:N:487:PHE:CD2  | 1:N:489:MET:HG3  | 2.42                     | 0.55              |
| 1:O:216:ASN:ND2  | 1:P:194:GLU:OE2  | 2.40                     | 0.55              |
| 1:O:412:GLU:OE1  | 1:O:414:GLN:N    | 2.40                     | 0.55              |
| 1:O:557:LYS:HZ2  | 1:O:1223:GLN:HG3 | 1.71                     | 0.55              |
| 1:O:984:LEU:HD12 | 1:O:1022:ALA:HB2 | 1.88                     | 0.55              |
| 1:A:353:ILE:HD11 | 1:A:427:LEU:HA   | 1.89                     | 0.54              |
| 1:A:487:PHE:CD2  | 1:A:489:MET:HG3  | 2.42                     | 0.54              |
| 1:A:767:GLY:HA2  | 1:A:783:THR:HG22 | 1.89                     | 0.54              |
| 1:B:150:ASP:OD1  | 1:B:151:GLY:N    | 2.41                     | 0.54              |
| 1:C:410:LEU:HD22 | 1:C:413:LYS:HA   | 1.88                     | 0.54              |
| 1:C:538:LEU:CG   | 1:C:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:D:410:LEU:HD22 | 1:D:413:LYS:HA   | 1.88                     | 0.54              |
| 1:E:538:LEU:CG   | 1:E:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:E:946:ARG:HG3  | 1:E:947:GLU:H    | 1.71                     | 0.54              |
| 1:F:150:ASP:OD1  | 1:F:151:GLY:N    | 2.40                     | 0.54              |
| 1:F:442:SER:O    | 1:F:446:HIS:CG   | 2.55                     | 0.54              |
| 1:F:557:LYS:CE   | 1:F:1224:LEU:O   | 2.50                     | 0.54              |
| 1:G:487:PHE:CD2  | 1:G:489:MET:HG3  | 2.42                     | 0.54              |
| 1:G:538:LEU:CG   | 1:G:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:G:951:VAL:HA   | 1:G:987:VAL:HG11 | 1.87                     | 0.54              |
| 1:I:388:LEU:HB2  | 1:I:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:I:538:LEU:CD1  | 1:I:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:I:563:ARG:NH1  | 1:I:591:THR:O    | 2.40                     | 0.54              |
| 1:J:447:TYR:O    | 1:J:450:PRO:HD2  | 2.07                     | 0.54              |
| 1:J:538:LEU:CG   | 1:J:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:K:487:PHE:CD2  | 1:K:489:MET:HG3  | 2.42                     | 0.54              |
| 1:K:538:LEU:CD1  | 1:K:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:L:301:LEU:HD23 | 1:L:313:PRO:HD2  | 1.89                     | 0.54              |
| 1:L:368:MET:HE1  | 1:L:401:VAL:HG21 | 1.88                     | 0.54              |
| 1:L:538:LEU:CD1  | 1:L:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:M:150:ASP:OD1  | 1:M:151:GLY:N    | 2.41                     | 0.54              |
| 1:M:368:MET:HE1  | 1:M:401:VAL:HG21 | 1.88                     | 0.54              |
| 1:M:516:ASN:O    | 1:M:517:THR:HG22 | 2.06                     | 0.54              |
| 1:M:767:GLY:HA2  | 1:M:783:THR:HG22 | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:N:767:GLY:HA2   | 1:N:783:THR:HG22 | 1.89                     | 0.54              |
| 1:P:150:ASP:OD1   | 1:P:151:GLY:N    | 2.40                     | 0.54              |
| 1:P:423:PRO:O     | 1:P:424:SER:HB3  | 2.05                     | 0.54              |
| 1:P:487:PHE:CD2   | 1:P:489:MET:HG3  | 2.42                     | 0.54              |
| 1:P:951:VAL:HA    | 1:P:987:VAL:HG11 | 1.87                     | 0.54              |
| 1:A:516:ASN:O     | 1:A:517:THR:HG22 | 2.06                     | 0.54              |
| 1:A:946:ARG:HG3   | 1:A:947:GLU:H    | 1.71                     | 0.54              |
| 1:C:317:LEU:CD2   | 1:C:341:TRP:CH2  | 2.90                     | 0.54              |
| 1:C:538:LEU:CD1   | 1:C:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:D:114:TYR:O     | 1:D:117:ASN:N    | 2.36                     | 0.54              |
| 1:D:317:LEU:CD2   | 1:D:341:TRP:CH2  | 2.90                     | 0.54              |
| 1:D:538:LEU:CD1   | 1:D:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:E:365:TYR:O     | 1:E:368:MET:N    | 2.21                     | 0.54              |
| 1:E:397:ASP:HA    | 1:E:400:VAL:HB   | 1.89                     | 0.54              |
| 1:E:1195:VAL:HG11 | 1:E:1241:PHE:HZ  | 1.72                     | 0.54              |
| 1:F:458:LEU:CG    | 1:F:587:ARG:HH21 | 2.19                     | 0.54              |
| 1:G:388:LEU:HB2   | 1:G:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:G:397:ASP:HA    | 1:G:400:VAL:HB   | 1.89                     | 0.54              |
| 1:G:510:ALA:O     | 1:G:511:SER:HB2  | 2.07                     | 0.54              |
| 1:H:317:LEU:HD22  | 1:H:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:H:388:LEU:HB2   | 1:H:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:H:397:ASP:HA    | 1:H:400:VAL:HB   | 1.89                     | 0.54              |
| 1:H:984:LEU:HD12  | 1:H:1022:ALA:HB2 | 1.88                     | 0.54              |
| 1:I:124:ASN:H     | 1:I:303:LYS:HZ3  | 1.55                     | 0.54              |
| 1:J:317:LEU:HD22  | 1:J:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:K:317:LEU:CD2   | 1:K:341:TRP:CH2  | 2.90                     | 0.54              |
| 1:L:317:LEU:CD2   | 1:L:341:TRP:CH2  | 2.90                     | 0.54              |
| 1:L:353:ILE:HD11  | 1:L:427:LEU:HA   | 1.89                     | 0.54              |
| 1:L:412:GLU:OE1   | 1:L:414:GLN:N    | 2.40                     | 0.54              |
| 1:N:516:ASN:O     | 1:N:517:THR:HG22 | 2.06                     | 0.54              |
| 1:O:301:LEU:HD23  | 1:O:313:PRO:HD2  | 1.89                     | 0.54              |
| 1:O:317:LEU:HD22  | 1:O:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:O:397:ASP:HA    | 1:O:400:VAL:HB   | 1.89                     | 0.54              |
| 1:P:120:PHE:HE1   | 1:P:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:P:124:ASN:H     | 1:P:303:LYS:HZ3  | 1.55                     | 0.54              |
| 1:P:388:LEU:HB2   | 1:P:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:P:397:ASP:HA    | 1:P:400:VAL:HB   | 1.89                     | 0.54              |
| 1:P:538:LEU:CG    | 1:P:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:P:984:LEU:HD12  | 1:P:1022:ALA:HB2 | 1.88                     | 0.54              |
| 1:C:91:PRO:O      | 1:C:94:THR:OG1   | 2.21                     | 0.54              |
| 1:C:317:LEU:HD22  | 1:C:341:TRP:CH2  | 2.42                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:353:ILE:HD11  | 1:C:427:LEU:HA   | 1.90                     | 0.54              |
| 1:C:368:MET:HA    | 1:C:390:TRP:HE1  | 1.73                     | 0.54              |
| 1:D:100:SER:O     | 1:D:103:THR:N    | 2.41                     | 0.54              |
| 1:D:350:THR:HA    | 1:D:353:ILE:HG22 | 1.88                     | 0.54              |
| 1:E:458:LEU:CG    | 1:E:587:ARG:HH21 | 2.19                     | 0.54              |
| 1:F:563:ARG:NH1   | 1:F:591:THR:O    | 2.40                     | 0.54              |
| 1:G:120:PHE:HE1   | 1:G:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:G:150:ASP:OD1   | 1:G:151:GLY:N    | 2.41                     | 0.54              |
| 1:G:412:GLU:OE1   | 1:G:414:GLN:N    | 2.40                     | 0.54              |
| 1:G:423:PRO:O     | 1:G:424:SER:HB3  | 2.05                     | 0.54              |
| 1:G:984:LEU:HD12  | 1:G:1022:ALA:HB2 | 1.88                     | 0.54              |
| 1:I:383:THR:N     | 1:I:419:THR:HA   | 2.21                     | 0.54              |
| 1:J:397:ASP:HA    | 1:J:400:VAL:HB   | 1.89                     | 0.54              |
| 1:J:1195:VAL:HG11 | 1:J:1241:PHE:HZ  | 1.73                     | 0.54              |
| 1:K:557:LYS:CB    | 1:K:1226:TYR:CE1 | 2.87                     | 0.54              |
| 1:L:124:ASN:H     | 1:L:303:LYS:HZ3  | 1.55                     | 0.54              |
| 1:L:383:THR:N     | 1:L:419:THR:HA   | 2.21                     | 0.54              |
| 1:M:124:ASN:H     | 1:M:303:LYS:HZ3  | 1.56                     | 0.54              |
| 1:M:317:LEU:HD22  | 1:M:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:M:353:ILE:HD11  | 1:M:427:LEU:HA   | 1.89                     | 0.54              |
| 1:M:487:PHE:HD2   | 1:M:489:MET:HG3  | 1.72                     | 0.54              |
| 1:M:538:LEU:CD1   | 1:M:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:N:124:ASN:H     | 1:N:303:LYS:HZ3  | 1.56                     | 0.54              |
| 1:O:487:PHE:HD2   | 1:O:489:MET:HG3  | 1.72                     | 0.54              |
| 1:P:100:SER:O     | 1:P:103:THR:N    | 2.41                     | 0.54              |
| 1:P:412:GLU:OE1   | 1:P:414:GLN:N    | 2.40                     | 0.54              |
| 1:P:538:LEU:HG    | 1:P:571:GLU:CD   | 2.33                     | 0.54              |
| 1:A:389:ILE:CD1   | 1:A:446:HIS:CD2  | 2.91                     | 0.54              |
| 1:A:538:LEU:CD1   | 1:A:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:B:317:LEU:HD22  | 1:B:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:B:353:ILE:HD11  | 1:B:427:LEU:HA   | 1.89                     | 0.54              |
| 1:B:487:PHE:HD2   | 1:B:489:MET:HG3  | 1.72                     | 0.54              |
| 1:B:538:LEU:CD1   | 1:B:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:C:100:SER:O     | 1:C:103:THR:N    | 2.41                     | 0.54              |
| 1:C:383:THR:N     | 1:C:419:THR:HA   | 2.21                     | 0.54              |
| 1:D:120:PHE:HE1   | 1:D:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:D:510:ALA:O     | 1:D:511:SER:HB2  | 2.07                     | 0.54              |
| 1:D:557:LYS:CB    | 1:D:1226:TYR:CE1 | 2.87                     | 0.54              |
| 1:D:1195:VAL:HG11 | 1:D:1241:PHE:HZ  | 1.73                     | 0.54              |
| 1:E:317:LEU:HD22  | 1:E:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:F:124:ASN:H     | 1:F:303:LYS:HZ3  | 1.55                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:388:LEU:HB2  | 1:F:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:F:538:LEU:CG   | 1:F:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:G:100:SER:O    | 1:G:103:THR:N    | 2.41                     | 0.54              |
| 1:G:538:LEU:HG   | 1:G:571:GLU:CD   | 2.33                     | 0.54              |
| 1:G:550:GLU:O    | 1:G:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:H:353:ILE:HD11 | 1:H:427:LEU:HA   | 1.89                     | 0.54              |
| 1:H:487:PHE:HD2  | 1:H:489:MET:HG3  | 1.72                     | 0.54              |
| 1:I:100:SER:O    | 1:I:103:THR:N    | 2.41                     | 0.54              |
| 1:I:150:ASP:OD1  | 1:I:151:GLY:N    | 2.40                     | 0.54              |
| 1:I:458:LEU:CG   | 1:I:587:ARG:HH21 | 2.19                     | 0.54              |
| 1:J:946:ARG:HG3  | 1:J:947:GLU:H    | 1.71                     | 0.54              |
| 1:K:100:SER:O    | 1:K:103:THR:N    | 2.41                     | 0.54              |
| 1:K:350:THR:HA   | 1:K:353:ILE:HG22 | 1.88                     | 0.54              |
| 1:K:412:GLU:OE1  | 1:K:414:GLN:N    | 2.40                     | 0.54              |
| 1:K:510:ALA:O    | 1:K:511:SER:HB2  | 2.07                     | 0.54              |
| 1:L:150:ASP:OD1  | 1:L:151:GLY:N    | 2.40                     | 0.54              |
| 1:N:389:ILE:CD1  | 1:N:446:HIS:CD2  | 2.91                     | 0.54              |
| 1:N:538:LEU:CD1  | 1:N:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:P:301:LEU:HD23 | 1:P:313:PRO:HD2  | 1.89                     | 0.54              |
| 1:P:510:ALA:O    | 1:P:511:SER:HB2  | 2.07                     | 0.54              |
| 1:P:550:GLU:O    | 1:P:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:P:767:GLY:HA2  | 1:P:783:THR:HG22 | 1.89                     | 0.54              |
| 1:A:388:LEU:HB2  | 1:A:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:B:124:ASN:H    | 1:B:303:LYS:HZ3  | 1.56                     | 0.54              |
| 1:C:504:ASP:CG   | 1:C:509:ASN:O    | 2.51                     | 0.54              |
| 1:D:124:ASN:H    | 1:D:303:LYS:HZ3  | 1.56                     | 0.54              |
| 1:D:317:LEU:HD22 | 1:D:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:D:767:GLY:HA2  | 1:D:783:THR:HG22 | 1.89                     | 0.54              |
| 1:E:538:LEU:HG   | 1:E:571:GLU:CD   | 2.33                     | 0.54              |
| 1:F:100:SER:O    | 1:F:103:THR:N    | 2.41                     | 0.54              |
| 1:F:368:MET:HE1  | 1:F:401:VAL:HG21 | 1.88                     | 0.54              |
| 1:F:550:GLU:O    | 1:F:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:G:301:LEU:HD23 | 1:G:313:PRO:HD2  | 1.89                     | 0.54              |
| 1:G:767:GLY:HA2  | 1:G:783:THR:HG22 | 1.89                     | 0.54              |
| 1:H:100:SER:O    | 1:H:103:THR:N    | 2.41                     | 0.54              |
| 1:H:301:LEU:CD2  | 1:H:313:PRO:CD   | 2.86                     | 0.54              |
| 1:H:538:LEU:CD1  | 1:H:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:H:541:ALA:O    | 1:H:544:ASP:N    | 2.30                     | 0.54              |
| 1:H:550:GLU:O    | 1:H:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:I:353:ILE:HD11 | 1:I:427:LEU:HA   | 1.89                     | 0.54              |
| 1:I:550:GLU:O    | 1:I:552:ASN:ND2  | 2.41                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:458:LEU:CG    | 1:J:587:ARG:HH21 | 2.19                     | 0.54              |
| 1:J:538:LEU:HG    | 1:J:571:GLU:CD   | 2.33                     | 0.54              |
| 1:K:124:ASN:H     | 1:K:303:LYS:HZ3  | 1.56                     | 0.54              |
| 1:K:538:LEU:CG    | 1:K:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:K:1195:VAL:HG11 | 1:K:1241:PHE:HZ  | 1.73                     | 0.54              |
| 1:L:100:SER:O     | 1:L:103:THR:N    | 2.41                     | 0.54              |
| 1:L:368:MET:HA    | 1:L:390:TRP:HE1  | 1.73                     | 0.54              |
| 1:L:538:LEU:CG    | 1:L:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:M:368:MET:HA    | 1:M:390:TRP:HE1  | 1.73                     | 0.54              |
| 1:N:388:LEU:HB2   | 1:N:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:N:946:ARG:HG3   | 1:N:947:GLU:H    | 1.71                     | 0.54              |
| 1:O:100:SER:O     | 1:O:103:THR:N    | 2.41                     | 0.54              |
| 1:O:353:ILE:HD11  | 1:O:427:LEU:HA   | 1.89                     | 0.54              |
| 1:O:388:LEU:HB2   | 1:O:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:O:516:ASN:O     | 1:O:517:THR:HG22 | 2.06                     | 0.54              |
| 1:O:538:LEU:CD1   | 1:O:571:GLU:HG2  | 2.38                     | 0.54              |
| 1:O:541:ALA:O     | 1:O:544:ASP:N    | 2.30                     | 0.54              |
| 1:O:550:GLU:O     | 1:O:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:P:410:LEU:HD22  | 1:P:413:LYS:HA   | 1.88                     | 0.54              |
| 1:P:516:ASN:O     | 1:P:517:THR:HG22 | 2.06                     | 0.54              |
| 1:A:120:PHE:HE1   | 1:A:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:A:150:ASP:OD1   | 1:A:151:GLY:N    | 2.40                     | 0.54              |
| 1:A:541:ALA:O     | 1:A:544:ASP:N    | 2.30                     | 0.54              |
| 1:B:368:MET:HA    | 1:B:390:TRP:HE1  | 1.73                     | 0.54              |
| 1:B:386:LEU:HD12  | 1:B:420:ILE:HD13 | 1.90                     | 0.54              |
| 1:C:389:ILE:CD1   | 1:C:446:HIS:CD2  | 2.91                     | 0.54              |
| 1:D:412:GLU:OE1   | 1:D:414:GLN:N    | 2.40                     | 0.54              |
| 1:E:120:PHE:HE1   | 1:E:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:F:156:GLY:HA2   | 2:F:1501:DTP:O2A | 2.08                     | 0.54              |
| 1:F:353:ILE:HD11  | 1:F:427:LEU:HA   | 1.89                     | 0.54              |
| 1:F:633:THR:HG21  | 1:F:643:TYR:CA   | 2.33                     | 0.54              |
| 1:G:119:VAL:HA    | 1:G:159:TRP:CH2  | 2.43                     | 0.54              |
| 1:G:301:LEU:CD2   | 1:G:313:PRO:CD   | 2.86                     | 0.54              |
| 1:G:317:LEU:HD22  | 1:G:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:G:516:ASN:O     | 1:G:517:THR:HG22 | 2.06                     | 0.54              |
| 1:H:516:ASN:O     | 1:H:517:THR:HG22 | 2.06                     | 0.54              |
| 1:I:368:MET:HE1   | 1:I:401:VAL:HG21 | 1.88                     | 0.54              |
| 1:I:557:LYS:CE    | 1:I:1224:LEU:O   | 2.50                     | 0.54              |
| 1:J:119:VAL:HA    | 1:J:159:TRP:CH2  | 2.43                     | 0.54              |
| 1:J:120:PHE:HE1   | 1:J:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:J:397:ASP:O     | 1:J:401:VAL:N    | 2.28                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:120:PHE:HE1   | 1:K:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:K:767:GLY:HA2   | 1:K:783:THR:HG22 | 1.89                     | 0.54              |
| 1:L:410:LEU:HD22  | 1:L:413:LYS:HA   | 1.88                     | 0.54              |
| 1:L:504:ASP:CG    | 1:L:509:ASN:O    | 2.51                     | 0.54              |
| 1:M:386:LEU:HD12  | 1:M:420:ILE:HD13 | 1.90                     | 0.54              |
| 1:M:538:LEU:CG    | 1:M:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:N:120:PHE:HE1   | 1:N:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:O:301:LEU:CD2   | 1:O:313:PRO:CD   | 2.86                     | 0.54              |
| 1:P:301:LEU:CD2   | 1:P:313:PRO:CD   | 2.86                     | 0.54              |
| 1:A:168:TYR:O     | 1:A:171:GLN:N    | 2.41                     | 0.54              |
| 1:A:538:LEU:CG    | 1:A:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:B:538:LEU:CG    | 1:B:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:C:150:ASP:OD1   | 1:C:151:GLY:N    | 2.41                     | 0.54              |
| 1:C:301:LEU:CD2   | 1:C:313:PRO:CD   | 2.86                     | 0.54              |
| 1:C:1182:GLU:O    | 1:C:1183:GLU:HG3 | 2.08                     | 0.54              |
| 1:D:168:TYR:O     | 1:D:171:GLN:N    | 2.41                     | 0.54              |
| 1:D:383:THR:N     | 1:D:419:THR:HA   | 2.21                     | 0.54              |
| 1:D:504:ASP:CG    | 1:D:509:ASN:O    | 2.51                     | 0.54              |
| 1:D:538:LEU:CG    | 1:D:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:H:168:TYR:O     | 1:H:171:GLN:N    | 2.41                     | 0.54              |
| 1:H:504:ASP:CG    | 1:H:509:ASN:O    | 2.51                     | 0.54              |
| 1:I:156:GLY:HA2   | 2:I:1501:DTP:O1A | 2.08                     | 0.54              |
| 1:I:1195:VAL:HG11 | 1:I:1241:PHE:HZ  | 1.73                     | 0.54              |
| 1:J:168:TYR:O     | 1:J:171:GLN:N    | 2.41                     | 0.54              |
| 1:K:114:TYR:O     | 1:K:117:ASN:N    | 2.36                     | 0.54              |
| 1:K:168:TYR:O     | 1:K:171:GLN:N    | 2.41                     | 0.54              |
| 1:K:222:HIS:CD2   | 1:L:198:LYS:HZ1  | 2.24                     | 0.54              |
| 1:K:317:LEU:HD22  | 1:K:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:K:504:ASP:CG    | 1:K:509:ASN:O    | 2.51                     | 0.54              |
| 1:L:389:ILE:CD1   | 1:L:446:HIS:CD2  | 2.91                     | 0.54              |
| 1:N:100:SER:O     | 1:N:103:THR:N    | 2.41                     | 0.54              |
| 1:N:150:ASP:OD1   | 1:N:151:GLY:N    | 2.40                     | 0.54              |
| 1:N:168:TYR:O     | 1:N:171:GLN:N    | 2.41                     | 0.54              |
| 1:O:168:TYR:O     | 1:O:171:GLN:N    | 2.41                     | 0.54              |
| 1:A:100:SER:O     | 1:A:103:THR:N    | 2.41                     | 0.54              |
| 1:A:317:LEU:HD22  | 1:A:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:A:388:LEU:CB    | 1:A:446:HIS:CE1  | 2.91                     | 0.54              |
| 1:A:442:SER:O     | 1:A:446:HIS:CG   | 2.55                     | 0.54              |
| 1:B:120:PHE:HE1   | 1:B:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:C:124:ASN:H     | 1:C:303:LYS:HZ3  | 1.56                     | 0.54              |
| 1:E:119:VAL:HA    | 1:E:159:TRP:CH2  | 2.43                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:388:LEU:HB2   | 1:E:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:E:487:PHE:CD2   | 1:E:489:MET:HG3  | 2.42                     | 0.54              |
| 1:F:337:THR:C     | 1:F:339:ASP:H    | 2.16                     | 0.54              |
| 1:F:383:THR:N     | 1:F:419:THR:HA   | 2.21                     | 0.54              |
| 1:F:397:ASP:HA    | 1:F:400:VAL:HB   | 1.89                     | 0.54              |
| 1:F:447:TYR:O     | 1:F:450:PRO:HD2  | 2.07                     | 0.54              |
| 1:G:410:LEU:HD22  | 1:G:413:LYS:HA   | 1.88                     | 0.54              |
| 1:H:156:GLY:HA2   | 2:H:1501:DTP:O2A | 2.08                     | 0.54              |
| 1:H:389:ILE:CD1   | 1:H:446:HIS:CD2  | 2.91                     | 0.54              |
| 1:I:447:TYR:O     | 1:I:450:PRO:HD2  | 2.07                     | 0.54              |
| 1:I:538:LEU:CG    | 1:I:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:I:633:THR:HG21  | 1:I:643:TYR:CA   | 2.33                     | 0.54              |
| 1:L:120:PHE:HE1   | 1:L:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:L:301:LEU:CD2   | 1:L:313:PRO:CD   | 2.86                     | 0.54              |
| 1:L:518:LEU:HD22  | 1:L:643:TYR:CE1  | 2.22                     | 0.54              |
| 1:L:541:ALA:O     | 1:L:544:ASP:N    | 2.30                     | 0.54              |
| 1:M:120:PHE:HE1   | 1:M:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:N:301:LEU:CD2   | 1:N:313:PRO:CD   | 2.86                     | 0.54              |
| 1:N:317:LEU:HD22  | 1:N:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:N:388:LEU:CB    | 1:N:446:HIS:CE1  | 2.91                     | 0.54              |
| 1:N:442:SER:O     | 1:N:446:HIS:CG   | 2.55                     | 0.54              |
| 1:N:538:LEU:CG    | 1:N:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:N:541:ALA:O     | 1:N:544:ASP:N    | 2.30                     | 0.54              |
| 1:P:119:VAL:HA    | 1:P:159:TRP:CH2  | 2.43                     | 0.54              |
| 1:P:317:LEU:HD22  | 1:P:341:TRP:CH2  | 2.42                     | 0.54              |
| 1:A:106:TYR:O     | 1:A:109:GLN:N    | 2.41                     | 0.54              |
| 1:A:122:LYS:HG3   | 1:B:276:SER:OG   | 2.07                     | 0.54              |
| 1:A:301:LEU:CD2   | 1:A:313:PRO:CD   | 2.86                     | 0.54              |
| 1:B:168:TYR:O     | 1:B:171:GLN:N    | 2.41                     | 0.54              |
| 1:B:388:LEU:HB2   | 1:B:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:C:120:PHE:HE1   | 1:C:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:C:510:ALA:O     | 1:C:511:SER:HB2  | 2.07                     | 0.54              |
| 1:C:550:GLU:O     | 1:C:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:C:1195:VAL:HG11 | 1:C:1241:PHE:HZ  | 1.72                     | 0.54              |
| 1:D:301:LEU:CD2   | 1:D:313:PRO:CD   | 2.86                     | 0.54              |
| 1:D:301:LEU:HD23  | 1:D:313:PRO:HD2  | 1.89                     | 0.54              |
| 1:D:368:MET:HA    | 1:D:390:TRP:HE1  | 1.73                     | 0.54              |
| 1:D:388:LEU:HB2   | 1:D:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:E:168:TYR:O     | 1:E:171:GLN:N    | 2.41                     | 0.54              |
| 1:F:120:PHE:HE1   | 1:F:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:F:301:LEU:HD23  | 1:F:313:PRO:HD2  | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:1195:VAL:HG11 | 1:F:1241:PHE:HZ  | 1.73                     | 0.54              |
| 1:G:106:TYR:O     | 1:G:109:GLN:N    | 2.41                     | 0.54              |
| 1:G:353:ILE:HD11  | 1:G:427:LEU:HA   | 1.89                     | 0.54              |
| 1:G:538:LEU:CD1   | 1:G:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:H:604:ASN:HB3   | 1:H:929:VAL:HG12 | 1.90                     | 0.54              |
| 1:I:120:PHE:HE1   | 1:I:159:TRP:CE3  | 2.26                     | 0.54              |
| 1:J:388:LEU:HB2   | 1:J:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:J:487:PHE:CD2   | 1:J:489:MET:HG3  | 2.42                     | 0.54              |
| 1:K:106:TYR:O     | 1:K:109:GLN:N    | 2.41                     | 0.54              |
| 1:K:301:LEU:HD23  | 1:K:313:PRO:HD2  | 1.89                     | 0.54              |
| 1:K:383:THR:N     | 1:K:419:THR:HA   | 2.21                     | 0.54              |
| 1:K:388:LEU:HB2   | 1:K:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:L:1182:GLU:O    | 1:L:1183:GLU:HG3 | 2.08                     | 0.54              |
| 1:L:1195:VAL:HG11 | 1:L:1241:PHE:HZ  | 1.73                     | 0.54              |
| 1:M:168:TYR:O     | 1:M:171:GLN:N    | 2.41                     | 0.54              |
| 1:M:301:LEU:CD2   | 1:M:313:PRO:CD   | 2.86                     | 0.54              |
| 1:M:383:THR:N     | 1:M:419:THR:HA   | 2.21                     | 0.54              |
| 1:M:388:LEU:HB2   | 1:M:446:HIS:CE1  | 2.43                     | 0.54              |
| 1:N:106:TYR:O     | 1:N:109:GLN:N    | 2.41                     | 0.54              |
| 1:O:156:GLY:HA2   | 2:O:1501:DTP:O1A | 2.08                     | 0.54              |
| 1:O:389:ILE:CD1   | 1:O:446:HIS:CD2  | 2.91                     | 0.54              |
| 1:O:504:ASP:CG    | 1:O:509:ASN:O    | 2.51                     | 0.54              |
| 1:O:510:ALA:O     | 1:O:511:SER:HB2  | 2.07                     | 0.54              |
| 1:O:604:ASN:HB3   | 1:O:929:VAL:HG12 | 1.90                     | 0.54              |
| 1:P:353:ILE:HD11  | 1:P:427:LEU:HA   | 1.89                     | 0.54              |
| 1:A:487:PHE:HD2   | 1:A:489:MET:HG3  | 1.72                     | 0.54              |
| 1:A:550:GLU:O     | 1:A:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:B:301:LEU:CD2   | 1:B:313:PRO:CD   | 2.86                     | 0.54              |
| 1:B:383:THR:N     | 1:B:419:THR:HA   | 2.21                     | 0.54              |
| 1:B:1182:GLU:O    | 1:B:1183:GLU:HG3 | 2.08                     | 0.54              |
| 1:C:106:TYR:O     | 1:C:109:GLN:N    | 2.41                     | 0.54              |
| 1:C:119:VAL:HA    | 1:C:159:TRP:CH2  | 2.43                     | 0.54              |
| 1:D:106:TYR:O     | 1:D:109:GLN:N    | 2.41                     | 0.54              |
| 1:D:119:VAL:HA    | 1:D:159:TRP:CH2  | 2.43                     | 0.54              |
| 1:E:100:SER:O     | 1:E:103:THR:N    | 2.41                     | 0.54              |
| 1:E:557:LYS:CB    | 1:E:1226:TYR:CE1 | 2.87                     | 0.54              |
| 1:F:301:LEU:CD2   | 1:F:313:PRO:CD   | 2.86                     | 0.54              |
| 1:F:767:GLY:HA2   | 1:F:783:THR:HG22 | 1.89                     | 0.54              |
| 1:H:150:ASP:OD1   | 1:H:151:GLY:N    | 2.40                     | 0.54              |
| 1:H:388:LEU:CB    | 1:H:446:HIS:CE1  | 2.91                     | 0.54              |
| 1:H:538:LEU:HG    | 1:H:571:GLU:CD   | 2.33                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:538:LEU:CG   | 1:H:571:GLU:HG2  | 2.37                     | 0.54              |
| 1:I:301:LEU:HD23 | 1:I:313:PRO:HD2  | 1.89                     | 0.54              |
| 1:I:388:LEU:CB   | 1:I:446:HIS:CE1  | 2.91                     | 0.54              |
| 1:I:538:LEU:HG   | 1:I:571:GLU:CD   | 2.33                     | 0.54              |
| 1:J:337:THR:C    | 1:J:339:ASP:H    | 2.16                     | 0.54              |
| 1:K:119:VAL:HA   | 1:K:159:TRP:CH2  | 2.43                     | 0.54              |
| 1:K:301:LEU:CD2  | 1:K:313:PRO:CD   | 2.86                     | 0.54              |
| 1:K:368:MET:HA   | 1:K:390:TRP:HE1  | 1.73                     | 0.54              |
| 1:L:106:TYR:O    | 1:L:109:GLN:N    | 2.41                     | 0.54              |
| 1:N:550:GLU:O    | 1:N:552:ASN:ND2  | 2.41                     | 0.54              |
| 1:O:150:ASP:OD1  | 1:O:151:GLY:N    | 2.40                     | 0.54              |
| 1:O:538:LEU:HG   | 1:O:571:GLU:CD   | 2.33                     | 0.54              |
| 1:P:106:TYR:O    | 1:P:109:GLN:N    | 2.41                     | 0.54              |
| 1:P:557:LYS:CE   | 1:P:1224:LEU:O   | 2.50                     | 0.54              |
| 1:A:368:MET:HA   | 1:A:390:TRP:HE1  | 1.73                     | 0.53              |
| 1:A:510:ALA:O    | 1:A:511:SER:HB2  | 2.07                     | 0.53              |
| 1:A:538:LEU:HG   | 1:A:571:GLU:CD   | 2.33                     | 0.53              |
| 1:B:120:PHE:CZ   | 1:B:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:B:743:ILE:HG22 | 1:B:762:LYS:HA   | 1.91                     | 0.53              |
| 1:E:150:ASP:OD1  | 1:E:151:GLY:N    | 2.40                     | 0.53              |
| 1:E:337:THR:C    | 1:E:339:ASP:H    | 2.16                     | 0.53              |
| 1:E:538:LEU:CD1  | 1:E:571:GLU:HG2  | 2.38                     | 0.53              |
| 1:F:386:LEU:HD12 | 1:F:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:F:504:ASP:CG   | 1:F:509:ASN:O    | 2.51                     | 0.53              |
| 1:H:120:PHE:CZ   | 1:H:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:H:510:ALA:O    | 1:H:511:SER:HB2  | 2.07                     | 0.53              |
| 1:I:487:PHE:CD2  | 1:I:489:MET:HG3  | 2.42                     | 0.53              |
| 1:I:504:ASP:CG   | 1:I:509:ASN:O    | 2.51                     | 0.53              |
| 1:J:100:SER:O    | 1:J:103:THR:N    | 2.41                     | 0.53              |
| 1:J:171:GLN:HE22 | 1:J:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:J:557:LYS:CB   | 1:J:1226:TYR:CE1 | 2.87                     | 0.53              |
| 1:J:767:GLY:HA2  | 1:J:783:THR:HG22 | 1.89                     | 0.53              |
| 1:L:538:LEU:HG   | 1:L:571:GLU:CD   | 2.33                     | 0.53              |
| 1:L:550:GLU:O    | 1:L:552:ASN:ND2  | 2.41                     | 0.53              |
| 1:L:557:LYS:CB   | 1:L:1226:TYR:CE1 | 2.87                     | 0.53              |
| 1:M:114:TYR:O    | 1:M:117:ASN:N    | 2.36                     | 0.53              |
| 1:M:120:PHE:CZ   | 1:M:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:M:1182:GLU:O   | 1:M:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:N:386:LEU:HD12 | 1:N:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:N:510:ALA:O    | 1:N:511:SER:HB2  | 2.07                     | 0.53              |
| 1:N:538:LEU:HG   | 1:N:571:GLU:CD   | 2.33                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:538:LEU:CD1  | 1:P:571:GLU:HG2  | 2.38                     | 0.53              |
| 1:P:604:ASN:HB3  | 1:P:929:VAL:HG12 | 1.90                     | 0.53              |
| 1:A:504:ASP:CG   | 1:A:509:ASN:O    | 2.51                     | 0.53              |
| 1:B:100:SER:O    | 1:B:103:THR:N    | 2.41                     | 0.53              |
| 1:B:114:TYR:O    | 1:B:117:ASN:N    | 2.36                     | 0.53              |
| 1:B:171:GLN:HE22 | 1:B:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:B:389:ILE:CD1  | 1:B:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:D:120:PHE:HZ   | 1:D:162:LEU:HB2  | 1.73                     | 0.53              |
| 1:E:386:LEU:HD12 | 1:E:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:E:487:PHE:HD2  | 1:E:489:MET:HG3  | 1.72                     | 0.53              |
| 1:E:767:GLY:HA2  | 1:E:783:THR:HG22 | 1.89                     | 0.53              |
| 1:F:106:TYR:O    | 1:F:109:GLN:N    | 2.41                     | 0.53              |
| 1:F:1182:GLU:O   | 1:F:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:G:120:PHE:CZ   | 1:G:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:G:156:GLY:HA2  | 2:G:1501:DTP:O2A | 2.08                     | 0.53              |
| 1:G:168:TYR:O    | 1:G:171:GLN:N    | 2.41                     | 0.53              |
| 1:G:557:LYS:CE   | 1:G:1224:LEU:O   | 2.51                     | 0.53              |
| 1:G:604:ASN:HB3  | 1:G:929:VAL:HG12 | 1.90                     | 0.53              |
| 1:I:301:LEU:CD2  | 1:I:313:PRO:CD   | 2.86                     | 0.53              |
| 1:I:337:THR:C    | 1:I:339:ASP:H    | 2.16                     | 0.53              |
| 1:J:120:PHE:HZ   | 1:J:162:LEU:HB2  | 1.73                     | 0.53              |
| 1:J:150:ASP:OD1  | 1:J:151:GLY:N    | 2.40                     | 0.53              |
| 1:J:386:LEU:HD12 | 1:J:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:J:538:LEU:CD1  | 1:J:571:GLU:HG2  | 2.38                     | 0.53              |
| 1:K:120:PHE:HZ   | 1:K:162:LEU:HB2  | 1.73                     | 0.53              |
| 1:L:119:VAL:HA   | 1:L:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:M:100:SER:O    | 1:M:103:THR:N    | 2.41                     | 0.53              |
| 1:M:171:GLN:HE22 | 1:M:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:M:389:ILE:CD1  | 1:M:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:N:119:VAL:HA   | 1:N:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:N:504:ASP:CG   | 1:N:509:ASN:O    | 2.51                     | 0.53              |
| 1:O:120:PHE:CZ   | 1:O:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:O:388:LEU:CB   | 1:O:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:O:538:LEU:CG   | 1:O:571:GLU:HG2  | 2.37                     | 0.53              |
| 1:P:156:GLY:HA2  | 2:P:1501:DTP:O1A | 2.08                     | 0.53              |
| 1:P:168:TYR:O    | 1:P:171:GLN:N    | 2.41                     | 0.53              |
| 1:A:119:VAL:HA   | 1:A:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:A:120:PHE:CZ   | 1:A:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:A:386:LEU:HD12 | 1:A:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:A:548:LYS:HZ2  | 1:A:601:GLN:H    | 1.56                     | 0.53              |
| 1:B:388:LEU:CB   | 1:B:446:HIS:CE1  | 2.91                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:14:ASP:CG    | 1:D:142:ARG:HH12 | 2.15                     | 0.53              |
| 1:C:388:LEU:HB2  | 1:C:446:HIS:CE1  | 2.43                     | 0.53              |
| 1:E:120:PHE:HZ   | 1:E:162:LEU:HB2  | 1.73                     | 0.53              |
| 1:E:171:GLN:HE22 | 1:E:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:E:388:LEU:CB   | 1:E:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:F:388:LEU:CB   | 1:F:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:F:487:PHE:CD2  | 1:F:489:MET:HG3  | 2.42                     | 0.53              |
| 1:G:450:PRO:HG2  | 1:G:471:ILE:HD11 | 1.90                     | 0.53              |
| 1:I:106:TYR:O    | 1:I:109:GLN:N    | 2.41                     | 0.53              |
| 1:I:548:LYS:HZ2  | 1:I:601:GLN:H    | 1.53                     | 0.53              |
| 1:I:767:GLY:HA2  | 1:I:783:THR:HG22 | 1.89                     | 0.53              |
| 1:I:1182:GLU:O   | 1:I:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:J:388:LEU:CB   | 1:J:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:J:487:PHE:HD2  | 1:J:489:MET:HG3  | 1.72                     | 0.53              |
| 1:J:504:ASP:CG   | 1:J:509:ASN:O    | 2.51                     | 0.53              |
| 1:K:150:ASP:OD1  | 1:K:151:GLY:N    | 2.40                     | 0.53              |
| 1:L:637:LEU:O    | 1:L:638:GLU:CB   | 2.43                     | 0.53              |
| 1:M:388:LEU:CB   | 1:M:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:M:743:ILE:HG22 | 1:M:762:LYS:HA   | 1.91                     | 0.53              |
| 1:N:368:MET:HA   | 1:N:390:TRP:HE1  | 1.73                     | 0.53              |
| 1:N:397:ASP:HA   | 1:N:400:VAL:HB   | 1.89                     | 0.53              |
| 1:N:487:PHE:HD2  | 1:N:489:MET:HG3  | 1.72                     | 0.53              |
| 1:P:120:PHE:CZ   | 1:P:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:P:450:PRO:HG2  | 1:P:471:ILE:HD11 | 1.90                     | 0.53              |
| 1:B:106:TYR:O    | 1:B:109:GLN:N    | 2.41                     | 0.53              |
| 1:B:119:VAL:HA   | 1:B:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:B:313:PRO:HA   | 1:B:338:TRP:HH2  | 1.63                     | 0.53              |
| 1:C:156:GLY:HA2  | 2:C:1501:DTP:O2A | 2.08                     | 0.53              |
| 1:C:557:LYS:CB   | 1:C:1226:TYR:CE1 | 2.87                     | 0.53              |
| 1:D:156:GLY:HA2  | 2:D:1501:DTP:O2A | 2.08                     | 0.53              |
| 1:D:550:GLU:O    | 1:D:552:ASN:ND2  | 2.41                     | 0.53              |
| 1:E:301:LEU:CD2  | 1:E:313:PRO:CD   | 2.86                     | 0.53              |
| 1:E:301:LEU:HD23 | 1:E:313:PRO:HD2  | 1.89                     | 0.53              |
| 1:E:504:ASP:CG   | 1:E:509:ASN:O    | 2.51                     | 0.53              |
| 1:E:743:ILE:HG22 | 1:E:762:LYS:HA   | 1.91                     | 0.53              |
| 1:G:388:LEU:CB   | 1:G:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:G:389:ILE:CD1  | 1:G:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:G:394:ILE:HD12 | 1:G:395:LYS:HE3  | 1.91                     | 0.53              |
| 1:G:504:ASP:CG   | 1:G:509:ASN:O    | 2.51                     | 0.53              |
| 1:H:450:PRO:HG2  | 1:H:471:ILE:HD11 | 1.91                     | 0.53              |
| 1:I:168:TYR:O    | 1:I:171:GLN:N    | 2.41                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:386:LEU:HD12  | 1:I:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:I:397:ASP:HA    | 1:I:400:VAL:HB   | 1.89                     | 0.53              |
| 1:J:301:LEU:CD2   | 1:J:313:PRO:CD   | 2.86                     | 0.53              |
| 1:J:743:ILE:HG22  | 1:J:762:LYS:HA   | 1.91                     | 0.53              |
| 1:K:156:GLY:HA2   | 2:K:1501:DTP:O1A | 2.08                     | 0.53              |
| 1:K:389:ILE:CD1   | 1:K:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:L:388:LEU:HB2   | 1:L:446:HIS:CE1  | 2.43                     | 0.53              |
| 1:M:106:TYR:O     | 1:M:109:GLN:N    | 2.41                     | 0.53              |
| 1:N:156:GLY:HA2   | 2:N:1501:DTP:O1A | 2.08                     | 0.53              |
| 1:P:388:LEU:CB    | 1:P:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:P:389:ILE:CD1   | 1:P:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:A:604:ASN:HB3   | 1:A:929:VAL:HG12 | 1.90                     | 0.53              |
| 1:B:510:ALA:O     | 1:B:511:SER:HB2  | 2.07                     | 0.53              |
| 1:C:114:TYR:O     | 1:C:117:ASN:N    | 2.36                     | 0.53              |
| 1:C:168:TYR:O     | 1:C:171:GLN:N    | 2.41                     | 0.53              |
| 1:C:386:LEU:HD12  | 1:C:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:C:538:LEU:HG    | 1:C:571:GLU:CD   | 2.33                     | 0.53              |
| 1:C:631:LEU:HD22  | 1:C:680:LEU:HD22 | 1.91                     | 0.53              |
| 1:C:743:ILE:HG22  | 1:C:762:LYS:HA   | 1.91                     | 0.53              |
| 1:D:150:ASP:OD1   | 1:D:151:GLY:N    | 2.41                     | 0.53              |
| 1:D:389:ILE:CD1   | 1:D:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:E:368:MET:HA    | 1:E:390:TRP:HE1  | 1.73                     | 0.53              |
| 1:F:538:LEU:HG    | 1:F:571:GLU:CD   | 2.33                     | 0.53              |
| 1:G:171:GLN:HE22  | 1:G:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:H:106:TYR:O     | 1:H:109:GLN:N    | 2.41                     | 0.53              |
| 1:H:119:VAL:HA    | 1:H:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:I:120:PHE:HZ    | 1:I:162:LEU:HB2  | 1.73                     | 0.53              |
| 1:I:631:LEU:HD22  | 1:I:680:LEU:HD22 | 1.91                     | 0.53              |
| 1:J:301:LEU:HD23  | 1:J:313:PRO:HD2  | 1.89                     | 0.53              |
| 1:J:410:LEU:HD22  | 1:J:413:LYS:HA   | 1.88                     | 0.53              |
| 1:K:550:GLU:O     | 1:K:552:ASN:ND2  | 2.41                     | 0.53              |
| 1:L:510:ALA:O     | 1:L:511:SER:HB2  | 2.07                     | 0.53              |
| 1:M:119:VAL:HA    | 1:M:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:M:313:PRO:HA    | 1:M:338:TRP:HH2  | 1.63                     | 0.53              |
| 1:N:120:PHE:CZ    | 1:N:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:N:548:LYS:HZ2   | 1:N:601:GLN:H    | 1.56                     | 0.53              |
| 1:O:106:TYR:O     | 1:O:109:GLN:N    | 2.41                     | 0.53              |
| 1:O:386:LEU:HD12  | 1:O:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:P:1195:VAL:HG11 | 1:P:1241:PHE:HZ  | 1.73                     | 0.53              |
| 1:A:156:GLY:HA2   | 2:A:1501:DTP:O2A | 2.08                     | 0.53              |
| 1:A:397:ASP:HA    | 1:A:400:VAL:HB   | 1.89                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:388:LEU:CB    | 1:C:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:C:487:PHE:HD2   | 1:C:489:MET:HG3  | 1.72                     | 0.53              |
| 1:F:119:VAL:HA    | 1:F:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:F:631:LEU:HD22  | 1:F:680:LEU:HD22 | 1.91                     | 0.53              |
| 1:F:743:ILE:HG22  | 1:F:762:LYS:HA   | 1.91                     | 0.53              |
| 1:H:368:MET:HA    | 1:H:390:TRP:HE1  | 1.72                     | 0.53              |
| 1:H:1182:GLU:O    | 1:H:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:J:368:MET:HA    | 1:J:390:TRP:HE1  | 1.73                     | 0.53              |
| 1:L:397:ASP:HA    | 1:L:400:VAL:HB   | 1.89                     | 0.53              |
| 1:L:631:LEU:HD22  | 1:L:680:LEU:HD22 | 1.91                     | 0.53              |
| 1:M:397:ASP:HA    | 1:M:400:VAL:HB   | 1.89                     | 0.53              |
| 1:M:510:ALA:O     | 1:M:511:SER:HB2  | 2.07                     | 0.53              |
| 1:N:604:ASN:HB3   | 1:N:929:VAL:HG12 | 1.90                     | 0.53              |
| 1:O:119:VAL:HA    | 1:O:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:O:450:PRO:HG2   | 1:O:471:ILE:HD11 | 1.91                     | 0.53              |
| 1:O:616:LEU:HD23  | 1:O:620:PHE:HB2  | 1.91                     | 0.53              |
| 1:O:1182:GLU:O    | 1:O:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:P:171:GLN:HE22  | 1:P:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:P:394:ILE:HD12  | 1:P:395:LYS:HE3  | 1.91                     | 0.53              |
| 1:P:504:ASP:CG    | 1:P:509:ASN:O    | 2.51                     | 0.53              |
| 1:A:1182:GLU:O    | 1:A:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:B:156:GLY:HA2   | 2:B:1501:DTP:O2A | 2.08                     | 0.53              |
| 1:B:397:ASP:HA    | 1:B:400:VAL:HB   | 1.89                     | 0.53              |
| 1:C:397:ASP:HA    | 1:C:400:VAL:HB   | 1.89                     | 0.53              |
| 1:D:388:LEU:CB    | 1:D:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:E:410:LEU:HD22  | 1:E:413:LYS:HA   | 1.88                     | 0.53              |
| 1:F:120:PHE:HZ    | 1:F:162:LEU:HB2  | 1.73                     | 0.53              |
| 1:F:120:PHE:CZ    | 1:F:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:F:171:GLN:HE22  | 1:F:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:G:337:THR:C     | 1:G:339:ASP:H    | 2.16                     | 0.53              |
| 1:G:1195:VAL:HG11 | 1:G:1241:PHE:HZ  | 1.73                     | 0.53              |
| 1:H:386:LEU:HD12  | 1:H:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:H:394:ILE:HD12  | 1:H:395:LYS:HE3  | 1.91                     | 0.53              |
| 1:H:616:LEU:HD23  | 1:H:620:PHE:HB2  | 1.91                     | 0.53              |
| 1:I:743:ILE:HG22  | 1:I:762:LYS:HA   | 1.91                     | 0.53              |
| 1:K:388:LEU:CB    | 1:K:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:K:487:PHE:HD2   | 1:K:489:MET:HG3  | 1.72                     | 0.53              |
| 1:L:388:LEU:CB    | 1:L:446:HIS:CE1  | 2.91                     | 0.53              |
| 1:M:156:GLY:HA2   | 2:M:1501:DTP:O1A | 2.08                     | 0.53              |
| 1:O:120:PHE:HE1   | 1:O:159:TRP:CE3  | 2.26                     | 0.53              |
| 1:P:337:THR:C     | 1:P:339:ASP:H    | 2.16                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1195:VAL:HG11 | 1:A:1241:PHE:HZ  | 1.73                     | 0.53              |
| 1:D:1182:GLU:O    | 1:D:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:F:14:ASP:OD2    | 1:G:142:ARG:CZ   | 2.55                     | 0.53              |
| 1:F:168:TYR:O     | 1:F:171:GLN:N    | 2.41                     | 0.53              |
| 1:F:487:PHE:HD2   | 1:F:489:MET:HG3  | 1.72                     | 0.53              |
| 1:J:550:GLU:O     | 1:J:552:ASN:ND2  | 2.41                     | 0.53              |
| 1:L:156:GLY:HA2   | 2:L:1501:DTP:O1A | 2.08                     | 0.53              |
| 1:L:168:TYR:O     | 1:L:171:GLN:N    | 2.41                     | 0.53              |
| 1:L:487:PHE:HD2   | 1:L:489:MET:HG3  | 1.72                     | 0.53              |
| 1:N:743:ILE:HG22  | 1:N:762:LYS:HA   | 1.91                     | 0.53              |
| 1:N:1182:GLU:O    | 1:N:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:N:1195:VAL:HG11 | 1:N:1241:PHE:HZ  | 1.73                     | 0.53              |
| 1:O:368:MET:HA    | 1:O:390:TRP:HE1  | 1.73                     | 0.53              |
| 1:O:394:ILE:HD12  | 1:O:395:LYS:HE3  | 1.91                     | 0.53              |
| 1:A:992:ARG:HH12  | 1:A:1029:GLU:HG2 | 1.74                     | 0.53              |
| 1:B:550:GLU:O     | 1:B:552:ASN:ND2  | 2.41                     | 0.53              |
| 1:D:487:PHE:HD2   | 1:D:489:MET:HG3  | 1.72                     | 0.53              |
| 1:E:156:GLY:HA2   | 2:E:1501:DTP:O2A | 2.08                     | 0.53              |
| 1:E:389:ILE:CD1   | 1:E:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:E:550:GLU:O     | 1:E:552:ASN:ND2  | 2.41                     | 0.53              |
| 1:E:616:LEU:HD23  | 1:E:620:PHE:HB2  | 1.91                     | 0.53              |
| 1:F:188:SER:N     | 1:F:251:APK:O2P  | 2.31                     | 0.53              |
| 1:F:394:ILE:HD12  | 1:F:395:LYS:HE3  | 1.91                     | 0.53              |
| 1:F:604:ASN:HB3   | 1:F:929:VAL:HG12 | 1.90                     | 0.53              |
| 1:H:120:PHE:HE1   | 1:H:159:TRP:CE3  | 2.26                     | 0.53              |
| 1:H:1195:VAL:HG11 | 1:H:1241:PHE:HZ  | 1.72                     | 0.53              |
| 1:I:119:VAL:HA    | 1:I:159:TRP:CH2  | 2.43                     | 0.53              |
| 1:I:120:PHE:CZ    | 1:I:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:J:120:PHE:CZ    | 1:J:162:LEU:HB2  | 2.43                     | 0.53              |
| 1:J:156:GLY:HA2   | 2:J:1501:DTP:O1A | 2.08                     | 0.53              |
| 1:J:389:ILE:CD1   | 1:J:446:HIS:CD2  | 2.91                     | 0.53              |
| 1:K:1182:GLU:O    | 1:K:1183:GLU:HG3 | 2.08                     | 0.53              |
| 1:L:386:LEU:HD12  | 1:L:420:ILE:HD13 | 1.90                     | 0.53              |
| 1:L:743:ILE:HG22  | 1:L:762:LYS:HA   | 1.91                     | 0.53              |
| 1:M:504:ASP:CG    | 1:M:509:ASN:O    | 2.51                     | 0.53              |
| 1:N:171:GLN:HE22  | 1:N:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:N:992:ARG:HH12  | 1:N:1029:GLU:HG2 | 1.74                     | 0.53              |
| 1:O:992:ARG:HH12  | 1:O:1029:GLU:HG2 | 1.74                     | 0.53              |
| 1:C:171:GLN:HE22  | 1:C:178:ILE:HD12 | 1.74                     | 0.53              |
| 1:C:337:THR:C     | 1:C:339:ASP:H    | 2.16                     | 0.53              |
| 1:D:604:ASN:HB3   | 1:D:929:VAL:HG12 | 1.90                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:616:LEU:HD23  | 1:D:620:PHE:HB2   | 1.91                     | 0.53              |
| 1:D:631:LEU:HD22  | 1:D:680:LEU:HD22  | 1.91                     | 0.53              |
| 1:E:106:TYR:O     | 1:E:109:GLN:N     | 2.41                     | 0.53              |
| 1:E:120:PHE:CZ    | 1:E:162:LEU:HB2   | 2.43                     | 0.53              |
| 1:G:487:PHE:HD2   | 1:G:489:MET:HG3   | 1.72                     | 0.53              |
| 1:G:992:ARG:HH12  | 1:G:1029:GLU:HG2  | 1.74                     | 0.53              |
| 1:H:992:ARG:HH12  | 1:H:1029:GLU:HG2  | 1.74                     | 0.53              |
| 1:I:171:GLN:HE22  | 1:I:178:ILE:HD12  | 1.74                     | 0.53              |
| 1:I:450:PRO:HG2   | 1:I:471:ILE:HD11  | 1.90                     | 0.53              |
| 1:I:836:VAL:HG21  | 1:I:876:LEU:HD22  | 1.91                     | 0.53              |
| 1:J:616:LEU:HD23  | 1:J:620:PHE:HB2   | 1.91                     | 0.53              |
| 1:J:836:VAL:HG21  | 1:J:876:LEU:HD22  | 1.91                     | 0.53              |
| 1:J:1086:LYS:O    | 1:J:1087:ILE:HG13 | 2.09                     | 0.53              |
| 1:K:604:ASN:HB3   | 1:K:929:VAL:HG12  | 1.90                     | 0.53              |
| 1:K:616:LEU:HD23  | 1:K:620:PHE:HB2   | 1.91                     | 0.53              |
| 1:M:538:LEU:HG    | 1:M:571:GLU:CD    | 2.33                     | 0.53              |
| 1:M:550:GLU:O     | 1:M:552:ASN:ND2   | 2.41                     | 0.53              |
| 1:M:604:ASN:HB3   | 1:M:929:VAL:HG12  | 1.90                     | 0.53              |
| 1:N:337:THR:C     | 1:N:339:ASP:H     | 2.16                     | 0.53              |
| 1:O:1195:VAL:HG11 | 1:O:1241:PHE:HZ   | 1.73                     | 0.53              |
| 1:P:616:LEU:HD23  | 1:P:620:PHE:HB2   | 1.91                     | 0.53              |
| 1:P:992:ARG:HH12  | 1:P:1029:GLU:HG2  | 1.74                     | 0.53              |
| 1:A:743:ILE:HG22  | 1:A:762:LYS:HA    | 1.91                     | 0.52              |
| 1:B:337:THR:C     | 1:B:339:ASP:H     | 2.16                     | 0.52              |
| 1:B:538:LEU:HG    | 1:B:571:GLU:CD    | 2.33                     | 0.52              |
| 1:E:394:ILE:HD12  | 1:E:395:LYS:HE3   | 1.91                     | 0.52              |
| 1:E:836:VAL:HG21  | 1:E:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:E:1182:GLU:O    | 1:E:1183:GLU:HG3  | 2.08                     | 0.52              |
| 1:G:616:LEU:HD23  | 1:G:620:PHE:HB2   | 1.91                     | 0.52              |
| 1:H:337:THR:C     | 1:H:339:ASP:H     | 2.16                     | 0.52              |
| 1:I:394:ILE:HD12  | 1:I:395:LYS:HE3   | 1.91                     | 0.52              |
| 1:I:604:ASN:HB3   | 1:I:929:VAL:HG12  | 1.90                     | 0.52              |
| 1:J:394:ILE:HD12  | 1:J:395:LYS:HE3   | 1.91                     | 0.52              |
| 1:J:1182:GLU:O    | 1:J:1183:GLU:HG3  | 2.08                     | 0.52              |
| 1:K:538:LEU:HG    | 1:K:571:GLU:CD    | 2.33                     | 0.52              |
| 1:K:631:LEU:HD22  | 1:K:680:LEU:HD22  | 1.91                     | 0.52              |
| 1:L:188:SER:N     | 1:L:251:APK:O2P   | 2.31                     | 0.52              |
| 1:M:337:THR:C     | 1:M:339:ASP:H     | 2.16                     | 0.52              |
| 1:M:992:ARG:HH12  | 1:M:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:N:378:SER:H     | 1:N:422:ILE:HD13  | 1.62                     | 0.52              |
| 1:O:337:THR:C     | 1:O:339:ASP:H     | 2.16                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:518:LEU:HD22  | 1:P:643:TYR:CE1   | 2.22                     | 0.52              |
| 1:A:171:GLN:HE22  | 1:A:178:ILE:HD12  | 1.74                     | 0.52              |
| 1:A:337:THR:C     | 1:A:339:ASP:H     | 2.16                     | 0.52              |
| 1:A:450:PRO:HG2   | 1:A:471:ILE:HD11  | 1.90                     | 0.52              |
| 1:A:912:ASP:OD2   | 1:A:921:CYS:SG    | 2.68                     | 0.52              |
| 1:B:553:LEU:HB3   | 1:B:556:SER:HG    | 1.72                     | 0.52              |
| 1:B:992:ARG:HH12  | 1:B:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:B:1195:VAL:HG11 | 1:B:1241:PHE:HZ   | 1.73                     | 0.52              |
| 1:C:120:PHE:CZ    | 1:C:162:LEU:HB2   | 2.43                     | 0.52              |
| 1:D:538:LEU:HG    | 1:D:571:GLU:CD    | 2.33                     | 0.52              |
| 1:D:1086:LYS:O    | 1:D:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:E:912:ASP:OD2   | 1:E:921:CYS:SG    | 2.68                     | 0.52              |
| 1:E:1086:LYS:O    | 1:E:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:F:389:ILE:CD1   | 1:F:446:HIS:CD2   | 2.91                     | 0.52              |
| 1:F:625:LEU:HD22  | 1:F:629:GLN:HA    | 1.92                     | 0.52              |
| 1:G:386:LEU:HD12  | 1:G:420:ILE:HD13  | 1.90                     | 0.52              |
| 1:G:518:LEU:HD22  | 1:G:643:TYR:CE1   | 2.22                     | 0.52              |
| 1:G:631:LEU:HD22  | 1:G:680:LEU:HD22  | 1.91                     | 0.52              |
| 1:G:1182:GLU:O    | 1:G:1183:GLU:HG3  | 2.08                     | 0.52              |
| 1:I:487:PHE:HD2   | 1:I:489:MET:HG3   | 1.72                     | 0.52              |
| 1:J:106:TYR:O     | 1:J:109:GLN:N     | 2.41                     | 0.52              |
| 1:J:912:ASP:OD2   | 1:J:921:CYS:SG    | 2.68                     | 0.52              |
| 1:J:1177:TYR:CE2  | 1:K:916:LYS:CE    | 2.91                     | 0.52              |
| 1:K:171:GLN:HE22  | 1:K:178:ILE:HD12  | 1.74                     | 0.52              |
| 1:K:450:PRO:HG2   | 1:K:471:ILE:HD11  | 1.90                     | 0.52              |
| 1:K:1086:LYS:O    | 1:K:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:L:120:PHE:HZ    | 1:L:162:LEU:HB2   | 1.73                     | 0.52              |
| 1:M:557:LYS:HZ2   | 1:M:1223:GLN:HG3  | 1.73                     | 0.52              |
| 1:N:912:ASP:OD2   | 1:N:921:CYS:SG    | 2.68                     | 0.52              |
| 1:O:171:GLN:HE22  | 1:O:178:ILE:HD12  | 1.74                     | 0.52              |
| 1:P:631:LEU:HD22  | 1:P:680:LEU:HD22  | 1.91                     | 0.52              |
| 1:A:120:PHE:HZ    | 1:A:162:LEU:HB2   | 1.73                     | 0.52              |
| 1:A:616:LEU:HD23  | 1:A:620:PHE:HB2   | 1.91                     | 0.52              |
| 1:B:604:ASN:HB3   | 1:B:929:VAL:HG12  | 1.90                     | 0.52              |
| 1:B:912:ASP:OD2   | 1:B:921:CYS:SG    | 2.68                     | 0.52              |
| 1:D:346:CYS:O     | 1:D:350:THR:N     | 2.25                     | 0.52              |
| 1:D:397:ASP:HA    | 1:D:400:VAL:HB    | 1.89                     | 0.52              |
| 1:D:450:PRO:HG2   | 1:D:471:ILE:HD11  | 1.90                     | 0.52              |
| 1:D:836:VAL:HG21  | 1:D:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:E:434:GLU:C     | 1:E:436:GLU:H     | 2.18                     | 0.52              |
| 1:E:625:LEU:HD22  | 1:E:629:GLN:HA    | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:183:LEU:HD11  | 1:F:256:PHE:HE2   | 1.75                     | 0.52              |
| 1:F:450:PRO:HG2   | 1:F:471:ILE:HD11  | 1.90                     | 0.52              |
| 1:F:836:VAL:HG21  | 1:F:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:F:1086:LYS:O    | 1:F:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:G:397:ASP:O     | 1:G:401:VAL:N     | 2.28                     | 0.52              |
| 1:H:171:GLN:HE22  | 1:H:178:ILE:HD12  | 1.74                     | 0.52              |
| 1:I:912:ASP:OD2   | 1:I:921:CYS:SG    | 2.68                     | 0.52              |
| 1:K:397:ASP:HA    | 1:K:400:VAL:HB    | 1.89                     | 0.52              |
| 1:K:836:VAL:HG21  | 1:K:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:M:631:LEU:HD22  | 1:M:680:LEU:HD22  | 1.91                     | 0.52              |
| 1:M:912:ASP:OD2   | 1:M:921:CYS:SG    | 2.68                     | 0.52              |
| 1:O:743:ILE:HG22  | 1:O:762:LYS:HA    | 1.91                     | 0.52              |
| 1:P:386:LEU:HD12  | 1:P:420:ILE:HD13  | 1.90                     | 0.52              |
| 1:P:397:ASP:O     | 1:P:401:VAL:N     | 2.28                     | 0.52              |
| 1:P:487:PHE:HD2   | 1:P:489:MET:HG3   | 1.72                     | 0.52              |
| 1:B:504:ASP:CG    | 1:B:509:ASN:O     | 2.51                     | 0.52              |
| 1:C:120:PHE:HZ    | 1:C:162:LEU:HB2   | 1.73                     | 0.52              |
| 1:C:1086:LYS:O    | 1:C:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:E:631:LEU:HD22  | 1:E:680:LEU:HD22  | 1.91                     | 0.52              |
| 1:F:992:ARG:HH12  | 1:F:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:G:120:PHE:HZ    | 1:G:162:LEU:HB2   | 1.73                     | 0.52              |
| 1:H:743:ILE:HG22  | 1:H:762:LYS:HA    | 1.91                     | 0.52              |
| 1:I:183:LEU:HD11  | 1:I:256:PHE:HE2   | 1.75                     | 0.52              |
| 1:I:625:LEU:HD22  | 1:I:629:GLN:HA    | 1.92                     | 0.52              |
| 1:I:992:ARG:HH12  | 1:I:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:I:1086:LYS:O    | 1:I:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:J:36:PRO:O      | 1:J:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:J:434:GLU:C     | 1:J:436:GLU:H     | 2.18                     | 0.52              |
| 1:J:625:LEU:HD22  | 1:J:629:GLN:HA    | 1.92                     | 0.52              |
| 1:J:631:LEU:HD22  | 1:J:680:LEU:HD22  | 1.91                     | 0.52              |
| 1:K:276:SER:OG    | 1:L:122:LYS:CG    | 2.57                     | 0.52              |
| 1:K:337:THR:C     | 1:K:339:ASP:H     | 2.16                     | 0.52              |
| 1:L:36:PRO:O      | 1:L:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:L:337:THR:C     | 1:L:339:ASP:H     | 2.16                     | 0.52              |
| 1:L:346:CYS:O     | 1:L:350:THR:N     | 2.25                     | 0.52              |
| 1:L:557:LYS:HZ2   | 1:L:1223:GLN:HG3  | 1.74                     | 0.52              |
| 1:M:1195:VAL:HG11 | 1:M:1241:PHE:HZ   | 1.73                     | 0.52              |
| 1:N:120:PHE:HZ    | 1:N:162:LEU:HB2   | 1.73                     | 0.52              |
| 1:N:450:PRO:HG2   | 1:N:471:ILE:HD11  | 1.90                     | 0.52              |
| 1:P:1182:GLU:O    | 1:P:1183:GLU:HG3  | 2.08                     | 0.52              |
| 1:A:378:SER:H     | 1:A:422:ILE:HD13  | 1.62                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:394:ILE:HD12 | 1:A:395:LYS:HE3  | 1.91                     | 0.52              |
| 1:B:631:LEU:HD22 | 1:B:680:LEU:HD22 | 1.91                     | 0.52              |
| 1:C:14:ASP:OD2   | 1:D:142:ARG:CZ   | 2.57                     | 0.52              |
| 1:C:36:PRO:O     | 1:C:39:ILE:HG22  | 2.10                     | 0.52              |
| 1:C:122:LYS:HG3  | 1:D:276:SER:HB2  | 1.91                     | 0.52              |
| 1:C:188:SER:N    | 1:C:251:APK:O2P  | 2.31                     | 0.52              |
| 1:D:518:LEU:HD22 | 1:D:643:TYR:CE1  | 2.22                     | 0.52              |
| 1:D:625:LEU:HD22 | 1:D:629:GLN:HA   | 1.92                     | 0.52              |
| 1:E:36:PRO:O     | 1:E:39:ILE:HG22  | 2.10                     | 0.52              |
| 1:F:912:ASP:OD2  | 1:F:921:CYS:SG   | 2.68                     | 0.52              |
| 1:K:625:LEU:HD22 | 1:K:629:GLN:HA   | 1.92                     | 0.52              |
| 1:L:120:PHE:CZ   | 1:L:162:LEU:HB2  | 2.43                     | 0.52              |
| 1:L:171:GLN:HE22 | 1:L:178:ILE:HD12 | 1.74                     | 0.52              |
| 1:N:394:ILE:HD12 | 1:N:395:LYS:HE3  | 1.91                     | 0.52              |
| 1:N:434:GLU:C    | 1:N:436:GLU:H    | 2.18                     | 0.52              |
| 1:N:616:LEU:HD23 | 1:N:620:PHE:HB2  | 1.91                     | 0.52              |
| 1:N:625:LEU:HD22 | 1:N:629:GLN:HA   | 1.92                     | 0.52              |
| 1:P:162:LEU:O    | 1:P:165:CYS:N    | 2.43                     | 0.52              |
| 1:A:434:GLU:C    | 1:A:436:GLU:H    | 2.18                     | 0.52              |
| 1:A:625:LEU:HD22 | 1:A:629:GLN:HA   | 1.92                     | 0.52              |
| 1:C:346:CYS:O    | 1:C:350:THR:N    | 2.25                     | 0.52              |
| 1:D:171:GLN:HE22 | 1:D:178:ILE:HD12 | 1.74                     | 0.52              |
| 1:D:337:THR:C    | 1:D:339:ASP:H    | 2.16                     | 0.52              |
| 1:D:992:ARG:HH12 | 1:D:1029:GLU:HG2 | 1.74                     | 0.52              |
| 1:G:548:LYS:HZ2  | 1:G:601:GLN:H    | 1.54                     | 0.52              |
| 1:G:743:ILE:HG22 | 1:G:762:LYS:HA   | 1.91                     | 0.52              |
| 1:H:162:LEU:O    | 1:H:165:CYS:N    | 2.43                     | 0.52              |
| 1:K:120:PHE:CZ   | 1:K:162:LEU:HB2  | 2.43                     | 0.52              |
| 1:K:346:CYS:O    | 1:K:350:THR:N    | 2.25                     | 0.52              |
| 1:L:450:PRO:HG2  | 1:L:471:ILE:HD11 | 1.91                     | 0.52              |
| 1:N:518:LEU:HD12 | 1:N:518:LEU:N    | 2.20                     | 0.52              |
| 1:O:162:LEU:O    | 1:O:165:CYS:N    | 2.43                     | 0.52              |
| 1:O:375:PHE:CD2  | 1:O:381:ILE:HG12 | 2.45                     | 0.52              |
| 1:A:183:LEU:HD11 | 1:A:256:PHE:HE2  | 1.75                     | 0.52              |
| 1:A:836:VAL:HG21 | 1:A:876:LEU:HD22 | 1.91                     | 0.52              |
| 1:B:616:LEU:HD23 | 1:B:620:PHE:HB2  | 1.91                     | 0.52              |
| 1:B:631:LEU:H    | 1:B:646:ARG:HB3  | 1.74                     | 0.52              |
| 1:C:450:PRO:HG2  | 1:C:471:ILE:HD11 | 1.91                     | 0.52              |
| 1:C:631:LEU:H    | 1:C:646:ARG:HB3  | 1.74                     | 0.52              |
| 1:C:992:ARG:HH12 | 1:C:1029:GLU:HG2 | 1.74                     | 0.52              |
| 1:D:120:PHE:CZ   | 1:D:162:LEU:HB2  | 2.43                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:912:ASP:OD2  | 1:D:921:CYS:SG    | 2.68                     | 0.52              |
| 1:E:553:LEU:HB3  | 1:E:556:SER:HG    | 1.75                     | 0.52              |
| 1:F:883:ILE:HA   | 1:F:898:VAL:HB    | 1.92                     | 0.52              |
| 1:G:162:LEU:O    | 1:G:165:CYS:N     | 2.43                     | 0.52              |
| 1:G:1086:LYS:O   | 1:G:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:H:375:PHE:CD2  | 1:H:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:H:631:LEU:H    | 1:H:646:ARG:HB3   | 1.74                     | 0.52              |
| 1:I:389:ILE:CD1  | 1:I:446:HIS:CD2   | 2.91                     | 0.52              |
| 1:I:883:ILE:HA   | 1:I:898:VAL:HB    | 1.92                     | 0.52              |
| 1:J:183:LEU:HD11 | 1:J:256:PHE:HE2   | 1.75                     | 0.52              |
| 1:J:604:ASN:HB3  | 1:J:929:VAL:HG12  | 1.90                     | 0.52              |
| 1:K:36:PRO:O     | 1:K:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:K:375:PHE:CD2  | 1:K:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:K:992:ARG:HH12 | 1:K:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:L:1086:LYS:O   | 1:L:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:N:183:LEU:HD11 | 1:N:256:PHE:HE2   | 1.75                     | 0.52              |
| 1:O:63:TRP:CZ3   | 1:O:126:SER:HB2   | 2.45                     | 0.52              |
| 1:O:434:GLU:C    | 1:O:436:GLU:H     | 2.18                     | 0.52              |
| 1:O:631:LEU:H    | 1:O:646:ARG:HB3   | 1.74                     | 0.52              |
| 1:P:120:PHE:HZ   | 1:P:162:LEU:HB2   | 1.73                     | 0.52              |
| 1:P:548:LYS:HZ2  | 1:P:601:GLN:H     | 1.54                     | 0.52              |
| 1:P:743:ILE:HG22 | 1:P:762:LYS:HA    | 1.91                     | 0.52              |
| 1:P:1086:LYS:O   | 1:P:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:A:373:SER:HB3  | 1:A:433:LEU:CG    | 2.40                     | 0.52              |
| 1:A:518:LEU:HD12 | 1:A:518:LEU:N     | 2.20                     | 0.52              |
| 1:C:394:ILE:HD12 | 1:C:395:LYS:HE3   | 1.91                     | 0.52              |
| 1:D:36:PRO:O     | 1:D:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:D:375:PHE:CD2  | 1:D:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:E:183:LEU:HD11 | 1:E:256:PHE:HE2   | 1.75                     | 0.52              |
| 1:E:450:PRO:HG2  | 1:E:471:ILE:HD11  | 1.90                     | 0.52              |
| 1:E:604:ASN:HB3  | 1:E:929:VAL:HG12  | 1.90                     | 0.52              |
| 1:F:162:LEU:O    | 1:F:165:CYS:N     | 2.43                     | 0.52              |
| 1:F:375:PHE:CD2  | 1:F:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:H:434:GLU:C    | 1:H:436:GLU:H     | 2.18                     | 0.52              |
| 1:H:912:ASP:OD2  | 1:H:921:CYS:SG    | 2.68                     | 0.52              |
| 1:I:162:LEU:O    | 1:I:165:CYS:N     | 2.43                     | 0.52              |
| 1:I:188:SER:N    | 1:I:251:APK:O2P   | 2.31                     | 0.52              |
| 1:J:375:PHE:CD2  | 1:J:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:J:553:LEU:HB3  | 1:J:556:SER:HG    | 1.75                     | 0.52              |
| 1:K:518:LEU:HD22 | 1:K:643:TYR:CE1   | 2.22                     | 0.52              |
| 1:K:912:ASP:OD2  | 1:K:921:CYS:SG    | 2.68                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:373:SER:HB3  | 1:L:433:LEU:CG    | 2.40                     | 0.52              |
| 1:L:375:PHE:CD2  | 1:L:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:L:616:LEU:HD23 | 1:L:620:PHE:HB2   | 1.91                     | 0.52              |
| 1:L:992:ARG:HH12 | 1:L:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:N:162:LEU:O    | 1:N:165:CYS:N     | 2.43                     | 0.52              |
| 1:N:373:SER:HB3  | 1:N:433:LEU:CG    | 2.40                     | 0.52              |
| 1:N:836:VAL:HG21 | 1:N:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:O:912:ASP:OD2  | 1:O:921:CYS:SG    | 2.68                     | 0.52              |
| 1:P:368:MET:HA   | 1:P:390:TRP:HE1   | 1.73                     | 0.52              |
| 1:A:162:LEU:O    | 1:A:165:CYS:N     | 2.43                     | 0.52              |
| 1:A:467:PHE:HD1  | 1:A:471:ILE:HD12  | 1.75                     | 0.52              |
| 1:B:36:PRO:O     | 1:B:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:B:1086:LYS:O   | 1:B:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:C:162:LEU:O    | 1:C:165:CYS:N     | 2.43                     | 0.52              |
| 1:C:373:SER:HB3  | 1:C:433:LEU:CG    | 2.40                     | 0.52              |
| 1:C:467:PHE:HD1  | 1:C:471:ILE:HD12  | 1.75                     | 0.52              |
| 1:D:394:ILE:HD12 | 1:D:395:LYS:HE3   | 1.91                     | 0.52              |
| 1:D:434:GLU:C    | 1:D:436:GLU:H     | 2.18                     | 0.52              |
| 1:E:63:TRP:CZ3   | 1:E:126:SER:HB2   | 2.45                     | 0.52              |
| 1:E:375:PHE:CD2  | 1:E:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:E:992:ARG:HH12 | 1:E:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:F:36:PRO:O     | 1:F:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:G:36:PRO:O     | 1:G:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:H:63:TRP:CZ3   | 1:H:126:SER:HB2   | 2.45                     | 0.52              |
| 1:J:450:PRO:HG2  | 1:J:471:ILE:HD11  | 1.91                     | 0.52              |
| 1:J:992:ARG:HH12 | 1:J:1029:GLU:HG2  | 1.74                     | 0.52              |
| 1:K:394:ILE:HD12 | 1:K:395:LYS:HE3   | 1.91                     | 0.52              |
| 1:K:883:ILE:HA   | 1:K:898:VAL:HB    | 1.92                     | 0.52              |
| 1:M:36:PRO:O     | 1:M:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:M:631:LEU:H    | 1:M:646:ARG:HB3   | 1.74                     | 0.52              |
| 1:M:1086:LYS:O   | 1:M:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:N:64:THR:O     | 1:N:67:SER:OG     | 2.27                     | 0.52              |
| 1:N:467:PHE:HD1  | 1:N:471:ILE:HD12  | 1.75                     | 0.52              |
| 1:N:1086:LYS:O   | 1:N:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:P:36:PRO:O     | 1:P:39:ILE:HG22   | 2.10                     | 0.52              |
| 1:P:836:VAL:HG21 | 1:P:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:A:198:LYS:HZ1  | 1:B:222:HIS:CG    | 2.28                     | 0.52              |
| 1:A:336:ALA:C    | 1:A:338:TRP:H     | 2.17                     | 0.52              |
| 1:B:492:LEU:HD11 | 1:B:561:LEU:CD2   | 2.40                     | 0.52              |
| 1:C:375:PHE:CD2  | 1:C:381:ILE:HG12  | 2.45                     | 0.52              |
| 1:C:557:LYS:HZ2  | 1:C:1223:GLN:HG3  | 1.74                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:604:ASN:HB3  | 1:C:929:VAL:HG12  | 1.90                     | 0.52              |
| 1:E:209:SER:OG   | 1:F:212:ASP:CG    | 2.48                     | 0.52              |
| 1:E:373:SER:HB3  | 1:E:433:LEU:CG    | 2.40                     | 0.52              |
| 1:F:548:LYS:HZ2  | 1:F:601:GLN:H     | 1.54                     | 0.52              |
| 1:G:117:ASN:O    | 1:G:118:GLN:C     | 2.53                     | 0.52              |
| 1:G:625:LEU:HD22 | 1:G:629:GLN:HA    | 1.92                     | 0.52              |
| 1:G:836:VAL:HG21 | 1:G:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:H:1086:LYS:O   | 1:H:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:J:63:TRP:CZ3   | 1:J:126:SER:HB2   | 2.45                     | 0.52              |
| 1:J:373:SER:HB3  | 1:J:433:LEU:CG    | 2.40                     | 0.52              |
| 1:L:467:PHE:HD1  | 1:L:471:ILE:HD12  | 1.75                     | 0.52              |
| 1:L:604:ASN:HB3  | 1:L:929:VAL:HG12  | 1.90                     | 0.52              |
| 1:L:836:VAL:HG21 | 1:L:876:LEU:HD22  | 1.91                     | 0.52              |
| 1:M:492:LEU:HD11 | 1:M:561:LEU:CD2   | 2.40                     | 0.52              |
| 1:M:616:LEU:HD23 | 1:M:620:PHE:HB2   | 1.91                     | 0.52              |
| 1:N:386:LEU:HD21 | 1:N:390:TRP:HZ3   | 1.75                     | 0.52              |
| 1:N:661:ASN:OD1  | 1:N:662:GLN:N     | 2.43                     | 0.52              |
| 1:O:661:ASN:OD1  | 1:O:662:GLN:N     | 2.44                     | 0.52              |
| 1:O:1086:LYS:O   | 1:O:1087:ILE:HG13 | 2.09                     | 0.52              |
| 1:P:117:ASN:O    | 1:P:118:GLN:C     | 2.53                     | 0.52              |
| 1:P:373:SER:HB3  | 1:P:433:LEU:CG    | 2.40                     | 0.52              |
| 1:P:625:LEU:HD22 | 1:P:629:GLN:HA    | 1.92                     | 0.52              |
| 1:A:386:LEU:HD21 | 1:A:390:TRP:HZ3   | 1.76                     | 0.51              |
| 1:A:661:ASN:OD1  | 1:A:662:GLN:N     | 2.44                     | 0.51              |
| 1:A:1086:LYS:O   | 1:A:1087:ILE:HG13 | 2.09                     | 0.51              |
| 1:C:492:LEU:HD11 | 1:C:561:LEU:CD2   | 2.40                     | 0.51              |
| 1:C:616:LEU:HD23 | 1:C:620:PHE:HB2   | 1.91                     | 0.51              |
| 1:D:386:LEU:HD21 | 1:D:390:TRP:HZ3   | 1.75                     | 0.51              |
| 1:D:883:ILE:HA   | 1:D:898:VAL:HB    | 1.92                     | 0.51              |
| 1:G:368:MET:HA   | 1:G:390:TRP:HE1   | 1.73                     | 0.51              |
| 1:G:373:SER:HB3  | 1:G:433:LEU:CG    | 2.40                     | 0.51              |
| 1:G:661:ASN:OD1  | 1:G:662:GLN:N     | 2.44                     | 0.51              |
| 1:G:912:ASP:OD2  | 1:G:921:CYS:SG    | 2.68                     | 0.51              |
| 1:H:36:PRO:O     | 1:H:39:ILE:HG22   | 2.10                     | 0.51              |
| 1:H:631:LEU:HD22 | 1:H:680:LEU:HD22  | 1.91                     | 0.51              |
| 1:H:661:ASN:OD1  | 1:H:662:GLN:N     | 2.44                     | 0.51              |
| 1:I:36:PRO:O     | 1:I:39:ILE:HG22   | 2.10                     | 0.51              |
| 1:I:373:SER:HB3  | 1:I:433:LEU:CG    | 2.40                     | 0.51              |
| 1:I:375:PHE:CD2  | 1:I:381:ILE:HG12  | 2.45                     | 0.51              |
| 1:K:386:LEU:HD21 | 1:K:390:TRP:HZ3   | 1.76                     | 0.51              |
| 1:L:162:LEU:O    | 1:L:165:CYS:N     | 2.43                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:394:ILE:HD12 | 1:L:395:LYS:HE3   | 1.91                     | 0.51              |
| 1:M:63:TRP:CZ3   | 1:M:126:SER:HB2   | 2.45                     | 0.51              |
| 1:N:336:ALA:C    | 1:N:338:TRP:H     | 2.18                     | 0.51              |
| 1:O:36:PRO:O     | 1:O:39:ILE:HG22   | 2.10                     | 0.51              |
| 1:O:365:TYR:O    | 1:O:368:MET:N     | 2.21                     | 0.51              |
| 1:P:661:ASN:OD1  | 1:P:662:GLN:N     | 2.43                     | 0.51              |
| 1:P:912:ASP:OD2  | 1:P:921:CYS:SG    | 2.68                     | 0.51              |
| 1:A:557:LYS:HZ2  | 1:A:1223:GLN:HG3  | 1.74                     | 0.51              |
| 1:A:557:LYS:CB   | 1:A:1226:TYR:CE1  | 2.87                     | 0.51              |
| 1:B:488:ARG:HA   | 1:B:491:PHE:H     | 1.75                     | 0.51              |
| 1:B:625:LEU:HD22 | 1:B:629:GLN:HA    | 1.92                     | 0.51              |
| 1:B:661:ASN:OD1  | 1:B:662:GLN:N     | 2.44                     | 0.51              |
| 1:B:994:HIS:HE1  | 1:B:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:C:115:ASN:HB3  | 1:D:257:ASN:HD21  | 1.75                     | 0.51              |
| 1:C:488:ARG:HA   | 1:C:491:PHE:H     | 1.75                     | 0.51              |
| 1:D:286:ASP:OD1  | 1:D:287:HIS:N     | 2.44                     | 0.51              |
| 1:D:661:ASN:OD1  | 1:D:662:GLN:N     | 2.43                     | 0.51              |
| 1:D:994:HIS:HE1  | 1:D:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:F:373:SER:HB3  | 1:F:433:LEU:CG    | 2.40                     | 0.51              |
| 1:F:480:HIS:HB2  | 1:F:481:PRO:HD3   | 1.92                     | 0.51              |
| 1:G:479:GLU:HB3  | 1:G:482:GLU:HB3   | 1.92                     | 0.51              |
| 1:H:836:VAL:HG21 | 1:H:876:LEU:HD22  | 1.91                     | 0.51              |
| 1:I:63:TRP:CZ3   | 1:I:126:SER:HB2   | 2.45                     | 0.51              |
| 1:I:336:ALA:C    | 1:I:338:TRP:H     | 2.18                     | 0.51              |
| 1:I:557:LYS:CB   | 1:I:1226:TYR:CE1  | 2.87                     | 0.51              |
| 1:I:994:HIS:HE1  | 1:I:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:J:117:ASN:O    | 1:J:118:GLN:C     | 2.53                     | 0.51              |
| 1:K:661:ASN:OD1  | 1:K:662:GLN:N     | 2.44                     | 0.51              |
| 1:L:434:GLU:C    | 1:L:436:GLU:H     | 2.18                     | 0.51              |
| 1:L:553:LEU:HB3  | 1:L:556:SER:HG    | 1.76                     | 0.51              |
| 1:M:373:SER:HB3  | 1:M:433:LEU:CG    | 2.40                     | 0.51              |
| 1:M:625:LEU:HD22 | 1:M:629:GLN:HA    | 1.92                     | 0.51              |
| 1:M:661:ASN:OD1  | 1:M:662:GLN:N     | 2.43                     | 0.51              |
| 1:N:631:LEU:H    | 1:N:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:O:120:PHE:HZ   | 1:O:162:LEU:HB2   | 1.73                     | 0.51              |
| 1:O:631:LEU:HD22 | 1:O:680:LEU:HD22  | 1.91                     | 0.51              |
| 1:O:836:VAL:HG21 | 1:O:876:LEU:HD22  | 1.91                     | 0.51              |
| 1:B:63:TRP:CZ3   | 1:B:126:SER:HB2   | 2.45                     | 0.51              |
| 1:B:117:ASN:O    | 1:B:118:GLN:C     | 2.53                     | 0.51              |
| 1:B:375:PHE:CD2  | 1:B:381:ILE:HG12  | 2.45                     | 0.51              |
| 1:B:434:GLU:C    | 1:B:436:GLU:H     | 2.18                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:479:GLU:HB3  | 1:C:482:GLU:HB3   | 1.92                     | 0.51              |
| 1:C:553:LEU:HB3  | 1:C:556:SER:HG    | 1.76                     | 0.51              |
| 1:C:625:LEU:HD22 | 1:C:629:GLN:HA    | 1.92                     | 0.51              |
| 1:E:117:ASN:O    | 1:E:118:GLN:C     | 2.53                     | 0.51              |
| 1:E:631:LEU:H    | 1:E:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:E:994:HIS:HE1  | 1:E:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:F:63:TRP:CZ3   | 1:F:126:SER:HB2   | 2.45                     | 0.51              |
| 1:F:368:MET:HA   | 1:F:390:TRP:HE1   | 1.73                     | 0.51              |
| 1:G:431:VAL:HB   | 1:G:432:LYS:HB2   | 1.93                     | 0.51              |
| 1:H:183:LEU:HD11 | 1:H:256:PHE:HE2   | 1.75                     | 0.51              |
| 1:I:368:MET:HA   | 1:I:390:TRP:HE1   | 1.73                     | 0.51              |
| 1:I:553:LEU:HB3  | 1:I:556:SER:HG    | 1.76                     | 0.51              |
| 1:I:631:LEU:H    | 1:I:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:K:286:ASP:OD1  | 1:K:287:HIS:N     | 2.44                     | 0.51              |
| 1:K:386:LEU:HD12 | 1:K:420:ILE:HD13  | 1.90                     | 0.51              |
| 1:K:434:GLU:C    | 1:K:436:GLU:H     | 2.18                     | 0.51              |
| 1:K:743:ILE:HG22 | 1:K:762:LYS:HA    | 1.91                     | 0.51              |
| 1:K:994:HIS:HE1  | 1:K:1023:ILE:HG23 | 1.76                     | 0.51              |
| 1:L:63:TRP:CZ3   | 1:L:126:SER:HB2   | 2.45                     | 0.51              |
| 1:L:492:LEU:HD11 | 1:L:561:LEU:CD2   | 2.40                     | 0.51              |
| 1:L:625:LEU:HD22 | 1:L:629:GLN:HA    | 1.92                     | 0.51              |
| 1:L:631:LEU:H    | 1:L:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:L:912:ASP:OD2  | 1:L:921:CYS:SG    | 2.68                     | 0.51              |
| 1:M:375:PHE:CD2  | 1:M:381:ILE:HG12  | 2.45                     | 0.51              |
| 1:M:450:PRO:HG2  | 1:M:471:ILE:HD11  | 1.90                     | 0.51              |
| 1:M:488:ARG:HA   | 1:M:491:PHE:H     | 1.75                     | 0.51              |
| 1:M:994:HIS:HE1  | 1:M:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:N:36:PRO:O     | 1:N:39:ILE:HG22   | 2.10                     | 0.51              |
| 1:O:183:LEU:HD11 | 1:O:256:PHE:HE2   | 1.75                     | 0.51              |
| 1:O:625:LEU:HD22 | 1:O:629:GLN:HA    | 1.92                     | 0.51              |
| 1:P:375:PHE:CD2  | 1:P:381:ILE:HG12  | 2.45                     | 0.51              |
| 1:P:431:VAL:HB   | 1:P:432:LYS:HB2   | 1.93                     | 0.51              |
| 1:A:36:PRO:O     | 1:A:39:ILE:HG22   | 2.10                     | 0.51              |
| 1:A:117:ASN:O    | 1:A:118:GLN:C     | 2.53                     | 0.51              |
| 1:A:307:CYS:HB3  | 1:A:311:ASP:OD2   | 2.11                     | 0.51              |
| 1:A:631:LEU:H    | 1:A:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:A:994:HIS:HE1  | 1:A:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:B:336:ALA:C    | 1:B:338:TRP:H     | 2.17                     | 0.51              |
| 1:B:373:SER:HB3  | 1:B:433:LEU:CG    | 2.40                     | 0.51              |
| 1:B:450:PRO:HG2  | 1:B:471:ILE:HD11  | 1.90                     | 0.51              |
| 1:B:557:LYS:CB   | 1:B:1226:TYR:CE1  | 2.87                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:301:LEU:CD2  | 1:C:313:PRO:CG    | 2.87                     | 0.51              |
| 1:C:836:VAL:HG21 | 1:C:876:LEU:HD22  | 1.91                     | 0.51              |
| 1:C:912:ASP:OD2  | 1:C:921:CYS:SG    | 2.68                     | 0.51              |
| 1:D:386:LEU:HD12 | 1:D:420:ILE:HD13  | 1.90                     | 0.51              |
| 1:E:661:ASN:OD1  | 1:E:662:GLN:N     | 2.44                     | 0.51              |
| 1:F:314:ARG:C    | 1:F:315:GLU:CG    | 2.81                     | 0.51              |
| 1:F:336:ALA:C    | 1:F:338:TRP:H     | 2.18                     | 0.51              |
| 1:F:553:LEU:HB3  | 1:F:556:SER:HG    | 1.76                     | 0.51              |
| 1:F:631:LEU:H    | 1:F:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:G:307:CYS:HB3  | 1:G:311:ASP:OD2   | 2.11                     | 0.51              |
| 1:G:375:PHE:CD2  | 1:G:381:ILE:HG12  | 2.45                     | 0.51              |
| 1:H:120:PHE:HZ   | 1:H:162:LEU:HB2   | 1.73                     | 0.51              |
| 1:H:480:HIS:HB2  | 1:H:481:PRO:HD3   | 1.93                     | 0.51              |
| 1:H:625:LEU:HD22 | 1:H:629:GLN:HA    | 1.92                     | 0.51              |
| 1:I:253:TRP:CH2  | 1:I:262:ILE:HD11  | 2.46                     | 0.51              |
| 1:I:480:HIS:HB2  | 1:I:481:PRO:HD3   | 1.93                     | 0.51              |
| 1:I:492:LEU:HD11 | 1:I:561:LEU:CD2   | 2.40                     | 0.51              |
| 1:J:286:ASP:OD1  | 1:J:287:HIS:N     | 2.44                     | 0.51              |
| 1:J:467:PHE:HD1  | 1:J:471:ILE:HD12  | 1.75                     | 0.51              |
| 1:J:631:LEU:H    | 1:J:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:J:661:ASN:OD1  | 1:J:662:GLN:N     | 2.43                     | 0.51              |
| 1:J:994:HIS:HE1  | 1:J:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:M:117:ASN:O    | 1:M:118:GLN:C     | 2.53                     | 0.51              |
| 1:M:434:GLU:C    | 1:M:436:GLU:H     | 2.18                     | 0.51              |
| 1:M:557:LYS:CB   | 1:M:1226:TYR:CE1  | 2.87                     | 0.51              |
| 1:N:994:HIS:HE1  | 1:N:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:O:480:HIS:HB2  | 1:O:481:PRO:HD3   | 1.93                     | 0.51              |
| 1:O:638:GLU:OE1  | 1:O:640:GLU:N     | 2.42                     | 0.51              |
| 1:P:307:CYS:HB3  | 1:P:311:ASP:OD2   | 2.11                     | 0.51              |
| 1:P:434:GLU:C    | 1:P:436:GLU:H     | 2.18                     | 0.51              |
| 1:A:253:TRP:CH2  | 1:A:262:ILE:HD11  | 2.46                     | 0.51              |
| 1:B:162:LEU:O    | 1:B:165:CYS:N     | 2.43                     | 0.51              |
| 1:B:394:ILE:HD12 | 1:B:395:LYS:HE3   | 1.91                     | 0.51              |
| 1:B:397:ASP:O    | 1:B:401:VAL:N     | 2.28                     | 0.51              |
| 1:B:901:HIS:CG   | 1:B:902:ILE:H     | 2.29                     | 0.51              |
| 1:C:63:TRP:CZ3   | 1:C:126:SER:HB2   | 2.45                     | 0.51              |
| 1:C:307:CYS:HB3  | 1:C:311:ASP:OD2   | 2.11                     | 0.51              |
| 1:D:183:LEU:HD11 | 1:D:256:PHE:HE2   | 1.75                     | 0.51              |
| 1:D:373:SER:HB3  | 1:D:433:LEU:CG    | 2.40                     | 0.51              |
| 1:D:551:GLU:HB3  | 1:D:605:LEU:O     | 2.11                     | 0.51              |
| 1:D:743:ILE:HG22 | 1:D:762:LYS:HA    | 1.91                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:901:HIS:CG   | 1:D:902:ILE:H    | 2.29                     | 0.51              |
| 1:E:286:ASP:OD1  | 1:E:287:HIS:N    | 2.44                     | 0.51              |
| 1:F:317:LEU:C    | 1:F:318:THR:HG1  | 1.94                     | 0.51              |
| 1:F:467:PHE:HD1  | 1:F:471:ILE:HD12 | 1.75                     | 0.51              |
| 1:F:492:LEU:HD11 | 1:F:561:LEU:CD2  | 2.40                     | 0.51              |
| 1:G:901:HIS:CG   | 1:G:902:ILE:H    | 2.29                     | 0.51              |
| 1:H:253:TRP:CH2  | 1:H:262:ILE:HD11 | 2.46                     | 0.51              |
| 1:H:365:TYR:O    | 1:H:368:MET:N    | 2.21                     | 0.51              |
| 1:H:638:GLU:OE1  | 1:H:640:GLU:N    | 2.42                     | 0.51              |
| 1:I:467:PHE:HD1  | 1:I:471:ILE:HD12 | 1.75                     | 0.51              |
| 1:I:901:HIS:CG   | 1:I:902:ILE:H    | 2.29                     | 0.51              |
| 1:K:183:LEU:HD11 | 1:K:256:PHE:HE2  | 1.75                     | 0.51              |
| 1:K:551:GLU:HB3  | 1:K:605:LEU:O    | 2.11                     | 0.51              |
| 1:K:901:HIS:CG   | 1:K:902:ILE:H    | 2.29                     | 0.51              |
| 1:L:307:CYS:HB3  | 1:L:311:ASP:OD2  | 2.11                     | 0.51              |
| 1:M:162:LEU:O    | 1:M:165:CYS:N    | 2.43                     | 0.51              |
| 1:M:463:LEU:HD22 | 1:M:467:PHE:HD2  | 1.74                     | 0.51              |
| 1:M:901:HIS:CG   | 1:M:902:ILE:H    | 2.29                     | 0.51              |
| 1:N:117:ASN:O    | 1:N:118:GLN:C    | 2.53                     | 0.51              |
| 1:N:253:TRP:CH2  | 1:N:262:ILE:HD11 | 2.46                     | 0.51              |
| 1:N:307:CYS:HB3  | 1:N:311:ASP:OD2  | 2.11                     | 0.51              |
| 1:O:253:TRP:CH2  | 1:O:262:ILE:HD11 | 2.46                     | 0.51              |
| 1:P:479:GLU:HB3  | 1:P:482:GLU:HB3  | 1.92                     | 0.51              |
| 1:A:883:ILE:HA   | 1:A:898:VAL:HB   | 1.92                     | 0.51              |
| 1:B:120:PHE:HZ   | 1:B:162:LEU:HB2  | 1.73                     | 0.51              |
| 1:B:463:LEU:HD22 | 1:B:467:PHE:HD2  | 1.74                     | 0.51              |
| 1:B:836:VAL:HG21 | 1:B:876:LEU:HD22 | 1.91                     | 0.51              |
| 1:B:883:ILE:HA   | 1:B:898:VAL:HB   | 1.92                     | 0.51              |
| 1:C:286:ASP:OD1  | 1:C:287:HIS:N    | 2.44                     | 0.51              |
| 1:E:162:LEU:O    | 1:E:165:CYS:N    | 2.43                     | 0.51              |
| 1:E:467:PHE:HD1  | 1:E:471:ILE:HD12 | 1.75                     | 0.51              |
| 1:F:253:TRP:CH2  | 1:F:262:ILE:HD11 | 2.46                     | 0.51              |
| 1:F:386:LEU:HD21 | 1:F:390:TRP:HZ3  | 1.75                     | 0.51              |
| 1:F:458:LEU:CG   | 1:F:587:ARG:NH2  | 2.74                     | 0.51              |
| 1:F:557:LYS:CB   | 1:F:1226:TYR:CE1 | 2.87                     | 0.51              |
| 1:F:616:LEU:HD23 | 1:F:620:PHE:HB2  | 1.91                     | 0.51              |
| 1:F:901:HIS:CG   | 1:F:902:ILE:H    | 2.29                     | 0.51              |
| 1:F:916:LYS:HE3  | 1:G:1177:TYR:CE2 | 2.42                     | 0.51              |
| 1:G:63:TRP:CZ3   | 1:G:126:SER:HB2  | 2.45                     | 0.51              |
| 1:G:434:GLU:C    | 1:G:436:GLU:H    | 2.18                     | 0.51              |
| 1:G:541:ALA:O    | 1:G:544:ASP:N    | 2.30                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:631:LEU:H    | 1:G:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:G:638:GLU:OE1  | 1:G:640:GLU:N     | 2.42                     | 0.51              |
| 1:H:463:LEU:HD22 | 1:H:467:PHE:HD2   | 1.74                     | 0.51              |
| 1:H:553:LEU:HB3  | 1:H:556:SER:HG    | 1.75                     | 0.51              |
| 1:I:551:GLU:HB3  | 1:I:605:LEU:O     | 2.11                     | 0.51              |
| 1:J:162:LEU:O    | 1:J:165:CYS:N     | 2.43                     | 0.51              |
| 1:K:431:VAL:HB   | 1:K:432:LYS:HB2   | 1.93                     | 0.51              |
| 1:L:386:LEU:HD21 | 1:L:390:TRP:HZ3   | 1.75                     | 0.51              |
| 1:L:463:LEU:CD2  | 1:L:467:PHE:CD2   | 2.92                     | 0.51              |
| 1:L:488:ARG:HA   | 1:L:491:PHE:H     | 1.75                     | 0.51              |
| 1:M:336:ALA:C    | 1:M:338:TRP:H     | 2.17                     | 0.51              |
| 1:M:394:ILE:HD12 | 1:M:395:LYS:HE3   | 1.91                     | 0.51              |
| 1:N:557:LYS:CB   | 1:N:1226:TYR:CE1  | 2.87                     | 0.51              |
| 1:O:463:LEU:HD22 | 1:O:467:PHE:HD2   | 1.74                     | 0.51              |
| 1:P:467:PHE:HD1  | 1:P:471:ILE:HD12  | 1.75                     | 0.51              |
| 1:P:541:ALA:O    | 1:P:544:ASP:N     | 2.30                     | 0.51              |
| 1:P:638:GLU:OE1  | 1:P:640:GLU:N     | 2.42                     | 0.51              |
| 1:P:901:HIS:CG   | 1:P:902:ILE:H     | 2.29                     | 0.51              |
| 1:B:183:LEU:HD11 | 1:B:256:PHE:HE2   | 1.75                     | 0.51              |
| 1:D:63:TRP:CZ3   | 1:D:126:SER:HB2   | 2.45                     | 0.51              |
| 1:D:187:ASN:HA   | 1:D:249:ASN:ND2   | 2.23                     | 0.51              |
| 1:D:336:ALA:C    | 1:D:338:TRP:H     | 2.18                     | 0.51              |
| 1:E:479:GLU:HB3  | 1:E:482:GLU:HB3   | 1.92                     | 0.51              |
| 1:F:551:GLU:HB3  | 1:F:605:LEU:O     | 2.11                     | 0.51              |
| 1:F:994:HIS:HE1  | 1:F:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:G:253:TRP:CH2  | 1:G:262:ILE:HD11  | 2.46                     | 0.51              |
| 1:G:467:PHE:HD1  | 1:G:471:ILE:HD12  | 1.76                     | 0.51              |
| 1:H:336:ALA:C    | 1:H:338:TRP:H     | 2.17                     | 0.51              |
| 1:H:994:HIS:HE1  | 1:H:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:I:386:LEU:HD21 | 1:I:390:TRP:HZ3   | 1.76                     | 0.51              |
| 1:I:431:VAL:HB   | 1:I:432:LYS:HB2   | 1.93                     | 0.51              |
| 1:I:434:GLU:C    | 1:I:436:GLU:H     | 2.18                     | 0.51              |
| 1:I:458:LEU:CG   | 1:I:587:ARG:NH2   | 2.74                     | 0.51              |
| 1:J:313:PRO:HA   | 1:J:338:TRP:HH2   | 1.63                     | 0.51              |
| 1:J:322:ARG:C    | 1:J:324:LEU:H     | 2.19                     | 0.51              |
| 1:J:479:GLU:HB3  | 1:J:482:GLU:HB3   | 1.92                     | 0.51              |
| 1:K:63:TRP:CZ3   | 1:K:126:SER:HB2   | 2.45                     | 0.51              |
| 1:K:187:ASN:HA   | 1:K:249:ASN:ND2   | 2.23                     | 0.51              |
| 1:K:336:ALA:C    | 1:K:338:TRP:H     | 2.17                     | 0.51              |
| 1:K:373:SER:HB3  | 1:K:433:LEU:CG    | 2.40                     | 0.51              |
| 1:L:286:ASP:OD1  | 1:L:287:HIS:N     | 2.44                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:479:GLU:HB3  | 1:L:482:GLU:HB3   | 1.92                     | 0.51              |
| 1:L:661:ASN:OD1  | 1:L:662:GLN:N     | 2.44                     | 0.51              |
| 1:M:120:PHE:HZ   | 1:M:162:LEU:HB2   | 1.73                     | 0.51              |
| 1:M:183:LEU:HD11 | 1:M:256:PHE:HE2   | 1.75                     | 0.51              |
| 1:M:286:ASP:OD1  | 1:M:287:HIS:N     | 2.44                     | 0.51              |
| 1:M:397:ASP:O    | 1:M:401:VAL:N     | 2.28                     | 0.51              |
| 1:M:883:ILE:HA   | 1:M:898:VAL:HB    | 1.92                     | 0.51              |
| 1:N:883:ILE:HA   | 1:N:898:VAL:HB    | 1.92                     | 0.51              |
| 1:O:336:ALA:C    | 1:O:338:TRP:H     | 2.17                     | 0.51              |
| 1:O:553:LEU:HB3  | 1:O:556:SER:HG    | 1.76                     | 0.51              |
| 1:P:63:TRP:CZ3   | 1:P:126:SER:HB2   | 2.45                     | 0.51              |
| 1:P:253:TRP:CH2  | 1:P:262:ILE:HD11  | 2.46                     | 0.51              |
| 1:P:631:LEU:H    | 1:P:646:ARG:HB3   | 1.74                     | 0.51              |
| 1:A:551:GLU:HB3  | 1:A:605:LEU:O     | 2.11                     | 0.51              |
| 1:A:631:LEU:HD22 | 1:A:680:LEU:HD22  | 1.91                     | 0.51              |
| 1:B:286:ASP:OD1  | 1:B:287:HIS:N     | 2.44                     | 0.51              |
| 1:C:386:LEU:HD21 | 1:C:390:TRP:HZ3   | 1.76                     | 0.51              |
| 1:D:91:PRO:O     | 1:D:94:THR:OG1    | 2.21                     | 0.51              |
| 1:D:122:LYS:HG3  | 1:E:276:SER:OG    | 2.11                     | 0.51              |
| 1:D:162:LEU:O    | 1:D:165:CYS:N     | 2.43                     | 0.51              |
| 1:D:431:VAL:HB   | 1:D:432:LYS:HB2   | 1.93                     | 0.51              |
| 1:D:467:PHE:HD1  | 1:D:471:ILE:HD12  | 1.75                     | 0.51              |
| 1:D:916:LYS:HE2  | 1:E:1177:TYR:CE2  | 2.43                     | 0.51              |
| 1:E:180:TRP:C    | 1:E:181:LEU:HD12  | 2.36                     | 0.51              |
| 1:F:248:GLN:NE2  | 1:F:268:PHE:CZ    | 2.79                     | 0.51              |
| 1:G:183:LEU:HD11 | 1:G:256:PHE:HE2   | 1.75                     | 0.51              |
| 1:G:386:LEU:HD21 | 1:G:390:TRP:HZ3   | 1.76                     | 0.51              |
| 1:H:557:LYS:HZ2  | 1:H:1223:GLN:HG3  | 1.75                     | 0.51              |
| 1:H:1075:SER:OG  | 1:H:1094:ASP:O    | 2.29                     | 0.51              |
| 1:I:286:ASP:OD1  | 1:I:287:HIS:N     | 2.44                     | 0.51              |
| 1:I:661:ASN:OD1  | 1:I:662:GLN:N     | 2.43                     | 0.51              |
| 1:J:64:THR:O     | 1:J:67:SER:OG     | 2.27                     | 0.51              |
| 1:K:162:LEU:O    | 1:K:165:CYS:N     | 2.43                     | 0.51              |
| 1:M:253:TRP:CH2  | 1:M:262:ILE:HD11  | 2.46                     | 0.51              |
| 1:M:836:VAL:HG21 | 1:M:876:LEU:HD22  | 1.91                     | 0.51              |
| 1:N:551:GLU:HB3  | 1:N:605:LEU:O     | 2.11                     | 0.51              |
| 1:N:631:LEU:HD22 | 1:N:680:LEU:HD22  | 1.91                     | 0.51              |
| 1:O:994:HIS:HE1  | 1:O:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:O:1075:SER:OG  | 1:O:1094:ASP:O    | 2.29                     | 0.51              |
| 1:A:375:PHE:CD2  | 1:A:381:ILE:HG12  | 2.45                     | 0.51              |
| 1:C:336:ALA:C    | 1:C:338:TRP:H     | 2.18                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:661:ASN:OD1  | 1:C:662:GLN:N     | 2.44                     | 0.51              |
| 1:D:64:THR:O     | 1:D:67:SER:OG     | 2.27                     | 0.51              |
| 1:D:488:ARG:HA   | 1:D:491:PHE:H     | 1.75                     | 0.51              |
| 1:E:307:CYS:HB3  | 1:E:311:ASP:OD2   | 2.11                     | 0.51              |
| 1:E:322:ARG:C    | 1:E:324:LEU:H     | 2.19                     | 0.51              |
| 1:E:336:ALA:C    | 1:E:338:TRP:H     | 2.18                     | 0.51              |
| 1:E:431:VAL:HB   | 1:E:432:LYS:HB2   | 1.93                     | 0.51              |
| 1:G:248:GLN:NE2  | 1:G:268:PHE:CZ    | 2.79                     | 0.51              |
| 1:H:551:GLU:HB3  | 1:H:605:LEU:O     | 2.11                     | 0.51              |
| 1:I:248:GLN:NE2  | 1:I:268:PHE:CZ    | 2.79                     | 0.51              |
| 1:J:180:TRP:C    | 1:J:181:LEU:HD12  | 2.36                     | 0.51              |
| 1:K:91:PRO:O     | 1:K:94:THR:OG1    | 2.22                     | 0.51              |
| 1:K:488:ARG:HA   | 1:K:491:PHE:H     | 1.75                     | 0.51              |
| 1:L:994:HIS:HE1  | 1:L:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:N:375:PHE:CD2  | 1:N:381:ILE:HG12  | 2.45                     | 0.51              |
| 1:O:117:ASN:O    | 1:O:118:GLN:C     | 2.53                     | 0.51              |
| 1:O:467:PHE:HD1  | 1:O:471:ILE:HD12  | 1.75                     | 0.51              |
| 1:O:551:GLU:HB3  | 1:O:605:LEU:O     | 2.11                     | 0.51              |
| 1:P:183:LEU:HD11 | 1:P:256:PHE:HE2   | 1.75                     | 0.51              |
| 1:P:336:ALA:C    | 1:P:338:TRP:H     | 2.17                     | 0.51              |
| 1:P:386:LEU:HD21 | 1:P:390:TRP:HZ3   | 1.76                     | 0.51              |
| 1:B:253:TRP:CH2  | 1:B:262:ILE:HD11  | 2.46                     | 0.51              |
| 1:B:479:GLU:HB3  | 1:B:482:GLU:HB3   | 1.92                     | 0.51              |
| 1:C:463:LEU:CD2  | 1:C:467:PHE:CD2   | 2.92                     | 0.51              |
| 1:C:994:HIS:HE1  | 1:C:1023:ILE:HG23 | 1.75                     | 0.51              |
| 1:E:64:THR:O     | 1:E:67:SER:OG     | 2.27                     | 0.51              |
| 1:E:346:CYS:O    | 1:E:350:THR:N     | 2.25                     | 0.51              |
| 1:E:551:GLU:HB3  | 1:E:605:LEU:O     | 2.11                     | 0.51              |
| 1:E:883:ILE:HA   | 1:E:898:VAL:HB    | 1.92                     | 0.51              |
| 1:F:286:ASP:OD1  | 1:F:287:HIS:N     | 2.44                     | 0.51              |
| 1:F:431:VAL:HB   | 1:F:432:LYS:HB2   | 1.93                     | 0.51              |
| 1:F:518:LEU:HD22 | 1:F:643:TYR:CE1   | 2.22                     | 0.51              |
| 1:F:661:ASN:OD1  | 1:F:662:GLN:N     | 2.44                     | 0.51              |
| 1:F:901:HIS:CD2  | 1:F:902:ILE:H     | 2.29                     | 0.51              |
| 1:G:180:TRP:C    | 1:G:181:LEU:HD12  | 2.36                     | 0.51              |
| 1:G:336:ALA:C    | 1:G:338:TRP:H     | 2.17                     | 0.51              |
| 1:G:492:LEU:HD11 | 1:G:561:LEU:CD2   | 2.40                     | 0.51              |
| 1:H:705:PHE:HB3  | 1:H:706:ILE:HD12  | 1.93                     | 0.51              |
| 1:I:479:GLU:HB3  | 1:I:482:GLU:HB3   | 1.92                     | 0.51              |
| 1:I:616:LEU:HD23 | 1:I:620:PHE:HB2   | 1.91                     | 0.51              |
| 1:I:901:HIS:CD2  | 1:I:902:ILE:H     | 2.29                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:307:CYS:HB3  | 1:J:311:ASP:OD2  | 2.11                     | 0.51              |
| 1:J:386:LEU:HD21 | 1:J:390:TRP:HZ3  | 1.75                     | 0.51              |
| 1:J:431:VAL:HB   | 1:J:432:LYS:HB2  | 1.93                     | 0.51              |
| 1:J:539:VAL:O    | 1:J:543:LEU:HG   | 2.11                     | 0.51              |
| 1:J:551:GLU:HB3  | 1:J:605:LEU:O    | 2.11                     | 0.51              |
| 1:K:467:PHE:HD1  | 1:K:471:ILE:HD12 | 1.75                     | 0.51              |
| 1:L:336:ALA:C    | 1:L:338:TRP:H    | 2.17                     | 0.51              |
| 1:M:479:GLU:HB3  | 1:M:482:GLU:HB3  | 1.92                     | 0.51              |
| 1:N:286:ASP:OD1  | 1:N:287:HIS:N    | 2.44                     | 0.51              |
| 1:O:180:TRP:C    | 1:O:181:LEU:HD12 | 2.36                     | 0.51              |
| 1:O:386:LEU:HD21 | 1:O:390:TRP:HZ3  | 1.75                     | 0.51              |
| 1:P:180:TRP:C    | 1:P:181:LEU:HD12 | 2.36                     | 0.51              |
| 1:P:187:ASN:HA   | 1:P:249:ASN:ND2  | 2.23                     | 0.51              |
| 1:P:248:GLN:NE2  | 1:P:268:PHE:CZ   | 2.79                     | 0.51              |
| 1:P:492:LEU:HD11 | 1:P:561:LEU:CD2  | 2.40                     | 0.51              |
| 1:A:63:TRP:CZ3   | 1:A:126:SER:HB2  | 2.45                     | 0.50              |
| 1:A:480:HIS:HB2  | 1:A:481:PRO:HD3  | 1.93                     | 0.50              |
| 1:A:539:VAL:O    | 1:A:543:LEU:HG   | 2.12                     | 0.50              |
| 1:B:301:LEU:CD2  | 1:B:313:PRO:CG   | 2.87                     | 0.50              |
| 1:B:307:CYS:HB3  | 1:B:311:ASP:OD2  | 2.11                     | 0.50              |
| 1:C:183:LEU:HD11 | 1:C:256:PHE:HE2  | 1.75                     | 0.50              |
| 1:E:248:GLN:NE2  | 1:E:268:PHE:CZ   | 2.79                     | 0.50              |
| 1:E:386:LEU:HD21 | 1:E:390:TRP:HZ3  | 1.76                     | 0.50              |
| 1:E:539:VAL:O    | 1:E:543:LEU:HG   | 2.12                     | 0.50              |
| 1:F:539:VAL:O    | 1:F:543:LEU:HG   | 2.12                     | 0.50              |
| 1:G:187:ASN:HA   | 1:G:249:ASN:ND2  | 2.23                     | 0.50              |
| 1:H:117:ASN:O    | 1:H:118:GLN:C    | 2.53                     | 0.50              |
| 1:H:286:ASP:OD1  | 1:H:287:HIS:N    | 2.44                     | 0.50              |
| 1:H:488:ARG:HA   | 1:H:491:PHE:H    | 1.75                     | 0.50              |
| 1:H:883:ILE:HA   | 1:H:898:VAL:HB   | 1.92                     | 0.50              |
| 1:I:378:SER:H    | 1:I:422:ILE:HD13 | 1.62                     | 0.50              |
| 1:I:539:VAL:O    | 1:I:543:LEU:HG   | 2.11                     | 0.50              |
| 1:J:336:ALA:C    | 1:J:338:TRP:H    | 2.18                     | 0.50              |
| 1:K:322:ARG:C    | 1:K:324:LEU:H    | 2.19                     | 0.50              |
| 1:L:183:LEU:HD11 | 1:L:256:PHE:HE2  | 1.75                     | 0.50              |
| 1:N:539:VAL:O    | 1:N:543:LEU:HG   | 2.11                     | 0.50              |
| 1:O:479:GLU:HB3  | 1:O:482:GLU:HB3  | 1.92                     | 0.50              |
| 1:O:488:ARG:HA   | 1:O:491:PHE:H    | 1.75                     | 0.50              |
| 1:O:705:PHE:HB3  | 1:O:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:O:883:ILE:HA   | 1:O:898:VAL:HB   | 1.92                     | 0.50              |
| 1:P:921:CYS:HA   | 1:P:930:HIS:O    | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:994:HIS:HE1   | 1:P:1023:ILE:HG23 | 1.75                     | 0.50              |
| 1:A:286:ASP:OD1   | 1:A:287:HIS:N     | 2.44                     | 0.50              |
| 1:A:479:GLU:HB3   | 1:A:482:GLU:HB3   | 1.92                     | 0.50              |
| 1:B:386:LEU:HD21  | 1:B:390:TRP:HZ3   | 1.75                     | 0.50              |
| 1:C:117:ASN:O     | 1:C:118:GLN:C     | 2.53                     | 0.50              |
| 1:D:322:ARG:C     | 1:D:324:LEU:H     | 2.19                     | 0.50              |
| 1:D:458:LEU:CG    | 1:D:587:ARG:NH2   | 2.74                     | 0.50              |
| 1:D:479:GLU:HB3   | 1:D:482:GLU:HB3   | 1.92                     | 0.50              |
| 1:D:631:LEU:H     | 1:D:646:ARG:HB3   | 1.74                     | 0.50              |
| 1:E:14:ASP:OD2    | 1:F:142:ARG:NH1   | 2.44                     | 0.50              |
| 1:E:488:ARG:HA    | 1:E:491:PHE:H     | 1.75                     | 0.50              |
| 1:F:705:PHE:HB3   | 1:F:706:ILE:HD12  | 1.94                     | 0.50              |
| 1:G:994:HIS:HE1   | 1:G:1023:ILE:HG23 | 1.75                     | 0.50              |
| 1:H:180:TRP:C     | 1:H:181:LEU:HD12  | 2.36                     | 0.50              |
| 1:H:386:LEU:HD21  | 1:H:390:TRP:HZ3   | 1.75                     | 0.50              |
| 1:H:467:PHE:HD1   | 1:H:471:ILE:HD12  | 1.75                     | 0.50              |
| 1:H:539:VAL:O     | 1:H:543:LEU:HG    | 2.11                     | 0.50              |
| 1:H:901:HIS:CG    | 1:H:902:ILE:H     | 2.29                     | 0.50              |
| 1:I:322:ARG:C     | 1:I:324:LEU:H     | 2.19                     | 0.50              |
| 1:I:488:ARG:HA    | 1:I:491:PHE:H     | 1.75                     | 0.50              |
| 1:J:248:GLN:NE2   | 1:J:268:PHE:CZ    | 2.79                     | 0.50              |
| 1:J:488:ARG:HA    | 1:J:491:PHE:H     | 1.75                     | 0.50              |
| 1:J:538:LEU:HD12  | 1:J:571:GLU:HG2   | 1.94                     | 0.50              |
| 1:K:307:CYS:HB3   | 1:K:311:ASP:OD2   | 2.11                     | 0.50              |
| 1:K:631:LEU:H     | 1:K:646:ARG:HB3   | 1.74                     | 0.50              |
| 1:K:921:CYS:HA    | 1:K:930:HIS:O     | 2.11                     | 0.50              |
| 1:L:253:TRP:CH2   | 1:L:262:ILE:HD11  | 2.46                     | 0.50              |
| 1:M:301:LEU:CD2   | 1:M:313:PRO:CG    | 2.87                     | 0.50              |
| 1:M:307:CYS:HB3   | 1:M:311:ASP:OD2   | 2.11                     | 0.50              |
| 1:N:63:TRP:CZ3    | 1:N:126:SER:HB2   | 2.45                     | 0.50              |
| 1:N:479:GLU:HB3   | 1:N:482:GLU:HB3   | 1.92                     | 0.50              |
| 1:N:1192:SER:OG   | 1:N:1208:GLU:OE2  | 2.28                     | 0.50              |
| 1:O:286:ASP:OD1   | 1:O:287:HIS:N     | 2.44                     | 0.50              |
| 1:O:1058:ILE:HG13 | 1:O:1059:ASP:N    | 2.27                     | 0.50              |
| 1:A:99:PRO:HB2    | 1:A:104:ARG:HG3   | 1.93                     | 0.50              |
| 1:B:557:LYS:HZ2   | 1:B:1223:GLN:HG3  | 1.75                     | 0.50              |
| 1:C:463:LEU:HD22  | 1:C:467:PHE:HD2   | 1.74                     | 0.50              |
| 1:D:180:TRP:C     | 1:D:181:LEU:HD12  | 2.36                     | 0.50              |
| 1:D:253:TRP:CH2   | 1:D:262:ILE:HD11  | 2.46                     | 0.50              |
| 1:D:307:CYS:HB3   | 1:D:311:ASP:OD2   | 2.11                     | 0.50              |
| 1:E:313:PRO:HA    | 1:E:338:TRP:HH2   | 1.63                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:538:LEU:HD12  | 1:E:571:GLU:HG2  | 1.94                     | 0.50              |
| 1:F:488:ARG:HA    | 1:F:491:PHE:H    | 1.75                     | 0.50              |
| 1:G:921:CYS:HA    | 1:G:930:HIS:O    | 2.11                     | 0.50              |
| 1:H:373:SER:HB3   | 1:H:433:LEU:CG   | 2.40                     | 0.50              |
| 1:H:479:GLU:HB3   | 1:H:482:GLU:HB3  | 1.92                     | 0.50              |
| 1:H:538:LEU:HD12  | 1:H:571:GLU:HG2  | 1.94                     | 0.50              |
| 1:H:1058:ILE:HG13 | 1:H:1059:ASP:N   | 2.27                     | 0.50              |
| 1:I:705:PHE:HB3   | 1:I:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:J:883:ILE:HA    | 1:J:898:VAL:HB   | 1.92                     | 0.50              |
| 1:K:180:TRP:C     | 1:K:181:LEU:HD12 | 2.36                     | 0.50              |
| 1:K:458:LEU:CG    | 1:K:587:ARG:NH2  | 2.74                     | 0.50              |
| 1:K:479:GLU:HB3   | 1:K:482:GLU:HB3  | 1.92                     | 0.50              |
| 1:N:180:TRP:C     | 1:N:181:LEU:HD12 | 2.36                     | 0.50              |
| 1:N:480:HIS:HB2   | 1:N:481:PRO:HD3  | 1.93                     | 0.50              |
| 1:O:492:LEU:HD11  | 1:O:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:O:538:LEU:HD12  | 1:O:571:GLU:HG2  | 1.94                     | 0.50              |
| 1:O:539:VAL:O     | 1:O:543:LEU:HG   | 2.12                     | 0.50              |
| 1:O:901:HIS:CG    | 1:O:902:ILE:H    | 2.29                     | 0.50              |
| 1:A:222:HIS:CG    | 1:H:198:LYS:HZ1  | 2.29                     | 0.50              |
| 1:A:222:HIS:CG    | 1:H:198:LYS:NZ   | 2.79                     | 0.50              |
| 1:A:553:LEU:HB3   | 1:A:556:SER:HG   | 1.76                     | 0.50              |
| 1:A:916:LYS:CE    | 1:B:1177:TYR:CE2 | 2.93                     | 0.50              |
| 1:B:551:GLU:HB3   | 1:B:605:LEU:O    | 2.11                     | 0.50              |
| 1:C:434:GLU:C     | 1:C:436:GLU:H    | 2.18                     | 0.50              |
| 1:C:551:GLU:HB3   | 1:C:605:LEU:O    | 2.11                     | 0.50              |
| 1:D:921:CYS:HA    | 1:D:930:HIS:O    | 2.11                     | 0.50              |
| 1:F:322:ARG:C     | 1:F:324:LEU:H    | 2.19                     | 0.50              |
| 1:F:434:GLU:C     | 1:F:436:GLU:H    | 2.18                     | 0.50              |
| 1:G:286:ASP:OD1   | 1:G:287:HIS:N    | 2.44                     | 0.50              |
| 1:G:539:VAL:O     | 1:G:543:LEU:HG   | 2.12                     | 0.50              |
| 1:H:492:LEU:HD11  | 1:H:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:I:64:THR:O      | 1:I:67:SER:OG    | 2.27                     | 0.50              |
| 1:I:518:LEU:HD22  | 1:I:643:TYR:CE1  | 2.22                     | 0.50              |
| 1:K:253:TRP:CH2   | 1:K:262:ILE:HD11 | 2.46                     | 0.50              |
| 1:K:492:LEU:HD11  | 1:K:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:M:386:LEU:HD21  | 1:M:390:TRP:HZ3  | 1.75                     | 0.50              |
| 1:M:551:GLU:HB3   | 1:M:605:LEU:O    | 2.11                     | 0.50              |
| 1:N:99:PRO:HB2    | 1:N:104:ARG:HG3  | 1.93                     | 0.50              |
| 1:N:313:PRO:HA    | 1:N:338:TRP:HH2  | 1.63                     | 0.50              |
| 1:N:553:LEU:HB3   | 1:N:556:SER:HG   | 1.75                     | 0.50              |
| 1:O:307:CYS:HB3   | 1:O:311:ASP:OD2  | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:O:373:SER:HB3   | 1:O:433:LEU:CG   | 2.40                     | 0.50              |
| 1:P:1240:LEU:HD12 | 1:P:1250:SER:HB2 | 1.93                     | 0.50              |
| 1:A:152:VAL:O     | 1:A:155:SER:OG   | 2.29                     | 0.50              |
| 1:A:313:PRO:HA    | 1:A:338:TRP:HH2  | 1.63                     | 0.50              |
| 1:A:901:HIS:CD2   | 1:A:902:ILE:H    | 2.29                     | 0.50              |
| 1:A:1192:SER:OG   | 1:A:1208:GLU:OE2 | 2.28                     | 0.50              |
| 1:B:467:PHE:HD1   | 1:B:471:ILE:HD12 | 1.75                     | 0.50              |
| 1:B:638:GLU:OE1   | 1:B:640:GLU:N    | 2.42                     | 0.50              |
| 1:C:478:ILE:HG22  | 1:C:479:GLU:H    | 1.77                     | 0.50              |
| 1:C:883:ILE:HA    | 1:C:898:VAL:HB   | 1.92                     | 0.50              |
| 1:D:478:ILE:HG22  | 1:D:479:GLU:H    | 1.77                     | 0.50              |
| 1:D:492:LEU:HD11  | 1:D:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:D:1058:ILE:HG13 | 1:D:1059:ASP:N   | 2.27                     | 0.50              |
| 1:E:705:PHE:HB3   | 1:E:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:E:901:HIS:CD2   | 1:E:902:ILE:H    | 2.29                     | 0.50              |
| 1:E:901:HIS:CG    | 1:E:902:ILE:H    | 2.29                     | 0.50              |
| 1:F:180:TRP:C     | 1:F:181:LEU:HD12 | 2.36                     | 0.50              |
| 1:F:479:GLU:HB3   | 1:F:482:GLU:HB3  | 1.92                     | 0.50              |
| 1:F:538:LEU:HD12  | 1:F:571:GLU:HG2  | 1.94                     | 0.50              |
| 1:F:1240:LEU:HD12 | 1:F:1250:SER:HB2 | 1.93                     | 0.50              |
| 1:G:538:LEU:HG    | 1:G:571:GLU:CG   | 2.42                     | 0.50              |
| 1:H:307:CYS:HB3   | 1:H:311:ASP:OD2  | 2.11                     | 0.50              |
| 1:H:478:ILE:HG22  | 1:H:479:GLU:H    | 1.77                     | 0.50              |
| 1:H:557:LYS:CB    | 1:H:1226:TYR:CE1 | 2.87                     | 0.50              |
| 1:H:901:HIS:CD2   | 1:H:902:ILE:H    | 2.29                     | 0.50              |
| 1:I:317:LEU:C     | 1:I:318:THR:HG1  | 1.95                     | 0.50              |
| 1:J:492:LEU:HD11  | 1:J:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:J:705:PHE:HB3   | 1:J:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:K:478:ILE:HG22  | 1:K:479:GLU:H    | 1.77                     | 0.50              |
| 1:K:1075:SER:OG   | 1:K:1094:ASP:O   | 2.29                     | 0.50              |
| 1:L:478:ILE:HG22  | 1:L:479:GLU:H    | 1.77                     | 0.50              |
| 1:L:1058:ILE:HG13 | 1:L:1059:ASP:N   | 2.27                     | 0.50              |
| 1:M:91:PRO:O      | 1:M:94:THR:OG1   | 2.22                     | 0.50              |
| 1:M:467:PHE:HD1   | 1:M:471:ILE:HD12 | 1.75                     | 0.50              |
| 1:N:901:HIS:CD2   | 1:N:902:ILE:H    | 2.29                     | 0.50              |
| 1:O:478:ILE:HG22  | 1:O:479:GLU:H    | 1.77                     | 0.50              |
| 1:P:286:ASP:OD1   | 1:P:287:HIS:N    | 2.44                     | 0.50              |
| 1:P:539:VAL:O     | 1:P:543:LEU:HG   | 2.12                     | 0.50              |
| 1:P:551:GLU:HB3   | 1:P:605:LEU:O    | 2.11                     | 0.50              |
| 1:P:883:ILE:HA    | 1:P:898:VAL:HB   | 1.92                     | 0.50              |
| 1:A:180:TRP:C     | 1:A:181:LEU:HD12 | 2.36                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:431:VAL:HB    | 1:A:432:LYS:HB2  | 1.93                     | 0.50              |
| 1:A:488:ARG:HA    | 1:A:491:PHE:H    | 1.75                     | 0.50              |
| 1:A:538:LEU:HD12  | 1:A:571:GLU:HG2  | 1.94                     | 0.50              |
| 1:B:91:PRO:O      | 1:B:94:THR:OG1   | 2.22                     | 0.50              |
| 1:B:99:PRO:HB2    | 1:B:104:ARG:HG3  | 1.93                     | 0.50              |
| 1:C:253:TRP:CH2   | 1:C:262:ILE:HD11 | 2.46                     | 0.50              |
| 1:C:1058:ILE:HG13 | 1:C:1059:ASP:N   | 2.27                     | 0.50              |
| 1:D:275:LEU:HD23  | 1:D:280:THR:HG21 | 1.93                     | 0.50              |
| 1:E:99:PRO:HB2    | 1:E:104:ARG:HG3  | 1.93                     | 0.50              |
| 1:E:114:TYR:O     | 1:E:117:ASN:N    | 2.36                     | 0.50              |
| 1:E:538:LEU:HG    | 1:E:571:GLU:CG   | 2.42                     | 0.50              |
| 1:G:480:HIS:HB2   | 1:G:481:PRO:HD3  | 1.92                     | 0.50              |
| 1:G:551:GLU:HB3   | 1:G:605:LEU:O    | 2.11                     | 0.50              |
| 1:G:883:ILE:HA    | 1:G:898:VAL:HB   | 1.92                     | 0.50              |
| 1:G:1240:LEU:HD12 | 1:G:1250:SER:HB2 | 1.93                     | 0.50              |
| 1:H:248:GLN:NE2   | 1:H:268:PHE:CZ   | 2.79                     | 0.50              |
| 1:H:322:ARG:C     | 1:H:324:LEU:H    | 2.19                     | 0.50              |
| 1:I:117:ASN:O     | 1:I:118:GLN:C    | 2.53                     | 0.50              |
| 1:I:231:LEU:O     | 1:I:234:SER:OG   | 2.26                     | 0.50              |
| 1:I:478:ILE:HG22  | 1:I:479:GLU:H    | 1.77                     | 0.50              |
| 1:I:496:PHE:HE2   | 1:I:555:CYS:HG   | 1.55                     | 0.50              |
| 1:I:638:GLU:OE1   | 1:I:640:GLU:N    | 2.42                     | 0.50              |
| 1:J:114:TYR:O     | 1:J:117:ASN:N    | 2.36                     | 0.50              |
| 1:J:253:TRP:CH2   | 1:J:262:ILE:HD11 | 2.46                     | 0.50              |
| 1:J:901:HIS:CD2   | 1:J:902:ILE:H    | 2.29                     | 0.50              |
| 1:J:901:HIS:CG    | 1:J:902:ILE:H    | 2.29                     | 0.50              |
| 1:K:508:TRP:C     | 1:K:606:GLY:N    | 2.70                     | 0.50              |
| 1:K:553:LEU:HB3   | 1:K:556:SER:HG   | 1.75                     | 0.50              |
| 1:K:988:ASP:OD1   | 1:K:989:SER:N    | 2.43                     | 0.50              |
| 1:K:1058:ILE:HG13 | 1:K:1059:ASP:N   | 2.27                     | 0.50              |
| 1:L:551:GLU:HB3   | 1:L:605:LEU:O    | 2.11                     | 0.50              |
| 1:M:99:PRO:HB2    | 1:M:104:ARG:HG3  | 1.93                     | 0.50              |
| 1:M:480:HIS:HB2   | 1:M:481:PRO:HD3  | 1.93                     | 0.50              |
| 1:N:431:VAL:HB    | 1:N:432:LYS:HB2  | 1.93                     | 0.50              |
| 1:N:538:LEU:HD12  | 1:N:571:GLU:HG2  | 1.94                     | 0.50              |
| 1:N:921:CYS:HA    | 1:N:930:HIS:O    | 2.11                     | 0.50              |
| 1:O:248:GLN:NE2   | 1:O:268:PHE:CZ   | 2.79                     | 0.50              |
| 1:O:901:HIS:CD2   | 1:O:902:ILE:H    | 2.29                     | 0.50              |
| 1:P:538:LEU:HG    | 1:P:571:GLU:CG   | 2.42                     | 0.50              |
| 1:P:863:THR:HA    | 1:P:907:ILE:HG13 | 1.93                     | 0.50              |
| 1:A:322:ARG:C     | 1:A:324:LEU:H    | 2.19                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:458:LEU:HG    | 1:A:587:ARG:HH21 | 1.77                     | 0.50              |
| 1:B:180:TRP:C     | 1:B:181:LEU:HD12 | 2.36                     | 0.50              |
| 1:C:539:VAL:O     | 1:C:543:LEU:HG   | 2.12                     | 0.50              |
| 1:C:604:ASN:ND2   | 1:C:929:VAL:H    | 2.04                     | 0.50              |
| 1:C:863:THR:HA    | 1:C:907:ILE:HG13 | 1.94                     | 0.50              |
| 1:D:508:TRP:C     | 1:D:606:GLY:N    | 2.70                     | 0.50              |
| 1:D:988:ASP:OD1   | 1:D:989:SER:N    | 2.43                     | 0.50              |
| 1:E:492:LEU:HD11  | 1:E:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:G:863:THR:HA    | 1:G:907:ILE:HG13 | 1.94                     | 0.50              |
| 1:H:921:CYS:HA    | 1:H:930:HIS:O    | 2.11                     | 0.50              |
| 1:I:1240:LEU:HD12 | 1:I:1250:SER:HB2 | 1.93                     | 0.50              |
| 1:J:99:PRO:HB2    | 1:J:104:ARG:HG3  | 1.93                     | 0.50              |
| 1:J:538:LEU:HG    | 1:J:571:GLU:CG   | 2.42                     | 0.50              |
| 1:K:275:LEU:HD23  | 1:K:280:THR:HG21 | 1.93                     | 0.50              |
| 1:K:539:VAL:O     | 1:K:543:LEU:HG   | 2.11                     | 0.50              |
| 1:L:117:ASN:O     | 1:L:118:GLN:C    | 2.53                     | 0.50              |
| 1:M:322:ARG:C     | 1:M:324:LEU:H    | 2.19                     | 0.50              |
| 1:M:638:GLU:OE1   | 1:M:640:GLU:N    | 2.42                     | 0.50              |
| 1:M:1240:LEU:HD12 | 1:M:1250:SER:HB2 | 1.93                     | 0.50              |
| 1:N:458:LEU:HG    | 1:N:587:ARG:HH21 | 1.77                     | 0.50              |
| 1:O:382:PRO:HA    | 1:O:419:THR:CG2  | 2.36                     | 0.50              |
| 1:O:538:LEU:HD21  | 1:O:573:ILE:HD11 | 1.94                     | 0.50              |
| 1:O:548:LYS:HZ2   | 1:O:601:GLN:H    | 1.56                     | 0.50              |
| 1:P:705:PHE:HB3   | 1:P:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:A:492:LEU:HD11  | 1:A:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:A:921:CYS:HA    | 1:A:930:HIS:O    | 2.11                     | 0.50              |
| 1:B:248:GLN:NE2   | 1:B:268:PHE:CZ   | 2.79                     | 0.50              |
| 1:B:480:HIS:HB2   | 1:B:481:PRO:HD3  | 1.93                     | 0.50              |
| 1:B:518:LEU:HD12  | 1:B:518:LEU:N    | 2.20                     | 0.50              |
| 1:B:539:VAL:O     | 1:B:543:LEU:HG   | 2.12                     | 0.50              |
| 1:B:921:CYS:HA    | 1:B:930:HIS:O    | 2.11                     | 0.50              |
| 1:B:1058:ILE:HG13 | 1:B:1059:ASP:N   | 2.27                     | 0.50              |
| 1:B:1240:LEU:HD12 | 1:B:1250:SER:HB2 | 1.93                     | 0.50              |
| 1:C:901:HIS:CG    | 1:C:902:ILE:H    | 2.29                     | 0.50              |
| 1:D:20:GLU:O      | 1:D:23:PHE:N     | 2.45                     | 0.50              |
| 1:D:480:HIS:HB2   | 1:D:481:PRO:HD3  | 1.92                     | 0.50              |
| 1:D:553:LEU:HB3   | 1:D:556:SER:HG   | 1.75                     | 0.50              |
| 1:D:705:PHE:HB3   | 1:D:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:E:253:TRP:CH2   | 1:E:262:ILE:HD11 | 2.46                     | 0.50              |
| 1:E:507:ALA:N     | 1:E:608:ASN:HB2  | 2.27                     | 0.50              |
| 1:E:921:CYS:HA    | 1:E:930:HIS:O    | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:863:THR:HA    | 1:F:907:ILE:HG13 | 1.93                     | 0.50              |
| 1:G:705:PHE:HB3   | 1:G:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:G:901:HIS:CD2   | 1:G:902:ILE:H    | 2.29                     | 0.50              |
| 1:H:275:LEU:HD23  | 1:H:280:THR:HG21 | 1.94                     | 0.50              |
| 1:H:538:LEU:HD21  | 1:H:573:ILE:HD11 | 1.94                     | 0.50              |
| 1:I:99:PRO:HB2    | 1:I:104:ARG:HG3  | 1.93                     | 0.50              |
| 1:I:307:CYS:HB3   | 1:I:311:ASP:OD2  | 2.11                     | 0.50              |
| 1:J:20:GLU:O      | 1:J:23:PHE:N     | 2.45                     | 0.50              |
| 1:J:507:ALA:N     | 1:J:608:ASN:HB2  | 2.27                     | 0.50              |
| 1:J:921:CYS:HA    | 1:J:930:HIS:O    | 2.11                     | 0.50              |
| 1:J:1058:ILE:HG13 | 1:J:1059:ASP:N   | 2.27                     | 0.50              |
| 1:J:1192:SER:OG   | 1:J:1208:GLU:OE2 | 2.28                     | 0.50              |
| 1:K:480:HIS:HB2   | 1:K:481:PRO:HD3  | 1.92                     | 0.50              |
| 1:K:705:PHE:HB3   | 1:K:706:ILE:HD12 | 1.94                     | 0.50              |
| 1:K:1192:SER:OG   | 1:K:1208:GLU:OE2 | 2.28                     | 0.50              |
| 1:L:64:THR:O      | 1:L:67:SER:OG    | 2.27                     | 0.50              |
| 1:L:480:HIS:HB2   | 1:L:481:PRO:HD3  | 1.93                     | 0.50              |
| 1:M:180:TRP:C     | 1:M:181:LEU:HD12 | 2.36                     | 0.50              |
| 1:M:248:GLN:NE2   | 1:M:268:PHE:CZ   | 2.79                     | 0.50              |
| 1:M:458:LEU:HG    | 1:M:587:ARG:HH21 | 1.77                     | 0.50              |
| 1:M:539:VAL:O     | 1:M:543:LEU:HG   | 2.12                     | 0.50              |
| 1:M:1058:ILE:HG13 | 1:M:1059:ASP:N   | 2.27                     | 0.50              |
| 1:N:322:ARG:C     | 1:N:324:LEU:H    | 2.19                     | 0.50              |
| 1:N:488:ARG:HA    | 1:N:491:PHE:H    | 1.75                     | 0.50              |
| 1:N:492:LEU:HD11  | 1:N:561:LEU:CD2  | 2.40                     | 0.50              |
| 1:O:64:THR:O      | 1:O:67:SER:OG    | 2.27                     | 0.50              |
| 1:O:275:LEU:HD23  | 1:O:280:THR:HG21 | 1.94                     | 0.50              |
| 1:O:557:LYS:CB    | 1:O:1226:TYR:CE1 | 2.87                     | 0.50              |
| 1:O:921:CYS:HA    | 1:O:930:HIS:O    | 2.11                     | 0.50              |
| 1:P:480:HIS:HB2   | 1:P:481:PRO:HD3  | 1.93                     | 0.50              |
| 1:P:901:HIS:CD2   | 1:P:902:ILE:H    | 2.29                     | 0.50              |
| 1:A:275:LEU:HD23  | 1:A:280:THR:HG21 | 1.93                     | 0.50              |
| 1:A:1058:ILE:HG13 | 1:A:1059:ASP:N   | 2.27                     | 0.50              |
| 1:B:458:LEU:HG    | 1:B:587:ARG:HH21 | 1.77                     | 0.50              |
| 1:C:20:GLU:O      | 1:C:23:PHE:N     | 2.45                     | 0.50              |
| 1:C:480:HIS:HB2   | 1:C:481:PRO:HD3  | 1.93                     | 0.50              |
| 1:D:463:LEU:CD2   | 1:D:467:PHE:CD2  | 2.92                     | 0.50              |
| 1:D:539:VAL:O     | 1:D:543:LEU:HG   | 2.11                     | 0.50              |
| 1:D:541:ALA:O     | 1:D:544:ASP:N    | 2.30                     | 0.50              |
| 1:E:20:GLU:O      | 1:E:23:PHE:N     | 2.45                     | 0.50              |
| 1:E:541:ALA:O     | 1:E:544:ASP:N    | 2.30                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:1192:SER:OG   | 1:E:1208:GLU:OE2 | 2.28                     | 0.50              |
| 1:F:99:PRO:HB2    | 1:F:104:ARG:HG3  | 1.93                     | 0.50              |
| 1:F:651:SER:O     | 1:F:654:ILE:HG23 | 2.12                     | 0.50              |
| 1:G:1058:ILE:HG13 | 1:G:1059:ASP:N   | 2.27                     | 0.50              |
| 1:H:20:GLU:O      | 1:H:23:PHE:N     | 2.45                     | 0.50              |
| 1:H:382:PRO:HA    | 1:H:419:THR:CG2  | 2.36                     | 0.50              |
| 1:H:548:LYS:HZ2   | 1:H:601:GLN:H    | 1.56                     | 0.50              |
| 1:I:180:TRP:C     | 1:I:181:LEU:HD12 | 2.36                     | 0.50              |
| 1:I:538:LEU:HD12  | 1:I:571:GLU:HG2  | 1.94                     | 0.50              |
| 1:I:863:THR:HA    | 1:I:907:ILE:HG13 | 1.93                     | 0.50              |
| 1:J:541:ALA:O     | 1:J:544:ASP:N    | 2.30                     | 0.50              |
| 1:J:1240:LEU:HD12 | 1:J:1250:SER:HB2 | 1.93                     | 0.50              |
| 1:K:20:GLU:O      | 1:K:23:PHE:N     | 2.45                     | 0.50              |
| 1:K:117:ASN:O     | 1:K:118:GLN:C    | 2.53                     | 0.50              |
| 1:K:563:ARG:HH11  | 1:K:593:HIS:HA   | 1.77                     | 0.50              |
| 1:L:431:VAL:HB    | 1:L:432:LYS:HB2  | 1.93                     | 0.50              |
| 1:L:863:THR:HA    | 1:L:907:ILE:HG13 | 1.93                     | 0.50              |
| 1:L:883:ILE:HA    | 1:L:898:VAL:HB   | 1.92                     | 0.50              |
| 1:M:518:LEU:HD12  | 1:M:518:LEU:N    | 2.20                     | 0.50              |
| 1:M:553:LEU:HB3   | 1:M:556:SER:HG   | 1.76                     | 0.50              |
| 1:M:705:PHE:HB3   | 1:M:706:ILE:HD12 | 1.93                     | 0.50              |
| 1:M:901:HIS:CD2   | 1:M:902:ILE:H    | 2.29                     | 0.50              |
| 1:M:921:CYS:HA    | 1:M:930:HIS:O    | 2.11                     | 0.50              |
| 1:N:1058:ILE:HG13 | 1:N:1059:ASP:N   | 2.27                     | 0.50              |
| 1:O:20:GLU:O      | 1:O:23:PHE:N     | 2.45                     | 0.50              |
| 1:A:563:ARG:HH11  | 1:A:593:HIS:HA   | 1.77                     | 0.49              |
| 1:B:322:ARG:C     | 1:B:324:LEU:H    | 2.19                     | 0.49              |
| 1:B:538:LEU:HD12  | 1:B:571:GLU:HG2  | 1.94                     | 0.49              |
| 1:B:901:HIS:CD2   | 1:B:902:ILE:H    | 2.29                     | 0.49              |
| 1:C:180:TRP:C     | 1:C:181:LEU:HD12 | 2.36                     | 0.49              |
| 1:C:198:LYS:NZ    | 1:D:222:HIS:CG   | 2.80                     | 0.49              |
| 1:C:248:GLN:NE2   | 1:C:268:PHE:CZ   | 2.79                     | 0.49              |
| 1:D:117:ASN:O     | 1:D:118:GLN:C    | 2.53                     | 0.49              |
| 1:D:507:ALA:N     | 1:D:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:D:563:ARG:HH11  | 1:D:593:HIS:HA   | 1.78                     | 0.49              |
| 1:D:1192:SER:OG   | 1:D:1208:GLU:OE2 | 2.28                     | 0.49              |
| 1:E:478:ILE:HG22  | 1:E:479:GLU:H    | 1.77                     | 0.49              |
| 1:E:518:LEU:HD22  | 1:E:643:TYR:CE1  | 2.22                     | 0.49              |
| 1:E:563:ARG:HH11  | 1:E:593:HIS:HA   | 1.77                     | 0.49              |
| 1:E:1058:ILE:HG13 | 1:E:1059:ASP:N   | 2.27                     | 0.49              |
| 1:E:1240:LEU:HD12 | 1:E:1250:SER:HB2 | 1.93                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:307:CYS:HB3   | 1:F:311:ASP:OD2  | 2.11                     | 0.49              |
| 1:F:478:ILE:HG22  | 1:F:479:GLU:H    | 1.77                     | 0.49              |
| 1:F:538:LEU:HD21  | 1:F:573:ILE:HD11 | 1.94                     | 0.49              |
| 1:G:322:ARG:C     | 1:G:324:LEU:H    | 2.19                     | 0.49              |
| 1:H:64:THR:O      | 1:H:67:SER:OG    | 2.27                     | 0.49              |
| 1:I:20:GLU:O      | 1:I:23:PHE:N     | 2.45                     | 0.49              |
| 1:I:538:LEU:HD21  | 1:I:573:ILE:HD11 | 1.94                     | 0.49              |
| 1:I:651:SER:O     | 1:I:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:J:651:SER:O     | 1:J:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:K:248:GLN:NE2   | 1:K:268:PHE:CZ   | 2.79                     | 0.49              |
| 1:K:463:LEU:CD2   | 1:K:467:PHE:CD2  | 2.92                     | 0.49              |
| 1:K:538:LEU:HD12  | 1:K:571:GLU:HG2  | 1.93                     | 0.49              |
| 1:L:180:TRP:C     | 1:L:181:LEU:HD12 | 2.36                     | 0.49              |
| 1:L:322:ARG:C     | 1:L:324:LEU:H    | 2.19                     | 0.49              |
| 1:N:275:LEU:HD23  | 1:N:280:THR:HG21 | 1.94                     | 0.49              |
| 1:N:301:LEU:CD2   | 1:N:313:PRO:CG   | 2.87                     | 0.49              |
| 1:N:563:ARG:HH11  | 1:N:593:HIS:HA   | 1.77                     | 0.49              |
| 1:O:322:ARG:C     | 1:O:324:LEU:H    | 2.19                     | 0.49              |
| 1:O:431:VAL:HB    | 1:O:432:LYS:HB2  | 1.93                     | 0.49              |
| 1:O:507:ALA:N     | 1:O:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:P:275:LEU:HD23  | 1:P:280:THR:HG21 | 1.93                     | 0.49              |
| 1:P:322:ARG:C     | 1:P:324:LEU:H    | 2.19                     | 0.49              |
| 1:P:1058:ILE:HG13 | 1:P:1059:ASP:N   | 2.27                     | 0.49              |
| 1:A:508:TRP:C     | 1:A:606:GLY:N    | 2.70                     | 0.49              |
| 1:B:705:PHE:HB3   | 1:B:706:ILE:HD12 | 1.94                     | 0.49              |
| 1:C:518:LEU:HD12  | 1:C:518:LEU:N    | 2.20                     | 0.49              |
| 1:C:1240:LEU:HD12 | 1:C:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:D:99:PRO:HB2    | 1:D:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:D:248:GLN:NE2   | 1:D:268:PHE:CZ   | 2.79                     | 0.49              |
| 1:D:248:GLN:HE22  | 1:D:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:E:651:SER:O     | 1:E:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:E:863:THR:HA    | 1:E:907:ILE:HG13 | 1.93                     | 0.49              |
| 1:F:117:ASN:O     | 1:F:118:GLN:C    | 2.53                     | 0.49              |
| 1:F:248:GLN:HE22  | 1:F:268:PHE:HZ   | 1.60                     | 0.49              |
| 1:G:162:LEU:HD23  | 1:G:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:G:275:LEU:HD23  | 1:G:280:THR:HG21 | 1.94                     | 0.49              |
| 1:H:507:ALA:N     | 1:H:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:I:563:ARG:HH11  | 1:I:593:HIS:HA   | 1.77                     | 0.49              |
| 1:I:921:CYS:HA    | 1:I:930:HIS:O    | 2.11                     | 0.49              |
| 1:J:563:ARG:HH11  | 1:J:593:HIS:HA   | 1.77                     | 0.49              |
| 1:J:863:THR:HA    | 1:J:907:ILE:HG13 | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:99:PRO:HB2    | 1:K:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:K:248:GLN:HE22  | 1:K:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:K:507:ALA:N     | 1:K:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:L:463:LEU:HD22  | 1:L:467:PHE:HD2  | 1.74                     | 0.49              |
| 1:L:539:VAL:O     | 1:L:543:LEU:HG   | 2.12                     | 0.49              |
| 1:M:431:VAL:HB    | 1:M:432:LYS:HB2  | 1.93                     | 0.49              |
| 1:M:538:LEU:HD12  | 1:M:571:GLU:HG2  | 1.94                     | 0.49              |
| 1:N:20:GLU:O      | 1:N:23:PHE:N     | 2.45                     | 0.49              |
| 1:N:705:PHE:HB3   | 1:N:706:ILE:HD12 | 1.93                     | 0.49              |
| 1:O:515:LEU:HD12  | 1:O:517:THR:H    | 1.78                     | 0.49              |
| 1:P:557:LYS:CB    | 1:P:1226:TYR:CE1 | 2.87                     | 0.49              |
| 1:A:162:LEU:HD23  | 1:A:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:A:248:GLN:NE2   | 1:A:268:PHE:CZ   | 2.79                     | 0.49              |
| 1:A:301:LEU:CD2   | 1:A:313:PRO:CG   | 2.87                     | 0.49              |
| 1:A:347:ASP:OD1   | 1:A:348:LYS:N    | 2.37                     | 0.49              |
| 1:A:901:HIS:CG    | 1:A:902:ILE:H    | 2.29                     | 0.49              |
| 1:A:1240:LEU:HD12 | 1:A:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:B:162:LEU:HD23  | 1:B:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:C:64:THR:O      | 1:C:67:SER:OG    | 2.27                     | 0.49              |
| 1:C:431:VAL:HB    | 1:C:432:LYS:HB2  | 1.93                     | 0.49              |
| 1:C:563:ARG:HH11  | 1:C:593:HIS:HA   | 1.77                     | 0.49              |
| 1:C:1252:ALA:HB1  | 1:C:1256:CYS:HB2 | 1.95                     | 0.49              |
| 1:D:538:LEU:HD12  | 1:D:571:GLU:HG2  | 1.94                     | 0.49              |
| 1:E:248:GLN:HE22  | 1:E:268:PHE:HZ   | 1.60                     | 0.49              |
| 1:F:20:GLU:O      | 1:F:23:PHE:N     | 2.45                     | 0.49              |
| 1:F:162:LEU:HD23  | 1:F:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:F:541:ALA:O     | 1:F:544:ASP:N    | 2.30                     | 0.49              |
| 1:F:563:ARG:HH11  | 1:F:593:HIS:HA   | 1.77                     | 0.49              |
| 1:G:488:ARG:HA    | 1:G:491:PHE:H    | 1.75                     | 0.49              |
| 1:G:538:LEU:HD12  | 1:G:571:GLU:HG2  | 1.94                     | 0.49              |
| 1:G:557:LYS:CB    | 1:G:1226:TYR:CE1 | 2.87                     | 0.49              |
| 1:G:660:PHE:HZ    | 1:G:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:J:478:ILE:HG22  | 1:J:479:GLU:H    | 1.77                     | 0.49              |
| 1:K:293:THR:O     | 1:K:296:GLU:N    | 2.40                     | 0.49              |
| 1:L:20:GLU:O      | 1:L:23:PHE:N     | 2.45                     | 0.49              |
| 1:L:275:LEU:HD23  | 1:L:280:THR:HG21 | 1.93                     | 0.49              |
| 1:L:293:THR:O     | 1:L:296:GLU:N    | 2.40                     | 0.49              |
| 1:L:563:ARG:HH11  | 1:L:593:HIS:HA   | 1.78                     | 0.49              |
| 1:L:604:ASN:ND2   | 1:L:929:VAL:H    | 2.04                     | 0.49              |
| 1:L:651:SER:O     | 1:L:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:L:705:PHE:HB3   | 1:L:706:ILE:HD12 | 1.93                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:901:HIS:CD2   | 1:L:902:ILE:H    | 2.29                     | 0.49              |
| 1:L:901:HIS:CG    | 1:L:902:ILE:H    | 2.29                     | 0.49              |
| 1:L:1252:ALA:HB1  | 1:L:1256:CYS:HB2 | 1.94                     | 0.49              |
| 1:M:162:LEU:HD23  | 1:M:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:N:508:TRP:C     | 1:N:606:GLY:N    | 2.70                     | 0.49              |
| 1:N:556:SER:O     | 1:N:557:LYS:HB2  | 2.13                     | 0.49              |
| 1:O:99:PRO:HB2    | 1:O:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:O:162:LEU:HD23  | 1:O:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:P:162:LEU:HD23  | 1:P:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:A:20:GLU:O      | 1:A:23:PHE:N     | 2.45                     | 0.49              |
| 1:A:556:SER:O     | 1:A:557:LYS:HB2  | 2.13                     | 0.49              |
| 1:A:705:PHE:HB3   | 1:A:706:ILE:HD12 | 1.93                     | 0.49              |
| 1:B:431:VAL:HB    | 1:B:432:LYS:HB2  | 1.93                     | 0.49              |
| 1:C:248:GLN:HE22  | 1:C:268:PHE:HZ   | 1.60                     | 0.49              |
| 1:C:275:LEU:HD23  | 1:C:280:THR:HG21 | 1.94                     | 0.49              |
| 1:C:293:THR:O     | 1:C:296:GLU:N    | 2.40                     | 0.49              |
| 1:C:322:ARG:C     | 1:C:324:LEU:H    | 2.19                     | 0.49              |
| 1:C:508:TRP:C     | 1:C:606:GLY:N    | 2.70                     | 0.49              |
| 1:C:1075:SER:OG   | 1:C:1094:ASP:O   | 2.29                     | 0.49              |
| 1:D:221:ILE:HG13  | 1:D:222:HIS:N    | 2.28                     | 0.49              |
| 1:D:882:LEU:HB2   | 1:D:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:D:1240:LEU:HD12 | 1:D:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:F:221:ILE:HG13  | 1:F:222:HIS:N    | 2.28                     | 0.49              |
| 1:F:921:CYS:HA    | 1:F:930:HIS:O    | 2.11                     | 0.49              |
| 1:G:450:PRO:O     | 1:G:452:THR:N    | 2.46                     | 0.49              |
| 1:G:458:LEU:CG    | 1:G:587:ARG:NH2  | 2.74                     | 0.49              |
| 1:H:162:LEU:HD23  | 1:H:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:H:431:VAL:HB    | 1:H:432:LYS:HB2  | 1.93                     | 0.49              |
| 1:I:221:ILE:HG13  | 1:I:222:HIS:N    | 2.28                     | 0.49              |
| 1:J:187:ASN:HA    | 1:J:249:ASN:ND2  | 2.24                     | 0.49              |
| 1:J:248:GLN:HE22  | 1:J:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:K:221:ILE:HG13  | 1:K:222:HIS:N    | 2.28                     | 0.49              |
| 1:K:882:LEU:HB2   | 1:K:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:L:248:GLN:HE22  | 1:L:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:L:1240:LEU:HD12 | 1:L:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:M:64:THR:O      | 1:M:67:SER:OG    | 2.27                     | 0.49              |
| 1:M:450:PRO:O     | 1:M:452:THR:N    | 2.46                     | 0.49              |
| 1:N:162:LEU:HD23  | 1:N:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:N:901:HIS:CG    | 1:N:902:ILE:H    | 2.29                     | 0.49              |
| 1:P:488:ARG:HA    | 1:P:491:PHE:H    | 1.75                     | 0.49              |
| 1:P:538:LEU:HD12  | 1:P:571:GLU:HG2  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:P:660:PHE:HZ    | 1:P:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:A:651:SER:O     | 1:A:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:B:450:PRO:O     | 1:B:452:THR:N    | 2.46                     | 0.49              |
| 1:B:563:ARG:HH11  | 1:B:593:HIS:HA   | 1.77                     | 0.49              |
| 1:C:538:LEU:HD12  | 1:C:571:GLU:HG2  | 1.94                     | 0.49              |
| 1:C:901:HIS:CD2   | 1:C:902:ILE:H    | 2.29                     | 0.49              |
| 1:C:946:ARG:HG3   | 1:C:947:GLU:N    | 2.28                     | 0.49              |
| 1:D:293:THR:O     | 1:D:296:GLU:N    | 2.40                     | 0.49              |
| 1:D:515:LEU:HD12  | 1:D:517:THR:H    | 1.78                     | 0.49              |
| 1:D:901:HIS:CD2   | 1:D:902:ILE:H    | 2.29                     | 0.49              |
| 1:E:187:ASN:HA    | 1:E:249:ASN:ND2  | 2.23                     | 0.49              |
| 1:G:248:GLN:HE22  | 1:G:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:G:507:ALA:N     | 1:G:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:G:517:THR:HA    | 1:G:520:GLN:CG   | 2.43                     | 0.49              |
| 1:G:882:LEU:HB2   | 1:G:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:H:99:PRO:HB2    | 1:H:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:H:511:SER:HB3   | 1:H:645:LEU:HD21 | 1.94                     | 0.49              |
| 1:I:162:LEU:HD23  | 1:I:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:I:248:GLN:HE22  | 1:I:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:J:480:HIS:HB2   | 1:J:481:PRO:HD3  | 1.93                     | 0.49              |
| 1:K:541:ALA:O     | 1:K:544:ASP:N    | 2.30                     | 0.49              |
| 1:K:901:HIS:CD2   | 1:K:902:ILE:H    | 2.30                     | 0.49              |
| 1:K:1240:LEU:HD12 | 1:K:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:L:538:LEU:HD12  | 1:L:571:GLU:HG2  | 1.94                     | 0.49              |
| 1:M:988:ASP:OD1   | 1:M:989:SER:N    | 2.43                     | 0.49              |
| 1:N:507:ALA:N     | 1:N:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:N:651:SER:O     | 1:N:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:N:1240:LEU:HD12 | 1:N:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:O:187:ASN:HA    | 1:O:249:ASN:ND2  | 2.23                     | 0.49              |
| 1:O:946:ARG:HG3   | 1:O:947:GLU:N    | 2.28                     | 0.49              |
| 1:P:221:ILE:HG13  | 1:P:222:HIS:N    | 2.28                     | 0.49              |
| 1:P:248:GLN:HE22  | 1:P:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:P:450:PRO:O     | 1:P:452:THR:N    | 2.46                     | 0.49              |
| 1:P:458:LEU:CG    | 1:P:587:ARG:NH2  | 2.74                     | 0.49              |
| 1:P:507:ALA:N     | 1:P:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:P:517:THR:HA    | 1:P:520:GLN:CG   | 2.43                     | 0.49              |
| 1:P:563:ARG:HH11  | 1:P:593:HIS:HA   | 1.77                     | 0.49              |
| 1:P:882:LEU:HB2   | 1:P:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:A:450:PRO:O     | 1:A:452:THR:N    | 2.46                     | 0.49              |
| 1:A:507:ALA:N     | 1:A:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:A:517:THR:HA    | 1:A:520:GLN:CG   | 2.43                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:64:THR:O      | 1:B:67:SER:OG    | 2.27                     | 0.49              |
| 1:B:478:ILE:HG22  | 1:B:479:GLU:H    | 1.77                     | 0.49              |
| 1:B:507:ALA:N     | 1:B:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:B:517:THR:HA    | 1:B:520:GLN:CG   | 2.43                     | 0.49              |
| 1:B:660:PHE:HZ    | 1:B:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:B:863:THR:HA    | 1:B:907:ILE:HG13 | 1.93                     | 0.49              |
| 1:B:988:ASP:OD1   | 1:B:989:SER:N    | 2.43                     | 0.49              |
| 1:C:507:ALA:N     | 1:C:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:C:517:THR:HA    | 1:C:520:GLN:CG   | 2.43                     | 0.49              |
| 1:E:480:HIS:HB2   | 1:E:481:PRO:HD3  | 1.93                     | 0.49              |
| 1:E:1252:ALA:HB1  | 1:E:1256:CYS:HB2 | 1.94                     | 0.49              |
| 1:F:175:ASP:O     | 1:F:177:LYS:HG2  | 2.13                     | 0.49              |
| 1:F:882:LEU:HB2   | 1:F:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:G:99:PRO:HB2    | 1:G:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:G:221:ILE:HG13  | 1:G:222:HIS:N    | 2.28                     | 0.49              |
| 1:G:451:LYS:CD    | 1:G:486:LEU:HD21 | 2.33                     | 0.49              |
| 1:H:515:LEU:HD12  | 1:H:517:THR:H    | 1.78                     | 0.49              |
| 1:H:651:SER:O     | 1:H:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:I:538:LEU:HG    | 1:I:571:GLU:CG   | 2.42                     | 0.49              |
| 1:I:1058:ILE:HG13 | 1:I:1059:ASP:N   | 2.27                     | 0.49              |
| 1:K:515:LEU:HD12  | 1:K:517:THR:H    | 1.78                     | 0.49              |
| 1:K:604:ASN:ND2   | 1:K:929:VAL:H    | 2.04                     | 0.49              |
| 1:L:162:LEU:HD23  | 1:L:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:M:398:VAL:HG23  | 1:M:399:MET:N    | 2.28                     | 0.49              |
| 1:M:478:ILE:HG22  | 1:M:479:GLU:H    | 1.77                     | 0.49              |
| 1:M:507:ALA:N     | 1:M:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:M:563:ARG:HH11  | 1:M:593:HIS:HA   | 1.77                     | 0.49              |
| 1:M:660:PHE:HZ    | 1:M:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:M:863:THR:HA    | 1:M:907:ILE:HG13 | 1.93                     | 0.49              |
| 1:N:347:ASP:OD1   | 1:N:348:LYS:N    | 2.37                     | 0.49              |
| 1:O:863:THR:HA    | 1:O:907:ILE:HG13 | 1.93                     | 0.49              |
| 1:A:187:ASN:HA    | 1:A:249:ASN:ND2  | 2.23                     | 0.49              |
| 1:A:346:CYS:O     | 1:A:350:THR:N    | 2.25                     | 0.49              |
| 1:A:478:ILE:HG22  | 1:A:479:GLU:H    | 1.77                     | 0.49              |
| 1:A:863:THR:HA    | 1:A:907:ILE:HG13 | 1.93                     | 0.49              |
| 1:B:346:CYS:O     | 1:B:350:THR:N    | 2.25                     | 0.49              |
| 1:B:398:VAL:HG23  | 1:B:399:MET:N    | 2.28                     | 0.49              |
| 1:C:99:PRO:HB2    | 1:C:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:C:162:LEU:HD23  | 1:C:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:C:336:ALA:C     | 1:C:337:THR:HG1  | 2.20                     | 0.49              |
| 1:C:651:SER:O     | 1:C:654:ILE:HG23 | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:604:ASN:ND2   | 1:D:929:VAL:H    | 2.04                     | 0.49              |
| 1:D:651:SER:O     | 1:D:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:F:275:LEU:HD23  | 1:F:280:THR:HG21 | 1.93                     | 0.49              |
| 1:F:346:CYS:O     | 1:F:350:THR:N    | 2.25                     | 0.49              |
| 1:F:443:ILE:HG21  | 1:F:477:ASN:ND2  | 2.24                     | 0.49              |
| 1:F:517:THR:HA    | 1:F:520:GLN:CG   | 2.43                     | 0.49              |
| 1:G:90:SER:HG     | 1:G:91:PRO:HD3   | 1.77                     | 0.49              |
| 1:G:563:ARG:HH11  | 1:G:593:HIS:HA   | 1.78                     | 0.49              |
| 1:G:946:ARG:HG3   | 1:G:947:GLU:N    | 2.28                     | 0.49              |
| 1:H:187:ASN:HA    | 1:H:249:ASN:ND2  | 2.23                     | 0.49              |
| 1:H:248:GLN:HE22  | 1:H:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:H:863:THR:HA    | 1:H:907:ILE:HG13 | 1.93                     | 0.49              |
| 1:H:946:ARG:HG3   | 1:H:947:GLU:N    | 2.28                     | 0.49              |
| 1:H:1240:LEU:HD12 | 1:H:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:I:175:ASP:O     | 1:I:177:LYS:HG2  | 2.13                     | 0.49              |
| 1:I:275:LEU:HD23  | 1:I:280:THR:HG21 | 1.94                     | 0.49              |
| 1:I:517:THR:HA    | 1:I:520:GLN:CG   | 2.43                     | 0.49              |
| 1:I:882:LEU:HB2   | 1:I:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:J:1252:ALA:HB1  | 1:J:1256:CYS:HB2 | 1.95                     | 0.49              |
| 1:K:651:SER:O     | 1:K:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:L:507:ALA:N     | 1:L:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:L:515:LEU:HD12  | 1:L:517:THR:H    | 1.78                     | 0.49              |
| 1:L:517:THR:HA    | 1:L:520:GLN:CG   | 2.43                     | 0.49              |
| 1:L:921:CYS:HA    | 1:L:930:HIS:O    | 2.11                     | 0.49              |
| 1:M:517:THR:HA    | 1:M:520:GLN:CG   | 2.43                     | 0.49              |
| 1:N:187:ASN:HA    | 1:N:249:ASN:ND2  | 2.24                     | 0.49              |
| 1:N:450:PRO:O     | 1:N:452:THR:N    | 2.46                     | 0.49              |
| 1:N:517:THR:HA    | 1:N:520:GLN:CG   | 2.43                     | 0.49              |
| 1:O:511:SER:HB3   | 1:O:645:LEU:HD21 | 1.95                     | 0.49              |
| 1:O:517:THR:HA    | 1:O:520:GLN:CG   | 2.43                     | 0.49              |
| 1:O:556:SER:O     | 1:O:557:LYS:HB2  | 2.13                     | 0.49              |
| 1:O:651:SER:O     | 1:O:654:ILE:HG23 | 2.12                     | 0.49              |
| 1:P:90:SER:HG     | 1:P:91:PRO:HD3   | 1.77                     | 0.49              |
| 1:P:99:PRO:HB2    | 1:P:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:P:946:ARG:HG3   | 1:P:947:GLU:N    | 2.28                     | 0.49              |
| 1:A:248:GLN:HE22  | 1:A:268:PHE:HZ   | 1.60                     | 0.49              |
| 1:B:248:GLN:HE22  | 1:B:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:B:556:SER:O     | 1:B:557:LYS:HB2  | 2.13                     | 0.49              |
| 1:B:946:ARG:HG3   | 1:B:947:GLU:N    | 2.28                     | 0.49              |
| 1:C:921:CYS:HA    | 1:C:930:HIS:O    | 2.11                     | 0.49              |
| 1:D:450:PRO:O     | 1:D:452:THR:N    | 2.46                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:799:ASN:C     | 1:D:800:THR:CG2  | 2.86                     | 0.49              |
| 1:E:660:PHE:HZ    | 1:E:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:F:122:LYS:HG2   | 1:G:276:SER:OG   | 2.13                     | 0.49              |
| 1:F:450:PRO:O     | 1:F:452:THR:N    | 2.46                     | 0.49              |
| 1:F:1058:ILE:HG13 | 1:F:1059:ASP:N   | 2.27                     | 0.49              |
| 1:H:517:THR:HA    | 1:H:520:GLN:CG   | 2.43                     | 0.49              |
| 1:H:556:SER:O     | 1:H:557:LYS:HB2  | 2.13                     | 0.49              |
| 1:I:198:LYS:NZ    | 1:P:222:HIS:CD2  | 2.81                     | 0.49              |
| 1:I:507:ALA:N     | 1:I:608:ASN:HB2  | 2.27                     | 0.49              |
| 1:I:541:ALA:O     | 1:I:544:ASP:N    | 2.30                     | 0.49              |
| 1:K:450:PRO:O     | 1:K:452:THR:N    | 2.46                     | 0.49              |
| 1:K:799:ASN:C     | 1:K:800:THR:CG2  | 2.86                     | 0.49              |
| 1:L:99:PRO:HB2    | 1:L:104:ARG:HG3  | 1.93                     | 0.49              |
| 1:L:799:ASN:C     | 1:L:800:THR:CG2  | 2.86                     | 0.49              |
| 1:L:1192:SER:OG   | 1:L:1208:GLU:OE2 | 2.28                     | 0.49              |
| 1:M:556:SER:O     | 1:M:557:LYS:HB2  | 2.13                     | 0.49              |
| 1:O:248:GLN:HE22  | 1:O:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:P:451:LYS:CD    | 1:P:486:LEU:HD21 | 2.33                     | 0.49              |
| 1:B:122:LYS:O     | 1:B:303:LYS:NZ   | 2.38                     | 0.49              |
| 1:C:705:PHE:HB3   | 1:C:706:ILE:HD12 | 1.93                     | 0.49              |
| 1:D:162:LEU:HD23  | 1:D:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:D:946:ARG:HG3   | 1:D:947:GLU:N    | 2.28                     | 0.49              |
| 1:E:162:LEU:HD23  | 1:E:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:E:462:TYR:CZ    | 1:E:467:PHE:HB3  | 2.48                     | 0.49              |
| 1:F:462:TYR:CZ    | 1:F:467:PHE:HB3  | 2.48                     | 0.49              |
| 1:F:538:LEU:HG    | 1:F:571:GLU:CG   | 2.42                     | 0.49              |
| 1:G:799:ASN:C     | 1:G:800:THR:CG2  | 2.86                     | 0.49              |
| 1:I:518:LEU:HD12  | 1:I:518:LEU:N    | 2.20                     | 0.49              |
| 1:I:523:PHE:HD1   | 1:I:527:TYR:CE2  | 2.28                     | 0.49              |
| 1:I:1192:SER:OG   | 1:I:1208:GLU:OE2 | 2.28                     | 0.49              |
| 1:K:162:LEU:HD23  | 1:K:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:L:248:GLN:NE2   | 1:L:268:PHE:CZ   | 2.79                     | 0.49              |
| 1:L:946:ARG:HG3   | 1:L:947:GLU:N    | 2.28                     | 0.49              |
| 1:M:122:LYS:O     | 1:M:303:LYS:NZ   | 2.38                     | 0.49              |
| 1:M:248:GLN:HE22  | 1:M:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:M:275:LEU:HD23  | 1:M:280:THR:HG21 | 1.93                     | 0.49              |
| 1:M:346:CYS:O     | 1:M:350:THR:N    | 2.25                     | 0.49              |
| 1:N:248:GLN:NE2   | 1:N:268:PHE:CZ   | 2.79                     | 0.49              |
| 1:N:478:ILE:HG22  | 1:N:479:GLU:H    | 1.77                     | 0.49              |
| 1:O:347:ASP:OD1   | 1:O:348:LYS:N    | 2.37                     | 0.49              |
| 1:O:450:PRO:O     | 1:O:452:THR:N    | 2.46                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:882:LEU:HB2  | 1:O:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:P:799:ASN:C    | 1:P:800:THR:CG2  | 2.86                     | 0.49              |
| 1:A:511:SER:HB3  | 1:A:645:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:515:LEU:HD12 | 1:A:517:THR:H    | 1.78                     | 0.49              |
| 1:B:20:GLU:O     | 1:B:23:PHE:N     | 2.45                     | 0.49              |
| 1:B:275:LEU:HD23 | 1:B:280:THR:HG21 | 1.93                     | 0.49              |
| 1:B:538:LEU:HD21 | 1:B:573:ILE:HD11 | 1.94                     | 0.49              |
| 1:B:604:ASN:ND2  | 1:B:929:VAL:H    | 2.04                     | 0.49              |
| 1:B:1252:ALA:HB1 | 1:B:1256:CYS:HB2 | 1.94                     | 0.49              |
| 1:C:175:ASP:O    | 1:C:177:LYS:HG2  | 2.13                     | 0.49              |
| 1:C:799:ASN:C    | 1:C:800:THR:CG2  | 2.86                     | 0.49              |
| 1:D:517:THR:HA   | 1:D:520:GLN:CG   | 2.43                     | 0.49              |
| 1:D:660:PHE:HZ   | 1:D:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:D:863:THR:HA   | 1:D:907:ILE:HG13 | 1.93                     | 0.49              |
| 1:E:517:THR:HA   | 1:E:520:GLN:CG   | 2.43                     | 0.49              |
| 1:E:799:ASN:C    | 1:E:800:THR:CG2  | 2.86                     | 0.49              |
| 1:F:523:PHE:HD1  | 1:F:527:TYR:CE2  | 2.28                     | 0.49              |
| 1:F:660:PHE:HZ   | 1:F:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:F:799:ASN:C    | 1:F:800:THR:CG2  | 2.86                     | 0.49              |
| 1:G:175:ASP:O    | 1:G:177:LYS:HG2  | 2.13                     | 0.49              |
| 1:G:462:TYR:CZ   | 1:G:467:PHE:HB3  | 2.48                     | 0.49              |
| 1:G:463:LEU:CD2  | 1:G:467:PHE:CD2  | 2.92                     | 0.49              |
| 1:G:538:LEU:HD21 | 1:G:573:ILE:HD11 | 1.94                     | 0.49              |
| 1:H:221:ILE:HG13 | 1:H:222:HIS:N    | 2.28                     | 0.49              |
| 1:H:347:ASP:OD1  | 1:H:348:LYS:N    | 2.37                     | 0.49              |
| 1:H:882:LEU:HB2  | 1:H:901:HIS:CE1  | 2.48                     | 0.49              |
| 1:I:450:PRO:O    | 1:I:452:THR:N    | 2.46                     | 0.49              |
| 1:I:462:TYR:CZ   | 1:I:467:PHE:HB3  | 2.48                     | 0.49              |
| 1:I:660:PHE:HZ   | 1:I:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:I:799:ASN:C    | 1:I:800:THR:CG2  | 2.86                     | 0.49              |
| 1:J:162:LEU:HD23 | 1:J:180:TRP:CH2  | 2.48                     | 0.49              |
| 1:J:517:THR:HA   | 1:J:520:GLN:CG   | 2.43                     | 0.49              |
| 1:J:660:PHE:HZ   | 1:J:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:J:799:ASN:C    | 1:J:800:THR:CG2  | 2.86                     | 0.49              |
| 1:K:517:THR:HA   | 1:K:520:GLN:CG   | 2.43                     | 0.49              |
| 1:K:660:PHE:HZ   | 1:K:731:GLN:HG3  | 1.78                     | 0.49              |
| 1:K:946:ARG:HG3  | 1:K:947:GLU:N    | 2.28                     | 0.49              |
| 1:M:538:LEU:HG   | 1:M:571:GLU:CG   | 2.42                     | 0.49              |
| 1:M:538:LEU:HD21 | 1:M:573:ILE:HD11 | 1.94                     | 0.49              |
| 1:M:946:ARG:HG3  | 1:M:947:GLU:N    | 2.28                     | 0.49              |
| 1:M:1252:ALA:HB1 | 1:M:1256:CYS:HB2 | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:N:248:GLN:HE22  | 1:N:268:PHE:HZ   | 1.61                     | 0.49              |
| 1:N:511:SER:HB3   | 1:N:645:LEU:HD21 | 1.94                     | 0.49              |
| 1:N:515:LEU:HD12  | 1:N:517:THR:H    | 1.78                     | 0.49              |
| 1:O:1240:LEU:HD12 | 1:O:1250:SER:HB2 | 1.93                     | 0.49              |
| 1:P:175:ASP:O     | 1:P:177:LYS:HG2  | 2.13                     | 0.49              |
| 1:P:462:TYR:CZ    | 1:P:467:PHE:HB3  | 2.48                     | 0.49              |
| 1:P:511:SER:HB3   | 1:P:645:LEU:HD21 | 1.94                     | 0.49              |
| 1:P:538:LEU:HD21  | 1:P:573:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:253:TRP:CZ3   | 1:A:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:A:462:TYR:CZ    | 1:A:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:A:538:LEU:HG    | 1:A:571:GLU:CG   | 2.42                     | 0.48              |
| 1:A:1252:ALA:HB1  | 1:A:1256:CYS:HB2 | 1.94                     | 0.48              |
| 1:B:538:LEU:HG    | 1:B:571:GLU:CG   | 2.42                     | 0.48              |
| 1:C:515:LEU:HD12  | 1:C:517:THR:H    | 1.78                     | 0.48              |
| 1:G:478:ILE:HG22  | 1:G:479:GLU:H    | 1.77                     | 0.48              |
| 1:G:511:SER:HB3   | 1:G:645:LEU:HD21 | 1.94                     | 0.48              |
| 1:H:175:ASP:O     | 1:H:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:H:450:PRO:O     | 1:H:452:THR:N    | 2.46                     | 0.48              |
| 1:H:462:TYR:CZ    | 1:H:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:H:900:GLU:HB2   | 1:H:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:I:499:GLN:CD    | 1:I:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:J:462:TYR:CZ    | 1:J:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:K:538:LEU:HG    | 1:K:571:GLU:CG   | 2.42                     | 0.48              |
| 1:L:175:ASP:O     | 1:L:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:L:450:PRO:O     | 1:L:452:THR:N    | 2.46                     | 0.48              |
| 1:M:20:GLU:O      | 1:M:23:PHE:N     | 2.45                     | 0.48              |
| 1:M:499:GLN:CD    | 1:M:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:M:604:ASN:ND2   | 1:M:929:VAL:H    | 2.04                     | 0.48              |
| 1:N:253:TRP:CZ3   | 1:N:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:N:346:CYS:O     | 1:N:350:THR:N    | 2.25                     | 0.48              |
| 1:N:863:THR:HA    | 1:N:907:ILE:HG13 | 1.94                     | 0.48              |
| 1:O:221:ILE:HG13  | 1:O:222:HIS:N    | 2.28                     | 0.48              |
| 1:O:462:TYR:CZ    | 1:O:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:O:988:ASP:OD1   | 1:O:989:SER:N    | 2.43                     | 0.48              |
| 1:P:463:LEU:CD2   | 1:P:467:PHE:CD2  | 2.92                     | 0.48              |
| 1:P:478:ILE:HG22  | 1:P:479:GLU:H    | 1.77                     | 0.48              |
| 1:A:900:GLU:HB2   | 1:A:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:B:253:TRP:CZ3   | 1:B:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:B:499:GLN:CD    | 1:B:516:ASN:HB3  | 2.39                     | 0.48              |
| 1:C:408:TYR:O     | 1:C:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:C:1192:SER:OG   | 1:C:1208:GLU:OE2 | 2.28                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:175:ASP:O    | 1:D:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:D:900:GLU:HB2  | 1:D:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:E:636:SER:O    | 1:E:637:LEU:O    | 2.31                     | 0.48              |
| 1:E:946:ARG:HG3  | 1:E:947:GLU:N    | 2.28                     | 0.48              |
| 1:F:499:GLN:CD   | 1:F:516:ASN:HB3  | 2.39                     | 0.48              |
| 1:F:507:ALA:N    | 1:F:608:ASN:HB2  | 2.27                     | 0.48              |
| 1:F:946:ARG:HG3  | 1:F:947:GLU:N    | 2.28                     | 0.48              |
| 1:G:64:THR:O     | 1:G:67:SER:OG    | 2.27                     | 0.48              |
| 1:G:651:SER:O    | 1:G:654:ILE:HG23 | 2.12                     | 0.48              |
| 1:H:346:CYS:O    | 1:H:350:THR:N    | 2.25                     | 0.48              |
| 1:H:408:TYR:O    | 1:H:411:VAL:HG22 | 2.13                     | 0.48              |
| 1:H:538:LEU:HG   | 1:H:571:GLU:CG   | 2.42                     | 0.48              |
| 1:H:660:PHE:HZ   | 1:H:731:GLN:HG3  | 1.78                     | 0.48              |
| 1:I:443:ILE:HG21 | 1:I:477:ASN:ND2  | 2.24                     | 0.48              |
| 1:I:946:ARG:HG3  | 1:I:947:GLU:N    | 2.28                     | 0.48              |
| 1:J:636:SER:O    | 1:J:637:LEU:O    | 2.31                     | 0.48              |
| 1:K:175:ASP:O    | 1:K:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:K:863:THR:HA   | 1:K:907:ILE:HG13 | 1.93                     | 0.48              |
| 1:K:900:GLU:HB2  | 1:K:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:L:408:TYR:O    | 1:L:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:L:518:LEU:HD12 | 1:L:518:LEU:N    | 2.20                     | 0.48              |
| 1:M:508:TRP:C    | 1:M:606:GLY:N    | 2.70                     | 0.48              |
| 1:N:462:TYR:CZ   | 1:N:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:N:538:LEU:HG   | 1:N:571:GLU:CG   | 2.42                     | 0.48              |
| 1:N:660:PHE:HZ   | 1:N:731:GLN:HG3  | 1.78                     | 0.48              |
| 1:N:882:LEU:HB2  | 1:N:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:N:900:GLU:HB2  | 1:N:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:O:175:ASP:O    | 1:O:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:O:231:LEU:O    | 1:O:234:SER:OG   | 2.26                     | 0.48              |
| 1:O:799:ASN:C    | 1:O:800:THR:CG2  | 2.86                     | 0.48              |
| 1:P:20:GLU:O     | 1:P:23:PHE:N     | 2.45                     | 0.48              |
| 1:A:499:GLN:CD   | 1:A:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:A:660:PHE:HZ   | 1:A:731:GLN:HG3  | 1.78                     | 0.48              |
| 1:B:201:TYR:CZ   | 1:C:223:SER:OG   | 2.64                     | 0.48              |
| 1:B:293:THR:O    | 1:B:296:GLU:N    | 2.40                     | 0.48              |
| 1:B:508:TRP:C    | 1:B:606:GLY:N    | 2.70                     | 0.48              |
| 1:B:651:SER:O    | 1:B:654:ILE:HG23 | 2.12                     | 0.48              |
| 1:B:799:ASN:C    | 1:B:800:THR:CG2  | 2.86                     | 0.48              |
| 1:B:1075:SER:OG  | 1:B:1094:ASP:O   | 2.29                     | 0.48              |
| 1:C:462:TYR:CZ   | 1:C:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:C:511:SER:HB3  | 1:C:645:LEU:HD21 | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:538:LEU:HG   | 1:C:571:GLU:CG   | 2.42                     | 0.48              |
| 1:C:660:PHE:HZ   | 1:C:731:GLN:HG3  | 1.78                     | 0.48              |
| 1:D:462:TYR:CZ   | 1:D:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:E:882:LEU:HB2  | 1:E:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:F:1192:SER:OG  | 1:F:1208:GLU:OE2 | 2.28                     | 0.48              |
| 1:G:20:GLU:O     | 1:G:23:PHE:N     | 2.45                     | 0.48              |
| 1:H:799:ASN:C    | 1:H:800:THR:CG2  | 2.86                     | 0.48              |
| 1:J:275:LEU:HD23 | 1:J:280:THR:HG21 | 1.94                     | 0.48              |
| 1:J:538:LEU:HD21 | 1:J:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:J:882:LEU:HB2  | 1:J:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:J:946:ARG:HG3  | 1:J:947:GLU:N    | 2.28                     | 0.48              |
| 1:K:462:TYR:CZ   | 1:K:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:K:538:LEU:HD21 | 1:K:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:K:636:SER:O    | 1:K:637:LEU:O    | 2.31                     | 0.48              |
| 1:M:253:TRP:CZ3  | 1:M:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:M:293:THR:O    | 1:M:296:GLU:N    | 2.40                     | 0.48              |
| 1:M:462:TYR:CZ   | 1:M:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:M:651:SER:O    | 1:M:654:ILE:HG23 | 2.12                     | 0.48              |
| 1:M:1075:SER:OG  | 1:M:1094:ASP:O   | 2.29                     | 0.48              |
| 1:N:463:LEU:HD22 | 1:N:467:PHE:HD2  | 1.74                     | 0.48              |
| 1:N:1252:ALA:HB1 | 1:N:1256:CYS:HB2 | 1.95                     | 0.48              |
| 1:O:142:ARG:HH22 | 1:P:14:ASP:CG    | 2.21                     | 0.48              |
| 1:O:900:GLU:HB2  | 1:O:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:P:515:LEU:HD12 | 1:P:517:THR:H    | 1.78                     | 0.48              |
| 1:P:651:SER:O    | 1:P:654:ILE:HG23 | 2.12                     | 0.48              |
| 1:P:900:GLU:HB2  | 1:P:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:A:90:SER:HG    | 1:A:91:PRO:HD3   | 1.78                     | 0.48              |
| 1:A:882:LEU:HB2  | 1:A:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:B:462:TYR:CZ   | 1:B:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:B:882:LEU:HB2  | 1:B:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:C:253:TRP:CZ3  | 1:C:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:C:337:THR:HG1  | 1:C:340:ASN:H    | 1.61                     | 0.48              |
| 1:C:900:GLU:HB2  | 1:C:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:D:253:TRP:CZ3  | 1:D:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:D:538:LEU:HG   | 1:D:571:GLU:CG   | 2.42                     | 0.48              |
| 1:D:538:LEU:HD21 | 1:D:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:D:636:SER:O    | 1:D:637:LEU:O    | 2.31                     | 0.48              |
| 1:E:175:ASP:O    | 1:E:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:E:654:ILE:HG22 | 1:E:670:HIS:HD2  | 1.79                     | 0.48              |
| 1:F:64:THR:O     | 1:F:67:SER:OG    | 2.27                     | 0.48              |
| 1:F:187:ASN:HA   | 1:F:249:ASN:ND2  | 2.23                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:515:LEU:HD12 | 1:G:517:THR:H    | 1.78                     | 0.48              |
| 1:G:900:GLU:HB2  | 1:G:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:H:563:ARG:HH11 | 1:H:593:HIS:HA   | 1.77                     | 0.48              |
| 1:H:988:ASP:OD1  | 1:H:989:SER:N    | 2.43                     | 0.48              |
| 1:I:187:ASN:HA   | 1:I:249:ASN:ND2  | 2.23                     | 0.48              |
| 1:I:636:SER:O    | 1:I:637:LEU:O    | 2.31                     | 0.48              |
| 1:I:654:ILE:HG22 | 1:I:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:J:398:VAL:HG23 | 1:J:399:MET:N    | 2.28                     | 0.48              |
| 1:J:654:ILE:HG22 | 1:J:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:K:1252:ALA:HB1 | 1:K:1256:CYS:HB2 | 1.95                     | 0.48              |
| 1:L:221:ILE:HG13 | 1:L:222:HIS:N    | 2.28                     | 0.48              |
| 1:L:511:SER:HB3  | 1:L:645:LEU:HD21 | 1.94                     | 0.48              |
| 1:L:882:LEU:HB2  | 1:L:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:M:799:ASN:C    | 1:M:800:THR:CG2  | 2.86                     | 0.48              |
| 1:M:882:LEU:HB2  | 1:M:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:N:946:ARG:HG3  | 1:N:947:GLU:N    | 2.28                     | 0.48              |
| 1:O:253:TRP:CZ3  | 1:O:264:LEU:HD11 | 2.48                     | 0.48              |
| 1:O:408:TYR:O    | 1:O:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:O:499:GLN:CD   | 1:O:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:O:538:LEU:HG   | 1:O:571:GLU:CG   | 2.42                     | 0.48              |
| 1:O:563:ARG:HH11 | 1:O:593:HIS:HA   | 1.77                     | 0.48              |
| 1:O:660:PHE:HZ   | 1:O:731:GLN:HG3  | 1.78                     | 0.48              |
| 1:A:946:ARG:HG3  | 1:A:947:GLU:N    | 2.28                     | 0.48              |
| 1:B:324:LEU:HD12 | 1:B:324:LEU:HA   | 1.61                     | 0.48              |
| 1:B:515:LEU:HD12 | 1:B:517:THR:H    | 1.78                     | 0.48              |
| 1:C:450:PRO:O    | 1:C:452:THR:N    | 2.46                     | 0.48              |
| 1:D:408:TYR:O    | 1:D:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:D:1252:ALA:HB1 | 1:D:1256:CYS:HB2 | 1.94                     | 0.48              |
| 1:E:275:LEU:HD23 | 1:E:280:THR:HG21 | 1.93                     | 0.48              |
| 1:E:398:VAL:HG23 | 1:E:399:MET:N    | 2.28                     | 0.48              |
| 1:E:515:LEU:HD12 | 1:E:517:THR:H    | 1.78                     | 0.48              |
| 1:E:538:LEU:HD21 | 1:E:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:F:654:ILE:HG22 | 1:F:670:HIS:HD2  | 1.79                     | 0.48              |
| 1:G:499:GLN:HG3  | 1:G:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:G:641:ASP:OD1  | 1:G:642:THR:N    | 2.45                     | 0.48              |
| 1:H:231:LEU:O    | 1:H:234:SER:OG   | 2.26                     | 0.48              |
| 1:H:247:VAL:HG21 | 1:H:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:H:253:TRP:CZ3  | 1:H:264:LEU:HD11 | 2.49                     | 0.48              |
| 1:H:499:GLN:CD   | 1:H:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:I:515:LEU:HD12 | 1:I:517:THR:H    | 1.78                     | 0.48              |
| 1:J:175:ASP:O    | 1:J:177:LYS:HG2  | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:515:LEU:HD12 | 1:J:517:THR:H    | 1.78                     | 0.48              |
| 1:L:462:TYR:CZ   | 1:L:467:PHE:HB3  | 2.48                     | 0.48              |
| 1:L:900:GLU:HB2  | 1:L:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:M:175:ASP:O    | 1:M:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:M:324:LEU:HD12 | 1:M:324:LEU:HA   | 1.61                     | 0.48              |
| 1:N:221:ILE:HG13 | 1:N:222:HIS:N    | 2.28                     | 0.48              |
| 1:N:499:GLN:CD   | 1:N:516:ASN:HB3  | 2.39                     | 0.48              |
| 1:N:538:LEU:HD21 | 1:N:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:O:499:GLN:HG3  | 1:O:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:P:499:GLN:HG3  | 1:P:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:A:463:LEU:HD22 | 1:A:467:PHE:HD2  | 1.74                     | 0.48              |
| 1:A:799:ASN:C    | 1:A:800:THR:CG2  | 2.86                     | 0.48              |
| 1:C:499:GLN:HG3  | 1:C:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:D:373:SER:CB   | 1:D:433:LEU:CD1  | 2.73                     | 0.48              |
| 1:E:293:THR:O    | 1:E:296:GLU:N    | 2.40                     | 0.48              |
| 1:E:450:PRO:O    | 1:E:452:THR:N    | 2.46                     | 0.48              |
| 1:E:511:SER:HB3  | 1:E:645:LEU:HD21 | 1.95                     | 0.48              |
| 1:F:636:SER:O    | 1:F:637:LEU:O    | 2.31                     | 0.48              |
| 1:F:965:LEU:HD11 | 1:F:993:ILE:HG12 | 1.96                     | 0.48              |
| 1:G:347:ASP:OD1  | 1:G:348:LYS:N    | 2.37                     | 0.48              |
| 1:H:499:GLN:HG3  | 1:H:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:K:253:TRP:CZ3  | 1:K:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:K:408:TYR:O    | 1:K:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:K:875:LEU:CD1  | 1:K:911:PHE:HD2  | 2.07                     | 0.48              |
| 1:L:538:LEU:HG   | 1:L:571:GLU:CG   | 2.42                     | 0.48              |
| 1:M:515:LEU:HD12 | 1:M:517:THR:H    | 1.78                     | 0.48              |
| 1:M:654:ILE:HG22 | 1:M:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:N:90:SER:HG    | 1:N:91:PRO:HD3   | 1.78                     | 0.48              |
| 1:N:799:ASN:C    | 1:N:800:THR:CG2  | 2.86                     | 0.48              |
| 1:O:247:VAL:HG21 | 1:O:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:P:347:ASP:OD1  | 1:P:348:LYS:N    | 2.37                     | 0.48              |
| 1:P:463:LEU:HD22 | 1:P:467:PHE:HD2  | 1.74                     | 0.48              |
| 1:P:641:ASP:OD1  | 1:P:642:THR:N    | 2.45                     | 0.48              |
| 1:P:965:LEU:HD11 | 1:P:993:ILE:HG12 | 1.96                     | 0.48              |
| 1:A:90:SER:OG    | 1:A:91:PRO:HD3   | 2.14                     | 0.48              |
| 1:A:221:ILE:HG13 | 1:A:222:HIS:N    | 2.28                     | 0.48              |
| 1:B:175:ASP:O    | 1:B:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:B:253:TRP:CZ3  | 1:B:264:LEU:HD11 | 2.49                     | 0.48              |
| 1:B:408:TYR:O    | 1:B:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:B:654:ILE:HG22 | 1:B:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:C:221:ILE:HG13 | 1:C:222:HIS:N    | 2.28                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:882:LEU:HB2  | 1:C:901:HIS:CE1  | 2.48                     | 0.48              |
| 1:D:556:SER:O    | 1:D:557:LYS:HB2  | 2.13                     | 0.48              |
| 1:D:654:ILE:HG22 | 1:D:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:E:253:TRP:CZ3  | 1:E:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:E:317:LEU:C    | 1:E:318:THR:HG1  | 1.95                     | 0.48              |
| 1:E:458:LEU:CG   | 1:E:587:ARG:NH2  | 2.74                     | 0.48              |
| 1:F:383:THR:O    | 1:F:386:LEU:HB3  | 2.14                     | 0.48              |
| 1:F:499:GLN:HG3  | 1:F:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:G:965:LEU:HD11 | 1:G:993:ILE:HG12 | 1.96                     | 0.48              |
| 1:I:317:LEU:O    | 1:I:318:THR:CB   | 2.61                     | 0.48              |
| 1:I:346:CYS:O    | 1:I:350:THR:N    | 2.25                     | 0.48              |
| 1:I:383:THR:O    | 1:I:386:LEU:HB3  | 2.14                     | 0.48              |
| 1:J:293:THR:O    | 1:J:296:GLU:N    | 2.40                     | 0.48              |
| 1:J:450:PRO:O    | 1:J:452:THR:N    | 2.46                     | 0.48              |
| 1:J:511:SER:HB3  | 1:J:645:LEU:HD21 | 1.95                     | 0.48              |
| 1:K:398:VAL:HG23 | 1:K:399:MET:N    | 2.28                     | 0.48              |
| 1:K:499:GLN:CD   | 1:K:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:L:187:ASN:HA   | 1:L:249:ASN:ND2  | 2.24                     | 0.48              |
| 1:L:253:TRP:CZ3  | 1:L:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:L:499:GLN:HG3  | 1:L:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:L:636:SER:O    | 1:L:637:LEU:O    | 2.31                     | 0.48              |
| 1:L:660:PHE:HZ   | 1:L:731:GLN:HG3  | 1.78                     | 0.48              |
| 1:M:247:VAL:HG21 | 1:M:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:M:408:TYR:O    | 1:M:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:N:90:SER:OG    | 1:N:91:PRO:HD3   | 2.14                     | 0.48              |
| 1:N:499:GLN:HG3  | 1:N:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:O:346:CYS:O    | 1:O:350:THR:N    | 2.25                     | 0.48              |
| 1:A:175:ASP:O    | 1:A:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:A:499:GLN:HG3  | 1:A:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:B:247:VAL:HG21 | 1:B:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:B:499:GLN:HG3  | 1:B:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:B:511:SER:HB3  | 1:B:645:LEU:HD21 | 1.95                     | 0.48              |
| 1:B:900:GLU:HB2  | 1:B:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:C:538:LEU:HD21 | 1:C:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:C:654:ILE:HG22 | 1:C:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:D:499:GLN:CD   | 1:D:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:D:499:GLN:HG3  | 1:D:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:D:875:LEU:CD1  | 1:D:911:PHE:HD2  | 2.07                     | 0.48              |
| 1:E:121:ALA:CB   | 1:F:276:SER:CB   | 2.79                     | 0.48              |
| 1:E:221:ILE:HG13 | 1:E:222:HIS:N    | 2.28                     | 0.48              |
| 1:E:408:TYR:O    | 1:E:411:VAL:HG22 | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:90:SER:OG    | 1:F:91:PRO:HD3   | 2.14                     | 0.48              |
| 1:F:247:VAL:HG21 | 1:F:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:F:398:VAL:HG23 | 1:F:399:MET:N    | 2.28                     | 0.48              |
| 1:F:463:LEU:HD22 | 1:F:467:PHE:HD2  | 1.74                     | 0.48              |
| 1:F:511:SER:HB3  | 1:F:645:LEU:HD21 | 1.94                     | 0.48              |
| 1:G:1252:ALA:HB1 | 1:G:1256:CYS:HB2 | 1.94                     | 0.48              |
| 1:I:398:VAL:HG23 | 1:I:399:MET:N    | 2.28                     | 0.48              |
| 1:J:408:TYR:O    | 1:J:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:K:499:GLN:HG3  | 1:K:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:K:511:SER:HB3  | 1:K:645:LEU:HD21 | 1.94                     | 0.48              |
| 1:K:556:SER:O    | 1:K:557:LYS:HB2  | 2.13                     | 0.48              |
| 1:K:654:ILE:HG22 | 1:K:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:M:253:TRP:CZ3  | 1:M:264:LEU:HD11 | 2.49                     | 0.48              |
| 1:M:511:SER:HB3  | 1:M:645:LEU:HD21 | 1.94                     | 0.48              |
| 1:M:900:GLU:HB2  | 1:M:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:N:398:VAL:HG23 | 1:N:399:MET:N    | 2.28                     | 0.48              |
| 1:P:408:TYR:O    | 1:P:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:P:1252:ALA:HB1 | 1:P:1256:CYS:HB2 | 1.94                     | 0.48              |
| 1:A:253:TRP:CZ3  | 1:A:264:LEU:HD11 | 2.48                     | 0.48              |
| 1:A:398:VAL:HG23 | 1:A:399:MET:N    | 2.28                     | 0.48              |
| 1:A:538:LEU:HD21 | 1:A:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:A:552:ASN:HB3  | 1:A:1226:TYR:CE1 | 2.48                     | 0.48              |
| 1:B:392:ASP:OD1  | 1:B:393:VAL:N    | 2.47                     | 0.48              |
| 1:C:253:TRP:CZ3  | 1:C:264:LEU:HD11 | 2.49                     | 0.48              |
| 1:D:317:LEU:O    | 1:D:318:THR:CB   | 2.61                     | 0.48              |
| 1:D:511:SER:HB3  | 1:D:645:LEU:HD21 | 1.95                     | 0.48              |
| 1:E:463:LEU:CD2  | 1:E:467:PHE:CD2  | 2.92                     | 0.48              |
| 1:E:510:ALA:HB1  | 1:E:515:LEU:HA   | 1.96                     | 0.48              |
| 1:E:604:ASN:ND2  | 1:E:929:VAL:H    | 2.04                     | 0.48              |
| 1:E:900:GLU:HB2  | 1:E:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:F:317:LEU:O    | 1:F:318:THR:CB   | 2.61                     | 0.48              |
| 1:F:510:ALA:HB1  | 1:F:515:LEU:HA   | 1.96                     | 0.48              |
| 1:F:515:LEU:HD12 | 1:F:517:THR:H    | 1.78                     | 0.48              |
| 1:G:383:THR:O    | 1:G:386:LEU:HB3  | 2.14                     | 0.48              |
| 1:G:408:TYR:O    | 1:G:411:VAL:HG22 | 2.14                     | 0.48              |
| 1:G:463:LEU:HD22 | 1:G:467:PHE:HD2  | 1.74                     | 0.48              |
| 1:G:499:GLN:CD   | 1:G:516:ASN:HB3  | 2.39                     | 0.48              |
| 1:H:383:THR:O    | 1:H:386:LEU:HB3  | 2.14                     | 0.48              |
| 1:I:90:SER:OG    | 1:I:91:PRO:HD3   | 2.14                     | 0.48              |
| 1:I:499:GLN:HG3  | 1:I:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:I:965:LEU:HD11 | 1:I:993:ILE:HG12 | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:91:PRO:O     | 1:J:94:THR:OG1   | 2.21                     | 0.48              |
| 1:J:253:TRP:CZ3  | 1:J:262:ILE:HD11 | 2.48                     | 0.48              |
| 1:J:458:LEU:CG   | 1:J:587:ARG:NH2  | 2.74                     | 0.48              |
| 1:J:510:ALA:HB1  | 1:J:515:LEU:HA   | 1.96                     | 0.48              |
| 1:J:604:ASN:ND2  | 1:J:929:VAL:H    | 2.04                     | 0.48              |
| 1:J:900:GLU:HB2  | 1:J:930:HIS:CD2  | 2.48                     | 0.48              |
| 1:J:965:LEU:HD11 | 1:J:993:ILE:HG12 | 1.96                     | 0.48              |
| 1:K:317:LEU:O    | 1:K:318:THR:CB   | 2.61                     | 0.48              |
| 1:L:180:TRP:O    | 1:L:181:LEU:HD12 | 2.14                     | 0.48              |
| 1:L:654:ILE:HG22 | 1:L:670:HIS:HD2  | 1.79                     | 0.48              |
| 1:M:90:SER:OG    | 1:M:91:PRO:HD3   | 2.14                     | 0.48              |
| 1:M:499:GLN:HG3  | 1:M:502:ARG:HB2  | 1.96                     | 0.48              |
| 1:N:253:TRP:CZ3  | 1:N:264:LEU:HD11 | 2.49                     | 0.48              |
| 1:N:552:ASN:HB3  | 1:N:1226:TYR:CE1 | 2.48                     | 0.48              |
| 1:N:654:ILE:HG22 | 1:N:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:O:383:THR:O    | 1:O:386:LEU:HB3  | 2.14                     | 0.48              |
| 1:O:965:LEU:HD11 | 1:O:993:ILE:HG12 | 1.96                     | 0.48              |
| 1:P:383:THR:O    | 1:P:386:LEU:HB3  | 2.14                     | 0.48              |
| 1:P:499:GLN:CD   | 1:P:516:ASN:HB3  | 2.38                     | 0.48              |
| 1:A:198:LYS:NZ   | 1:B:222:HIS:CG   | 2.81                     | 0.48              |
| 1:A:502:ARG:HD3  | 1:A:516:ASN:HA   | 1.96                     | 0.48              |
| 1:A:654:ILE:HG22 | 1:A:670:HIS:HD2  | 1.78                     | 0.48              |
| 1:B:90:SER:OG    | 1:B:91:PRO:HD3   | 2.14                     | 0.48              |
| 1:B:441:ARG:O    | 1:B:445:ASP:HB3  | 2.14                     | 0.48              |
| 1:C:180:TRP:O    | 1:C:181:LEU:HD12 | 2.14                     | 0.48              |
| 1:C:247:VAL:HG21 | 1:C:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:383:THR:O    | 1:C:386:LEU:HB3  | 2.14                     | 0.48              |
| 1:C:441:ARG:O    | 1:C:445:ASP:HB3  | 2.14                     | 0.48              |
| 1:C:556:SER:O    | 1:C:557:LYS:HB2  | 2.13                     | 0.48              |
| 1:C:604:ASN:ND2  | 1:C:928:VAL:HB   | 2.29                     | 0.48              |
| 1:D:180:TRP:O    | 1:D:181:LEU:HD12 | 2.14                     | 0.48              |
| 1:D:398:VAL:HG23 | 1:D:399:MET:N    | 2.28                     | 0.48              |
| 1:D:447:TYR:O    | 1:D:447:TYR:CG   | 2.67                     | 0.48              |
| 1:E:180:TRP:O    | 1:E:181:LEU:HD12 | 2.14                     | 0.48              |
| 1:E:965:LEU:HD11 | 1:E:993:ILE:HG12 | 1.96                     | 0.48              |
| 1:I:11:GLN:O     | 1:I:14:ASP:N     | 2.46                     | 0.48              |
| 1:I:247:VAL:HG21 | 1:I:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:I:510:ALA:HB1  | 1:I:515:LEU:HA   | 1.96                     | 0.48              |
| 1:J:142:ARG:HH22 | 1:K:14:ASP:CG    | 2.22                     | 0.48              |
| 1:J:221:ILE:HG13 | 1:J:222:HIS:N    | 2.28                     | 0.48              |
| 1:J:382:PRO:HA   | 1:J:419:THR:CG2  | 2.36                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:247:VAL:HG21 | 1:K:264:LEU:HD22 | 1.96                     | 0.48              |
| 1:K:441:ARG:O    | 1:K:445:ASP:HB3  | 2.14                     | 0.48              |
| 1:K:447:TYR:O    | 1:K:447:TYR:CG   | 2.67                     | 0.48              |
| 1:L:152:VAL:O    | 1:L:155:SER:OG   | 2.29                     | 0.48              |
| 1:L:441:ARG:O    | 1:L:445:ASP:HB3  | 2.14                     | 0.48              |
| 1:L:447:TYR:O    | 1:L:447:TYR:CG   | 2.67                     | 0.48              |
| 1:L:538:LEU:HD21 | 1:L:573:ILE:HD11 | 1.94                     | 0.48              |
| 1:L:604:ASN:ND2  | 1:L:928:VAL:HB   | 2.29                     | 0.48              |
| 1:M:441:ARG:O    | 1:M:445:ASP:HB3  | 2.14                     | 0.48              |
| 1:N:175:ASP:O    | 1:N:177:LYS:HG2  | 2.13                     | 0.48              |
| 1:N:502:ARG:HD3  | 1:N:516:ASN:HA   | 1.96                     | 0.48              |
| 1:O:496:PHE:HE2  | 1:O:555:CYS:HG   | 1.59                     | 0.48              |
| 1:P:510:ALA:HB1  | 1:P:515:LEU:HA   | 1.96                     | 0.48              |
| 1:A:463:LEU:CD2  | 1:A:467:PHE:CD2  | 2.92                     | 0.47              |
| 1:A:965:LEU:HD11 | 1:A:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:A:1075:SER:OG  | 1:A:1094:ASP:O   | 2.29                     | 0.47              |
| 1:B:194:GLU:OE2  | 1:C:216:ASN:ND2  | 2.47                     | 0.47              |
| 1:B:478:ILE:HG22 | 1:B:479:GLU:N    | 2.29                     | 0.47              |
| 1:C:447:TYR:O    | 1:C:447:TYR:CG   | 2.67                     | 0.47              |
| 1:C:636:SER:O    | 1:C:637:LEU:O    | 2.31                     | 0.47              |
| 1:D:243:VAL:C    | 1:D:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:D:441:ARG:O    | 1:D:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:E:117:ASN:O    | 1:E:119:VAL:N    | 2.47                     | 0.47              |
| 1:E:124:ASN:C    | 1:E:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:E:478:ILE:HG22 | 1:E:479:GLU:N    | 2.29                     | 0.47              |
| 1:F:253:TRP:CZ3  | 1:F:262:ILE:HD11 | 2.48                     | 0.47              |
| 1:G:510:ALA:HB1  | 1:G:515:LEU:HA   | 1.96                     | 0.47              |
| 1:G:654:ILE:HG22 | 1:G:670:HIS:HD2  | 1.78                     | 0.47              |
| 1:H:253:TRP:CZ3  | 1:H:262:ILE:HD11 | 2.48                     | 0.47              |
| 1:H:965:LEU:HD11 | 1:H:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:I:253:TRP:CZ3  | 1:I:262:ILE:HD11 | 2.48                     | 0.47              |
| 1:J:117:ASN:O    | 1:J:119:VAL:N    | 2.47                     | 0.47              |
| 1:J:180:TRP:O    | 1:J:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:J:556:SER:O    | 1:J:557:LYS:HB2  | 2.13                     | 0.47              |
| 1:K:180:TRP:O    | 1:K:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:K:243:VAL:C    | 1:K:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:K:373:SER:CB   | 1:K:433:LEU:CD1  | 2.73                     | 0.47              |
| 1:L:247:VAL:HG21 | 1:L:264:LEU:HD22 | 1.96                     | 0.47              |
| 1:L:253:TRP:CZ3  | 1:L:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:N:965:LEU:HD11 | 1:N:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:O:11:GLN:O     | 1:O:14:ASP:N     | 2.46                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:1192:SER:OG  | 1:O:1208:GLU:OE2 | 2.28                     | 0.47              |
| 1:O:1252:ALA:HB1 | 1:O:1256:CYS:HB2 | 1.94                     | 0.47              |
| 1:P:604:ASN:ND2  | 1:P:928:VAL:HB   | 2.29                     | 0.47              |
| 1:P:654:ILE:HG22 | 1:P:670:HIS:HD2  | 1.78                     | 0.47              |
| 1:A:117:ASN:O    | 1:A:119:VAL:N    | 2.47                     | 0.47              |
| 1:A:604:ASN:ND2  | 1:A:928:VAL:HB   | 2.29                     | 0.47              |
| 1:A:638:GLU:OE1  | 1:A:640:GLU:N    | 2.42                     | 0.47              |
| 1:B:117:ASN:O    | 1:B:119:VAL:N    | 2.47                     | 0.47              |
| 1:B:180:TRP:O    | 1:B:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:C:365:TYR:OH   | 1:C:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:D:124:ASN:C    | 1:D:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:D:247:VAL:HG21 | 1:D:264:LEU:HD22 | 1.96                     | 0.47              |
| 1:D:376:PRO:HG3  | 1:D:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:D:496:PHE:HE2  | 1:D:555:CYS:HG   | 1.58                     | 0.47              |
| 1:D:552:ASN:HB3  | 1:D:1226:TYR:CE1 | 2.48                     | 0.47              |
| 1:D:875:LEU:CD2  | 1:D:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:E:247:VAL:HG21 | 1:E:264:LEU:HD22 | 1.96                     | 0.47              |
| 1:E:382:PRO:HA   | 1:E:419:THR:CG2  | 2.36                     | 0.47              |
| 1:E:441:ARG:O    | 1:E:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:E:453:PHE:CE2  | 1:E:460:PRO:HB3  | 2.49                     | 0.47              |
| 1:E:556:SER:O    | 1:E:557:LYS:HB2  | 2.13                     | 0.47              |
| 1:E:875:LEU:CD2  | 1:E:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:F:376:PRO:HG3  | 1:F:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:F:408:TYR:O    | 1:F:411:VAL:HG22 | 2.14                     | 0.47              |
| 1:G:253:TRP:CZ3  | 1:G:262:ILE:HD11 | 2.48                     | 0.47              |
| 1:G:462:TYR:OH   | 1:G:494:PHE:CZ   | 2.66                     | 0.47              |
| 1:G:502:ARG:HD3  | 1:G:516:ASN:HA   | 1.96                     | 0.47              |
| 1:G:556:SER:O    | 1:G:557:LYS:HB2  | 2.13                     | 0.47              |
| 1:G:602:ILE:HD12 | 1:G:900:GLU:HG2  | 1.96                     | 0.47              |
| 1:G:604:ASN:ND2  | 1:G:928:VAL:HB   | 2.29                     | 0.47              |
| 1:H:478:ILE:HG22 | 1:H:479:GLU:N    | 2.29                     | 0.47              |
| 1:H:554:ILE:O    | 1:H:556:SER:N    | 2.45                     | 0.47              |
| 1:H:1252:ALA:HB1 | 1:H:1256:CYS:HB2 | 1.94                     | 0.47              |
| 1:I:180:TRP:O    | 1:I:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:I:243:VAL:C    | 1:I:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:I:511:SER:HB3  | 1:I:645:LEU:HD21 | 1.95                     | 0.47              |
| 1:J:441:ARG:O    | 1:J:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:J:453:PHE:CE2  | 1:J:460:PRO:HB3  | 2.49                     | 0.47              |
| 1:J:478:ILE:HG22 | 1:J:479:GLU:N    | 2.30                     | 0.47              |
| 1:J:875:LEU:CD2  | 1:J:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:K:124:ASN:C    | 1:K:124:ASN:OD1  | 2.58                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:376:PRO:HG3  | 1:K:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:K:875:LEU:CD2  | 1:K:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:L:602:ILE:HD12 | 1:L:900:GLU:HG2  | 1.97                     | 0.47              |
| 1:M:180:TRP:O    | 1:M:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:M:187:ASN:HA   | 1:M:249:ASN:ND2  | 2.24                     | 0.47              |
| 1:M:478:ILE:HG22 | 1:M:479:GLU:N    | 2.30                     | 0.47              |
| 1:N:463:LEU:CD2  | 1:N:467:PHE:CD2  | 2.92                     | 0.47              |
| 1:N:604:ASN:ND2  | 1:N:928:VAL:HB   | 2.29                     | 0.47              |
| 1:O:253:TRP:CZ3  | 1:O:262:ILE:HD11 | 2.48                     | 0.47              |
| 1:O:1177:TYR:CE2 | 1:P:916:LYS:CE   | 2.97                     | 0.47              |
| 1:P:253:TRP:CZ3  | 1:P:262:ILE:HD11 | 2.48                     | 0.47              |
| 1:P:602:ILE:HD12 | 1:P:900:GLU:HG2  | 1.97                     | 0.47              |
| 1:A:64:THR:O     | 1:A:67:SER:OG    | 2.27                     | 0.47              |
| 1:B:365:TYR:OH   | 1:B:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:B:447:TYR:O    | 1:B:447:TYR:CG   | 2.67                     | 0.47              |
| 1:C:90:SER:OG    | 1:C:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:C:187:ASN:HA   | 1:C:249:ASN:ND2  | 2.24                     | 0.47              |
| 1:C:502:ARG:HD3  | 1:C:516:ASN:HA   | 1.96                     | 0.47              |
| 1:D:510:ALA:HB1  | 1:D:515:LEU:HA   | 1.96                     | 0.47              |
| 1:E:447:TYR:O    | 1:E:447:TYR:CG   | 2.67                     | 0.47              |
| 1:F:180:TRP:O    | 1:F:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:F:243:VAL:C    | 1:F:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:F:604:ASN:ND2  | 1:F:928:VAL:HB   | 2.29                     | 0.47              |
| 1:G:11:GLN:O     | 1:G:14:ASP:N     | 2.46                     | 0.47              |
| 1:G:253:TRP:CZ3  | 1:G:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:G:552:ASN:HB3  | 1:G:1226:TYR:CE1 | 2.48                     | 0.47              |
| 1:H:11:GLN:O     | 1:H:14:ASP:N     | 2.46                     | 0.47              |
| 1:I:376:PRO:HG3  | 1:I:473:HIS:CD2  | 2.50                     | 0.47              |
| 1:I:408:TYR:O    | 1:I:411:VAL:HG22 | 2.13                     | 0.47              |
| 1:I:463:LEU:HD22 | 1:I:467:PHE:HD2  | 1.74                     | 0.47              |
| 1:I:875:LEU:CD2  | 1:I:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:J:124:ASN:C    | 1:J:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:J:499:GLN:HG3  | 1:J:502:ARG:HB2  | 1.96                     | 0.47              |
| 1:J:602:ILE:HD12 | 1:J:900:GLU:HG2  | 1.97                     | 0.47              |
| 1:K:496:PHE:HE2  | 1:K:555:CYS:HG   | 1.58                     | 0.47              |
| 1:K:965:LEU:HD11 | 1:K:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:L:243:VAL:C    | 1:L:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:L:365:TYR:OH   | 1:L:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:L:383:THR:O    | 1:L:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:L:483:ARG:O    | 1:L:486:LEU:N    | 2.48                     | 0.47              |
| 1:M:117:ASN:O    | 1:M:119:VAL:N    | 2.48                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:447:TYR:O    | 1:M:447:TYR:CG   | 2.67                     | 0.47              |
| 1:N:117:ASN:O    | 1:N:119:VAL:N    | 2.47                     | 0.47              |
| 1:O:324:LEU:HD12 | 1:O:324:LEU:HA   | 1.61                     | 0.47              |
| 1:O:554:ILE:O    | 1:O:556:SER:N    | 2.45                     | 0.47              |
| 1:P:11:GLN:O     | 1:P:14:ASP:N     | 2.46                     | 0.47              |
| 1:P:253:TRP:CZ3  | 1:P:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:A:376:PRO:HG3  | 1:A:473:HIS:CD2  | 2.50                     | 0.47              |
| 1:A:443:ILE:HG21 | 1:A:477:ASN:ND2  | 2.24                     | 0.47              |
| 1:A:875:LEU:CD2  | 1:A:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:B:187:ASN:HA   | 1:B:249:ASN:ND2  | 2.24                     | 0.47              |
| 1:C:198:LYS:HZ1  | 1:D:222:HIS:CG   | 2.32                     | 0.47              |
| 1:C:483:ARG:O    | 1:C:486:LEU:N    | 2.48                     | 0.47              |
| 1:C:523:PHE:HD1  | 1:C:527:TYR:CE2  | 2.28                     | 0.47              |
| 1:C:602:ILE:HD12 | 1:C:900:GLU:HG2  | 1.97                     | 0.47              |
| 1:D:90:SER:OG    | 1:D:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:D:122:LYS:O    | 1:D:303:LYS:NZ   | 2.38                     | 0.47              |
| 1:D:511:SER:C    | 1:D:513:SER:N    | 2.60                     | 0.47              |
| 1:D:965:LEU:HD11 | 1:D:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:E:90:SER:OG    | 1:E:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:E:243:VAL:C    | 1:E:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:E:499:GLN:HG3  | 1:E:502:ARG:HB2  | 1.96                     | 0.47              |
| 1:E:602:ILE:HD12 | 1:E:900:GLU:HG2  | 1.97                     | 0.47              |
| 1:F:124:ASN:C    | 1:F:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:F:451:LYS:CD   | 1:F:486:LEU:HD21 | 2.33                     | 0.47              |
| 1:F:875:LEU:CD2  | 1:F:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:I:124:ASN:C    | 1:I:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:I:462:TYR:OH   | 1:I:494:PHE:CZ   | 2.66                     | 0.47              |
| 1:I:1252:ALA:HB1 | 1:I:1256:CYS:HB2 | 1.94                     | 0.47              |
| 1:J:243:VAL:C    | 1:J:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:J:247:VAL:HG21 | 1:J:264:LEU:HD22 | 1.96                     | 0.47              |
| 1:J:447:TYR:O    | 1:J:447:TYR:CG   | 2.67                     | 0.47              |
| 1:J:463:LEU:CD2  | 1:J:467:PHE:CD2  | 2.92                     | 0.47              |
| 1:K:510:ALA:HB1  | 1:K:515:LEU:HA   | 1.96                     | 0.47              |
| 1:L:124:ASN:C    | 1:L:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:M:365:TYR:OH   | 1:M:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:N:376:PRO:HG3  | 1:N:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:N:523:PHE:HD1  | 1:N:527:TYR:CE2  | 2.28                     | 0.47              |
| 1:N:875:LEU:CD2  | 1:N:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:O:478:ILE:HG22 | 1:O:479:GLU:N    | 2.30                     | 0.47              |
| 1:P:90:SER:OG    | 1:P:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:P:502:ARG:HD3  | 1:P:516:ASN:HA   | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:552:ASN:HB3  | 1:P:1226:TYR:CE1 | 2.48                     | 0.47              |
| 1:P:556:SER:O    | 1:P:557:LYS:HB2  | 2.13                     | 0.47              |
| 1:A:383:THR:O    | 1:A:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:A:408:TYR:O    | 1:A:411:VAL:HG22 | 2.14                     | 0.47              |
| 1:B:636:SER:O    | 1:B:637:LEU:O    | 2.31                     | 0.47              |
| 1:B:965:LEU:HD11 | 1:B:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:C:124:ASN:C    | 1:C:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:C:152:VAL:O    | 1:C:155:SER:OG   | 2.29                     | 0.47              |
| 1:C:317:LEU:C    | 1:C:318:THR:HG1  | 1.95                     | 0.47              |
| 1:C:478:ILE:HG22 | 1:C:479:GLU:N    | 2.29                     | 0.47              |
| 1:E:483:ARG:O    | 1:E:486:LEU:N    | 2.48                     | 0.47              |
| 1:F:11:GLN:O     | 1:F:14:ASP:N     | 2.46                     | 0.47              |
| 1:F:253:TRP:CZ3  | 1:F:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:F:365:TYR:OH   | 1:F:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:F:483:ARG:O    | 1:F:486:LEU:N    | 2.48                     | 0.47              |
| 1:F:1252:ALA:HB1 | 1:F:1256:CYS:HB2 | 1.95                     | 0.47              |
| 1:G:90:SER:OG    | 1:G:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:G:636:SER:O    | 1:G:637:LEU:O    | 2.31                     | 0.47              |
| 1:H:510:ALA:HB1  | 1:H:515:LEU:HA   | 1.96                     | 0.47              |
| 1:H:875:LEU:CD2  | 1:H:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:H:1192:SER:OG  | 1:H:1208:GLU:OE2 | 2.28                     | 0.47              |
| 1:I:478:ILE:HG22 | 1:I:479:GLU:N    | 2.29                     | 0.47              |
| 1:I:604:ASN:ND2  | 1:I:928:VAL:HB   | 2.29                     | 0.47              |
| 1:J:483:ARG:O    | 1:J:486:LEU:N    | 2.48                     | 0.47              |
| 1:J:604:ASN:ND2  | 1:J:928:VAL:HB   | 2.29                     | 0.47              |
| 1:J:988:ASP:OD1  | 1:J:989:SER:N    | 2.43                     | 0.47              |
| 1:K:552:ASN:HB3  | 1:K:1226:TYR:CE1 | 2.48                     | 0.47              |
| 1:L:392:ASP:OD1  | 1:L:393:VAL:N    | 2.47                     | 0.47              |
| 1:L:502:ARG:HD3  | 1:L:516:ASN:HA   | 1.96                     | 0.47              |
| 1:L:556:SER:O    | 1:L:557:LYS:HB2  | 2.13                     | 0.47              |
| 1:L:965:LEU:HD11 | 1:L:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:M:221:ILE:HG13 | 1:M:222:HIS:N    | 2.28                     | 0.47              |
| 1:M:636:SER:O    | 1:M:637:LEU:O    | 2.31                     | 0.47              |
| 1:M:875:LEU:CD2  | 1:M:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:M:965:LEU:HD11 | 1:M:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:N:365:TYR:OH   | 1:N:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:N:383:THR:O    | 1:N:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:O:636:SER:O    | 1:O:637:LEU:O    | 2.31                     | 0.47              |
| 1:P:636:SER:O    | 1:P:637:LEU:O    | 2.31                     | 0.47              |
| 1:A:365:TYR:OH   | 1:A:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:A:604:ASN:ND2  | 1:A:929:VAL:H    | 2.04                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:916:LYS:HE2  | 1:B:1177:TYR:CE2 | 2.47                     | 0.47              |
| 1:B:221:ILE:HG13 | 1:B:222:HIS:N    | 2.28                     | 0.47              |
| 1:B:383:THR:O    | 1:B:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:B:615:TYR:CD1  | 1:B:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:B:875:LEU:CD2  | 1:B:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:C:499:GLN:CD   | 1:C:516:ASN:HB3  | 2.39                     | 0.47              |
| 1:C:965:LEU:HD11 | 1:C:993:ILE:HG12 | 1.96                     | 0.47              |
| 1:D:352:ILE:O    | 1:D:356:SER:OG   | 2.29                     | 0.47              |
| 1:E:383:THR:O    | 1:E:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:E:463:LEU:HD22 | 1:E:467:PHE:HD2  | 1.74                     | 0.47              |
| 1:E:604:ASN:ND2  | 1:E:928:VAL:HB   | 2.29                     | 0.47              |
| 1:F:615:TYR:CD1  | 1:F:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:G:615:TYR:CD1  | 1:G:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:H:636:SER:O    | 1:H:637:LEU:O    | 2.31                     | 0.47              |
| 1:H:811:ASP:OD1  | 1:H:812:THR:N    | 2.47                     | 0.47              |
| 1:I:483:ARG:O    | 1:I:486:LEU:N    | 2.48                     | 0.47              |
| 1:I:900:GLU:HB2  | 1:I:930:HIS:CD2  | 2.48                     | 0.47              |
| 1:J:90:SER:OG    | 1:J:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:J:463:LEU:HD22 | 1:J:467:PHE:HD2  | 1.74                     | 0.47              |
| 1:K:90:SER:OG    | 1:K:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:L:90:SER:OG    | 1:L:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:L:170:VAL:O    | 1:L:173:LYS:N    | 2.48                     | 0.47              |
| 1:L:478:ILE:HG22 | 1:L:479:GLU:N    | 2.29                     | 0.47              |
| 1:L:499:GLN:CD   | 1:L:516:ASN:HB3  | 2.38                     | 0.47              |
| 1:M:615:TYR:CD1  | 1:M:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:N:408:TYR:O    | 1:N:411:VAL:HG22 | 2.14                     | 0.47              |
| 1:N:638:GLU:OE1  | 1:N:640:GLU:N    | 2.42                     | 0.47              |
| 1:O:376:PRO:HG3  | 1:O:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:O:811:ASP:OD1  | 1:O:812:THR:N    | 2.46                     | 0.47              |
| 1:O:875:LEU:CD2  | 1:O:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:P:615:TYR:CD1  | 1:P:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:A:441:ARG:O    | 1:A:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:A:447:TYR:O    | 1:A:447:TYR:CG   | 2.67                     | 0.47              |
| 1:A:523:PHE:HD1  | 1:A:527:TYR:CE2  | 2.28                     | 0.47              |
| 1:A:602:ILE:HD12 | 1:A:900:GLU:HG2  | 1.97                     | 0.47              |
| 1:A:615:TYR:CD1  | 1:A:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:A:636:SER:O    | 1:A:637:LEU:O    | 2.31                     | 0.47              |
| 1:B:376:PRO:HG3  | 1:B:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:B:1074:HIS:O   | 1:B:1075:SER:OG  | 2.33                     | 0.47              |
| 1:C:115:ASN:HB3  | 1:D:257:ASN:OD1  | 2.14                     | 0.47              |
| 1:C:117:ASN:O    | 1:C:119:VAL:N    | 2.47                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:170:VAL:O    | 1:C:173:LYS:N    | 2.48                     | 0.47              |
| 1:C:243:VAL:C    | 1:C:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:C:392:ASP:OD1  | 1:C:393:VAL:N    | 2.47                     | 0.47              |
| 1:D:117:ASN:O    | 1:D:119:VAL:N    | 2.47                     | 0.47              |
| 1:D:253:TRP:CZ3  | 1:D:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:D:483:ARG:O    | 1:D:486:LEU:N    | 2.48                     | 0.47              |
| 1:D:604:ASN:ND2  | 1:D:928:VAL:HB   | 2.29                     | 0.47              |
| 1:E:170:VAL:O    | 1:E:173:LYS:N    | 2.48                     | 0.47              |
| 1:E:499:GLN:CD   | 1:E:516:ASN:HB3  | 2.38                     | 0.47              |
| 1:E:554:ILE:O    | 1:E:556:SER:N    | 2.45                     | 0.47              |
| 1:E:988:ASP:OD1  | 1:E:989:SER:N    | 2.43                     | 0.47              |
| 1:F:170:VAL:O    | 1:F:173:LYS:N    | 2.48                     | 0.47              |
| 1:F:441:ARG:O    | 1:F:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:F:478:ILE:HG22 | 1:F:479:GLU:N    | 2.30                     | 0.47              |
| 1:F:556:SER:O    | 1:F:557:LYS:HB2  | 2.13                     | 0.47              |
| 1:F:900:GLU:HB2  | 1:F:930:HIS:CD2  | 2.48                     | 0.47              |
| 1:G:117:ASN:O    | 1:G:119:VAL:N    | 2.47                     | 0.47              |
| 1:G:243:VAL:C    | 1:G:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:G:331:ILE:HG21 | 1:G:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:G:346:CYS:O    | 1:G:350:THR:N    | 2.25                     | 0.47              |
| 1:G:441:ARG:O    | 1:G:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:G:483:ARG:O    | 1:G:486:LEU:N    | 2.48                     | 0.47              |
| 1:G:537:ARG:HA   | 1:G:540:ASN:HB2  | 1.97                     | 0.47              |
| 1:G:875:LEU:CD2  | 1:G:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:H:90:SER:OG    | 1:H:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:H:243:VAL:C    | 1:H:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:H:376:PRO:HG3  | 1:H:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:H:441:ARG:O    | 1:H:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:H:447:TYR:O    | 1:H:447:TYR:CG   | 2.67                     | 0.47              |
| 1:H:508:TRP:C    | 1:H:606:GLY:N    | 2.70                     | 0.47              |
| 1:H:537:ARG:HA   | 1:H:540:ASN:HB2  | 1.97                     | 0.47              |
| 1:I:253:TRP:CZ3  | 1:I:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:I:365:TYR:OH   | 1:I:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:I:556:SER:O    | 1:I:557:LYS:HB2  | 2.13                     | 0.47              |
| 1:I:615:TYR:CD1  | 1:I:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:J:170:VAL:O    | 1:J:173:LYS:N    | 2.48                     | 0.47              |
| 1:J:499:GLN:CD   | 1:J:516:ASN:HB3  | 2.39                     | 0.47              |
| 1:K:122:LYS:O    | 1:K:303:LYS:NZ   | 2.38                     | 0.47              |
| 1:K:331:ILE:HG21 | 1:K:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:K:482:GLU:C    | 1:K:485:THR:HG1  | 2.23                     | 0.47              |
| 1:K:604:ASN:ND2  | 1:K:928:VAL:HB   | 2.29                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:212:ASP:OD2  | 1:M:209:SER:CB   | 2.57                     | 0.47              |
| 1:L:510:ALA:HB1  | 1:L:515:LEU:HA   | 1.96                     | 0.47              |
| 1:L:523:PHE:HD1  | 1:L:527:TYR:CE2  | 2.28                     | 0.47              |
| 1:L:635:VAL:HB   | 1:L:641:ASP:CG   | 2.40                     | 0.47              |
| 1:L:875:LEU:CD2  | 1:L:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:M:376:PRO:HG3  | 1:M:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:M:383:THR:O    | 1:M:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:N:122:LYS:O    | 1:N:303:LYS:NZ   | 2.37                     | 0.47              |
| 1:N:441:ARG:O    | 1:N:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:N:443:ILE:HG21 | 1:N:477:ASN:ND2  | 2.24                     | 0.47              |
| 1:N:602:ILE:HD12 | 1:N:900:GLU:HG2  | 1.97                     | 0.47              |
| 1:N:604:ASN:ND2  | 1:N:929:VAL:H    | 2.04                     | 0.47              |
| 1:N:615:TYR:CD1  | 1:N:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:N:1074:HIS:O   | 1:N:1075:SER:OG  | 2.33                     | 0.47              |
| 1:O:243:VAL:C    | 1:O:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:O:441:ARG:O    | 1:O:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:O:447:TYR:O    | 1:O:447:TYR:CG   | 2.67                     | 0.47              |
| 1:O:508:TRP:C    | 1:O:606:GLY:N    | 2.70                     | 0.47              |
| 1:O:510:ALA:HB1  | 1:O:515:LEU:HA   | 1.96                     | 0.47              |
| 1:O:537:ARG:HA   | 1:O:540:ASN:HB2  | 1.97                     | 0.47              |
| 1:O:615:TYR:CD1  | 1:O:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:O:654:ILE:HG22 | 1:O:670:HIS:HD2  | 1.78                     | 0.47              |
| 1:P:117:ASN:O    | 1:P:119:VAL:N    | 2.48                     | 0.47              |
| 1:P:331:ILE:HG21 | 1:P:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:P:441:ARG:O    | 1:P:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:P:483:ARG:O    | 1:P:486:LEU:N    | 2.48                     | 0.47              |
| 1:P:537:ARG:HA   | 1:P:540:ASN:HB2  | 1.97                     | 0.47              |
| 1:P:875:LEU:CD2  | 1:P:911:PHE:CE2  | 2.97                     | 0.47              |
| 1:A:510:ALA:HB1  | 1:A:515:LEU:HA   | 1.96                     | 0.47              |
| 1:B:604:ASN:ND2  | 1:B:928:VAL:HB   | 2.29                     | 0.47              |
| 1:C:615:TYR:CD1  | 1:C:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:C:1074:HIS:O   | 1:C:1075:SER:OG  | 2.33                     | 0.47              |
| 1:E:331:ILE:HG21 | 1:E:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:E:615:TYR:CD1  | 1:E:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:F:293:THR:O    | 1:F:296:GLU:N    | 2.40                     | 0.47              |
| 1:F:331:ILE:HG21 | 1:F:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:F:641:ASP:OD1  | 1:F:642:THR:N    | 2.45                     | 0.47              |
| 1:G:124:ASN:C    | 1:G:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:H:483:ARG:O    | 1:H:486:LEU:N    | 2.47                     | 0.47              |
| 1:H:615:TYR:CD1  | 1:H:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:H:654:ILE:HG22 | 1:H:670:HIS:HD2  | 1.79                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:170:VAL:O    | 1:I:173:LYS:N    | 2.48                     | 0.47              |
| 1:I:508:TRP:C    | 1:I:606:GLY:N    | 2.70                     | 0.47              |
| 1:J:331:ILE:HG21 | 1:J:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:J:383:THR:O    | 1:J:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:J:615:TYR:CD1  | 1:J:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:K:253:TRP:CZ3  | 1:K:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:K:483:ARG:O    | 1:K:486:LEU:N    | 2.48                     | 0.47              |
| 1:L:117:ASN:O    | 1:L:119:VAL:N    | 2.47                     | 0.47              |
| 1:L:337:THR:HG1  | 1:L:340:ASN:H    | 1.63                     | 0.47              |
| 1:L:482:GLU:C    | 1:L:485:THR:HG1  | 2.23                     | 0.47              |
| 1:L:615:TYR:CD1  | 1:L:622:LEU:HD13 | 2.50                     | 0.47              |
| 1:M:222:HIS:CG   | 1:N:198:LYS:HZ1  | 2.33                     | 0.47              |
| 1:M:458:LEU:HA   | 1:M:587:ARG:HH21 | 1.80                     | 0.47              |
| 1:M:635:VAL:HB   | 1:M:641:ASP:CG   | 2.40                     | 0.47              |
| 1:M:1074:HIS:O   | 1:M:1075:SER:OG  | 2.33                     | 0.47              |
| 1:N:247:VAL:HG21 | 1:N:264:LEU:HD22 | 1.96                     | 0.47              |
| 1:N:447:TYR:O    | 1:N:447:TYR:CG   | 2.67                     | 0.47              |
| 1:N:557:LYS:HZ2  | 1:N:1223:GLN:HG3 | 1.79                     | 0.47              |
| 1:O:90:SER:OG    | 1:O:91:PRO:HD3   | 2.14                     | 0.47              |
| 1:O:483:ARG:O    | 1:O:486:LEU:N    | 2.48                     | 0.47              |
| 1:P:1075:SER:OG  | 1:P:1094:ASP:O   | 2.29                     | 0.47              |
| 1:A:180:TRP:O    | 1:A:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:A:247:VAL:HG21 | 1:A:264:LEU:HD22 | 1.96                     | 0.47              |
| 1:A:1074:HIS:O   | 1:A:1075:SER:OG  | 2.33                     | 0.47              |
| 1:B:483:ARG:O    | 1:B:486:LEU:N    | 2.48                     | 0.47              |
| 1:B:635:VAL:HB   | 1:B:641:ASP:CG   | 2.40                     | 0.47              |
| 1:C:371:ARG:HB3  | 1:C:389:ILE:CG2  | 2.45                     | 0.47              |
| 1:C:482:GLU:C    | 1:C:485:THR:HG1  | 2.23                     | 0.47              |
| 1:D:293:THR:HG22 | 1:D:295:ASP:H    | 1.80                     | 0.47              |
| 1:D:331:ILE:HG21 | 1:D:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:D:453:PHE:CE2  | 1:D:460:PRO:HB3  | 2.49                     | 0.47              |
| 1:E:293:THR:HG22 | 1:E:295:ASP:H    | 1.80                     | 0.47              |
| 1:G:496:PHE:HE2  | 1:G:555:CYS:HG   | 1.61                     | 0.47              |
| 1:H:331:ILE:HG21 | 1:H:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:I:301:LEU:CD2  | 1:I:313:PRO:CG   | 2.87                     | 0.47              |
| 1:I:635:VAL:HB   | 1:I:641:ASP:CG   | 2.40                     | 0.47              |
| 1:J:554:ILE:O    | 1:J:556:SER:N    | 2.46                     | 0.47              |
| 1:K:117:ASN:O    | 1:K:119:VAL:N    | 2.48                     | 0.47              |
| 1:K:293:THR:HG22 | 1:K:295:ASP:H    | 1.80                     | 0.47              |
| 1:K:635:VAL:HB   | 1:K:641:ASP:CG   | 2.40                     | 0.47              |
| 1:M:483:ARG:O    | 1:M:486:LEU:N    | 2.48                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:604:ASN:ND2  | 1:M:928:VAL:HB   | 2.29                     | 0.47              |
| 1:N:312:LEU:HD23 | 1:N:312:LEU:C    | 2.40                     | 0.47              |
| 1:N:478:ILE:HG22 | 1:N:479:GLU:N    | 2.30                     | 0.47              |
| 1:N:483:ARG:O    | 1:N:486:LEU:N    | 2.48                     | 0.47              |
| 1:N:510:ALA:HB1  | 1:N:515:LEU:HA   | 1.96                     | 0.47              |
| 1:N:636:SER:O    | 1:N:637:LEU:O    | 2.31                     | 0.47              |
| 1:O:331:ILE:HG21 | 1:O:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:P:124:ASN:C    | 1:P:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:P:243:VAL:C    | 1:P:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:P:346:CYS:O    | 1:P:350:THR:N    | 2.25                     | 0.47              |
| 1:P:496:PHE:HE2  | 1:P:555:CYS:HG   | 1.61                     | 0.47              |
| 1:A:243:VAL:C    | 1:A:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:A:293:THR:O    | 1:A:296:GLU:N    | 2.40                     | 0.47              |
| 1:A:312:LEU:HD23 | 1:A:312:LEU:C    | 2.40                     | 0.47              |
| 1:A:478:ILE:HG22 | 1:A:479:GLU:N    | 2.30                     | 0.47              |
| 1:A:483:ARG:O    | 1:A:486:LEU:N    | 2.48                     | 0.47              |
| 1:B:124:ASN:C    | 1:B:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:B:243:VAL:C    | 1:B:244:LEU:HD12 | 2.39                     | 0.47              |
| 1:B:811:ASP:OD1  | 1:B:812:THR:N    | 2.46                     | 0.47              |
| 1:C:122:LYS:HG3  | 1:D:276:SER:CB   | 2.45                     | 0.47              |
| 1:C:443:ILE:HG21 | 1:C:477:ASN:ND2  | 2.24                     | 0.47              |
| 1:C:451:LYS:CD   | 1:C:486:LEU:HD21 | 2.33                     | 0.47              |
| 1:D:54:ALA:O     | 1:D:58:THR:N     | 2.48                     | 0.47              |
| 1:D:365:TYR:OH   | 1:D:404:LYS:HG2  | 2.15                     | 0.47              |
| 1:D:383:THR:O    | 1:D:386:LEU:HB3  | 2.14                     | 0.47              |
| 1:D:443:ILE:HG21 | 1:D:477:ASN:ND2  | 2.24                     | 0.47              |
| 1:D:463:LEU:HD22 | 1:D:467:PHE:HD2  | 1.74                     | 0.47              |
| 1:D:478:ILE:HG22 | 1:D:479:GLU:N    | 2.30                     | 0.47              |
| 1:D:635:VAL:HB   | 1:D:641:ASP:CG   | 2.40                     | 0.47              |
| 1:D:811:ASP:OD1  | 1:D:812:THR:N    | 2.46                     | 0.47              |
| 1:E:253:TRP:CZ3  | 1:E:264:LEU:HD11 | 2.49                     | 0.47              |
| 1:F:447:TYR:O    | 1:F:447:TYR:CG   | 2.67                     | 0.47              |
| 1:F:552:ASN:HB3  | 1:F:1226:TYR:CE1 | 2.48                     | 0.47              |
| 1:F:635:VAL:HB   | 1:F:641:ASP:CG   | 2.40                     | 0.47              |
| 1:G:312:LEU:HD23 | 1:G:312:LEU:C    | 2.40                     | 0.47              |
| 1:I:331:ILE:HG21 | 1:I:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:I:441:ARG:O    | 1:I:445:ASP:HB3  | 2.14                     | 0.47              |
| 1:I:447:TYR:O    | 1:I:447:TYR:CG   | 2.67                     | 0.47              |
| 1:I:508:TRP:O    | 1:I:606:GLY:CA   | 2.63                     | 0.47              |
| 1:J:293:THR:HG22 | 1:J:295:ASP:H    | 1.80                     | 0.47              |
| 1:K:54:ALA:O     | 1:K:58:THR:N     | 2.48                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:64:THR:O     | 1:K:67:SER:OG    | 2.27                     | 0.47              |
| 1:K:453:PHE:CE2  | 1:K:460:PRO:HB3  | 2.49                     | 0.47              |
| 1:K:478:ILE:HG22 | 1:K:479:GLU:N    | 2.29                     | 0.47              |
| 1:K:504:ASP:CG   | 1:K:608:ASN:ND2  | 2.69                     | 0.47              |
| 1:K:511:SER:C    | 1:K:513:SER:N    | 2.61                     | 0.47              |
| 1:L:331:ILE:HG21 | 1:L:338:TRP:HB2  | 1.97                     | 0.47              |
| 1:L:371:ARG:HB3  | 1:L:389:ILE:CG2  | 2.45                     | 0.47              |
| 1:L:376:PRO:HG3  | 1:L:473:HIS:CD2  | 2.49                     | 0.47              |
| 1:L:811:ASP:OD1  | 1:L:812:THR:N    | 2.46                     | 0.47              |
| 1:M:124:ASN:C    | 1:M:124:ASN:OD1  | 2.58                     | 0.47              |
| 1:M:510:ALA:HB1  | 1:M:515:LEU:HA   | 1.96                     | 0.47              |
| 1:N:180:TRP:O    | 1:N:181:LEU:HD12 | 2.14                     | 0.47              |
| 1:N:293:THR:O    | 1:N:296:GLU:N    | 2.40                     | 0.47              |
| 1:O:117:ASN:O    | 1:O:119:VAL:N    | 2.47                     | 0.47              |
| 1:P:312:LEU:HD23 | 1:P:312:LEU:C    | 2.40                     | 0.47              |
| 1:A:811:ASP:OD1  | 1:A:812:THR:N    | 2.46                     | 0.46              |
| 1:B:458:LEU:HA   | 1:B:587:ARG:HH21 | 1.80                     | 0.46              |
| 1:B:510:ALA:HB1  | 1:B:515:LEU:HA   | 1.96                     | 0.46              |
| 1:C:635:VAL:HB   | 1:C:641:ASP:CG   | 2.40                     | 0.46              |
| 1:C:875:LEU:CD2  | 1:C:911:PHE:CE2  | 2.97                     | 0.46              |
| 1:D:504:ASP:CG   | 1:D:608:ASN:ND2  | 2.69                     | 0.46              |
| 1:E:201:TYR:CZ   | 1:F:223:SER:OG   | 2.65                     | 0.46              |
| 1:E:358:ASN:HA   | 1:E:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:F:508:TRP:C    | 1:F:606:GLY:N    | 2.70                     | 0.46              |
| 1:H:117:ASN:O    | 1:H:119:VAL:N    | 2.48                     | 0.46              |
| 1:H:462:TYR:OH   | 1:H:494:PHE:CZ   | 2.66                     | 0.46              |
| 1:I:117:ASN:O    | 1:I:119:VAL:N    | 2.47                     | 0.46              |
| 1:J:635:VAL:HB   | 1:J:641:ASP:CG   | 2.40                     | 0.46              |
| 1:K:317:LEU:C    | 1:K:318:THR:HG1  | 1.95                     | 0.46              |
| 1:K:383:THR:O    | 1:K:386:LEU:HB3  | 2.14                     | 0.46              |
| 1:K:638:GLU:OE1  | 1:K:640:GLU:N    | 2.42                     | 0.46              |
| 1:K:811:ASP:OD1  | 1:K:812:THR:N    | 2.46                     | 0.46              |
| 1:L:1074:HIS:O   | 1:L:1075:SER:OG  | 2.33                     | 0.46              |
| 1:N:811:ASP:OD1  | 1:N:812:THR:N    | 2.46                     | 0.46              |
| 1:O:365:TYR:OH   | 1:O:404:LYS:HG2  | 2.15                     | 0.46              |
| 1:O:462:TYR:OH   | 1:O:494:PHE:CZ   | 2.66                     | 0.46              |
| 1:O:502:ARG:HD3  | 1:O:516:ASN:HA   | 1.96                     | 0.46              |
| 1:P:247:VAL:HG21 | 1:P:264:LEU:HD22 | 1.96                     | 0.46              |
| 1:P:376:PRO:HG3  | 1:P:473:HIS:CD2  | 2.49                     | 0.46              |
| 1:A:122:LYS:HG3  | 1:B:276:SER:CB   | 2.44                     | 0.46              |
| 1:A:293:THR:HG22 | 1:A:295:ASP:H    | 1.80                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:331:ILE:HG21 | 1:A:338:TRP:HB2  | 1.97                     | 0.46              |
| 1:A:458:LEU:HA   | 1:A:587:ARG:HH21 | 1.80                     | 0.46              |
| 1:A:537:ARG:HA   | 1:A:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:A:635:VAL:HB   | 1:A:641:ASP:CG   | 2.40                     | 0.46              |
| 1:B:504:ASP:CG   | 1:B:608:ASN:ND2  | 2.69                     | 0.46              |
| 1:C:376:PRO:HG3  | 1:C:473:HIS:CD2  | 2.49                     | 0.46              |
| 1:C:462:TYR:OH   | 1:C:494:PHE:CZ   | 2.66                     | 0.46              |
| 1:C:504:ASP:CG   | 1:C:608:ASN:ND2  | 2.69                     | 0.46              |
| 1:C:510:ALA:HB1  | 1:C:515:LEU:HA   | 1.96                     | 0.46              |
| 1:D:543:LEU:O    | 1:D:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:D:615:TYR:CD1  | 1:D:622:LEU:HD13 | 2.50                     | 0.46              |
| 1:D:638:GLU:OE1  | 1:D:640:GLU:N    | 2.42                     | 0.46              |
| 1:E:502:ARG:HD3  | 1:E:516:ASN:HA   | 1.96                     | 0.46              |
| 1:F:508:TRP:O    | 1:F:606:GLY:CA   | 2.63                     | 0.46              |
| 1:F:543:LEU:O    | 1:F:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:G:247:VAL:HG21 | 1:G:264:LEU:HD22 | 1.96                     | 0.46              |
| 1:G:365:TYR:OH   | 1:G:404:LYS:HG2  | 2.15                     | 0.46              |
| 1:G:447:TYR:O    | 1:G:447:TYR:CG   | 2.67                     | 0.46              |
| 1:H:251:APK:H2'  | 1:H:251:APK:H8   | 1.74                     | 0.46              |
| 1:H:365:TYR:OH   | 1:H:404:LYS:HG2  | 2.15                     | 0.46              |
| 1:H:604:ASN:ND2  | 1:H:928:VAL:HB   | 2.29                     | 0.46              |
| 1:I:293:THR:O    | 1:I:296:GLU:N    | 2.40                     | 0.46              |
| 1:I:602:ILE:HD12 | 1:I:900:GLU:HG2  | 1.97                     | 0.46              |
| 1:J:253:TRP:CZ3  | 1:J:264:LEU:HD11 | 2.49                     | 0.46              |
| 1:J:352:ILE:O    | 1:J:356:SER:OG   | 2.29                     | 0.46              |
| 1:K:463:LEU:HD22 | 1:K:467:PHE:HD2  | 1.74                     | 0.46              |
| 1:K:615:TYR:CD1  | 1:K:622:LEU:HD13 | 2.50                     | 0.46              |
| 1:L:504:ASP:CG   | 1:L:608:ASN:ND2  | 2.69                     | 0.46              |
| 1:L:537:ARG:HA   | 1:L:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:M:811:ASP:OD1  | 1:M:812:THR:N    | 2.47                     | 0.46              |
| 1:N:243:VAL:C    | 1:N:244:LEU:HD12 | 2.39                     | 0.46              |
| 1:N:293:THR:HG22 | 1:N:295:ASP:H    | 1.80                     | 0.46              |
| 1:N:458:LEU:HA   | 1:N:587:ARG:HH21 | 1.80                     | 0.46              |
| 1:N:537:ARG:HA   | 1:N:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:O:504:ASP:CG   | 1:O:608:ASN:ND2  | 2.69                     | 0.46              |
| 1:O:1201:THR:OG1 | 1:O:1202:MET:N   | 2.48                     | 0.46              |
| 1:P:447:TYR:O    | 1:P:447:TYR:CG   | 2.67                     | 0.46              |
| 1:P:478:ILE:HG22 | 1:P:479:GLU:N    | 2.29                     | 0.46              |
| 1:P:508:TRP:O    | 1:P:606:GLY:CA   | 2.63                     | 0.46              |
| 1:P:1192:SER:OG  | 1:P:1208:GLU:OE2 | 2.28                     | 0.46              |
| 1:A:133:LYS:O    | 1:A:136:GLN:HB3  | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:502:ARG:HD3  | 1:B:516:ASN:HA   | 1.96                     | 0.46              |
| 1:C:54:ALA:O     | 1:C:58:THR:N     | 2.48                     | 0.46              |
| 1:C:312:LEU:HD23 | 1:C:312:LEU:C    | 2.40                     | 0.46              |
| 1:C:331:ILE:HG21 | 1:C:338:TRP:HB2  | 1.97                     | 0.46              |
| 1:C:811:ASP:OD1  | 1:C:812:THR:N    | 2.46                     | 0.46              |
| 1:D:537:ARG:HA   | 1:D:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:E:225:GLN:HG3  | 1:E:258:LEU:HD22 | 1.98                     | 0.46              |
| 1:E:376:PRO:HG3  | 1:E:473:HIS:CD2  | 2.49                     | 0.46              |
| 1:E:635:VAL:HB   | 1:E:641:ASP:CG   | 2.40                     | 0.46              |
| 1:E:811:ASP:OD1  | 1:E:812:THR:N    | 2.46                     | 0.46              |
| 1:F:537:ARG:HA   | 1:F:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:F:602:ILE:HD12 | 1:F:900:GLU:HG2  | 1.96                     | 0.46              |
| 1:G:133:LYS:O    | 1:G:136:GLN:HB3  | 2.16                     | 0.46              |
| 1:G:376:PRO:HG3  | 1:G:473:HIS:CD2  | 2.50                     | 0.46              |
| 1:G:508:TRP:O    | 1:G:606:GLY:CA   | 2.63                     | 0.46              |
| 1:G:811:ASP:OD1  | 1:G:812:THR:N    | 2.47                     | 0.46              |
| 1:G:1192:SER:OG  | 1:G:1208:GLU:OE2 | 2.28                     | 0.46              |
| 1:H:502:ARG:HD3  | 1:H:516:ASN:HA   | 1.96                     | 0.46              |
| 1:H:504:ASP:CG   | 1:H:608:ASN:ND2  | 2.69                     | 0.46              |
| 1:I:543:LEU:O    | 1:I:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:I:552:ASN:HB3  | 1:I:1226:TYR:CE1 | 2.48                     | 0.46              |
| 1:J:358:ASN:HA   | 1:J:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:K:365:TYR:OH   | 1:K:404:LYS:HG2  | 2.15                     | 0.46              |
| 1:K:443:ILE:HG21 | 1:K:477:ASN:ND2  | 2.24                     | 0.46              |
| 1:K:537:ARG:HA   | 1:K:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:K:543:LEU:O    | 1:K:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:L:54:ALA:O     | 1:L:58:THR:N     | 2.48                     | 0.46              |
| 1:L:443:ILE:HG21 | 1:L:477:ASN:ND2  | 2.24                     | 0.46              |
| 1:M:243:VAL:C    | 1:M:244:LEU:HD12 | 2.39                     | 0.46              |
| 1:M:331:ILE:HG21 | 1:M:338:TRP:HB2  | 1.97                     | 0.46              |
| 1:M:443:ILE:HG21 | 1:M:477:ASN:ND2  | 2.24                     | 0.46              |
| 1:N:331:ILE:HG21 | 1:N:338:TRP:HB2  | 1.97                     | 0.46              |
| 1:O:602:ILE:HD12 | 1:O:900:GLU:HG2  | 1.97                     | 0.46              |
| 1:O:604:ASN:ND2  | 1:O:928:VAL:HB   | 2.29                     | 0.46              |
| 1:P:133:LYS:O    | 1:P:136:GLN:HB3  | 2.16                     | 0.46              |
| 1:P:170:VAL:O    | 1:P:173:LYS:N    | 2.48                     | 0.46              |
| 1:P:365:TYR:OH   | 1:P:404:LYS:HG2  | 2.15                     | 0.46              |
| 1:P:811:ASP:OD1  | 1:P:812:THR:N    | 2.46                     | 0.46              |
| 1:A:543:LEU:O    | 1:A:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:B:331:ILE:HG21 | 1:B:338:TRP:HB2  | 1.97                     | 0.46              |
| 1:C:537:ARG:HA   | 1:C:540:ASN:HB2  | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:14:ASP:CG    | 1:E:142:ARG:HH22 | 2.22                     | 0.46              |
| 1:D:198:LYS:NZ   | 1:E:222:HIS:CG   | 2.83                     | 0.46              |
| 1:E:312:LEU:HD23 | 1:E:312:LEU:C    | 2.40                     | 0.46              |
| 1:F:133:LYS:O    | 1:F:136:GLN:HB3  | 2.16                     | 0.46              |
| 1:F:301:LEU:CD2  | 1:F:313:PRO:CG   | 2.87                     | 0.46              |
| 1:F:358:ASN:HA   | 1:F:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:G:170:VAL:O    | 1:G:173:LYS:N    | 2.48                     | 0.46              |
| 1:G:293:THR:HG22 | 1:G:295:ASP:H    | 1.80                     | 0.46              |
| 1:G:478:ILE:HG22 | 1:G:479:GLU:N    | 2.30                     | 0.46              |
| 1:H:180:TRP:O    | 1:H:181:LEU:HD12 | 2.14                     | 0.46              |
| 1:H:1201:THR:OG1 | 1:H:1202:MET:N   | 2.48                     | 0.46              |
| 1:I:133:LYS:O    | 1:I:136:GLN:HB3  | 2.16                     | 0.46              |
| 1:I:537:ARG:HA   | 1:I:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:J:301:LEU:CD2  | 1:J:313:PRO:CG   | 2.87                     | 0.46              |
| 1:J:376:PRO:HG3  | 1:J:473:HIS:CD2  | 2.49                     | 0.46              |
| 1:J:502:ARG:HD3  | 1:J:516:ASN:HA   | 1.96                     | 0.46              |
| 1:J:638:GLU:OE1  | 1:J:640:GLU:N    | 2.42                     | 0.46              |
| 1:K:301:LEU:CD2  | 1:K:313:PRO:CG   | 2.87                     | 0.46              |
| 1:K:392:ASP:OD1  | 1:K:393:VAL:N    | 2.47                     | 0.46              |
| 1:K:554:ILE:O    | 1:K:556:SER:N    | 2.45                     | 0.46              |
| 1:L:312:LEU:HD23 | 1:L:312:LEU:C    | 2.41                     | 0.46              |
| 1:L:358:ASN:HA   | 1:L:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:N:133:LYS:O    | 1:N:136:GLN:HB3  | 2.16                     | 0.46              |
| 1:N:222:HIS:CG   | 1:O:198:LYS:NZ   | 2.84                     | 0.46              |
| 1:N:543:LEU:O    | 1:N:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:N:635:VAL:HB   | 1:N:641:ASP:CG   | 2.40                     | 0.46              |
| 1:O:180:TRP:O    | 1:O:181:LEU:HD12 | 2.14                     | 0.46              |
| 1:P:293:THR:HG22 | 1:P:295:ASP:H    | 1.80                     | 0.46              |
| 1:C:207:TRP:CH2  | 1:C:209:SER:HA   | 2.51                     | 0.46              |
| 1:C:458:LEU:HA   | 1:C:587:ARG:HH21 | 1.80                     | 0.46              |
| 1:D:358:ASN:HA   | 1:D:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:D:392:ASP:OD1  | 1:D:393:VAL:N    | 2.47                     | 0.46              |
| 1:D:554:ILE:O    | 1:D:556:SER:N    | 2.45                     | 0.46              |
| 1:E:638:GLU:OE1  | 1:E:640:GLU:N    | 2.42                     | 0.46              |
| 1:F:117:ASN:O    | 1:F:119:VAL:N    | 2.47                     | 0.46              |
| 1:F:371:ARG:HB3  | 1:F:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:G:358:ASN:HA   | 1:G:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:G:371:ARG:HB3  | 1:G:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:H:207:TRP:CH2  | 1:H:209:SER:HA   | 2.51                     | 0.46              |
| 1:H:458:LEU:CG   | 1:H:587:ARG:NH2  | 2.74                     | 0.46              |
| 1:I:127:ARG:HD3  | 1:I:292:LEU:HD12 | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:451:LYS:CD    | 1:I:486:LEU:HD21 | 2.33                     | 0.46              |
| 1:J:225:GLN:HG3   | 1:J:258:LEU:HD22 | 1.98                     | 0.46              |
| 1:J:312:LEU:HD23  | 1:J:312:LEU:C    | 2.41                     | 0.46              |
| 1:J:365:TYR:OH    | 1:J:404:LYS:HG2  | 2.15                     | 0.46              |
| 1:J:392:ASP:OD1   | 1:J:393:VAL:N    | 2.47                     | 0.46              |
| 1:J:811:ASP:OD1   | 1:J:812:THR:N    | 2.46                     | 0.46              |
| 1:K:225:GLN:HG3   | 1:K:258:LEU:HD22 | 1.98                     | 0.46              |
| 1:K:358:ASN:HA    | 1:K:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:L:207:TRP:CH2   | 1:L:209:SER:HA   | 2.51                     | 0.46              |
| 1:L:336:ALA:C     | 1:L:338:TRP:N    | 2.74                     | 0.46              |
| 1:L:398:VAL:HG23  | 1:L:399:MET:N    | 2.28                     | 0.46              |
| 1:M:502:ARG:HD3   | 1:M:516:ASN:HA   | 1.96                     | 0.46              |
| 1:N:170:VAL:O     | 1:N:173:LYS:N    | 2.48                     | 0.46              |
| 1:N:1201:THR:OG1  | 1:N:1202:MET:N   | 2.48                     | 0.46              |
| 1:O:508:TRP:O     | 1:O:606:GLY:CA   | 2.63                     | 0.46              |
| 1:P:180:TRP:O     | 1:P:181:LEU:HD12 | 2.14                     | 0.46              |
| 1:P:361:GLU:HB2   | 1:P:364:GLU:HB3  | 1.98                     | 0.46              |
| 1:P:371:ARG:HB3   | 1:P:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:P:635:VAL:HB    | 1:P:641:ASP:CG   | 2.40                     | 0.46              |
| 1:A:170:VAL:O     | 1:A:173:LYS:N    | 2.48                     | 0.46              |
| 1:A:371:ARG:HB3   | 1:A:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:C:293:THR:HG22  | 1:C:295:ASP:H    | 1.80                     | 0.46              |
| 1:C:866:LYS:HE2   | 1:C:872:ARG:HH11 | 1.81                     | 0.46              |
| 1:D:225:GLN:HG3   | 1:D:258:LEU:HD22 | 1.98                     | 0.46              |
| 1:D:1059:ASP:HB3  | 1:D:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:E:301:LEU:CD2   | 1:E:313:PRO:CG   | 2.87                     | 0.46              |
| 1:E:365:TYR:OH    | 1:E:404:LYS:HG2  | 2.15                     | 0.46              |
| 1:E:1074:HIS:O    | 1:E:1075:SER:OG  | 2.33                     | 0.46              |
| 1:F:127:ARG:HD3   | 1:F:292:LEU:HD12 | 1.98                     | 0.46              |
| 1:G:180:TRP:O     | 1:G:181:LEU:HD12 | 2.14                     | 0.46              |
| 1:G:361:GLU:HB2   | 1:G:364:GLU:HB3  | 1.98                     | 0.46              |
| 1:G:1074:HIS:O    | 1:G:1075:SER:OG  | 2.33                     | 0.46              |
| 1:H:170:VAL:O     | 1:H:173:LYS:N    | 2.48                     | 0.46              |
| 1:H:336:ALA:C     | 1:H:338:TRP:N    | 2.74                     | 0.46              |
| 1:H:602:ILE:HD12  | 1:H:900:GLU:HG2  | 1.97                     | 0.46              |
| 1:H:635:VAL:HB    | 1:H:641:ASP:CG   | 2.40                     | 0.46              |
| 1:H:1036:VAL:HG12 | 1:H:1037:ASP:N   | 2.31                     | 0.46              |
| 1:I:80:VAL:HA     | 1:I:83:ILE:HD12  | 1.98                     | 0.46              |
| 1:I:358:ASN:HA    | 1:I:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:I:641:ASP:OD1   | 1:I:642:THR:N    | 2.45                     | 0.46              |
| 1:J:317:LEU:O     | 1:J:318:THR:CB   | 2.61                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:462:TYR:OH    | 1:J:494:PHE:CZ   | 2.66                     | 0.46              |
| 1:J:1074:HIS:O    | 1:J:1075:SER:OG  | 2.33                     | 0.46              |
| 1:L:293:THR:HG22  | 1:L:295:ASP:H    | 1.80                     | 0.46              |
| 1:L:866:LYS:HE2   | 1:L:872:ARG:HH11 | 1.81                     | 0.46              |
| 1:O:207:TRP:CH2   | 1:O:209:SER:HA   | 2.51                     | 0.46              |
| 1:O:336:ALA:C     | 1:O:338:TRP:N    | 2.74                     | 0.46              |
| 1:A:482:GLU:C     | 1:A:485:THR:HG1  | 2.23                     | 0.46              |
| 1:A:1201:THR:OG1  | 1:A:1202:MET:N   | 2.48                     | 0.46              |
| 1:B:482:GLU:C     | 1:B:485:THR:HG1  | 2.24                     | 0.46              |
| 1:B:543:LEU:O     | 1:B:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:B:1059:ASP:HB3  | 1:B:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:C:641:ASP:OD1   | 1:C:642:THR:N    | 2.45                     | 0.46              |
| 1:D:133:LYS:O     | 1:D:136:GLN:HB3  | 2.16                     | 0.46              |
| 1:D:301:LEU:CD2   | 1:D:313:PRO:CG   | 2.87                     | 0.46              |
| 1:D:482:GLU:C     | 1:D:485:THR:HG1  | 2.24                     | 0.46              |
| 1:D:602:ILE:HD12  | 1:D:900:GLU:HG2  | 1.97                     | 0.46              |
| 1:D:1074:HIS:O    | 1:D:1075:SER:OG  | 2.33                     | 0.46              |
| 1:E:371:ARG:HB3   | 1:E:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:E:392:ASP:OD1   | 1:E:393:VAL:N    | 2.47                     | 0.46              |
| 1:F:458:LEU:HA    | 1:F:587:ARG:HH21 | 1.80                     | 0.46              |
| 1:G:80:VAL:HA     | 1:G:83:ILE:HD12  | 1.98                     | 0.46              |
| 1:G:635:VAL:HB    | 1:G:641:ASP:CG   | 2.40                     | 0.46              |
| 1:H:371:ARG:HB3   | 1:H:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:H:508:TRP:O     | 1:H:606:GLY:CA   | 2.63                     | 0.46              |
| 1:I:85:TYR:HB2    | 1:I:87:PHE:CE2   | 2.51                     | 0.46              |
| 1:I:371:ARG:HB3   | 1:I:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:J:537:ARG:HA    | 1:J:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:J:1036:VAL:HG12 | 1:J:1037:ASP:N   | 2.31                     | 0.46              |
| 1:K:133:LYS:O     | 1:K:136:GLN:HB3  | 2.16                     | 0.46              |
| 1:K:602:ILE:HD12  | 1:K:900:GLU:HG2  | 1.97                     | 0.46              |
| 1:L:458:LEU:HA    | 1:L:587:ARG:HH21 | 1.80                     | 0.46              |
| 1:M:1059:ASP:HB3  | 1:M:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:N:371:ARG:HB3   | 1:N:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:O:170:VAL:O     | 1:O:173:LYS:N    | 2.48                     | 0.46              |
| 1:O:371:ARG:HB3   | 1:O:389:ILE:CG2  | 2.45                     | 0.46              |
| 1:O:398:VAL:HG23  | 1:O:399:MET:N    | 2.28                     | 0.46              |
| 1:O:635:VAL:HB    | 1:O:641:ASP:CG   | 2.40                     | 0.46              |
| 1:O:1036:VAL:HG12 | 1:O:1037:ASP:N   | 2.31                     | 0.46              |
| 1:P:358:ASN:HA    | 1:P:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:P:1074:HIS:O    | 1:P:1075:SER:OG  | 2.33                     | 0.46              |
| 1:A:207:TRP:CH2   | 1:A:209:SER:HA   | 2.51                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1059:ASP:HB3  | 1:A:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:B:537:ARG:HA    | 1:B:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:C:11:GLN:O      | 1:C:14:ASP:N     | 2.46                     | 0.46              |
| 1:C:115:ASN:HB3   | 1:D:257:ASN:ND2  | 2.31                     | 0.46              |
| 1:C:250:ALA:C     | 1:C:251:APK:O    | 2.59                     | 0.46              |
| 1:C:336:ALA:C     | 1:C:338:TRP:N    | 2.74                     | 0.46              |
| 1:C:358:ASN:HA    | 1:C:366:ARG:NH2  | 2.31                     | 0.46              |
| 1:D:146:ASN:HB2   | 1:D:280:THR:HG22 | 1.98                     | 0.46              |
| 1:D:170:VAL:O     | 1:D:173:LYS:N    | 2.48                     | 0.46              |
| 1:E:85:TYR:HB2    | 1:E:87:PHE:CE2   | 2.51                     | 0.46              |
| 1:E:361:GLU:HB2   | 1:E:364:GLU:HB3  | 1.98                     | 0.46              |
| 1:E:1036:VAL:HG12 | 1:E:1037:ASP:N   | 2.31                     | 0.46              |
| 1:F:85:TYR:HB2    | 1:F:87:PHE:CE2   | 2.51                     | 0.46              |
| 1:F:312:LEU:HD23  | 1:F:312:LEU:C    | 2.41                     | 0.46              |
| 1:G:453:PHE:CE1   | 1:G:460:PRO:HB3  | 2.51                     | 0.46              |
| 1:H:124:ASN:OD1   | 1:H:124:ASN:C    | 2.57                     | 0.46              |
| 1:H:398:VAL:HG23  | 1:H:399:MET:N    | 2.28                     | 0.46              |
| 1:H:543:LEU:O     | 1:H:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:I:1074:HIS:O    | 1:I:1075:SER:OG  | 2.33                     | 0.46              |
| 1:J:54:ALA:O      | 1:J:58:THR:N     | 2.48                     | 0.46              |
| 1:J:85:TYR:HB2    | 1:J:87:PHE:CE2   | 2.51                     | 0.46              |
| 1:J:1059:ASP:HB3  | 1:J:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:K:170:VAL:O     | 1:K:173:LYS:N    | 2.48                     | 0.46              |
| 1:K:336:ALA:C     | 1:K:338:TRP:N    | 2.74                     | 0.46              |
| 1:K:1059:ASP:HB3  | 1:K:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:K:1074:HIS:O    | 1:K:1075:SER:OG  | 2.33                     | 0.46              |
| 1:L:146:ASN:HB2   | 1:L:280:THR:HG22 | 1.98                     | 0.46              |
| 1:L:250:ALA:C     | 1:L:251:APK:O    | 2.59                     | 0.46              |
| 1:L:451:LYS:CD    | 1:L:486:LEU:HD21 | 2.33                     | 0.46              |
| 1:M:482:GLU:C     | 1:M:485:THR:HG1  | 2.24                     | 0.46              |
| 1:M:543:LEU:O     | 1:M:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:N:207:TRP:CH2   | 1:N:209:SER:HA   | 2.51                     | 0.46              |
| 1:N:453:PHE:CE1   | 1:N:460:PRO:HB3  | 2.51                     | 0.46              |
| 1:N:1075:SER:OG   | 1:N:1094:ASP:O   | 2.29                     | 0.46              |
| 1:O:458:LEU:CG    | 1:O:587:ARG:NH2  | 2.74                     | 0.46              |
| 1:P:225:GLN:HG3   | 1:P:258:LEU:HD22 | 1.98                     | 0.46              |
| 1:P:317:LEU:O     | 1:P:318:THR:CB   | 2.61                     | 0.46              |
| 1:P:543:LEU:O     | 1:P:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:A:453:PHE:CE1   | 1:A:460:PRO:HB3  | 2.51                     | 0.46              |
| 1:A:656:ARG:HG2   | 1:A:657:MET:H    | 1.81                     | 0.46              |
| 1:C:85:TYR:HB2    | 1:C:87:PHE:CE2   | 2.51                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:146:ASN:HB2   | 1:C:280:THR:HG22 | 1.98                     | 0.46              |
| 1:C:398:VAL:HG23  | 1:C:399:MET:N    | 2.28                     | 0.46              |
| 1:C:458:LEU:CG    | 1:C:587:ARG:NH2  | 2.74                     | 0.46              |
| 1:D:85:TYR:HB2    | 1:D:87:PHE:CE2   | 2.51                     | 0.46              |
| 1:D:336:ALA:C     | 1:D:338:TRP:N    | 2.74                     | 0.46              |
| 1:D:1201:THR:OG1  | 1:D:1202:MET:N   | 2.48                     | 0.46              |
| 1:E:54:ALA:O      | 1:E:58:THR:N     | 2.48                     | 0.46              |
| 1:E:146:ASN:HB2   | 1:E:280:THR:HG22 | 1.98                     | 0.46              |
| 1:E:317:LEU:O     | 1:E:318:THR:CB   | 2.61                     | 0.46              |
| 1:E:537:ARG:HA    | 1:E:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:F:80:VAL:HA     | 1:F:83:ILE:HD12  | 1.98                     | 0.46              |
| 1:F:121:ALA:CB    | 1:G:276:SER:HB3  | 2.29                     | 0.46              |
| 1:F:207:TRP:CH2   | 1:F:209:SER:HA   | 2.51                     | 0.46              |
| 1:F:293:THR:HG22  | 1:F:295:ASP:H    | 1.81                     | 0.46              |
| 1:G:225:GLN:HG3   | 1:G:258:LEU:HD22 | 1.98                     | 0.46              |
| 1:G:317:LEU:O     | 1:G:318:THR:CB   | 2.61                     | 0.46              |
| 1:H:458:LEU:HA    | 1:H:587:ARG:HH21 | 1.80                     | 0.46              |
| 1:I:14:ASP:CG     | 1:P:142:ARG:HH22 | 2.24                     | 0.46              |
| 1:I:293:THR:HG22  | 1:I:295:ASP:H    | 1.80                     | 0.46              |
| 1:I:392:ASP:OD1   | 1:I:393:VAL:N    | 2.47                     | 0.46              |
| 1:I:475:LEU:HA    | 1:I:478:ILE:HD12 | 1.98                     | 0.46              |
| 1:J:146:ASN:HB2   | 1:J:280:THR:HG22 | 1.98                     | 0.46              |
| 1:J:361:GLU:HB2   | 1:J:364:GLU:HB3  | 1.98                     | 0.46              |
| 1:K:85:TYR:HB2    | 1:K:87:PHE:CE2   | 2.51                     | 0.46              |
| 1:K:146:ASN:HB2   | 1:K:280:THR:HG22 | 1.98                     | 0.46              |
| 1:K:403:ASN:CG    | 1:L:333:ASP:OD2  | 2.58                     | 0.46              |
| 1:K:633:THR:HG22  | 1:K:643:TYR:HA   | 1.97                     | 0.46              |
| 1:K:1201:THR:OG1  | 1:K:1202:MET:N   | 2.48                     | 0.46              |
| 1:L:458:LEU:HG    | 1:L:587:ARG:HH22 | 1.81                     | 0.46              |
| 1:M:602:ILE:HD12  | 1:M:900:GLU:HG2  | 1.97                     | 0.46              |
| 1:M:1177:TYR:HE2  | 1:N:916:LYS:HE2  | 1.81                     | 0.46              |
| 1:N:482:GLU:C     | 1:N:485:THR:HG1  | 2.23                     | 0.46              |
| 1:N:554:ILE:O     | 1:N:556:SER:N    | 2.45                     | 0.46              |
| 1:N:1059:ASP:HB3  | 1:N:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:O:543:LEU:O     | 1:O:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:P:80:VAL:HA     | 1:P:83:ILE:HD12  | 1.98                     | 0.46              |
| 1:P:1036:VAL:HG12 | 1:P:1037:ASP:N   | 2.31                     | 0.46              |
| 1:A:475:LEU:HA    | 1:A:478:ILE:HD12 | 1.98                     | 0.46              |
| 1:A:597:HIS:CD2   | 1:A:598:GLN:H    | 2.34                     | 0.46              |
| 1:A:866:LYS:HE2   | 1:A:872:ARG:HH11 | 1.81                     | 0.46              |
| 1:B:250:ALA:C     | 1:B:251:APK:O    | 2.59                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:602:ILE:HD12  | 1:B:900:GLU:HG2  | 1.97                     | 0.46              |
| 1:C:127:ARG:HD3   | 1:C:292:LEU:HD12 | 1.98                     | 0.46              |
| 1:C:1059:ASP:HB3  | 1:C:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:D:633:THR:HG22  | 1:D:643:TYR:HA   | 1.97                     | 0.46              |
| 1:E:207:TRP:CH2   | 1:E:209:SER:HA   | 2.51                     | 0.46              |
| 1:E:1059:ASP:HB3  | 1:E:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:G:475:LEU:HA    | 1:G:478:ILE:HD12 | 1.98                     | 0.46              |
| 1:G:543:LEU:O     | 1:G:547:PRO:HD2  | 2.16                     | 0.46              |
| 1:G:1036:VAL:HG12 | 1:G:1037:ASP:N   | 2.31                     | 0.46              |
| 1:H:361:GLU:HB2   | 1:H:364:GLU:HB3  | 1.98                     | 0.46              |
| 1:J:523:PHE:HD1   | 1:J:527:TYR:CE2  | 2.28                     | 0.46              |
| 1:J:656:ARG:HG2   | 1:J:657:MET:H    | 1.81                     | 0.46              |
| 1:J:866:LYS:HE2   | 1:J:872:ARG:HH11 | 1.81                     | 0.46              |
| 1:L:85:TYR:HB2    | 1:L:87:PHE:CE2   | 2.51                     | 0.46              |
| 1:L:458:LEU:CG    | 1:L:587:ARG:NH2  | 2.74                     | 0.46              |
| 1:L:554:ILE:O     | 1:L:556:SER:N    | 2.46                     | 0.46              |
| 1:L:1036:VAL:HG12 | 1:L:1037:ASP:N   | 2.31                     | 0.46              |
| 1:L:1059:ASP:HB3  | 1:L:1071:ALA:HB3 | 1.98                     | 0.46              |
| 1:M:207:TRP:CH2   | 1:M:209:SER:HA   | 2.51                     | 0.46              |
| 1:M:537:ARG:HA    | 1:M:540:ASN:HB2  | 1.97                     | 0.46              |
| 1:N:475:LEU:HA    | 1:N:478:ILE:HD12 | 1.98                     | 0.46              |
| 1:O:124:ASN:OD1   | 1:O:124:ASN:C    | 2.58                     | 0.46              |
| 1:P:231:LEU:O     | 1:P:234:SER:OG   | 2.26                     | 0.46              |
| 1:A:85:TYR:HB2    | 1:A:87:PHE:CE2   | 2.51                     | 0.45              |
| 1:A:491:PHE:N     | 1:A:491:PHE:CD1  | 2.83                     | 0.45              |
| 1:B:207:TRP:CH2   | 1:B:209:SER:HA   | 2.51                     | 0.45              |
| 1:B:352:ILE:O     | 1:B:356:SER:OG   | 2.29                     | 0.45              |
| 1:B:656:ARG:HG2   | 1:B:657:MET:H    | 1.81                     | 0.45              |
| 1:C:36:PRO:HG2    | 1:C:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:D:502:ARG:HD3   | 1:D:516:ASN:HA   | 1.96                     | 0.45              |
| 1:D:1036:VAL:HG12 | 1:D:1037:ASP:N   | 2.31                     | 0.45              |
| 1:E:36:PRO:HG2    | 1:E:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:E:458:LEU:HA    | 1:E:587:ARG:HH21 | 1.80                     | 0.45              |
| 1:E:552:ASN:HB3   | 1:E:1226:TYR:CE1 | 2.48                     | 0.45              |
| 1:E:656:ARG:HG2   | 1:E:657:MET:H    | 1.81                     | 0.45              |
| 1:E:866:LYS:HE2   | 1:E:872:ARG:HH11 | 1.81                     | 0.45              |
| 1:F:475:LEU:HA    | 1:F:478:ILE:HD12 | 1.99                     | 0.45              |
| 1:F:1074:HIS:O    | 1:F:1075:SER:OG  | 2.33                     | 0.45              |
| 1:F:1201:THR:OG1  | 1:F:1202:MET:N   | 2.48                     | 0.45              |
| 1:H:597:HIS:CD2   | 1:H:598:GLN:H    | 2.34                     | 0.45              |
| 1:H:604:ASN:ND2   | 1:H:929:VAL:H    | 2.04                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:H:841:PHE:O     | 1:H:842:LEU:HB2  | 2.16                     | 0.45              |
| 1:I:91:PRO:O      | 1:I:94:THR:OG1   | 2.21                     | 0.45              |
| 1:I:207:TRP:CH2   | 1:I:209:SER:HA   | 2.51                     | 0.45              |
| 1:I:453:PHE:CE1   | 1:I:460:PRO:HB3  | 2.51                     | 0.45              |
| 1:I:502:ARG:HD3   | 1:I:516:ASN:HA   | 1.96                     | 0.45              |
| 1:I:656:ARG:HG2   | 1:I:657:MET:H    | 1.81                     | 0.45              |
| 1:I:1201:THR:OG1  | 1:I:1202:MET:N   | 2.48                     | 0.45              |
| 1:J:36:PRO:HG2    | 1:J:39:ILE:CG2   | 2.47                     | 0.45              |
| 1:J:207:TRP:CH2   | 1:J:209:SER:HA   | 2.51                     | 0.45              |
| 1:K:480:HIS:O     | 1:K:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:K:1036:VAL:HG12 | 1:K:1037:ASP:N   | 2.31                     | 0.45              |
| 1:L:91:PRO:O      | 1:L:94:THR:OG1   | 2.22                     | 0.45              |
| 1:L:133:LYS:O     | 1:L:136:GLN:HB3  | 2.16                     | 0.45              |
| 1:L:231:LEU:O     | 1:L:234:SER:OG   | 2.26                     | 0.45              |
| 1:L:317:LEU:C     | 1:L:318:THR:HG1  | 1.95                     | 0.45              |
| 1:L:428:GLU:C     | 1:L:430:LYS:N    | 2.74                     | 0.45              |
| 1:L:453:PHE:CE2   | 1:L:460:PRO:HB3  | 2.49                     | 0.45              |
| 1:L:875:LEU:CD1   | 1:L:911:PHE:HD2  | 2.07                     | 0.45              |
| 1:M:146:ASN:HB2   | 1:M:280:THR:HG22 | 1.98                     | 0.45              |
| 1:M:222:HIS:CG    | 1:N:198:LYS:NZ   | 2.84                     | 0.45              |
| 1:M:250:ALA:C     | 1:M:251:APK:O    | 2.59                     | 0.45              |
| 1:M:352:ILE:O     | 1:M:356:SER:OG   | 2.29                     | 0.45              |
| 1:M:358:ASN:HA    | 1:M:366:ARG:NH2  | 2.31                     | 0.45              |
| 1:M:656:ARG:HG2   | 1:M:657:MET:H    | 1.81                     | 0.45              |
| 1:N:85:TYR:HB2    | 1:N:87:PHE:CE2   | 2.51                     | 0.45              |
| 1:N:124:ASN:OD1   | 1:N:124:ASN:C    | 2.58                     | 0.45              |
| 1:N:336:ALA:C     | 1:N:338:TRP:N    | 2.74                     | 0.45              |
| 1:N:508:TRP:O     | 1:N:606:GLY:CA   | 2.63                     | 0.45              |
| 1:N:597:HIS:CD2   | 1:N:598:GLN:H    | 2.34                     | 0.45              |
| 1:N:656:ARG:HG2   | 1:N:657:MET:H    | 1.81                     | 0.45              |
| 1:O:36:PRO:HG2    | 1:O:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:O:80:VAL:HA     | 1:O:83:ILE:HD12  | 1.98                     | 0.45              |
| 1:O:361:GLU:HB2   | 1:O:364:GLU:HB3  | 1.98                     | 0.45              |
| 1:O:458:LEU:HA    | 1:O:587:ARG:HH21 | 1.80                     | 0.45              |
| 1:O:597:HIS:CD2   | 1:O:598:GLN:H    | 2.34                     | 0.45              |
| 1:O:604:ASN:ND2   | 1:O:929:VAL:H    | 2.04                     | 0.45              |
| 1:P:64:THR:O      | 1:P:67:SER:OG    | 2.27                     | 0.45              |
| 1:P:85:TYR:HB2    | 1:P:87:PHE:CE2   | 2.51                     | 0.45              |
| 1:P:475:LEU:HA    | 1:P:478:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:36:PRO:HG2    | 1:A:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:A:124:ASN:OD1   | 1:A:124:ASN:C    | 2.58                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:146:ASN:HB2   | 1:A:280:THR:HG22  | 1.98                     | 0.45              |
| 1:A:336:ALA:C     | 1:A:338:TRP:N     | 2.74                     | 0.45              |
| 1:A:508:TRP:O     | 1:A:606:GLY:CA    | 2.63                     | 0.45              |
| 1:A:554:ILE:O     | 1:A:556:SER:N     | 2.46                     | 0.45              |
| 1:B:312:LEU:HD23  | 1:B:312:LEU:C     | 2.40                     | 0.45              |
| 1:B:358:ASN:HA    | 1:B:366:ARG:NH2   | 2.31                     | 0.45              |
| 1:B:1036:VAL:HG12 | 1:B:1037:ASP:N    | 2.31                     | 0.45              |
| 1:C:80:VAL:HA     | 1:C:83:ILE:HD12   | 1.98                     | 0.45              |
| 1:C:633:THR:HG22  | 1:C:643:TYR:HA    | 1.97                     | 0.45              |
| 1:D:458:LEU:HG    | 1:D:587:ARG:HH22  | 1.81                     | 0.45              |
| 1:D:480:HIS:O     | 1:D:483:ARG:HG2   | 2.16                     | 0.45              |
| 1:D:557:LYS:CD    | 1:D:1223:GLN:HE21 | 2.30                     | 0.45              |
| 1:D:841:PHE:O     | 1:D:842:LEU:HB2   | 2.17                     | 0.45              |
| 1:E:428:GLU:C     | 1:E:430:LYS:N     | 2.74                     | 0.45              |
| 1:E:523:PHE:HD1   | 1:E:527:TYR:CE2   | 2.28                     | 0.45              |
| 1:F:604:ASN:ND2   | 1:F:929:VAL:H     | 2.03                     | 0.45              |
| 1:F:656:ARG:HG2   | 1:F:657:MET:H     | 1.81                     | 0.45              |
| 1:F:1036:VAL:HG12 | 1:F:1037:ASP:N    | 2.31                     | 0.45              |
| 1:F:1075:SER:OG   | 1:F:1094:ASP:O    | 2.29                     | 0.45              |
| 1:G:85:TYR:HB2    | 1:G:87:PHE:CE2    | 2.51                     | 0.45              |
| 1:G:127:ARG:HD3   | 1:G:292:LEU:HD12  | 1.98                     | 0.45              |
| 1:G:597:HIS:CD2   | 1:G:598:GLN:H     | 2.34                     | 0.45              |
| 1:G:633:THR:HG22  | 1:G:643:TYR:HA    | 1.97                     | 0.45              |
| 1:H:475:LEU:HA    | 1:H:478:ILE:HD12  | 1.98                     | 0.45              |
| 1:I:811:ASP:OD1   | 1:I:812:THR:N     | 2.46                     | 0.45              |
| 1:J:133:LYS:O     | 1:J:136:GLN:HB3   | 2.16                     | 0.45              |
| 1:J:222:HIS:CG    | 1:K:198:LYS:HZ1   | 2.35                     | 0.45              |
| 1:J:428:GLU:C     | 1:J:430:LYS:N     | 2.75                     | 0.45              |
| 1:J:841:PHE:O     | 1:J:842:LEU:HB2   | 2.16                     | 0.45              |
| 1:K:382:PRO:HA    | 1:K:419:THR:CG2   | 2.36                     | 0.45              |
| 1:K:557:LYS:CD    | 1:K:1223:GLN:HE21 | 2.30                     | 0.45              |
| 1:L:11:GLN:O      | 1:L:14:ASP:N      | 2.46                     | 0.45              |
| 1:M:312:LEU:HD23  | 1:M:312:LEU:C     | 2.41                     | 0.45              |
| 1:M:475:LEU:HA    | 1:M:478:ILE:HD12  | 1.98                     | 0.45              |
| 1:M:597:HIS:CD2   | 1:M:598:GLN:H     | 2.34                     | 0.45              |
| 1:M:866:LYS:HE2   | 1:M:872:ARG:HH11  | 1.81                     | 0.45              |
| 1:N:146:ASN:HB2   | 1:N:280:THR:HG22  | 1.98                     | 0.45              |
| 1:N:361:GLU:HB2   | 1:N:364:GLU:HB3   | 1.98                     | 0.45              |
| 1:N:458:LEU:CG    | 1:N:587:ARG:NH2   | 2.74                     | 0.45              |
| 1:N:557:LYS:NZ    | 1:N:1223:GLN:HG3  | 2.32                     | 0.45              |
| 1:N:866:LYS:HE2   | 1:N:872:ARG:HH11  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:O:389:ILE:CD1   | 1:O:446:HIS:HE2  | 2.14                     | 0.45              |
| 1:O:475:LEU:HA    | 1:O:478:ILE:HD12 | 1.98                     | 0.45              |
| 1:O:841:PHE:O     | 1:O:842:LEU:HB2  | 2.17                     | 0.45              |
| 1:P:102:MET:O     | 1:P:105:MET:N    | 2.46                     | 0.45              |
| 1:P:633:THR:HG22  | 1:P:643:TYR:HA   | 1.97                     | 0.45              |
| 1:B:127:ARG:HD3   | 1:B:292:LEU:HD12 | 1.98                     | 0.45              |
| 1:B:146:ASN:HB2   | 1:B:280:THR:HG22 | 1.98                     | 0.45              |
| 1:B:428:GLU:C     | 1:B:430:LYS:N    | 2.74                     | 0.45              |
| 1:B:552:ASN:HB3   | 1:B:1226:TYR:CE1 | 2.48                     | 0.45              |
| 1:B:597:HIS:CD2   | 1:B:598:GLN:H    | 2.34                     | 0.45              |
| 1:B:866:LYS:HE2   | 1:B:872:ARG:HH11 | 1.81                     | 0.45              |
| 1:B:1035:TYR:HA   | 1:B:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:C:231:LEU:O     | 1:C:234:SER:OG   | 2.26                     | 0.45              |
| 1:C:428:GLU:C     | 1:C:430:LYS:N    | 2.75                     | 0.45              |
| 1:C:475:LEU:HA    | 1:C:478:ILE:HD12 | 1.98                     | 0.45              |
| 1:C:557:LYS:NZ    | 1:C:1223:GLN:HG3 | 2.31                     | 0.45              |
| 1:C:1036:VAL:HG12 | 1:C:1037:ASP:N   | 2.31                     | 0.45              |
| 1:D:207:TRP:CH2   | 1:D:209:SER:HA   | 2.51                     | 0.45              |
| 1:E:133:LYS:O     | 1:E:136:GLN:HB3  | 2.16                     | 0.45              |
| 1:E:336:ALA:C     | 1:E:338:TRP:N    | 2.74                     | 0.45              |
| 1:E:480:HIS:O     | 1:E:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:F:146:ASN:HB2   | 1:F:280:THR:HG22 | 1.98                     | 0.45              |
| 1:F:458:LEU:HG    | 1:F:587:ARG:HH22 | 1.81                     | 0.45              |
| 1:F:597:HIS:CD2   | 1:F:598:GLN:H    | 2.34                     | 0.45              |
| 1:G:231:LEU:O     | 1:G:234:SER:OG   | 2.26                     | 0.45              |
| 1:H:36:PRO:HG2    | 1:H:39:ILE:CG2   | 2.47                     | 0.45              |
| 1:H:80:VAL:HA     | 1:H:83:ILE:HD12  | 1.98                     | 0.45              |
| 1:H:127:ARG:HD3   | 1:H:292:LEU:HD12 | 1.98                     | 0.45              |
| 1:H:225:GLN:HG3   | 1:H:258:LEU:HD22 | 1.98                     | 0.45              |
| 1:H:389:ILE:CD1   | 1:H:446:HIS:HE2  | 2.14                     | 0.45              |
| 1:H:491:PHE:CD1   | 1:H:491:PHE:N    | 2.83                     | 0.45              |
| 1:H:1059:ASP:HB3  | 1:H:1071:ALA:HB3 | 1.98                     | 0.45              |
| 1:I:458:LEU:HG    | 1:I:587:ARG:HH22 | 1.81                     | 0.45              |
| 1:J:475:LEU:HA    | 1:J:478:ILE:HD12 | 1.98                     | 0.45              |
| 1:K:458:LEU:HG    | 1:K:587:ARG:HH22 | 1.81                     | 0.45              |
| 1:K:841:PHE:O     | 1:K:842:LEU:HB2  | 2.17                     | 0.45              |
| 1:L:542:ILE:HA    | 1:L:545:PHE:HD2  | 1.82                     | 0.45              |
| 1:L:557:LYS:NZ    | 1:L:1223:GLN:HG3 | 2.31                     | 0.45              |
| 1:L:633:THR:HG22  | 1:L:643:TYR:HA   | 1.97                     | 0.45              |
| 1:M:127:ARG:HD3   | 1:M:292:LEU:HD12 | 1.98                     | 0.45              |
| 1:M:542:ILE:HA    | 1:M:545:PHE:HD2  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:M:552:ASN:HB3   | 1:M:1226:TYR:CE1 | 2.48                     | 0.45              |
| 1:M:1036:VAL:HG12 | 1:M:1037:ASP:N   | 2.31                     | 0.45              |
| 1:N:491:PHE:N     | 1:N:491:PHE:CD1  | 2.83                     | 0.45              |
| 1:O:127:ARG:HD3   | 1:O:292:LEU:HD12 | 1.98                     | 0.45              |
| 1:O:293:THR:HG22  | 1:O:295:ASP:H    | 1.80                     | 0.45              |
| 1:O:480:HIS:O     | 1:O:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:O:491:PHE:N     | 1:O:491:PHE:CD1  | 2.83                     | 0.45              |
| 1:P:382:PRO:HA    | 1:P:419:THR:CG2  | 2.36                     | 0.45              |
| 1:P:523:PHE:HD1   | 1:P:527:TYR:CE2  | 2.28                     | 0.45              |
| 1:P:656:ARG:HG2   | 1:P:657:MET:H    | 1.81                     | 0.45              |
| 1:P:841:PHE:O     | 1:P:842:LEU:HB2  | 2.17                     | 0.45              |
| 1:A:458:LEU:CG    | 1:A:587:ARG:NH2  | 2.74                     | 0.45              |
| 1:A:662:GLN:O     | 1:A:663:GLN:HG2  | 2.17                     | 0.45              |
| 1:B:80:VAL:HA     | 1:B:83:ILE:HD12  | 1.98                     | 0.45              |
| 1:B:85:TYR:HB2    | 1:B:87:PHE:CE2   | 2.51                     | 0.45              |
| 1:B:475:LEU:HA    | 1:B:478:ILE:HD12 | 1.98                     | 0.45              |
| 1:B:542:ILE:HA    | 1:B:545:PHE:HD2  | 1.82                     | 0.45              |
| 1:B:898:VAL:HG13  | 1:B:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:C:133:LYS:O     | 1:C:136:GLN:HB3  | 2.16                     | 0.45              |
| 1:C:453:PHE:CE2   | 1:C:460:PRO:HB3  | 2.49                     | 0.45              |
| 1:C:543:LEU:O     | 1:C:547:PRO:HD2  | 2.16                     | 0.45              |
| 1:C:597:HIS:CD2   | 1:C:598:GLN:H    | 2.34                     | 0.45              |
| 1:C:898:VAL:HG13  | 1:C:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:D:458:LEU:HA    | 1:D:587:ARG:HH21 | 1.80                     | 0.45              |
| 1:D:866:LYS:HE2   | 1:D:872:ARG:HH11 | 1.81                     | 0.45              |
| 1:E:80:VAL:HA     | 1:E:83:ILE:HD12  | 1.98                     | 0.45              |
| 1:E:597:HIS:CD2   | 1:E:598:GLN:H    | 2.34                     | 0.45              |
| 1:E:902:ILE:HD13  | 1:E:930:HIS:CE1  | 2.43                     | 0.45              |
| 1:E:1201:THR:OG1  | 1:E:1202:MET:N   | 2.48                     | 0.45              |
| 1:F:36:PRO:HG2    | 1:F:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:F:336:ALA:C     | 1:F:338:TRP:N    | 2.74                     | 0.45              |
| 1:F:392:ASP:OD1   | 1:F:393:VAL:N    | 2.47                     | 0.45              |
| 1:F:453:PHE:CE1   | 1:F:460:PRO:HB3  | 2.51                     | 0.45              |
| 1:F:502:ARG:HD3   | 1:F:516:ASN:HA   | 1.96                     | 0.45              |
| 1:F:811:ASP:OD1   | 1:F:812:THR:N    | 2.47                     | 0.45              |
| 1:G:102:MET:O     | 1:G:105:MET:N    | 2.46                     | 0.45              |
| 1:G:293:THR:O     | 1:G:296:GLU:N    | 2.40                     | 0.45              |
| 1:H:146:ASN:HB2   | 1:H:280:THR:HG22 | 1.98                     | 0.45              |
| 1:H:293:THR:O     | 1:H:296:GLU:N    | 2.40                     | 0.45              |
| 1:H:480:HIS:O     | 1:H:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:H:557:LYS:NZ    | 1:H:1223:GLN:HG3 | 2.31                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:1036:VAL:HG12 | 1:I:1037:ASP:N    | 2.31                     | 0.45              |
| 1:J:80:VAL:HA     | 1:J:83:ILE:HD12   | 1.97                     | 0.45              |
| 1:J:336:ALA:C     | 1:J:338:TRP:N     | 2.74                     | 0.45              |
| 1:J:552:ASN:HB3   | 1:J:1226:TYR:CE1  | 2.48                     | 0.45              |
| 1:J:557:LYS:CD    | 1:J:1223:GLN:HE21 | 2.30                     | 0.45              |
| 1:K:207:TRP:CH2   | 1:K:209:SER:HA    | 2.51                     | 0.45              |
| 1:K:502:ARG:HD3   | 1:K:516:ASN:HA    | 1.96                     | 0.45              |
| 1:L:36:PRO:HG2    | 1:L:39:ILE:CG2    | 2.47                     | 0.45              |
| 1:L:80:VAL:HA     | 1:L:83:ILE:HD12   | 1.97                     | 0.45              |
| 1:L:557:LYS:CD    | 1:L:1223:GLN:HE21 | 2.30                     | 0.45              |
| 1:L:898:VAL:HG13  | 1:L:930:HIS:CD2   | 2.52                     | 0.45              |
| 1:M:28:ASP:HB2    | 1:M:31:ASP:CG     | 2.42                     | 0.45              |
| 1:M:80:VAL:HA     | 1:M:83:ILE:HD12   | 1.98                     | 0.45              |
| 1:M:376:PRO:HA    | 1:M:377:PRO:HD3   | 1.89                     | 0.45              |
| 1:M:428:GLU:C     | 1:M:430:LYS:N     | 2.74                     | 0.45              |
| 1:M:898:VAL:HG13  | 1:M:930:HIS:CD2   | 2.52                     | 0.45              |
| 1:N:36:PRO:HG2    | 1:N:39:ILE:CG2    | 2.47                     | 0.45              |
| 1:N:496:PHE:HE2   | 1:N:555:CYS:HG    | 1.64                     | 0.45              |
| 1:N:662:GLN:O     | 1:N:663:GLN:HG2   | 2.17                     | 0.45              |
| 1:N:1035:TYR:HA   | 1:N:1057:PRO:HG2  | 1.99                     | 0.45              |
| 1:O:225:GLN:HG3   | 1:O:258:LEU:HD22  | 1.98                     | 0.45              |
| 1:O:523:PHE:HD1   | 1:O:527:TYR:CE2   | 2.28                     | 0.45              |
| 1:O:1059:ASP:HB3  | 1:O:1071:ALA:HB3  | 1.98                     | 0.45              |
| 1:P:127:ARG:HD3   | 1:P:292:LEU:HD12  | 1.98                     | 0.45              |
| 1:P:293:THR:O     | 1:P:296:GLU:N     | 2.40                     | 0.45              |
| 1:P:597:HIS:CD2   | 1:P:598:GLN:H     | 2.34                     | 0.45              |
| 1:A:361:GLU:HB2   | 1:A:364:GLU:HB3   | 1.98                     | 0.45              |
| 1:B:28:ASP:HB2    | 1:B:31:ASP:CG     | 2.42                     | 0.45              |
| 1:B:557:LYS:NZ    | 1:B:1223:GLN:HG3  | 2.31                     | 0.45              |
| 1:C:542:ILE:HA    | 1:C:545:PHE:HD2   | 1.82                     | 0.45              |
| 1:C:1035:TYR:HA   | 1:C:1057:PRO:HG2  | 1.99                     | 0.45              |
| 1:D:382:PRO:HA    | 1:D:419:THR:CG2   | 2.36                     | 0.45              |
| 1:D:475:LEU:HA    | 1:D:478:ILE:HD12  | 1.98                     | 0.45              |
| 1:D:597:HIS:CD2   | 1:D:598:GLN:H     | 2.34                     | 0.45              |
| 1:E:443:ILE:HG21  | 1:E:477:ASN:ND2   | 2.24                     | 0.45              |
| 1:E:475:LEU:HA    | 1:E:478:ILE:HD12  | 1.99                     | 0.45              |
| 1:E:543:LEU:O     | 1:E:547:PRO:HD2   | 2.16                     | 0.45              |
| 1:E:557:LYS:CD    | 1:E:1223:GLN:HE21 | 2.30                     | 0.45              |
| 1:E:841:PHE:O     | 1:E:842:LEU:HB2   | 2.17                     | 0.45              |
| 1:F:91:PRO:O      | 1:F:94:THR:OG1    | 2.21                     | 0.45              |
| 1:G:557:LYS:NZ    | 1:G:1223:GLN:HG3  | 2.31                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:584:PHE:HB3   | 1:G:585:ASP:H    | 1.61                     | 0.45              |
| 1:G:656:ARG:HG2   | 1:G:657:MET:H    | 1.81                     | 0.45              |
| 1:G:841:PHE:O     | 1:G:842:LEU:HB2  | 2.17                     | 0.45              |
| 1:H:293:THR:HG22  | 1:H:295:ASP:H    | 1.80                     | 0.45              |
| 1:I:146:ASN:HB2   | 1:I:280:THR:HG22 | 1.98                     | 0.45              |
| 1:I:597:HIS:CD2   | 1:I:598:GLN:H    | 2.34                     | 0.45              |
| 1:J:336:ALA:O     | 1:J:337:THR:OG1  | 2.35                     | 0.45              |
| 1:J:597:HIS:CD2   | 1:J:598:GLN:H    | 2.34                     | 0.45              |
| 1:J:1201:THR:OG1  | 1:J:1202:MET:N   | 2.48                     | 0.45              |
| 1:K:11:GLN:O      | 1:K:14:ASP:N     | 2.46                     | 0.45              |
| 1:K:371:ARG:HB3   | 1:K:389:ILE:CG2  | 2.45                     | 0.45              |
| 1:K:597:HIS:CD2   | 1:K:598:GLN:H    | 2.34                     | 0.45              |
| 1:K:656:ARG:HG2   | 1:K:657:MET:H    | 1.81                     | 0.45              |
| 1:K:866:LYS:HE2   | 1:K:872:ARG:HH11 | 1.81                     | 0.45              |
| 1:L:28:ASP:HB2    | 1:L:31:ASP:CG    | 2.42                     | 0.45              |
| 1:L:127:ARG:HD3   | 1:L:292:LEU:HD12 | 1.98                     | 0.45              |
| 1:L:480:HIS:O     | 1:L:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:L:543:LEU:O     | 1:L:547:PRO:HD2  | 2.16                     | 0.45              |
| 1:L:597:HIS:CD2   | 1:L:598:GLN:H    | 2.34                     | 0.45              |
| 1:M:85:TYR:HB2    | 1:M:87:PHE:CE2   | 2.51                     | 0.45              |
| 1:N:1036:VAL:HG12 | 1:N:1037:ASP:N   | 2.31                     | 0.45              |
| 1:N:1177:TYR:HE2  | 1:O:916:LYS:HE2  | 1.81                     | 0.45              |
| 1:O:146:ASN:HB2   | 1:O:280:THR:HG22 | 1.98                     | 0.45              |
| 1:O:293:THR:O     | 1:O:296:GLU:N    | 2.40                     | 0.45              |
| 1:O:312:LEU:HD23  | 1:O:312:LEU:C    | 2.40                     | 0.45              |
| 1:P:146:ASN:HB2   | 1:P:280:THR:HG22 | 1.98                     | 0.45              |
| 1:P:557:LYS:NZ    | 1:P:1223:GLN:HG3 | 2.31                     | 0.45              |
| 1:P:604:ASN:ND2   | 1:P:929:VAL:H    | 2.04                     | 0.45              |
| 1:A:269:LYS:HB3   | 1:A:407:LYS:O    | 2.17                     | 0.45              |
| 1:A:898:VAL:HG13  | 1:A:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:A:1035:TYR:HA   | 1:A:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:A:1036:VAL:HG12 | 1:A:1037:ASP:N   | 2.31                     | 0.45              |
| 1:B:376:PRO:HA    | 1:B:377:PRO:HD3  | 1.89                     | 0.45              |
| 1:B:641:ASP:OD1   | 1:B:642:THR:N    | 2.45                     | 0.45              |
| 1:C:28:ASP:HB2    | 1:C:31:ASP:CG    | 2.42                     | 0.45              |
| 1:D:11:GLN:O      | 1:D:14:ASP:N     | 2.46                     | 0.45              |
| 1:D:250:ALA:C     | 1:D:251:APK:O    | 2.59                     | 0.45              |
| 1:D:312:LEU:HD23  | 1:D:312:LEU:C    | 2.40                     | 0.45              |
| 1:D:336:ALA:O     | 1:D:337:THR:OG1  | 2.35                     | 0.45              |
| 1:E:336:ALA:O     | 1:E:337:THR:OG1  | 2.35                     | 0.45              |
| 1:E:633:THR:HG22  | 1:E:643:TYR:HA   | 1.97                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:999:ALA:HA   | 1:E:1019:LYS:HA  | 1.98                     | 0.45              |
| 1:F:898:VAL:HG13 | 1:F:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:F:1059:ASP:HB3 | 1:F:1071:ALA:HB3 | 1.98                     | 0.45              |
| 1:G:146:ASN:HB2  | 1:G:280:THR:HG22 | 1.98                     | 0.45              |
| 1:G:523:PHE:HD1  | 1:G:527:TYR:CE2  | 2.28                     | 0.45              |
| 1:G:604:ASN:ND2  | 1:G:929:VAL:H    | 2.04                     | 0.45              |
| 1:G:1035:TYR:HA  | 1:G:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:G:1201:THR:OG1 | 1:G:1202:MET:N   | 2.48                     | 0.45              |
| 1:H:133:LYS:O    | 1:H:136:GLN:HB3  | 2.16                     | 0.45              |
| 1:H:898:VAL:HG13 | 1:H:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:H:1035:TYR:HA  | 1:H:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:I:28:ASP:HB2   | 1:I:31:ASP:CG    | 2.42                     | 0.45              |
| 1:I:36:PRO:HG2   | 1:I:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:I:225:GLN:HG3  | 1:I:258:LEU:HD22 | 1.98                     | 0.45              |
| 1:I:1059:ASP:HB3 | 1:I:1071:ALA:HB3 | 1.98                     | 0.45              |
| 1:I:1075:SER:OG  | 1:I:1094:ASP:O   | 2.29                     | 0.45              |
| 1:J:480:HIS:O    | 1:J:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:J:543:LEU:O    | 1:J:547:PRO:HD2  | 2.16                     | 0.45              |
| 1:J:999:ALA:HA   | 1:J:1019:LYS:HA  | 1.98                     | 0.45              |
| 1:K:250:ALA:C    | 1:K:251:APK:O    | 2.59                     | 0.45              |
| 1:K:475:LEU:HA   | 1:K:478:ILE:HD12 | 1.98                     | 0.45              |
| 1:L:475:LEU:HA   | 1:L:478:ILE:HD12 | 1.98                     | 0.45              |
| 1:M:170:VAL:O    | 1:M:173:LYS:N    | 2.48                     | 0.45              |
| 1:M:225:GLN:HG3  | 1:M:258:LEU:HD22 | 1.98                     | 0.45              |
| 1:M:641:ASP:OD1  | 1:M:642:THR:N    | 2.45                     | 0.45              |
| 1:M:1035:TYR:HA  | 1:M:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:N:457:ASP:OD2  | 1:N:458:LEU:HB2  | 2.17                     | 0.45              |
| 1:N:898:VAL:HG13 | 1:N:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:O:133:LYS:O    | 1:O:136:GLN:HB3  | 2.16                     | 0.45              |
| 1:O:249:ASN:O    | 1:O:251:APK:O    | 2.35                     | 0.45              |
| 1:O:898:VAL:HG13 | 1:O:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:O:1035:TYR:HA  | 1:O:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:P:1035:TYR:HA  | 1:P:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:P:1201:THR:OG1 | 1:P:1202:MET:N   | 2.48                     | 0.45              |
| 1:A:28:ASP:HB2   | 1:A:31:ASP:CG    | 2.42                     | 0.45              |
| 1:A:225:GLN:HG3  | 1:A:258:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:249:ASN:O    | 1:A:251:APK:O    | 2.35                     | 0.45              |
| 1:A:457:ASP:OD2  | 1:A:458:LEU:HB2  | 2.17                     | 0.45              |
| 1:A:480:HIS:O    | 1:A:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:A:782:CYS:HB3  | 1:A:816:LEU:HD13 | 1.99                     | 0.45              |
| 1:B:170:VAL:O    | 1:B:173:LYS:N    | 2.48                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:225:GLN:HG3  | 1:B:258:LEU:HD22  | 1.98                     | 0.45              |
| 1:B:480:HIS:O    | 1:B:483:ARG:HG2   | 2.16                     | 0.45              |
| 1:C:111:ASP:HB3  | 1:D:144:ALA:HB3   | 1.97                     | 0.45              |
| 1:C:554:ILE:O    | 1:C:556:SER:N     | 2.45                     | 0.45              |
| 1:C:557:LYS:CD   | 1:C:1223:GLN:HE21 | 2.30                     | 0.45              |
| 1:D:269:LYS:HB3  | 1:D:407:LYS:O     | 2.17                     | 0.45              |
| 1:D:371:ARG:HB3  | 1:D:389:ILE:CG2   | 2.45                     | 0.45              |
| 1:D:557:LYS:NZ   | 1:D:1223:GLN:HG3  | 2.31                     | 0.45              |
| 1:D:656:ARG:HG2  | 1:D:657:MET:H     | 1.81                     | 0.45              |
| 1:E:337:THR:OG1  | 1:E:340:ASN:N     | 2.50                     | 0.45              |
| 1:G:336:ALA:O    | 1:G:337:THR:OG1   | 2.35                     | 0.45              |
| 1:G:458:LEU:HG   | 1:G:587:ARG:HH22  | 1.81                     | 0.45              |
| 1:G:914:VAL:O    | 1:G:915:TYR:C     | 2.60                     | 0.45              |
| 1:G:1059:ASP:HB3 | 1:G:1071:ALA:HB3  | 1.98                     | 0.45              |
| 1:H:28:ASP:HB2   | 1:H:31:ASP:CG     | 2.42                     | 0.45              |
| 1:H:249:ASN:O    | 1:H:251:APK:O     | 2.35                     | 0.45              |
| 1:H:358:ASN:HA   | 1:H:366:ARG:NH2   | 2.31                     | 0.45              |
| 1:H:523:PHE:HD1  | 1:H:527:TYR:CE2   | 2.28                     | 0.45              |
| 1:H:662:GLN:O    | 1:H:663:GLN:HG2   | 2.17                     | 0.45              |
| 1:I:336:ALA:O    | 1:I:337:THR:OG1   | 2.35                     | 0.45              |
| 1:I:336:ALA:C    | 1:I:338:TRP:N     | 2.74                     | 0.45              |
| 1:I:604:ASN:ND2  | 1:I:929:VAL:H     | 2.04                     | 0.45              |
| 1:I:999:ALA:HA   | 1:I:1019:LYS:HA   | 1.98                     | 0.45              |
| 1:I:1035:TYR:HA  | 1:I:1057:PRO:HG2  | 1.99                     | 0.45              |
| 1:J:222:HIS:CG   | 1:K:198:LYS:NZ    | 2.84                     | 0.45              |
| 1:J:337:THR:OG1  | 1:J:340:ASN:N     | 2.50                     | 0.45              |
| 1:J:443:ILE:HG21 | 1:J:477:ASN:ND2   | 2.24                     | 0.45              |
| 1:J:633:THR:HG22 | 1:J:643:TYR:HA    | 1.97                     | 0.45              |
| 1:J:1188:LYS:HG3 | 1:J:1189:ALA:H    | 1.82                     | 0.45              |
| 1:K:222:HIS:CD2  | 1:L:198:LYS:HG2   | 2.52                     | 0.45              |
| 1:K:336:ALA:O    | 1:K:337:THR:OG1   | 2.35                     | 0.45              |
| 1:L:1035:TYR:HA  | 1:L:1057:PRO:HG2  | 1.99                     | 0.45              |
| 1:M:480:HIS:O    | 1:M:483:ARG:HG2   | 2.16                     | 0.45              |
| 1:M:1201:THR:OG1 | 1:M:1202:MET:N    | 2.48                     | 0.45              |
| 1:N:28:ASP:HB2   | 1:N:31:ASP:CG     | 2.42                     | 0.45              |
| 1:N:249:ASN:O    | 1:N:251:APK:O     | 2.35                     | 0.45              |
| 1:N:269:LYS:HB3  | 1:N:407:LYS:O     | 2.17                     | 0.45              |
| 1:N:480:HIS:O    | 1:N:483:ARG:HG2   | 2.16                     | 0.45              |
| 1:N:782:CYS:HB3  | 1:N:816:LEU:HD13  | 1.99                     | 0.45              |
| 1:O:28:ASP:HB2   | 1:O:31:ASP:CG     | 2.42                     | 0.45              |
| 1:O:269:LYS:HB3  | 1:O:407:LYS:O     | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:O:557:LYS:NZ   | 1:O:1223:GLN:HG3  | 2.31                     | 0.45              |
| 1:A:841:PHE:O    | 1:A:842:LEU:HB2   | 2.17                     | 0.45              |
| 1:B:662:GLN:O    | 1:B:663:GLN:HG2   | 2.17                     | 0.45              |
| 1:B:782:CYS:HB3  | 1:B:816:LEU:HD13  | 1.99                     | 0.45              |
| 1:B:1098:LEU:HG  | 1:B:1111:GLU:HG2  | 1.98                     | 0.45              |
| 1:B:1201:THR:OG1 | 1:B:1202:MET:N    | 2.48                     | 0.45              |
| 1:D:127:ARG:HD3  | 1:D:292:LEU:HD12  | 1.98                     | 0.45              |
| 1:D:337:THR:OG1  | 1:D:340:ASN:N     | 2.50                     | 0.45              |
| 1:D:542:ILE:HA   | 1:D:545:PHE:HD2   | 1.82                     | 0.45              |
| 1:E:250:ALA:C    | 1:E:251:APK:O     | 2.59                     | 0.45              |
| 1:E:451:LYS:CD   | 1:E:486:LEU:HD21  | 2.33                     | 0.45              |
| 1:E:457:ASP:OD2  | 1:E:458:LEU:HB2   | 2.17                     | 0.45              |
| 1:E:1188:LYS:HG3 | 1:E:1189:ALA:H    | 1.82                     | 0.45              |
| 1:F:336:ALA:O    | 1:F:337:THR:OG1   | 2.35                     | 0.45              |
| 1:F:480:HIS:O    | 1:F:483:ARG:HG2   | 2.16                     | 0.45              |
| 1:F:1035:TYR:HA  | 1:F:1057:PRO:HG2  | 1.99                     | 0.45              |
| 1:G:382:PRO:HA   | 1:G:419:THR:CG2   | 2.36                     | 0.45              |
| 1:G:491:PHE:N    | 1:G:491:PHE:CD1   | 2.83                     | 0.45              |
| 1:H:269:LYS:HB3  | 1:H:407:LYS:O     | 2.17                     | 0.45              |
| 1:H:312:LEU:HD23 | 1:H:312:LEU:C     | 2.41                     | 0.45              |
| 1:H:656:ARG:HG2  | 1:H:657:MET:H     | 1.81                     | 0.45              |
| 1:H:999:ALA:HA   | 1:H:1019:LYS:HA   | 1.98                     | 0.45              |
| 1:I:557:LYS:CD   | 1:I:1223:GLN:HE21 | 2.30                     | 0.45              |
| 1:J:28:ASP:HB2   | 1:J:31:ASP:CG     | 2.42                     | 0.45              |
| 1:J:457:ASP:OD2  | 1:J:458:LEU:HB2   | 2.17                     | 0.45              |
| 1:K:28:ASP:HB2   | 1:K:31:ASP:CG     | 2.42                     | 0.45              |
| 1:K:127:ARG:HD3  | 1:K:292:LEU:HD12  | 1.98                     | 0.45              |
| 1:K:269:LYS:HB3  | 1:K:407:LYS:O     | 2.17                     | 0.45              |
| 1:K:312:LEU:HD23 | 1:K:312:LEU:C     | 2.40                     | 0.45              |
| 1:K:458:LEU:HA   | 1:K:587:ARG:HH21  | 1.80                     | 0.45              |
| 1:K:542:ILE:HA   | 1:K:545:PHE:HD2   | 1.82                     | 0.45              |
| 1:K:557:LYS:NZ   | 1:K:1223:GLN:HG3  | 2.31                     | 0.45              |
| 1:L:225:GLN:HG3  | 1:L:258:LEU:HD22  | 1.98                     | 0.45              |
| 1:L:361:GLU:HB2  | 1:L:364:GLU:HB3   | 1.98                     | 0.45              |
| 1:L:638:GLU:OE1  | 1:L:640:GLU:N     | 2.42                     | 0.45              |
| 1:L:641:ASP:OD1  | 1:L:642:THR:N     | 2.45                     | 0.45              |
| 1:L:782:CYS:HB3  | 1:L:816:LEU:HD13  | 1.99                     | 0.45              |
| 1:L:841:PHE:O    | 1:L:842:LEU:HB2   | 2.17                     | 0.45              |
| 1:M:269:LYS:HB3  | 1:M:407:LYS:O     | 2.17                     | 0.45              |
| 1:M:557:LYS:NZ   | 1:M:1223:GLN:HG3  | 2.32                     | 0.45              |
| 1:M:662:GLN:O    | 1:M:663:GLN:HG2   | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:782:CYS:HB3  | 1:M:816:LEU:HD13 | 1.99                     | 0.45              |
| 1:N:225:GLN:HG3  | 1:N:258:LEU:HD22 | 1.98                     | 0.45              |
| 1:N:462:TYR:OH   | 1:N:494:PHE:CZ   | 2.66                     | 0.45              |
| 1:O:85:TYR:HB2   | 1:O:87:PHE:CE2   | 2.51                     | 0.45              |
| 1:O:662:GLN:O    | 1:O:663:GLN:HG2  | 2.17                     | 0.45              |
| 1:O:999:ALA:HA   | 1:O:1019:LYS:HA  | 1.98                     | 0.45              |
| 1:P:336:ALA:O    | 1:P:337:THR:OG1  | 2.35                     | 0.45              |
| 1:P:458:LEU:HG   | 1:P:587:ARG:HH22 | 1.81                     | 0.45              |
| 1:P:584:PHE:HB3  | 1:P:585:ASP:H    | 1.61                     | 0.45              |
| 1:P:914:VAL:O    | 1:P:915:TYR:C    | 2.60                     | 0.45              |
| 1:P:1059:ASP:HB3 | 1:P:1071:ALA:HB3 | 1.98                     | 0.45              |
| 1:A:198:LYS:NZ   | 1:B:222:HIS:CD2  | 2.85                     | 0.45              |
| 1:A:542:ILE:HA   | 1:A:545:PHE:HD2  | 1.82                     | 0.45              |
| 1:A:999:ALA:HA   | 1:A:1019:LYS:HA  | 1.98                     | 0.45              |
| 1:B:54:ALA:O     | 1:B:58:THR:N     | 2.48                     | 0.45              |
| 1:B:336:ALA:O    | 1:B:337:THR:OG1  | 2.35                     | 0.45              |
| 1:B:457:ASP:OD2  | 1:B:458:LEU:HB2  | 2.17                     | 0.45              |
| 1:C:324:LEU:HD12 | 1:C:324:LEU:HA   | 1.61                     | 0.45              |
| 1:C:782:CYS:HB3  | 1:C:816:LEU:HD13 | 1.99                     | 0.45              |
| 1:C:841:PHE:O    | 1:C:842:LEU:HB2  | 2.17                     | 0.45              |
| 1:D:28:ASP:HB2   | 1:D:31:ASP:CG    | 2.42                     | 0.45              |
| 1:D:428:GLU:C    | 1:D:430:LYS:N    | 2.74                     | 0.45              |
| 1:D:491:PHE:N    | 1:D:491:PHE:CD1  | 2.83                     | 0.45              |
| 1:E:28:ASP:HB2   | 1:E:31:ASP:CG    | 2.42                     | 0.45              |
| 1:E:249:ASN:O    | 1:E:251:APK:O    | 2.35                     | 0.45              |
| 1:E:458:LEU:HG   | 1:E:587:ARG:HH22 | 1.81                     | 0.45              |
| 1:E:584:PHE:HB3  | 1:E:585:ASP:H    | 1.61                     | 0.45              |
| 1:E:1035:TYR:HA  | 1:E:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:E:1158:TYR:HE2 | 1:E:1160:ASN:HB2 | 1.82                     | 0.45              |
| 1:F:225:GLN:HG3  | 1:F:258:LEU:HD22 | 1.98                     | 0.45              |
| 1:F:231:LEU:O    | 1:F:234:SER:OG   | 2.26                     | 0.45              |
| 1:F:914:VAL:O    | 1:F:915:TYR:C    | 2.60                     | 0.45              |
| 1:F:999:ALA:HA   | 1:F:1019:LYS:HA  | 1.98                     | 0.45              |
| 1:G:1188:LYS:HG3 | 1:G:1189:ALA:H   | 1.82                     | 0.45              |
| 1:I:898:VAL:HG13 | 1:I:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:J:249:ASN:O    | 1:J:251:APK:O    | 2.35                     | 0.45              |
| 1:J:250:ALA:C    | 1:J:251:APK:O    | 2.59                     | 0.45              |
| 1:J:542:ILE:HA   | 1:J:545:PHE:HD2  | 1.82                     | 0.45              |
| 1:J:898:VAL:HG13 | 1:J:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:J:1035:TYR:HA  | 1:J:1057:PRO:HG2 | 1.99                     | 0.45              |
| 1:K:80:VAL:HA    | 1:K:83:ILE:HD12  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:337:THR:OG1  | 1:K:340:ASN:N    | 2.50                     | 0.45              |
| 1:K:457:ASP:OD2  | 1:K:458:LEU:HB2  | 2.17                     | 0.45              |
| 1:K:491:PHE:CD1  | 1:K:491:PHE:N    | 2.83                     | 0.45              |
| 1:L:269:LYS:HB3  | 1:L:407:LYS:O    | 2.17                     | 0.45              |
| 1:M:336:ALA:O    | 1:M:337:THR:OG1  | 2.35                     | 0.45              |
| 1:M:337:THR:OG1  | 1:M:340:ASN:N    | 2.50                     | 0.45              |
| 1:M:457:ASP:OD2  | 1:M:458:LEU:HB2  | 2.17                     | 0.45              |
| 1:N:542:ILE:HA   | 1:N:545:PHE:HD2  | 1.81                     | 0.45              |
| 1:N:841:PHE:O    | 1:N:842:LEU:HB2  | 2.17                     | 0.45              |
| 1:O:102:MET:O    | 1:O:105:MET:N    | 2.46                     | 0.45              |
| 1:O:358:ASN:HA   | 1:O:366:ARG:NH2  | 2.31                     | 0.45              |
| 1:P:491:PHE:CD1  | 1:P:491:PHE:N    | 2.83                     | 0.45              |
| 1:A:127:ARG:HD3  | 1:A:292:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:341:TRP:O    | 1:A:341:TRP:CE3  | 2.70                     | 0.45              |
| 1:A:458:LEU:CA   | 1:A:587:ARG:HH21 | 2.30                     | 0.45              |
| 1:A:462:TYR:OH   | 1:A:494:PHE:CZ   | 2.66                     | 0.45              |
| 1:A:641:ASP:OD1  | 1:A:642:THR:N    | 2.45                     | 0.45              |
| 1:B:11:GLN:O     | 1:B:14:ASP:N     | 2.46                     | 0.45              |
| 1:B:36:PRO:HG2   | 1:B:39:ILE:CG2   | 2.47                     | 0.45              |
| 1:B:154:GLY:O    | 1:B:155:SER:OG   | 2.35                     | 0.45              |
| 1:B:269:LYS:HB3  | 1:B:407:LYS:O    | 2.17                     | 0.45              |
| 1:B:337:THR:OG1  | 1:B:340:ASN:N    | 2.50                     | 0.45              |
| 1:B:462:TYR:OH   | 1:B:494:PHE:CZ   | 2.66                     | 0.45              |
| 1:C:15:ILE:HD11  | 1:C:103:THR:HG21 | 1.99                     | 0.45              |
| 1:C:225:GLN:HG3  | 1:C:258:LEU:HD22 | 1.98                     | 0.45              |
| 1:C:269:LYS:HB3  | 1:C:407:LYS:O    | 2.17                     | 0.45              |
| 1:C:901:HIS:HB2  | 1:C:1230:GLU:CD  | 2.42                     | 0.45              |
| 1:D:249:ASN:O    | 1:D:251:APK:O    | 2.35                     | 0.45              |
| 1:D:898:VAL:HG13 | 1:D:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:E:542:ILE:HA   | 1:E:545:PHE:HD2  | 1.82                     | 0.45              |
| 1:E:662:GLN:O    | 1:E:663:GLN:HG2  | 2.17                     | 0.45              |
| 1:E:898:VAL:HG13 | 1:E:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:F:28:ASP:HB2   | 1:F:31:ASP:CG    | 2.42                     | 0.45              |
| 1:F:1158:TYR:HE2 | 1:F:1160:ASN:HB2 | 1.82                     | 0.45              |
| 1:G:508:TRP:C    | 1:G:606:GLY:N    | 2.70                     | 0.45              |
| 1:G:866:LYS:HE2  | 1:G:872:ARG:HH11 | 1.81                     | 0.45              |
| 1:H:85:TYR:HB2   | 1:H:87:PHE:CE2   | 2.51                     | 0.45              |
| 1:H:250:ALA:C    | 1:H:251:APK:O    | 2.59                     | 0.45              |
| 1:H:292:LEU:HB2  | 1:H:319:THR:HB   | 1.99                     | 0.45              |
| 1:H:336:ALA:O    | 1:H:337:THR:OG1  | 2.35                     | 0.45              |
| 1:H:1098:LEU:HG  | 1:H:1111:GLU:HG2 | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:1158:TYR:HE2 | 1:H:1160:ASN:HB2 | 1.82                     | 0.45              |
| 1:I:312:LEU:HD23 | 1:I:312:LEU:C    | 2.40                     | 0.45              |
| 1:I:914:VAL:O    | 1:I:915:TYR:C    | 2.60                     | 0.45              |
| 1:I:1158:TYR:HE2 | 1:I:1160:ASN:HB2 | 1.83                     | 0.45              |
| 1:J:662:GLN:O    | 1:J:663:GLN:HG2  | 2.17                     | 0.45              |
| 1:K:15:ILE:HD11  | 1:K:103:THR:HG21 | 1.99                     | 0.45              |
| 1:K:249:ASN:O    | 1:K:251:APK:O    | 2.35                     | 0.45              |
| 1:K:898:VAL:HG13 | 1:K:930:HIS:CD2  | 2.52                     | 0.45              |
| 1:K:1158:TYR:HE2 | 1:K:1160:ASN:HB2 | 1.82                     | 0.45              |
| 1:L:142:ARG:NH1  | 1:M:14:ASP:OD2   | 2.48                     | 0.45              |
| 1:L:656:ARG:HG2  | 1:L:657:MET:H    | 1.81                     | 0.45              |
| 1:L:901:HIS:HB2  | 1:L:1230:GLU:CD  | 2.42                     | 0.45              |
| 1:M:36:PRO:HG2   | 1:M:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:M:54:ALA:O     | 1:M:58:THR:N     | 2.48                     | 0.45              |
| 1:M:133:LYS:O    | 1:M:136:GLN:HB3  | 2.16                     | 0.45              |
| 1:M:154:GLY:O    | 1:M:155:SER:OG   | 2.35                     | 0.45              |
| 1:M:249:ASN:O    | 1:M:251:APK:O    | 2.35                     | 0.45              |
| 1:M:371:ARG:HB3  | 1:M:389:ILE:CG2  | 2.45                     | 0.45              |
| 1:M:458:LEU:CA   | 1:M:587:ARG:HH21 | 2.30                     | 0.45              |
| 1:M:462:TYR:OH   | 1:M:494:PHE:CZ   | 2.66                     | 0.45              |
| 1:N:458:LEU:CA   | 1:N:587:ARG:HH21 | 2.30                     | 0.45              |
| 1:N:999:ALA:HA   | 1:N:1019:LYS:HA  | 1.98                     | 0.45              |
| 1:O:250:ALA:C    | 1:O:251:APK:O    | 2.59                     | 0.45              |
| 1:O:292:LEU:HB2  | 1:O:319:THR:HB   | 1.99                     | 0.45              |
| 1:O:656:ARG:HG2  | 1:O:657:MET:H    | 1.81                     | 0.45              |
| 1:O:866:LYS:HE2  | 1:O:872:ARG:HH11 | 1.81                     | 0.45              |
| 1:O:1098:LEU:HG  | 1:O:1111:GLU:HG2 | 1.99                     | 0.45              |
| 1:O:1158:TYR:HE2 | 1:O:1160:ASN:HB2 | 1.82                     | 0.45              |
| 1:P:458:LEU:CA   | 1:P:587:ARG:HH21 | 2.30                     | 0.45              |
| 1:P:480:HIS:O    | 1:P:483:ARG:HG2  | 2.16                     | 0.45              |
| 1:P:508:TRP:C    | 1:P:606:GLY:N    | 2.70                     | 0.45              |
| 1:P:866:LYS:HE2  | 1:P:872:ARG:HH11 | 1.81                     | 0.45              |
| 1:P:901:HIS:HB2  | 1:P:1230:GLU:CD  | 2.42                     | 0.45              |
| 1:A:80:VAL:HA    | 1:A:83:ILE:HD12  | 1.98                     | 0.44              |
| 1:A:157:LYS:N    | 2:A:1501:DTP:O2B | 2.51                     | 0.44              |
| 1:A:388:LEU:HB3  | 1:A:446:HIS:CE1  | 2.52                     | 0.44              |
| 1:B:249:ASN:O    | 1:B:251:APK:O    | 2.35                     | 0.44              |
| 1:B:371:ARG:HB3  | 1:B:389:ILE:CG2  | 2.45                     | 0.44              |
| 1:B:373:SER:C    | 1:B:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:B:388:LEU:HB3  | 1:B:446:HIS:CE1  | 2.52                     | 0.44              |
| 1:B:491:PHE:N    | 1:B:491:PHE:CD1  | 2.83                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1158:TYR:HE2 | 1:B:1160:ASN:HB2 | 1.83                     | 0.44              |
| 1:C:154:GLY:O    | 1:C:155:SER:OG   | 2.35                     | 0.44              |
| 1:C:207:TRP:CD1  | 1:C:227:GLU:CD   | 2.95                     | 0.44              |
| 1:C:317:LEU:O    | 1:C:318:THR:CB   | 2.61                     | 0.44              |
| 1:C:361:GLU:HB2  | 1:C:364:GLU:HB3  | 1.98                     | 0.44              |
| 1:C:638:GLU:OE1  | 1:C:640:GLU:N    | 2.42                     | 0.44              |
| 1:C:1158:TYR:HE2 | 1:C:1160:ASN:HB2 | 1.82                     | 0.44              |
| 1:D:15:ILE:HD11  | 1:D:103:THR:HG21 | 1.99                     | 0.44              |
| 1:D:80:VAL:HA    | 1:D:83:ILE:HD12  | 1.98                     | 0.44              |
| 1:D:457:ASP:OD2  | 1:D:458:LEU:HB2  | 2.17                     | 0.44              |
| 1:D:641:ASP:OD1  | 1:D:642:THR:N    | 2.45                     | 0.44              |
| 1:D:1198:ASP:CG  | 1:D:1199:ASP:H   | 2.25                     | 0.44              |
| 1:E:269:LYS:HB3  | 1:E:407:LYS:O    | 2.17                     | 0.44              |
| 1:E:341:TRP:CE3  | 1:E:341:TRP:O    | 2.70                     | 0.44              |
| 1:E:491:PHE:N    | 1:E:491:PHE:CD1  | 2.83                     | 0.44              |
| 1:F:54:ALA:O     | 1:F:58:THR:N     | 2.48                     | 0.44              |
| 1:F:250:ALA:C    | 1:F:251:APK:O    | 2.59                     | 0.44              |
| 1:F:269:LYS:HB3  | 1:F:407:LYS:O    | 2.17                     | 0.44              |
| 1:F:361:GLU:HB2  | 1:F:364:GLU:HB3  | 1.98                     | 0.44              |
| 1:F:557:LYS:NZ   | 1:F:1223:GLN:HG3 | 2.31                     | 0.44              |
| 1:F:1188:LYS:HG3 | 1:F:1189:ALA:H   | 1.82                     | 0.44              |
| 1:G:15:ILE:HD11  | 1:G:103:THR:HG21 | 1.99                     | 0.44              |
| 1:G:36:PRO:HG2   | 1:G:39:ILE:CG2   | 2.47                     | 0.44              |
| 1:G:157:LYS:N    | 2:G:1501:DTP:O2B | 2.51                     | 0.44              |
| 1:G:207:TRP:CH2  | 1:G:209:SER:HA   | 2.51                     | 0.44              |
| 1:G:336:ALA:C    | 1:G:338:TRP:N    | 2.74                     | 0.44              |
| 1:G:373:SER:C    | 1:G:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:G:392:ASP:OD1  | 1:G:393:VAL:N    | 2.47                     | 0.44              |
| 1:G:458:LEU:CA   | 1:G:587:ARG:HH21 | 2.31                     | 0.44              |
| 1:G:901:HIS:HB2  | 1:G:1230:GLU:CD  | 2.43                     | 0.44              |
| 1:I:250:ALA:C    | 1:I:251:APK:O    | 2.59                     | 0.44              |
| 1:I:361:GLU:HB2  | 1:I:364:GLU:HB3  | 1.98                     | 0.44              |
| 1:I:413:LYS:CD   | 1:I:422:ILE:O    | 2.61                     | 0.44              |
| 1:I:480:HIS:O    | 1:I:483:ARG:HG2  | 2.16                     | 0.44              |
| 1:I:1188:LYS:HG3 | 1:I:1189:ALA:H   | 1.82                     | 0.44              |
| 1:J:269:LYS:HB3  | 1:J:407:LYS:O    | 2.17                     | 0.44              |
| 1:J:292:LEU:HB2  | 1:J:319:THR:HB   | 1.99                     | 0.44              |
| 1:J:458:LEU:HG   | 1:J:587:ARG:HH22 | 1.81                     | 0.44              |
| 1:J:1158:TYR:HE2 | 1:J:1160:ASN:HB2 | 1.83                     | 0.44              |
| 1:K:36:PRO:HG2   | 1:K:39:ILE:CG2   | 2.46                     | 0.44              |
| 1:K:782:CYS:HB3  | 1:K:816:LEU:HD13 | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:15:ILE:HD11  | 1:L:103:THR:HG21 | 1.99                     | 0.44              |
| 1:L:157:LYS:N    | 2:L:1501:DTP:O1B | 2.51                     | 0.44              |
| 1:L:914:VAL:O    | 1:L:915:TYR:C    | 2.60                     | 0.44              |
| 1:L:988:ASP:OD1  | 1:L:989:SER:N    | 2.43                     | 0.44              |
| 1:M:11:GLN:O     | 1:M:14:ASP:N     | 2.46                     | 0.44              |
| 1:M:373:SER:C    | 1:M:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:M:1098:LEU:HG  | 1:M:1111:GLU:HG2 | 1.99                     | 0.44              |
| 1:M:1158:TYR:HE2 | 1:M:1160:ASN:HB2 | 1.82                     | 0.44              |
| 1:N:80:VAL:HA    | 1:N:83:ILE:HD12  | 1.98                     | 0.44              |
| 1:N:127:ARG:HD3  | 1:N:292:LEU:HD12 | 1.98                     | 0.44              |
| 1:N:157:LYS:N    | 2:N:1501:DTP:O1B | 2.51                     | 0.44              |
| 1:N:341:TRP:O    | 1:N:341:TRP:CE3  | 2.71                     | 0.44              |
| 1:N:358:ASN:HA   | 1:N:366:ARG:NH2  | 2.31                     | 0.44              |
| 1:N:641:ASP:OD1  | 1:N:642:THR:N    | 2.45                     | 0.44              |
| 1:N:1158:TYR:HE2 | 1:N:1160:ASN:HB2 | 1.82                     | 0.44              |
| 1:O:336:ALA:O    | 1:O:337:THR:OG1  | 2.35                     | 0.44              |
| 1:O:511:SER:C    | 1:O:513:SER:N    | 2.61                     | 0.44              |
| 1:O:914:VAL:O    | 1:O:915:TYR:C    | 2.60                     | 0.44              |
| 1:P:15:ILE:HD11  | 1:P:103:THR:HG21 | 1.99                     | 0.44              |
| 1:P:36:PRO:HG2   | 1:P:39:ILE:CG2   | 2.46                     | 0.44              |
| 1:P:207:TRP:CH2  | 1:P:209:SER:HA   | 2.51                     | 0.44              |
| 1:P:392:ASP:OD1  | 1:P:393:VAL:N    | 2.47                     | 0.44              |
| 1:P:1158:TYR:HE2 | 1:P:1160:ASN:HB2 | 1.82                     | 0.44              |
| 1:P:1188:LYS:HG3 | 1:P:1189:ALA:H   | 1.82                     | 0.44              |
| 1:A:194:GLU:OE2  | 1:B:216:ASN:ND2  | 2.50                     | 0.44              |
| 1:A:336:ALA:O    | 1:A:337:THR:OG1  | 2.35                     | 0.44              |
| 1:A:1158:TYR:HE2 | 1:A:1160:ASN:HB2 | 1.83                     | 0.44              |
| 1:B:133:LYS:O    | 1:B:136:GLN:HB3  | 2.16                     | 0.44              |
| 1:B:293:THR:HG22 | 1:B:295:ASP:H    | 1.80                     | 0.44              |
| 1:B:341:TRP:O    | 1:B:341:TRP:CE3  | 2.71                     | 0.44              |
| 1:B:361:GLU:HB2  | 1:B:364:GLU:HB3  | 1.98                     | 0.44              |
| 1:B:458:LEU:CA   | 1:B:587:ARG:HH21 | 2.31                     | 0.44              |
| 1:B:841:PHE:O    | 1:B:842:LEU:HB2  | 2.17                     | 0.44              |
| 1:B:1192:SER:OG  | 1:B:1208:GLU:OE2 | 2.28                     | 0.44              |
| 1:C:480:HIS:O    | 1:C:483:ARG:HG2  | 2.16                     | 0.44              |
| 1:C:656:ARG:HG2  | 1:C:657:MET:H    | 1.81                     | 0.44              |
| 1:C:662:GLN:O    | 1:C:663:GLN:HG2  | 2.17                     | 0.44              |
| 1:D:1035:TYR:HA  | 1:D:1057:PRO:HG2 | 1.99                     | 0.44              |
| 1:D:1158:TYR:HE2 | 1:D:1160:ASN:HB2 | 1.83                     | 0.44              |
| 1:E:292:LEU:HB2  | 1:E:319:THR:HB   | 1.99                     | 0.44              |
| 1:E:641:ASP:OD1  | 1:E:642:THR:N    | 2.45                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:15:ILE:HD11  | 1:F:103:THR:HG21  | 1.99                     | 0.44              |
| 1:F:207:TRP:CD1  | 1:F:227:GLU:CD    | 2.95                     | 0.44              |
| 1:F:557:LYS:CD   | 1:F:1223:GLN:HE21 | 2.30                     | 0.44              |
| 1:G:337:THR:OG1  | 1:G:340:ASN:N     | 2.50                     | 0.44              |
| 1:G:480:HIS:O    | 1:G:483:ARG:HG2   | 2.16                     | 0.44              |
| 1:G:1158:TYR:HE2 | 1:G:1160:ASN:HB2  | 1.82                     | 0.44              |
| 1:H:15:ILE:HD11  | 1:H:103:THR:HG21  | 1.99                     | 0.44              |
| 1:H:102:MET:O    | 1:H:105:MET:N     | 2.46                     | 0.44              |
| 1:H:341:TRP:CE3  | 1:H:341:TRP:O     | 2.71                     | 0.44              |
| 1:H:782:CYS:HB3  | 1:H:816:LEU:HD13  | 1.99                     | 0.44              |
| 1:H:866:LYS:HE2  | 1:H:872:ARG:HH11  | 1.81                     | 0.44              |
| 1:H:1188:LYS:HG3 | 1:H:1189:ALA:H    | 1.82                     | 0.44              |
| 1:I:249:ASN:O    | 1:I:251:APK:O     | 2.35                     | 0.44              |
| 1:I:269:LYS:HB3  | 1:I:407:LYS:O     | 2.17                     | 0.44              |
| 1:I:629:GLN:HG2  | 1:I:651:SER:H     | 1.83                     | 0.44              |
| 1:J:15:ILE:HD11  | 1:J:103:THR:HG21  | 1.99                     | 0.44              |
| 1:J:341:TRP:O    | 1:J:341:TRP:CE3   | 2.71                     | 0.44              |
| 1:J:491:PHE:N    | 1:J:491:PHE:CD1   | 2.83                     | 0.44              |
| 1:J:1098:LEU:HG  | 1:J:1111:GLU:HG2  | 1.99                     | 0.44              |
| 1:J:1198:ASP:CG  | 1:J:1199:ASP:H    | 2.25                     | 0.44              |
| 1:K:144:ALA:HB3  | 1:L:111:ASP:HB3   | 1.99                     | 0.44              |
| 1:K:1035:TYR:HA  | 1:K:1057:PRO:HG2  | 1.99                     | 0.44              |
| 1:K:1198:ASP:CG  | 1:K:1199:ASP:H    | 2.25                     | 0.44              |
| 1:L:154:GLY:O    | 1:L:155:SER:OG    | 2.35                     | 0.44              |
| 1:L:207:TRP:CD1  | 1:L:227:GLU:CD    | 2.95                     | 0.44              |
| 1:L:285:LEU:HD23 | 1:L:285:LEU:HA    | 1.74                     | 0.44              |
| 1:L:1158:TYR:HE2 | 1:L:1160:ASN:HB2  | 1.82                     | 0.44              |
| 1:M:388:LEU:HB3  | 1:M:446:HIS:CE1   | 2.53                     | 0.44              |
| 1:M:491:PHE:N    | 1:M:491:PHE:CD1   | 2.83                     | 0.44              |
| 1:M:508:TRP:O    | 1:M:606:GLY:CA    | 2.63                     | 0.44              |
| 1:M:1192:SER:OG  | 1:M:1208:GLU:OE2  | 2.28                     | 0.44              |
| 1:N:336:ALA:O    | 1:N:337:THR:OG1   | 2.35                     | 0.44              |
| 1:N:388:LEU:HB3  | 1:N:446:HIS:CE1   | 2.52                     | 0.44              |
| 1:N:1098:LEU:HG  | 1:N:1111:GLU:HG2  | 1.98                     | 0.44              |
| 1:O:120:PHE:CE1  | 1:O:159:TRP:CE3   | 3.05                     | 0.44              |
| 1:P:157:LYS:N    | 2:P:1501:DTP:O1B  | 2.51                     | 0.44              |
| 1:P:207:TRP:CD1  | 1:P:227:GLU:CD    | 2.95                     | 0.44              |
| 1:P:269:LYS:HB3  | 1:P:407:LYS:O     | 2.17                     | 0.44              |
| 1:P:336:ALA:C    | 1:P:338:TRP:N     | 2.74                     | 0.44              |
| 1:P:337:THR:OG1  | 1:P:340:ASN:N     | 2.50                     | 0.44              |
| 1:P:373:SER:C    | 1:P:433:LEU:HD12  | 2.43                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:999:ALA:HA   | 1:P:1019:LYS:HA   | 1.98                     | 0.44              |
| 1:A:122:LYS:HG3  | 1:B:276:SER:HB2   | 1.99                     | 0.44              |
| 1:A:337:THR:OG1  | 1:A:340:ASN:N     | 2.50                     | 0.44              |
| 1:A:358:ASN:HA   | 1:A:366:ARG:NH2   | 2.31                     | 0.44              |
| 1:A:557:LYS:NZ   | 1:A:1223:GLN:HG3  | 2.32                     | 0.44              |
| 1:A:629:GLN:HG2  | 1:A:651:SER:H     | 1.83                     | 0.44              |
| 1:B:15:ILE:HD11  | 1:B:103:THR:HG21  | 1.99                     | 0.44              |
| 1:B:292:LEU:HB2  | 1:B:319:THR:HB    | 1.99                     | 0.44              |
| 1:B:504:ASP:CG   | 1:B:608:ASN:HD22  | 2.26                     | 0.44              |
| 1:B:508:TRP:O    | 1:B:606:GLY:CA    | 2.63                     | 0.44              |
| 1:C:157:LYS:N    | 2:C:1501:DTP:O2B  | 2.51                     | 0.44              |
| 1:C:292:LEU:HB2  | 1:C:319:THR:HB    | 1.99                     | 0.44              |
| 1:C:914:VAL:O    | 1:C:915:TYR:C     | 2.60                     | 0.44              |
| 1:C:988:ASP:OD1  | 1:C:989:SER:N     | 2.43                     | 0.44              |
| 1:D:36:PRO:HG2   | 1:D:39:ILE:CG2    | 2.46                     | 0.44              |
| 1:D:341:TRP:O    | 1:D:341:TRP:CE3   | 2.70                     | 0.44              |
| 1:D:417:GLU:O    | 1:D:417:GLU:HG2   | 2.18                     | 0.44              |
| 1:D:782:CYS:HB3  | 1:D:816:LEU:HD13  | 1.99                     | 0.44              |
| 1:E:15:ILE:HD11  | 1:E:103:THR:HG21  | 1.99                     | 0.44              |
| 1:E:504:ASP:CG   | 1:E:608:ASN:HD22  | 2.26                     | 0.44              |
| 1:E:511:SER:C    | 1:E:513:SER:N     | 2.60                     | 0.44              |
| 1:E:1098:LEU:HG  | 1:E:1111:GLU:HG2  | 1.99                     | 0.44              |
| 1:E:1198:ASP:CG  | 1:E:1199:ASP:H    | 2.25                     | 0.44              |
| 1:F:266:THR:HG22 | 1:F:268:PHE:N     | 2.33                     | 0.44              |
| 1:F:413:LYS:CD   | 1:F:422:ILE:O     | 2.61                     | 0.44              |
| 1:F:457:ASP:OD2  | 1:F:458:LEU:HB2   | 2.17                     | 0.44              |
| 1:F:629:GLN:HG2  | 1:F:651:SER:H     | 1.83                     | 0.44              |
| 1:F:957:ILE:HG13 | 1:F:1248:LEU:HD22 | 1.99                     | 0.44              |
| 1:G:207:TRP:CD1  | 1:G:227:GLU:CD    | 2.95                     | 0.44              |
| 1:G:251:APK:H8   | 1:G:251:APK:H2'   | 1.74                     | 0.44              |
| 1:G:341:TRP:O    | 1:G:341:TRP:CE3   | 2.70                     | 0.44              |
| 1:G:428:GLU:C    | 1:G:430:LYS:N     | 2.74                     | 0.44              |
| 1:G:440:HIS:O    | 1:G:444:VAL:HG23  | 2.18                     | 0.44              |
| 1:G:999:ALA:HA   | 1:G:1019:LYS:HA   | 1.98                     | 0.44              |
| 1:H:914:VAL:O    | 1:H:915:TYR:C     | 2.60                     | 0.44              |
| 1:I:54:ALA:O     | 1:I:58:THR:N      | 2.48                     | 0.44              |
| 1:I:122:LYS:HG3  | 1:P:276:SER:OG    | 2.16                     | 0.44              |
| 1:I:266:THR:HG22 | 1:I:268:PHE:N     | 2.33                     | 0.44              |
| 1:I:440:HIS:O    | 1:I:444:VAL:HG23  | 2.18                     | 0.44              |
| 1:I:662:GLN:O    | 1:I:663:GLN:HG2   | 2.17                     | 0.44              |
| 1:I:841:PHE:O    | 1:I:842:LEU:HB2   | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:957:ILE:HG13 | 1:I:1248:LEU:HD22 | 1.99                     | 0.44              |
| 1:J:200:LEU:HD12 | 1:J:200:LEU:HA    | 1.74                     | 0.44              |
| 1:J:451:LYS:CD   | 1:J:486:LEU:HD21  | 2.33                     | 0.44              |
| 1:J:504:ASP:CG   | 1:J:608:ASN:HD22  | 2.26                     | 0.44              |
| 1:J:584:PHE:HB3  | 1:J:585:ASP:H     | 1.61                     | 0.44              |
| 1:K:341:TRP:CE3  | 1:K:341:TRP:O     | 2.70                     | 0.44              |
| 1:K:417:GLU:HG2  | 1:K:417:GLU:O     | 2.18                     | 0.44              |
| 1:K:641:ASP:OD1  | 1:K:642:THR:N     | 2.45                     | 0.44              |
| 1:K:999:ALA:HA   | 1:K:1019:LYS:HA   | 1.98                     | 0.44              |
| 1:K:1098:LEU:HG  | 1:K:1111:GLU:HG2  | 1.99                     | 0.44              |
| 1:L:249:ASN:O    | 1:L:251:APK:O     | 2.35                     | 0.44              |
| 1:L:457:ASP:OD2  | 1:L:458:LEU:HB2   | 2.17                     | 0.44              |
| 1:L:662:GLN:O    | 1:L:663:GLN:HG2   | 2.17                     | 0.44              |
| 1:M:20:GLU:HG3   | 1:M:21:ASP:N      | 2.33                     | 0.44              |
| 1:M:292:LEU:HB2  | 1:M:319:THR:HB    | 1.99                     | 0.44              |
| 1:M:293:THR:HG22 | 1:M:295:ASP:H     | 1.80                     | 0.44              |
| 1:M:313:PRO:CG   | 1:M:338:TRP:CE2   | 2.94                     | 0.44              |
| 1:M:341:TRP:CE3  | 1:M:341:TRP:O     | 2.71                     | 0.44              |
| 1:M:361:GLU:HB2  | 1:M:364:GLU:HB3   | 1.98                     | 0.44              |
| 1:M:504:ASP:CG   | 1:M:608:ASN:HD22  | 2.26                     | 0.44              |
| 1:M:633:THR:HG22 | 1:M:643:TYR:HA    | 1.97                     | 0.44              |
| 1:M:841:PHE:O    | 1:M:842:LEU:HB2   | 2.17                     | 0.44              |
| 1:N:629:GLN:HG2  | 1:N:651:SER:H     | 1.83                     | 0.44              |
| 1:N:1188:LYS:HG3 | 1:N:1189:ALA:H    | 1.82                     | 0.44              |
| 1:O:341:TRP:O    | 1:O:341:TRP:CE3   | 2.71                     | 0.44              |
| 1:P:28:ASP:HB2   | 1:P:31:ASP:CG     | 2.42                     | 0.44              |
| 1:P:341:TRP:CE3  | 1:P:341:TRP:O     | 2.70                     | 0.44              |
| 1:P:428:GLU:C    | 1:P:430:LYS:N     | 2.74                     | 0.44              |
| 1:A:120:PHE:CE1  | 1:A:159:TRP:CE3   | 3.05                     | 0.44              |
| 1:A:154:GLY:O    | 1:A:155:SER:OG    | 2.35                     | 0.44              |
| 1:A:250:ALA:C    | 1:A:251:APK:O     | 2.59                     | 0.44              |
| 1:A:1098:LEU:HG  | 1:A:1111:GLU:HG2  | 1.99                     | 0.44              |
| 1:B:20:GLU:HG3   | 1:B:21:ASP:N      | 2.33                     | 0.44              |
| 1:B:313:PRO:CG   | 1:B:338:TRP:CE2   | 2.94                     | 0.44              |
| 1:B:463:LEU:CD2  | 1:B:467:PHE:CD2   | 2.92                     | 0.44              |
| 1:B:557:LYS:CD   | 1:B:1223:GLN:HE21 | 2.30                     | 0.44              |
| 1:B:633:THR:HG22 | 1:B:643:TYR:HA    | 1.97                     | 0.44              |
| 1:C:266:THR:HG22 | 1:C:268:PHE:N     | 2.33                     | 0.44              |
| 1:C:457:ASP:OD2  | 1:C:458:LEU:HB2   | 2.17                     | 0.44              |
| 1:D:154:GLY:O    | 1:D:155:SER:OG    | 2.35                     | 0.44              |
| 1:D:373:SER:C    | 1:D:433:LEU:HD12  | 2.43                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:462:TYR:CZ   | 1:D:494:PHE:CZ    | 3.03                     | 0.44              |
| 1:D:999:ALA:HA   | 1:D:1019:LYS:HA   | 1.98                     | 0.44              |
| 1:D:1098:LEU:HG  | 1:D:1111:GLU:HG2  | 1.99                     | 0.44              |
| 1:E:234:SER:OG   | 1:E:235:LYS:N     | 2.51                     | 0.44              |
| 1:E:458:LEU:CA   | 1:E:587:ARG:HH21  | 2.31                     | 0.44              |
| 1:E:629:GLN:HG2  | 1:E:651:SER:H     | 1.83                     | 0.44              |
| 1:E:782:CYS:HB3  | 1:E:816:LEU:HD13  | 1.99                     | 0.44              |
| 1:F:249:ASN:O    | 1:F:251:APK:O     | 2.35                     | 0.44              |
| 1:F:292:LEU:HB2  | 1:F:319:THR:HB    | 1.99                     | 0.44              |
| 1:F:440:HIS:O    | 1:F:444:VAL:HG23  | 2.18                     | 0.44              |
| 1:G:28:ASP:HB2   | 1:G:31:ASP:CG     | 2.42                     | 0.44              |
| 1:G:54:ALA:O     | 1:G:58:THR:N      | 2.48                     | 0.44              |
| 1:G:249:ASN:O    | 1:G:251:APK:O     | 2.35                     | 0.44              |
| 1:G:269:LYS:HB3  | 1:G:407:LYS:O     | 2.17                     | 0.44              |
| 1:G:292:LEU:HB2  | 1:G:319:THR:HB    | 1.99                     | 0.44              |
| 1:H:120:PHE:CE1  | 1:H:159:TRP:CE3   | 3.05                     | 0.44              |
| 1:H:388:LEU:HB3  | 1:H:446:HIS:CE1   | 2.52                     | 0.44              |
| 1:H:463:LEU:CD2  | 1:H:467:PHE:CD2   | 2.92                     | 0.44              |
| 1:H:901:HIS:HB2  | 1:H:1230:GLU:CD   | 2.42                     | 0.44              |
| 1:I:15:ILE:HD11  | 1:I:103:THR:HG21  | 1.99                     | 0.44              |
| 1:I:207:TRP:CD1  | 1:I:227:GLU:CD    | 2.95                     | 0.44              |
| 1:I:292:LEU:HB2  | 1:I:319:THR:HB    | 1.99                     | 0.44              |
| 1:I:458:LEU:HA   | 1:I:587:ARG:HH21  | 1.80                     | 0.44              |
| 1:I:557:LYS:NZ   | 1:I:1223:GLN:HG3  | 2.31                     | 0.44              |
| 1:I:1098:LEU:HG  | 1:I:1111:GLU:HG2  | 1.99                     | 0.44              |
| 1:J:127:ARG:HD3  | 1:J:292:LEU:HD12  | 1.98                     | 0.44              |
| 1:J:234:SER:OG   | 1:J:235:LYS:N     | 2.51                     | 0.44              |
| 1:J:440:HIS:O    | 1:J:444:VAL:HG23  | 2.18                     | 0.44              |
| 1:J:458:LEU:CA   | 1:J:587:ARG:HH21  | 2.31                     | 0.44              |
| 1:J:782:CYS:HB3  | 1:J:816:LEU:HD13  | 1.99                     | 0.44              |
| 1:K:154:GLY:O    | 1:K:155:SER:OG    | 2.35                     | 0.44              |
| 1:L:292:LEU:HB2  | 1:L:319:THR:HB    | 2.00                     | 0.44              |
| 1:L:1188:LYS:HG3 | 1:L:1189:ALA:H    | 1.82                     | 0.44              |
| 1:L:1198:ASP:CG  | 1:L:1199:ASP:H    | 2.25                     | 0.44              |
| 1:M:15:ILE:HD11  | 1:M:103:THR:HG21  | 1.99                     | 0.44              |
| 1:M:463:LEU:CD2  | 1:M:467:PHE:CD2   | 2.92                     | 0.44              |
| 1:M:557:LYS:CD   | 1:M:1223:GLN:HE21 | 2.30                     | 0.44              |
| 1:M:875:LEU:CD1  | 1:M:911:PHE:HD2   | 2.07                     | 0.44              |
| 1:M:1177:TYR:HE2 | 1:N:916:LYS:CE    | 2.30                     | 0.44              |
| 1:N:15:ILE:HD11  | 1:N:103:THR:HG21  | 1.99                     | 0.44              |
| 1:N:20:GLU:HG3   | 1:N:21:ASP:N      | 2.33                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:120:PHE:CE1  | 1:N:159:TRP:CE3  | 3.05                     | 0.44              |
| 1:N:250:ALA:C    | 1:N:251:APK:O    | 2.59                     | 0.44              |
| 1:N:337:THR:OG1  | 1:N:340:ASN:N    | 2.50                     | 0.44              |
| 1:N:504:ASP:CG   | 1:N:608:ASN:ND2  | 2.69                     | 0.44              |
| 1:N:988:ASP:OD1  | 1:N:989:SER:N    | 2.43                     | 0.44              |
| 1:O:15:ILE:HD11  | 1:O:103:THR:HG21 | 2.00                     | 0.44              |
| 1:O:388:LEU:HB3  | 1:O:446:HIS:CE1  | 2.52                     | 0.44              |
| 1:O:457:ASP:OD2  | 1:O:458:LEU:HB2  | 2.17                     | 0.44              |
| 1:P:292:LEU:HB2  | 1:P:319:THR:HB   | 1.99                     | 0.44              |
| 1:P:440:HIS:O    | 1:P:444:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:15:ILE:HD11  | 1:A:103:THR:HG21 | 1.99                     | 0.44              |
| 1:A:20:GLU:HG3   | 1:A:21:ASP:N     | 2.33                     | 0.44              |
| 1:A:1188:LYS:HG3 | 1:A:1189:ALA:H   | 1.82                     | 0.44              |
| 1:B:120:PHE:CE1  | 1:B:159:TRP:CE3  | 3.05                     | 0.44              |
| 1:C:337:THR:OG1  | 1:C:340:ASN:N    | 2.50                     | 0.44              |
| 1:C:1198:ASP:CG  | 1:C:1199:ASP:H   | 2.25                     | 0.44              |
| 1:D:409:SER:O    | 1:D:411:VAL:N    | 2.51                     | 0.44              |
| 1:D:462:TYR:OH   | 1:D:494:PHE:CZ   | 2.66                     | 0.44              |
| 1:E:20:GLU:HG3   | 1:E:21:ASP:N     | 2.33                     | 0.44              |
| 1:E:127:ARG:HD3  | 1:E:292:LEU:HD12 | 1.97                     | 0.44              |
| 1:E:417:GLU:HG2  | 1:E:417:GLU:O    | 2.18                     | 0.44              |
| 1:E:440:HIS:O    | 1:E:444:VAL:HG23 | 2.18                     | 0.44              |
| 1:F:234:SER:OG   | 1:F:235:LYS:N    | 2.51                     | 0.44              |
| 1:F:662:GLN:O    | 1:F:663:GLN:HG2  | 2.17                     | 0.44              |
| 1:F:1098:LEU:HG  | 1:F:1111:GLU:HG2 | 1.99                     | 0.44              |
| 1:G:398:VAL:HG23 | 1:G:399:MET:N    | 2.28                     | 0.44              |
| 1:G:898:VAL:HG13 | 1:G:930:HIS:CD2  | 2.52                     | 0.44              |
| 1:H:157:LYS:N    | 2:H:1501:DTP:O2B | 2.51                     | 0.44              |
| 1:H:207:TRP:CD1  | 1:H:227:GLU:CD   | 2.95                     | 0.44              |
| 1:H:266:THR:HG22 | 1:H:268:PHE:N    | 2.33                     | 0.44              |
| 1:I:337:THR:OG1  | 1:I:340:ASN:N    | 2.50                     | 0.44              |
| 1:I:373:SER:C    | 1:I:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:J:557:LYS:NZ   | 1:J:1223:GLN:HG3 | 2.31                     | 0.44              |
| 1:K:462:TYR:CZ   | 1:K:494:PHE:CZ   | 3.03                     | 0.44              |
| 1:K:662:GLN:O    | 1:K:663:GLN:HG2  | 2.17                     | 0.44              |
| 1:L:317:LEU:O    | 1:L:318:THR:CB   | 2.61                     | 0.44              |
| 1:L:388:LEU:HB3  | 1:L:446:HIS:CE1  | 2.52                     | 0.44              |
| 1:L:409:SER:O    | 1:L:411:VAL:N    | 2.51                     | 0.44              |
| 1:L:417:GLU:O    | 1:L:417:GLU:HG2  | 2.18                     | 0.44              |
| 1:M:120:PHE:CE1  | 1:M:159:TRP:CE3  | 3.05                     | 0.44              |
| 1:N:154:GLY:O    | 1:N:155:SER:OG   | 2.35                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:20:GLU:HG3    | 1:O:21:ASP:N      | 2.33                     | 0.44              |
| 1:O:157:LYS:N     | 2:O:1501:DTP:O1B  | 2.51                     | 0.44              |
| 1:O:266:THR:HG22  | 1:O:268:PHE:N     | 2.33                     | 0.44              |
| 1:O:782:CYS:HB3   | 1:O:816:LEU:HD13  | 1.99                     | 0.44              |
| 1:O:1188:LYS:HG3  | 1:O:1189:ALA:H    | 1.82                     | 0.44              |
| 1:O:1198:ASP:CG   | 1:O:1199:ASP:H    | 2.25                     | 0.44              |
| 1:P:249:ASN:O     | 1:P:251:APK:O     | 2.35                     | 0.44              |
| 1:P:251:APK:H8    | 1:P:251:APK:H2'   | 1.73                     | 0.44              |
| 1:P:398:VAL:HG23  | 1:P:399:MET:N     | 2.28                     | 0.44              |
| 1:P:782:CYS:HB3   | 1:P:816:LEU:HD13  | 1.99                     | 0.44              |
| 1:P:988:ASP:OD1   | 1:P:989:SER:N     | 2.43                     | 0.44              |
| 1:A:451:LYS:CD    | 1:A:486:LEU:HD21  | 2.33                     | 0.44              |
| 1:A:504:ASP:CG    | 1:A:608:ASN:ND2   | 2.69                     | 0.44              |
| 1:A:557:LYS:CD    | 1:A:1223:GLN:HE21 | 2.30                     | 0.44              |
| 1:A:914:VAL:O     | 1:A:915:TYR:C     | 2.60                     | 0.44              |
| 1:B:336:ALA:C     | 1:B:338:TRP:N     | 2.74                     | 0.44              |
| 1:B:453:PHE:CE2   | 1:B:460:PRO:HB3   | 2.49                     | 0.44              |
| 1:B:554:ILE:O     | 1:B:556:SER:N     | 2.46                     | 0.44              |
| 1:B:875:LEU:CD1   | 1:B:911:PHE:HD2   | 2.07                     | 0.44              |
| 1:B:901:HIS:HB2   | 1:B:1230:GLU:CD   | 2.42                     | 0.44              |
| 1:C:249:ASN:O     | 1:C:251:APK:O     | 2.35                     | 0.44              |
| 1:C:373:SER:C     | 1:C:433:LEU:HD12  | 2.43                     | 0.44              |
| 1:C:409:SER:O     | 1:C:411:VAL:N     | 2.51                     | 0.44              |
| 1:C:905:VAL:HG13  | 1:C:906:ASP:N     | 2.33                     | 0.44              |
| 1:C:957:ILE:HG13  | 1:C:1248:LEU:HD22 | 1.99                     | 0.44              |
| 1:C:1000:ILE:HD11 | 1:C:1014:ALA:HB3  | 2.00                     | 0.44              |
| 1:C:1098:LEU:HG   | 1:C:1111:GLU:HG2  | 1.99                     | 0.44              |
| 1:D:207:TRP:CD1   | 1:D:227:GLU:CD    | 2.95                     | 0.44              |
| 1:D:231:LEU:O     | 1:D:234:SER:OG    | 2.26                     | 0.44              |
| 1:D:440:HIS:O     | 1:D:444:VAL:HG23  | 2.18                     | 0.44              |
| 1:D:458:LEU:CA    | 1:D:587:ARG:HH21  | 2.30                     | 0.44              |
| 1:E:901:HIS:HB2   | 1:E:1230:GLU:CD   | 2.43                     | 0.44              |
| 1:F:157:LYS:N     | 2:F:1501:DTP:O2B  | 2.51                     | 0.44              |
| 1:F:373:SER:C     | 1:F:433:LEU:HD12  | 2.43                     | 0.44              |
| 1:F:463:LEU:CD2   | 1:F:467:PHE:CD2   | 2.92                     | 0.44              |
| 1:F:491:PHE:N     | 1:F:491:PHE:CD1   | 2.83                     | 0.44              |
| 1:F:782:CYS:HB3   | 1:F:816:LEU:HD13  | 1.99                     | 0.44              |
| 1:F:841:PHE:O     | 1:F:842:LEU:HB2   | 2.16                     | 0.44              |
| 1:G:409:SER:O     | 1:G:411:VAL:N     | 2.51                     | 0.44              |
| 1:G:457:ASP:OD2   | 1:G:458:LEU:HB2   | 2.17                     | 0.44              |
| 1:G:542:ILE:HA    | 1:G:545:PHE:HD2   | 1.82                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:988:ASP:OD1   | 1:G:989:SER:N    | 2.43                     | 0.44              |
| 1:H:337:THR:OG1   | 1:H:340:ASN:N    | 2.50                     | 0.44              |
| 1:H:417:GLU:HG2   | 1:H:417:GLU:O    | 2.18                     | 0.44              |
| 1:H:457:ASP:OD2   | 1:H:458:LEU:HB2  | 2.17                     | 0.44              |
| 1:H:458:LEU:CA    | 1:H:587:ARG:HH21 | 2.31                     | 0.44              |
| 1:H:1198:ASP:CG   | 1:H:1199:ASP:H   | 2.25                     | 0.44              |
| 1:I:157:LYS:N     | 2:I:1501:DTP:O1B | 2.51                     | 0.44              |
| 1:I:234:SER:OG    | 1:I:235:LYS:N    | 2.51                     | 0.44              |
| 1:I:457:ASP:OD2   | 1:I:458:LEU:HB2  | 2.17                     | 0.44              |
| 1:I:782:CYS:HB3   | 1:I:816:LEU:HD13 | 1.99                     | 0.44              |
| 1:J:629:GLN:HG2   | 1:J:651:SER:H    | 1.83                     | 0.44              |
| 1:J:641:ASP:OD1   | 1:J:642:THR:N    | 2.45                     | 0.44              |
| 1:J:901:HIS:HB2   | 1:J:1230:GLU:CD  | 2.42                     | 0.44              |
| 1:K:207:TRP:CD1   | 1:K:227:GLU:CD   | 2.95                     | 0.44              |
| 1:K:373:SER:C     | 1:K:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:K:409:SER:O     | 1:K:411:VAL:N    | 2.51                     | 0.44              |
| 1:K:428:GLU:C     | 1:K:430:LYS:N    | 2.74                     | 0.44              |
| 1:K:440:HIS:O     | 1:K:444:VAL:HG23 | 2.18                     | 0.44              |
| 1:K:462:TYR:OH    | 1:K:494:PHE:CZ   | 2.66                     | 0.44              |
| 1:L:182:ASN:HD22  | 1:L:245:LEU:HB2  | 1.83                     | 0.44              |
| 1:L:266:THR:HG22  | 1:L:268:PHE:N    | 2.33                     | 0.44              |
| 1:L:346:CYS:HG    | 1:L:350:THR:HG1  | 1.62                     | 0.44              |
| 1:L:373:SER:C     | 1:L:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:L:1000:ILE:HD11 | 1:L:1014:ALA:HB3 | 2.00                     | 0.44              |
| 1:M:554:ILE:O     | 1:M:556:SER:N    | 2.46                     | 0.44              |
| 1:N:54:ALA:O      | 1:N:58:THR:N     | 2.48                     | 0.44              |
| 1:N:373:SER:C     | 1:N:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:O:207:TRP:CD1   | 1:O:227:GLU:CD   | 2.95                     | 0.44              |
| 1:O:417:GLU:O     | 1:O:417:GLU:HG2  | 2.18                     | 0.44              |
| 1:O:453:PHE:CE1   | 1:O:460:PRO:HB3  | 2.51                     | 0.44              |
| 1:O:458:LEU:CA    | 1:O:587:ARG:HH21 | 2.30                     | 0.44              |
| 1:P:54:ALA:O      | 1:P:58:THR:N     | 2.48                     | 0.44              |
| 1:P:457:ASP:OD2   | 1:P:458:LEU:HB2  | 2.17                     | 0.44              |
| 1:A:54:ALA:O      | 1:A:58:THR:N     | 2.48                     | 0.44              |
| 1:A:901:HIS:HB2   | 1:A:1230:GLU:CD  | 2.42                     | 0.44              |
| 1:B:266:THR:HG22  | 1:B:268:PHE:N    | 2.33                     | 0.44              |
| 1:B:999:ALA:HA    | 1:B:1019:LYS:HA  | 1.98                     | 0.44              |
| 1:B:1036:VAL:HG12 | 1:B:1037:ASP:H   | 1.83                     | 0.44              |
| 1:C:102:MET:O     | 1:C:105:MET:N    | 2.46                     | 0.44              |
| 1:C:182:ASN:HD22  | 1:C:245:LEU:HB2  | 1.83                     | 0.44              |
| 1:D:264:LEU:HD23  | 1:D:264:LEU:HA   | 1.74                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:451:LYS:CD    | 1:D:486:LEU:HD21 | 2.33                     | 0.44              |
| 1:E:120:PHE:CE1   | 1:E:159:TRP:CE3  | 3.05                     | 0.44              |
| 1:E:157:LYS:N     | 2:E:1501:DTP:O2B | 2.51                     | 0.44              |
| 1:E:409:SER:O     | 1:E:411:VAL:N    | 2.51                     | 0.44              |
| 1:G:443:ILE:HG21  | 1:G:477:ASN:ND2  | 2.24                     | 0.44              |
| 1:G:662:GLN:O     | 1:G:663:GLN:HG2  | 2.17                     | 0.44              |
| 1:G:782:CYS:HB3   | 1:G:816:LEU:HD13 | 1.99                     | 0.44              |
| 1:G:1198:ASP:CG   | 1:G:1199:ASP:H   | 2.25                     | 0.44              |
| 1:H:20:GLU:HG3    | 1:H:21:ASP:N     | 2.33                     | 0.44              |
| 1:H:453:PHE:CE1   | 1:H:460:PRO:HB3  | 2.51                     | 0.44              |
| 1:I:90:SER:HG     | 1:I:91:PRO:HD3   | 1.82                     | 0.44              |
| 1:I:148:LEU:HD23  | 1:I:264:LEU:HB2  | 2.00                     | 0.44              |
| 1:I:198:LYS:HZ2   | 1:P:222:HIS:CG   | 2.36                     | 0.44              |
| 1:I:409:SER:O     | 1:I:411:VAL:N    | 2.51                     | 0.44              |
| 1:I:458:LEU:CA    | 1:I:587:ARG:HH21 | 2.30                     | 0.44              |
| 1:I:866:LYS:HE2   | 1:I:872:ARG:HH11 | 1.81                     | 0.44              |
| 1:I:1198:ASP:CG   | 1:I:1199:ASP:H   | 2.25                     | 0.44              |
| 1:J:20:GLU:HG3    | 1:J:21:ASP:N     | 2.33                     | 0.44              |
| 1:J:120:PHE:CE1   | 1:J:159:TRP:CE3  | 3.05                     | 0.44              |
| 1:J:417:GLU:HG2   | 1:J:417:GLU:O    | 2.18                     | 0.44              |
| 1:K:231:LEU:O     | 1:K:234:SER:OG   | 2.26                     | 0.44              |
| 1:K:914:VAL:O     | 1:K:915:TYR:C    | 2.60                     | 0.44              |
| 1:L:341:TRP:O     | 1:L:341:TRP:CE3  | 2.70                     | 0.44              |
| 1:L:905:VAL:HG13  | 1:L:906:ASP:N    | 2.33                     | 0.44              |
| 1:M:266:THR:HG22  | 1:M:268:PHE:N    | 2.33                     | 0.44              |
| 1:M:901:HIS:HB2   | 1:M:1230:GLU:CD  | 2.43                     | 0.44              |
| 1:M:1036:VAL:HG12 | 1:M:1037:ASP:H   | 1.83                     | 0.44              |
| 1:N:207:TRP:CD1   | 1:N:227:GLU:CD   | 2.95                     | 0.44              |
| 1:N:901:HIS:HB2   | 1:N:1230:GLU:CD  | 2.42                     | 0.44              |
| 1:N:902:ILE:HD13  | 1:N:930:HIS:CE1  | 2.43                     | 0.44              |
| 1:N:1036:VAL:HG12 | 1:N:1037:ASP:H   | 1.83                     | 0.44              |
| 1:O:879:SER:N     | 1:O:880:GLU:OE1  | 2.51                     | 0.44              |
| 1:O:901:HIS:HB2   | 1:O:1230:GLU:CD  | 2.42                     | 0.44              |
| 1:P:409:SER:O     | 1:P:411:VAL:N    | 2.51                     | 0.44              |
| 1:P:443:ILE:HG21  | 1:P:477:ASN:ND2  | 2.24                     | 0.44              |
| 1:P:662:GLN:O     | 1:P:663:GLN:HG2  | 2.17                     | 0.44              |
| 1:P:898:VAL:HG13  | 1:P:930:HIS:CD2  | 2.52                     | 0.44              |
| 1:A:373:SER:C     | 1:A:433:LEU:HD12 | 2.43                     | 0.44              |
| 1:A:461:PRO:O     | 1:A:461:PRO:HG2  | 2.18                     | 0.44              |
| 1:A:988:ASP:OD1   | 1:A:989:SER:N    | 2.43                     | 0.44              |
| 1:C:97:ARG:HH22   | 1:L:97:ARG:NH2   | 2.14                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:157:LYS:N     | 2:D:1501:DTP:O2B | 2.51                     | 0.44              |
| 1:D:244:LEU:HD21  | 1:D:256:PHE:CD2  | 2.50                     | 0.44              |
| 1:D:662:GLN:O     | 1:D:663:GLN:HG2  | 2.17                     | 0.44              |
| 1:D:914:VAL:O     | 1:D:915:TYR:C    | 2.60                     | 0.44              |
| 1:D:1000:ILE:HD11 | 1:D:1014:ALA:HB3 | 2.00                     | 0.44              |
| 1:D:1036:VAL:HG12 | 1:D:1037:ASP:H   | 1.83                     | 0.44              |
| 1:E:266:THR:HG22  | 1:E:268:PHE:N    | 2.33                     | 0.44              |
| 1:E:463:LEU:CD2   | 1:E:467:PHE:HD2  | 2.31                     | 0.44              |
| 1:E:879:SER:N     | 1:E:880:GLU:OE1  | 2.51                     | 0.44              |
| 1:F:337:THR:OG1   | 1:F:340:ASN:N    | 2.50                     | 0.44              |
| 1:F:388:LEU:HB3   | 1:F:446:HIS:CE1  | 2.52                     | 0.44              |
| 1:F:866:LYS:HE2   | 1:F:872:ARG:HH11 | 1.81                     | 0.44              |
| 1:G:20:GLU:HG3    | 1:G:21:ASP:N     | 2.33                     | 0.44              |
| 1:G:388:LEU:HB3   | 1:G:446:HIS:CE1  | 2.52                     | 0.44              |
| 1:H:54:ALA:O      | 1:H:58:THR:N     | 2.48                     | 0.44              |
| 1:H:409:SER:O     | 1:H:411:VAL:N    | 2.51                     | 0.44              |
| 1:H:428:GLU:C     | 1:H:430:LYS:H    | 2.26                     | 0.44              |
| 1:H:440:HIS:O     | 1:H:444:VAL:HG23 | 2.18                     | 0.44              |
| 1:H:542:ILE:HA    | 1:H:545:PHE:HD2  | 1.82                     | 0.44              |
| 1:H:879:SER:N     | 1:H:880:GLU:OE1  | 2.51                     | 0.44              |
| 1:I:222:HIS:CG    | 1:J:198:LYS:NZ   | 2.86                     | 0.44              |
| 1:I:901:HIS:HB2   | 1:I:1230:GLU:CD  | 2.42                     | 0.44              |
| 1:I:988:ASP:OD1   | 1:I:989:SER:N    | 2.43                     | 0.44              |
| 1:J:157:LYS:N     | 2:J:1501:DTP:O1B | 2.51                     | 0.44              |
| 1:J:266:THR:HG22  | 1:J:268:PHE:N    | 2.33                     | 0.44              |
| 1:J:371:ARG:HB3   | 1:J:389:ILE:CG2  | 2.45                     | 0.44              |
| 1:J:409:SER:O     | 1:J:411:VAL:N    | 2.51                     | 0.44              |
| 1:J:879:SER:N     | 1:J:880:GLU:OE1  | 2.51                     | 0.44              |
| 1:K:157:LYS:N     | 2:K:1501:DTP:O1B | 2.51                     | 0.44              |
| 1:K:234:SER:OG    | 1:K:235:LYS:N    | 2.51                     | 0.44              |
| 1:K:458:LEU:CA    | 1:K:587:ARG:HH21 | 2.31                     | 0.44              |
| 1:K:629:GLN:HG2   | 1:K:651:SER:H    | 1.83                     | 0.44              |
| 1:K:1036:VAL:HG12 | 1:K:1037:ASP:H   | 1.83                     | 0.44              |
| 1:L:337:THR:OG1   | 1:L:340:ASN:N    | 2.50                     | 0.44              |
| 1:L:999:ALA:HA    | 1:L:1019:LYS:HA  | 1.98                     | 0.44              |
| 1:M:336:ALA:C     | 1:M:338:TRP:N    | 2.74                     | 0.44              |
| 1:M:453:PHE:CE2   | 1:M:460:PRO:HB3  | 2.49                     | 0.44              |
| 1:M:461:PRO:HG2   | 1:M:461:PRO:O    | 2.18                     | 0.44              |
| 1:M:879:SER:N     | 1:M:880:GLU:OE1  | 2.51                     | 0.44              |
| 1:M:999:ALA:HA    | 1:M:1019:LYS:HA  | 1.98                     | 0.44              |
| 1:N:251:APK:H2'   | 1:N:251:APK:H8   | 1.74                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:276:SER:OG    | 1:O:122:LYS:HG3   | 2.18                     | 0.44              |
| 1:N:382:PRO:HA    | 1:N:419:THR:CG2   | 2.36                     | 0.44              |
| 1:N:461:PRO:O     | 1:N:461:PRO:HG2   | 2.18                     | 0.44              |
| 1:N:557:LYS:CD    | 1:N:1223:GLN:HE21 | 2.30                     | 0.44              |
| 1:N:914:VAL:O     | 1:N:915:TYR:C     | 2.60                     | 0.44              |
| 1:O:54:ALA:O      | 1:O:58:THR:N      | 2.48                     | 0.44              |
| 1:O:337:THR:OG1   | 1:O:340:ASN:N     | 2.50                     | 0.44              |
| 1:O:409:SER:O     | 1:O:411:VAL:N     | 2.51                     | 0.44              |
| 1:O:428:GLU:C     | 1:O:430:LYS:H     | 2.26                     | 0.44              |
| 1:O:463:LEU:CD2   | 1:O:467:PHE:CD2   | 2.92                     | 0.44              |
| 1:O:1036:VAL:HG12 | 1:O:1037:ASP:H    | 1.83                     | 0.44              |
| 1:P:20:GLU:HG3    | 1:P:21:ASP:N      | 2.33                     | 0.44              |
| 1:P:504:ASP:CG    | 1:P:608:ASN:HD22  | 2.26                     | 0.44              |
| 1:P:554:ILE:C     | 1:P:556:SER:N     | 2.76                     | 0.44              |
| 1:P:905:VAL:HG13  | 1:P:906:ASP:N     | 2.33                     | 0.44              |
| 1:P:1198:ASP:CG   | 1:P:1199:ASP:H    | 2.25                     | 0.44              |
| 1:A:207:TRP:CD1   | 1:A:227:GLU:CD    | 2.95                     | 0.44              |
| 1:A:440:HIS:O     | 1:A:444:VAL:HG23  | 2.18                     | 0.44              |
| 1:A:496:PHE:HE2   | 1:A:555:CYS:HG    | 1.66                     | 0.44              |
| 1:A:902:ILE:HD13  | 1:A:930:HIS:CE1   | 2.43                     | 0.44              |
| 1:A:1036:VAL:HG12 | 1:A:1037:ASP:H    | 1.83                     | 0.44              |
| 1:B:317:LEU:O     | 1:B:318:THR:CB    | 2.61                     | 0.44              |
| 1:B:401:VAL:O     | 1:B:402:VAL:C     | 2.61                     | 0.44              |
| 1:B:409:SER:O     | 1:B:411:VAL:N     | 2.51                     | 0.44              |
| 1:B:879:SER:N     | 1:B:880:GLU:OE1   | 2.51                     | 0.44              |
| 1:C:341:TRP:CE3   | 1:C:341:TRP:O     | 2.70                     | 0.44              |
| 1:C:388:LEU:HB3   | 1:C:446:HIS:CE1   | 2.52                     | 0.44              |
| 1:C:417:GLU:HG2   | 1:C:417:GLU:O     | 2.18                     | 0.44              |
| 1:C:461:PRO:O     | 1:C:461:PRO:HG2   | 2.18                     | 0.44              |
| 1:C:862:ILE:HG23  | 1:C:863:THR:H     | 1.83                     | 0.44              |
| 1:C:879:SER:N     | 1:C:880:GLU:OE1   | 2.51                     | 0.44              |
| 1:D:234:SER:OG    | 1:D:235:LYS:N     | 2.51                     | 0.44              |
| 1:D:266:THR:HG22  | 1:D:268:PHE:N     | 2.33                     | 0.44              |
| 1:D:629:GLN:HG2   | 1:D:651:SER:H     | 1.83                     | 0.44              |
| 1:E:154:GLY:O     | 1:E:155:SER:OG    | 2.35                     | 0.44              |
| 1:E:207:TRP:CD1   | 1:E:227:GLU:CD    | 2.95                     | 0.44              |
| 1:E:373:SER:CB    | 1:E:433:LEU:CD1   | 2.73                     | 0.44              |
| 1:E:373:SER:C     | 1:E:433:LEU:HD12  | 2.43                     | 0.44              |
| 1:E:646:ARG:HG3   | 1:E:648:GLU:HG3   | 2.00                     | 0.44              |
| 1:F:409:SER:O     | 1:F:411:VAL:N     | 2.51                     | 0.44              |
| 1:F:458:LEU:CA    | 1:F:587:ARG:HH21  | 2.30                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1198:ASP:CG   | 1:F:1199:ASP:H    | 2.25                     | 0.44              |
| 1:G:91:PRO:O      | 1:G:94:THR:OG1    | 2.21                     | 0.44              |
| 1:G:148:LEU:HD23  | 1:G:264:LEU:HB2   | 2.00                     | 0.44              |
| 1:G:250:ALA:C     | 1:G:251:APK:O     | 2.59                     | 0.44              |
| 1:G:504:ASP:CG    | 1:G:608:ASN:HD22  | 2.26                     | 0.44              |
| 1:G:554:ILE:C     | 1:G:556:SER:N     | 2.76                     | 0.44              |
| 1:G:629:GLN:HG2   | 1:G:651:SER:H     | 1.83                     | 0.44              |
| 1:G:905:VAL:HG13  | 1:G:906:ASP:N     | 2.33                     | 0.44              |
| 1:H:148:LEU:HD23  | 1:H:264:LEU:HB2   | 2.00                     | 0.44              |
| 1:H:182:ASN:HD22  | 1:H:245:LEU:HB2   | 1.83                     | 0.44              |
| 1:I:248:GLN:CD    | 1:I:268:PHE:CZ    | 2.96                     | 0.44              |
| 1:I:491:PHE:N     | 1:I:491:PHE:CD1   | 2.83                     | 0.44              |
| 1:I:905:VAL:HG13  | 1:I:906:ASP:N     | 2.33                     | 0.44              |
| 1:J:154:GLY:O     | 1:J:155:SER:OG    | 2.35                     | 0.44              |
| 1:J:276:SER:OG    | 1:K:122:LYS:HG3   | 2.18                     | 0.44              |
| 1:J:373:SER:C     | 1:J:433:LEU:HD12  | 2.43                     | 0.44              |
| 1:J:463:LEU:CD2   | 1:J:467:PHE:HD2   | 2.31                     | 0.44              |
| 1:J:646:ARG:HG3   | 1:J:648:GLU:HG3   | 2.00                     | 0.44              |
| 1:K:463:LEU:CD2   | 1:K:467:PHE:HD2   | 2.31                     | 0.44              |
| 1:K:901:HIS:HB2   | 1:K:1230:GLU:CD   | 2.43                     | 0.44              |
| 1:K:1000:ILE:HD11 | 1:K:1014:ALA:HB3  | 2.00                     | 0.44              |
| 1:K:1188:LYS:HG3  | 1:K:1189:ALA:H    | 1.82                     | 0.44              |
| 1:L:862:ILE:HG23  | 1:L:863:THR:H     | 1.83                     | 0.44              |
| 1:L:957:ILE:HG13  | 1:L:1248:LEU:HD22 | 1.99                     | 0.44              |
| 1:M:317:LEU:O     | 1:M:318:THR:CB    | 2.61                     | 0.44              |
| 1:M:401:VAL:O     | 1:M:402:VAL:C     | 2.61                     | 0.44              |
| 1:M:453:PHE:CE1   | 1:M:460:PRO:HB3   | 2.51                     | 0.44              |
| 1:N:504:ASP:CG    | 1:N:608:ASN:HD22  | 2.26                     | 0.44              |
| 1:N:1198:ASP:CG   | 1:N:1199:ASP:H    | 2.25                     | 0.44              |
| 1:O:148:LEU:HD23  | 1:O:264:LEU:HB2   | 2.00                     | 0.44              |
| 1:O:182:ASN:HD22  | 1:O:245:LEU:HB2   | 1.83                     | 0.44              |
| 1:O:243:VAL:HG13  | 1:O:263:LEU:HD22  | 2.00                     | 0.44              |
| 1:O:440:HIS:O     | 1:O:444:VAL:HG23  | 2.18                     | 0.44              |
| 1:P:388:LEU:HB3   | 1:P:446:HIS:CE1   | 2.52                     | 0.44              |
| 1:P:417:GLU:HG2   | 1:P:417:GLU:O     | 2.18                     | 0.44              |
| 1:P:458:LEU:HA    | 1:P:587:ARG:HH21  | 1.80                     | 0.44              |
| 1:P:542:ILE:HA    | 1:P:545:PHE:HD2   | 1.82                     | 0.44              |
| 1:A:504:ASP:CG    | 1:A:608:ASN:HD22  | 2.26                     | 0.43              |
| 1:A:1198:ASP:CG   | 1:A:1199:ASP:H    | 2.25                     | 0.43              |
| 1:B:243:VAL:HG13  | 1:B:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:B:461:PRO:HG2   | 1:B:461:PRO:O     | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:20:GLU:HG3    | 1:C:21:ASP:N     | 2.33                     | 0.43              |
| 1:C:120:PHE:CE1   | 1:C:159:TRP:CE3  | 3.05                     | 0.43              |
| 1:C:243:VAL:HG13  | 1:C:263:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:491:PHE:N     | 1:C:491:PHE:CD1  | 2.83                     | 0.43              |
| 1:C:543:LEU:HA    | 1:C:546:LEU:CD1  | 2.48                     | 0.43              |
| 1:C:915:TYR:CE2   | 1:C:916:LYS:HE3  | 2.53                     | 0.43              |
| 1:C:1188:LYS:HG3  | 1:C:1189:ALA:H   | 1.82                     | 0.43              |
| 1:D:182:ASN:HD22  | 1:D:245:LEU:HB2  | 1.83                     | 0.43              |
| 1:D:463:LEU:CD2   | 1:D:467:PHE:HD2  | 2.31                     | 0.43              |
| 1:D:901:HIS:HB2   | 1:D:1230:GLU:CD  | 2.43                     | 0.43              |
| 1:D:905:VAL:HG13  | 1:D:906:ASP:N    | 2.33                     | 0.43              |
| 1:D:1188:LYS:HG3  | 1:D:1189:ALA:H   | 1.82                     | 0.43              |
| 1:E:200:LEU:HD12  | 1:E:200:LEU:HA   | 1.74                     | 0.43              |
| 1:E:201:TYR:CE2   | 1:F:223:SER:OG   | 2.70                     | 0.43              |
| 1:E:1000:ILE:HD11 | 1:E:1014:ALA:HB3 | 2.00                     | 0.43              |
| 1:F:148:LEU:HD23  | 1:F:264:LEU:HB2  | 2.00                     | 0.43              |
| 1:F:341:TRP:O     | 1:F:341:TRP:CE3  | 2.71                     | 0.43              |
| 1:G:458:LEU:HA    | 1:G:587:ARG:HH21 | 1.80                     | 0.43              |
| 1:G:1036:VAL:HG12 | 1:G:1037:ASP:H   | 1.83                     | 0.43              |
| 1:G:1098:LEU:HG   | 1:G:1111:GLU:HG2 | 1.99                     | 0.43              |
| 1:H:373:SER:C     | 1:H:433:LEU:HD12 | 2.43                     | 0.43              |
| 1:H:1036:VAL:HG12 | 1:H:1037:ASP:H   | 1.83                     | 0.43              |
| 1:H:1074:HIS:O    | 1:H:1075:SER:OG  | 2.33                     | 0.43              |
| 1:I:341:TRP:O     | 1:I:341:TRP:CE3  | 2.71                     | 0.43              |
| 1:J:862:ILE:HG23  | 1:J:863:THR:H    | 1.83                     | 0.43              |
| 1:J:1000:ILE:HD11 | 1:J:1014:ALA:HB3 | 2.00                     | 0.43              |
| 1:K:244:LEU:HD21  | 1:K:256:PHE:CD2  | 2.51                     | 0.43              |
| 1:K:905:VAL:HG13  | 1:K:906:ASP:N    | 2.33                     | 0.43              |
| 1:L:243:VAL:HG13  | 1:L:263:LEU:HD22 | 2.00                     | 0.43              |
| 1:L:491:PHE:N     | 1:L:491:PHE:CD1  | 2.83                     | 0.43              |
| 1:L:879:SER:N     | 1:L:880:GLU:OE1  | 2.51                     | 0.43              |
| 1:L:915:TYR:CE2   | 1:L:916:LYS:HE3  | 2.53                     | 0.43              |
| 1:M:157:LYS:N     | 2:M:1501:DTP:O1B | 2.51                     | 0.43              |
| 1:M:243:VAL:HG13  | 1:M:263:LEU:HD22 | 2.00                     | 0.43              |
| 1:M:409:SER:O     | 1:M:411:VAL:N    | 2.51                     | 0.43              |
| 1:N:102:MET:O     | 1:N:105:MET:N    | 2.46                     | 0.43              |
| 1:N:428:GLU:C     | 1:N:430:LYS:N    | 2.75                     | 0.43              |
| 1:N:440:HIS:O     | 1:N:444:VAL:HG23 | 2.18                     | 0.43              |
| 1:O:373:SER:C     | 1:O:433:LEU:HD12 | 2.43                     | 0.43              |
| 1:O:542:ILE:HA    | 1:O:545:PHE:HD2  | 1.82                     | 0.43              |
| 1:P:148:LEU:HD23  | 1:P:264:LEU:HB2  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:244:LEU:HD21  | 1:P:256:PHE:CD2   | 2.51                     | 0.43              |
| 1:P:250:ALA:C     | 1:P:251:APK:O     | 2.59                     | 0.43              |
| 1:P:629:GLN:HG2   | 1:P:651:SER:H     | 1.83                     | 0.43              |
| 1:P:1036:VAL:HG12 | 1:P:1037:ASP:H    | 1.83                     | 0.43              |
| 1:A:292:LEU:HB2   | 1:A:319:THR:HB    | 1.99                     | 0.43              |
| 1:A:428:GLU:C     | 1:A:430:LYS:N     | 2.74                     | 0.43              |
| 1:A:957:ILE:HG13  | 1:A:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:157:LYS:N     | 2:B:1501:DTP:O2B  | 2.51                     | 0.43              |
| 1:B:453:PHE:CE1   | 1:B:460:PRO:HB3   | 2.51                     | 0.43              |
| 1:B:543:LEU:HA    | 1:B:546:LEU:CD1   | 2.49                     | 0.43              |
| 1:B:629:GLN:HG2   | 1:B:651:SER:H     | 1.83                     | 0.43              |
| 1:B:905:VAL:HG13  | 1:B:906:ASP:N     | 2.33                     | 0.43              |
| 1:B:957:ILE:HG13  | 1:B:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:1198:ASP:CG   | 1:B:1199:ASP:H    | 2.25                     | 0.43              |
| 1:C:401:VAL:O     | 1:C:402:VAL:C     | 2.61                     | 0.43              |
| 1:C:999:ALA:HA    | 1:C:1019:LYS:HA   | 1.98                     | 0.43              |
| 1:D:97:ARG:NH2    | 1:M:97:ARG:NH2    | 2.66                     | 0.43              |
| 1:D:122:LYS:HG3   | 1:E:276:SER:CB    | 2.49                     | 0.43              |
| 1:E:182:ASN:HD22  | 1:E:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:E:388:LEU:HB3   | 1:E:446:HIS:CE1   | 2.52                     | 0.43              |
| 1:E:557:LYS:NZ    | 1:E:1223:GLN:HG3  | 2.31                     | 0.43              |
| 1:E:862:ILE:HG23  | 1:E:863:THR:H     | 1.84                     | 0.43              |
| 1:E:957:ILE:HG13  | 1:E:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:E:1036:VAL:HG12 | 1:E:1037:ASP:H    | 1.83                     | 0.43              |
| 1:F:122:LYS:O     | 1:F:303:LYS:NZ    | 2.38                     | 0.43              |
| 1:F:200:LEU:HA    | 1:F:200:LEU:HD12  | 1.74                     | 0.43              |
| 1:F:428:GLU:C     | 1:F:430:LYS:H     | 2.26                     | 0.43              |
| 1:F:554:ILE:O     | 1:F:556:SER:N     | 2.45                     | 0.43              |
| 1:F:902:ILE:HD13  | 1:F:930:HIS:CE1   | 2.43                     | 0.43              |
| 1:F:905:VAL:HG13  | 1:F:906:ASP:N     | 2.33                     | 0.43              |
| 1:F:915:TYR:CE2   | 1:F:916:LYS:HE3   | 2.54                     | 0.43              |
| 1:G:234:SER:OG    | 1:G:235:LYS:N     | 2.51                     | 0.43              |
| 1:G:244:LEU:HD21  | 1:G:256:PHE:CD2   | 2.51                     | 0.43              |
| 1:G:417:GLU:O     | 1:G:417:GLU:HG2   | 2.18                     | 0.43              |
| 1:G:428:GLU:C     | 1:G:430:LYS:H     | 2.26                     | 0.43              |
| 1:G:557:LYS:CD    | 1:G:1223:GLN:HE21 | 2.30                     | 0.43              |
| 1:H:152:VAL:O     | 1:H:155:SER:OG    | 2.29                     | 0.43              |
| 1:H:243:VAL:HG13  | 1:H:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:H:392:ASP:OD1   | 1:H:393:VAL:N     | 2.47                     | 0.43              |
| 1:I:120:PHE:CE1   | 1:I:159:TRP:CE3   | 3.05                     | 0.43              |
| 1:I:182:ASN:HD22  | 1:I:245:LEU:HB2   | 1.83                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:443:ILE:HG13  | 1:I:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:I:463:LEU:CD2   | 1:I:467:PHE:CD2   | 2.92                     | 0.43              |
| 1:I:915:TYR:CE2   | 1:I:916:LYS:HE3   | 2.53                     | 0.43              |
| 1:J:182:ASN:HD22  | 1:J:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:J:207:TRP:CD1   | 1:J:227:GLU:CD    | 2.95                     | 0.43              |
| 1:J:388:LEU:HB3   | 1:J:446:HIS:CE1   | 2.52                     | 0.43              |
| 1:J:957:ILE:HG13  | 1:J:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:K:20:GLU:HG3    | 1:K:21:ASP:N      | 2.33                     | 0.43              |
| 1:K:73:VAL:O      | 1:K:76:PHE:N      | 2.52                     | 0.43              |
| 1:K:182:ASN:HD22  | 1:K:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:K:231:LEU:HD23  | 1:K:231:LEU:C     | 2.43                     | 0.43              |
| 1:K:264:LEU:HD23  | 1:K:264:LEU:HA    | 1.74                     | 0.43              |
| 1:K:266:THR:HG22  | 1:K:268:PHE:N     | 2.33                     | 0.43              |
| 1:L:120:PHE:CE1   | 1:L:159:TRP:CE3   | 3.05                     | 0.43              |
| 1:L:443:ILE:HG13  | 1:L:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:L:461:PRO:HG2   | 1:L:461:PRO:O     | 2.18                     | 0.43              |
| 1:L:543:LEU:HA    | 1:L:546:LEU:CD1   | 2.48                     | 0.43              |
| 1:L:1098:LEU:HG   | 1:L:1111:GLU:HG2  | 1.99                     | 0.43              |
| 1:M:443:ILE:HG13  | 1:M:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:M:629:GLN:HG2   | 1:M:651:SER:H     | 1.83                     | 0.43              |
| 1:M:905:VAL:HG13  | 1:M:906:ASP:N     | 2.33                     | 0.43              |
| 1:M:957:ILE:HG13  | 1:M:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:N:148:LEU:HD23  | 1:N:264:LEU:HB2   | 2.00                     | 0.43              |
| 1:N:266:THR:HG22  | 1:N:268:PHE:N     | 2.33                     | 0.43              |
| 1:N:401:VAL:O     | 1:N:402:VAL:C     | 2.61                     | 0.43              |
| 1:N:451:LYS:CD    | 1:N:486:LEU:HD21  | 2.33                     | 0.43              |
| 1:N:957:ILE:HG13  | 1:N:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:N:1000:ILE:HD11 | 1:N:1014:ALA:HB3  | 2.00                     | 0.43              |
| 1:P:154:GLY:O     | 1:P:155:SER:OG    | 2.35                     | 0.43              |
| 1:P:234:SER:OG    | 1:P:235:LYS:N     | 2.51                     | 0.43              |
| 1:P:428:GLU:C     | 1:P:430:LYS:H     | 2.26                     | 0.43              |
| 1:P:1098:LEU:HG   | 1:P:1111:GLU:HG2  | 1.99                     | 0.43              |
| 1:A:102:MET:O     | 1:A:105:MET:N     | 2.46                     | 0.43              |
| 1:A:243:VAL:HG13  | 1:A:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:A:266:THR:HG22  | 1:A:268:PHE:N     | 2.33                     | 0.43              |
| 1:A:285:LEU:HD23  | 1:A:285:LEU:HA    | 1.74                     | 0.43              |
| 1:A:382:PRO:HA    | 1:A:419:THR:CG2   | 2.36                     | 0.43              |
| 1:A:401:VAL:O     | 1:A:402:VAL:C     | 2.61                     | 0.43              |
| 1:A:879:SER:N     | 1:A:880:GLU:OE1   | 2.51                     | 0.43              |
| 1:A:1000:ILE:HD11 | 1:A:1014:ALA:HB3  | 2.00                     | 0.43              |
| 1:B:443:ILE:HG13  | 1:B:477:ASN:ND2   | 2.34                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:248:GLN:CD    | 1:C:268:PHE:CZ    | 2.96                     | 0.43              |
| 1:C:443:ILE:HG13  | 1:C:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:C:875:LEU:CD1   | 1:C:911:PHE:HD2   | 2.07                     | 0.43              |
| 1:D:73:VAL:O      | 1:D:76:PHE:N      | 2.52                     | 0.43              |
| 1:D:231:LEU:HD23  | 1:D:231:LEU:C     | 2.43                     | 0.43              |
| 1:E:148:LEU:HD23  | 1:E:264:LEU:HB2   | 2.00                     | 0.43              |
| 1:E:905:VAL:HG13  | 1:E:906:ASP:N     | 2.33                     | 0.43              |
| 1:F:120:PHE:CE1   | 1:F:159:TRP:CE3   | 3.05                     | 0.43              |
| 1:F:443:ILE:HG13  | 1:F:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:F:542:ILE:HA    | 1:F:545:PHE:HD2   | 1.82                     | 0.43              |
| 1:F:638:GLU:OE1   | 1:F:640:GLU:N     | 2.42                     | 0.43              |
| 1:F:1036:VAL:HG12 | 1:F:1037:ASP:H    | 1.83                     | 0.43              |
| 1:G:154:GLY:O     | 1:G:155:SER:OG    | 2.35                     | 0.43              |
| 1:G:200:LEU:HA    | 1:G:200:LEU:HD12  | 1.74                     | 0.43              |
| 1:H:443:ILE:HG13  | 1:H:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:H:553:LEU:HD23  | 1:H:553:LEU:HA    | 1.90                     | 0.43              |
| 1:H:557:LYS:CD    | 1:H:1223:GLN:HE21 | 2.30                     | 0.43              |
| 1:I:200:LEU:HD12  | 1:I:200:LEU:HA    | 1.74                     | 0.43              |
| 1:J:461:PRO:HG2   | 1:J:461:PRO:O     | 2.18                     | 0.43              |
| 1:J:905:VAL:HG13  | 1:J:906:ASP:N     | 2.33                     | 0.43              |
| 1:J:914:VAL:O     | 1:J:915:TYR:C     | 2.60                     | 0.43              |
| 1:J:1036:VAL:HG12 | 1:J:1037:ASP:H    | 1.83                     | 0.43              |
| 1:K:504:ASP:CG    | 1:K:608:ASN:HD22  | 2.26                     | 0.43              |
| 1:L:200:LEU:HA    | 1:L:200:LEU:HD12  | 1.74                     | 0.43              |
| 1:M:543:LEU:HA    | 1:M:546:LEU:CD1   | 2.49                     | 0.43              |
| 1:M:1198:ASP:CG   | 1:M:1199:ASP:H    | 2.25                     | 0.43              |
| 1:N:243:VAL:HG13  | 1:N:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:N:543:LEU:HA    | 1:N:546:LEU:CD1   | 2.48                     | 0.43              |
| 1:O:392:ASP:OD1   | 1:O:393:VAL:N     | 2.47                     | 0.43              |
| 1:O:443:ILE:HG13  | 1:O:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:O:957:ILE:HG13  | 1:O:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:P:557:LYS:CD    | 1:P:1223:GLN:HE21 | 2.30                     | 0.43              |
| 1:P:879:SER:N     | 1:P:880:GLU:OE1   | 2.51                     | 0.43              |
| 1:A:182:ASN:HD22  | 1:A:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:A:417:GLU:O     | 1:A:417:GLU:HG2   | 2.18                     | 0.43              |
| 1:A:543:LEU:HA    | 1:A:546:LEU:CD1   | 2.49                     | 0.43              |
| 1:C:428:GLU:C     | 1:C:430:LYS:H     | 2.26                     | 0.43              |
| 1:C:901:HIS:O     | 1:C:902:ILE:HB    | 2.18                     | 0.43              |
| 1:D:20:GLU:HG3    | 1:D:21:ASP:N      | 2.33                     | 0.43              |
| 1:D:361:GLU:HB2   | 1:D:364:GLU:HB3   | 1.98                     | 0.43              |
| 1:D:388:LEU:HB3   | 1:D:446:HIS:CE1   | 2.52                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:504:ASP:CG    | 1:D:608:ASN:HD22  | 2.26                     | 0.43              |
| 1:D:879:SER:N     | 1:D:880:GLU:OE1   | 2.51                     | 0.43              |
| 1:E:54:ALA:O      | 1:E:57:GLY:N      | 2.52                     | 0.43              |
| 1:E:73:VAL:O      | 1:E:76:PHE:N      | 2.52                     | 0.43              |
| 1:E:914:VAL:O     | 1:E:915:TYR:C     | 2.60                     | 0.43              |
| 1:E:1075:SER:OG   | 1:E:1094:ASP:O    | 2.29                     | 0.43              |
| 1:F:182:ASN:HD22  | 1:F:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:F:248:GLN:CD    | 1:F:268:PHE:CZ    | 2.96                     | 0.43              |
| 1:F:251:APK:H8    | 1:F:251:APK:H2'   | 1.73                     | 0.43              |
| 1:F:496:PHE:HE2   | 1:F:555:CYS:HG    | 1.64                     | 0.43              |
| 1:F:1000:ILE:HD11 | 1:F:1014:ALA:HB3  | 2.00                     | 0.43              |
| 1:G:266:THR:HG22  | 1:G:268:PHE:N     | 2.33                     | 0.43              |
| 1:G:453:PHE:CE2   | 1:G:460:PRO:HB3   | 2.49                     | 0.43              |
| 1:G:903:GLU:HG3   | 1:G:904:CYS:H     | 1.84                     | 0.43              |
| 1:H:451:LYS:CD    | 1:H:486:LEU:HD21  | 2.33                     | 0.43              |
| 1:H:461:PRO:O     | 1:H:461:PRO:HG2   | 2.18                     | 0.43              |
| 1:H:543:LEU:HA    | 1:H:546:LEU:CD1   | 2.49                     | 0.43              |
| 1:H:957:ILE:HG13  | 1:H:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:I:54:ALA:O      | 1:I:57:GLY:N      | 2.52                     | 0.43              |
| 1:I:73:VAL:O      | 1:I:76:PHE:N      | 2.52                     | 0.43              |
| 1:I:388:LEU:HB3   | 1:I:446:HIS:CE1   | 2.52                     | 0.43              |
| 1:I:542:ILE:HA    | 1:I:545:PHE:HD2   | 1.82                     | 0.43              |
| 1:I:1036:VAL:HG12 | 1:I:1037:ASP:H    | 1.83                     | 0.43              |
| 1:J:54:ALA:O      | 1:J:57:GLY:N      | 2.52                     | 0.43              |
| 1:J:73:VAL:O      | 1:J:76:PHE:N      | 2.52                     | 0.43              |
| 1:J:148:LEU:HD23  | 1:J:264:LEU:HB2   | 2.00                     | 0.43              |
| 1:K:292:LEU:HB2   | 1:K:319:THR:HB    | 2.00                     | 0.43              |
| 1:K:361:GLU:HB2   | 1:K:364:GLU:HB3   | 1.98                     | 0.43              |
| 1:K:388:LEU:HB3   | 1:K:446:HIS:CE1   | 2.52                     | 0.43              |
| 1:K:399:MET:HG3   | 1:L:335:LEU:HD21  | 1.99                     | 0.43              |
| 1:K:879:SER:N     | 1:K:880:GLU:OE1   | 2.51                     | 0.43              |
| 1:L:73:VAL:O      | 1:L:76:PHE:N      | 2.52                     | 0.43              |
| 1:L:102:MET:O     | 1:L:105:MET:N     | 2.46                     | 0.43              |
| 1:L:124:ASN:HA    | 2:L:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:L:440:HIS:O     | 1:L:444:VAL:HG23  | 2.18                     | 0.43              |
| 1:M:231:LEU:O     | 1:M:234:SER:OG    | 2.26                     | 0.43              |
| 1:N:54:ALA:O      | 1:N:57:GLY:N      | 2.52                     | 0.43              |
| 1:N:292:LEU:HB2   | 1:N:319:THR:HB    | 1.99                     | 0.43              |
| 1:N:417:GLU:O     | 1:N:417:GLU:HG2   | 2.18                     | 0.43              |
| 1:N:428:GLU:C     | 1:N:430:LYS:H     | 2.26                     | 0.43              |
| 1:N:879:SER:N     | 1:N:880:GLU:OE1   | 2.51                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:903:GLU:HG3   | 1:N:904:CYS:H     | 1.84                     | 0.43              |
| 1:N:1177:TYR:HE2  | 1:O:916:LYS:CE    | 2.30                     | 0.43              |
| 1:O:154:GLY:O     | 1:O:155:SER:OG    | 2.35                     | 0.43              |
| 1:O:301:LEU:CD2   | 1:O:313:PRO:CG    | 2.87                     | 0.43              |
| 1:O:461:PRO:HG2   | 1:O:461:PRO:O     | 2.18                     | 0.43              |
| 1:O:557:LYS:CD    | 1:O:1223:GLN:HE21 | 2.30                     | 0.43              |
| 1:O:905:VAL:HG13  | 1:O:906:ASP:N     | 2.33                     | 0.43              |
| 1:P:200:LEU:HA    | 1:P:200:LEU:HD12  | 1.74                     | 0.43              |
| 1:A:54:ALA:O      | 1:A:57:GLY:N      | 2.52                     | 0.43              |
| 1:A:148:LEU:HD23  | 1:A:264:LEU:HB2   | 2.00                     | 0.43              |
| 1:A:428:GLU:C     | 1:A:430:LYS:H     | 2.26                     | 0.43              |
| 1:A:511:SER:C     | 1:A:513:SER:N     | 2.60                     | 0.43              |
| 1:A:535:TYR:O     | 1:A:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:A:903:GLU:HG3   | 1:A:904:CYS:H     | 1.84                     | 0.43              |
| 1:B:535:TYR:O     | 1:B:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:B:584:PHE:HB3   | 1:B:585:ASP:H     | 1.61                     | 0.43              |
| 1:B:1000:ILE:HD11 | 1:B:1014:ALA:HB3  | 2.00                     | 0.43              |
| 1:C:382:PRO:HA    | 1:C:419:THR:CG2   | 2.36                     | 0.43              |
| 1:C:629:GLN:HG2   | 1:C:651:SER:H     | 1.83                     | 0.43              |
| 1:D:243:VAL:HG13  | 1:D:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:D:543:LEU:HA    | 1:D:546:LEU:CD1   | 2.48                     | 0.43              |
| 1:E:124:ASN:HA    | 2:E:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:E:243:VAL:HG13  | 1:E:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:E:535:TYR:O     | 1:E:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:E:554:ILE:C     | 1:E:556:SER:N     | 2.76                     | 0.43              |
| 1:F:20:GLU:HG3    | 1:F:21:ASP:N      | 2.33                     | 0.43              |
| 1:F:73:VAL:O      | 1:F:76:PHE:N      | 2.52                     | 0.43              |
| 1:F:121:ALA:HB1   | 1:G:276:SER:CB    | 2.31                     | 0.43              |
| 1:F:542:ILE:HA    | 1:F:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:G:73:VAL:O      | 1:G:76:PHE:N      | 2.52                     | 0.43              |
| 1:G:182:ASN:HD22  | 1:G:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:G:879:SER:N     | 1:G:880:GLU:OE1   | 2.51                     | 0.43              |
| 1:H:905:VAL:HG13  | 1:H:906:ASP:N     | 2.33                     | 0.43              |
| 1:I:264:LEU:HD23  | 1:I:264:LEU:HA    | 1.74                     | 0.43              |
| 1:I:1000:ILE:HD11 | 1:I:1014:ALA:HB3  | 2.00                     | 0.43              |
| 1:I:1195:VAL:HG11 | 1:I:1241:PHE:CZ   | 2.54                     | 0.43              |
| 1:J:243:VAL:HG13  | 1:J:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:J:511:SER:C     | 1:J:513:SER:N     | 2.60                     | 0.43              |
| 1:J:535:TYR:O     | 1:J:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:K:243:VAL:HG13  | 1:K:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:K:251:APK:H8    | 1:K:251:APK:H2'   | 1.73                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:376:PRO:HA   | 1:K:377:PRO:HD3   | 1.89                     | 0.43              |
| 1:K:451:LYS:CD   | 1:K:486:LEU:HD21  | 2.33                     | 0.43              |
| 1:K:461:PRO:O    | 1:K:461:PRO:HG2   | 2.18                     | 0.43              |
| 1:K:481:PRO:O    | 1:K:485:THR:HG23  | 2.19                     | 0.43              |
| 1:K:543:LEU:HA   | 1:K:546:LEU:CD1   | 2.48                     | 0.43              |
| 1:L:234:SER:OG   | 1:L:235:LYS:N     | 2.51                     | 0.43              |
| 1:L:382:PRO:HA   | 1:L:419:THR:CG2   | 2.36                     | 0.43              |
| 1:L:401:VAL:O    | 1:L:402:VAL:C     | 2.61                     | 0.43              |
| 1:M:535:TYR:O    | 1:M:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:N:182:ASN:HD22 | 1:N:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:N:511:SER:C    | 1:N:513:SER:N     | 2.60                     | 0.43              |
| 1:N:535:TYR:O    | 1:N:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:N:554:ILE:C    | 1:N:556:SER:N     | 2.76                     | 0.43              |
| 1:O:186:CYS:C    | 1:O:249:ASN:HD21  | 2.27                     | 0.43              |
| 1:O:543:LEU:HA   | 1:O:546:LEU:CD1   | 2.49                     | 0.43              |
| 1:P:73:VAL:O     | 1:P:76:PHE:N      | 2.52                     | 0.43              |
| 1:P:147:VAL:HG12 | 1:P:281:THR:OG1   | 2.19                     | 0.43              |
| 1:P:266:THR:HG22 | 1:P:268:PHE:N     | 2.33                     | 0.43              |
| 1:P:453:PHE:CE2  | 1:P:460:PRO:HB3   | 2.49                     | 0.43              |
| 1:P:903:GLU:HG3  | 1:P:904:CYS:H     | 1.84                     | 0.43              |
| 1:A:409:SER:O    | 1:A:411:VAL:N     | 2.51                     | 0.43              |
| 1:A:443:ILE:HG13 | 1:A:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:A:453:PHE:CE2  | 1:A:460:PRO:HB3   | 2.49                     | 0.43              |
| 1:A:554:ILE:C    | 1:A:556:SER:N     | 2.76                     | 0.43              |
| 1:A:905:VAL:HG13 | 1:A:906:ASP:N     | 2.33                     | 0.43              |
| 1:B:54:ALA:O     | 1:B:57:GLY:N      | 2.52                     | 0.43              |
| 1:B:231:LEU:O    | 1:B:234:SER:OG    | 2.26                     | 0.43              |
| 1:B:481:PRO:O    | 1:B:485:THR:HG23  | 2.19                     | 0.43              |
| 1:C:73:VAL:O     | 1:C:76:PHE:N      | 2.52                     | 0.43              |
| 1:C:124:ASN:HA   | 2:C:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:C:481:PRO:O    | 1:C:485:THR:HG23  | 2.19                     | 0.43              |
| 1:C:903:GLU:HG3  | 1:C:904:CYS:H     | 1.84                     | 0.43              |
| 1:C:1158:TYR:HB3 | 1:C:1162:ILE:HG23 | 2.01                     | 0.43              |
| 1:D:376:PRO:HA   | 1:D:377:PRO:HD3   | 1.89                     | 0.43              |
| 1:D:428:GLU:C    | 1:D:430:LYS:H     | 2.26                     | 0.43              |
| 1:D:443:ILE:HG13 | 1:D:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:D:461:PRO:HG2  | 1:D:461:PRO:O     | 2.18                     | 0.43              |
| 1:D:481:PRO:O    | 1:D:485:THR:HG23  | 2.19                     | 0.43              |
| 1:D:535:TYR:O    | 1:D:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:D:646:ARG:HG3  | 1:D:648:GLU:HG3   | 2.00                     | 0.43              |
| 1:E:14:ASP:CG    | 1:F:142:ARG:HH22  | 2.27                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:401:VAL:O     | 1:E:402:VAL:C     | 2.61                     | 0.43              |
| 1:E:461:PRO:O     | 1:E:461:PRO:HG2   | 2.18                     | 0.43              |
| 1:E:901:HIS:O     | 1:E:902:ILE:HB    | 2.18                     | 0.43              |
| 1:F:154:GLY:O     | 1:F:155:SER:OG    | 2.35                     | 0.43              |
| 1:F:417:GLU:O     | 1:F:417:GLU:HG2   | 2.18                     | 0.43              |
| 1:F:901:HIS:HB2   | 1:F:1230:GLU:CD   | 2.42                     | 0.43              |
| 1:F:988:ASP:OD1   | 1:F:989:SER:N     | 2.43                     | 0.43              |
| 1:G:147:VAL:HG12  | 1:G:281:THR:OG1   | 2.19                     | 0.43              |
| 1:G:186:CYS:C     | 1:G:249:ASN:HD21  | 2.27                     | 0.43              |
| 1:G:264:LEU:HD23  | 1:G:264:LEU:HA    | 1.74                     | 0.43              |
| 1:G:957:ILE:HG13  | 1:G:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:H:154:GLY:O     | 1:H:155:SER:OG    | 2.36                     | 0.43              |
| 1:H:285:LEU:HA    | 1:H:285:LEU:HD23  | 1.74                     | 0.43              |
| 1:H:301:LEU:CD2   | 1:H:313:PRO:CG    | 2.87                     | 0.43              |
| 1:H:324:LEU:HD12  | 1:H:324:LEU:HA    | 1.61                     | 0.43              |
| 1:H:903:GLU:HG3   | 1:H:904:CYS:H     | 1.84                     | 0.43              |
| 1:I:542:ILE:HA    | 1:I:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:I:1177:TYR:HE2  | 1:J:916:LYS:HE2   | 1.83                     | 0.43              |
| 1:J:124:ASN:HA    | 2:J:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:J:231:LEU:O     | 1:J:234:SER:OG    | 2.26                     | 0.43              |
| 1:J:373:SER:CB    | 1:J:433:LEU:CD1   | 2.73                     | 0.43              |
| 1:J:554:ILE:C     | 1:J:556:SER:N     | 2.76                     | 0.43              |
| 1:K:428:GLU:C     | 1:K:430:LYS:H     | 2.26                     | 0.43              |
| 1:K:535:TYR:O     | 1:K:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:K:646:ARG:HG3   | 1:K:648:GLU:HG3   | 2.00                     | 0.43              |
| 1:L:113:LEU:HA    | 1:L:113:LEU:HD12  | 1.83                     | 0.43              |
| 1:L:428:GLU:C     | 1:L:430:LYS:H     | 2.26                     | 0.43              |
| 1:L:901:HIS:O     | 1:L:902:ILE:HB    | 2.18                     | 0.43              |
| 1:L:1075:SER:OG   | 1:L:1094:ASP:O    | 2.29                     | 0.43              |
| 1:M:54:ALA:O      | 1:M:57:GLY:N      | 2.52                     | 0.43              |
| 1:M:182:ASN:HD22  | 1:M:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:M:207:TRP:CD1   | 1:M:227:GLU:CD    | 2.95                     | 0.43              |
| 1:M:231:LEU:C     | 1:M:231:LEU:HD23  | 2.43                     | 0.43              |
| 1:M:417:GLU:HG2   | 1:M:417:GLU:O     | 2.18                     | 0.43              |
| 1:M:481:PRO:O     | 1:M:485:THR:HG23  | 2.19                     | 0.43              |
| 1:M:1000:ILE:HD11 | 1:M:1014:ALA:HB3  | 2.00                     | 0.43              |
| 1:N:392:ASP:OD1   | 1:N:393:VAL:N     | 2.47                     | 0.43              |
| 1:N:443:ILE:HG13  | 1:N:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:N:905:VAL:HG13  | 1:N:906:ASP:N     | 2.33                     | 0.43              |
| 1:O:152:VAL:O     | 1:O:155:SER:OG    | 2.29                     | 0.43              |
| 1:O:629:GLN:HG2   | 1:O:651:SER:H     | 1.83                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:141:LEU:HD12 | 1:P:141:LEU:O     | 2.19                     | 0.43              |
| 1:P:182:ASN:HD22 | 1:P:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:P:957:ILE:HG13 | 1:P:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:A:141:LEU:HD12 | 1:A:141:LEU:O     | 2.19                     | 0.43              |
| 1:A:324:LEU:HD12 | 1:A:324:LEU:HA    | 1.61                     | 0.43              |
| 1:A:553:LEU:HD23 | 1:A:553:LEU:HA    | 1.90                     | 0.43              |
| 1:A:799:ASN:O    | 1:A:800:THR:CG2   | 2.67                     | 0.43              |
| 1:A:1158:TYR:HB3 | 1:A:1162:ILE:HG23 | 2.01                     | 0.43              |
| 1:B:207:TRP:CD1  | 1:B:227:GLU:CD    | 2.95                     | 0.43              |
| 1:B:231:LEU:C    | 1:B:231:LEU:HD23  | 2.43                     | 0.43              |
| 1:B:342:LYS:HG3  | 1:B:343:HIS:N     | 2.34                     | 0.43              |
| 1:B:417:GLU:HG2  | 1:B:417:GLU:O     | 2.18                     | 0.43              |
| 1:B:428:GLU:C    | 1:B:430:LYS:H     | 2.26                     | 0.43              |
| 1:B:1158:TYR:HB3 | 1:B:1162:ILE:HG23 | 2.01                     | 0.43              |
| 1:B:1188:LYS:HG3 | 1:B:1189:ALA:H    | 1.82                     | 0.43              |
| 1:C:244:LEU:HD21 | 1:C:256:PHE:CD2   | 2.51                     | 0.43              |
| 1:C:799:ASN:O    | 1:C:800:THR:CG2   | 2.67                     | 0.43              |
| 1:D:141:LEU:HD12 | 1:D:141:LEU:O     | 2.19                     | 0.43              |
| 1:D:292:LEU:HB2  | 1:D:319:THR:HB    | 1.99                     | 0.43              |
| 1:D:541:ALA:O    | 1:D:543:LEU:N     | 2.52                     | 0.43              |
| 1:E:11:GLN:O     | 1:E:12:TYR:C      | 2.62                     | 0.43              |
| 1:E:541:ALA:O    | 1:E:543:LEU:N     | 2.52                     | 0.43              |
| 1:F:54:ALA:O     | 1:F:57:GLY:N      | 2.52                     | 0.43              |
| 1:F:147:VAL:HG12 | 1:F:281:THR:OG1   | 2.19                     | 0.43              |
| 1:F:186:CYS:C    | 1:F:249:ASN:HD21  | 2.27                     | 0.43              |
| 1:G:542:ILE:HA   | 1:G:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:G:1075:SER:OG  | 1:G:1094:ASP:O    | 2.29                     | 0.43              |
| 1:H:231:LEU:HD23 | 1:H:231:LEU:C     | 2.43                     | 0.43              |
| 1:H:629:GLN:HG2  | 1:H:651:SER:H     | 1.83                     | 0.43              |
| 1:H:799:ASN:O    | 1:H:800:THR:CG2   | 2.67                     | 0.43              |
| 1:I:122:LYS:O    | 1:I:303:LYS:NZ    | 2.38                     | 0.43              |
| 1:I:147:VAL:HG12 | 1:I:281:THR:OG1   | 2.19                     | 0.43              |
| 1:I:154:GLY:O    | 1:I:155:SER:OG    | 2.35                     | 0.43              |
| 1:I:428:GLU:C    | 1:I:430:LYS:H     | 2.26                     | 0.43              |
| 1:I:508:TRP:CD1  | 1:I:604:ASN:HB2   | 2.54                     | 0.43              |
| 1:I:554:ILE:C    | 1:I:556:SER:N     | 2.76                     | 0.43              |
| 1:I:879:SER:N    | 1:I:880:GLU:OE1   | 2.51                     | 0.43              |
| 1:J:11:GLN:O     | 1:J:12:TYR:C      | 2.62                     | 0.43              |
| 1:J:458:LEU:HA   | 1:J:587:ARG:HH21  | 1.80                     | 0.43              |
| 1:J:541:ALA:O    | 1:J:543:LEU:N     | 2.52                     | 0.43              |
| 1:K:54:ALA:O     | 1:K:57:GLY:N      | 2.52                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:257:ASN:OD1  | 1:L:115:ASN:HB3   | 2.19                     | 0.43              |
| 1:K:443:ILE:HG13 | 1:K:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:K:541:ALA:O    | 1:K:543:LEU:N     | 2.52                     | 0.43              |
| 1:L:20:GLU:HG3   | 1:L:21:ASP:N      | 2.33                     | 0.43              |
| 1:L:481:PRO:O    | 1:L:485:THR:HG23  | 2.19                     | 0.43              |
| 1:L:629:GLN:HG2  | 1:L:651:SER:H     | 1.83                     | 0.43              |
| 1:L:903:GLU:HG3  | 1:L:904:CYS:H     | 1.84                     | 0.43              |
| 1:M:1188:LYS:HG3 | 1:M:1189:ALA:H    | 1.82                     | 0.43              |
| 1:N:141:LEU:O    | 1:N:141:LEU:HD12  | 2.19                     | 0.43              |
| 1:N:285:LEU:HD23 | 1:N:285:LEU:HA    | 1.74                     | 0.43              |
| 1:N:409:SER:O    | 1:N:411:VAL:N     | 2.51                     | 0.43              |
| 1:N:633:THR:HG22 | 1:N:643:TYR:HA    | 1.97                     | 0.43              |
| 1:N:862:ILE:HG23 | 1:N:863:THR:H     | 1.83                     | 0.43              |
| 1:N:1158:TYR:HB3 | 1:N:1162:ILE:HG23 | 2.01                     | 0.43              |
| 1:O:147:VAL:HG12 | 1:O:281:THR:OG1   | 2.19                     | 0.43              |
| 1:O:641:ASP:OD1  | 1:O:642:THR:N     | 2.45                     | 0.43              |
| 1:O:799:ASN:O    | 1:O:800:THR:CG2   | 2.67                     | 0.43              |
| 1:P:186:CYS:C    | 1:P:249:ASN:HD21  | 2.27                     | 0.43              |
| 1:P:463:LEU:CD2  | 1:P:467:PHE:HD2   | 2.31                     | 0.43              |
| 1:P:543:LEU:HA   | 1:P:546:LEU:CD1   | 2.48                     | 0.43              |
| 1:P:862:ILE:HG23 | 1:P:863:THR:H     | 1.83                     | 0.43              |
| 1:A:392:ASP:OD1  | 1:A:393:VAL:N     | 2.47                     | 0.43              |
| 1:A:862:ILE:HG23 | 1:A:863:THR:H     | 1.83                     | 0.43              |
| 1:B:248:GLN:CD   | 1:B:268:PHE:CZ    | 2.96                     | 0.43              |
| 1:B:903:GLU:HG3  | 1:B:904:CYS:H     | 1.84                     | 0.43              |
| 1:C:148:LEU:HD23 | 1:C:264:LEU:HB2   | 2.00                     | 0.43              |
| 1:C:440:HIS:O    | 1:C:444:VAL:HG23  | 2.18                     | 0.43              |
| 1:D:54:ALA:O     | 1:D:57:GLY:N      | 2.52                     | 0.43              |
| 1:D:342:LYS:HG3  | 1:D:343:HIS:N     | 2.34                     | 0.43              |
| 1:D:915:TYR:CE2  | 1:D:916:LYS:HE3   | 2.54                     | 0.43              |
| 1:E:244:LEU:HD21 | 1:E:256:PHE:CD2   | 2.51                     | 0.43              |
| 1:E:410:LEU:CD2  | 1:E:413:LYS:HA    | 2.49                     | 0.43              |
| 1:E:542:ILE:HA   | 1:E:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:F:141:LEU:O    | 1:F:141:LEU:HD12  | 2.19                     | 0.43              |
| 1:F:428:GLU:C    | 1:F:430:LYS:N     | 2.74                     | 0.43              |
| 1:F:508:TRP:CD1  | 1:F:604:ASN:HB2   | 2.54                     | 0.43              |
| 1:F:879:SER:N    | 1:F:880:GLU:OE1   | 2.51                     | 0.43              |
| 1:G:124:ASN:HA   | 2:G:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:G:141:LEU:HD12 | 1:G:141:LEU:O     | 2.19                     | 0.43              |
| 1:G:443:ILE:HG13 | 1:G:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:G:543:LEU:HA   | 1:G:546:LEU:CD1   | 2.49                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:862:ILE:HG23 | 1:G:863:THR:H     | 1.83                     | 0.43              |
| 1:H:124:ASN:HA   | 2:H:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:H:147:VAL:HG12 | 1:H:281:THR:OG1   | 2.19                     | 0.43              |
| 1:H:453:PHE:CE2  | 1:H:460:PRO:HB3   | 2.49                     | 0.43              |
| 1:H:535:TYR:O    | 1:H:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:H:542:ILE:HA   | 1:H:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:H:641:ASP:OD1  | 1:H:642:THR:N     | 2.45                     | 0.43              |
| 1:I:417:GLU:O    | 1:I:417:GLU:HG2   | 2.18                     | 0.43              |
| 1:I:428:GLU:C    | 1:I:430:LYS:N     | 2.74                     | 0.43              |
| 1:I:541:ALA:O    | 1:I:543:LEU:N     | 2.52                     | 0.43              |
| 1:I:633:THR:HG22 | 1:I:643:TYR:HA    | 1.97                     | 0.43              |
| 1:J:244:LEU:HD21 | 1:J:256:PHE:CD2   | 2.51                     | 0.43              |
| 1:J:403:ASN:CG   | 1:K:333:ASP:OD2   | 2.60                     | 0.43              |
| 1:J:410:LEU:CD2  | 1:J:413:LYS:HA    | 2.49                     | 0.43              |
| 1:J:508:TRP:CD1  | 1:J:604:ASN:HB2   | 2.54                     | 0.43              |
| 1:J:518:LEU:N    | 1:J:518:LEU:CD1   | 2.81                     | 0.43              |
| 1:J:542:ILE:HA   | 1:J:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:K:102:MET:O    | 1:K:105:MET:N     | 2.46                     | 0.43              |
| 1:K:141:LEU:HD12 | 1:K:141:LEU:O     | 2.19                     | 0.43              |
| 1:K:222:HIS:HD2  | 1:L:198:LYS:HG2   | 1.84                     | 0.43              |
| 1:L:141:LEU:HD12 | 1:L:141:LEU:O     | 2.19                     | 0.43              |
| 1:L:231:LEU:HD23 | 1:L:231:LEU:C     | 2.43                     | 0.43              |
| 1:L:248:GLN:CD   | 1:L:268:PHE:CZ    | 2.96                     | 0.43              |
| 1:L:1158:TYR:HB3 | 1:L:1162:ILE:HG23 | 2.01                     | 0.43              |
| 1:M:152:VAL:O    | 1:M:155:SER:OG    | 2.29                     | 0.43              |
| 1:M:248:GLN:CD   | 1:M:268:PHE:CZ    | 2.96                     | 0.43              |
| 1:M:342:LYS:HG3  | 1:M:343:HIS:N     | 2.34                     | 0.43              |
| 1:M:428:GLU:C    | 1:M:430:LYS:H     | 2.26                     | 0.43              |
| 1:M:584:PHE:HB3  | 1:M:585:ASP:H     | 1.61                     | 0.43              |
| 1:M:1158:TYR:HB3 | 1:M:1162:ILE:HG23 | 2.01                     | 0.43              |
| 1:N:514:ILE:HG22 | 1:N:515:LEU:O     | 2.19                     | 0.43              |
| 1:N:553:LEU:HD23 | 1:N:553:LEU:HA    | 1.90                     | 0.43              |
| 1:N:799:ASN:O    | 1:N:800:THR:CG2   | 2.67                     | 0.43              |
| 1:N:901:HIS:O    | 1:N:902:ILE:HB    | 2.18                     | 0.43              |
| 1:O:231:LEU:HD23 | 1:O:231:LEU:C     | 2.43                     | 0.43              |
| 1:O:514:ILE:HG22 | 1:O:515:LEU:O     | 2.19                     | 0.43              |
| 1:O:517:THR:HA   | 1:O:520:GLN:OE1   | 2.18                     | 0.43              |
| 1:O:517:THR:CG2  | 1:O:518:LEU:N     | 2.81                     | 0.43              |
| 1:O:535:TYR:O    | 1:O:538:LEU:HB3   | 2.19                     | 0.43              |
| 1:O:553:LEU:HD23 | 1:O:553:LEU:HA    | 1.91                     | 0.43              |
| 1:O:903:GLU:HG3  | 1:O:904:CYS:H     | 1.84                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:443:ILE:HG13 | 1:P:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:P:508:TRP:CD1  | 1:P:604:ASN:HB2   | 2.54                     | 0.43              |
| 1:P:542:ILE:HA   | 1:P:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:A:251:APK:H2'  | 1:A:251:APK:H8    | 1.74                     | 0.43              |
| 1:A:514:ILE:HG22 | 1:A:515:LEU:O     | 2.19                     | 0.43              |
| 1:A:901:HIS:O    | 1:A:902:ILE:HB    | 2.18                     | 0.43              |
| 1:A:915:TYR:CE2  | 1:A:916:LYS:HE3   | 2.53                     | 0.43              |
| 1:B:124:ASN:HA   | 2:B:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:B:182:ASN:HD22 | 1:B:245:LEU:HB2   | 1.83                     | 0.43              |
| 1:B:252:ALA:HB3  | 1:B:253:TRP:H     | 1.70                     | 0.43              |
| 1:B:410:LEU:CD2  | 1:B:413:LYS:HA    | 2.49                     | 0.43              |
| 1:B:799:ASN:O    | 1:B:800:THR:CG2   | 2.67                     | 0.43              |
| 1:C:141:LEU:HD12 | 1:C:141:LEU:O     | 2.19                     | 0.43              |
| 1:C:231:LEU:HD23 | 1:C:231:LEU:C     | 2.43                     | 0.43              |
| 1:C:1201:THR:OG1 | 1:C:1202:MET:N    | 2.48                     | 0.43              |
| 1:D:102:MET:O    | 1:D:105:MET:N     | 2.46                     | 0.43              |
| 1:D:148:LEU:HD23 | 1:D:264:LEU:HB2   | 2.00                     | 0.43              |
| 1:D:285:LEU:HD23 | 1:D:285:LEU:HA    | 1.74                     | 0.43              |
| 1:D:957:ILE:HG13 | 1:D:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:E:11:GLN:O     | 1:E:14:ASP:N      | 2.46                     | 0.43              |
| 1:E:231:LEU:O    | 1:E:234:SER:OG    | 2.26                     | 0.43              |
| 1:E:518:LEU:N    | 1:E:518:LEU:CD1   | 2.81                     | 0.43              |
| 1:F:541:ALA:O    | 1:F:543:LEU:N     | 2.52                     | 0.43              |
| 1:F:633:THR:HG22 | 1:F:643:TYR:HA    | 1.97                     | 0.43              |
| 1:G:54:ALA:O     | 1:G:57:GLY:N      | 2.52                     | 0.43              |
| 1:G:243:VAL:HG13 | 1:G:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:G:463:LEU:CD2  | 1:G:467:PHE:HD2   | 2.31                     | 0.43              |
| 1:G:989:SER:HB2  | 1:G:1027:ASN:HA   | 2.01                     | 0.43              |
| 1:H:428:GLU:C    | 1:H:430:LYS:N     | 2.74                     | 0.43              |
| 1:H:481:PRO:O    | 1:H:485:THR:HG23  | 2.19                     | 0.43              |
| 1:H:511:SER:C    | 1:H:513:SER:N     | 2.60                     | 0.43              |
| 1:H:514:ILE:HG22 | 1:H:515:LEU:O     | 2.19                     | 0.43              |
| 1:H:517:THR:HA   | 1:H:520:GLN:OE1   | 2.18                     | 0.43              |
| 1:H:541:ALA:O    | 1:H:543:LEU:N     | 2.52                     | 0.43              |
| 1:H:554:ILE:C    | 1:H:556:SER:N     | 2.76                     | 0.43              |
| 1:I:11:GLN:O     | 1:I:12:TYR:C      | 2.62                     | 0.43              |
| 1:I:20:GLU:HG3   | 1:I:21:ASP:N      | 2.33                     | 0.43              |
| 1:I:141:LEU:O    | 1:I:141:LEU:HD12  | 2.19                     | 0.43              |
| 1:I:243:VAL:HG13 | 1:I:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:J:11:GLN:O     | 1:J:14:ASP:N      | 2.46                     | 0.43              |
| 1:J:901:HIS:O    | 1:J:902:ILE:HB    | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:915:TYR:CE2  | 1:K:916:LYS:HE3   | 2.54                     | 0.43              |
| 1:K:957:ILE:HG13 | 1:K:1248:LEU:HD22 | 1.99                     | 0.43              |
| 1:L:244:LEU:HD21 | 1:L:256:PHE:CD2   | 2.50                     | 0.43              |
| 1:L:324:LEU:HD12 | 1:L:324:LEU:HA    | 1.61                     | 0.43              |
| 1:L:412:GLU:CD   | 1:L:412:GLU:C     | 2.87                     | 0.43              |
| 1:L:517:THR:HA   | 1:L:520:GLN:OE1   | 2.18                     | 0.43              |
| 1:L:1201:THR:OG1 | 1:L:1202:MET:N    | 2.48                     | 0.43              |
| 1:M:132:LEU:HD12 | 1:M:132:LEU:HA    | 1.79                     | 0.43              |
| 1:M:410:LEU:CD2  | 1:M:413:LYS:HA    | 2.49                     | 0.43              |
| 1:M:903:GLU:HG3  | 1:M:904:CYS:H     | 1.84                     | 0.43              |
| 1:N:124:ASN:HA   | 2:N:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:N:453:PHE:CE2  | 1:N:460:PRO:HB3   | 2.49                     | 0.43              |
| 1:O:54:ALA:O     | 1:O:57:GLY:N      | 2.52                     | 0.43              |
| 1:O:124:ASN:HA   | 2:O:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:O:234:SER:OG   | 1:O:235:LYS:N     | 2.51                     | 0.43              |
| 1:O:428:GLU:C    | 1:O:430:LYS:N     | 2.74                     | 0.43              |
| 1:O:443:ILE:HG21 | 1:O:477:ASN:ND2   | 2.24                     | 0.43              |
| 1:O:451:LYS:CD   | 1:O:486:LEU:HD21  | 2.33                     | 0.43              |
| 1:O:541:ALA:O    | 1:O:543:LEU:N     | 2.52                     | 0.43              |
| 1:O:542:ILE:HA   | 1:O:545:PHE:CD2   | 2.54                     | 0.43              |
| 1:P:124:ASN:HA   | 2:P:1501:DTP:C2   | 2.49                     | 0.43              |
| 1:P:231:LEU:HD23 | 1:P:231:LEU:C     | 2.43                     | 0.43              |
| 1:P:243:VAL:HG13 | 1:P:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:P:264:LEU:HD23 | 1:P:264:LEU:HA    | 1.75                     | 0.43              |
| 1:P:461:PRO:O    | 1:P:461:PRO:HG2   | 2.18                     | 0.43              |
| 1:B:132:LEU:HD12 | 1:B:132:LEU:HA    | 1.79                     | 0.43              |
| 1:B:463:LEU:CD2  | 1:B:467:PHE:HD2   | 2.31                     | 0.43              |
| 1:C:234:SER:OG   | 1:C:235:LYS:N     | 2.51                     | 0.43              |
| 1:C:412:GLU:C    | 1:C:412:GLU:CD    | 2.87                     | 0.43              |
| 1:D:401:VAL:O    | 1:D:402:VAL:C     | 2.61                     | 0.43              |
| 1:D:412:GLU:CD   | 1:D:412:GLU:C     | 2.87                     | 0.43              |
| 1:E:231:LEU:C    | 1:E:231:LEU:HD23  | 2.43                     | 0.43              |
| 1:E:333:ASP:OD2  | 1:F:403:ASN:CG    | 2.57                     | 0.43              |
| 1:E:428:GLU:C    | 1:E:430:LYS:H     | 2.26                     | 0.43              |
| 1:E:443:ILE:HG13 | 1:E:477:ASN:ND2   | 2.34                     | 0.43              |
| 1:E:508:TRP:CD1  | 1:E:604:ASN:HB2   | 2.54                     | 0.43              |
| 1:F:243:VAL:HG13 | 1:F:263:LEU:HD22  | 2.00                     | 0.43              |
| 1:F:543:LEU:HA   | 1:F:546:LEU:CD1   | 2.48                     | 0.43              |
| 1:F:554:ILE:C    | 1:F:556:SER:N     | 2.76                     | 0.43              |
| 1:F:799:ASN:O    | 1:F:800:THR:CG2   | 2.67                     | 0.43              |
| 1:F:901:HIS:O    | 1:F:902:ILE:HB    | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:231:LEU:HD23  | 1:G:231:LEU:C    | 2.43                     | 0.43              |
| 1:G:248:GLN:CD    | 1:G:268:PHE:CZ   | 2.96                     | 0.43              |
| 1:G:461:PRO:HG2   | 1:G:461:PRO:O    | 2.18                     | 0.43              |
| 1:G:508:TRP:CD1   | 1:G:604:ASN:HB2  | 2.54                     | 0.43              |
| 1:G:1000:ILE:HD11 | 1:G:1014:ALA:HB3 | 2.00                     | 0.43              |
| 1:H:54:ALA:O      | 1:H:57:GLY:N     | 2.52                     | 0.43              |
| 1:H:305:LEU:HD23  | 1:H:305:LEU:HA   | 1.84                     | 0.43              |
| 1:H:410:LEU:CD2   | 1:H:413:LYS:HA   | 2.49                     | 0.43              |
| 1:H:443:ILE:HG21  | 1:H:477:ASN:ND2  | 2.24                     | 0.43              |
| 1:H:517:THR:CG2   | 1:H:518:LEU:N    | 2.81                     | 0.43              |
| 1:H:1198:ASP:OD1  | 1:H:1199:ASP:N   | 2.50                     | 0.43              |
| 1:I:122:LYS:HG3   | 1:P:276:SER:CB   | 2.49                     | 0.43              |
| 1:I:186:CYS:C     | 1:I:249:ASN:HD21 | 2.27                     | 0.43              |
| 1:I:481:PRO:O     | 1:I:485:THR:HG23 | 2.19                     | 0.43              |
| 1:J:305:LEU:HD23  | 1:J:305:LEU:HA   | 1.84                     | 0.43              |
| 1:J:443:ILE:HG13  | 1:J:477:ASN:ND2  | 2.34                     | 0.43              |
| 1:K:342:LYS:HG3   | 1:K:343:HIS:N    | 2.34                     | 0.43              |
| 1:L:376:PRO:HA    | 1:L:377:PRO:HD3  | 1.89                     | 0.43              |
| 1:L:410:LEU:CD2   | 1:L:413:LYS:HA   | 2.49                     | 0.43              |
| 1:L:535:TYR:O     | 1:L:538:LEU:HB3  | 2.19                     | 0.43              |
| 1:L:799:ASN:O     | 1:L:800:THR:CG2  | 2.67                     | 0.43              |
| 1:L:1036:VAL:HG12 | 1:L:1037:ASP:H   | 1.83                     | 0.43              |
| 1:M:124:ASN:HA    | 2:M:1501:DTP:C2  | 2.49                     | 0.43              |
| 1:M:463:LEU:CD2   | 1:M:467:PHE:HD2  | 2.31                     | 0.43              |
| 1:M:517:THR:CG2   | 1:M:518:LEU:N    | 2.81                     | 0.43              |
| 1:M:799:ASN:O     | 1:M:800:THR:CG2  | 2.67                     | 0.43              |
| 1:M:914:VAL:O     | 1:M:915:TYR:C    | 2.60                     | 0.43              |
| 1:N:222:HIS:CG    | 1:O:198:LYS:HZ1  | 2.37                     | 0.43              |
| 1:N:915:TYR:CE2   | 1:N:916:LYS:HE3  | 2.53                     | 0.43              |
| 1:O:73:VAL:O      | 1:O:76:PHE:N     | 2.52                     | 0.43              |
| 1:O:410:LEU:CD2   | 1:O:413:LYS:HA   | 2.49                     | 0.43              |
| 1:O:481:PRO:O     | 1:O:485:THR:HG23 | 2.19                     | 0.43              |
| 1:O:554:ILE:C     | 1:O:556:SER:N    | 2.76                     | 0.43              |
| 1:P:482:GLU:C     | 1:P:485:THR:HG1  | 2.26                     | 0.43              |
| 1:P:646:ARG:HG3   | 1:P:648:GLU:HG3  | 2.00                     | 0.43              |
| 1:P:989:SER:HB2   | 1:P:1027:ASN:HA  | 2.01                     | 0.43              |
| 1:P:1000:ILE:HD11 | 1:P:1014:ALA:HB3 | 2.00                     | 0.43              |
| 1:A:124:ASN:HA    | 2:A:1501:DTP:C2  | 2.49                     | 0.42              |
| 1:A:376:PRO:HA    | 1:A:377:PRO:HD3  | 1.89                     | 0.42              |
| 1:A:1195:VAL:HG11 | 1:A:1241:PHE:CZ  | 2.54                     | 0.42              |
| 1:B:148:LEU:HD23  | 1:B:264:LEU:HB2  | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:541:ALA:O     | 1:B:543:LEU:N    | 2.52                     | 0.42              |
| 1:B:914:VAL:O     | 1:B:915:TYR:C    | 2.60                     | 0.42              |
| 1:B:950:TRP:CZ3   | 1:B:952:HIS:HA   | 2.54                     | 0.42              |
| 1:C:54:ALA:O      | 1:C:57:GLY:N     | 2.52                     | 0.42              |
| 1:C:342:LYS:HG3   | 1:C:343:HIS:N    | 2.34                     | 0.42              |
| 1:C:376:PRO:HA    | 1:C:377:PRO:HD3  | 1.89                     | 0.42              |
| 1:C:535:TYR:O     | 1:C:538:LEU:HB3  | 2.19                     | 0.42              |
| 1:C:1036:VAL:HG12 | 1:C:1037:ASP:H   | 1.83                     | 0.42              |
| 1:E:514:ILE:HG22  | 1:E:515:LEU:O    | 2.19                     | 0.42              |
| 1:E:517:THR:HA    | 1:E:520:GLN:OE1  | 2.19                     | 0.42              |
| 1:F:11:GLN:O      | 1:F:12:TYR:C     | 2.62                     | 0.42              |
| 1:F:481:PRO:O     | 1:F:485:THR:HG23 | 2.19                     | 0.42              |
| 1:F:517:THR:HA    | 1:F:520:GLN:OE1  | 2.18                     | 0.42              |
| 1:G:514:ILE:HG22  | 1:G:515:LEU:O    | 2.19                     | 0.42              |
| 1:G:646:ARG:HG3   | 1:G:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:H:73:VAL:O      | 1:H:76:PHE:N     | 2.52                     | 0.42              |
| 1:H:234:SER:OG    | 1:H:235:LYS:N    | 2.51                     | 0.42              |
| 1:H:646:ARG:HG3   | 1:H:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:H:724:GLY:HA3   | 1:H:730:ILE:HD12 | 2.01                     | 0.42              |
| 1:I:554:ILE:O     | 1:I:556:SER:N    | 2.45                     | 0.42              |
| 1:I:799:ASN:O     | 1:I:800:THR:CG2  | 2.67                     | 0.42              |
| 1:I:901:HIS:O     | 1:I:902:ILE:HB   | 2.18                     | 0.42              |
| 1:J:231:LEU:C     | 1:J:231:LEU:HD23 | 2.43                     | 0.42              |
| 1:J:514:ILE:HG22  | 1:J:515:LEU:O    | 2.19                     | 0.42              |
| 1:J:903:GLU:HG3   | 1:J:904:CYS:H    | 1.84                     | 0.42              |
| 1:K:148:LEU:HD23  | 1:K:264:LEU:HB2  | 2.00                     | 0.42              |
| 1:K:285:LEU:HD23  | 1:K:285:LEU:HA   | 1.74                     | 0.42              |
| 1:K:401:VAL:O     | 1:K:402:VAL:C    | 2.61                     | 0.42              |
| 1:L:54:ALA:O      | 1:L:57:GLY:N     | 2.52                     | 0.42              |
| 1:L:148:LEU:HD23  | 1:L:264:LEU:HB2  | 2.00                     | 0.42              |
| 1:L:458:LEU:CA    | 1:L:587:ARG:HH21 | 2.31                     | 0.42              |
| 1:L:514:ILE:HG22  | 1:L:515:LEU:O    | 2.19                     | 0.42              |
| 1:M:148:LEU:HD23  | 1:M:264:LEU:HB2  | 2.00                     | 0.42              |
| 1:M:187:ASN:CA    | 1:M:249:ASN:HD21 | 2.27                     | 0.42              |
| 1:M:514:ILE:HG22  | 1:M:515:LEU:O    | 2.19                     | 0.42              |
| 1:N:324:LEU:HD12  | 1:N:324:LEU:HA   | 1.61                     | 0.42              |
| 1:O:305:LEU:HD23  | 1:O:305:LEU:HA   | 1.84                     | 0.42              |
| 1:O:453:PHE:CE2   | 1:O:460:PRO:HB3  | 2.49                     | 0.42              |
| 1:O:646:ARG:HG3   | 1:O:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:O:724:GLY:HA3   | 1:O:730:ILE:HD12 | 2.01                     | 0.42              |
| 1:O:950:TRP:CZ3   | 1:O:952:HIS:HA   | 2.54                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:O:1198:ASP:OD1  | 1:O:1199:ASP:N   | 2.50                     | 0.42              |
| 1:P:54:ALA:O      | 1:P:57:GLY:N     | 2.52                     | 0.42              |
| 1:P:248:GLN:CD    | 1:P:268:PHE:CZ   | 2.96                     | 0.42              |
| 1:P:324:LEU:HD12  | 1:P:324:LEU:HA   | 1.61                     | 0.42              |
| 1:P:514:ILE:HG22  | 1:P:515:LEU:O    | 2.19                     | 0.42              |
| 1:P:535:TYR:O     | 1:P:538:LEU:HB3  | 2.19                     | 0.42              |
| 1:P:950:TRP:CZ3   | 1:P:952:HIS:HA   | 2.54                     | 0.42              |
| 1:A:122:LYS:CG    | 1:B:276:SER:OG   | 2.67                     | 0.42              |
| 1:A:248:GLN:CD    | 1:A:268:PHE:CZ   | 2.96                     | 0.42              |
| 1:A:633:THR:HG22  | 1:A:643:TYR:HA   | 1.97                     | 0.42              |
| 1:B:187:ASN:CA    | 1:B:249:ASN:HD21 | 2.27                     | 0.42              |
| 1:B:443:ILE:HG21  | 1:B:477:ASN:ND2  | 2.24                     | 0.42              |
| 1:B:514:ILE:HG22  | 1:B:515:LEU:O    | 2.19                     | 0.42              |
| 1:B:517:THR:CG2   | 1:B:518:LEU:N    | 2.81                     | 0.42              |
| 1:B:901:HIS:O     | 1:B:902:ILE:HB   | 2.18                     | 0.42              |
| 1:B:1195:VAL:HG11 | 1:B:1241:PHE:CZ  | 2.54                     | 0.42              |
| 1:C:458:LEU:CA    | 1:C:587:ARG:HH21 | 2.30                     | 0.42              |
| 1:E:903:GLU:HG3   | 1:E:904:CYS:H    | 1.84                     | 0.42              |
| 1:G:535:TYR:O     | 1:G:538:LEU:HB3  | 2.19                     | 0.42              |
| 1:G:541:ALA:O     | 1:G:543:LEU:N    | 2.52                     | 0.42              |
| 1:G:950:TRP:CZ3   | 1:G:952:HIS:HA   | 2.54                     | 0.42              |
| 1:G:1195:VAL:HG11 | 1:G:1241:PHE:CZ  | 2.54                     | 0.42              |
| 1:H:401:VAL:O     | 1:H:402:VAL:C    | 2.61                     | 0.42              |
| 1:H:950:TRP:CZ3   | 1:H:952:HIS:HA   | 2.54                     | 0.42              |
| 1:I:231:LEU:HD23  | 1:I:231:LEU:C    | 2.43                     | 0.42              |
| 1:I:461:PRO:O     | 1:I:461:PRO:HG2  | 2.18                     | 0.42              |
| 1:I:646:ARG:HG3   | 1:I:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:J:162:LEU:O     | 1:J:163:ASP:C    | 2.62                     | 0.42              |
| 1:J:517:THR:HA    | 1:J:520:GLN:OE1  | 2.19                     | 0.42              |
| 1:K:412:GLU:C     | 1:K:412:GLU:CD   | 2.87                     | 0.42              |
| 1:K:428:GLU:OE1   | 1:K:429:LEU:HA   | 2.20                     | 0.42              |
| 1:L:132:LEU:HD12  | 1:L:132:LEU:HA   | 1.79                     | 0.42              |
| 1:L:342:LYS:HG3   | 1:L:343:HIS:N    | 2.34                     | 0.42              |
| 1:L:950:TRP:CZ3   | 1:L:952:HIS:HA   | 2.54                     | 0.42              |
| 1:M:541:ALA:O     | 1:M:543:LEU:N    | 2.52                     | 0.42              |
| 1:M:950:TRP:CZ3   | 1:M:952:HIS:HA   | 2.54                     | 0.42              |
| 1:M:1195:VAL:HG11 | 1:M:1241:PHE:CZ  | 2.54                     | 0.42              |
| 1:N:234:SER:OG    | 1:N:235:LYS:N    | 2.51                     | 0.42              |
| 1:N:248:GLN:CD    | 1:N:268:PHE:CZ   | 2.96                     | 0.42              |
| 1:N:517:THR:HA    | 1:N:520:GLN:OE1  | 2.18                     | 0.42              |
| 1:N:950:TRP:CZ3   | 1:N:952:HIS:HA   | 2.54                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:1195:VAL:HG11 | 1:N:1241:PHE:CZ   | 2.54                     | 0.42              |
| 1:O:401:VAL:O     | 1:O:402:VAL:C     | 2.61                     | 0.42              |
| 1:O:508:TRP:CD1   | 1:O:604:ASN:HB2   | 2.54                     | 0.42              |
| 1:O:901:HIS:O     | 1:O:902:ILE:HB    | 2.18                     | 0.42              |
| 1:P:541:ALA:O     | 1:P:543:LEU:N     | 2.52                     | 0.42              |
| 1:P:1195:VAL:HG11 | 1:P:1241:PHE:CZ   | 2.54                     | 0.42              |
| 1:A:516:ASN:O     | 1:A:517:THR:CB    | 2.67                     | 0.42              |
| 1:B:73:VAL:O      | 1:B:76:PHE:N      | 2.52                     | 0.42              |
| 1:B:234:SER:OG    | 1:B:235:LYS:N     | 2.51                     | 0.42              |
| 1:B:412:GLU:CD    | 1:B:412:GLU:C     | 2.87                     | 0.42              |
| 1:C:147:VAL:HG12  | 1:C:281:THR:OG1   | 2.19                     | 0.42              |
| 1:C:251:APK:H8    | 1:C:251:APK:H2'   | 1.74                     | 0.42              |
| 1:C:314:ARG:C     | 1:C:315:GLU:CG    | 2.81                     | 0.42              |
| 1:C:428:GLU:OE1   | 1:C:429:LEU:HA    | 2.20                     | 0.42              |
| 1:C:517:THR:HA    | 1:C:520:GLN:OE1   | 2.18                     | 0.42              |
| 1:C:545:PHE:O     | 1:C:549:ILE:HG22  | 2.20                     | 0.42              |
| 1:D:11:GLN:O      | 1:D:12:TYR:C      | 2.62                     | 0.42              |
| 1:D:124:ASN:HA    | 2:D:1501:DTP:C2   | 2.49                     | 0.42              |
| 1:D:251:APK:H8    | 1:D:251:APK:H2'   | 1.74                     | 0.42              |
| 1:D:428:GLU:OE1   | 1:D:429:LEU:HA    | 2.20                     | 0.42              |
| 1:D:799:ASN:O     | 1:D:800:THR:CG2   | 2.67                     | 0.42              |
| 1:D:950:TRP:CZ3   | 1:D:952:HIS:HA    | 2.54                     | 0.42              |
| 1:E:162:LEU:O     | 1:E:163:ASP:C     | 2.62                     | 0.42              |
| 1:E:186:CYS:C     | 1:E:249:ASN:HD21  | 2.27                     | 0.42              |
| 1:E:342:LYS:HG3   | 1:E:343:HIS:N     | 2.34                     | 0.42              |
| 1:E:412:GLU:C     | 1:E:412:GLU:CD    | 2.87                     | 0.42              |
| 1:E:482:GLU:C     | 1:E:485:THR:HG1   | 2.27                     | 0.42              |
| 1:E:543:LEU:HA    | 1:E:546:LEU:CD1   | 2.48                     | 0.42              |
| 1:F:231:LEU:HD23  | 1:F:231:LEU:C     | 2.43                     | 0.42              |
| 1:F:453:PHE:CE2   | 1:F:460:PRO:HB3   | 2.49                     | 0.42              |
| 1:F:463:LEU:CD2   | 1:F:467:PHE:HD2   | 2.31                     | 0.42              |
| 1:G:79:GLU:OE2    | 1:G:83:ILE:HD11   | 2.20                     | 0.42              |
| 1:G:120:PHE:CE1   | 1:G:159:TRP:CE3   | 3.05                     | 0.42              |
| 1:G:324:LEU:HA    | 1:G:324:LEU:HD12  | 1.61                     | 0.42              |
| 1:G:553:LEU:HD23  | 1:G:553:LEU:HA    | 1.91                     | 0.42              |
| 1:H:516:ASN:O     | 1:H:517:THR:CB    | 2.67                     | 0.42              |
| 1:H:901:HIS:O     | 1:H:902:ILE:HB    | 2.18                     | 0.42              |
| 1:H:1000:ILE:HD11 | 1:H:1014:ALA:HB3  | 2.00                     | 0.42              |
| 1:H:1158:TYR:HB3  | 1:H:1162:ILE:HG23 | 2.01                     | 0.42              |
| 1:I:514:ILE:HG22  | 1:I:515:LEU:O     | 2.19                     | 0.42              |
| 1:J:141:LEU:HD12  | 1:J:141:LEU:O     | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:186:CYS:C     | 1:J:249:ASN:HD21 | 2.27                     | 0.42              |
| 1:J:342:LYS:HG3   | 1:J:343:HIS:N    | 2.34                     | 0.42              |
| 1:J:428:GLU:C     | 1:J:430:LYS:H    | 2.26                     | 0.42              |
| 1:J:543:LEU:HA    | 1:J:546:LEU:CD1  | 2.49                     | 0.42              |
| 1:J:1075:SER:OG   | 1:J:1094:ASP:O   | 2.29                     | 0.42              |
| 1:K:124:ASN:HA    | 2:K:1501:DTP:C2  | 2.49                     | 0.42              |
| 1:K:514:ILE:HG22  | 1:K:515:LEU:O    | 2.19                     | 0.42              |
| 1:K:799:ASN:O     | 1:K:800:THR:CG2  | 2.67                     | 0.42              |
| 1:K:950:TRP:CZ3   | 1:K:952:HIS:HA   | 2.54                     | 0.42              |
| 1:L:507:ALA:O     | 1:L:608:ASN:CB   | 2.61                     | 0.42              |
| 1:L:508:TRP:O     | 1:L:606:GLY:CA   | 2.63                     | 0.42              |
| 1:L:545:PHE:O     | 1:L:549:ILE:HG22 | 2.19                     | 0.42              |
| 1:L:646:ARG:HG3   | 1:L:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:M:73:VAL:O      | 1:M:76:PHE:N     | 2.52                     | 0.42              |
| 1:M:234:SER:OG    | 1:M:235:LYS:N    | 2.51                     | 0.42              |
| 1:M:517:THR:HA    | 1:M:520:GLN:OE1  | 2.18                     | 0.42              |
| 1:M:901:HIS:O     | 1:M:902:ILE:HB   | 2.18                     | 0.42              |
| 1:N:251:APK:O     | 1:N:253:TRP:HB3  | 2.20                     | 0.42              |
| 1:O:285:LEU:HA    | 1:O:285:LEU:HD23 | 1.74                     | 0.42              |
| 1:O:317:LEU:O     | 1:O:318:THR:CB   | 2.61                     | 0.42              |
| 1:O:516:ASN:O     | 1:O:517:THR:CB   | 2.67                     | 0.42              |
| 1:O:1000:ILE:HD11 | 1:O:1014:ALA:HB3 | 2.00                     | 0.42              |
| 1:P:79:GLU:OE2    | 1:P:83:ILE:HD11  | 2.20                     | 0.42              |
| 1:P:120:PHE:CE1   | 1:P:159:TRP:CE3  | 3.05                     | 0.42              |
| 1:A:14:ASP:CG     | 1:B:142:ARG:HH22 | 2.28                     | 0.42              |
| 1:A:234:SER:OG    | 1:A:235:LYS:N    | 2.51                     | 0.42              |
| 1:A:517:THR:HA    | 1:A:520:GLN:OE1  | 2.18                     | 0.42              |
| 1:A:646:ARG:HG3   | 1:A:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:A:724:GLY:HA3   | 1:A:730:ILE:HD12 | 2.01                     | 0.42              |
| 1:A:950:TRP:CZ3   | 1:A:952:HIS:HA   | 2.54                     | 0.42              |
| 1:B:39:ILE:HG23   | 1:B:40:LEU:HG    | 2.02                     | 0.42              |
| 1:B:440:HIS:O     | 1:B:444:VAL:HG23 | 2.18                     | 0.42              |
| 1:B:724:GLY:HA3   | 1:B:730:ILE:HD12 | 2.01                     | 0.42              |
| 1:C:507:ALA:O     | 1:C:608:ASN:CB   | 2.61                     | 0.42              |
| 1:C:508:TRP:O     | 1:C:606:GLY:CA   | 2.63                     | 0.42              |
| 1:C:514:ILE:HG22  | 1:C:515:LEU:O    | 2.19                     | 0.42              |
| 1:C:542:ILE:HA    | 1:C:545:PHE:CD2  | 2.54                     | 0.42              |
| 1:C:646:ARG:HG3   | 1:C:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:D:248:GLN:CD    | 1:D:268:PHE:CZ   | 2.96                     | 0.42              |
| 1:D:410:LEU:CD2   | 1:D:413:LYS:HA   | 2.49                     | 0.42              |
| 1:D:514:ILE:HG22  | 1:D:515:LEU:O    | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:862:ILE:HG23 | 1:D:863:THR:H     | 1.84                     | 0.42              |
| 1:F:115:ASN:HB3  | 1:G:257:ASN:HD21  | 1.84                     | 0.42              |
| 1:F:514:ILE:HG22 | 1:F:515:LEU:O     | 2.19                     | 0.42              |
| 1:F:862:ILE:HG23 | 1:F:863:THR:H     | 1.84                     | 0.42              |
| 1:G:39:ILE:HG23  | 1:G:40:LEU:HG     | 2.02                     | 0.42              |
| 1:G:470:HIS:O    | 1:G:473:HIS:N     | 2.53                     | 0.42              |
| 1:G:482:GLU:C    | 1:G:485:THR:HG1   | 2.26                     | 0.42              |
| 1:H:11:GLN:O     | 1:H:12:TYR:C      | 2.62                     | 0.42              |
| 1:H:508:TRP:CD1  | 1:H:604:ASN:HB2   | 2.54                     | 0.42              |
| 1:H:545:PHE:O    | 1:H:549:ILE:HG22  | 2.19                     | 0.42              |
| 1:I:162:LEU:O    | 1:I:163:ASP:C     | 2.62                     | 0.42              |
| 1:I:517:THR:HA   | 1:I:520:GLN:OE1   | 2.18                     | 0.42              |
| 1:I:543:LEU:HA   | 1:I:546:LEU:CD1   | 2.48                     | 0.42              |
| 1:J:413:LYS:CD   | 1:J:422:ILE:O     | 2.61                     | 0.42              |
| 1:K:11:GLN:O     | 1:K:12:TYR:C      | 2.62                     | 0.42              |
| 1:K:545:PHE:O    | 1:K:549:ILE:HG22  | 2.19                     | 0.42              |
| 1:L:90:SER:HG    | 1:L:91:PRO:HD3    | 1.83                     | 0.42              |
| 1:L:541:ALA:O    | 1:L:543:LEU:N     | 2.52                     | 0.42              |
| 1:M:39:ILE:HG23  | 1:M:40:LEU:HG     | 2.02                     | 0.42              |
| 1:M:412:GLU:C    | 1:M:412:GLU:CD    | 2.87                     | 0.42              |
| 1:M:458:LEU:CG   | 1:M:587:ARG:NH2   | 2.74                     | 0.42              |
| 1:M:470:HIS:O    | 1:M:473:HIS:N     | 2.53                     | 0.42              |
| 1:M:553:LEU:HD23 | 1:M:553:LEU:HA    | 1.90                     | 0.42              |
| 1:M:724:GLY:HA3  | 1:M:730:ILE:HD12  | 2.01                     | 0.42              |
| 1:N:376:PRO:HA   | 1:N:377:PRO:HD3   | 1.89                     | 0.42              |
| 1:N:516:ASN:O    | 1:N:517:THR:CB    | 2.67                     | 0.42              |
| 1:N:724:GLY:HA3  | 1:N:730:ILE:HD12  | 2.01                     | 0.42              |
| 1:O:91:PRO:O     | 1:O:94:THR:OG1    | 2.21                     | 0.42              |
| 1:O:1158:TYR:HB3 | 1:O:1162:ILE:HG23 | 2.01                     | 0.42              |
| 1:P:39:ILE:HG23  | 1:P:40:LEU:HG     | 2.02                     | 0.42              |
| 1:P:902:ILE:HD13 | 1:P:930:HIS:CE1   | 2.43                     | 0.42              |
| 1:A:39:ILE:HG23  | 1:A:40:LEU:HG     | 2.02                     | 0.42              |
| 1:A:79:GLU:OE2   | 1:A:83:ILE:HD11   | 2.19                     | 0.42              |
| 1:A:251:APK:O    | 1:A:253:TRP:HB3   | 2.20                     | 0.42              |
| 1:A:481:PRO:O    | 1:A:485:THR:HG23  | 2.19                     | 0.42              |
| 1:A:508:TRP:CD1  | 1:A:604:ASN:HB2   | 2.54                     | 0.42              |
| 1:B:458:LEU:CG   | 1:B:587:ARG:NH2   | 2.74                     | 0.42              |
| 1:B:470:HIS:O    | 1:B:473:HIS:N     | 2.53                     | 0.42              |
| 1:B:488:ARG:HG2  | 1:B:491:PHE:CG    | 2.55                     | 0.42              |
| 1:B:517:THR:HA   | 1:B:520:GLN:OE1   | 2.18                     | 0.42              |
| 1:B:542:ILE:HA   | 1:B:545:PHE:CD2   | 2.54                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:553:LEU:HD23 | 1:B:553:LEU:HA   | 1.91                     | 0.42              |
| 1:C:312:LEU:CD2  | 1:C:313:PRO:CD   | 2.86                     | 0.42              |
| 1:C:346:CYS:HG   | 1:C:350:THR:HG1  | 1.64                     | 0.42              |
| 1:C:553:LEU:HD23 | 1:C:553:LEU:HA   | 1.90                     | 0.42              |
| 1:D:488:ARG:HG2  | 1:D:491:PHE:CG   | 2.55                     | 0.42              |
| 1:D:508:TRP:CD1  | 1:D:604:ASN:HB2  | 2.54                     | 0.42              |
| 1:D:545:PHE:O    | 1:D:549:ILE:HG22 | 2.20                     | 0.42              |
| 1:D:557:LYS:HZ2  | 1:D:1223:GLN:CG  | 2.32                     | 0.42              |
| 1:E:141:LEU:HD12 | 1:E:141:LEU:O    | 2.19                     | 0.42              |
| 1:E:147:VAL:HG12 | 1:E:281:THR:OG1  | 2.19                     | 0.42              |
| 1:F:410:LEU:CD2  | 1:F:413:LYS:HA   | 2.49                     | 0.42              |
| 1:F:461:PRO:O    | 1:F:461:PRO:HG2  | 2.18                     | 0.42              |
| 1:F:516:ASN:O    | 1:F:517:THR:CB   | 2.67                     | 0.42              |
| 1:F:903:GLU:HG3  | 1:F:904:CYS:H    | 1.84                     | 0.42              |
| 1:G:517:THR:HA   | 1:G:520:GLN:OE1  | 2.18                     | 0.42              |
| 1:G:901:HIS:O    | 1:G:902:ILE:HB   | 2.18                     | 0.42              |
| 1:H:39:ILE:HG23  | 1:H:40:LEU:HG    | 2.02                     | 0.42              |
| 1:H:463:LEU:CD2  | 1:H:467:PHE:HD2  | 2.31                     | 0.42              |
| 1:H:989:SER:HB2  | 1:H:1027:ASN:HA  | 2.01                     | 0.42              |
| 1:I:463:LEU:CD2  | 1:I:467:PHE:HD2  | 2.31                     | 0.42              |
| 1:I:504:ASP:CG   | 1:I:608:ASN:ND2  | 2.69                     | 0.42              |
| 1:I:535:TYR:O    | 1:I:538:LEU:HB3  | 2.19                     | 0.42              |
| 1:J:113:LEU:HA   | 1:J:113:LEU:HD12 | 1.83                     | 0.42              |
| 1:J:412:GLU:CD   | 1:J:412:GLU:C    | 2.87                     | 0.42              |
| 1:K:79:GLU:OE2   | 1:K:83:ILE:HD11  | 2.19                     | 0.42              |
| 1:K:162:LEU:O    | 1:K:163:ASP:C    | 2.62                     | 0.42              |
| 1:K:248:GLN:CD   | 1:K:268:PHE:CZ   | 2.96                     | 0.42              |
| 1:K:488:ARG:HG2  | 1:K:491:PHE:CG   | 2.55                     | 0.42              |
| 1:K:517:THR:CG2  | 1:K:518:LEU:N    | 2.81                     | 0.42              |
| 1:K:542:ILE:HA   | 1:K:545:PHE:CD2  | 2.54                     | 0.42              |
| 1:K:901:HIS:O    | 1:K:902:ILE:HB   | 2.18                     | 0.42              |
| 1:L:147:VAL:HG12 | 1:L:281:THR:OG1  | 2.19                     | 0.42              |
| 1:L:542:ILE:HA   | 1:L:545:PHE:CD2  | 2.54                     | 0.42              |
| 1:L:553:LEU:HD23 | 1:L:553:LEU:HA   | 1.90                     | 0.42              |
| 1:M:440:HIS:O    | 1:M:444:VAL:HG23 | 2.18                     | 0.42              |
| 1:M:542:ILE:HA   | 1:M:545:PHE:CD2  | 2.54                     | 0.42              |
| 1:M:646:ARG:HG3  | 1:M:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:N:147:VAL:HG12 | 1:N:281:THR:OG1  | 2.19                     | 0.42              |
| 1:N:342:LYS:HG3  | 1:N:343:HIS:N    | 2.34                     | 0.42              |
| 1:N:508:TRP:CD1  | 1:N:604:ASN:HB2  | 2.54                     | 0.42              |
| 1:N:542:ILE:HA   | 1:N:545:PHE:CD2  | 2.54                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:11:GLN:O     | 1:O:12:TYR:C     | 2.62                     | 0.42              |
| 1:O:545:PHE:O    | 1:O:549:ILE:HG22 | 2.20                     | 0.42              |
| 1:O:989:SER:HB2  | 1:O:1027:ASN:HA  | 2.01                     | 0.42              |
| 1:P:470:HIS:O    | 1:P:473:HIS:N    | 2.53                     | 0.42              |
| 1:P:517:THR:HA   | 1:P:520:GLN:OE1  | 2.18                     | 0.42              |
| 1:P:901:HIS:O    | 1:P:902:ILE:HB   | 2.18                     | 0.42              |
| 1:A:342:LYS:HG3  | 1:A:343:HIS:N    | 2.34                     | 0.42              |
| 1:A:542:ILE:HA   | 1:A:545:PHE:CD2  | 2.54                     | 0.42              |
| 1:A:545:PHE:O    | 1:A:549:ILE:HG22 | 2.20                     | 0.42              |
| 1:B:13:LYS:HE3   | 1:B:13:LYS:HB2   | 1.87                     | 0.42              |
| 1:B:545:PHE:O    | 1:B:549:ILE:HG22 | 2.20                     | 0.42              |
| 1:C:39:ILE:HG23  | 1:C:40:LEU:HG    | 2.02                     | 0.42              |
| 1:C:552:ASN:HB3  | 1:C:1226:TYR:CE1 | 2.48                     | 0.42              |
| 1:C:950:TRP:CZ3  | 1:C:952:HIS:HA   | 2.54                     | 0.42              |
| 1:C:1127:ASP:OD1 | 1:C:1128:ILE:N   | 2.50                     | 0.42              |
| 1:D:120:PHE:CE1  | 1:D:159:TRP:CE3  | 3.05                     | 0.42              |
| 1:D:162:LEU:O    | 1:D:163:ASP:C    | 2.62                     | 0.42              |
| 1:D:517:THR:CG2  | 1:D:518:LEU:N    | 2.81                     | 0.42              |
| 1:D:542:ILE:HA   | 1:D:545:PHE:CD2  | 2.54                     | 0.42              |
| 1:D:901:HIS:O    | 1:D:902:ILE:HB   | 2.18                     | 0.42              |
| 1:E:39:ILE:HG23  | 1:E:40:LEU:HG    | 2.02                     | 0.42              |
| 1:E:413:LYS:CD   | 1:E:422:ILE:O    | 2.61                     | 0.42              |
| 1:E:481:PRO:O    | 1:E:485:THR:HG23 | 2.19                     | 0.42              |
| 1:E:950:TRP:CZ3  | 1:E:952:HIS:HA   | 2.54                     | 0.42              |
| 1:F:124:ASN:HA   | 2:F:1501:DTP:C2  | 2.49                     | 0.42              |
| 1:F:162:LEU:O    | 1:F:163:ASP:C    | 2.62                     | 0.42              |
| 1:F:535:TYR:O    | 1:F:538:LEU:HB3  | 2.19                     | 0.42              |
| 1:F:646:ARG:HG3  | 1:F:648:GLU:HG3  | 2.00                     | 0.42              |
| 1:G:915:TYR:CE2  | 1:G:916:LYS:HE3  | 2.54                     | 0.42              |
| 1:H:79:GLU:OE2   | 1:H:83:ILE:HD11  | 2.19                     | 0.42              |
| 1:H:248:GLN:CD   | 1:H:268:PHE:CZ   | 2.96                     | 0.42              |
| 1:H:317:LEU:O    | 1:H:318:THR:CB   | 2.61                     | 0.42              |
| 1:H:488:ARG:HG2  | 1:H:491:PHE:CG   | 2.55                     | 0.42              |
| 1:I:122:LYS:HG3  | 1:P:276:SER:HB2  | 2.00                     | 0.42              |
| 1:I:401:VAL:O    | 1:I:402:VAL:C    | 2.61                     | 0.42              |
| 1:I:453:PHE:CE2  | 1:I:460:PRO:HB3  | 2.49                     | 0.42              |
| 1:I:516:ASN:O    | 1:I:517:THR:CB   | 2.67                     | 0.42              |
| 1:J:147:VAL:HG12 | 1:J:281:THR:OG1  | 2.19                     | 0.42              |
| 1:J:428:GLU:OE1  | 1:J:429:LEU:HA   | 2.20                     | 0.42              |
| 1:J:481:PRO:O    | 1:J:485:THR:HG23 | 2.19                     | 0.42              |
| 1:J:950:TRP:CZ3  | 1:J:952:HIS:HA   | 2.54                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:120:PHE:CE1   | 1:K:159:TRP:CE3   | 3.05                     | 0.42              |
| 1:K:410:LEU:CD2   | 1:K:413:LYS:HA    | 2.49                     | 0.42              |
| 1:K:862:ILE:HG23  | 1:K:863:THR:H     | 1.84                     | 0.42              |
| 1:L:428:GLU:OE1   | 1:L:429:LEU:HA    | 2.20                     | 0.42              |
| 1:M:13:LYS:HE3    | 1:M:13:LYS:HB2    | 1.87                     | 0.42              |
| 1:M:488:ARG:HG2   | 1:M:491:PHE:CG    | 2.55                     | 0.42              |
| 1:M:545:PHE:O     | 1:M:549:ILE:HG22  | 2.20                     | 0.42              |
| 1:N:11:GLN:O      | 1:N:12:TYR:C      | 2.62                     | 0.42              |
| 1:N:11:GLN:O      | 1:N:14:ASP:N      | 2.46                     | 0.42              |
| 1:N:39:ILE:HG23   | 1:N:40:LEU:HG     | 2.02                     | 0.42              |
| 1:N:79:GLU:OE2    | 1:N:83:ILE:HD11   | 2.19                     | 0.42              |
| 1:N:264:LEU:HA    | 1:N:264:LEU:HD23  | 1.74                     | 0.42              |
| 1:O:39:ILE:HG23   | 1:O:40:LEU:HG     | 2.02                     | 0.42              |
| 1:O:248:GLN:CD    | 1:O:268:PHE:CZ    | 2.96                     | 0.42              |
| 1:O:463:LEU:CD2   | 1:O:467:PHE:HD2   | 2.31                     | 0.42              |
| 1:P:11:GLN:O      | 1:P:12:TYR:C      | 2.62                     | 0.42              |
| 1:P:410:LEU:CD2   | 1:P:413:LYS:HA    | 2.49                     | 0.42              |
| 1:P:553:LEU:HD23  | 1:P:553:LEU:HA    | 1.91                     | 0.42              |
| 1:A:11:GLN:O      | 1:A:12:TYR:C      | 2.62                     | 0.42              |
| 1:A:11:GLN:O      | 1:A:14:ASP:N      | 2.46                     | 0.42              |
| 1:A:147:VAL:HG12  | 1:A:281:THR:OG1   | 2.19                     | 0.42              |
| 1:C:200:LEU:HD12  | 1:C:200:LEU:HA    | 1.74                     | 0.42              |
| 1:C:554:ILE:C     | 1:C:556:SER:N     | 2.76                     | 0.42              |
| 1:C:1195:VAL:HG11 | 1:C:1241:PHE:CZ   | 2.54                     | 0.42              |
| 1:D:79:GLU:OE2    | 1:D:83:ILE:HD11   | 2.19                     | 0.42              |
| 1:D:453:PHE:CE1   | 1:D:460:PRO:HB3   | 2.51                     | 0.42              |
| 1:D:517:THR:HA    | 1:D:520:GLN:OE1   | 2.18                     | 0.42              |
| 1:D:523:PHE:HD1   | 1:D:527:TYR:CE2   | 2.28                     | 0.42              |
| 1:D:1158:TYR:HB3  | 1:D:1162:ILE:HG23 | 2.01                     | 0.42              |
| 1:E:504:ASP:CG    | 1:E:608:ASN:ND2   | 2.69                     | 0.42              |
| 1:E:507:ALA:O     | 1:E:608:ASN:CB    | 2.61                     | 0.42              |
| 1:F:39:ILE:HG23   | 1:F:40:LEU:HG     | 2.02                     | 0.42              |
| 1:F:769:ARG:NH1   | 1:F:771:PHE:HB2   | 2.35                     | 0.42              |
| 1:F:950:TRP:CZ3   | 1:F:952:HIS:HA    | 2.54                     | 0.42              |
| 1:G:11:GLN:O      | 1:G:12:TYR:C      | 2.62                     | 0.42              |
| 1:G:410:LEU:CD2   | 1:G:413:LYS:HA    | 2.49                     | 0.42              |
| 1:G:724:GLY:HA3   | 1:G:730:ILE:HD12  | 2.01                     | 0.42              |
| 1:G:902:ILE:HD13  | 1:G:930:HIS:CE1   | 2.43                     | 0.42              |
| 1:H:251:APK:O     | 1:H:253:TRP:HB3   | 2.20                     | 0.42              |
| 1:H:496:PHE:HE2   | 1:H:555:CYS:HG    | 1.66                     | 0.42              |
| 1:I:862:ILE:HG23  | 1:I:863:THR:H     | 1.83                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:39:ILE:HG23   | 1:J:40:LEU:HG     | 2.02                     | 0.42              |
| 1:J:504:ASP:CG    | 1:J:608:ASN:ND2   | 2.69                     | 0.42              |
| 1:K:453:PHE:CE1   | 1:K:460:PRO:HB3   | 2.51                     | 0.42              |
| 1:K:508:TRP:CD1   | 1:K:604:ASN:HB2   | 2.54                     | 0.42              |
| 1:K:517:THR:HA    | 1:K:520:GLN:OE1   | 2.19                     | 0.42              |
| 1:K:523:PHE:HD1   | 1:K:527:TYR:CE2   | 2.28                     | 0.42              |
| 1:K:1158:TYR:HB3  | 1:K:1162:ILE:HG23 | 2.01                     | 0.42              |
| 1:L:13:LYS:HE3    | 1:L:13:LYS:HB2    | 1.87                     | 0.42              |
| 1:L:39:ILE:HG23   | 1:L:40:LEU:HG     | 2.02                     | 0.42              |
| 1:L:508:TRP:CD1   | 1:L:604:ASN:HB2   | 2.54                     | 0.42              |
| 1:L:1195:VAL:HG11 | 1:L:1241:PHE:CZ   | 2.54                     | 0.42              |
| 1:N:481:PRO:O     | 1:N:485:THR:HG23  | 2.19                     | 0.42              |
| 1:N:545:PHE:O     | 1:N:549:ILE:HG22  | 2.20                     | 0.42              |
| 1:O:79:GLU:OE2    | 1:O:83:ILE:HD11   | 2.20                     | 0.42              |
| 1:O:488:ARG:HG2   | 1:O:491:PHE:CG    | 2.55                     | 0.42              |
| 1:P:915:TYR:CE2   | 1:P:916:LYS:HE3   | 2.54                     | 0.42              |
| 1:A:231:LEU:HD23  | 1:A:231:LEU:C     | 2.43                     | 0.42              |
| 1:A:276:SER:OG    | 1:H:122:LYS:HG3   | 2.20                     | 0.42              |
| 1:B:79:GLU:OE2    | 1:B:83:ILE:HD11   | 2.19                     | 0.42              |
| 1:B:989:SER:HB2   | 1:B:1027:ASN:HA   | 2.01                     | 0.42              |
| 1:C:115:ASN:O     | 1:D:257:ASN:ND2   | 2.52                     | 0.42              |
| 1:C:313:PRO:CG    | 1:C:338:TRP:CE2   | 2.94                     | 0.42              |
| 1:C:541:ALA:O     | 1:C:543:LEU:N     | 2.52                     | 0.42              |
| 1:D:39:ILE:HG23   | 1:D:40:LEU:HG     | 2.02                     | 0.42              |
| 1:D:186:CYS:C     | 1:D:249:ASN:HD21  | 2.27                     | 0.42              |
| 1:D:200:LEU:HA    | 1:D:200:LEU:HD12  | 1.74                     | 0.42              |
| 1:D:516:ASN:O     | 1:D:517:THR:CB    | 2.67                     | 0.42              |
| 1:E:119:VAL:HG23  | 1:E:120:PHE:N     | 2.28                     | 0.42              |
| 1:E:428:GLU:OE1   | 1:E:429:LEU:HA    | 2.20                     | 0.42              |
| 1:F:342:LYS:HG3   | 1:F:343:HIS:N     | 2.34                     | 0.42              |
| 1:G:412:GLU:CD    | 1:G:412:GLU:C     | 2.87                     | 0.42              |
| 1:H:141:LEU:HD12  | 1:H:141:LEU:O     | 2.19                     | 0.42              |
| 1:H:162:LEU:O     | 1:H:163:ASP:C     | 2.62                     | 0.42              |
| 1:H:283:ILE:HD13  | 1:H:283:ILE:HA    | 1.92                     | 0.42              |
| 1:H:412:GLU:C     | 1:H:412:GLU:CD    | 2.87                     | 0.42              |
| 1:I:39:ILE:HG23   | 1:I:40:LEU:HG     | 2.02                     | 0.42              |
| 1:I:251:APK:H8    | 1:I:251:APK:H2'   | 1.73                     | 0.42              |
| 1:I:410:LEU:CD2   | 1:I:413:LYS:HA    | 2.49                     | 0.42              |
| 1:I:517:THR:CG2   | 1:I:518:LEU:N     | 2.82                     | 0.42              |
| 1:J:79:GLU:OE2    | 1:J:83:ILE:HD11   | 2.19                     | 0.42              |
| 1:J:545:PHE:O     | 1:J:549:ILE:HG22  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:39:ILE:HG23  | 1:K:40:LEU:HG     | 2.02                     | 0.42              |
| 1:K:200:LEU:HA   | 1:K:200:LEU:HD12  | 1.74                     | 0.42              |
| 1:K:251:APK:O    | 1:K:253:TRP:HB3   | 2.20                     | 0.42              |
| 1:L:251:APK:H8   | 1:L:251:APK:H2'   | 1.74                     | 0.42              |
| 1:L:463:LEU:CD2  | 1:L:467:PHE:HD2   | 2.31                     | 0.42              |
| 1:L:549:ILE:HD12 | 1:L:550:GLU:H     | 1.85                     | 0.42              |
| 1:L:1177:TYR:HE2 | 1:M:916:LYS:CE    | 2.33                     | 0.42              |
| 1:M:79:GLU:OE2   | 1:M:83:ILE:HD11   | 2.19                     | 0.42              |
| 1:M:392:ASP:OD1  | 1:M:393:VAL:N     | 2.47                     | 0.42              |
| 1:M:523:PHE:HD1  | 1:M:527:TYR:CE2   | 2.28                     | 0.42              |
| 1:N:73:VAL:O     | 1:N:76:PHE:N      | 2.52                     | 0.42              |
| 1:N:231:LEU:HD23 | 1:N:231:LEU:C     | 2.43                     | 0.42              |
| 1:N:646:ARG:HG3  | 1:N:648:GLU:HG3   | 2.00                     | 0.42              |
| 1:O:90:SER:HG    | 1:O:91:PRO:HD3    | 1.85                     | 0.42              |
| 1:O:244:LEU:HD21 | 1:O:256:PHE:CD2   | 2.50                     | 0.42              |
| 1:O:470:HIS:O    | 1:O:473:HIS:N     | 2.53                     | 0.42              |
| 1:O:902:ILE:HD13 | 1:O:930:HIS:CE1   | 2.43                     | 0.42              |
| 1:P:481:PRO:O    | 1:P:485:THR:HG23  | 2.19                     | 0.42              |
| 1:P:799:ASN:O    | 1:P:800:THR:CG2   | 2.67                     | 0.42              |
| 1:A:73:VAL:O     | 1:A:76:PHE:N      | 2.52                     | 0.42              |
| 1:A:283:ILE:HD13 | 1:A:283:ILE:HA    | 1.92                     | 0.42              |
| 1:B:462:TYR:OH   | 1:B:494:PHE:CE1   | 2.72                     | 0.42              |
| 1:B:560:ASP:HA   | 1:B:592:ASN:ND2   | 2.29                     | 0.42              |
| 1:B:646:ARG:HG3  | 1:B:648:GLU:HG3   | 2.00                     | 0.42              |
| 1:B:833:LYS:HB3  | 1:B:834:TYR:H     | 1.63                     | 0.42              |
| 1:C:113:LEU:HA   | 1:C:113:LEU:HD12  | 1.83                     | 0.42              |
| 1:C:453:PHE:CE1  | 1:C:460:PRO:HB3   | 2.51                     | 0.42              |
| 1:C:463:LEU:CD2  | 1:C:467:PHE:HD2   | 2.31                     | 0.42              |
| 1:C:549:ILE:HD12 | 1:C:550:GLU:H     | 1.85                     | 0.42              |
| 1:D:59:LEU:HD21  | 1:D:63:TRP:CZ2    | 2.55                     | 0.42              |
| 1:D:251:APK:O    | 1:D:253:TRP:HB3   | 2.20                     | 0.42              |
| 1:D:903:GLU:HG3  | 1:D:904:CYS:H     | 1.84                     | 0.42              |
| 1:D:989:SER:HB2  | 1:D:1027:ASN:HA   | 2.01                     | 0.42              |
| 1:E:248:GLN:CD   | 1:E:268:PHE:CZ    | 2.96                     | 0.42              |
| 1:E:251:APK:H8   | 1:E:251:APK:H2'   | 1.74                     | 0.42              |
| 1:E:545:PHE:O    | 1:E:549:ILE:HG22  | 2.20                     | 0.42              |
| 1:E:989:SER:HB2  | 1:E:1027:ASN:HA   | 2.01                     | 0.42              |
| 1:E:1158:TYR:HB3 | 1:E:1162:ILE:HG23 | 2.01                     | 0.42              |
| 1:F:285:LEU:HA   | 1:F:285:LEU:HD23  | 1.74                     | 0.42              |
| 1:F:875:LEU:CG   | 1:F:911:PHE:CE2   | 2.86                     | 0.42              |
| 1:G:481:PRO:O    | 1:G:485:THR:HG23  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:799:ASN:O    | 1:G:800:THR:CG2  | 2.67                     | 0.42              |
| 1:H:91:PRO:O     | 1:H:94:THR:OG1   | 2.21                     | 0.42              |
| 1:H:470:HIS:O    | 1:H:473:HIS:N    | 2.53                     | 0.42              |
| 1:H:552:ASN:HB3  | 1:H:1226:TYR:CE1 | 2.48                     | 0.42              |
| 1:I:124:ASN:HA   | 2:I:1501:DTP:C2  | 2.49                     | 0.42              |
| 1:I:342:LYS:HG3  | 1:I:343:HIS:N    | 2.34                     | 0.42              |
| 1:I:488:ARG:HG2  | 1:I:491:PHE:CG   | 2.55                     | 0.42              |
| 1:I:545:PHE:CA   | 1:I:548:LYS:HB2  | 2.45                     | 0.42              |
| 1:I:769:ARG:NH1  | 1:I:771:PHE:HB2  | 2.35                     | 0.42              |
| 1:I:903:GLU:HG3  | 1:I:904:CYS:H    | 1.84                     | 0.42              |
| 1:J:119:VAL:HG23 | 1:J:120:PHE:N    | 2.28                     | 0.42              |
| 1:J:516:ASN:O    | 1:J:517:THR:CB   | 2.67                     | 0.42              |
| 1:J:545:PHE:CA   | 1:J:548:LYS:HB2  | 2.45                     | 0.42              |
| 1:J:989:SER:HB2  | 1:J:1027:ASN:HA  | 2.01                     | 0.42              |
| 1:K:59:LEU:HD21  | 1:K:63:TRP:CZ2   | 2.55                     | 0.42              |
| 1:K:222:HIS:CD2  | 1:L:198:LYS:HZ2  | 2.32                     | 0.42              |
| 1:K:516:ASN:O    | 1:K:517:THR:CB   | 2.67                     | 0.42              |
| 1:L:79:GLU:OE2   | 1:L:83:ILE:HD11  | 2.19                     | 0.42              |
| 1:M:276:SER:OG   | 1:N:122:LYS:HG3  | 2.19                     | 0.42              |
| 1:M:462:TYR:OH   | 1:M:494:PHE:CE1  | 2.72                     | 0.42              |
| 1:M:560:ASP:HA   | 1:M:592:ASN:ND2  | 2.29                     | 0.42              |
| 1:M:862:ILE:HG23 | 1:M:863:THR:H    | 1.83                     | 0.42              |
| 1:M:989:SER:HB2  | 1:M:1027:ASN:HA  | 2.01                     | 0.42              |
| 1:N:389:ILE:CD1  | 1:N:446:HIS:HE2  | 2.14                     | 0.42              |
| 1:N:463:LEU:CD2  | 1:N:467:PHE:HD2  | 2.31                     | 0.42              |
| 1:O:59:LEU:HD21  | 1:O:63:TRP:CZ2   | 2.55                     | 0.42              |
| 1:O:141:LEU:HD12 | 1:O:141:LEU:O    | 2.19                     | 0.42              |
| 1:O:251:APK:O    | 1:O:253:TRP:HB3  | 2.20                     | 0.42              |
| 1:O:412:GLU:CD   | 1:O:412:GLU:C    | 2.87                     | 0.42              |
| 1:P:724:GLY:HA3  | 1:P:730:ILE:HD12 | 2.01                     | 0.42              |
| 1:A:162:LEU:O    | 1:A:163:ASP:C    | 2.62                     | 0.42              |
| 1:A:406:HIS:ND1  | 1:A:414:GLN:HG3  | 2.35                     | 0.42              |
| 1:A:428:GLU:OE1  | 1:A:429:LEU:HA   | 2.20                     | 0.42              |
| 1:B:162:LEU:O    | 1:B:163:ASP:C    | 2.62                     | 0.42              |
| 1:B:347:ASP:CG   | 1:B:348:LYS:H    | 2.27                     | 0.42              |
| 1:B:523:PHE:HD1  | 1:B:527:TYR:CE2  | 2.28                     | 0.42              |
| 1:C:13:LYS:HE3   | 1:C:13:LYS:HB2   | 1.87                     | 0.42              |
| 1:C:406:HIS:ND1  | 1:C:414:GLN:HG3  | 2.35                     | 0.42              |
| 1:C:557:LYS:HD3  | 1:C:1223:GLN:NE2 | 2.35                     | 0.42              |
| 1:E:79:GLU:OE2   | 1:E:83:ILE:HD11  | 2.19                     | 0.42              |
| 1:E:113:LEU:HA   | 1:E:113:LEU:HD12 | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:516:ASN:O    | 1:E:517:THR:CB    | 2.67                     | 0.42              |
| 1:E:557:LYS:HD3  | 1:E:1223:GLN:NE2  | 2.35                     | 0.42              |
| 1:F:331:ILE:HD12 | 1:F:338:TRP:H     | 1.85                     | 0.42              |
| 1:F:401:VAL:O    | 1:F:402:VAL:C     | 2.61                     | 0.42              |
| 1:F:426:TYR:O    | 1:F:429:LEU:N     | 2.53                     | 0.42              |
| 1:F:470:HIS:O    | 1:F:473:HIS:N     | 2.53                     | 0.42              |
| 1:F:488:ARG:HG2  | 1:F:491:PHE:CG    | 2.55                     | 0.42              |
| 1:F:504:ASP:CG   | 1:F:608:ASN:ND2   | 2.69                     | 0.42              |
| 1:F:517:THR:CG2  | 1:F:518:LEU:N     | 2.81                     | 0.42              |
| 1:F:989:SER:HB2  | 1:F:1027:ASN:HA   | 2.01                     | 0.42              |
| 1:H:342:LYS:HG3  | 1:H:343:HIS:N     | 2.34                     | 0.42              |
| 1:H:557:LYS:HD3  | 1:H:1223:GLN:NE2  | 2.35                     | 0.42              |
| 1:I:59:LEU:HD21  | 1:I:63:TRP:CZ2    | 2.55                     | 0.42              |
| 1:I:504:ASP:CG   | 1:I:608:ASN:HD22  | 2.26                     | 0.42              |
| 1:I:989:SER:HB2  | 1:I:1027:ASN:HA   | 2.01                     | 0.42              |
| 1:J:248:GLN:CD   | 1:J:268:PHE:CZ    | 2.96                     | 0.42              |
| 1:J:1158:TYR:HB3 | 1:J:1162:ILE:HG23 | 2.01                     | 0.42              |
| 1:K:186:CYS:C    | 1:K:249:ASN:HD21  | 2.27                     | 0.42              |
| 1:K:903:GLU:HG3  | 1:K:904:CYS:H     | 1.84                     | 0.42              |
| 1:K:989:SER:HB2  | 1:K:1027:ASN:HA   | 2.01                     | 0.42              |
| 1:L:426:TYR:O    | 1:L:429:LEU:N     | 2.53                     | 0.42              |
| 1:L:453:PHE:CE1  | 1:L:460:PRO:HB3   | 2.51                     | 0.42              |
| 1:L:557:LYS:HD3  | 1:L:1223:GLN:NE2  | 2.35                     | 0.42              |
| 1:L:770:CYS:SG   | 1:L:781:VAL:HG13  | 2.60                     | 0.42              |
| 1:M:162:LEU:O    | 1:M:163:ASP:C     | 2.62                     | 0.42              |
| 1:M:208:THR:C    | 1:M:210:ARG:H     | 2.28                     | 0.42              |
| 1:N:59:LEU:HD21  | 1:N:63:TRP:CZ2    | 2.55                     | 0.42              |
| 1:N:162:LEU:O    | 1:N:163:ASP:C     | 2.62                     | 0.42              |
| 1:N:317:LEU:O    | 1:N:318:THR:CB    | 2.61                     | 0.42              |
| 1:N:406:HIS:ND1  | 1:N:414:GLN:HG3   | 2.35                     | 0.42              |
| 1:N:905:VAL:HG13 | 1:N:906:ASP:H     | 1.85                     | 0.42              |
| 1:O:162:LEU:O    | 1:O:163:ASP:C     | 2.62                     | 0.42              |
| 1:O:557:LYS:HD3  | 1:O:1223:GLN:NE2  | 2.35                     | 0.42              |
| 1:P:162:LEU:O    | 1:P:163:ASP:C     | 2.62                     | 0.42              |
| 1:P:412:GLU:C    | 1:P:412:GLU:CD    | 2.87                     | 0.42              |
| 1:P:453:PHE:CE1  | 1:P:460:PRO:HB3   | 2.51                     | 0.42              |
| 1:A:59:LEU:HD21  | 1:A:63:TRP:CZ2    | 2.55                     | 0.41              |
| 1:A:463:LEU:CD2  | 1:A:467:PHE:HD2   | 2.31                     | 0.41              |
| 1:A:905:VAL:HG13 | 1:A:906:ASP:H     | 1.85                     | 0.41              |
| 1:A:989:SER:HB2  | 1:A:1027:ASN:HA   | 2.01                     | 0.41              |
| 1:B:141:LEU:HD12 | 1:B:141:LEU:O     | 2.19                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:208:THR:C    | 1:B:210:ARG:H    | 2.28                     | 0.41              |
| 1:B:331:ILE:HD12 | 1:B:338:TRP:H    | 1.85                     | 0.41              |
| 1:B:426:TYR:O    | 1:B:429:LEU:N    | 2.53                     | 0.41              |
| 1:B:516:ASN:O    | 1:B:517:THR:CB   | 2.67                     | 0.41              |
| 1:B:862:ILE:HG23 | 1:B:863:THR:H    | 1.83                     | 0.41              |
| 1:C:79:GLU:OE2   | 1:C:83:ILE:HD11  | 2.20                     | 0.41              |
| 1:C:331:ILE:HD12 | 1:C:338:TRP:H    | 1.85                     | 0.41              |
| 1:D:406:HIS:ND1  | 1:D:414:GLN:HG3  | 2.35                     | 0.41              |
| 1:D:770:CYS:SG   | 1:D:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:E:331:ILE:HD12 | 1:E:338:TRP:H    | 1.85                     | 0.41              |
| 1:E:545:PHE:CA   | 1:E:548:LYS:HB2  | 2.45                     | 0.41              |
| 1:E:549:ILE:HD12 | 1:E:550:GLU:H    | 1.85                     | 0.41              |
| 1:E:799:ASN:O    | 1:E:800:THR:CG2  | 2.67                     | 0.41              |
| 1:F:59:LEU:HD21  | 1:F:63:TRP:CZ2   | 2.55                     | 0.41              |
| 1:F:468:TYR:HE1  | 1:F:497:LEU:HB2  | 1.85                     | 0.41              |
| 1:F:504:ASP:CG   | 1:F:608:ASN:HD22 | 2.26                     | 0.41              |
| 1:G:162:LEU:O    | 1:G:163:ASP:C    | 2.62                     | 0.41              |
| 1:G:462:TYR:OH   | 1:G:494:PHE:CE1  | 2.72                     | 0.41              |
| 1:G:516:ASN:O    | 1:G:517:THR:CB   | 2.67                     | 0.41              |
| 1:H:13:LYS:HB2   | 1:H:13:LYS:HE3   | 1.87                     | 0.41              |
| 1:H:59:LEU:HD21  | 1:H:63:TRP:CZ2   | 2.55                     | 0.41              |
| 1:I:244:LEU:HD21 | 1:I:256:PHE:CD2  | 2.50                     | 0.41              |
| 1:I:346:CYS:SG   | 1:I:350:THR:OG1  | 2.76                     | 0.41              |
| 1:I:389:ILE:CD1  | 1:I:446:HIS:HE2  | 2.14                     | 0.41              |
| 1:I:426:TYR:O    | 1:I:429:LEU:N    | 2.53                     | 0.41              |
| 1:I:549:ILE:HD12 | 1:I:550:GLU:H    | 1.85                     | 0.41              |
| 1:I:950:TRP:CZ3  | 1:I:952:HIS:HA   | 2.54                     | 0.41              |
| 1:J:331:ILE:HD12 | 1:J:338:TRP:H    | 1.85                     | 0.41              |
| 1:J:507:ALA:O    | 1:J:608:ASN:CB   | 2.61                     | 0.41              |
| 1:J:508:TRP:C    | 1:J:606:GLY:N    | 2.70                     | 0.41              |
| 1:J:549:ILE:HD12 | 1:J:550:GLU:H    | 1.85                     | 0.41              |
| 1:J:557:LYS:HD3  | 1:J:1223:GLN:NE2 | 2.35                     | 0.41              |
| 1:J:799:ASN:O    | 1:J:800:THR:CG2  | 2.67                     | 0.41              |
| 1:K:257:ASN:ND2  | 1:L:115:ASN:O    | 2.51                     | 0.41              |
| 1:K:406:HIS:ND1  | 1:K:414:GLN:HG3  | 2.35                     | 0.41              |
| 1:L:313:PRO:CG   | 1:L:338:TRP:CE2  | 2.94                     | 0.41              |
| 1:L:768:ILE:HG23 | 1:L:769:ARG:N    | 2.36                     | 0.41              |
| 1:L:989:SER:HB2  | 1:L:1027:ASN:HA  | 2.01                     | 0.41              |
| 1:M:141:LEU:HD12 | 1:M:141:LEU:O    | 2.19                     | 0.41              |
| 1:M:347:ASP:CG   | 1:M:348:LYS:H    | 2.27                     | 0.41              |
| 1:M:382:PRO:HA   | 1:M:419:THR:CG2  | 2.36                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:406:HIS:ND1  | 1:M:414:GLN:HG3   | 2.35                     | 0.41              |
| 1:M:516:ASN:O    | 1:M:517:THR:CB    | 2.67                     | 0.41              |
| 1:N:428:GLU:OE1  | 1:N:429:LEU:HA    | 2.20                     | 0.41              |
| 1:N:989:SER:HB2  | 1:N:1027:ASN:HA   | 2.01                     | 0.41              |
| 1:N:1026:PHE:HD1 | 1:N:1062:LYS:HG2  | 1.86                     | 0.41              |
| 1:N:1051:GLN:HG3 | 1:N:1053:PHE:CD2  | 2.55                     | 0.41              |
| 1:O:342:LYS:HG3  | 1:O:343:HIS:N     | 2.34                     | 0.41              |
| 1:P:462:TYR:OH   | 1:P:494:PHE:CE1   | 2.72                     | 0.41              |
| 1:A:264:LEU:HA   | 1:A:264:LEU:HD23  | 1.74                     | 0.41              |
| 1:A:317:LEU:O    | 1:A:318:THR:CB    | 2.61                     | 0.41              |
| 1:A:389:ILE:CD1  | 1:A:446:HIS:HE2   | 2.14                     | 0.41              |
| 1:A:410:LEU:CD2  | 1:A:413:LYS:HA    | 2.49                     | 0.41              |
| 1:A:541:ALA:O    | 1:A:543:LEU:N     | 2.52                     | 0.41              |
| 1:A:1026:PHE:HD1 | 1:A:1062:LYS:HG2  | 1.86                     | 0.41              |
| 1:A:1051:GLN:HG3 | 1:A:1053:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:1198:ASP:OD1 | 1:A:1199:ASP:N    | 2.50                     | 0.41              |
| 1:B:147:VAL:HG12 | 1:B:281:THR:OG1   | 2.19                     | 0.41              |
| 1:B:428:GLU:OE1  | 1:B:429:LEU:HA    | 2.20                     | 0.41              |
| 1:B:768:ILE:HG23 | 1:B:769:ARG:N     | 2.35                     | 0.41              |
| 1:C:132:LEU:HD12 | 1:C:132:LEU:HA    | 1.79                     | 0.41              |
| 1:C:426:TYR:O    | 1:C:429:LEU:N     | 2.53                     | 0.41              |
| 1:C:508:TRP:CD1  | 1:C:604:ASN:HB2   | 2.54                     | 0.41              |
| 1:C:724:GLY:HA3  | 1:C:730:ILE:HD12  | 2.01                     | 0.41              |
| 1:C:768:ILE:HG23 | 1:C:769:ARG:N     | 2.36                     | 0.41              |
| 1:C:770:CYS:SG   | 1:C:781:VAL:HG13  | 2.60                     | 0.41              |
| 1:C:989:SER:HB2  | 1:C:1027:ASN:HA   | 2.01                     | 0.41              |
| 1:C:1051:GLN:HG3 | 1:C:1053:PHE:CD2  | 2.55                     | 0.41              |
| 1:D:450:PRO:C    | 1:D:452:THR:N     | 2.78                     | 0.41              |
| 1:D:470:HIS:O    | 1:D:473:HIS:N     | 2.53                     | 0.41              |
| 1:D:560:ASP:O    | 1:D:564:ILE:HG12  | 2.21                     | 0.41              |
| 1:E:59:LEU:HD21  | 1:E:63:TRP:CZ2    | 2.55                     | 0.41              |
| 1:E:324:LEU:HA   | 1:E:324:LEU:HD12  | 1.61                     | 0.41              |
| 1:E:406:HIS:ND1  | 1:E:414:GLN:HG3   | 2.35                     | 0.41              |
| 1:F:244:LEU:HD21 | 1:F:256:PHE:CD2   | 2.50                     | 0.41              |
| 1:F:335:LEU:HD21 | 1:G:399:MET:HG3   | 2.01                     | 0.41              |
| 1:F:389:ILE:CD1  | 1:F:446:HIS:HE2   | 2.14                     | 0.41              |
| 1:F:1139:ASP:O   | 1:F:1140:SER:OG   | 2.35                     | 0.41              |
| 1:G:1158:TYR:HB3 | 1:G:1162:ILE:HG23 | 2.01                     | 0.41              |
| 1:H:244:LEU:HD21 | 1:H:256:PHE:CD2   | 2.51                     | 0.41              |
| 1:H:406:HIS:ND1  | 1:H:414:GLN:HG3   | 2.35                     | 0.41              |
| 1:H:770:CYS:SG   | 1:H:781:VAL:HG13  | 2.60                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:276:SER:OG   | 1:J:122:LYS:HG3   | 2.20                     | 0.41              |
| 1:I:412:GLU:C    | 1:I:412:GLU:CD    | 2.87                     | 0.41              |
| 1:I:468:TYR:HE1  | 1:I:497:LEU:HB2   | 1.85                     | 0.41              |
| 1:I:470:HIS:O    | 1:I:473:HIS:N     | 2.53                     | 0.41              |
| 1:J:406:HIS:ND1  | 1:J:414:GLN:HG3   | 2.35                     | 0.41              |
| 1:K:450:PRO:C    | 1:K:452:THR:N     | 2.78                     | 0.41              |
| 1:K:554:ILE:C    | 1:K:556:SER:N     | 2.76                     | 0.41              |
| 1:L:406:HIS:ND1  | 1:L:414:GLN:HG3   | 2.35                     | 0.41              |
| 1:L:519:GLN:HG2  | 1:L:523:PHE:HE2   | 1.84                     | 0.41              |
| 1:L:552:ASN:HB3  | 1:L:1226:TYR:CE1  | 2.48                     | 0.41              |
| 1:M:147:VAL:HG12 | 1:M:281:THR:OG1   | 2.19                     | 0.41              |
| 1:M:331:ILE:HD12 | 1:M:338:TRP:H     | 1.85                     | 0.41              |
| 1:M:426:TYR:O    | 1:M:429:LEU:N     | 2.53                     | 0.41              |
| 1:M:428:GLU:OE1  | 1:M:429:LEU:HA    | 2.20                     | 0.41              |
| 1:M:557:LYS:HD3  | 1:M:1223:GLN:NE2  | 2.35                     | 0.41              |
| 1:M:833:LYS:HB3  | 1:M:834:TYR:H     | 1.63                     | 0.41              |
| 1:N:1198:ASP:OD1 | 1:N:1199:ASP:N    | 2.50                     | 0.41              |
| 1:O:406:HIS:ND1  | 1:O:414:GLN:HG3   | 2.35                     | 0.41              |
| 1:P:516:ASN:O    | 1:P:517:THR:CB    | 2.67                     | 0.41              |
| 1:P:545:PHE:O    | 1:P:549:ILE:HG22  | 2.19                     | 0.41              |
| 1:P:1158:TYR:HB3 | 1:P:1162:ILE:HG23 | 2.01                     | 0.41              |
| 1:A:208:THR:C    | 1:A:210:ARG:H     | 2.28                     | 0.41              |
| 1:A:331:ILE:HD12 | 1:A:338:TRP:H     | 1.85                     | 0.41              |
| 1:A:412:GLU:C    | 1:A:412:GLU:CD    | 2.87                     | 0.41              |
| 1:A:549:ILE:HD12 | 1:A:550:GLU:H     | 1.85                     | 0.41              |
| 1:A:584:PHE:HB3  | 1:A:585:ASP:H     | 1.61                     | 0.41              |
| 1:A:769:ARG:NH1  | 1:A:771:PHE:HB2   | 2.35                     | 0.41              |
| 1:B:11:GLN:O     | 1:B:12:TYR:C      | 2.62                     | 0.41              |
| 1:B:312:LEU:CD2  | 1:B:313:PRO:CD    | 2.86                     | 0.41              |
| 1:B:406:HIS:ND1  | 1:B:414:GLN:HG3   | 2.35                     | 0.41              |
| 1:B:442:SER:C    | 1:B:446:HIS:CD2   | 2.92                     | 0.41              |
| 1:B:557:LYS:HD3  | 1:B:1223:GLN:NE2  | 2.35                     | 0.41              |
| 1:C:162:LEU:O    | 1:C:163:ASP:C     | 2.62                     | 0.41              |
| 1:C:208:THR:C    | 1:C:210:ARG:H     | 2.28                     | 0.41              |
| 1:C:285:LEU:HD23 | 1:C:285:LEU:HA    | 1.74                     | 0.41              |
| 1:D:13:LYS:HE3   | 1:D:13:LYS:HB2    | 1.87                     | 0.41              |
| 1:D:113:LEU:HD12 | 1:D:113:LEU:HA    | 1.83                     | 0.41              |
| 1:D:345:ASN:O    | 1:D:346:CYS:C     | 2.64                     | 0.41              |
| 1:D:426:TYR:O    | 1:D:429:LEU:N     | 2.53                     | 0.41              |
| 1:D:554:ILE:C    | 1:D:556:SER:N     | 2.76                     | 0.41              |
| 1:D:768:ILE:HG23 | 1:D:769:ARG:N     | 2.36                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:1075:SER:OG  | 1:D:1094:ASP:O   | 2.29                     | 0.41              |
| 1:E:508:TRP:C    | 1:E:606:GLY:N    | 2.70                     | 0.41              |
| 1:F:271:VAL:O    | 1:F:274:PHE:N    | 2.54                     | 0.41              |
| 1:F:412:GLU:C    | 1:F:412:GLU:CD   | 2.87                     | 0.41              |
| 1:F:549:ILE:HD12 | 1:F:550:GLU:H    | 1.85                     | 0.41              |
| 1:F:557:LYS:HD3  | 1:F:1223:GLN:NE2 | 2.35                     | 0.41              |
| 1:G:342:LYS:HG3  | 1:G:343:HIS:N    | 2.34                     | 0.41              |
| 1:G:545:PHE:O    | 1:G:549:ILE:HG22 | 2.19                     | 0.41              |
| 1:G:770:CYS:SG   | 1:G:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:H:113:LEU:HD12 | 1:H:113:LEU:HA   | 1.84                     | 0.41              |
| 1:H:271:VAL:O    | 1:H:274:PHE:N    | 2.54                     | 0.41              |
| 1:H:331:ILE:HD12 | 1:H:338:TRP:H    | 1.85                     | 0.41              |
| 1:I:79:GLU:OE2   | 1:I:83:ILE:HD11  | 2.19                     | 0.41              |
| 1:I:119:VAL:HG23 | 1:I:120:PHE:N    | 2.29                     | 0.41              |
| 1:I:770:CYS:SG   | 1:I:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:J:59:LEU:HD21  | 1:J:63:TRP:CZ2   | 2.55                     | 0.41              |
| 1:J:90:SER:HG    | 1:J:91:PRO:HD3   | 1.85                     | 0.41              |
| 1:J:346:CYS:SG   | 1:J:350:THR:OG1  | 2.76                     | 0.41              |
| 1:K:147:VAL:HG12 | 1:K:281:THR:OG1  | 2.19                     | 0.41              |
| 1:K:325:SER:O    | 1:K:329:GLU:N    | 2.42                     | 0.41              |
| 1:K:413:LYS:CD   | 1:K:422:ILE:O    | 2.60                     | 0.41              |
| 1:K:426:TYR:O    | 1:K:429:LEU:N    | 2.53                     | 0.41              |
| 1:K:470:HIS:O    | 1:K:473:HIS:N    | 2.53                     | 0.41              |
| 1:K:560:ASP:O    | 1:K:564:ILE:HG12 | 2.21                     | 0.41              |
| 1:K:768:ILE:HG23 | 1:K:769:ARG:N    | 2.36                     | 0.41              |
| 1:K:770:CYS:SG   | 1:K:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:K:1051:GLN:HG3 | 1:K:1053:PHE:CD2 | 2.55                     | 0.41              |
| 1:L:219:LEU:HD11 | 1:M:201:TYR:HE2  | 1.86                     | 0.41              |
| 1:L:504:ASP:CG   | 1:L:608:ASN:HD22 | 2.26                     | 0.41              |
| 1:L:554:ILE:C    | 1:L:556:SER:N    | 2.76                     | 0.41              |
| 1:L:724:GLY:HA3  | 1:L:730:ILE:HD12 | 2.01                     | 0.41              |
| 1:L:1051:GLN:HG3 | 1:L:1053:PHE:CD2 | 2.56                     | 0.41              |
| 1:M:11:GLN:O     | 1:M:12:TYR:C     | 2.62                     | 0.41              |
| 1:M:251:APK:O    | 1:M:253:TRP:HB3  | 2.20                     | 0.41              |
| 1:M:768:ILE:HG23 | 1:M:769:ARG:N    | 2.36                     | 0.41              |
| 1:M:770:CYS:SG   | 1:M:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:M:1026:PHE:HD1 | 1:M:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:N:410:LEU:CD2  | 1:N:413:LYS:HA   | 2.49                     | 0.41              |
| 1:N:412:GLU:C    | 1:N:412:GLU:CD   | 2.87                     | 0.41              |
| 1:N:426:TYR:O    | 1:N:429:LEU:N    | 2.53                     | 0.41              |
| 1:O:283:ILE:HD13 | 1:O:283:ILE:HA   | 1.92                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:331:ILE:HD12 | 1:O:338:TRP:H    | 1.85                     | 0.41              |
| 1:O:552:ASN:HB3  | 1:O:1226:TYR:CE1 | 2.48                     | 0.41              |
| 1:O:770:CYS:SG   | 1:O:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:P:342:LYS:HG3  | 1:P:343:HIS:N    | 2.34                     | 0.41              |
| 1:P:346:CYS:SG   | 1:P:350:THR:OG1  | 2.76                     | 0.41              |
| 1:P:446:HIS:C    | 1:P:448:ASN:H    | 2.29                     | 0.41              |
| 1:P:504:ASP:CG   | 1:P:608:ASN:ND2  | 2.69                     | 0.41              |
| 1:P:770:CYS:SG   | 1:P:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:A:488:ARG:HG2  | 1:A:491:PHE:CG   | 2.55                     | 0.41              |
| 1:B:102:MET:O    | 1:B:105:MET:N    | 2.46                     | 0.41              |
| 1:B:251:APK:O    | 1:B:253:TRP:HB3  | 2.20                     | 0.41              |
| 1:B:770:CYS:SG   | 1:B:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:B:915:TYR:CE2  | 1:B:916:LYS:HE3  | 2.53                     | 0.41              |
| 1:B:1026:PHE:HD1 | 1:B:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:C:413:LYS:CD   | 1:C:422:ILE:O    | 2.61                     | 0.41              |
| 1:C:450:PRO:C    | 1:C:452:THR:N    | 2.78                     | 0.41              |
| 1:C:504:ASP:CG   | 1:C:608:ASN:HD22 | 2.26                     | 0.41              |
| 1:D:147:VAL:HG12 | 1:D:281:THR:OG1  | 2.19                     | 0.41              |
| 1:D:325:SER:O    | 1:D:329:GLU:N    | 2.42                     | 0.41              |
| 1:D:413:LYS:CD   | 1:D:422:ILE:O    | 2.61                     | 0.41              |
| 1:D:1026:PHE:HD1 | 1:D:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:D:1051:GLN:HG3 | 1:D:1053:PHE:CD2 | 2.55                     | 0.41              |
| 1:F:545:PHE:CA   | 1:F:548:LYS:HB2  | 2.45                     | 0.41              |
| 1:F:833:LYS:HB3  | 1:F:834:TYR:H    | 1.63                     | 0.41              |
| 1:G:346:CYS:SG   | 1:G:350:THR:OG1  | 2.76                     | 0.41              |
| 1:G:1051:GLN:HG3 | 1:G:1053:PHE:CD2 | 2.55                     | 0.41              |
| 1:H:902:ILE:HD13 | 1:H:930:HIS:CE1  | 2.43                     | 0.41              |
| 1:H:1026:PHE:HD1 | 1:H:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:I:331:ILE:HD12 | 1:I:338:TRP:H    | 1.85                     | 0.41              |
| 1:I:428:GLU:OE1  | 1:I:429:LEU:HA   | 2.20                     | 0.41              |
| 1:I:511:SER:C    | 1:I:513:SER:N    | 2.60                     | 0.41              |
| 1:I:545:PHE:O    | 1:I:549:ILE:HG22 | 2.20                     | 0.41              |
| 1:I:1177:TYR:HE2 | 1:J:916:LYS:CE   | 2.32                     | 0.41              |
| 1:J:251:APK:O    | 1:J:253:TRP:HB3  | 2.20                     | 0.41              |
| 1:J:401:VAL:O    | 1:J:402:VAL:C    | 2.61                     | 0.41              |
| 1:K:13:LYS:HE3   | 1:K:13:LYS:HB2   | 1.87                     | 0.41              |
| 1:K:345:ASN:O    | 1:K:346:CYS:C    | 2.64                     | 0.41              |
| 1:K:724:GLY:HA3  | 1:K:730:ILE:HD12 | 2.01                     | 0.41              |
| 1:K:902:ILE:HD13 | 1:K:930:HIS:CE1  | 2.43                     | 0.41              |
| 1:K:1026:PHE:HD1 | 1:K:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:L:251:APK:O    | 1:L:253:TRP:HB3  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:331:ILE:HD12  | 1:L:338:TRP:H     | 1.86                     | 0.41              |
| 1:L:518:LEU:N     | 1:L:518:LEU:CD1   | 2.81                     | 0.41              |
| 1:L:1026:PHE:HD1  | 1:L:1062:LYS:HG2  | 1.85                     | 0.41              |
| 1:M:102:MET:O     | 1:M:105:MET:N     | 2.46                     | 0.41              |
| 1:M:113:LEU:HA    | 1:M:113:LEU:HD12  | 1.83                     | 0.41              |
| 1:M:442:SER:C     | 1:M:446:HIS:CD2   | 2.92                     | 0.41              |
| 1:M:902:ILE:HD13  | 1:M:930:HIS:CE1   | 2.43                     | 0.41              |
| 1:N:119:VAL:HG23  | 1:N:120:PHE:N     | 2.28                     | 0.41              |
| 1:N:208:THR:C     | 1:N:210:ARG:H     | 2.28                     | 0.41              |
| 1:N:283:ILE:HD13  | 1:N:283:ILE:HA    | 1.92                     | 0.41              |
| 1:N:331:ILE:HD12  | 1:N:338:TRP:H     | 1.85                     | 0.41              |
| 1:N:541:ALA:O     | 1:N:543:LEU:N     | 2.52                     | 0.41              |
| 1:N:549:ILE:HD12  | 1:N:550:GLU:H     | 1.85                     | 0.41              |
| 1:O:549:ILE:HD12  | 1:O:550:GLU:H     | 1.85                     | 0.41              |
| 1:O:915:TYR:CE2   | 1:O:916:LYS:HE3   | 2.53                     | 0.41              |
| 1:O:1026:PHE:HD1  | 1:O:1062:LYS:HG2  | 1.86                     | 0.41              |
| 1:P:59:LEU:HD21   | 1:P:63:TRP:CZ2    | 2.55                     | 0.41              |
| 1:P:142:ARG:H     | 1:P:142:ARG:HG2   | 1.73                     | 0.41              |
| 1:P:251:APK:O     | 1:P:253:TRP:HB3   | 2.20                     | 0.41              |
| 1:P:905:VAL:HG13  | 1:P:906:ASP:H     | 1.85                     | 0.41              |
| 1:A:426:TYR:O     | 1:A:429:LEU:N     | 2.53                     | 0.41              |
| 1:A:768:ILE:HG23  | 1:A:769:ARG:N     | 2.36                     | 0.41              |
| 1:B:285:LEU:HD23  | 1:B:285:LEU:HA    | 1.74                     | 0.41              |
| 1:B:382:PRO:HA    | 1:B:419:THR:CG2   | 2.36                     | 0.41              |
| 1:B:451:LYS:CD    | 1:B:486:LEU:HD21  | 2.33                     | 0.41              |
| 1:B:508:TRP:CD1   | 1:B:604:ASN:HB2   | 2.54                     | 0.41              |
| 1:C:251:APK:O     | 1:C:253:TRP:HB3   | 2.20                     | 0.41              |
| 1:C:345:ASN:O     | 1:C:346:CYS:C     | 2.64                     | 0.41              |
| 1:C:519:GLN:HG2   | 1:C:523:PHE:HE2   | 1.84                     | 0.41              |
| 1:D:468:TYR:HE1   | 1:D:497:LEU:HB2   | 1.85                     | 0.41              |
| 1:D:724:GLY:HA3   | 1:D:730:ILE:HD12  | 2.01                     | 0.41              |
| 1:D:829:LEU:HD21  | 1:D:874:LEU:HD22  | 2.03                     | 0.41              |
| 1:E:446:HIS:C     | 1:E:448:ASN:H     | 2.29                     | 0.41              |
| 1:E:768:ILE:HG23  | 1:E:769:ARG:N     | 2.35                     | 0.41              |
| 1:E:1009:ILE:HG13 | 1:E:1011:PRO:HD3  | 2.03                     | 0.41              |
| 1:F:428:GLU:OE1   | 1:F:429:LEU:HA    | 2.20                     | 0.41              |
| 1:F:545:PHE:O     | 1:F:549:ILE:HG22  | 2.19                     | 0.41              |
| 1:F:603:ILE:HD11  | 1:F:635:VAL:HG11  | 2.03                     | 0.41              |
| 1:F:770:CYS:SG    | 1:F:781:VAL:HG13  | 2.61                     | 0.41              |
| 1:F:1158:TYR:HB3  | 1:F:1162:ILE:HG23 | 2.01                     | 0.41              |
| 1:G:59:LEU:HD21   | 1:G:63:TRP:CZ2    | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:251:APK:O     | 1:G:253:TRP:HB3  | 2.20                     | 0.41              |
| 1:G:446:HIS:C     | 1:G:448:ASN:H    | 2.29                     | 0.41              |
| 1:G:504:ASP:CG    | 1:G:608:ASN:ND2  | 2.69                     | 0.41              |
| 1:G:507:ALA:O     | 1:G:608:ASN:CB   | 2.61                     | 0.41              |
| 1:H:915:TYR:CE2   | 1:H:916:LYS:HE3  | 2.53                     | 0.41              |
| 1:I:557:LYS:HD3   | 1:I:1223:GLN:NE2 | 2.35                     | 0.41              |
| 1:J:157:LYS:H     | 1:J:157:LYS:HG2  | 1.68                     | 0.41              |
| 1:J:251:APK:H8    | 1:J:251:APK:H2'  | 1.74                     | 0.41              |
| 1:J:1009:ILE:HG13 | 1:J:1011:PRO:HD3 | 2.03                     | 0.41              |
| 1:K:468:TYR:HE1   | 1:K:497:LEU:HB2  | 1.85                     | 0.41              |
| 1:K:519:GLN:HG2   | 1:K:523:PHE:HE2  | 1.84                     | 0.41              |
| 1:K:829:LEU:HD21  | 1:K:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:L:208:THR:C     | 1:L:210:ARG:H    | 2.29                     | 0.41              |
| 1:L:345:ASN:O     | 1:L:346:CYS:C    | 2.64                     | 0.41              |
| 1:L:450:PRO:C     | 1:L:452:THR:N    | 2.78                     | 0.41              |
| 1:M:312:LEU:CD2   | 1:M:313:PRO:CD   | 2.86                     | 0.41              |
| 1:M:508:TRP:CD1   | 1:M:604:ASN:HB2  | 2.54                     | 0.41              |
| 1:M:519:GLN:HG2   | 1:M:523:PHE:HE2  | 1.84                     | 0.41              |
| 1:M:915:TYR:CE2   | 1:M:916:LYS:HE3  | 2.53                     | 0.41              |
| 1:N:768:ILE:HG23  | 1:N:769:ARG:N    | 2.36                     | 0.41              |
| 1:N:769:ARG:NH1   | 1:N:771:PHE:HB2  | 2.35                     | 0.41              |
| 1:O:271:VAL:O     | 1:O:274:PHE:N    | 2.54                     | 0.41              |
| 1:O:413:LYS:CD    | 1:O:422:ILE:O    | 2.61                     | 0.41              |
| 1:O:862:ILE:HG23  | 1:O:863:THR:H    | 1.83                     | 0.41              |
| 1:P:406:HIS:ND1   | 1:P:414:GLN:HG3  | 2.35                     | 0.41              |
| 1:P:1051:GLN:HG3  | 1:P:1053:PHE:CD2 | 2.55                     | 0.41              |
| 1:A:15:ILE:HD12   | 1:A:15:ILE:HA    | 1.92                     | 0.41              |
| 1:A:557:LYS:HD3   | 1:A:1223:GLN:NE2 | 2.35                     | 0.41              |
| 1:A:829:LEU:HD21  | 1:A:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:833:LYS:HB3   | 1:A:834:TYR:H    | 1.63                     | 0.41              |
| 1:B:519:GLN:HG2   | 1:B:523:PHE:HE2  | 1.84                     | 0.41              |
| 1:B:902:ILE:HD13  | 1:B:930:HIS:CE1  | 2.43                     | 0.41              |
| 1:C:122:LYS:O     | 1:C:303:LYS:NZ   | 2.38                     | 0.41              |
| 1:C:560:ASP:O     | 1:C:564:ILE:HG12 | 2.21                     | 0.41              |
| 1:C:829:LEU:HD21  | 1:C:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:C:905:VAL:HG13  | 1:C:906:ASP:H    | 1.85                     | 0.41              |
| 1:D:324:LEU:HD12  | 1:D:324:LEU:HA   | 1.61                     | 0.41              |
| 1:D:1195:VAL:HG11 | 1:D:1241:PHE:CZ  | 2.54                     | 0.41              |
| 1:E:346:CYS:SG    | 1:E:350:THR:OG1  | 2.76                     | 0.41              |
| 1:F:79:GLU:OE2    | 1:F:83:ILE:HD11  | 2.20                     | 0.41              |
| 1:F:346:CYS:SG    | 1:F:350:THR:OG1  | 2.76                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:724:GLY:HA3   | 1:F:730:ILE:HD12 | 2.01                     | 0.41              |
| 1:G:198:LYS:NZ    | 1:H:222:HIS:CG   | 2.88                     | 0.41              |
| 1:G:406:HIS:ND1   | 1:G:414:GLN:HG3  | 2.35                     | 0.41              |
| 1:G:905:VAL:HG13  | 1:G:906:ASP:H    | 1.86                     | 0.41              |
| 1:H:468:TYR:HE1   | 1:H:497:LEU:HB2  | 1.85                     | 0.41              |
| 1:H:549:ILE:HD12  | 1:H:550:GLU:H    | 1.85                     | 0.41              |
| 1:H:833:LYS:HB3   | 1:H:834:TYR:H    | 1.63                     | 0.41              |
| 1:H:862:ILE:HG23  | 1:H:863:THR:H    | 1.83                     | 0.41              |
| 1:I:142:ARG:HH22  | 1:J:14:ASP:CG    | 2.28                     | 0.41              |
| 1:I:271:VAL:O     | 1:I:274:PHE:N    | 2.54                     | 0.41              |
| 1:I:406:HIS:ND1   | 1:I:414:GLN:HG3  | 2.35                     | 0.41              |
| 1:I:724:GLY:HA3   | 1:I:730:ILE:HD12 | 2.01                     | 0.41              |
| 1:I:1009:ILE:HG13 | 1:I:1011:PRO:HD3 | 2.03                     | 0.41              |
| 1:I:1026:PHE:HD1  | 1:I:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:J:426:TYR:O     | 1:J:429:LEU:N    | 2.53                     | 0.41              |
| 1:J:468:TYR:HE1   | 1:J:497:LEU:HB2  | 1.85                     | 0.41              |
| 1:J:768:ILE:HG23  | 1:J:769:ARG:N    | 2.35                     | 0.41              |
| 1:K:147:VAL:HG23  | 1:K:263:LEU:HG   | 2.03                     | 0.41              |
| 1:L:516:ASN:O     | 1:L:517:THR:CB   | 2.67                     | 0.41              |
| 1:L:560:ASP:O     | 1:L:564:ILE:HG12 | 2.21                     | 0.41              |
| 1:M:142:ARG:HH22  | 1:N:14:ASP:CG    | 2.28                     | 0.41              |
| 1:M:147:VAL:HG23  | 1:M:263:LEU:HG   | 2.03                     | 0.41              |
| 1:N:829:LEU:HD21  | 1:N:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:O:446:HIS:C     | 1:O:448:ASN:H    | 2.29                     | 0.41              |
| 1:O:468:TYR:HE1   | 1:O:497:LEU:HB2  | 1.85                     | 0.41              |
| 1:A:470:HIS:O     | 1:A:473:HIS:N    | 2.53                     | 0.41              |
| 1:B:147:VAL:HG23  | 1:B:263:LEU:HG   | 2.03                     | 0.41              |
| 1:B:271:VAL:O     | 1:B:274:PHE:N    | 2.54                     | 0.41              |
| 1:C:186:CYS:C     | 1:C:249:ASN:HD21 | 2.27                     | 0.41              |
| 1:C:516:ASN:O     | 1:C:517:THR:CB   | 2.67                     | 0.41              |
| 1:D:20:GLU:O      | 1:D:21:ASP:C     | 2.63                     | 0.41              |
| 1:D:147:VAL:HG23  | 1:D:263:LEU:HG   | 2.03                     | 0.41              |
| 1:D:1009:ILE:HG13 | 1:D:1011:PRO:HD3 | 2.03                     | 0.41              |
| 1:E:153:LEU:CD2   | 1:E:267:ARG:HD3  | 2.51                     | 0.41              |
| 1:E:251:APK:O     | 1:E:253:TRP:HB3  | 2.20                     | 0.41              |
| 1:E:829:LEU:HD21  | 1:E:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:E:1198:ASP:OD1  | 1:E:1199:ASP:N   | 2.50                     | 0.41              |
| 1:F:251:APK:O     | 1:F:253:TRP:HB3  | 2.20                     | 0.41              |
| 1:F:450:PRO:C     | 1:F:452:THR:N    | 2.78                     | 0.41              |
| 1:F:768:ILE:HG23  | 1:F:769:ARG:N    | 2.35                     | 0.41              |
| 1:F:1026:PHE:HD1  | 1:F:1062:LYS:HG2 | 1.86                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:488:ARG:HG2  | 1:G:491:PHE:CG    | 2.55                     | 0.41              |
| 1:G:557:LYS:HD3  | 1:G:1223:GLN:NE2  | 2.35                     | 0.41              |
| 1:I:603:ILE:HD11 | 1:I:635:VAL:HG11  | 2.03                     | 0.41              |
| 1:I:1158:TYR:HB3 | 1:I:1162:ILE:HG23 | 2.01                     | 0.41              |
| 1:J:153:LEU:CD2  | 1:J:267:ARG:HD3   | 2.51                     | 0.41              |
| 1:J:446:HIS:C    | 1:J:448:ASN:H     | 2.29                     | 0.41              |
| 1:J:453:PHE:CE1  | 1:J:460:PRO:HB3   | 2.51                     | 0.41              |
| 1:J:829:LEU:HD21 | 1:J:874:LEU:HD22  | 2.03                     | 0.41              |
| 1:K:20:GLU:O     | 1:K:21:ASP:C      | 2.63                     | 0.41              |
| 1:K:208:THR:C    | 1:K:210:ARG:H     | 2.28                     | 0.41              |
| 1:L:11:GLN:O     | 1:L:12:TYR:C      | 2.62                     | 0.41              |
| 1:L:162:LEU:O    | 1:L:163:ASP:C     | 2.62                     | 0.41              |
| 1:L:314:ARG:C    | 1:L:315:GLU:CG    | 2.82                     | 0.41              |
| 1:L:488:ARG:HG2  | 1:L:491:PHE:CG    | 2.55                     | 0.41              |
| 1:L:829:LEU:HD21 | 1:L:874:LEU:HD22  | 2.03                     | 0.41              |
| 1:L:905:VAL:HG13 | 1:L:906:ASP:H     | 1.85                     | 0.41              |
| 1:M:271:VAL:O    | 1:M:274:PHE:N     | 2.54                     | 0.41              |
| 1:N:470:HIS:O    | 1:N:473:HIS:N     | 2.53                     | 0.41              |
| 1:N:488:ARG:HG2  | 1:N:491:PHE:CG    | 2.55                     | 0.41              |
| 1:N:770:CYS:SG   | 1:N:781:VAL:HG13  | 2.60                     | 0.41              |
| 1:O:426:TYR:O    | 1:O:429:LEU:N     | 2.53                     | 0.41              |
| 1:O:428:GLU:OE1  | 1:O:429:LEU:HA    | 2.20                     | 0.41              |
| 1:O:504:ASP:CG   | 1:O:608:ASN:HD22  | 2.26                     | 0.41              |
| 1:P:507:ALA:O    | 1:P:608:ASN:CB    | 2.61                     | 0.41              |
| 1:P:557:LYS:HD3  | 1:P:1223:GLN:NE2  | 2.35                     | 0.41              |
| 1:A:119:VAL:HG23 | 1:A:120:PHE:N     | 2.29                     | 0.41              |
| 1:A:147:VAL:HG23 | 1:A:263:LEU:HG    | 2.03                     | 0.41              |
| 1:A:770:CYS:SG   | 1:A:781:VAL:HG13  | 2.60                     | 0.41              |
| 1:B:113:LEU:HA   | 1:B:113:LEU:HD12  | 1.83                     | 0.41              |
| 1:B:554:ILE:C    | 1:B:556:SER:N     | 2.76                     | 0.41              |
| 1:C:322:ARG:C    | 1:C:324:LEU:N     | 2.79                     | 0.41              |
| 1:C:488:ARG:HG2  | 1:C:491:PHE:CG    | 2.55                     | 0.41              |
| 1:C:587:ARG:CG   | 1:C:588:VAL:H     | 2.33                     | 0.41              |
| 1:C:1026:PHE:HD1 | 1:C:1062:LYS:HG2  | 1.86                     | 0.41              |
| 1:D:208:THR:C    | 1:D:210:ARG:H     | 2.28                     | 0.41              |
| 1:D:519:GLN:HG2  | 1:D:523:PHE:HE2   | 1.85                     | 0.41              |
| 1:E:426:TYR:O    | 1:E:429:LEU:N     | 2.53                     | 0.41              |
| 1:E:468:TYR:HE1  | 1:E:497:LEU:HB2   | 1.85                     | 0.41              |
| 1:F:119:VAL:HG23 | 1:F:120:PHE:N     | 2.28                     | 0.41              |
| 1:G:271:VAL:O    | 1:G:274:PHE:N     | 2.54                     | 0.41              |
| 1:G:426:TYR:O    | 1:G:429:LEU:N     | 2.53                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:H:208:THR:C     | 1:H:210:ARG:H    | 2.28                     | 0.41              |
| 1:H:413:LYS:CD    | 1:H:422:ILE:O    | 2.61                     | 0.41              |
| 1:H:426:TYR:O     | 1:H:429:LEU:N    | 2.53                     | 0.41              |
| 1:H:446:HIS:C     | 1:H:448:ASN:H    | 2.29                     | 0.41              |
| 1:H:905:VAL:HG13  | 1:H:906:ASP:H    | 1.85                     | 0.41              |
| 1:I:153:LEU:CD2   | 1:I:267:ARG:HD3  | 2.51                     | 0.41              |
| 1:I:285:LEU:HA    | 1:I:285:LEU:HD23 | 1.74                     | 0.41              |
| 1:I:450:PRO:C     | 1:I:452:THR:N    | 2.78                     | 0.41              |
| 1:I:616:LEU:HG    | 1:I:618:ASN:H    | 1.86                     | 0.41              |
| 1:J:324:LEU:HA    | 1:J:324:LEU:HD12 | 1.61                     | 0.41              |
| 1:J:488:ARG:HG2   | 1:J:491:PHE:CG   | 2.55                     | 0.41              |
| 1:J:1177:TYR:CE2  | 1:K:916:LYS:HE2  | 2.49                     | 0.41              |
| 1:K:153:LEU:CD2   | 1:K:267:ARG:HD3  | 2.51                     | 0.41              |
| 1:K:428:GLU:OE1   | 1:K:429:LEU:N    | 2.54                     | 0.41              |
| 1:K:1009:ILE:HG13 | 1:K:1011:PRO:HD3 | 2.03                     | 0.41              |
| 1:K:1195:VAL:HG11 | 1:K:1241:PHE:CZ  | 2.54                     | 0.41              |
| 1:L:20:GLU:O      | 1:L:21:ASP:C     | 2.63                     | 0.41              |
| 1:L:1198:ASP:OD1  | 1:L:1199:ASP:N   | 2.50                     | 0.41              |
| 1:M:451:LYS:CD    | 1:M:486:LEU:HD21 | 2.33                     | 0.41              |
| 1:M:554:ILE:C     | 1:M:556:SER:N    | 2.76                     | 0.41              |
| 1:N:142:ARG:HH22  | 1:O:14:ASP:CG    | 2.28                     | 0.41              |
| 1:N:147:VAL:HG23  | 1:N:263:LEU:HG   | 2.03                     | 0.41              |
| 1:N:557:LYS:HD3   | 1:N:1223:GLN:NE2 | 2.35                     | 0.41              |
| 1:O:113:LEU:HD12  | 1:O:113:LEU:HA   | 1.83                     | 0.41              |
| 1:O:768:ILE:HG23  | 1:O:769:ARG:N    | 2.36                     | 0.41              |
| 1:O:829:LEU:HD21  | 1:O:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:P:401:VAL:O     | 1:P:402:VAL:C    | 2.61                     | 0.41              |
| 1:P:426:TYR:O     | 1:P:429:LEU:N    | 2.53                     | 0.41              |
| 1:P:428:GLU:OE1   | 1:P:429:LEU:HA   | 2.20                     | 0.41              |
| 1:P:488:ARG:HG2   | 1:P:491:PHE:CG   | 2.55                     | 0.41              |
| 1:A:231:LEU:O     | 1:A:234:SER:OG   | 2.26                     | 0.41              |
| 1:A:462:TYR:CZ    | 1:A:494:PHE:CZ   | 3.03                     | 0.41              |
| 1:A:519:GLN:HG2   | 1:A:523:PHE:HE2  | 1.84                     | 0.41              |
| 1:B:59:LEU:HD21   | 1:B:63:TRP:CZ2   | 2.55                     | 0.41              |
| 1:B:207:TRP:CZ2   | 1:B:224:ILE:HD11 | 2.56                     | 0.41              |
| 1:B:345:ASN:O     | 1:B:346:CYS:C    | 2.64                     | 0.41              |
| 1:B:361:GLU:O     | 1:B:365:TYR:N    | 2.53                     | 0.41              |
| 1:B:560:ASP:O     | 1:B:564:ILE:HG12 | 2.21                     | 0.41              |
| 1:B:829:LEU:HD21  | 1:B:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:B:905:VAL:HG13  | 1:B:906:ASP:H    | 1.85                     | 0.41              |
| 1:B:1051:GLN:HG3  | 1:B:1053:PHE:CD2 | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1198:ASP:OD1  | 1:B:1199:ASP:N   | 2.50                     | 0.41              |
| 1:C:20:GLU:O      | 1:C:21:ASP:C     | 2.63                     | 0.41              |
| 1:C:59:LEU:HD21   | 1:C:63:TRP:CZ2   | 2.55                     | 0.41              |
| 1:C:147:VAL:HG23  | 1:C:263:LEU:HG   | 2.03                     | 0.41              |
| 1:C:207:TRP:CZ2   | 1:C:224:ILE:HD11 | 2.56                     | 0.41              |
| 1:C:462:TYR:OH    | 1:C:494:PHE:CE1  | 2.72                     | 0.41              |
| 1:D:153:LEU:CD2   | 1:D:267:ARG:HD3  | 2.51                     | 0.41              |
| 1:D:428:GLU:OE1   | 1:D:429:LEU:N    | 2.54                     | 0.41              |
| 1:D:603:ILE:HD11  | 1:D:635:VAL:HG11 | 2.03                     | 0.41              |
| 1:D:616:LEU:HG    | 1:D:618:ASN:H    | 1.86                     | 0.41              |
| 1:D:902:ILE:HD13  | 1:D:930:HIS:CE1  | 2.43                     | 0.41              |
| 1:D:1198:ASP:OD1  | 1:D:1199:ASP:N   | 2.50                     | 0.41              |
| 1:E:20:GLU:O      | 1:E:21:ASP:C     | 2.63                     | 0.41              |
| 1:E:147:VAL:HG23  | 1:E:263:LEU:HG   | 2.03                     | 0.41              |
| 1:E:157:LYS:H     | 1:E:157:LYS:HG2  | 1.68                     | 0.41              |
| 1:E:208:THR:C     | 1:E:210:ARG:H    | 2.28                     | 0.41              |
| 1:E:447:TYR:OH    | 1:E:486:LEU:CD2  | 2.67                     | 0.41              |
| 1:E:453:PHE:CE1   | 1:E:460:PRO:HB3  | 2.51                     | 0.41              |
| 1:E:488:ARG:HG2   | 1:E:491:PHE:CG   | 2.55                     | 0.41              |
| 1:E:724:GLY:HA3   | 1:E:730:ILE:HD12 | 2.01                     | 0.41              |
| 1:E:915:TYR:CE2   | 1:E:916:LYS:HE3  | 2.54                     | 0.41              |
| 1:E:1051:GLN:HG3  | 1:E:1053:PHE:CD2 | 2.56                     | 0.41              |
| 1:F:14:ASP:CG     | 1:G:142:ARG:NH2  | 2.77                     | 0.41              |
| 1:F:153:LEU:CD2   | 1:F:267:ARG:HD3  | 2.51                     | 0.41              |
| 1:F:324:LEU:HD12  | 1:F:324:LEU:HA   | 1.61                     | 0.41              |
| 1:F:406:HIS:ND1   | 1:F:414:GLN:HG3  | 2.35                     | 0.41              |
| 1:F:428:GLU:OE1   | 1:F:429:LEU:N    | 2.54                     | 0.41              |
| 1:F:511:SER:C     | 1:F:513:SER:N    | 2.60                     | 0.41              |
| 1:F:616:LEU:HG    | 1:F:618:ASN:H    | 1.86                     | 0.41              |
| 1:F:1009:ILE:HG13 | 1:F:1011:PRO:HD3 | 2.03                     | 0.41              |
| 1:G:187:ASN:CA    | 1:G:249:ASN:HD21 | 2.27                     | 0.41              |
| 1:G:301:LEU:CD2   | 1:G:313:PRO:CG   | 2.87                     | 0.41              |
| 1:G:401:VAL:O     | 1:G:402:VAL:C    | 2.61                     | 0.41              |
| 1:G:428:GLU:OE1   | 1:G:429:LEU:N    | 2.54                     | 0.41              |
| 1:G:428:GLU:OE1   | 1:G:429:LEU:HA   | 2.20                     | 0.41              |
| 1:G:468:TYR:HE1   | 1:G:497:LEU:HB2  | 1.85                     | 0.41              |
| 1:G:768:ILE:HG23  | 1:G:769:ARG:N    | 2.36                     | 0.41              |
| 1:H:428:GLU:OE1   | 1:H:429:LEU:HA   | 2.20                     | 0.41              |
| 1:H:428:GLU:OE1   | 1:H:429:LEU:N    | 2.54                     | 0.41              |
| 1:H:504:ASP:CG    | 1:H:608:ASN:HD22 | 2.26                     | 0.41              |
| 1:H:511:SER:HA    | 1:H:514:ILE:H    | 1.86                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:H:768:ILE:HG23  | 1:H:769:ARG:N    | 2.36                     | 0.41              |
| 1:H:829:LEU:HD21  | 1:H:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:H:1051:GLN:HG3  | 1:H:1053:PHE:CD2 | 2.55                     | 0.41              |
| 1:H:1195:VAL:HG11 | 1:H:1241:PHE:CZ  | 2.54                     | 0.41              |
| 1:I:251:APK:O     | 1:I:253:TRP:HB3  | 2.20                     | 0.41              |
| 1:I:768:ILE:HG23  | 1:I:769:ARG:N    | 2.36                     | 0.41              |
| 1:I:1051:GLN:HG3  | 1:I:1053:PHE:CD2 | 2.55                     | 0.41              |
| 1:J:20:GLU:O      | 1:J:21:ASP:C     | 2.63                     | 0.41              |
| 1:J:147:VAL:HG23  | 1:J:263:LEU:HG   | 2.03                     | 0.41              |
| 1:J:447:TYR:OH    | 1:J:486:LEU:CD2  | 2.67                     | 0.41              |
| 1:J:770:CYS:SG    | 1:J:781:VAL:HG13 | 2.60                     | 0.41              |
| 1:J:915:TYR:CE2   | 1:J:916:LYS:HE3  | 2.53                     | 0.41              |
| 1:J:1051:GLN:HG3  | 1:J:1053:PHE:CD2 | 2.55                     | 0.41              |
| 1:K:89:MET:O      | 1:K:92:ILE:HG22  | 2.21                     | 0.41              |
| 1:K:113:LEU:HD12  | 1:K:113:LEU:HA   | 1.83                     | 0.41              |
| 1:K:324:LEU:HD12  | 1:K:324:LEU:HA   | 1.61                     | 0.41              |
| 1:K:346:CYS:SG    | 1:K:350:THR:OG1  | 2.76                     | 0.41              |
| 1:K:549:ILE:HD12  | 1:K:550:GLU:H    | 1.85                     | 0.41              |
| 1:K:616:LEU:HG    | 1:K:618:ASN:H    | 1.86                     | 0.41              |
| 1:K:1198:ASP:OD1  | 1:K:1199:ASP:N   | 2.50                     | 0.41              |
| 1:L:147:VAL:HG23  | 1:L:263:LEU:HG   | 2.03                     | 0.41              |
| 1:L:186:CYS:C     | 1:L:249:ASN:HD21 | 2.27                     | 0.41              |
| 1:L:207:TRP:CZ2   | 1:L:224:ILE:HD11 | 2.56                     | 0.41              |
| 1:L:312:LEU:CD2   | 1:L:313:PRO:CD   | 2.86                     | 0.41              |
| 1:L:322:ARG:C     | 1:L:324:LEU:N    | 2.79                     | 0.41              |
| 1:L:428:GLU:OE1   | 1:L:429:LEU:N    | 2.54                     | 0.41              |
| 1:L:587:ARG:CG    | 1:L:588:VAL:H    | 2.33                     | 0.41              |
| 1:M:207:TRP:CZ2   | 1:M:224:ILE:HD11 | 2.56                     | 0.41              |
| 1:M:285:LEU:HD23  | 1:M:285:LEU:HA   | 1.74                     | 0.41              |
| 1:M:345:ASN:O     | 1:M:346:CYS:C    | 2.64                     | 0.41              |
| 1:M:361:GLU:O     | 1:M:365:TYR:N    | 2.53                     | 0.41              |
| 1:M:504:ASP:CG    | 1:M:608:ASN:ND2  | 2.69                     | 0.41              |
| 1:M:560:ASP:O     | 1:M:564:ILE:HG12 | 2.21                     | 0.41              |
| 1:M:829:LEU:HD21  | 1:M:874:LEU:HD22 | 2.03                     | 0.41              |
| 1:M:905:VAL:HG13  | 1:M:906:ASP:H    | 1.85                     | 0.41              |
| 1:M:1051:GLN:HG3  | 1:M:1053:PHE:CD2 | 2.56                     | 0.41              |
| 1:M:1127:ASP:OD1  | 1:M:1128:ILE:N   | 2.50                     | 0.41              |
| 1:M:1198:ASP:OD1  | 1:M:1199:ASP:N   | 2.50                     | 0.41              |
| 1:N:519:GLN:HG2   | 1:N:523:PHE:HE2  | 1.84                     | 0.41              |
| 1:N:560:ASP:O     | 1:N:564:ILE:HG12 | 2.21                     | 0.41              |
| 1:N:584:PHE:HB3   | 1:N:585:ASP:H    | 1.61                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:603:ILE:HD11 | 1:N:635:VAL:HG11 | 2.03                     | 0.41              |
| 1:N:833:LYS:HB3  | 1:N:834:TYR:H    | 1.63                     | 0.41              |
| 1:O:208:THR:C    | 1:O:210:ARG:H    | 2.29                     | 0.41              |
| 1:O:428:GLU:OE1  | 1:O:429:LEU:N    | 2.54                     | 0.41              |
| 1:O:905:VAL:HG13 | 1:O:906:ASP:H    | 1.85                     | 0.41              |
| 1:P:122:LYS:O    | 1:P:303:LYS:NZ   | 2.38                     | 0.41              |
| 1:P:271:VAL:O    | 1:P:274:PHE:N    | 2.54                     | 0.41              |
| 1:P:301:LEU:CD2  | 1:P:313:PRO:CG   | 2.87                     | 0.41              |
| 1:P:428:GLU:OE1  | 1:P:429:LEU:N    | 2.54                     | 0.41              |
| 1:P:468:TYR:HE1  | 1:P:497:LEU:HB2  | 1.85                     | 0.41              |
| 1:P:768:ILE:HG23 | 1:P:769:ARG:N    | 2.36                     | 0.41              |
| 1:P:1026:PHE:HD1 | 1:P:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:A:271:VAL:O    | 1:A:274:PHE:N    | 2.54                     | 0.41              |
| 1:A:347:ASP:CG   | 1:A:348:LYS:H    | 2.27                     | 0.41              |
| 1:A:560:ASP:O    | 1:A:564:ILE:HG12 | 2.21                     | 0.41              |
| 1:B:322:ARG:C    | 1:B:324:LEU:N    | 2.79                     | 0.41              |
| 1:B:450:PRO:C    | 1:B:452:THR:N    | 2.78                     | 0.41              |
| 1:B:781:VAL:HG11 | 1:B:791:TRP:HZ3  | 1.87                     | 0.41              |
| 1:C:11:GLN:O     | 1:C:12:TYR:C     | 2.62                     | 0.41              |
| 1:C:361:GLU:O    | 1:C:365:TYR:N    | 2.53                     | 0.41              |
| 1:C:428:GLU:OE1  | 1:C:429:LEU:N    | 2.54                     | 0.41              |
| 1:D:322:ARG:C    | 1:D:324:LEU:N    | 2.79                     | 0.41              |
| 1:D:331:ILE:HD12 | 1:D:338:TRP:H    | 1.85                     | 0.41              |
| 1:D:346:CYS:SG   | 1:D:350:THR:OG1  | 2.76                     | 0.41              |
| 1:D:549:ILE:HD12 | 1:D:550:GLU:H    | 1.85                     | 0.41              |
| 1:D:717:PHE:HB2  | 1:D:771:PHE:HD1  | 1.86                     | 0.41              |
| 1:D:769:ARG:NH1  | 1:D:771:PHE:HB2  | 2.35                     | 0.41              |
| 1:E:271:VAL:O    | 1:E:274:PHE:N    | 2.54                     | 0.41              |
| 1:F:446:HIS:C    | 1:F:448:ASN:H    | 2.29                     | 0.41              |
| 1:G:545:PHE:CA   | 1:G:548:LYS:HB2  | 2.45                     | 0.41              |
| 1:G:1026:PHE:HD1 | 1:G:1062:LYS:HG2 | 1.86                     | 0.41              |
| 1:I:322:ARG:C    | 1:I:324:LEU:N    | 2.79                     | 0.41              |
| 1:I:428:GLU:OE1  | 1:I:429:LEU:N    | 2.54                     | 0.41              |
| 1:I:447:TYR:OH   | 1:I:486:LEU:CD2  | 2.67                     | 0.41              |
| 1:I:967:PRO:HD2  | 1:I:976:ASP:HB2  | 2.03                     | 0.41              |
| 1:J:208:THR:C    | 1:J:210:ARG:H    | 2.28                     | 0.41              |
| 1:J:271:VAL:O    | 1:J:274:PHE:N    | 2.54                     | 0.41              |
| 1:J:322:ARG:C    | 1:J:324:LEU:N    | 2.79                     | 0.41              |
| 1:J:389:ILE:CD1  | 1:J:446:HIS:HE2  | 2.14                     | 0.41              |
| 1:J:724:GLY:HA3  | 1:J:730:ILE:HD12 | 2.01                     | 0.41              |
| 1:J:1198:ASP:OD1 | 1:J:1199:ASP:N   | 2.50                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:322:ARG:C    | 1:K:324:LEU:N    | 2.79                     | 0.41              |
| 1:K:545:PHE:CA   | 1:K:548:LYS:HB2  | 2.45                     | 0.41              |
| 1:K:603:ILE:HD11 | 1:K:635:VAL:HG11 | 2.03                     | 0.41              |
| 1:M:59:LEU:HD21  | 1:M:63:TRP:CZ2   | 2.55                     | 0.41              |
| 1:M:781:VAL:HG11 | 1:M:791:TRP:HZ3  | 1.86                     | 0.41              |
| 1:N:231:LEU:O    | 1:N:234:SER:OG   | 2.26                     | 0.41              |
| 1:N:361:GLU:O    | 1:N:365:TYR:N    | 2.53                     | 0.41              |
| 1:P:545:PHE:CA   | 1:P:548:LYS:HB2  | 2.45                     | 0.41              |
| 1:A:142:ARG:HH22 | 1:H:14:ASP:CG    | 2.28                     | 0.40              |
| 1:A:361:GLU:O    | 1:A:365:TYR:N    | 2.53                     | 0.40              |
| 1:B:450:PRO:O    | 1:B:453:PHE:N    | 2.54                     | 0.40              |
| 1:B:1127:ASP:OD1 | 1:B:1128:ILE:N   | 2.50                     | 0.40              |
| 1:C:122:LYS:HG3  | 1:D:276:SER:OG   | 2.21                     | 0.40              |
| 1:C:207:TRP:NE1  | 1:C:227:GLU:CD   | 2.79                     | 0.40              |
| 1:D:89:MET:O     | 1:D:92:ILE:HG22  | 2.22                     | 0.40              |
| 1:D:450:PRO:O    | 1:D:453:PHE:N    | 2.55                     | 0.40              |
| 1:E:325:SER:O    | 1:E:326:ILE:C    | 2.64                     | 0.40              |
| 1:E:770:CYS:SG   | 1:E:781:VAL:HG13 | 2.60                     | 0.40              |
| 1:E:967:PRO:HD2  | 1:E:976:ASP:HB2  | 2.04                     | 0.40              |
| 1:F:42:LYS:HG3   | 1:F:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:F:560:ASP:O    | 1:F:564:ILE:HG12 | 2.21                     | 0.40              |
| 1:F:829:LEU:HD21 | 1:F:874:LEU:HD22 | 2.03                     | 0.40              |
| 1:G:560:ASP:O    | 1:G:564:ILE:HG12 | 2.21                     | 0.40              |
| 1:G:916:LYS:CE   | 1:H:1177:TYR:HE2 | 2.34                     | 0.40              |
| 1:I:146:ASN:HB2  | 1:I:280:THR:CG2  | 2.51                     | 0.40              |
| 1:I:208:THR:C    | 1:I:210:ARG:H    | 2.28                     | 0.40              |
| 1:I:345:ASN:O    | 1:I:346:CYS:C    | 2.64                     | 0.40              |
| 1:I:560:ASP:O    | 1:I:564:ILE:HG12 | 2.21                     | 0.40              |
| 1:I:833:LYS:HB3  | 1:I:834:TYR:H    | 1.63                     | 0.40              |
| 1:J:102:MET:O    | 1:J:105:MET:N    | 2.46                     | 0.40              |
| 1:J:967:PRO:HD2  | 1:J:976:ASP:HB2  | 2.04                     | 0.40              |
| 1:K:119:VAL:HG23 | 1:K:120:PHE:N    | 2.28                     | 0.40              |
| 1:K:331:ILE:HD12 | 1:K:338:TRP:H    | 1.86                     | 0.40              |
| 1:K:508:TRP:O    | 1:K:606:GLY:CA   | 2.63                     | 0.40              |
| 1:K:769:ARG:NH1  | 1:K:771:PHE:HB2  | 2.35                     | 0.40              |
| 1:L:42:LYS:HG3   | 1:L:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:L:59:LEU:HD21  | 1:L:63:TRP:CZ2   | 2.55                     | 0.40              |
| 1:L:301:LEU:CD2  | 1:L:313:PRO:CG   | 2.87                     | 0.40              |
| 1:L:361:GLU:O    | 1:L:365:TYR:N    | 2.53                     | 0.40              |
| 1:L:450:PRO:O    | 1:L:453:PHE:N    | 2.54                     | 0.40              |
| 1:L:462:TYR:OH   | 1:L:494:PHE:CE1  | 2.73                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:545:PHE:CE1  | 1:L:565:ALA:HA   | 2.55                     | 0.40              |
| 1:M:207:TRP:NE1  | 1:M:227:GLU:CD   | 2.79                     | 0.40              |
| 1:M:322:ARG:C    | 1:M:324:LEU:N    | 2.79                     | 0.40              |
| 1:M:450:PRO:C    | 1:M:452:THR:N    | 2.78                     | 0.40              |
| 1:N:271:VAL:O    | 1:N:274:PHE:N    | 2.54                     | 0.40              |
| 1:N:462:TYR:CZ   | 1:N:494:PHE:CZ   | 3.03                     | 0.40              |
| 1:N:717:PHE:HB2  | 1:N:771:PHE:HD1  | 1.86                     | 0.40              |
| 1:O:352:ILE:O    | 1:O:356:SER:OG   | 2.29                     | 0.40              |
| 1:O:511:SER:HA   | 1:O:514:ILE:H    | 1.87                     | 0.40              |
| 1:O:1051:GLN:HG3 | 1:O:1053:PHE:CD2 | 2.56                     | 0.40              |
| 1:P:829:LEU:HD21 | 1:P:874:LEU:HD22 | 2.03                     | 0.40              |
| 1:A:207:TRP:CZ2  | 1:A:224:ILE:HD11 | 2.56                     | 0.40              |
| 1:B:207:TRP:NE1  | 1:B:227:GLU:CD   | 2.79                     | 0.40              |
| 1:B:468:TYR:HE1  | 1:B:497:LEU:HB2  | 1.85                     | 0.40              |
| 1:C:42:LYS:HG3   | 1:C:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:C:152:VAL:O    | 1:C:153:LEU:C    | 2.65                     | 0.40              |
| 1:C:450:PRO:O    | 1:C:453:PHE:N    | 2.54                     | 0.40              |
| 1:C:1198:ASP:OD1 | 1:C:1199:ASP:N   | 2.50                     | 0.40              |
| 1:D:122:LYS:HG3  | 1:E:276:SER:HB2  | 2.04                     | 0.40              |
| 1:D:207:TRP:CZ2  | 1:D:224:ILE:HD11 | 2.56                     | 0.40              |
| 1:D:271:VAL:O    | 1:D:274:PHE:N    | 2.54                     | 0.40              |
| 1:D:325:SER:O    | 1:D:326:ILE:C    | 2.64                     | 0.40              |
| 1:D:508:TRP:O    | 1:D:606:GLY:CA   | 2.63                     | 0.40              |
| 1:D:545:PHE:CA   | 1:D:548:LYS:HB2  | 2.45                     | 0.40              |
| 1:E:102:MET:O    | 1:E:105:MET:N    | 2.46                     | 0.40              |
| 1:E:322:ARG:C    | 1:E:324:LEU:N    | 2.79                     | 0.40              |
| 1:E:389:ILE:CD1  | 1:E:446:HIS:HE2  | 2.14                     | 0.40              |
| 1:E:450:PRO:C    | 1:E:452:THR:N    | 2.78                     | 0.40              |
| 1:F:89:MET:O     | 1:F:92:ILE:HG22  | 2.21                     | 0.40              |
| 1:F:207:TRP:CZ2  | 1:F:224:ILE:HD11 | 2.56                     | 0.40              |
| 1:F:322:ARG:C    | 1:F:324:LEU:N    | 2.79                     | 0.40              |
| 1:F:447:TYR:OH   | 1:F:486:LEU:CD2  | 2.67                     | 0.40              |
| 1:F:1198:ASP:OD1 | 1:F:1199:ASP:N   | 2.50                     | 0.40              |
| 1:G:42:LYS:HG3   | 1:G:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:G:322:ARG:C    | 1:G:324:LEU:N    | 2.79                     | 0.40              |
| 1:G:345:ASN:O    | 1:G:346:CYS:C    | 2.64                     | 0.40              |
| 1:G:829:LEU:HD21 | 1:G:874:LEU:HD22 | 2.03                     | 0.40              |
| 1:H:560:ASP:O    | 1:H:564:ILE:HG12 | 2.21                     | 0.40              |
| 1:H:781:VAL:HG11 | 1:H:791:TRP:HZ3  | 1.86                     | 0.40              |
| 1:I:207:TRP:CZ2  | 1:I:224:ILE:HD11 | 2.56                     | 0.40              |
| 1:I:829:LEU:HD21 | 1:I:874:LEU:HD22 | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:325:SER:O     | 1:J:326:ILE:C    | 2.64                     | 0.40              |
| 1:J:428:GLU:OE1   | 1:J:429:LEU:N    | 2.54                     | 0.40              |
| 1:J:450:PRO:C     | 1:J:452:THR:N    | 2.78                     | 0.40              |
| 1:K:207:TRP:NE1   | 1:K:227:GLU:CD   | 2.79                     | 0.40              |
| 1:K:207:TRP:CZ2   | 1:K:224:ILE:HD11 | 2.56                     | 0.40              |
| 1:K:271:VAL:O     | 1:K:274:PHE:N    | 2.54                     | 0.40              |
| 1:K:446:HIS:C     | 1:K:448:ASN:H    | 2.29                     | 0.40              |
| 1:K:450:PRO:O     | 1:K:453:PHE:N    | 2.55                     | 0.40              |
| 1:L:153:LEU:CD2   | 1:L:267:ARG:HD3  | 2.51                     | 0.40              |
| 1:L:207:TRP:NE1   | 1:L:227:GLU:CD   | 2.79                     | 0.40              |
| 1:L:305:LEU:HD23  | 1:L:305:LEU:HA   | 1.84                     | 0.40              |
| 1:L:413:LYS:CD    | 1:L:422:ILE:O    | 2.61                     | 0.40              |
| 1:L:468:TYR:HE1   | 1:L:497:LEU:HB2  | 1.85                     | 0.40              |
| 1:M:450:PRO:O     | 1:M:453:PHE:N    | 2.55                     | 0.40              |
| 1:M:468:TYR:HE1   | 1:M:497:LEU:HB2  | 1.85                     | 0.40              |
| 1:N:146:ASN:HB2   | 1:N:280:THR:CG2  | 2.51                     | 0.40              |
| 1:N:207:TRP:CZ2   | 1:N:224:ILE:HD11 | 2.56                     | 0.40              |
| 1:N:347:ASP:CG    | 1:N:348:LYS:H    | 2.27                     | 0.40              |
| 1:O:560:ASP:O     | 1:O:564:ILE:HG12 | 2.21                     | 0.40              |
| 1:O:1195:VAL:HG11 | 1:O:1241:PHE:CZ  | 2.54                     | 0.40              |
| 1:P:322:ARG:C     | 1:P:324:LEU:N    | 2.79                     | 0.40              |
| 1:P:345:ASN:O     | 1:P:346:CYS:C    | 2.64                     | 0.40              |
| 1:P:560:ASP:HA    | 1:P:592:ASN:ND2  | 2.29                     | 0.40              |
| 1:P:560:ASP:O     | 1:P:564:ILE:HG12 | 2.21                     | 0.40              |
| 1:P:717:PHE:HB2   | 1:P:771:PHE:HD1  | 1.86                     | 0.40              |
| 1:A:20:GLU:O      | 1:A:21:ASP:C     | 2.63                     | 0.40              |
| 1:A:428:GLU:OE1   | 1:A:429:LEU:N    | 2.54                     | 0.40              |
| 1:A:468:TYR:HE1   | 1:A:497:LEU:HB2  | 1.85                     | 0.40              |
| 1:A:717:PHE:HB2   | 1:A:771:PHE:HD1  | 1.86                     | 0.40              |
| 1:B:89:MET:O      | 1:B:92:ILE:HG22  | 2.21                     | 0.40              |
| 1:B:325:SER:O     | 1:B:326:ILE:C    | 2.64                     | 0.40              |
| 1:C:146:ASN:HB2   | 1:C:280:THR:CG2  | 2.51                     | 0.40              |
| 1:C:967:PRO:HD2   | 1:C:976:ASP:HB2  | 2.03                     | 0.40              |
| 1:C:1247:LEU:HD12 | 1:C:1263:MET:HG2 | 2.04                     | 0.40              |
| 1:D:42:LYS:HG3    | 1:D:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:D:207:TRP:NE1   | 1:D:227:GLU:CD   | 2.79                     | 0.40              |
| 1:D:781:VAL:HG11  | 1:D:791:TRP:HZ3  | 1.86                     | 0.40              |
| 1:D:967:PRO:HD2   | 1:D:976:ASP:HB2  | 2.04                     | 0.40              |
| 1:E:146:ASN:HB2   | 1:E:280:THR:CG2  | 2.51                     | 0.40              |
| 1:E:428:GLU:OE1   | 1:E:429:LEU:N    | 2.54                     | 0.40              |
| 1:E:616:LEU:HG    | 1:E:618:ASN:H    | 1.86                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:20:GLU:O      | 1:F:21:ASP:C      | 2.63                     | 0.40              |
| 1:F:146:ASN:HB2   | 1:F:280:THR:CG2   | 2.51                     | 0.40              |
| 1:F:208:THR:C     | 1:F:210:ARG:H     | 2.28                     | 0.40              |
| 1:F:511:SER:HA    | 1:F:514:ILE:H     | 1.87                     | 0.40              |
| 1:F:553:LEU:HD23  | 1:F:553:LEU:HA    | 1.90                     | 0.40              |
| 1:F:967:PRO:HD2   | 1:F:976:ASP:HB2   | 2.04                     | 0.40              |
| 1:G:208:THR:C     | 1:G:210:ARG:H     | 2.28                     | 0.40              |
| 1:G:549:ILE:HD12  | 1:G:550:GLU:H     | 1.85                     | 0.40              |
| 1:G:560:ASP:HA    | 1:G:592:ASN:ND2   | 2.29                     | 0.40              |
| 1:G:717:PHE:HB2   | 1:G:771:PHE:HD1   | 1.86                     | 0.40              |
| 1:G:768:ILE:HG23  | 1:G:769:ARG:H     | 1.87                     | 0.40              |
| 1:G:994:HIS:CE1   | 1:G:1023:ILE:HG23 | 2.56                     | 0.40              |
| 1:H:20:GLU:O      | 1:H:21:ASP:C      | 2.63                     | 0.40              |
| 1:H:89:MET:O      | 1:H:92:ILE:HG22   | 2.22                     | 0.40              |
| 1:H:147:VAL:HG23  | 1:H:263:LEU:HG    | 2.03                     | 0.40              |
| 1:H:458:LEU:HD23  | 1:H:459:ILE:N     | 2.27                     | 0.40              |
| 1:I:20:GLU:O      | 1:I:21:ASP:C      | 2.63                     | 0.40              |
| 1:I:42:LYS:HG3    | 1:I:46:ASP:OD2    | 2.22                     | 0.40              |
| 1:J:146:ASN:HB2   | 1:J:280:THR:CG2   | 2.51                     | 0.40              |
| 1:J:207:TRP:NE1   | 1:J:227:GLU:CD    | 2.79                     | 0.40              |
| 1:J:519:GLN:HG2   | 1:J:523:PHE:HE2   | 1.84                     | 0.40              |
| 1:J:560:ASP:HA    | 1:J:592:ASN:ND2   | 2.29                     | 0.40              |
| 1:J:616:LEU:HG    | 1:J:618:ASN:H     | 1.86                     | 0.40              |
| 1:K:42:LYS:HG3    | 1:K:46:ASP:OD2    | 2.21                     | 0.40              |
| 1:K:152:VAL:O     | 1:K:153:LEU:C     | 2.65                     | 0.40              |
| 1:K:325:SER:O     | 1:K:326:ILE:C     | 2.64                     | 0.40              |
| 1:K:399:MET:HG3   | 1:L:335:LEU:CD2   | 2.52                     | 0.40              |
| 1:K:656:ARG:HG2   | 1:K:657:MET:N     | 2.37                     | 0.40              |
| 1:K:717:PHE:HB2   | 1:K:771:PHE:HD1   | 1.86                     | 0.40              |
| 1:K:967:PRO:HD2   | 1:K:976:ASP:HB2   | 2.04                     | 0.40              |
| 1:L:146:ASN:HB2   | 1:L:280:THR:CG2   | 2.51                     | 0.40              |
| 1:L:152:VAL:O     | 1:L:153:LEU:C     | 2.64                     | 0.40              |
| 1:L:446:HIS:C     | 1:L:448:ASN:H     | 2.29                     | 0.40              |
| 1:L:462:TYR:OH    | 1:L:494:PHE:CZ    | 2.66                     | 0.40              |
| 1:L:1009:ILE:HG13 | 1:L:1011:PRO:HD3  | 2.03                     | 0.40              |
| 1:L:1247:LEU:HD12 | 1:L:1263:MET:HG2  | 2.04                     | 0.40              |
| 1:M:89:MET:O      | 1:M:92:ILE:HG22   | 2.22                     | 0.40              |
| 1:M:244:LEU:HD21  | 1:M:256:PHE:CD2   | 2.51                     | 0.40              |
| 1:M:511:SER:HA    | 1:M:514:ILE:H     | 1.86                     | 0.40              |
| 1:M:717:PHE:HB2   | 1:M:771:PHE:HD1   | 1.86                     | 0.40              |
| 1:N:113:LEU:HA    | 1:N:113:LEU:HD12  | 1.84                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:89:MET:O      | 1:O:92:ILE:HG22   | 2.22                     | 0.40              |
| 1:O:146:ASN:HB2   | 1:O:280:THR:CG2   | 2.51                     | 0.40              |
| 1:O:147:VAL:HG23  | 1:O:263:LEU:HG    | 2.03                     | 0.40              |
| 1:O:458:LEU:HD23  | 1:O:459:ILE:N     | 2.27                     | 0.40              |
| 1:O:519:GLN:HG2   | 1:O:523:PHE:HE2   | 1.84                     | 0.40              |
| 1:O:781:VAL:HG11  | 1:O:791:TRP:HZ3   | 1.86                     | 0.40              |
| 1:O:833:LYS:HB3   | 1:O:834:TYR:H     | 1.63                     | 0.40              |
| 1:P:42:LYS:HG3    | 1:P:46:ASP:OD2    | 2.22                     | 0.40              |
| 1:P:462:TYR:OH    | 1:P:494:PHE:CZ    | 2.66                     | 0.40              |
| 1:P:549:ILE:HD12  | 1:P:550:GLU:H     | 1.85                     | 0.40              |
| 1:P:656:ARG:HG2   | 1:P:657:MET:N     | 2.37                     | 0.40              |
| 1:P:994:HIS:CE1   | 1:P:1023:ILE:HG23 | 2.56                     | 0.40              |
| 1:A:186:CYS:C     | 1:A:249:ASN:ND2   | 2.80                     | 0.40              |
| 1:A:447:TYR:OH    | 1:A:486:LEU:CD2   | 2.67                     | 0.40              |
| 1:A:464:ASP:O     | 1:A:468:TYR:CD2   | 2.75                     | 0.40              |
| 1:A:1009:ILE:HG13 | 1:A:1011:PRO:HD3  | 2.03                     | 0.40              |
| 1:B:20:GLU:O      | 1:B:21:ASP:C      | 2.63                     | 0.40              |
| 1:B:244:LEU:HD21  | 1:B:256:PHE:CD2   | 2.51                     | 0.40              |
| 1:B:616:LEU:HG    | 1:B:618:ASN:H     | 1.86                     | 0.40              |
| 1:B:717:PHE:HB2   | 1:B:771:PHE:HD1   | 1.86                     | 0.40              |
| 1:B:967:PRO:HD2   | 1:B:976:ASP:HB2   | 2.04                     | 0.40              |
| 1:B:1247:LEU:HD12 | 1:B:1263:MET:HG2  | 2.04                     | 0.40              |
| 1:C:153:LEU:CD2   | 1:C:267:ARG:HD3   | 2.51                     | 0.40              |
| 1:C:446:HIS:C     | 1:C:448:ASN:H     | 2.29                     | 0.40              |
| 1:C:468:TYR:HE1   | 1:C:497:LEU:HB2   | 1.85                     | 0.40              |
| 1:C:545:PHE:CE1   | 1:C:565:ALA:HA    | 2.55                     | 0.40              |
| 1:D:119:VAL:HG23  | 1:D:120:PHE:N     | 2.29                     | 0.40              |
| 1:D:152:VAL:O     | 1:D:153:LEU:C     | 2.65                     | 0.40              |
| 1:D:656:ARG:HG2   | 1:D:657:MET:N     | 2.37                     | 0.40              |
| 1:E:905:VAL:HG13  | 1:E:906:ASP:H     | 1.85                     | 0.40              |
| 1:F:147:VAL:HG23  | 1:F:263:LEU:HG    | 2.03                     | 0.40              |
| 1:F:345:ASN:O     | 1:F:346:CYS:C     | 2.64                     | 0.40              |
| 1:F:1051:GLN:HG3  | 1:F:1053:PHE:CD2  | 2.55                     | 0.40              |
| 1:G:146:ASN:HB2   | 1:G:280:THR:CG2   | 2.51                     | 0.40              |
| 1:G:207:TRP:NE1   | 1:G:227:GLU:CD    | 2.79                     | 0.40              |
| 1:G:207:TRP:CZ2   | 1:G:224:ILE:HD11  | 2.56                     | 0.40              |
| 1:G:331:ILE:HD12  | 1:G:338:TRP:H     | 1.85                     | 0.40              |
| 1:G:603:ILE:HD11  | 1:G:635:VAL:HG11  | 2.03                     | 0.40              |
| 1:G:656:ARG:HG2   | 1:G:657:MET:N     | 2.37                     | 0.40              |
| 1:G:833:LYS:HB3   | 1:G:834:TYR:H     | 1.63                     | 0.40              |
| 1:G:1247:LEU:HD12 | 1:G:1263:MET:HG2  | 2.04                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:H:146:ASN:HB2   | 1:H:280:THR:CG2  | 2.51                     | 0.40              |
| 1:H:464:ASP:O     | 1:H:468:TYR:CD2  | 2.75                     | 0.40              |
| 1:H:519:GLN:HG2   | 1:H:523:PHE:HE2  | 1.84                     | 0.40              |
| 1:H:822:ARG:HH12  | 1:H:838:ARG:NH2  | 2.20                     | 0.40              |
| 1:I:222:HIS:CG    | 1:J:198:LYS:HZ1  | 2.39                     | 0.40              |
| 1:I:361:GLU:CB    | 1:I:364:GLU:HB3  | 2.52                     | 0.40              |
| 1:I:446:HIS:C     | 1:I:448:ASN:H    | 2.29                     | 0.40              |
| 1:I:511:SER:HA    | 1:I:514:ILE:H    | 1.86                     | 0.40              |
| 1:I:555:CYS:HA    | 1:I:558:TYR:HB2  | 2.04                     | 0.40              |
| 1:L:271:VAL:O     | 1:L:274:PHE:N    | 2.54                     | 0.40              |
| 1:L:967:PRO:HD2   | 1:L:976:ASP:HB2  | 2.04                     | 0.40              |
| 1:M:20:GLU:O      | 1:M:21:ASP:C     | 2.63                     | 0.40              |
| 1:M:42:LYS:HG3    | 1:M:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:M:325:SER:O     | 1:M:326:ILE:C    | 2.64                     | 0.40              |
| 1:M:361:GLU:CB    | 1:M:364:GLU:HB3  | 2.52                     | 0.40              |
| 1:M:967:PRO:HD2   | 1:M:976:ASP:HB2  | 2.04                     | 0.40              |
| 1:N:20:GLU:O      | 1:N:21:ASP:C     | 2.63                     | 0.40              |
| 1:N:345:ASN:O     | 1:N:346:CYS:C    | 2.64                     | 0.40              |
| 1:N:428:GLU:OE1   | 1:N:429:LEU:N    | 2.54                     | 0.40              |
| 1:N:1009:ILE:HG13 | 1:N:1011:PRO:HD3 | 2.03                     | 0.40              |
| 1:O:42:LYS:HG3    | 1:O:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:O:464:ASP:O     | 1:O:468:TYR:CD2  | 2.75                     | 0.40              |
| 1:O:633:THR:HG22  | 1:O:643:TYR:HA   | 1.97                     | 0.40              |
| 1:O:1247:LEU:HD12 | 1:O:1263:MET:HG2 | 2.04                     | 0.40              |
| 1:P:146:ASN:HB2   | 1:P:280:THR:CG2  | 2.51                     | 0.40              |
| 1:P:207:TRP:NE1   | 1:P:227:GLU:CD   | 2.79                     | 0.40              |
| 1:P:207:TRP:CZ2   | 1:P:224:ILE:HD11 | 2.56                     | 0.40              |
| 1:P:768:ILE:HG23  | 1:P:769:ARG:H    | 1.87                     | 0.40              |
| 1:P:822:ARG:HH12  | 1:P:838:ARG:NH2  | 2.20                     | 0.40              |
| 1:P:1247:LEU:HD12 | 1:P:1263:MET:HG2 | 2.04                     | 0.40              |
| 1:A:146:ASN:HB2   | 1:A:280:THR:CG2  | 2.51                     | 0.40              |
| 1:A:322:ARG:C     | 1:A:324:LEU:N    | 2.79                     | 0.40              |
| 1:B:42:LYS:HG3    | 1:B:46:ASP:OD2   | 2.22                     | 0.40              |
| 1:B:186:CYS:C     | 1:B:249:ASN:HD21 | 2.27                     | 0.40              |
| 1:B:361:GLU:CB    | 1:B:364:GLU:HB3  | 2.52                     | 0.40              |
| 1:B:549:ILE:HD12  | 1:B:550:GLU:H    | 1.85                     | 0.40              |
| 1:C:271:VAL:O     | 1:C:274:PHE:N    | 2.54                     | 0.40              |
| 1:C:470:HIS:O     | 1:C:473:HIS:N    | 2.53                     | 0.40              |
| 1:C:1009:ILE:HG13 | 1:C:1011:PRO:HD3 | 2.03                     | 0.40              |
| 1:D:557:LYS:HD3   | 1:D:1223:GLN:NE2 | 2.35                     | 0.40              |
| 1:E:207:TRP:NE1   | 1:E:227:GLU:CD   | 2.79                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:207:TRP:CZ2   | 1:E:224:ILE:HD11  | 2.56                     | 0.40              |
| 1:E:515:LEU:O     | 1:E:516:ASN:OD1   | 2.40                     | 0.40              |
| 1:E:560:ASP:O     | 1:E:564:ILE:HG12  | 2.21                     | 0.40              |
| 1:E:822:ARG:HH12  | 1:E:838:ARG:NH2   | 2.20                     | 0.40              |
| 1:F:325:SER:O     | 1:F:326:ILE:C     | 2.64                     | 0.40              |
| 1:F:347:ASP:CG    | 1:F:348:LYS:H     | 2.27                     | 0.40              |
| 1:F:361:GLU:CB    | 1:F:364:GLU:HB3   | 2.52                     | 0.40              |
| 1:F:555:CYS:HA    | 1:F:558:TYR:HB2   | 2.04                     | 0.40              |
| 1:F:822:ARG:HH12  | 1:F:838:ARG:NH2   | 2.20                     | 0.40              |
| 1:G:14:ASP:CG     | 1:H:142:ARG:HH22  | 2.29                     | 0.40              |
| 1:G:822:ARG:HH12  | 1:G:838:ARG:NH2   | 2.20                     | 0.40              |
| 1:G:996:ILE:HD11  | 1:G:1020:ILE:HG23 | 2.04                     | 0.40              |
| 1:H:42:LYS:HG3    | 1:H:46:ASP:OD2    | 2.22                     | 0.40              |
| 1:H:951:VAL:HB    | 1:H:958:SER:HB3   | 2.04                     | 0.40              |
| 1:I:89:MET:O      | 1:I:92:ILE:HG22   | 2.22                     | 0.40              |
| 1:I:147:VAL:HG23  | 1:I:263:LEU:HG    | 2.03                     | 0.40              |
| 1:I:347:ASP:CG    | 1:I:348:LYS:H     | 2.27                     | 0.40              |
| 1:I:560:ASP:HA    | 1:I:592:ASN:ND2   | 2.29                     | 0.40              |
| 1:I:656:ARG:HG2   | 1:I:657:MET:N     | 2.37                     | 0.40              |
| 1:J:515:LEU:O     | 1:J:516:ASN:OD1   | 2.40                     | 0.40              |
| 1:K:781:VAL:HG11  | 1:K:791:TRP:HZ3   | 1.87                     | 0.40              |
| 1:L:616:LEU:HG    | 1:L:618:ASN:H     | 1.86                     | 0.40              |
| 1:M:1247:LEU:HD12 | 1:M:1263:MET:HG2  | 2.04                     | 0.40              |
| 1:N:447:TYR:OH    | 1:N:486:LEU:CD2   | 2.67                     | 0.40              |
| 1:N:464:ASP:O     | 1:N:468:TYR:CD2   | 2.75                     | 0.40              |
| 1:O:345:ASN:O     | 1:O:346:CYS:C     | 2.64                     | 0.40              |
| 1:O:951:VAL:HB    | 1:O:958:SER:HB3   | 2.04                     | 0.40              |
| 1:P:20:GLU:O      | 1:P:21:ASP:C      | 2.63                     | 0.40              |
| 1:P:125:VAL:O     | 1:P:125:VAL:HG23  | 2.22                     | 0.40              |
| 1:P:208:THR:C     | 1:P:210:ARG:H     | 2.29                     | 0.40              |
| 1:P:331:ILE:HD12  | 1:P:338:TRP:H     | 1.85                     | 0.40              |
| 1:P:603:ILE:HD11  | 1:P:635:VAL:HG11  | 2.03                     | 0.40              |
| 1:P:996:ILE:HD11  | 1:P:1020:ILE:HG23 | 2.03                     | 0.40              |
| 1:P:1009:ILE:HG13 | 1:P:1011:PRO:HD3  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | B     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | C     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | D     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | E     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | F     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | G     | 1224/1440 (85%)   | 989 (81%)   | 202 (16%)  | 33 (3%)  | 4           | 25 |
| 1   | H     | 1224/1440 (85%)   | 988 (81%)   | 204 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | I     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | J     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | K     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | L     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | M     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | N     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| 1   | O     | 1224/1440 (85%)   | 988 (81%)   | 203 (17%)  | 33 (3%)  | 4           | 25 |
| 1   | P     | 1224/1440 (85%)   | 989 (81%)   | 203 (17%)  | 32 (3%)  | 4           | 25 |
| All | All   | 19584/23040 (85%) | 15822 (81%) | 3248 (17%) | 514 (3%) | 6           | 25 |

All (514) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 252 | ALA  |
| 1   | A     | 315 | GLU  |
| 1   | A     | 517 | THR  |
| 1   | A     | 638 | GLU  |
| 1   | A     | 760 | VAL  |
| 1   | A     | 914 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 252 | ALA  |
| 1   | B     | 315 | GLU  |
| 1   | B     | 517 | THR  |
| 1   | B     | 638 | GLU  |
| 1   | B     | 760 | VAL  |
| 1   | B     | 914 | VAL  |
| 1   | C     | 252 | ALA  |
| 1   | C     | 315 | GLU  |
| 1   | C     | 517 | THR  |
| 1   | C     | 638 | GLU  |
| 1   | C     | 760 | VAL  |
| 1   | C     | 914 | VAL  |
| 1   | D     | 252 | ALA  |
| 1   | D     | 315 | GLU  |
| 1   | D     | 517 | THR  |
| 1   | D     | 638 | GLU  |
| 1   | D     | 760 | VAL  |
| 1   | D     | 914 | VAL  |
| 1   | E     | 252 | ALA  |
| 1   | E     | 315 | GLU  |
| 1   | E     | 517 | THR  |
| 1   | E     | 638 | GLU  |
| 1   | E     | 760 | VAL  |
| 1   | E     | 914 | VAL  |
| 1   | F     | 252 | ALA  |
| 1   | F     | 315 | GLU  |
| 1   | F     | 517 | THR  |
| 1   | F     | 638 | GLU  |
| 1   | F     | 760 | VAL  |
| 1   | F     | 914 | VAL  |
| 1   | G     | 252 | ALA  |
| 1   | G     | 315 | GLU  |
| 1   | G     | 517 | THR  |
| 1   | G     | 638 | GLU  |
| 1   | G     | 760 | VAL  |
| 1   | G     | 914 | VAL  |
| 1   | H     | 252 | ALA  |
| 1   | H     | 315 | GLU  |
| 1   | H     | 517 | THR  |
| 1   | H     | 638 | GLU  |
| 1   | H     | 760 | VAL  |
| 1   | H     | 914 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 252 | ALA  |
| 1   | I     | 315 | GLU  |
| 1   | I     | 517 | THR  |
| 1   | I     | 638 | GLU  |
| 1   | I     | 760 | VAL  |
| 1   | I     | 914 | VAL  |
| 1   | J     | 252 | ALA  |
| 1   | J     | 315 | GLU  |
| 1   | J     | 517 | THR  |
| 1   | J     | 638 | GLU  |
| 1   | J     | 760 | VAL  |
| 1   | J     | 914 | VAL  |
| 1   | K     | 252 | ALA  |
| 1   | K     | 315 | GLU  |
| 1   | K     | 517 | THR  |
| 1   | K     | 638 | GLU  |
| 1   | K     | 760 | VAL  |
| 1   | K     | 914 | VAL  |
| 1   | L     | 252 | ALA  |
| 1   | L     | 315 | GLU  |
| 1   | L     | 517 | THR  |
| 1   | L     | 638 | GLU  |
| 1   | L     | 760 | VAL  |
| 1   | L     | 914 | VAL  |
| 1   | M     | 252 | ALA  |
| 1   | M     | 315 | GLU  |
| 1   | M     | 517 | THR  |
| 1   | M     | 638 | GLU  |
| 1   | M     | 760 | VAL  |
| 1   | M     | 914 | VAL  |
| 1   | N     | 252 | ALA  |
| 1   | N     | 315 | GLU  |
| 1   | N     | 517 | THR  |
| 1   | N     | 638 | GLU  |
| 1   | N     | 760 | VAL  |
| 1   | N     | 914 | VAL  |
| 1   | O     | 252 | ALA  |
| 1   | O     | 315 | GLU  |
| 1   | O     | 517 | THR  |
| 1   | O     | 638 | GLU  |
| 1   | O     | 760 | VAL  |
| 1   | O     | 914 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 252 | ALA  |
| 1   | P     | 315 | GLU  |
| 1   | P     | 517 | THR  |
| 1   | P     | 638 | GLU  |
| 1   | P     | 760 | VAL  |
| 1   | P     | 914 | VAL  |
| 1   | A     | 119 | VAL  |
| 1   | A     | 253 | TRP  |
| 1   | A     | 318 | THR  |
| 1   | A     | 410 | LEU  |
| 1   | A     | 511 | SER  |
| 1   | A     | 916 | LYS  |
| 1   | B     | 119 | VAL  |
| 1   | B     | 253 | TRP  |
| 1   | B     | 318 | THR  |
| 1   | B     | 511 | SER  |
| 1   | B     | 916 | LYS  |
| 1   | C     | 119 | VAL  |
| 1   | C     | 253 | TRP  |
| 1   | C     | 318 | THR  |
| 1   | C     | 410 | LEU  |
| 1   | C     | 511 | SER  |
| 1   | C     | 916 | LYS  |
| 1   | D     | 119 | VAL  |
| 1   | D     | 253 | TRP  |
| 1   | D     | 318 | THR  |
| 1   | D     | 511 | SER  |
| 1   | D     | 916 | LYS  |
| 1   | E     | 119 | VAL  |
| 1   | E     | 253 | TRP  |
| 1   | E     | 318 | THR  |
| 1   | E     | 410 | LEU  |
| 1   | E     | 511 | SER  |
| 1   | E     | 916 | LYS  |
| 1   | F     | 119 | VAL  |
| 1   | F     | 253 | TRP  |
| 1   | F     | 318 | THR  |
| 1   | F     | 511 | SER  |
| 1   | F     | 916 | LYS  |
| 1   | G     | 119 | VAL  |
| 1   | G     | 253 | TRP  |
| 1   | G     | 318 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 410 | LEU  |
| 1   | G     | 511 | SER  |
| 1   | G     | 916 | LYS  |
| 1   | H     | 119 | VAL  |
| 1   | H     | 253 | TRP  |
| 1   | H     | 318 | THR  |
| 1   | H     | 410 | LEU  |
| 1   | H     | 511 | SER  |
| 1   | H     | 916 | LYS  |
| 1   | I     | 119 | VAL  |
| 1   | I     | 253 | TRP  |
| 1   | I     | 318 | THR  |
| 1   | I     | 511 | SER  |
| 1   | I     | 916 | LYS  |
| 1   | J     | 119 | VAL  |
| 1   | J     | 253 | TRP  |
| 1   | J     | 318 | THR  |
| 1   | J     | 511 | SER  |
| 1   | J     | 916 | LYS  |
| 1   | K     | 119 | VAL  |
| 1   | K     | 253 | TRP  |
| 1   | K     | 318 | THR  |
| 1   | K     | 511 | SER  |
| 1   | K     | 916 | LYS  |
| 1   | L     | 119 | VAL  |
| 1   | L     | 253 | TRP  |
| 1   | L     | 318 | THR  |
| 1   | L     | 410 | LEU  |
| 1   | L     | 511 | SER  |
| 1   | L     | 916 | LYS  |
| 1   | M     | 119 | VAL  |
| 1   | M     | 253 | TRP  |
| 1   | M     | 318 | THR  |
| 1   | M     | 410 | LEU  |
| 1   | M     | 511 | SER  |
| 1   | M     | 916 | LYS  |
| 1   | N     | 119 | VAL  |
| 1   | N     | 253 | TRP  |
| 1   | N     | 318 | THR  |
| 1   | N     | 511 | SER  |
| 1   | N     | 916 | LYS  |
| 1   | O     | 119 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | O     | 253  | TRP  |
| 1   | O     | 318  | THR  |
| 1   | O     | 410  | LEU  |
| 1   | O     | 511  | SER  |
| 1   | O     | 916  | LYS  |
| 1   | P     | 119  | VAL  |
| 1   | P     | 253  | TRP  |
| 1   | P     | 318  | THR  |
| 1   | P     | 410  | LEU  |
| 1   | P     | 511  | SER  |
| 1   | P     | 916  | LYS  |
| 1   | A     | 341  | TRP  |
| 1   | A     | 430  | LYS  |
| 1   | A     | 902  | ILE  |
| 1   | A     | 1031 | ILE  |
| 1   | A     | 1169 | ILE  |
| 1   | B     | 341  | TRP  |
| 1   | B     | 410  | LEU  |
| 1   | B     | 430  | LYS  |
| 1   | B     | 902  | ILE  |
| 1   | B     | 1031 | ILE  |
| 1   | B     | 1169 | ILE  |
| 1   | C     | 341  | TRP  |
| 1   | C     | 430  | LYS  |
| 1   | C     | 902  | ILE  |
| 1   | C     | 1031 | ILE  |
| 1   | C     | 1169 | ILE  |
| 1   | D     | 341  | TRP  |
| 1   | D     | 410  | LEU  |
| 1   | D     | 430  | LYS  |
| 1   | D     | 902  | ILE  |
| 1   | D     | 1031 | ILE  |
| 1   | D     | 1169 | ILE  |
| 1   | E     | 341  | TRP  |
| 1   | E     | 430  | LYS  |
| 1   | E     | 902  | ILE  |
| 1   | E     | 1031 | ILE  |
| 1   | E     | 1169 | ILE  |
| 1   | F     | 341  | TRP  |
| 1   | F     | 410  | LEU  |
| 1   | F     | 430  | LYS  |
| 1   | F     | 902  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 1031 | ILE  |
| 1   | F     | 1169 | ILE  |
| 1   | G     | 341  | TRP  |
| 1   | G     | 430  | LYS  |
| 1   | G     | 902  | ILE  |
| 1   | G     | 1031 | ILE  |
| 1   | G     | 1169 | ILE  |
| 1   | H     | 341  | TRP  |
| 1   | H     | 430  | LYS  |
| 1   | H     | 902  | ILE  |
| 1   | H     | 1031 | ILE  |
| 1   | H     | 1169 | ILE  |
| 1   | I     | 341  | TRP  |
| 1   | I     | 410  | LEU  |
| 1   | I     | 430  | LYS  |
| 1   | I     | 902  | ILE  |
| 1   | I     | 1031 | ILE  |
| 1   | I     | 1169 | ILE  |
| 1   | J     | 341  | TRP  |
| 1   | J     | 410  | LEU  |
| 1   | J     | 430  | LYS  |
| 1   | J     | 902  | ILE  |
| 1   | J     | 1031 | ILE  |
| 1   | J     | 1169 | ILE  |
| 1   | K     | 341  | TRP  |
| 1   | K     | 410  | LEU  |
| 1   | K     | 430  | LYS  |
| 1   | K     | 902  | ILE  |
| 1   | K     | 1031 | ILE  |
| 1   | K     | 1169 | ILE  |
| 1   | L     | 341  | TRP  |
| 1   | L     | 430  | LYS  |
| 1   | L     | 902  | ILE  |
| 1   | L     | 1031 | ILE  |
| 1   | L     | 1169 | ILE  |
| 1   | M     | 341  | TRP  |
| 1   | M     | 430  | LYS  |
| 1   | M     | 902  | ILE  |
| 1   | M     | 1031 | ILE  |
| 1   | M     | 1169 | ILE  |
| 1   | N     | 341  | TRP  |
| 1   | N     | 410  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | N     | 430  | LYS  |
| 1   | N     | 902  | ILE  |
| 1   | N     | 1031 | ILE  |
| 1   | N     | 1169 | ILE  |
| 1   | O     | 341  | TRP  |
| 1   | O     | 430  | LYS  |
| 1   | O     | 902  | ILE  |
| 1   | O     | 1031 | ILE  |
| 1   | O     | 1169 | ILE  |
| 1   | P     | 341  | TRP  |
| 1   | P     | 430  | LYS  |
| 1   | P     | 902  | ILE  |
| 1   | P     | 1031 | ILE  |
| 1   | P     | 1169 | ILE  |
| 1   | A     | 415  | PRO  |
| 1   | A     | 432  | LYS  |
| 1   | A     | 439  | LEU  |
| 1   | A     | 512  | GLY  |
| 1   | A     | 518  | LEU  |
| 1   | A     | 706  | ILE  |
| 1   | A     | 915  | TYR  |
| 1   | B     | 415  | PRO  |
| 1   | B     | 432  | LYS  |
| 1   | B     | 439  | LEU  |
| 1   | B     | 512  | GLY  |
| 1   | B     | 518  | LEU  |
| 1   | B     | 706  | ILE  |
| 1   | B     | 915  | TYR  |
| 1   | C     | 415  | PRO  |
| 1   | C     | 432  | LYS  |
| 1   | C     | 439  | LEU  |
| 1   | C     | 512  | GLY  |
| 1   | C     | 518  | LEU  |
| 1   | C     | 706  | ILE  |
| 1   | C     | 915  | TYR  |
| 1   | D     | 415  | PRO  |
| 1   | D     | 432  | LYS  |
| 1   | D     | 439  | LEU  |
| 1   | D     | 512  | GLY  |
| 1   | D     | 518  | LEU  |
| 1   | D     | 706  | ILE  |
| 1   | D     | 915  | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 415 | PRO  |
| 1   | E     | 432 | LYS  |
| 1   | E     | 439 | LEU  |
| 1   | E     | 512 | GLY  |
| 1   | E     | 518 | LEU  |
| 1   | E     | 706 | ILE  |
| 1   | E     | 915 | TYR  |
| 1   | F     | 415 | PRO  |
| 1   | F     | 432 | LYS  |
| 1   | F     | 439 | LEU  |
| 1   | F     | 512 | GLY  |
| 1   | F     | 518 | LEU  |
| 1   | F     | 706 | ILE  |
| 1   | F     | 915 | TYR  |
| 1   | G     | 415 | PRO  |
| 1   | G     | 432 | LYS  |
| 1   | G     | 439 | LEU  |
| 1   | G     | 512 | GLY  |
| 1   | G     | 518 | LEU  |
| 1   | G     | 706 | ILE  |
| 1   | G     | 915 | TYR  |
| 1   | H     | 415 | PRO  |
| 1   | H     | 432 | LYS  |
| 1   | H     | 439 | LEU  |
| 1   | H     | 512 | GLY  |
| 1   | H     | 518 | LEU  |
| 1   | H     | 706 | ILE  |
| 1   | H     | 915 | TYR  |
| 1   | I     | 415 | PRO  |
| 1   | I     | 432 | LYS  |
| 1   | I     | 439 | LEU  |
| 1   | I     | 512 | GLY  |
| 1   | I     | 518 | LEU  |
| 1   | I     | 706 | ILE  |
| 1   | I     | 915 | TYR  |
| 1   | J     | 415 | PRO  |
| 1   | J     | 432 | LYS  |
| 1   | J     | 439 | LEU  |
| 1   | J     | 512 | GLY  |
| 1   | J     | 518 | LEU  |
| 1   | J     | 706 | ILE  |
| 1   | J     | 915 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 415 | PRO  |
| 1   | K     | 432 | LYS  |
| 1   | K     | 439 | LEU  |
| 1   | K     | 512 | GLY  |
| 1   | K     | 518 | LEU  |
| 1   | K     | 706 | ILE  |
| 1   | K     | 915 | TYR  |
| 1   | L     | 415 | PRO  |
| 1   | L     | 432 | LYS  |
| 1   | L     | 439 | LEU  |
| 1   | L     | 512 | GLY  |
| 1   | L     | 518 | LEU  |
| 1   | L     | 706 | ILE  |
| 1   | L     | 915 | TYR  |
| 1   | M     | 415 | PRO  |
| 1   | M     | 432 | LYS  |
| 1   | M     | 439 | LEU  |
| 1   | M     | 512 | GLY  |
| 1   | M     | 518 | LEU  |
| 1   | M     | 706 | ILE  |
| 1   | M     | 915 | TYR  |
| 1   | N     | 415 | PRO  |
| 1   | N     | 432 | LYS  |
| 1   | N     | 439 | LEU  |
| 1   | N     | 512 | GLY  |
| 1   | N     | 518 | LEU  |
| 1   | N     | 706 | ILE  |
| 1   | N     | 915 | TYR  |
| 1   | O     | 415 | PRO  |
| 1   | O     | 432 | LYS  |
| 1   | O     | 439 | LEU  |
| 1   | O     | 512 | GLY  |
| 1   | O     | 518 | LEU  |
| 1   | O     | 706 | ILE  |
| 1   | O     | 915 | TYR  |
| 1   | P     | 415 | PRO  |
| 1   | P     | 432 | LYS  |
| 1   | P     | 439 | LEU  |
| 1   | P     | 512 | GLY  |
| 1   | P     | 518 | LEU  |
| 1   | P     | 706 | ILE  |
| 1   | P     | 915 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 121  | ALA  |
| 1   | A     | 126  | SER  |
| 1   | A     | 316  | VAL  |
| 1   | A     | 424  | SER  |
| 1   | A     | 1228 | ILE  |
| 1   | B     | 121  | ALA  |
| 1   | B     | 126  | SER  |
| 1   | B     | 316  | VAL  |
| 1   | B     | 424  | SER  |
| 1   | B     | 1228 | ILE  |
| 1   | C     | 121  | ALA  |
| 1   | C     | 126  | SER  |
| 1   | C     | 316  | VAL  |
| 1   | C     | 424  | SER  |
| 1   | C     | 1228 | ILE  |
| 1   | D     | 121  | ALA  |
| 1   | D     | 126  | SER  |
| 1   | D     | 316  | VAL  |
| 1   | D     | 424  | SER  |
| 1   | D     | 1228 | ILE  |
| 1   | E     | 121  | ALA  |
| 1   | E     | 126  | SER  |
| 1   | E     | 316  | VAL  |
| 1   | E     | 424  | SER  |
| 1   | E     | 1228 | ILE  |
| 1   | F     | 121  | ALA  |
| 1   | F     | 126  | SER  |
| 1   | F     | 316  | VAL  |
| 1   | F     | 424  | SER  |
| 1   | F     | 1228 | ILE  |
| 1   | G     | 121  | ALA  |
| 1   | G     | 126  | SER  |
| 1   | G     | 316  | VAL  |
| 1   | G     | 424  | SER  |
| 1   | G     | 1228 | ILE  |
| 1   | H     | 121  | ALA  |
| 1   | H     | 126  | SER  |
| 1   | H     | 316  | VAL  |
| 1   | H     | 424  | SER  |
| 1   | H     | 1228 | ILE  |
| 1   | I     | 121  | ALA  |
| 1   | I     | 126  | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | I     | 316  | VAL  |
| 1   | I     | 424  | SER  |
| 1   | I     | 1228 | ILE  |
| 1   | J     | 121  | ALA  |
| 1   | J     | 126  | SER  |
| 1   | J     | 316  | VAL  |
| 1   | J     | 424  | SER  |
| 1   | J     | 1228 | ILE  |
| 1   | K     | 121  | ALA  |
| 1   | K     | 126  | SER  |
| 1   | K     | 316  | VAL  |
| 1   | K     | 424  | SER  |
| 1   | K     | 1228 | ILE  |
| 1   | L     | 121  | ALA  |
| 1   | L     | 126  | SER  |
| 1   | L     | 316  | VAL  |
| 1   | L     | 424  | SER  |
| 1   | L     | 1228 | ILE  |
| 1   | M     | 121  | ALA  |
| 1   | M     | 126  | SER  |
| 1   | M     | 316  | VAL  |
| 1   | M     | 424  | SER  |
| 1   | M     | 1228 | ILE  |
| 1   | N     | 121  | ALA  |
| 1   | N     | 126  | SER  |
| 1   | N     | 316  | VAL  |
| 1   | N     | 424  | SER  |
| 1   | N     | 1228 | ILE  |
| 1   | O     | 121  | ALA  |
| 1   | O     | 126  | SER  |
| 1   | O     | 316  | VAL  |
| 1   | O     | 424  | SER  |
| 1   | O     | 1228 | ILE  |
| 1   | P     | 121  | ALA  |
| 1   | P     | 126  | SER  |
| 1   | P     | 316  | VAL  |
| 1   | P     | 424  | SER  |
| 1   | P     | 1228 | ILE  |
| 1   | G     | 194  | GLU  |
| 1   | O     | 194  | GLU  |
| 1   | A     | 919  | VAL  |
| 1   | B     | 919  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 919 | VAL  |
| 1   | D     | 919 | VAL  |
| 1   | E     | 919 | VAL  |
| 1   | F     | 919 | VAL  |
| 1   | G     | 919 | VAL  |
| 1   | H     | 919 | VAL  |
| 1   | I     | 919 | VAL  |
| 1   | J     | 919 | VAL  |
| 1   | K     | 919 | VAL  |
| 1   | L     | 919 | VAL  |
| 1   | M     | 919 | VAL  |
| 1   | N     | 919 | VAL  |
| 1   | O     | 919 | VAL  |
| 1   | P     | 919 | VAL  |
| 1   | F     | 344 | VAL  |
| 1   | G     | 344 | VAL  |
| 1   | J     | 344 | VAL  |
| 1   | N     | 344 | VAL  |
| 1   | N     | 883 | ILE  |
| 1   | A     | 344 | VAL  |
| 1   | A     | 883 | ILE  |
| 1   | B     | 344 | VAL  |
| 1   | B     | 883 | ILE  |
| 1   | C     | 344 | VAL  |
| 1   | C     | 883 | ILE  |
| 1   | D     | 344 | VAL  |
| 1   | D     | 883 | ILE  |
| 1   | E     | 344 | VAL  |
| 1   | E     | 883 | ILE  |
| 1   | F     | 883 | ILE  |
| 1   | G     | 883 | ILE  |
| 1   | H     | 344 | VAL  |
| 1   | H     | 883 | ILE  |
| 1   | I     | 344 | VAL  |
| 1   | I     | 883 | ILE  |
| 1   | J     | 883 | ILE  |
| 1   | K     | 344 | VAL  |
| 1   | K     | 883 | ILE  |
| 1   | L     | 344 | VAL  |
| 1   | L     | 883 | ILE  |
| 1   | M     | 344 | VAL  |
| 1   | M     | 883 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 344 | VAL  |
| 1   | O     | 883 | ILE  |
| 1   | P     | 344 | VAL  |
| 1   | P     | 883 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | B     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | C     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | D     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | E     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | F     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | G     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | H     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | I     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | J     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | K     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | L     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | M     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | N     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | O     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| 1   | P     | 1138/1315 (86%)   | 1136 (100%)  | 2 (0%)   | 87          | 85 |
| All | All   | 18208/21040 (86%) | 18176 (100%) | 32 (0%)  | 85          | 85 |

All (32) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 258 | LEU  |
| 1   | A     | 914 | VAL  |
| 1   | B     | 258 | LEU  |
| 1   | B     | 914 | VAL  |
| 1   | C     | 258 | LEU  |
| 1   | C     | 914 | VAL  |
| 1   | D     | 258 | LEU  |
| 1   | D     | 914 | VAL  |
| 1   | E     | 258 | LEU  |
| 1   | E     | 914 | VAL  |
| 1   | F     | 258 | LEU  |
| 1   | F     | 914 | VAL  |
| 1   | G     | 258 | LEU  |
| 1   | G     | 914 | VAL  |
| 1   | H     | 258 | LEU  |
| 1   | H     | 914 | VAL  |
| 1   | I     | 258 | LEU  |
| 1   | I     | 914 | VAL  |
| 1   | J     | 258 | LEU  |
| 1   | J     | 914 | VAL  |
| 1   | K     | 258 | LEU  |
| 1   | K     | 914 | VAL  |
| 1   | L     | 258 | LEU  |
| 1   | L     | 914 | VAL  |
| 1   | M     | 258 | LEU  |
| 1   | M     | 914 | VAL  |
| 1   | N     | 258 | LEU  |
| 1   | N     | 914 | VAL  |
| 1   | O     | 258 | LEU  |
| 1   | O     | 914 | VAL  |
| 1   | P     | 258 | LEU  |
| 1   | P     | 914 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (490) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | GLN  |
| 1   | A     | 146 | ASN  |
| 1   | A     | 171 | GLN  |
| 1   | A     | 182 | ASN  |
| 1   | A     | 187 | ASN  |
| 1   | A     | 222 | HIS  |
| 1   | A     | 249 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 282  | HIS  |
| 1   | A     | 287  | HIS  |
| 1   | A     | 446  | HIS  |
| 1   | A     | 473  | HIS  |
| 1   | A     | 477  | ASN  |
| 1   | A     | 509  | ASN  |
| 1   | A     | 592  | ASN  |
| 1   | A     | 604  | ASN  |
| 1   | A     | 612  | HIS  |
| 1   | A     | 618  | ASN  |
| 1   | A     | 670  | HIS  |
| 1   | A     | 699  | ASN  |
| 1   | A     | 738  | ASN  |
| 1   | A     | 745  | ASN  |
| 1   | A     | 850  | GLN  |
| 1   | A     | 930  | HIS  |
| 1   | A     | 952  | HIS  |
| 1   | A     | 968  | ASN  |
| 1   | A     | 994  | HIS  |
| 1   | A     | 1027 | ASN  |
| 1   | A     | 1083 | GLN  |
| 1   | A     | 1173 | ASN  |
| 1   | A     | 1223 | GLN  |
| 1   | B     | 11   | GLN  |
| 1   | B     | 117  | ASN  |
| 1   | B     | 146  | ASN  |
| 1   | B     | 171  | GLN  |
| 1   | B     | 182  | ASN  |
| 1   | B     | 187  | ASN  |
| 1   | B     | 222  | HIS  |
| 1   | B     | 249  | ASN  |
| 1   | B     | 282  | HIS  |
| 1   | B     | 287  | HIS  |
| 1   | B     | 446  | HIS  |
| 1   | B     | 473  | HIS  |
| 1   | B     | 477  | ASN  |
| 1   | B     | 509  | ASN  |
| 1   | B     | 592  | ASN  |
| 1   | B     | 604  | ASN  |
| 1   | B     | 612  | HIS  |
| 1   | B     | 618  | ASN  |
| 1   | B     | 670  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 699  | ASN  |
| 1   | B     | 738  | ASN  |
| 1   | B     | 745  | ASN  |
| 1   | B     | 757  | HIS  |
| 1   | B     | 795  | ASN  |
| 1   | B     | 850  | GLN  |
| 1   | B     | 930  | HIS  |
| 1   | B     | 952  | HIS  |
| 1   | B     | 968  | ASN  |
| 1   | B     | 994  | HIS  |
| 1   | B     | 1027 | ASN  |
| 1   | B     | 1083 | GLN  |
| 1   | B     | 1173 | ASN  |
| 1   | B     | 1219 | ASN  |
| 1   | B     | 1223 | GLN  |
| 1   | C     | 11   | GLN  |
| 1   | C     | 146  | ASN  |
| 1   | C     | 171  | GLN  |
| 1   | C     | 182  | ASN  |
| 1   | C     | 187  | ASN  |
| 1   | C     | 249  | ASN  |
| 1   | C     | 282  | HIS  |
| 1   | C     | 287  | HIS  |
| 1   | C     | 446  | HIS  |
| 1   | C     | 473  | HIS  |
| 1   | C     | 477  | ASN  |
| 1   | C     | 509  | ASN  |
| 1   | C     | 592  | ASN  |
| 1   | C     | 604  | ASN  |
| 1   | C     | 612  | HIS  |
| 1   | C     | 618  | ASN  |
| 1   | C     | 670  | HIS  |
| 1   | C     | 699  | ASN  |
| 1   | C     | 738  | ASN  |
| 1   | C     | 745  | ASN  |
| 1   | C     | 850  | GLN  |
| 1   | C     | 930  | HIS  |
| 1   | C     | 952  | HIS  |
| 1   | C     | 968  | ASN  |
| 1   | C     | 994  | HIS  |
| 1   | C     | 1027 | ASN  |
| 1   | C     | 1083 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1173 | ASN  |
| 1   | C     | 1223 | GLN  |
| 1   | D     | 11   | GLN  |
| 1   | D     | 146  | ASN  |
| 1   | D     | 171  | GLN  |
| 1   | D     | 182  | ASN  |
| 1   | D     | 187  | ASN  |
| 1   | D     | 213  | HIS  |
| 1   | D     | 222  | HIS  |
| 1   | D     | 249  | ASN  |
| 1   | D     | 282  | HIS  |
| 1   | D     | 287  | HIS  |
| 1   | D     | 446  | HIS  |
| 1   | D     | 473  | HIS  |
| 1   | D     | 477  | ASN  |
| 1   | D     | 509  | ASN  |
| 1   | D     | 592  | ASN  |
| 1   | D     | 604  | ASN  |
| 1   | D     | 612  | HIS  |
| 1   | D     | 618  | ASN  |
| 1   | D     | 670  | HIS  |
| 1   | D     | 699  | ASN  |
| 1   | D     | 738  | ASN  |
| 1   | D     | 745  | ASN  |
| 1   | D     | 850  | GLN  |
| 1   | D     | 930  | HIS  |
| 1   | D     | 952  | HIS  |
| 1   | D     | 968  | ASN  |
| 1   | D     | 994  | HIS  |
| 1   | D     | 1027 | ASN  |
| 1   | D     | 1083 | GLN  |
| 1   | D     | 1173 | ASN  |
| 1   | D     | 1219 | ASN  |
| 1   | D     | 1223 | GLN  |
| 1   | E     | 11   | GLN  |
| 1   | E     | 146  | ASN  |
| 1   | E     | 171  | GLN  |
| 1   | E     | 182  | ASN  |
| 1   | E     | 187  | ASN  |
| 1   | E     | 222  | HIS  |
| 1   | E     | 249  | ASN  |
| 1   | E     | 282  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 287  | HIS  |
| 1   | E     | 446  | HIS  |
| 1   | E     | 473  | HIS  |
| 1   | E     | 477  | ASN  |
| 1   | E     | 509  | ASN  |
| 1   | E     | 592  | ASN  |
| 1   | E     | 604  | ASN  |
| 1   | E     | 612  | HIS  |
| 1   | E     | 618  | ASN  |
| 1   | E     | 699  | ASN  |
| 1   | E     | 738  | ASN  |
| 1   | E     | 745  | ASN  |
| 1   | E     | 785  | ASN  |
| 1   | E     | 795  | ASN  |
| 1   | E     | 850  | GLN  |
| 1   | E     | 930  | HIS  |
| 1   | E     | 952  | HIS  |
| 1   | E     | 968  | ASN  |
| 1   | E     | 994  | HIS  |
| 1   | E     | 1027 | ASN  |
| 1   | E     | 1130 | ASN  |
| 1   | E     | 1223 | GLN  |
| 1   | F     | 11   | GLN  |
| 1   | F     | 146  | ASN  |
| 1   | F     | 171  | GLN  |
| 1   | F     | 182  | ASN  |
| 1   | F     | 187  | ASN  |
| 1   | F     | 222  | HIS  |
| 1   | F     | 249  | ASN  |
| 1   | F     | 282  | HIS  |
| 1   | F     | 287  | HIS  |
| 1   | F     | 446  | HIS  |
| 1   | F     | 473  | HIS  |
| 1   | F     | 477  | ASN  |
| 1   | F     | 509  | ASN  |
| 1   | F     | 592  | ASN  |
| 1   | F     | 604  | ASN  |
| 1   | F     | 612  | HIS  |
| 1   | F     | 618  | ASN  |
| 1   | F     | 699  | ASN  |
| 1   | F     | 738  | ASN  |
| 1   | F     | 745  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 850  | GLN  |
| 1   | F     | 930  | HIS  |
| 1   | F     | 952  | HIS  |
| 1   | F     | 968  | ASN  |
| 1   | F     | 994  | HIS  |
| 1   | F     | 1027 | ASN  |
| 1   | F     | 1083 | GLN  |
| 1   | F     | 1130 | ASN  |
| 1   | F     | 1223 | GLN  |
| 1   | G     | 11   | GLN  |
| 1   | G     | 98   | GLN  |
| 1   | G     | 146  | ASN  |
| 1   | G     | 171  | GLN  |
| 1   | G     | 182  | ASN  |
| 1   | G     | 187  | ASN  |
| 1   | G     | 222  | HIS  |
| 1   | G     | 249  | ASN  |
| 1   | G     | 282  | HIS  |
| 1   | G     | 287  | HIS  |
| 1   | G     | 446  | HIS  |
| 1   | G     | 473  | HIS  |
| 1   | G     | 477  | ASN  |
| 1   | G     | 509  | ASN  |
| 1   | G     | 592  | ASN  |
| 1   | G     | 604  | ASN  |
| 1   | G     | 612  | HIS  |
| 1   | G     | 618  | ASN  |
| 1   | G     | 699  | ASN  |
| 1   | G     | 738  | ASN  |
| 1   | G     | 745  | ASN  |
| 1   | G     | 850  | GLN  |
| 1   | G     | 930  | HIS  |
| 1   | G     | 952  | HIS  |
| 1   | G     | 968  | ASN  |
| 1   | G     | 994  | HIS  |
| 1   | G     | 1027 | ASN  |
| 1   | G     | 1083 | GLN  |
| 1   | G     | 1173 | ASN  |
| 1   | G     | 1223 | GLN  |
| 1   | G     | 1254 | GLN  |
| 1   | H     | 11   | GLN  |
| 1   | H     | 146  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 171  | GLN  |
| 1   | H     | 182  | ASN  |
| 1   | H     | 187  | ASN  |
| 1   | H     | 222  | HIS  |
| 1   | H     | 249  | ASN  |
| 1   | H     | 282  | HIS  |
| 1   | H     | 287  | HIS  |
| 1   | H     | 446  | HIS  |
| 1   | H     | 473  | HIS  |
| 1   | H     | 477  | ASN  |
| 1   | H     | 509  | ASN  |
| 1   | H     | 592  | ASN  |
| 1   | H     | 604  | ASN  |
| 1   | H     | 612  | HIS  |
| 1   | H     | 618  | ASN  |
| 1   | H     | 699  | ASN  |
| 1   | H     | 738  | ASN  |
| 1   | H     | 745  | ASN  |
| 1   | H     | 850  | GLN  |
| 1   | H     | 930  | HIS  |
| 1   | H     | 952  | HIS  |
| 1   | H     | 968  | ASN  |
| 1   | H     | 994  | HIS  |
| 1   | H     | 1027 | ASN  |
| 1   | H     | 1083 | GLN  |
| 1   | H     | 1173 | ASN  |
| 1   | H     | 1223 | GLN  |
| 1   | I     | 11   | GLN  |
| 1   | I     | 146  | ASN  |
| 1   | I     | 171  | GLN  |
| 1   | I     | 182  | ASN  |
| 1   | I     | 187  | ASN  |
| 1   | I     | 222  | HIS  |
| 1   | I     | 249  | ASN  |
| 1   | I     | 282  | HIS  |
| 1   | I     | 287  | HIS  |
| 1   | I     | 446  | HIS  |
| 1   | I     | 473  | HIS  |
| 1   | I     | 477  | ASN  |
| 1   | I     | 509  | ASN  |
| 1   | I     | 592  | ASN  |
| 1   | I     | 604  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | I     | 612  | HIS  |
| 1   | I     | 618  | ASN  |
| 1   | I     | 699  | ASN  |
| 1   | I     | 738  | ASN  |
| 1   | I     | 745  | ASN  |
| 1   | I     | 850  | GLN  |
| 1   | I     | 930  | HIS  |
| 1   | I     | 952  | HIS  |
| 1   | I     | 968  | ASN  |
| 1   | I     | 994  | HIS  |
| 1   | I     | 1027 | ASN  |
| 1   | I     | 1083 | GLN  |
| 1   | I     | 1130 | ASN  |
| 1   | I     | 1223 | GLN  |
| 1   | J     | 11   | GLN  |
| 1   | J     | 146  | ASN  |
| 1   | J     | 171  | GLN  |
| 1   | J     | 182  | ASN  |
| 1   | J     | 187  | ASN  |
| 1   | J     | 222  | HIS  |
| 1   | J     | 249  | ASN  |
| 1   | J     | 282  | HIS  |
| 1   | J     | 287  | HIS  |
| 1   | J     | 446  | HIS  |
| 1   | J     | 473  | HIS  |
| 1   | J     | 477  | ASN  |
| 1   | J     | 509  | ASN  |
| 1   | J     | 592  | ASN  |
| 1   | J     | 604  | ASN  |
| 1   | J     | 612  | HIS  |
| 1   | J     | 618  | ASN  |
| 1   | J     | 699  | ASN  |
| 1   | J     | 738  | ASN  |
| 1   | J     | 745  | ASN  |
| 1   | J     | 785  | ASN  |
| 1   | J     | 795  | ASN  |
| 1   | J     | 850  | GLN  |
| 1   | J     | 930  | HIS  |
| 1   | J     | 952  | HIS  |
| 1   | J     | 968  | ASN  |
| 1   | J     | 994  | HIS  |
| 1   | J     | 1027 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 1130 | ASN  |
| 1   | J     | 1223 | GLN  |
| 1   | K     | 11   | GLN  |
| 1   | K     | 146  | ASN  |
| 1   | K     | 171  | GLN  |
| 1   | K     | 182  | ASN  |
| 1   | K     | 187  | ASN  |
| 1   | K     | 213  | HIS  |
| 1   | K     | 222  | HIS  |
| 1   | K     | 249  | ASN  |
| 1   | K     | 282  | HIS  |
| 1   | K     | 287  | HIS  |
| 1   | K     | 446  | HIS  |
| 1   | K     | 473  | HIS  |
| 1   | K     | 477  | ASN  |
| 1   | K     | 509  | ASN  |
| 1   | K     | 592  | ASN  |
| 1   | K     | 604  | ASN  |
| 1   | K     | 612  | HIS  |
| 1   | K     | 618  | ASN  |
| 1   | K     | 670  | HIS  |
| 1   | K     | 699  | ASN  |
| 1   | K     | 738  | ASN  |
| 1   | K     | 745  | ASN  |
| 1   | K     | 850  | GLN  |
| 1   | K     | 930  | HIS  |
| 1   | K     | 952  | HIS  |
| 1   | K     | 968  | ASN  |
| 1   | K     | 994  | HIS  |
| 1   | K     | 1017 | ASN  |
| 1   | K     | 1027 | ASN  |
| 1   | K     | 1063 | GLN  |
| 1   | K     | 1083 | GLN  |
| 1   | K     | 1173 | ASN  |
| 1   | K     | 1219 | ASN  |
| 1   | K     | 1223 | GLN  |
| 1   | L     | 11   | GLN  |
| 1   | L     | 146  | ASN  |
| 1   | L     | 171  | GLN  |
| 1   | L     | 182  | ASN  |
| 1   | L     | 187  | ASN  |
| 1   | L     | 249  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L     | 282  | HIS  |
| 1   | L     | 287  | HIS  |
| 1   | L     | 446  | HIS  |
| 1   | L     | 473  | HIS  |
| 1   | L     | 477  | ASN  |
| 1   | L     | 509  | ASN  |
| 1   | L     | 592  | ASN  |
| 1   | L     | 604  | ASN  |
| 1   | L     | 612  | HIS  |
| 1   | L     | 618  | ASN  |
| 1   | L     | 670  | HIS  |
| 1   | L     | 699  | ASN  |
| 1   | L     | 738  | ASN  |
| 1   | L     | 745  | ASN  |
| 1   | L     | 850  | GLN  |
| 1   | L     | 930  | HIS  |
| 1   | L     | 952  | HIS  |
| 1   | L     | 968  | ASN  |
| 1   | L     | 994  | HIS  |
| 1   | L     | 1017 | ASN  |
| 1   | L     | 1027 | ASN  |
| 1   | L     | 1083 | GLN  |
| 1   | L     | 1173 | ASN  |
| 1   | L     | 1223 | GLN  |
| 1   | M     | 11   | GLN  |
| 1   | M     | 146  | ASN  |
| 1   | M     | 171  | GLN  |
| 1   | M     | 182  | ASN  |
| 1   | M     | 187  | ASN  |
| 1   | M     | 213  | HIS  |
| 1   | M     | 222  | HIS  |
| 1   | M     | 249  | ASN  |
| 1   | M     | 282  | HIS  |
| 1   | M     | 287  | HIS  |
| 1   | M     | 446  | HIS  |
| 1   | M     | 473  | HIS  |
| 1   | M     | 477  | ASN  |
| 1   | M     | 509  | ASN  |
| 1   | M     | 592  | ASN  |
| 1   | M     | 604  | ASN  |
| 1   | M     | 612  | HIS  |
| 1   | M     | 618  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | M     | 670  | HIS  |
| 1   | M     | 699  | ASN  |
| 1   | M     | 738  | ASN  |
| 1   | M     | 745  | ASN  |
| 1   | M     | 757  | HIS  |
| 1   | M     | 795  | ASN  |
| 1   | M     | 850  | GLN  |
| 1   | M     | 930  | HIS  |
| 1   | M     | 952  | HIS  |
| 1   | M     | 968  | ASN  |
| 1   | M     | 994  | HIS  |
| 1   | M     | 1027 | ASN  |
| 1   | M     | 1083 | GLN  |
| 1   | M     | 1173 | ASN  |
| 1   | M     | 1219 | ASN  |
| 1   | M     | 1223 | GLN  |
| 1   | N     | 11   | GLN  |
| 1   | N     | 146  | ASN  |
| 1   | N     | 171  | GLN  |
| 1   | N     | 182  | ASN  |
| 1   | N     | 187  | ASN  |
| 1   | N     | 222  | HIS  |
| 1   | N     | 249  | ASN  |
| 1   | N     | 282  | HIS  |
| 1   | N     | 287  | HIS  |
| 1   | N     | 446  | HIS  |
| 1   | N     | 473  | HIS  |
| 1   | N     | 477  | ASN  |
| 1   | N     | 509  | ASN  |
| 1   | N     | 592  | ASN  |
| 1   | N     | 604  | ASN  |
| 1   | N     | 612  | HIS  |
| 1   | N     | 618  | ASN  |
| 1   | N     | 670  | HIS  |
| 1   | N     | 699  | ASN  |
| 1   | N     | 738  | ASN  |
| 1   | N     | 745  | ASN  |
| 1   | N     | 850  | GLN  |
| 1   | N     | 930  | HIS  |
| 1   | N     | 952  | HIS  |
| 1   | N     | 968  | ASN  |
| 1   | N     | 994  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | N     | 1027 | ASN  |
| 1   | N     | 1083 | GLN  |
| 1   | N     | 1173 | ASN  |
| 1   | N     | 1223 | GLN  |
| 1   | O     | 11   | GLN  |
| 1   | O     | 146  | ASN  |
| 1   | O     | 171  | GLN  |
| 1   | O     | 182  | ASN  |
| 1   | O     | 187  | ASN  |
| 1   | O     | 249  | ASN  |
| 1   | O     | 282  | HIS  |
| 1   | O     | 287  | HIS  |
| 1   | O     | 446  | HIS  |
| 1   | O     | 473  | HIS  |
| 1   | O     | 477  | ASN  |
| 1   | O     | 509  | ASN  |
| 1   | O     | 592  | ASN  |
| 1   | O     | 604  | ASN  |
| 1   | O     | 612  | HIS  |
| 1   | O     | 618  | ASN  |
| 1   | O     | 699  | ASN  |
| 1   | O     | 738  | ASN  |
| 1   | O     | 745  | ASN  |
| 1   | O     | 850  | GLN  |
| 1   | O     | 930  | HIS  |
| 1   | O     | 952  | HIS  |
| 1   | O     | 968  | ASN  |
| 1   | O     | 994  | HIS  |
| 1   | O     | 1027 | ASN  |
| 1   | O     | 1083 | GLN  |
| 1   | O     | 1173 | ASN  |
| 1   | O     | 1223 | GLN  |
| 1   | P     | 11   | GLN  |
| 1   | P     | 98   | GLN  |
| 1   | P     | 146  | ASN  |
| 1   | P     | 171  | GLN  |
| 1   | P     | 182  | ASN  |
| 1   | P     | 187  | ASN  |
| 1   | P     | 222  | HIS  |
| 1   | P     | 249  | ASN  |
| 1   | P     | 282  | HIS  |
| 1   | P     | 287  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | P     | 446  | HIS  |
| 1   | P     | 473  | HIS  |
| 1   | P     | 477  | ASN  |
| 1   | P     | 509  | ASN  |
| 1   | P     | 592  | ASN  |
| 1   | P     | 604  | ASN  |
| 1   | P     | 612  | HIS  |
| 1   | P     | 618  | ASN  |
| 1   | P     | 699  | ASN  |
| 1   | P     | 738  | ASN  |
| 1   | P     | 745  | ASN  |
| 1   | P     | 850  | GLN  |
| 1   | P     | 930  | HIS  |
| 1   | P     | 952  | HIS  |
| 1   | P     | 968  | ASN  |
| 1   | P     | 994  | HIS  |
| 1   | P     | 1027 | ASN  |
| 1   | P     | 1083 | GLN  |
| 1   | P     | 1173 | ASN  |
| 1   | P     | 1223 | GLN  |
| 1   | P     | 1254 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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 | $\# Z  > 2$ |
| 1   | APK  | P     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%)    | 41,47,47    | 3.30 | 16 (39%)    |
| 1   | APK  | N     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%)    | 41,47,47    | 3.29 | 16 (39%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | APK  | B     | 251 | 1    | 32,33,33     | 2.84 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | J     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.29 | 16 (39%) |
| 1   | APK  | E     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | L     | 251 | 1    | 32,33,33     | 2.84 | 13 (40%) | 41,47,47    | 3.29 | 16 (39%) |
| 1   | APK  | M     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.29 | 16 (39%) |
| 1   | APK  | A     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | H     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | D     | 251 | 1    | 32,33,33     | 2.84 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | I     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | F     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | C     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | K     | 251 | 1    | 32,33,33     | 2.84 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |
| 1   | APK  | O     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.29 | 16 (39%) |
| 1   | APK  | G     | 251 | 1    | 32,33,33     | 2.83 | 13 (40%) | 41,47,47    | 3.30 | 16 (39%) |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 1   | APK  | P     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | N     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | B     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | J     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | E     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | L     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | M     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | A     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | H     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | D     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | I     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | F     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | C     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | K     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |
| 1   | APK  | O     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 1   | APK  | G     | 251 | 1    | -       | 11/19/37/37 | 0/3/3/3 |

All (208) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 251 | APK  | C2'-C3' | -8.23 | 1.31        | 1.53     |
| 1   | B     | 251 | APK  | C2'-C3' | -8.22 | 1.31        | 1.53     |
| 1   | K     | 251 | APK  | C2'-C3' | -8.22 | 1.31        | 1.53     |
| 1   | G     | 251 | APK  | C2'-C3' | -8.21 | 1.31        | 1.53     |
| 1   | N     | 251 | APK  | C2'-C3' | -8.21 | 1.31        | 1.53     |
| 1   | F     | 251 | APK  | C2'-C3' | -8.20 | 1.31        | 1.53     |
| 1   | A     | 251 | APK  | C2'-C3' | -8.20 | 1.31        | 1.53     |
| 1   | E     | 251 | APK  | C2'-C3' | -8.20 | 1.31        | 1.53     |
| 1   | L     | 251 | APK  | C2'-C3' | -8.20 | 1.31        | 1.53     |
| 1   | D     | 251 | APK  | C2'-C3' | -8.19 | 1.31        | 1.53     |
| 1   | H     | 251 | APK  | C2'-C3' | -8.19 | 1.31        | 1.53     |
| 1   | I     | 251 | APK  | C2'-C3' | -8.19 | 1.31        | 1.53     |
| 1   | M     | 251 | APK  | C2'-C3' | -8.19 | 1.31        | 1.53     |
| 1   | O     | 251 | APK  | C2'-C3' | -8.19 | 1.31        | 1.53     |
| 1   | P     | 251 | APK  | C2'-C3' | -8.18 | 1.31        | 1.53     |
| 1   | J     | 251 | APK  | C2'-C3' | -8.17 | 1.31        | 1.53     |
| 1   | L     | 251 | APK  | P-NZ    | 6.40  | 1.69        | 1.61     |
| 1   | K     | 251 | APK  | P-NZ    | 6.38  | 1.69        | 1.61     |
| 1   | H     | 251 | APK  | P-NZ    | 6.37  | 1.69        | 1.61     |
| 1   | B     | 251 | APK  | P-NZ    | 6.37  | 1.69        | 1.61     |
| 1   | D     | 251 | APK  | P-NZ    | 6.36  | 1.69        | 1.61     |
| 1   | A     | 251 | APK  | P-NZ    | 6.33  | 1.69        | 1.61     |
| 1   | N     | 251 | APK  | P-NZ    | 6.33  | 1.69        | 1.61     |
| 1   | E     | 251 | APK  | P-NZ    | 6.32  | 1.69        | 1.61     |
| 1   | G     | 251 | APK  | P-NZ    | 6.32  | 1.69        | 1.61     |
| 1   | J     | 251 | APK  | P-NZ    | 6.32  | 1.69        | 1.61     |
| 1   | F     | 251 | APK  | P-NZ    | 6.32  | 1.69        | 1.61     |
| 1   | P     | 251 | APK  | P-NZ    | 6.31  | 1.69        | 1.61     |
| 1   | I     | 251 | APK  | P-NZ    | 6.30  | 1.69        | 1.61     |
| 1   | M     | 251 | APK  | P-NZ    | 6.30  | 1.69        | 1.61     |
| 1   | O     | 251 | APK  | P-NZ    | 6.30  | 1.69        | 1.61     |
| 1   | C     | 251 | APK  | P-NZ    | 6.27  | 1.69        | 1.61     |
| 1   | D     | 251 | APK  | O3'-C3' | 5.34  | 1.56        | 1.43     |
| 1   | F     | 251 | APK  | O3'-C3' | 5.34  | 1.56        | 1.43     |
| 1   | G     | 251 | APK  | O3'-C3' | 5.34  | 1.56        | 1.43     |
| 1   | I     | 251 | APK  | O3'-C3' | 5.34  | 1.56        | 1.43     |
| 1   | N     | 251 | APK  | O3'-C3' | 5.34  | 1.56        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | O     | 251 | APK  | O3'-C3' | 5.33 | 1.56        | 1.43     |
| 1   | A     | 251 | APK  | O3'-C3' | 5.32 | 1.56        | 1.43     |
| 1   | C     | 251 | APK  | O3'-C3' | 5.32 | 1.56        | 1.43     |
| 1   | L     | 251 | APK  | O3'-C3' | 5.32 | 1.56        | 1.43     |
| 1   | E     | 251 | APK  | O3'-C3' | 5.32 | 1.56        | 1.43     |
| 1   | P     | 251 | APK  | O3'-C3' | 5.32 | 1.56        | 1.43     |
| 1   | B     | 251 | APK  | O3'-C3' | 5.31 | 1.56        | 1.43     |
| 1   | J     | 251 | APK  | O3'-C3' | 5.30 | 1.56        | 1.43     |
| 1   | K     | 251 | APK  | O3'-C3' | 5.30 | 1.56        | 1.43     |
| 1   | H     | 251 | APK  | O3'-C3' | 5.30 | 1.56        | 1.43     |
| 1   | M     | 251 | APK  | O3'-C3' | 5.30 | 1.56        | 1.43     |
| 1   | K     | 251 | APK  | C6-N6   | 4.36 | 1.45        | 1.34     |
| 1   | H     | 251 | APK  | C6-N6   | 4.33 | 1.45        | 1.34     |
| 1   | L     | 251 | APK  | C6-N6   | 4.33 | 1.45        | 1.34     |
| 1   | E     | 251 | APK  | C6-N6   | 4.33 | 1.45        | 1.34     |
| 1   | F     | 251 | APK  | C6-N6   | 4.32 | 1.45        | 1.34     |
| 1   | D     | 251 | APK  | C6-N6   | 4.32 | 1.45        | 1.34     |
| 1   | J     | 251 | APK  | C6-N6   | 4.32 | 1.45        | 1.34     |
| 1   | C     | 251 | APK  | C6-N6   | 4.32 | 1.45        | 1.34     |
| 1   | A     | 251 | APK  | C6-N6   | 4.32 | 1.45        | 1.34     |
| 1   | P     | 251 | APK  | C6-N6   | 4.32 | 1.45        | 1.34     |
| 1   | B     | 251 | APK  | C6-N6   | 4.32 | 1.45        | 1.34     |
| 1   | I     | 251 | APK  | C6-N6   | 4.31 | 1.45        | 1.34     |
| 1   | M     | 251 | APK  | C6-N6   | 4.30 | 1.45        | 1.34     |
| 1   | N     | 251 | APK  | C6-N6   | 4.30 | 1.45        | 1.34     |
| 1   | G     | 251 | APK  | C6-N6   | 4.29 | 1.45        | 1.34     |
| 1   | O     | 251 | APK  | C6-N6   | 4.29 | 1.45        | 1.34     |
| 1   | D     | 251 | APK  | P-O1P   | 4.08 | 1.52        | 1.46     |
| 1   | C     | 251 | APK  | P-O1P   | 4.08 | 1.52        | 1.46     |
| 1   | G     | 251 | APK  | P-O1P   | 4.06 | 1.52        | 1.46     |
| 1   | A     | 251 | APK  | P-O1P   | 4.06 | 1.52        | 1.46     |
| 1   | K     | 251 | APK  | P-O1P   | 4.05 | 1.52        | 1.46     |
| 1   | H     | 251 | APK  | P-O1P   | 4.03 | 1.52        | 1.46     |
| 1   | I     | 251 | APK  | P-O1P   | 4.03 | 1.52        | 1.46     |
| 1   | N     | 251 | APK  | P-O1P   | 4.03 | 1.52        | 1.46     |
| 1   | M     | 251 | APK  | P-O1P   | 4.03 | 1.52        | 1.46     |
| 1   | O     | 251 | APK  | P-O1P   | 4.03 | 1.52        | 1.46     |
| 1   | P     | 251 | APK  | P-O1P   | 4.03 | 1.52        | 1.46     |
| 1   | L     | 251 | APK  | P-O1P   | 4.02 | 1.52        | 1.46     |
| 1   | J     | 251 | APK  | P-O1P   | 4.01 | 1.52        | 1.46     |
| 1   | B     | 251 | APK  | P-O1P   | 4.01 | 1.52        | 1.46     |
| 1   | E     | 251 | APK  | P-O1P   | 4.01 | 1.52        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 251 | APK  | P-O1P | 4.01  | 1.52        | 1.46     |
| 1   | B     | 251 | APK  | C4-N9 | -4.00 | 1.29        | 1.37     |
| 1   | D     | 251 | APK  | C4-N9 | -3.99 | 1.29        | 1.37     |
| 1   | P     | 251 | APK  | C4-N9 | -3.98 | 1.29        | 1.37     |
| 1   | O     | 251 | APK  | C5-N7 | -3.98 | 1.31        | 1.39     |
| 1   | G     | 251 | APK  | C4-N9 | -3.97 | 1.29        | 1.37     |
| 1   | N     | 251 | APK  | C4-N9 | -3.97 | 1.29        | 1.37     |
| 1   | E     | 251 | APK  | C4-N9 | -3.96 | 1.29        | 1.37     |
| 1   | C     | 251 | APK  | C5-N7 | -3.96 | 1.31        | 1.39     |
| 1   | H     | 251 | APK  | C4-N9 | -3.96 | 1.29        | 1.37     |
| 1   | I     | 251 | APK  | C4-N9 | -3.96 | 1.29        | 1.37     |
| 1   | O     | 251 | APK  | C4-N9 | -3.96 | 1.29        | 1.37     |
| 1   | A     | 251 | APK  | C4-N9 | -3.95 | 1.29        | 1.37     |
| 1   | J     | 251 | APK  | C4-N9 | -3.95 | 1.29        | 1.37     |
| 1   | K     | 251 | APK  | C4-N9 | -3.95 | 1.29        | 1.37     |
| 1   | C     | 251 | APK  | C4-N9 | -3.94 | 1.29        | 1.37     |
| 1   | M     | 251 | APK  | C4-N9 | -3.94 | 1.29        | 1.37     |
| 1   | J     | 251 | APK  | C5-N7 | -3.94 | 1.31        | 1.39     |
| 1   | F     | 251 | APK  | C4-N9 | -3.94 | 1.29        | 1.37     |
| 1   | P     | 251 | APK  | C5-N7 | -3.94 | 1.31        | 1.39     |
| 1   | G     | 251 | APK  | C5-N7 | -3.93 | 1.31        | 1.39     |
| 1   | L     | 251 | APK  | C4-N9 | -3.93 | 1.29        | 1.37     |
| 1   | L     | 251 | APK  | C5-N7 | -3.93 | 1.31        | 1.39     |
| 1   | F     | 251 | APK  | C5-N7 | -3.93 | 1.31        | 1.39     |
| 1   | A     | 251 | APK  | C5-N7 | -3.93 | 1.31        | 1.39     |
| 1   | E     | 251 | APK  | C5-N7 | -3.92 | 1.31        | 1.39     |
| 1   | N     | 251 | APK  | C5-N7 | -3.92 | 1.31        | 1.39     |
| 1   | B     | 251 | APK  | C5-N7 | -3.92 | 1.31        | 1.39     |
| 1   | K     | 251 | APK  | C5-N7 | -3.91 | 1.31        | 1.39     |
| 1   | H     | 251 | APK  | C5-N7 | -3.91 | 1.32        | 1.39     |
| 1   | I     | 251 | APK  | C5-N7 | -3.91 | 1.32        | 1.39     |
| 1   | M     | 251 | APK  | C5-N7 | -3.91 | 1.32        | 1.39     |
| 1   | D     | 251 | APK  | C5-N7 | -3.90 | 1.32        | 1.39     |
| 1   | D     | 251 | APK  | P-O2P | -3.11 | 1.48        | 1.56     |
| 1   | K     | 251 | APK  | P-O2P | -3.10 | 1.48        | 1.56     |
| 1   | E     | 251 | APK  | P-O2P | -3.09 | 1.48        | 1.56     |
| 1   | A     | 251 | APK  | P-O2P | -3.08 | 1.48        | 1.56     |
| 1   | C     | 251 | APK  | P-O2P | -3.08 | 1.48        | 1.56     |
| 1   | H     | 251 | APK  | P-O2P | -3.08 | 1.48        | 1.56     |
| 1   | I     | 251 | APK  | P-O2P | -3.08 | 1.48        | 1.56     |
| 1   | M     | 251 | APK  | P-O2P | -3.08 | 1.48        | 1.56     |
| 1   | O     | 251 | APK  | P-O2P | -3.08 | 1.48        | 1.56     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 251 | APK  | P-O2P | -3.07 | 1.48        | 1.56     |
| 1   | J     | 251 | APK  | P-O2P | -3.07 | 1.48        | 1.56     |
| 1   | N     | 251 | APK  | P-O2P | -3.07 | 1.48        | 1.56     |
| 1   | P     | 251 | APK  | P-O2P | -3.07 | 1.48        | 1.56     |
| 1   | G     | 251 | APK  | P-O2P | -3.07 | 1.48        | 1.56     |
| 1   | B     | 251 | APK  | P-O2P | -3.07 | 1.48        | 1.56     |
| 1   | L     | 251 | APK  | P-O2P | -3.06 | 1.48        | 1.56     |
| 1   | O     | 251 | APK  | C4-N3 | -2.91 | 1.29        | 1.34     |
| 1   | E     | 251 | APK  | C4-N3 | -2.89 | 1.29        | 1.34     |
| 1   | G     | 251 | APK  | C4-N3 | -2.89 | 1.29        | 1.34     |
| 1   | A     | 251 | APK  | C4-N3 | -2.89 | 1.29        | 1.34     |
| 1   | F     | 251 | APK  | C4-N3 | -2.89 | 1.29        | 1.34     |
| 1   | D     | 251 | APK  | C4-N3 | -2.88 | 1.29        | 1.34     |
| 1   | H     | 251 | APK  | C4-N3 | -2.88 | 1.29        | 1.34     |
| 1   | I     | 251 | APK  | C4-N3 | -2.88 | 1.29        | 1.34     |
| 1   | M     | 251 | APK  | C4-N3 | -2.88 | 1.29        | 1.34     |
| 1   | J     | 251 | APK  | C4-N3 | -2.88 | 1.29        | 1.34     |
| 1   | N     | 251 | APK  | C4-N3 | -2.88 | 1.29        | 1.34     |
| 1   | C     | 251 | APK  | C4-N3 | -2.88 | 1.29        | 1.34     |
| 1   | L     | 251 | APK  | C4-N3 | -2.87 | 1.29        | 1.34     |
| 1   | K     | 251 | APK  | C4-N3 | -2.87 | 1.29        | 1.34     |
| 1   | P     | 251 | APK  | C4-N3 | -2.86 | 1.29        | 1.34     |
| 1   | B     | 251 | APK  | C4-N3 | -2.84 | 1.29        | 1.34     |
| 1   | G     | 251 | APK  | C8-N9 | 2.70  | 1.42        | 1.37     |
| 1   | P     | 251 | APK  | C8-N9 | 2.69  | 1.42        | 1.37     |
| 1   | L     | 251 | APK  | C8-N9 | 2.68  | 1.42        | 1.37     |
| 1   | M     | 251 | APK  | C8-N9 | 2.68  | 1.42        | 1.37     |
| 1   | O     | 251 | APK  | C8-N9 | 2.68  | 1.42        | 1.37     |
| 1   | D     | 251 | APK  | C8-N9 | 2.68  | 1.42        | 1.37     |
| 1   | J     | 251 | APK  | C8-N9 | 2.68  | 1.42        | 1.37     |
| 1   | A     | 251 | APK  | C8-N9 | 2.67  | 1.42        | 1.37     |
| 1   | B     | 251 | APK  | C8-N9 | 2.66  | 1.42        | 1.37     |
| 1   | I     | 251 | APK  | C8-N9 | 2.66  | 1.42        | 1.37     |
| 1   | E     | 251 | APK  | C8-N9 | 2.66  | 1.42        | 1.37     |
| 1   | N     | 251 | APK  | C8-N9 | 2.66  | 1.42        | 1.37     |
| 1   | F     | 251 | APK  | C8-N9 | 2.65  | 1.42        | 1.37     |
| 1   | C     | 251 | APK  | C8-N9 | 2.65  | 1.42        | 1.37     |
| 1   | K     | 251 | APK  | C8-N9 | 2.64  | 1.42        | 1.37     |
| 1   | H     | 251 | APK  | C8-N9 | 2.63  | 1.42        | 1.37     |
| 1   | O     | 251 | APK  | CA-N  | -2.61 | 1.40        | 1.48     |
| 1   | L     | 251 | APK  | CA-N  | -2.61 | 1.40        | 1.48     |
| 1   | C     | 251 | APK  | CA-N  | -2.60 | 1.40        | 1.48     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 251 | APK  | CA-N    | -2.60 | 1.40        | 1.48     |
| 1   | F     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | M     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | A     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | B     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | K     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | P     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | H     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | I     | 251 | APK  | CA-N    | -2.59 | 1.40        | 1.48     |
| 1   | E     | 251 | APK  | CA-N    | -2.58 | 1.40        | 1.48     |
| 1   | J     | 251 | APK  | CA-N    | -2.57 | 1.40        | 1.48     |
| 1   | N     | 251 | APK  | CA-N    | -2.57 | 1.40        | 1.48     |
| 1   | D     | 251 | APK  | CA-N    | -2.55 | 1.40        | 1.48     |
| 1   | L     | 251 | APK  | C8-N7   | -2.54 | 1.26        | 1.31     |
| 1   | O     | 251 | APK  | C8-N7   | -2.54 | 1.26        | 1.31     |
| 1   | J     | 251 | APK  | C8-N7   | -2.54 | 1.26        | 1.31     |
| 1   | B     | 251 | APK  | C8-N7   | -2.53 | 1.26        | 1.31     |
| 1   | D     | 251 | APK  | C8-N7   | -2.53 | 1.26        | 1.31     |
| 1   | H     | 251 | APK  | C8-N7   | -2.52 | 1.26        | 1.31     |
| 1   | I     | 251 | APK  | C8-N7   | -2.52 | 1.26        | 1.31     |
| 1   | M     | 251 | APK  | C8-N7   | -2.52 | 1.26        | 1.31     |
| 1   | P     | 251 | APK  | C8-N7   | -2.51 | 1.26        | 1.31     |
| 1   | A     | 251 | APK  | C8-N7   | -2.51 | 1.26        | 1.31     |
| 1   | C     | 251 | APK  | C8-N7   | -2.51 | 1.26        | 1.31     |
| 1   | F     | 251 | APK  | C8-N7   | -2.51 | 1.26        | 1.31     |
| 1   | E     | 251 | APK  | C8-N7   | -2.50 | 1.26        | 1.31     |
| 1   | K     | 251 | APK  | C8-N7   | -2.49 | 1.26        | 1.31     |
| 1   | G     | 251 | APK  | C8-N7   | -2.49 | 1.26        | 1.31     |
| 1   | N     | 251 | APK  | C8-N7   | -2.49 | 1.26        | 1.31     |
| 1   | I     | 251 | APK  | O2'-C2' | 2.11  | 1.48        | 1.43     |
| 1   | F     | 251 | APK  | O2'-C2' | 2.10  | 1.48        | 1.43     |
| 1   | K     | 251 | APK  | O2'-C2' | 2.10  | 1.48        | 1.43     |
| 1   | L     | 251 | APK  | O2'-C2' | 2.09  | 1.48        | 1.43     |
| 1   | N     | 251 | APK  | O2'-C2' | 2.09  | 1.48        | 1.43     |
| 1   | M     | 251 | APK  | O2'-C2' | 2.09  | 1.48        | 1.43     |
| 1   | A     | 251 | APK  | O2'-C2' | 2.09  | 1.48        | 1.43     |
| 1   | D     | 251 | APK  | O2'-C2' | 2.08  | 1.48        | 1.43     |
| 1   | E     | 251 | APK  | O2'-C2' | 2.08  | 1.48        | 1.43     |
| 1   | C     | 251 | APK  | O2'-C2' | 2.08  | 1.48        | 1.43     |
| 1   | H     | 251 | APK  | O2'-C2' | 2.08  | 1.48        | 1.43     |
| 1   | O     | 251 | APK  | O2'-C2' | 2.08  | 1.48        | 1.43     |
| 1   | J     | 251 | APK  | O2'-C2' | 2.07  | 1.48        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | G     | 251 | APK  | O2'-C2' | 2.07 | 1.48        | 1.43     |
| 1   | B     | 251 | APK  | O2'-C2' | 2.06 | 1.48        | 1.43     |
| 1   | P     | 251 | APK  | O2'-C2' | 2.06 | 1.48        | 1.43     |

All (256) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 251 | APK  | C5-C4-N3  | -7.58 | 116.28      | 126.72   |
| 1   | E     | 251 | APK  | C5-C4-N3  | -7.57 | 116.29      | 126.72   |
| 1   | K     | 251 | APK  | C5-C4-N3  | -7.57 | 116.29      | 126.72   |
| 1   | B     | 251 | APK  | C5-C4-N3  | -7.57 | 116.29      | 126.72   |
| 1   | I     | 251 | APK  | C5-C4-N3  | -7.56 | 116.31      | 126.72   |
| 1   | F     | 251 | APK  | C5-C4-N3  | -7.55 | 116.32      | 126.72   |
| 1   | D     | 251 | APK  | C5-C4-N3  | -7.55 | 116.32      | 126.72   |
| 1   | P     | 251 | APK  | C5-C4-N3  | -7.55 | 116.32      | 126.72   |
| 1   | A     | 251 | APK  | C5-C4-N3  | -7.54 | 116.33      | 126.72   |
| 1   | M     | 251 | APK  | C5-C4-N3  | -7.54 | 116.33      | 126.72   |
| 1   | L     | 251 | APK  | C5-C4-N3  | -7.53 | 116.34      | 126.72   |
| 1   | C     | 251 | APK  | C5-C4-N3  | -7.53 | 116.35      | 126.72   |
| 1   | N     | 251 | APK  | C5-C4-N3  | -7.52 | 116.36      | 126.72   |
| 1   | O     | 251 | APK  | C5-C4-N3  | -7.52 | 116.36      | 126.72   |
| 1   | G     | 251 | APK  | C5-C4-N3  | -7.51 | 116.37      | 126.72   |
| 1   | J     | 251 | APK  | C5-C4-N3  | -7.49 | 116.40      | 126.72   |
| 1   | K     | 251 | APK  | N3-C4-N9  | 7.44  | 139.82      | 127.17   |
| 1   | E     | 251 | APK  | N3-C4-N9  | 7.43  | 139.81      | 127.17   |
| 1   | C     | 251 | APK  | N3-C4-N9  | 7.42  | 139.79      | 127.17   |
| 1   | F     | 251 | APK  | N3-C4-N9  | 7.41  | 139.78      | 127.17   |
| 1   | H     | 251 | APK  | N3-C4-N9  | 7.41  | 139.78      | 127.17   |
| 1   | I     | 251 | APK  | N3-C4-N9  | 7.41  | 139.78      | 127.17   |
| 1   | P     | 251 | APK  | N3-C4-N9  | 7.40  | 139.76      | 127.17   |
| 1   | A     | 251 | APK  | N3-C4-N9  | 7.40  | 139.75      | 127.17   |
| 1   | B     | 251 | APK  | N3-C4-N9  | 7.40  | 139.75      | 127.17   |
| 1   | O     | 251 | APK  | N3-C4-N9  | 7.39  | 139.74      | 127.17   |
| 1   | L     | 251 | APK  | N3-C4-N9  | 7.39  | 139.74      | 127.17   |
| 1   | M     | 251 | APK  | N3-C4-N9  | 7.39  | 139.73      | 127.17   |
| 1   | N     | 251 | APK  | N3-C4-N9  | 7.39  | 139.73      | 127.17   |
| 1   | G     | 251 | APK  | N3-C4-N9  | 7.38  | 139.73      | 127.17   |
| 1   | D     | 251 | APK  | N3-C4-N9  | 7.38  | 139.73      | 127.17   |
| 1   | J     | 251 | APK  | N3-C4-N9  | 7.37  | 139.70      | 127.17   |
| 1   | J     | 251 | APK  | C4-N9-C1' | 6.24  | 141.23      | 126.63   |
| 1   | A     | 251 | APK  | C4-N9-C1' | 6.24  | 141.23      | 126.63   |
| 1   | D     | 251 | APK  | C4-N9-C1' | 6.24  | 141.22      | 126.63   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | P     | 251 | APK  | C4-N9-C1' | 6.24  | 141.22      | 126.63   |
| 1   | B     | 251 | APK  | C4-N9-C1' | 6.24  | 141.21      | 126.63   |
| 1   | G     | 251 | APK  | C4-N9-C1' | 6.23  | 141.21      | 126.63   |
| 1   | O     | 251 | APK  | C4-N9-C1' | 6.23  | 141.21      | 126.63   |
| 1   | L     | 251 | APK  | C4-N9-C1' | 6.23  | 141.20      | 126.63   |
| 1   | N     | 251 | APK  | C4-N9-C1' | 6.23  | 141.19      | 126.63   |
| 1   | M     | 251 | APK  | C4-N9-C1' | 6.23  | 141.19      | 126.63   |
| 1   | H     | 251 | APK  | C4-N9-C1' | 6.22  | 141.17      | 126.63   |
| 1   | I     | 251 | APK  | C4-N9-C1' | 6.22  | 141.17      | 126.63   |
| 1   | F     | 251 | APK  | C4-N9-C1' | 6.21  | 141.16      | 126.63   |
| 1   | E     | 251 | APK  | C4-N9-C1' | 6.21  | 141.15      | 126.63   |
| 1   | C     | 251 | APK  | C4-N9-C1' | 6.20  | 141.13      | 126.63   |
| 1   | K     | 251 | APK  | C4-N9-C1' | 6.20  | 141.13      | 126.63   |
| 1   | C     | 251 | APK  | C4-C5-N7  | 6.13  | 117.59      | 110.58   |
| 1   | G     | 251 | APK  | C4-C5-N7  | 6.12  | 117.58      | 110.58   |
| 1   | P     | 251 | APK  | C4-C5-N7  | 6.11  | 117.57      | 110.58   |
| 1   | J     | 251 | APK  | C4-C5-N7  | 6.11  | 117.56      | 110.58   |
| 1   | N     | 251 | APK  | C4-C5-N7  | 6.10  | 117.56      | 110.58   |
| 1   | O     | 251 | APK  | C4-C5-N7  | 6.10  | 117.55      | 110.58   |
| 1   | A     | 251 | APK  | C4-C5-N7  | 6.08  | 117.53      | 110.58   |
| 1   | E     | 251 | APK  | C4-C5-N7  | 6.08  | 117.53      | 110.58   |
| 1   | F     | 251 | APK  | C4-C5-N7  | 6.07  | 117.53      | 110.58   |
| 1   | K     | 251 | APK  | C4-C5-N7  | 6.07  | 117.52      | 110.58   |
| 1   | L     | 251 | APK  | C4-C5-N7  | 6.07  | 117.52      | 110.58   |
| 1   | D     | 251 | APK  | C4-C5-N7  | 6.07  | 117.52      | 110.58   |
| 1   | I     | 251 | APK  | C4-C5-N7  | 6.06  | 117.51      | 110.58   |
| 1   | M     | 251 | APK  | C4-C5-N7  | 6.06  | 117.51      | 110.58   |
| 1   | B     | 251 | APK  | C4-C5-N7  | 6.03  | 117.48      | 110.58   |
| 1   | H     | 251 | APK  | C4-C5-N7  | 6.03  | 117.48      | 110.58   |
| 1   | P     | 251 | APK  | C6-C5-N7  | -5.43 | 121.62      | 132.09   |
| 1   | N     | 251 | APK  | C6-C5-N7  | -5.42 | 121.64      | 132.09   |
| 1   | C     | 251 | APK  | C6-C5-N7  | -5.42 | 121.65      | 132.09   |
| 1   | D     | 251 | APK  | C6-C5-N7  | -5.42 | 121.65      | 132.09   |
| 1   | G     | 251 | APK  | C6-C5-N7  | -5.41 | 121.66      | 132.09   |
| 1   | I     | 251 | APK  | C6-C5-N7  | -5.41 | 121.66      | 132.09   |
| 1   | F     | 251 | APK  | C6-C5-N7  | -5.40 | 121.67      | 132.09   |
| 1   | A     | 251 | APK  | C6-C5-N7  | -5.40 | 121.68      | 132.09   |
| 1   | H     | 251 | APK  | C6-C5-N7  | -5.40 | 121.68      | 132.09   |
| 1   | M     | 251 | APK  | C6-C5-N7  | -5.40 | 121.68      | 132.09   |
| 1   | J     | 251 | APK  | C6-C5-N7  | -5.40 | 121.68      | 132.09   |
| 1   | E     | 251 | APK  | C6-C5-N7  | -5.40 | 121.68      | 132.09   |
| 1   | O     | 251 | APK  | C6-C5-N7  | -5.40 | 121.69      | 132.09   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | K     | 251 | APK  | C6-C5-N7    | -5.39 | 121.70      | 132.09   |
| 1   | L     | 251 | APK  | C6-C5-N7    | -5.38 | 121.71      | 132.09   |
| 1   | B     | 251 | APK  | C6-C5-N7    | -5.38 | 121.72      | 132.09   |
| 1   | C     | 251 | APK  | N1-C2-N3    | -5.37 | 120.46      | 128.58   |
| 1   | D     | 251 | APK  | N1-C2-N3    | -5.36 | 120.47      | 128.58   |
| 1   | E     | 251 | APK  | N1-C2-N3    | -5.36 | 120.47      | 128.58   |
| 1   | F     | 251 | APK  | N1-C2-N3    | -5.36 | 120.47      | 128.58   |
| 1   | P     | 251 | APK  | N1-C2-N3    | -5.35 | 120.48      | 128.58   |
| 1   | H     | 251 | APK  | N1-C2-N3    | -5.34 | 120.49      | 128.58   |
| 1   | K     | 251 | APK  | N1-C2-N3    | -5.34 | 120.49      | 128.58   |
| 1   | M     | 251 | APK  | N1-C2-N3    | -5.34 | 120.49      | 128.58   |
| 1   | O     | 251 | APK  | N1-C2-N3    | -5.34 | 120.49      | 128.58   |
| 1   | A     | 251 | APK  | N1-C2-N3    | -5.34 | 120.50      | 128.58   |
| 1   | B     | 251 | APK  | N1-C2-N3    | -5.33 | 120.51      | 128.58   |
| 1   | L     | 251 | APK  | N1-C2-N3    | -5.33 | 120.51      | 128.58   |
| 1   | J     | 251 | APK  | N1-C2-N3    | -5.33 | 120.51      | 128.58   |
| 1   | N     | 251 | APK  | N1-C2-N3    | -5.33 | 120.51      | 128.58   |
| 1   | G     | 251 | APK  | N1-C2-N3    | -5.33 | 120.52      | 128.58   |
| 1   | I     | 251 | APK  | N1-C2-N3    | -5.32 | 120.53      | 128.58   |
| 1   | E     | 251 | APK  | C2-N3-C4    | 5.12  | 124.35      | 111.83   |
| 1   | C     | 251 | APK  | C2-N3-C4    | 5.11  | 124.31      | 111.83   |
| 1   | F     | 251 | APK  | C2-N3-C4    | 5.11  | 124.30      | 111.83   |
| 1   | D     | 251 | APK  | C2-N3-C4    | 5.10  | 124.29      | 111.83   |
| 1   | H     | 251 | APK  | C2-N3-C4    | 5.10  | 124.29      | 111.83   |
| 1   | B     | 251 | APK  | C2-N3-C4    | 5.10  | 124.28      | 111.83   |
| 1   | A     | 251 | APK  | C2-N3-C4    | 5.10  | 124.28      | 111.83   |
| 1   | K     | 251 | APK  | C2-N3-C4    | 5.10  | 124.28      | 111.83   |
| 1   | P     | 251 | APK  | C2-N3-C4    | 5.10  | 124.28      | 111.83   |
| 1   | M     | 251 | APK  | C2-N3-C4    | 5.09  | 124.27      | 111.83   |
| 1   | O     | 251 | APK  | C2-N3-C4    | 5.09  | 124.26      | 111.83   |
| 1   | L     | 251 | APK  | C2-N3-C4    | 5.09  | 124.25      | 111.83   |
| 1   | G     | 251 | APK  | C2-N3-C4    | 5.09  | 124.25      | 111.83   |
| 1   | I     | 251 | APK  | C2-N3-C4    | 5.09  | 124.25      | 111.83   |
| 1   | J     | 251 | APK  | C2-N3-C4    | 5.08  | 124.24      | 111.83   |
| 1   | N     | 251 | APK  | C2-N3-C4    | 5.08  | 124.24      | 111.83   |
| 1   | D     | 251 | APK  | C2'-C3'-C4' | 5.05  | 112.36      | 102.61   |
| 1   | G     | 251 | APK  | C2'-C3'-C4' | 5.04  | 112.35      | 102.61   |
| 1   | F     | 251 | APK  | C2'-C3'-C4' | 5.04  | 112.35      | 102.61   |
| 1   | P     | 251 | APK  | C2'-C3'-C4' | 5.04  | 112.35      | 102.61   |
| 1   | A     | 251 | APK  | C2'-C3'-C4' | 5.04  | 112.34      | 102.61   |
| 1   | K     | 251 | APK  | C2'-C3'-C4' | 5.04  | 112.34      | 102.61   |
| 1   | C     | 251 | APK  | C2'-C3'-C4' | 5.04  | 112.34      | 102.61   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | E     | 251 | APK  | C2'-C3'-C4' | 5.03  | 112.34      | 102.61   |
| 1   | B     | 251 | APK  | C2'-C3'-C4' | 5.03  | 112.34      | 102.61   |
| 1   | L     | 251 | APK  | C2'-C3'-C4' | 5.03  | 112.33      | 102.61   |
| 1   | N     | 251 | APK  | C2'-C3'-C4' | 5.03  | 112.33      | 102.61   |
| 1   | J     | 251 | APK  | C2'-C3'-C4' | 5.03  | 112.33      | 102.61   |
| 1   | I     | 251 | APK  | C2'-C3'-C4' | 5.02  | 112.31      | 102.61   |
| 1   | O     | 251 | APK  | C2'-C3'-C4' | 5.02  | 112.31      | 102.61   |
| 1   | H     | 251 | APK  | C2'-C3'-C4' | 5.01  | 112.30      | 102.61   |
| 1   | M     | 251 | APK  | C2'-C3'-C4' | 5.01  | 112.30      | 102.61   |
| 1   | K     | 251 | APK  | O4'-C4'-C3' | -4.83 | 95.57       | 105.15   |
| 1   | B     | 251 | APK  | O4'-C4'-C3' | -4.82 | 95.59       | 105.15   |
| 1   | J     | 251 | APK  | O4'-C4'-C3' | -4.82 | 95.59       | 105.15   |
| 1   | C     | 251 | APK  | O4'-C4'-C3' | -4.81 | 95.61       | 105.15   |
| 1   | G     | 251 | APK  | O4'-C4'-C3' | -4.81 | 95.61       | 105.15   |
| 1   | E     | 251 | APK  | O4'-C4'-C3' | -4.81 | 95.61       | 105.15   |
| 1   | P     | 251 | APK  | O4'-C4'-C3' | -4.80 | 95.62       | 105.15   |
| 1   | F     | 251 | APK  | O4'-C4'-C3' | -4.80 | 95.62       | 105.15   |
| 1   | A     | 251 | APK  | O4'-C4'-C3' | -4.80 | 95.62       | 105.15   |
| 1   | D     | 251 | APK  | O4'-C4'-C3' | -4.80 | 95.62       | 105.15   |
| 1   | I     | 251 | APK  | O4'-C4'-C3' | -4.80 | 95.62       | 105.15   |
| 1   | M     | 251 | APK  | O4'-C4'-C3' | -4.80 | 95.63       | 105.15   |
| 1   | N     | 251 | APK  | O4'-C4'-C3' | -4.80 | 95.63       | 105.15   |
| 1   | O     | 251 | APK  | O4'-C4'-C3' | -4.79 | 95.64       | 105.15   |
| 1   | H     | 251 | APK  | O4'-C4'-C3' | -4.79 | 95.65       | 105.15   |
| 1   | L     | 251 | APK  | O4'-C4'-C3' | -4.78 | 95.66       | 105.15   |
| 1   | G     | 251 | APK  | C1'-N9-C8   | -4.62 | 116.85      | 127.09   |
| 1   | A     | 251 | APK  | C1'-N9-C8   | -4.61 | 116.86      | 127.09   |
| 1   | P     | 251 | APK  | C5-N7-C8    | -4.61 | 96.20       | 103.45   |
| 1   | D     | 251 | APK  | C5-N7-C8    | -4.61 | 96.20       | 103.45   |
| 1   | N     | 251 | APK  | C1'-N9-C8   | -4.61 | 116.87      | 127.09   |
| 1   | J     | 251 | APK  | C5-N7-C8    | -4.61 | 96.21       | 103.45   |
| 1   | N     | 251 | APK  | C5-N7-C8    | -4.61 | 96.21       | 103.45   |
| 1   | P     | 251 | APK  | C1'-N9-C8   | -4.61 | 116.87      | 127.09   |
| 1   | B     | 251 | APK  | C1'-N9-C8   | -4.61 | 116.87      | 127.09   |
| 1   | J     | 251 | APK  | C1'-N9-C8   | -4.60 | 116.88      | 127.09   |
| 1   | O     | 251 | APK  | C1'-N9-C8   | -4.60 | 116.88      | 127.09   |
| 1   | D     | 251 | APK  | C1'-N9-C8   | -4.60 | 116.89      | 127.09   |
| 1   | G     | 251 | APK  | C5-N7-C8    | -4.60 | 96.22       | 103.45   |
| 1   | E     | 251 | APK  | C1'-N9-C8   | -4.60 | 116.89      | 127.09   |
| 1   | F     | 251 | APK  | C1'-N9-C8   | -4.60 | 116.89      | 127.09   |
| 1   | K     | 251 | APK  | C5-N7-C8    | -4.59 | 96.23       | 103.45   |
| 1   | I     | 251 | APK  | C1'-N9-C8   | -4.59 | 116.90      | 127.09   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 251 | APK  | C5-N7-C8  | -4.59 | 96.24       | 103.45   |
| 1   | C     | 251 | APK  | C1'-N9-C8 | -4.59 | 116.91      | 127.09   |
| 1   | A     | 251 | APK  | C5-N7-C8  | -4.59 | 96.24       | 103.45   |
| 1   | L     | 251 | APK  | C1'-N9-C8 | -4.59 | 116.91      | 127.09   |
| 1   | H     | 251 | APK  | C5-N7-C8  | -4.59 | 96.24       | 103.45   |
| 1   | I     | 251 | APK  | C5-N7-C8  | -4.59 | 96.24       | 103.45   |
| 1   | M     | 251 | APK  | C5-N7-C8  | -4.59 | 96.24       | 103.45   |
| 1   | C     | 251 | APK  | C5-N7-C8  | -4.59 | 96.24       | 103.45   |
| 1   | K     | 251 | APK  | C1'-N9-C8 | -4.59 | 116.92      | 127.09   |
| 1   | M     | 251 | APK  | C1'-N9-C8 | -4.59 | 116.92      | 127.09   |
| 1   | E     | 251 | APK  | C5-N7-C8  | -4.58 | 96.24       | 103.45   |
| 1   | H     | 251 | APK  | C1'-N9-C8 | -4.58 | 116.93      | 127.09   |
| 1   | L     | 251 | APK  | C5-N7-C8  | -4.57 | 96.26       | 103.45   |
| 1   | H     | 251 | APK  | N9-C8-N7  | 4.57  | 120.42      | 113.94   |
| 1   | O     | 251 | APK  | C5-N7-C8  | -4.57 | 96.26       | 103.45   |
| 1   | J     | 251 | APK  | N9-C8-N7  | 4.57  | 120.42      | 113.94   |
| 1   | D     | 251 | APK  | N9-C8-N7  | 4.57  | 120.42      | 113.94   |
| 1   | F     | 251 | APK  | C5-N7-C8  | -4.57 | 96.27       | 103.45   |
| 1   | M     | 251 | APK  | N9-C8-N7  | 4.57  | 120.41      | 113.94   |
| 1   | B     | 251 | APK  | N9-C8-N7  | 4.56  | 120.41      | 113.94   |
| 1   | I     | 251 | APK  | N9-C8-N7  | 4.56  | 120.40      | 113.94   |
| 1   | K     | 251 | APK  | N9-C8-N7  | 4.56  | 120.40      | 113.94   |
| 1   | L     | 251 | APK  | N9-C8-N7  | 4.55  | 120.39      | 113.94   |
| 1   | P     | 251 | APK  | N9-C8-N7  | 4.55  | 120.39      | 113.94   |
| 1   | A     | 251 | APK  | N9-C8-N7  | 4.55  | 120.39      | 113.94   |
| 1   | O     | 251 | APK  | N9-C8-N7  | 4.54  | 120.37      | 113.94   |
| 1   | N     | 251 | APK  | N9-C8-N7  | 4.54  | 120.37      | 113.94   |
| 1   | E     | 251 | APK  | N9-C8-N7  | 4.53  | 120.36      | 113.94   |
| 1   | G     | 251 | APK  | N9-C8-N7  | 4.52  | 120.35      | 113.94   |
| 1   | C     | 251 | APK  | N9-C8-N7  | 4.52  | 120.34      | 113.94   |
| 1   | F     | 251 | APK  | N9-C8-N7  | 4.51  | 120.34      | 113.94   |
| 1   | J     | 251 | APK  | C4-N9-C8  | -3.74 | 101.81      | 105.74   |
| 1   | M     | 251 | APK  | C4-N9-C8  | -3.74 | 101.82      | 105.74   |
| 1   | L     | 251 | APK  | C4-N9-C8  | -3.73 | 101.82      | 105.74   |
| 1   | D     | 251 | APK  | C4-N9-C8  | -3.73 | 101.82      | 105.74   |
| 1   | H     | 251 | APK  | C4-N9-C8  | -3.72 | 101.83      | 105.74   |
| 1   | O     | 251 | APK  | C4-N9-C8  | -3.72 | 101.84      | 105.74   |
| 1   | P     | 251 | APK  | C4-N9-C8  | -3.72 | 101.84      | 105.74   |
| 1   | B     | 251 | APK  | C4-N9-C8  | -3.71 | 101.84      | 105.74   |
| 1   | A     | 251 | APK  | C4-N9-C8  | -3.71 | 101.84      | 105.74   |
| 1   | I     | 251 | APK  | C4-N9-C8  | -3.70 | 101.85      | 105.74   |
| 1   | N     | 251 | APK  | C4-N9-C8  | -3.69 | 101.86      | 105.74   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 251 | APK  | C4-N9-C8    | -3.69 | 101.87      | 105.74   |
| 1   | F     | 251 | APK  | C4-N9-C8    | -3.68 | 101.87      | 105.74   |
| 1   | E     | 251 | APK  | C4-N9-C8    | -3.67 | 101.88      | 105.74   |
| 1   | K     | 251 | APK  | C4-N9-C8    | -3.67 | 101.88      | 105.74   |
| 1   | C     | 251 | APK  | C4-N9-C8    | -3.67 | 101.89      | 105.74   |
| 1   | D     | 251 | APK  | C3'-C2'-C1' | -3.66 | 94.54       | 101.46   |
| 1   | P     | 251 | APK  | C3'-C2'-C1' | -3.66 | 94.55       | 101.46   |
| 1   | J     | 251 | APK  | C3'-C2'-C1' | -3.65 | 94.55       | 101.46   |
| 1   | K     | 251 | APK  | C3'-C2'-C1' | -3.65 | 94.56       | 101.46   |
| 1   | H     | 251 | APK  | C3'-C2'-C1' | -3.65 | 94.57       | 101.46   |
| 1   | I     | 251 | APK  | C3'-C2'-C1' | -3.65 | 94.57       | 101.46   |
| 1   | O     | 251 | APK  | C3'-C2'-C1' | -3.65 | 94.57       | 101.46   |
| 1   | A     | 251 | APK  | C3'-C2'-C1' | -3.64 | 94.57       | 101.46   |
| 1   | F     | 251 | APK  | C3'-C2'-C1' | -3.64 | 94.58       | 101.46   |
| 1   | E     | 251 | APK  | C3'-C2'-C1' | -3.64 | 94.59       | 101.46   |
| 1   | M     | 251 | APK  | C3'-C2'-C1' | -3.63 | 94.59       | 101.46   |
| 1   | N     | 251 | APK  | C3'-C2'-C1' | -3.63 | 94.59       | 101.46   |
| 1   | C     | 251 | APK  | C3'-C2'-C1' | -3.63 | 94.60       | 101.46   |
| 1   | G     | 251 | APK  | C3'-C2'-C1' | -3.63 | 94.60       | 101.46   |
| 1   | B     | 251 | APK  | C3'-C2'-C1' | -3.62 | 94.61       | 101.46   |
| 1   | L     | 251 | APK  | C3'-C2'-C1' | -3.62 | 94.61       | 101.46   |
| 1   | G     | 251 | APK  | P-NZ-CE     | -3.57 | 119.63      | 124.61   |
| 1   | N     | 251 | APK  | P-NZ-CE     | -3.56 | 119.65      | 124.61   |
| 1   | L     | 251 | APK  | P-NZ-CE     | -3.55 | 119.66      | 124.61   |
| 1   | K     | 251 | APK  | P-NZ-CE     | -3.55 | 119.66      | 124.61   |
| 1   | A     | 251 | APK  | P-NZ-CE     | -3.54 | 119.67      | 124.61   |
| 1   | H     | 251 | APK  | P-NZ-CE     | -3.54 | 119.67      | 124.61   |
| 1   | B     | 251 | APK  | P-NZ-CE     | -3.54 | 119.67      | 124.61   |
| 1   | I     | 251 | APK  | P-NZ-CE     | -3.54 | 119.67      | 124.61   |
| 1   | M     | 251 | APK  | P-NZ-CE     | -3.54 | 119.67      | 124.61   |
| 1   | O     | 251 | APK  | P-NZ-CE     | -3.54 | 119.67      | 124.61   |
| 1   | F     | 251 | APK  | P-NZ-CE     | -3.54 | 119.67      | 124.61   |
| 1   | C     | 251 | APK  | P-NZ-CE     | -3.53 | 119.68      | 124.61   |
| 1   | D     | 251 | APK  | P-NZ-CE     | -3.53 | 119.68      | 124.61   |
| 1   | J     | 251 | APK  | P-NZ-CE     | -3.53 | 119.68      | 124.61   |
| 1   | P     | 251 | APK  | P-NZ-CE     | -3.53 | 119.69      | 124.61   |
| 1   | E     | 251 | APK  | P-NZ-CE     | -3.52 | 119.70      | 124.61   |
| 1   | H     | 251 | APK  | C6-C5-C4    | 2.66  | 120.81      | 117.18   |
| 1   | D     | 251 | APK  | C6-C5-C4    | 2.65  | 120.80      | 117.18   |
| 1   | I     | 251 | APK  | C6-C5-C4    | 2.65  | 120.79      | 117.18   |
| 1   | M     | 251 | APK  | C6-C5-C4    | 2.64  | 120.78      | 117.18   |
| 1   | P     | 251 | APK  | C6-C5-C4    | 2.63  | 120.78      | 117.18   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | B     | 251 | APK  | C6-C5-C4 | 2.63 | 120.77      | 117.18   |
| 1   | F     | 251 | APK  | C6-C5-C4 | 2.63 | 120.77      | 117.18   |
| 1   | N     | 251 | APK  | C6-C5-C4 | 2.62 | 120.76      | 117.18   |
| 1   | A     | 251 | APK  | C6-C5-C4 | 2.62 | 120.75      | 117.18   |
| 1   | E     | 251 | APK  | C6-C5-C4 | 2.62 | 120.75      | 117.18   |
| 1   | K     | 251 | APK  | C6-C5-C4 | 2.61 | 120.74      | 117.18   |
| 1   | G     | 251 | APK  | C6-C5-C4 | 2.60 | 120.73      | 117.18   |
| 1   | L     | 251 | APK  | C6-C5-C4 | 2.60 | 120.73      | 117.18   |
| 1   | O     | 251 | APK  | C6-C5-C4 | 2.60 | 120.73      | 117.18   |
| 1   | C     | 251 | APK  | C6-C5-C4 | 2.60 | 120.72      | 117.18   |
| 1   | J     | 251 | APK  | C6-C5-C4 | 2.59 | 120.72      | 117.18   |

There are no chirality outliers.

All (176) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 1   | A     | 251 | APK  | O-C-CA-CB     |
| 1   | A     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | A     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | B     | 251 | APK  | O-C-CA-CB     |
| 1   | B     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | B     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | C     | 251 | APK  | O-C-CA-CB     |
| 1   | C     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | C     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | D     | 251 | APK  | O-C-CA-CB     |
| 1   | D     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | D     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | E     | 251 | APK  | O-C-CA-CB     |
| 1   | E     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | E     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | F     | 251 | APK  | O-C-CA-CB     |
| 1   | F     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | F     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | G     | 251 | APK  | O-C-CA-CB     |
| 1   | G     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | G     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | H     | 251 | APK  | O-C-CA-CB     |
| 1   | H     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | H     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | I     | 251 | APK  | O-C-CA-CB     |
| 1   | I     | 251 | APK  | CG-CD-CE-NZ   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 1   | I     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | J     | 251 | APK  | O-C-CA-CB     |
| 1   | J     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | J     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | K     | 251 | APK  | O-C-CA-CB     |
| 1   | K     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | K     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | L     | 251 | APK  | O-C-CA-CB     |
| 1   | L     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | L     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | M     | 251 | APK  | O-C-CA-CB     |
| 1   | M     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | M     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | N     | 251 | APK  | O-C-CA-CB     |
| 1   | N     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | N     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | O     | 251 | APK  | O-C-CA-CB     |
| 1   | O     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | O     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | P     | 251 | APK  | O-C-CA-CB     |
| 1   | P     | 251 | APK  | CG-CD-CE-NZ   |
| 1   | P     | 251 | APK  | C5'-O5'-P-O2P |
| 1   | A     | 251 | APK  | CA-CB-CG-CD   |
| 1   | B     | 251 | APK  | CA-CB-CG-CD   |
| 1   | C     | 251 | APK  | CA-CB-CG-CD   |
| 1   | D     | 251 | APK  | CA-CB-CG-CD   |
| 1   | E     | 251 | APK  | CA-CB-CG-CD   |
| 1   | F     | 251 | APK  | CA-CB-CG-CD   |
| 1   | G     | 251 | APK  | CA-CB-CG-CD   |
| 1   | H     | 251 | APK  | CA-CB-CG-CD   |
| 1   | I     | 251 | APK  | CA-CB-CG-CD   |
| 1   | J     | 251 | APK  | CA-CB-CG-CD   |
| 1   | K     | 251 | APK  | CA-CB-CG-CD   |
| 1   | L     | 251 | APK  | CA-CB-CG-CD   |
| 1   | M     | 251 | APK  | CA-CB-CG-CD   |
| 1   | N     | 251 | APK  | CA-CB-CG-CD   |
| 1   | O     | 251 | APK  | CA-CB-CG-CD   |
| 1   | P     | 251 | APK  | CA-CB-CG-CD   |
| 1   | A     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | B     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | C     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | D     | 251 | APK  | C2'-C1'-N9-C8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 1   | E     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | F     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | G     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | H     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | I     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | J     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | K     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | L     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | M     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | N     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | O     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | P     | 251 | APK  | C2'-C1'-N9-C8 |
| 1   | A     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | B     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | C     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | D     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | E     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | F     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | G     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | H     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | I     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | J     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | K     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | L     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | M     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | N     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | O     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | P     | 251 | APK  | C4'-C5'-O5'-P |
| 1   | A     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | B     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | C     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | D     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | E     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | F     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | G     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | H     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | I     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | J     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | K     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | L     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | M     | 251 | APK  | C5'-O5'-P-NZ  |
| 1   | N     | 251 | APK  | C5'-O5'-P-NZ  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | O     | 251 | APK  | C5'-O5'-P-NZ    |
| 1   | P     | 251 | APK  | C5'-O5'-P-NZ    |
| 1   | A     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | B     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | C     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | D     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | E     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | F     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | G     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | H     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | I     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | J     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | K     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | L     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | M     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | N     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | O     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | P     | 251 | APK  | C2'-C1'-N9-C4   |
| 1   | A     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | B     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | C     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | D     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | E     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | F     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | G     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | H     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | I     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | J     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | K     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | L     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | M     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | N     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | O     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | P     | 251 | APK  | O4'-C1'-N9-C8   |
| 1   | A     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | B     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | C     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | D     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | E     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | F     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | G     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | H     | 251 | APK  | C3'-C4'-C5'-O5' |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | I     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | J     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | K     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | L     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | M     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | N     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | O     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | P     | 251 | APK  | C3'-C4'-C5'-O5' |
| 1   | A     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | B     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | C     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | D     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | E     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | F     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | G     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | H     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | I     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | J     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | K     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | L     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | M     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | N     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | O     | 251 | APK  | C5'-O5'-P-O1P   |
| 1   | P     | 251 | APK  | C5'-O5'-P-O1P   |

There are no ring outliers.

16 monomers are involved in 109 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | P     | 251 | APK  | 7       | 0            |
| 1   | N     | 251 | APK  | 7       | 0            |
| 1   | B     | 251 | APK  | 6       | 0            |
| 1   | J     | 251 | APK  | 7       | 0            |
| 1   | E     | 251 | APK  | 7       | 0            |
| 1   | L     | 251 | APK  | 7       | 0            |
| 1   | M     | 251 | APK  | 6       | 0            |
| 1   | A     | 251 | APK  | 7       | 0            |
| 1   | H     | 251 | APK  | 7       | 0            |
| 1   | D     | 251 | APK  | 7       | 0            |
| 1   | I     | 251 | APK  | 7       | 0            |
| 1   | F     | 251 | APK  | 7       | 0            |
| 1   | C     | 251 | APK  | 7       | 0            |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | K     | 251 | APK  | 7       | 0            |
| 1   | O     | 251 | APK  | 6       | 0            |
| 1   | G     | 251 | APK  | 7       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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   | DTP  | M     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.18 | 12 (26%)    |
| 2   | DTP  | A     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.20 | 13 (28%)    |
| 2   | DTP  | E     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.19 | 13 (28%)    |
| 2   | DTP  | G     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.19 | 13 (28%)    |
| 2   | DTP  | L     | 1501 | -    | 31,32,32     | 3.89 | 14 (45%)    | 46,50,50    | 2.19 | 12 (26%)    |
| 2   | DTP  | O     | 1501 | -    | 31,32,32     | 3.89 | 14 (45%)    | 46,50,50    | 2.18 | 12 (26%)    |
| 2   | DTP  | N     | 1501 | -    | 31,32,32     | 3.89 | 14 (45%)    | 46,50,50    | 2.18 | 12 (26%)    |
| 2   | DTP  | P     | 1501 | -    | 31,32,32     | 3.89 | 14 (45%)    | 46,50,50    | 2.18 | 12 (26%)    |
| 2   | DTP  | C     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.20 | 13 (28%)    |
| 2   | DTP  | F     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.20 | 13 (28%)    |
| 2   | DTP  | K     | 1501 | -    | 31,32,32     | 3.89 | 14 (45%)    | 46,50,50    | 2.18 | 12 (26%)    |
| 2   | DTP  | I     | 1501 | -    | 31,32,32     | 3.89 | 14 (45%)    | 46,50,50    | 2.18 | 12 (26%)    |
| 2   | DTP  | H     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.19 | 13 (28%)    |
| 2   | DTP  | D     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.20 | 13 (28%)    |
| 2   | DTP  | B     | 1501 | -    | 31,32,32     | 3.90 | 14 (45%)    | 46,50,50    | 2.19 | 13 (28%)    |
| 2   | DTP  | J     | 1501 | -    | 31,32,32     | 3.90 | 15 (48%)    | 46,50,50    | 2.18 | 12 (26%)    |

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   | DTP  | M     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 2   | DTP  | A     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | E     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | G     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | L     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 2   | DTP  | O     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 2   | DTP  | N     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 2   | DTP  | P     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 2   | DTP  | C     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | F     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | K     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 2   | DTP  | I     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 2   | DTP  | H     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | D     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | B     | 1501 | -    | -       | 5/22/34/34 | 0/3/3/3 |
| 2   | DTP  | J     | 1501 | -    | -       | 6/22/34/34 | 0/3/3/3 |

All (225) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2   | C     | 1501 | DTP  | C2'-C3' | -12.88 | 1.20        | 1.52     |
| 2   | D     | 1501 | DTP  | C2'-C3' | -12.88 | 1.20        | 1.52     |
| 2   | M     | 1501 | DTP  | C2'-C3' | -12.88 | 1.20        | 1.52     |
| 2   | G     | 1501 | DTP  | C2'-C3' | -12.87 | 1.20        | 1.52     |
| 2   | F     | 1501 | DTP  | C2'-C3' | -12.87 | 1.20        | 1.52     |
| 2   | B     | 1501 | DTP  | C2'-C3' | -12.87 | 1.20        | 1.52     |
| 2   | I     | 1501 | DTP  | C2'-C3' | -12.87 | 1.20        | 1.52     |
| 2   | O     | 1501 | DTP  | C2'-C3' | -12.87 | 1.20        | 1.52     |
| 2   | A     | 1501 | DTP  | C2'-C3' | -12.86 | 1.20        | 1.52     |
| 2   | L     | 1501 | DTP  | C2'-C3' | -12.86 | 1.20        | 1.52     |
| 2   | H     | 1501 | DTP  | C2'-C3' | -12.86 | 1.20        | 1.52     |
| 2   | J     | 1501 | DTP  | C2'-C3' | -12.86 | 1.20        | 1.52     |
| 2   | K     | 1501 | DTP  | C2'-C3' | -12.85 | 1.20        | 1.52     |
| 2   | E     | 1501 | DTP  | C2'-C3' | -12.85 | 1.20        | 1.52     |
| 2   | N     | 1501 | DTP  | C2'-C3' | -12.85 | 1.20        | 1.52     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2   | P     | 1501 | DTP  | C2'-C3' | -12.84 | 1.20        | 1.52     |
| 2   | G     | 1501 | DTP  | C1'-N9  | -9.83  | 1.27        | 1.46     |
| 2   | H     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | I     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | M     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | E     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | J     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | N     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | B     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | D     | 1501 | DTP  | C1'-N9  | -9.81  | 1.27        | 1.46     |
| 2   | C     | 1501 | DTP  | C1'-N9  | -9.80  | 1.27        | 1.46     |
| 2   | K     | 1501 | DTP  | C1'-N9  | -9.80  | 1.27        | 1.46     |
| 2   | A     | 1501 | DTP  | C1'-N9  | -9.80  | 1.27        | 1.46     |
| 2   | L     | 1501 | DTP  | C1'-N9  | -9.79  | 1.27        | 1.46     |
| 2   | P     | 1501 | DTP  | C1'-N9  | -9.78  | 1.27        | 1.46     |
| 2   | O     | 1501 | DTP  | C1'-N9  | -9.76  | 1.27        | 1.46     |
| 2   | F     | 1501 | DTP  | C1'-N9  | -9.76  | 1.27        | 1.46     |
| 2   | P     | 1501 | DTP  | O4'-C4' | -8.84  | 1.25        | 1.45     |
| 2   | C     | 1501 | DTP  | O4'-C4' | -8.83  | 1.25        | 1.45     |
| 2   | E     | 1501 | DTP  | O4'-C4' | -8.83  | 1.25        | 1.45     |
| 2   | B     | 1501 | DTP  | O4'-C4' | -8.82  | 1.25        | 1.45     |
| 2   | D     | 1501 | DTP  | O4'-C4' | -8.82  | 1.25        | 1.45     |
| 2   | H     | 1501 | DTP  | O4'-C4' | -8.82  | 1.25        | 1.45     |
| 2   | J     | 1501 | DTP  | O4'-C4' | -8.81  | 1.25        | 1.45     |
| 2   | K     | 1501 | DTP  | O4'-C4' | -8.81  | 1.25        | 1.45     |
| 2   | A     | 1501 | DTP  | O4'-C4' | -8.81  | 1.25        | 1.45     |
| 2   | G     | 1501 | DTP  | O4'-C4' | -8.80  | 1.25        | 1.45     |
| 2   | N     | 1501 | DTP  | O4'-C4' | -8.80  | 1.25        | 1.45     |
| 2   | I     | 1501 | DTP  | O4'-C4' | -8.80  | 1.25        | 1.45     |
| 2   | M     | 1501 | DTP  | O4'-C4' | -8.80  | 1.25        | 1.45     |
| 2   | F     | 1501 | DTP  | O4'-C4' | -8.79  | 1.25        | 1.45     |
| 2   | L     | 1501 | DTP  | O4'-C4' | -8.79  | 1.25        | 1.45     |
| 2   | O     | 1501 | DTP  | O4'-C4' | -8.78  | 1.25        | 1.45     |
| 2   | F     | 1501 | DTP  | PB-O3A  | -4.10  | 1.55        | 1.59     |
| 2   | K     | 1501 | DTP  | PB-O3A  | -4.05  | 1.55        | 1.59     |
| 2   | D     | 1501 | DTP  | PB-O3A  | -4.05  | 1.55        | 1.59     |
| 2   | H     | 1501 | DTP  | PB-O3A  | -4.05  | 1.55        | 1.59     |
| 2   | J     | 1501 | DTP  | PB-O3A  | -4.03  | 1.55        | 1.59     |
| 2   | B     | 1501 | DTP  | PB-O3A  | -4.02  | 1.55        | 1.59     |
| 2   | L     | 1501 | DTP  | PB-O3A  | -4.02  | 1.55        | 1.59     |
| 2   | I     | 1501 | DTP  | PB-O3A  | -4.02  | 1.55        | 1.59     |
| 2   | M     | 1501 | DTP  | PB-O3A  | -4.02  | 1.55        | 1.59     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1501 | DTP  | PB-O3A  | -4.01 | 1.55        | 1.59     |
| 2   | G     | 1501 | DTP  | PB-O3A  | -4.01 | 1.55        | 1.59     |
| 2   | O     | 1501 | DTP  | PB-O3A  | -4.00 | 1.55        | 1.59     |
| 2   | C     | 1501 | DTP  | PB-O3A  | -4.00 | 1.55        | 1.59     |
| 2   | N     | 1501 | DTP  | PB-O3A  | -4.00 | 1.55        | 1.59     |
| 2   | E     | 1501 | DTP  | PB-O3A  | -4.00 | 1.55        | 1.59     |
| 2   | P     | 1501 | DTP  | PB-O3A  | -3.97 | 1.55        | 1.59     |
| 2   | H     | 1501 | DTP  | C3'-C4' | 3.94  | 1.63        | 1.53     |
| 2   | O     | 1501 | DTP  | C3'-C4' | 3.93  | 1.63        | 1.53     |
| 2   | F     | 1501 | DTP  | C3'-C4' | 3.93  | 1.63        | 1.53     |
| 2   | G     | 1501 | DTP  | C3'-C4' | 3.93  | 1.63        | 1.53     |
| 2   | D     | 1501 | DTP  | C3'-C4' | 3.93  | 1.63        | 1.53     |
| 2   | M     | 1501 | DTP  | C3'-C4' | 3.93  | 1.63        | 1.53     |
| 2   | E     | 1501 | DTP  | C3'-C4' | 3.93  | 1.63        | 1.53     |
| 2   | B     | 1501 | DTP  | C3'-C4' | 3.92  | 1.63        | 1.53     |
| 2   | C     | 1501 | DTP  | C3'-C4' | 3.92  | 1.63        | 1.53     |
| 2   | A     | 1501 | DTP  | C3'-C4' | 3.92  | 1.63        | 1.53     |
| 2   | P     | 1501 | DTP  | C3'-C4' | 3.92  | 1.63        | 1.53     |
| 2   | L     | 1501 | DTP  | C3'-C4' | 3.91  | 1.63        | 1.53     |
| 2   | J     | 1501 | DTP  | C3'-C4' | 3.91  | 1.63        | 1.53     |
| 2   | K     | 1501 | DTP  | C3'-C4' | 3.91  | 1.63        | 1.53     |
| 2   | I     | 1501 | DTP  | C3'-C4' | 3.90  | 1.63        | 1.53     |
| 2   | N     | 1501 | DTP  | C3'-C4' | 3.89  | 1.63        | 1.53     |
| 2   | B     | 1501 | DTP  | C5-C4   | -3.77 | 1.32        | 1.39     |
| 2   | G     | 1501 | DTP  | C5-C4   | -3.75 | 1.32        | 1.39     |
| 2   | F     | 1501 | DTP  | C5-C4   | -3.75 | 1.32        | 1.39     |
| 2   | H     | 1501 | DTP  | C5-C4   | -3.75 | 1.32        | 1.39     |
| 2   | M     | 1501 | DTP  | C5-C4   | -3.75 | 1.32        | 1.39     |
| 2   | D     | 1501 | DTP  | C5-C4   | -3.74 | 1.32        | 1.39     |
| 2   | N     | 1501 | DTP  | C5-C4   | -3.74 | 1.32        | 1.39     |
| 2   | C     | 1501 | DTP  | C5-C4   | -3.72 | 1.32        | 1.39     |
| 2   | A     | 1501 | DTP  | C5-C4   | -3.72 | 1.32        | 1.39     |
| 2   | K     | 1501 | DTP  | C5-C4   | -3.72 | 1.32        | 1.39     |
| 2   | P     | 1501 | DTP  | C5-C4   | -3.71 | 1.32        | 1.39     |
| 2   | E     | 1501 | DTP  | C5-C4   | -3.71 | 1.32        | 1.39     |
| 2   | L     | 1501 | DTP  | C5-C4   | -3.70 | 1.32        | 1.39     |
| 2   | J     | 1501 | DTP  | C5-C4   | -3.70 | 1.32        | 1.39     |
| 2   | I     | 1501 | DTP  | C5-C4   | -3.69 | 1.32        | 1.39     |
| 2   | O     | 1501 | DTP  | C5-C4   | -3.69 | 1.32        | 1.39     |
| 2   | H     | 1501 | DTP  | PB-O3B  | -3.65 | 1.55        | 1.59     |
| 2   | J     | 1501 | DTP  | PB-O3B  | -3.64 | 1.55        | 1.59     |
| 2   | C     | 1501 | DTP  | PB-O3B  | -3.63 | 1.55        | 1.59     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | O     | 1501 | DTP  | PB-O3B  | -3.62 | 1.55        | 1.59     |
| 2   | A     | 1501 | DTP  | PB-O3B  | -3.61 | 1.55        | 1.59     |
| 2   | B     | 1501 | DTP  | PB-O3B  | -3.60 | 1.55        | 1.59     |
| 2   | D     | 1501 | DTP  | PB-O3B  | -3.59 | 1.55        | 1.59     |
| 2   | F     | 1501 | DTP  | PB-O3B  | -3.59 | 1.55        | 1.59     |
| 2   | P     | 1501 | DTP  | PB-O3B  | -3.58 | 1.55        | 1.59     |
| 2   | E     | 1501 | DTP  | PB-O3B  | -3.58 | 1.55        | 1.59     |
| 2   | N     | 1501 | DTP  | PB-O3B  | -3.58 | 1.55        | 1.59     |
| 2   | G     | 1501 | DTP  | PB-O3B  | -3.58 | 1.55        | 1.59     |
| 2   | O     | 1501 | DTP  | PA-O3A  | -3.57 | 1.55        | 1.59     |
| 2   | P     | 1501 | DTP  | PA-O3A  | -3.57 | 1.55        | 1.59     |
| 2   | M     | 1501 | DTP  | PB-O3B  | -3.56 | 1.55        | 1.59     |
| 2   | K     | 1501 | DTP  | PB-O3B  | -3.55 | 1.55        | 1.59     |
| 2   | L     | 1501 | DTP  | PB-O3B  | -3.55 | 1.55        | 1.59     |
| 2   | C     | 1501 | DTP  | PA-O3A  | -3.54 | 1.55        | 1.59     |
| 2   | M     | 1501 | DTP  | PA-O3A  | -3.54 | 1.55        | 1.59     |
| 2   | G     | 1501 | DTP  | PA-O3A  | -3.52 | 1.55        | 1.59     |
| 2   | D     | 1501 | DTP  | PA-O3A  | -3.51 | 1.55        | 1.59     |
| 2   | K     | 1501 | DTP  | PA-O3A  | -3.51 | 1.55        | 1.59     |
| 2   | A     | 1501 | DTP  | PA-O3A  | -3.51 | 1.55        | 1.59     |
| 2   | F     | 1501 | DTP  | PA-O3A  | -3.50 | 1.55        | 1.59     |
| 2   | I     | 1501 | DTP  | PB-O3B  | -3.50 | 1.55        | 1.59     |
| 2   | I     | 1501 | DTP  | PA-O3A  | -3.49 | 1.55        | 1.59     |
| 2   | E     | 1501 | DTP  | PA-O3A  | -3.48 | 1.55        | 1.59     |
| 2   | J     | 1501 | DTP  | PA-O3A  | -3.48 | 1.55        | 1.59     |
| 2   | N     | 1501 | DTP  | PA-O3A  | -3.48 | 1.55        | 1.59     |
| 2   | B     | 1501 | DTP  | PA-O3A  | -3.47 | 1.55        | 1.59     |
| 2   | L     | 1501 | DTP  | PA-O3A  | -3.46 | 1.55        | 1.59     |
| 2   | H     | 1501 | DTP  | PA-O3A  | -3.46 | 1.55        | 1.59     |
| 2   | I     | 1501 | DTP  | O4'-C1' | 3.34  | 1.49        | 1.42     |
| 2   | E     | 1501 | DTP  | O4'-C1' | 3.34  | 1.49        | 1.42     |
| 2   | G     | 1501 | DTP  | O4'-C1' | 3.33  | 1.49        | 1.42     |
| 2   | P     | 1501 | DTP  | O4'-C1' | 3.32  | 1.49        | 1.42     |
| 2   | C     | 1501 | DTP  | O4'-C1' | 3.31  | 1.49        | 1.42     |
| 2   | B     | 1501 | DTP  | O4'-C1' | 3.31  | 1.49        | 1.42     |
| 2   | A     | 1501 | DTP  | O4'-C1' | 3.31  | 1.49        | 1.42     |
| 2   | M     | 1501 | DTP  | O4'-C1' | 3.31  | 1.49        | 1.42     |
| 2   | J     | 1501 | DTP  | O4'-C1' | 3.30  | 1.49        | 1.42     |
| 2   | K     | 1501 | DTP  | O4'-C1' | 3.30  | 1.49        | 1.42     |
| 2   | O     | 1501 | DTP  | O4'-C1' | 3.30  | 1.49        | 1.42     |
| 2   | L     | 1501 | DTP  | O4'-C1' | 3.30  | 1.49        | 1.42     |
| 2   | D     | 1501 | DTP  | O4'-C1' | 3.30  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | F     | 1501 | DTP  | O4'-C1' | 3.30  | 1.49        | 1.42     |
| 2   | H     | 1501 | DTP  | O4'-C1' | 3.29  | 1.49        | 1.42     |
| 2   | N     | 1501 | DTP  | O4'-C1' | 3.28  | 1.49        | 1.42     |
| 2   | E     | 1501 | DTP  | C5-N7   | -2.98 | 1.33        | 1.39     |
| 2   | N     | 1501 | DTP  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 2   | L     | 1501 | DTP  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 2   | P     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | A     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | G     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | J     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | H     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | I     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | M     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | O     | 1501 | DTP  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 2   | F     | 1501 | DTP  | C5-N7   | -2.92 | 1.33        | 1.39     |
| 2   | B     | 1501 | DTP  | C5-N7   | -2.91 | 1.33        | 1.39     |
| 2   | K     | 1501 | DTP  | C5-N7   | -2.91 | 1.33        | 1.39     |
| 2   | D     | 1501 | DTP  | C5-N7   | -2.91 | 1.33        | 1.39     |
| 2   | C     | 1501 | DTP  | C5-N7   | -2.90 | 1.33        | 1.39     |
| 2   | H     | 1501 | DTP  | C8-N9   | -2.84 | 1.32        | 1.37     |
| 2   | M     | 1501 | DTP  | C8-N9   | -2.84 | 1.32        | 1.37     |
| 2   | D     | 1501 | DTP  | C8-N9   | -2.83 | 1.32        | 1.37     |
| 2   | J     | 1501 | DTP  | C8-N9   | -2.82 | 1.32        | 1.37     |
| 2   | N     | 1501 | DTP  | C8-N9   | -2.82 | 1.32        | 1.37     |
| 2   | C     | 1501 | DTP  | C8-N9   | -2.82 | 1.32        | 1.37     |
| 2   | L     | 1501 | DTP  | C8-N9   | -2.82 | 1.32        | 1.37     |
| 2   | A     | 1501 | DTP  | C8-N9   | -2.81 | 1.32        | 1.37     |
| 2   | E     | 1501 | DTP  | C8-N9   | -2.81 | 1.32        | 1.37     |
| 2   | P     | 1501 | DTP  | C8-N9   | -2.81 | 1.32        | 1.37     |
| 2   | I     | 1501 | DTP  | C8-N9   | -2.81 | 1.32        | 1.37     |
| 2   | O     | 1501 | DTP  | C8-N9   | -2.81 | 1.32        | 1.37     |
| 2   | K     | 1501 | DTP  | C8-N9   | -2.81 | 1.32        | 1.37     |
| 2   | F     | 1501 | DTP  | C8-N9   | -2.80 | 1.32        | 1.37     |
| 2   | B     | 1501 | DTP  | C8-N9   | -2.78 | 1.32        | 1.37     |
| 2   | G     | 1501 | DTP  | C8-N9   | -2.78 | 1.32        | 1.37     |
| 2   | I     | 1501 | DTP  | C6-N6   | 2.55  | 1.40        | 1.34     |
| 2   | O     | 1501 | DTP  | C6-N6   | 2.55  | 1.40        | 1.34     |
| 2   | P     | 1501 | DTP  | C6-N6   | 2.52  | 1.40        | 1.34     |
| 2   | A     | 1501 | DTP  | C6-N6   | 2.51  | 1.40        | 1.34     |
| 2   | E     | 1501 | DTP  | C6-N6   | 2.51  | 1.40        | 1.34     |
| 2   | K     | 1501 | DTP  | C6-N6   | 2.51  | 1.40        | 1.34     |
| 2   | G     | 1501 | DTP  | C6-N6   | 2.51  | 1.40        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | C     | 1501 | DTP  | C6-N6   | 2.50  | 1.40        | 1.34     |
| 2   | D     | 1501 | DTP  | C6-N6   | 2.50  | 1.40        | 1.34     |
| 2   | J     | 1501 | DTP  | C6-N6   | 2.50  | 1.40        | 1.34     |
| 2   | H     | 1501 | DTP  | C6-N6   | 2.50  | 1.40        | 1.34     |
| 2   | M     | 1501 | DTP  | C6-N6   | 2.50  | 1.40        | 1.34     |
| 2   | L     | 1501 | DTP  | C6-N6   | 2.50  | 1.40        | 1.34     |
| 2   | L     | 1501 | DTP  | O3'-C3' | 2.50  | 1.48        | 1.43     |
| 2   | B     | 1501 | DTP  | C6-N6   | 2.49  | 1.40        | 1.34     |
| 2   | I     | 1501 | DTP  | O3'-C3' | 2.48  | 1.48        | 1.43     |
| 2   | F     | 1501 | DTP  | C6-N6   | 2.47  | 1.40        | 1.34     |
| 2   | H     | 1501 | DTP  | O3'-C3' | 2.47  | 1.48        | 1.43     |
| 2   | M     | 1501 | DTP  | O3'-C3' | 2.47  | 1.48        | 1.43     |
| 2   | E     | 1501 | DTP  | O3'-C3' | 2.47  | 1.48        | 1.43     |
| 2   | G     | 1501 | DTP  | O3'-C3' | 2.47  | 1.48        | 1.43     |
| 2   | D     | 1501 | DTP  | O3'-C3' | 2.47  | 1.48        | 1.43     |
| 2   | J     | 1501 | DTP  | O3'-C3' | 2.47  | 1.48        | 1.43     |
| 2   | F     | 1501 | DTP  | O3'-C3' | 2.46  | 1.48        | 1.43     |
| 2   | A     | 1501 | DTP  | O3'-C3' | 2.46  | 1.48        | 1.43     |
| 2   | N     | 1501 | DTP  | C6-N6   | 2.46  | 1.40        | 1.34     |
| 2   | C     | 1501 | DTP  | O3'-C3' | 2.46  | 1.48        | 1.43     |
| 2   | B     | 1501 | DTP  | O3'-C3' | 2.46  | 1.48        | 1.43     |
| 2   | P     | 1501 | DTP  | O3'-C3' | 2.46  | 1.48        | 1.43     |
| 2   | N     | 1501 | DTP  | O3'-C3' | 2.45  | 1.48        | 1.43     |
| 2   | O     | 1501 | DTP  | O3'-C3' | 2.44  | 1.48        | 1.43     |
| 2   | K     | 1501 | DTP  | O3'-C3' | 2.42  | 1.48        | 1.43     |
| 2   | O     | 1501 | DTP  | C5-C6   | -2.09 | 1.35        | 1.41     |
| 2   | C     | 1501 | DTP  | C5-C6   | -2.09 | 1.35        | 1.41     |
| 2   | L     | 1501 | DTP  | C5-C6   | -2.08 | 1.35        | 1.41     |
| 2   | J     | 1501 | DTP  | C5-C6   | -2.08 | 1.35        | 1.41     |
| 2   | I     | 1501 | DTP  | C5-C6   | -2.07 | 1.35        | 1.41     |
| 2   | G     | 1501 | DTP  | C5-C6   | -2.07 | 1.35        | 1.41     |
| 2   | P     | 1501 | DTP  | C5-C6   | -2.06 | 1.35        | 1.41     |
| 2   | F     | 1501 | DTP  | C5-C6   | -2.06 | 1.35        | 1.41     |
| 2   | A     | 1501 | DTP  | C5-C6   | -2.06 | 1.35        | 1.41     |
| 2   | M     | 1501 | DTP  | C5-C6   | -2.06 | 1.35        | 1.41     |
| 2   | K     | 1501 | DTP  | C5-C6   | -2.05 | 1.35        | 1.41     |
| 2   | D     | 1501 | DTP  | C5-C6   | -2.05 | 1.35        | 1.41     |
| 2   | E     | 1501 | DTP  | C5-C6   | -2.05 | 1.35        | 1.41     |
| 2   | N     | 1501 | DTP  | C5-C6   | -2.05 | 1.35        | 1.41     |
| 2   | H     | 1501 | DTP  | C5-C6   | -2.04 | 1.35        | 1.41     |
| 2   | B     | 1501 | DTP  | C5-C6   | -2.04 | 1.35        | 1.41     |
| 2   | J     | 1501 | DTP  | C4-N9   | -2.01 | 1.33        | 1.37     |

All (200) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | O     | 1501 | DTP  | N6-C6-N1 | -5.31 | 106.55      | 118.38   |
| 2   | C     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.56      | 118.38   |
| 2   | J     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.57      | 118.38   |
| 2   | G     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.58      | 118.38   |
| 2   | B     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.58      | 118.38   |
| 2   | H     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.58      | 118.38   |
| 2   | M     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.58      | 118.38   |
| 2   | A     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.58      | 118.38   |
| 2   | L     | 1501 | DTP  | N6-C6-N1 | -5.30 | 106.58      | 118.38   |
| 2   | N     | 1501 | DTP  | N6-C6-N1 | -5.29 | 106.58      | 118.38   |
| 2   | D     | 1501 | DTP  | N6-C6-N1 | -5.29 | 106.59      | 118.38   |
| 2   | I     | 1501 | DTP  | N6-C6-N1 | -5.29 | 106.59      | 118.38   |
| 2   | E     | 1501 | DTP  | N6-C6-N1 | -5.28 | 106.61      | 118.38   |
| 2   | P     | 1501 | DTP  | N6-C6-N1 | -5.28 | 106.61      | 118.38   |
| 2   | F     | 1501 | DTP  | N6-C6-N1 | -5.28 | 106.62      | 118.38   |
| 2   | K     | 1501 | DTP  | N6-C6-N1 | -5.28 | 106.62      | 118.38   |
| 2   | P     | 1501 | DTP  | N3-C2-N1 | -4.97 | 121.06      | 128.58   |
| 2   | L     | 1501 | DTP  | N3-C2-N1 | -4.96 | 121.07      | 128.58   |
| 2   | H     | 1501 | DTP  | N3-C2-N1 | -4.96 | 121.08      | 128.58   |
| 2   | M     | 1501 | DTP  | N3-C2-N1 | -4.96 | 121.08      | 128.58   |
| 2   | E     | 1501 | DTP  | N3-C2-N1 | -4.96 | 121.08      | 128.58   |
| 2   | D     | 1501 | DTP  | N3-C2-N1 | -4.95 | 121.09      | 128.58   |
| 2   | K     | 1501 | DTP  | N3-C2-N1 | -4.94 | 121.10      | 128.58   |
| 2   | A     | 1501 | DTP  | N3-C2-N1 | -4.94 | 121.11      | 128.58   |
| 2   | J     | 1501 | DTP  | N3-C2-N1 | -4.94 | 121.11      | 128.58   |
| 2   | N     | 1501 | DTP  | N3-C2-N1 | -4.94 | 121.11      | 128.58   |
| 2   | I     | 1501 | DTP  | N3-C2-N1 | -4.93 | 121.11      | 128.58   |
| 2   | F     | 1501 | DTP  | N3-C2-N1 | -4.93 | 121.12      | 128.58   |
| 2   | J     | 1501 | DTP  | C5-C4-N3 | -4.93 | 119.93      | 126.72   |
| 2   | G     | 1501 | DTP  | N3-C2-N1 | -4.92 | 121.13      | 128.58   |
| 2   | P     | 1501 | DTP  | C5-C4-N3 | -4.92 | 119.94      | 126.72   |
| 2   | O     | 1501 | DTP  | N3-C2-N1 | -4.92 | 121.14      | 128.58   |
| 2   | D     | 1501 | DTP  | C5-C4-N3 | -4.92 | 119.95      | 126.72   |
| 2   | L     | 1501 | DTP  | C5-C4-N3 | -4.92 | 119.95      | 126.72   |
| 2   | C     | 1501 | DTP  | N3-C2-N1 | -4.91 | 121.14      | 128.58   |
| 2   | B     | 1501 | DTP  | N3-C2-N1 | -4.91 | 121.15      | 128.58   |
| 2   | I     | 1501 | DTP  | C5-C4-N3 | -4.91 | 119.96      | 126.72   |
| 2   | O     | 1501 | DTP  | C5-C4-N3 | -4.91 | 119.96      | 126.72   |
| 2   | K     | 1501 | DTP  | C5-C4-N3 | -4.90 | 119.96      | 126.72   |
| 2   | C     | 1501 | DTP  | C5-C4-N3 | -4.90 | 119.97      | 126.72   |
| 2   | G     | 1501 | DTP  | C5-C4-N3 | -4.90 | 119.97      | 126.72   |
| 2   | A     | 1501 | DTP  | C5-C4-N3 | -4.89 | 119.98      | 126.72   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | N     | 1501 | DTP  | C5-C4-N3   | -4.88 | 120.00      | 126.72   |
| 2   | M     | 1501 | DTP  | C5-C4-N3   | -4.88 | 120.00      | 126.72   |
| 2   | F     | 1501 | DTP  | C5-C4-N3   | -4.88 | 120.00      | 126.72   |
| 2   | H     | 1501 | DTP  | C5-C4-N3   | -4.88 | 120.00      | 126.72   |
| 2   | E     | 1501 | DTP  | C5-C4-N3   | -4.87 | 120.01      | 126.72   |
| 2   | B     | 1501 | DTP  | C5-C4-N3   | -4.86 | 120.02      | 126.72   |
| 2   | L     | 1501 | DTP  | N9-C8-N7   | -4.58 | 107.44      | 113.94   |
| 2   | I     | 1501 | DTP  | N9-C8-N7   | -4.57 | 107.46      | 113.94   |
| 2   | O     | 1501 | DTP  | N9-C8-N7   | -4.57 | 107.46      | 113.94   |
| 2   | F     | 1501 | DTP  | N9-C8-N7   | -4.56 | 107.47      | 113.94   |
| 2   | B     | 1501 | DTP  | N9-C8-N7   | -4.55 | 107.47      | 113.94   |
| 2   | C     | 1501 | DTP  | N9-C8-N7   | -4.55 | 107.48      | 113.94   |
| 2   | A     | 1501 | DTP  | N9-C8-N7   | -4.55 | 107.48      | 113.94   |
| 2   | P     | 1501 | DTP  | N9-C8-N7   | -4.55 | 107.48      | 113.94   |
| 2   | E     | 1501 | DTP  | N9-C8-N7   | -4.55 | 107.49      | 113.94   |
| 2   | K     | 1501 | DTP  | N9-C8-N7   | -4.55 | 107.49      | 113.94   |
| 2   | G     | 1501 | DTP  | N9-C8-N7   | -4.54 | 107.49      | 113.94   |
| 2   | J     | 1501 | DTP  | N9-C8-N7   | -4.54 | 107.49      | 113.94   |
| 2   | N     | 1501 | DTP  | N9-C8-N7   | -4.54 | 107.50      | 113.94   |
| 2   | M     | 1501 | DTP  | N9-C8-N7   | -4.53 | 107.50      | 113.94   |
| 2   | D     | 1501 | DTP  | N9-C8-N7   | -4.52 | 107.53      | 113.94   |
| 2   | H     | 1501 | DTP  | N9-C8-N7   | -4.50 | 107.55      | 113.94   |
| 2   | N     | 1501 | DTP  | C2'-C1'-N9 | -4.32 | 104.47      | 114.63   |
| 2   | O     | 1501 | DTP  | C2'-C1'-N9 | -4.32 | 104.48      | 114.63   |
| 2   | K     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.49      | 114.63   |
| 2   | F     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.50      | 114.63   |
| 2   | I     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.50      | 114.63   |
| 2   | L     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.50      | 114.63   |
| 2   | G     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.50      | 114.63   |
| 2   | H     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.50      | 114.63   |
| 2   | M     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.50      | 114.63   |
| 2   | J     | 1501 | DTP  | C2'-C1'-N9 | -4.31 | 104.51      | 114.63   |
| 2   | A     | 1501 | DTP  | C2'-C1'-N9 | -4.30 | 104.51      | 114.63   |
| 2   | B     | 1501 | DTP  | C2'-C1'-N9 | -4.30 | 104.52      | 114.63   |
| 2   | E     | 1501 | DTP  | C2'-C1'-N9 | -4.30 | 104.52      | 114.63   |
| 2   | D     | 1501 | DTP  | C2'-C1'-N9 | -4.30 | 104.53      | 114.63   |
| 2   | P     | 1501 | DTP  | C2'-C1'-N9 | -4.29 | 104.54      | 114.63   |
| 2   | C     | 1501 | DTP  | C2'-C1'-N9 | -4.29 | 104.55      | 114.63   |
| 2   | N     | 1501 | DTP  | C5-C6-N6   | 4.06  | 133.34      | 123.29   |
| 2   | B     | 1501 | DTP  | C5-C6-N6   | 4.06  | 133.33      | 123.29   |
| 2   | C     | 1501 | DTP  | C5-C6-N6   | 4.06  | 133.33      | 123.29   |
| 2   | M     | 1501 | DTP  | C5-C6-N6   | 4.06  | 133.33      | 123.29   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1501 | DTP  | C5-C6-N6    | 4.05  | 133.32      | 123.29   |
| 2   | F     | 1501 | DTP  | C5-C6-N6    | 4.05  | 133.31      | 123.29   |
| 2   | L     | 1501 | DTP  | C5-C6-N6    | 4.05  | 133.31      | 123.29   |
| 2   | J     | 1501 | DTP  | C5-C6-N6    | 4.04  | 133.30      | 123.29   |
| 2   | A     | 1501 | DTP  | C5-C6-N6    | 4.04  | 133.29      | 123.29   |
| 2   | H     | 1501 | DTP  | C5-C6-N6    | 4.04  | 133.29      | 123.29   |
| 2   | G     | 1501 | DTP  | C5-C6-N6    | 4.04  | 133.28      | 123.29   |
| 2   | K     | 1501 | DTP  | C5-C6-N6    | 4.03  | 133.27      | 123.29   |
| 2   | P     | 1501 | DTP  | C5-C6-N6    | 4.03  | 133.27      | 123.29   |
| 2   | O     | 1501 | DTP  | C5-C6-N6    | 4.02  | 133.25      | 123.29   |
| 2   | I     | 1501 | DTP  | C5-C6-N6    | 4.02  | 133.25      | 123.29   |
| 2   | E     | 1501 | DTP  | C5-C6-N6    | 4.02  | 133.24      | 123.29   |
| 2   | C     | 1501 | DTP  | C4'-O4'-C1' | -3.52 | 101.14      | 109.51   |
| 2   | B     | 1501 | DTP  | C4'-O4'-C1' | -3.52 | 101.14      | 109.51   |
| 2   | F     | 1501 | DTP  | C4'-O4'-C1' | -3.52 | 101.15      | 109.51   |
| 2   | E     | 1501 | DTP  | C4'-O4'-C1' | -3.51 | 101.16      | 109.51   |
| 2   | O     | 1501 | DTP  | C4'-O4'-C1' | -3.51 | 101.16      | 109.51   |
| 2   | I     | 1501 | DTP  | C4'-O4'-C1' | -3.51 | 101.17      | 109.51   |
| 2   | A     | 1501 | DTP  | C4'-O4'-C1' | -3.51 | 101.17      | 109.51   |
| 2   | P     | 1501 | DTP  | C4'-O4'-C1' | -3.51 | 101.18      | 109.51   |
| 2   | M     | 1501 | DTP  | C4'-O4'-C1' | -3.50 | 101.19      | 109.51   |
| 2   | K     | 1501 | DTP  | C4'-O4'-C1' | -3.50 | 101.19      | 109.51   |
| 2   | L     | 1501 | DTP  | C4'-O4'-C1' | -3.50 | 101.19      | 109.51   |
| 2   | D     | 1501 | DTP  | C4'-O4'-C1' | -3.50 | 101.20      | 109.51   |
| 2   | G     | 1501 | DTP  | C4'-O4'-C1' | -3.50 | 101.20      | 109.51   |
| 2   | H     | 1501 | DTP  | C4'-O4'-C1' | -3.50 | 101.20      | 109.51   |
| 2   | J     | 1501 | DTP  | C4'-O4'-C1' | -3.50 | 101.20      | 109.51   |
| 2   | N     | 1501 | DTP  | C4'-O4'-C1' | -3.49 | 101.23      | 109.51   |
| 2   | D     | 1501 | DTP  | N3-C4-N9    | 3.46  | 133.05      | 127.17   |
| 2   | P     | 1501 | DTP  | N3-C4-N9    | 3.45  | 133.04      | 127.17   |
| 2   | J     | 1501 | DTP  | N3-C4-N9    | 3.45  | 133.03      | 127.17   |
| 2   | M     | 1501 | DTP  | N3-C4-N9    | 3.44  | 133.02      | 127.17   |
| 2   | L     | 1501 | DTP  | N3-C4-N9    | 3.44  | 133.02      | 127.17   |
| 2   | C     | 1501 | DTP  | N3-C4-N9    | 3.44  | 133.01      | 127.17   |
| 2   | I     | 1501 | DTP  | N3-C4-N9    | 3.44  | 133.01      | 127.17   |
| 2   | O     | 1501 | DTP  | N3-C4-N9    | 3.44  | 133.01      | 127.17   |
| 2   | E     | 1501 | DTP  | N3-C4-N9    | 3.43  | 133.01      | 127.17   |
| 2   | A     | 1501 | DTP  | N3-C4-N9    | 3.43  | 133.01      | 127.17   |
| 2   | K     | 1501 | DTP  | N3-C4-N9    | 3.43  | 133.00      | 127.17   |
| 2   | H     | 1501 | DTP  | N3-C4-N9    | 3.42  | 132.98      | 127.17   |
| 2   | B     | 1501 | DTP  | N3-C4-N9    | 3.41  | 132.97      | 127.17   |
| 2   | N     | 1501 | DTP  | N3-C4-N9    | 3.41  | 132.97      | 127.17   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 2   | F     | 1501 | DTP  | N3-C4-N9   | 3.41 | 132.96      | 127.17   |
| 2   | G     | 1501 | DTP  | N3-C4-N9   | 3.41 | 132.96      | 127.17   |
| 2   | C     | 1501 | DTP  | O2B-PB-O3B | 3.22 | 115.98      | 107.27   |
| 2   | H     | 1501 | DTP  | O2B-PB-O3B | 3.21 | 115.96      | 107.27   |
| 2   | D     | 1501 | DTP  | O2B-PB-O3B | 3.21 | 115.96      | 107.27   |
| 2   | E     | 1501 | DTP  | O2B-PB-O3B | 3.21 | 115.96      | 107.27   |
| 2   | F     | 1501 | DTP  | O2B-PB-O3B | 3.21 | 115.95      | 107.27   |
| 2   | B     | 1501 | DTP  | O2B-PB-O3B | 3.21 | 115.95      | 107.27   |
| 2   | A     | 1501 | DTP  | O2B-PB-O3B | 3.21 | 115.94      | 107.27   |
| 2   | I     | 1501 | DTP  | C4-N9-C8   | 3.20 | 109.10      | 105.74   |
| 2   | O     | 1501 | DTP  | C4-N9-C8   | 3.20 | 109.10      | 105.74   |
| 2   | L     | 1501 | DTP  | C4-N9-C8   | 3.20 | 109.10      | 105.74   |
| 2   | K     | 1501 | DTP  | C4-N9-C8   | 3.19 | 109.09      | 105.74   |
| 2   | G     | 1501 | DTP  | O2B-PB-O3B | 3.19 | 115.89      | 107.27   |
| 2   | C     | 1501 | DTP  | C4-N9-C8   | 3.19 | 109.08      | 105.74   |
| 2   | J     | 1501 | DTP  | C4-N9-C8   | 3.18 | 109.08      | 105.74   |
| 2   | F     | 1501 | DTP  | C4-N9-C8   | 3.18 | 109.08      | 105.74   |
| 2   | A     | 1501 | DTP  | C4-N9-C8   | 3.18 | 109.08      | 105.74   |
| 2   | P     | 1501 | DTP  | C4-N9-C8   | 3.18 | 109.07      | 105.74   |
| 2   | D     | 1501 | DTP  | C4-N9-C8   | 3.17 | 109.07      | 105.74   |
| 2   | B     | 1501 | DTP  | C4-N9-C8   | 3.17 | 109.07      | 105.74   |
| 2   | E     | 1501 | DTP  | C4-N9-C8   | 3.16 | 109.06      | 105.74   |
| 2   | M     | 1501 | DTP  | C4-N9-C8   | 3.16 | 109.06      | 105.74   |
| 2   | N     | 1501 | DTP  | C4-N9-C8   | 3.16 | 109.05      | 105.74   |
| 2   | H     | 1501 | DTP  | C4-N9-C8   | 3.13 | 109.03      | 105.74   |
| 2   | G     | 1501 | DTP  | C4-N9-C8   | 3.13 | 109.02      | 105.74   |
| 2   | M     | 1501 | DTP  | C2-N3-C4   | 2.91 | 118.94      | 111.83   |
| 2   | D     | 1501 | DTP  | C2-N3-C4   | 2.91 | 118.94      | 111.83   |
| 2   | P     | 1501 | DTP  | C2-N3-C4   | 2.91 | 118.94      | 111.83   |
| 2   | J     | 1501 | DTP  | C2-N3-C4   | 2.91 | 118.93      | 111.83   |
| 2   | H     | 1501 | DTP  | C2-N3-C4   | 2.90 | 118.92      | 111.83   |
| 2   | L     | 1501 | DTP  | C2-N3-C4   | 2.90 | 118.92      | 111.83   |
| 2   | K     | 1501 | DTP  | C2-N3-C4   | 2.90 | 118.91      | 111.83   |
| 2   | E     | 1501 | DTP  | C2-N3-C4   | 2.90 | 118.91      | 111.83   |
| 2   | A     | 1501 | DTP  | C2-N3-C4   | 2.90 | 118.91      | 111.83   |
| 2   | N     | 1501 | DTP  | C2-N3-C4   | 2.89 | 118.89      | 111.83   |
| 2   | I     | 1501 | DTP  | C2-N3-C4   | 2.89 | 118.89      | 111.83   |
| 2   | C     | 1501 | DTP  | C2-N3-C4   | 2.89 | 118.88      | 111.83   |
| 2   | O     | 1501 | DTP  | C2-N3-C4   | 2.89 | 118.88      | 111.83   |
| 2   | G     | 1501 | DTP  | C2-N3-C4   | 2.89 | 118.88      | 111.83   |
| 2   | B     | 1501 | DTP  | C2-N3-C4   | 2.88 | 118.87      | 111.83   |
| 2   | F     | 1501 | DTP  | C2-N3-C4   | 2.88 | 118.86      | 111.83   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2   | F     | 1501 | DTP  | C6-C5-C4 | 2.87 | 121.10      | 117.18   |
| 2   | C     | 1501 | DTP  | C6-C5-C4 | 2.86 | 121.09      | 117.18   |
| 2   | D     | 1501 | DTP  | C6-C5-C4 | 2.86 | 121.08      | 117.18   |
| 2   | L     | 1501 | DTP  | C6-C5-C4 | 2.86 | 121.08      | 117.18   |
| 2   | K     | 1501 | DTP  | C6-C5-C4 | 2.86 | 121.08      | 117.18   |
| 2   | J     | 1501 | DTP  | C6-C5-C4 | 2.86 | 121.08      | 117.18   |
| 2   | N     | 1501 | DTP  | C6-C5-C4 | 2.86 | 121.08      | 117.18   |
| 2   | M     | 1501 | DTP  | C6-C5-C4 | 2.85 | 121.07      | 117.18   |
| 2   | P     | 1501 | DTP  | C6-C5-C4 | 2.84 | 121.06      | 117.18   |
| 2   | G     | 1501 | DTP  | C6-C5-C4 | 2.84 | 121.06      | 117.18   |
| 2   | O     | 1501 | DTP  | C6-C5-C4 | 2.84 | 121.06      | 117.18   |
| 2   | B     | 1501 | DTP  | C6-C5-C4 | 2.84 | 121.05      | 117.18   |
| 2   | I     | 1501 | DTP  | C6-C5-C4 | 2.84 | 121.05      | 117.18   |
| 2   | A     | 1501 | DTP  | C6-C5-C4 | 2.84 | 121.05      | 117.18   |
| 2   | H     | 1501 | DTP  | C6-C5-C4 | 2.82 | 121.03      | 117.18   |
| 2   | E     | 1501 | DTP  | C6-C5-C4 | 2.80 | 121.00      | 117.18   |
| 2   | L     | 1501 | DTP  | C5-N7-C8 | 2.58 | 107.51      | 103.45   |
| 2   | C     | 1501 | DTP  | C5-N7-C8 | 2.57 | 107.50      | 103.45   |
| 2   | M     | 1501 | DTP  | C5-N7-C8 | 2.57 | 107.48      | 103.45   |
| 2   | J     | 1501 | DTP  | C5-N7-C8 | 2.56 | 107.48      | 103.45   |
| 2   | P     | 1501 | DTP  | C5-N7-C8 | 2.56 | 107.48      | 103.45   |
| 2   | I     | 1501 | DTP  | C5-N7-C8 | 2.56 | 107.48      | 103.45   |
| 2   | O     | 1501 | DTP  | C5-N7-C8 | 2.56 | 107.48      | 103.45   |
| 2   | F     | 1501 | DTP  | C5-N7-C8 | 2.56 | 107.47      | 103.45   |
| 2   | A     | 1501 | DTP  | C5-N7-C8 | 2.56 | 107.47      | 103.45   |
| 2   | G     | 1501 | DTP  | C5-N7-C8 | 2.55 | 107.46      | 103.45   |
| 2   | E     | 1501 | DTP  | C5-N7-C8 | 2.55 | 107.46      | 103.45   |
| 2   | B     | 1501 | DTP  | C5-N7-C8 | 2.55 | 107.45      | 103.45   |
| 2   | K     | 1501 | DTP  | C5-N7-C8 | 2.54 | 107.45      | 103.45   |
| 2   | H     | 1501 | DTP  | C5-N7-C8 | 2.54 | 107.44      | 103.45   |
| 2   | N     | 1501 | DTP  | C5-N7-C8 | 2.54 | 107.44      | 103.45   |
| 2   | D     | 1501 | DTP  | C5-N7-C8 | 2.53 | 107.42      | 103.45   |

There are no chirality outliers.

All (88) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | B     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | C     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | D     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | E     | 1501 | DTP  | C3'-C4'-C5'-O5' |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | F     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | G     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | H     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | I     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | J     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | K     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | L     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | M     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | N     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | O     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | P     | 1501 | DTP  | C3'-C4'-C5'-O5' |
| 2   | A     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | B     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | C     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | D     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | E     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | F     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | G     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | H     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | I     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | J     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | K     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | L     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | M     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | N     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | O     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | P     | 1501 | DTP  | O4'-C4'-C5'-O5' |
| 2   | I     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | J     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | K     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | L     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | M     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | N     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | O     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | P     | 1501 | DTP  | C5'-O5'-PA-O1A  |
| 2   | A     | 1501 | DTP  | O4'-C1'-N9-C8   |
| 2   | B     | 1501 | DTP  | O4'-C1'-N9-C8   |
| 2   | C     | 1501 | DTP  | O4'-C1'-N9-C8   |
| 2   | D     | 1501 | DTP  | O4'-C1'-N9-C8   |
| 2   | E     | 1501 | DTP  | O4'-C1'-N9-C8   |
| 2   | F     | 1501 | DTP  | O4'-C1'-N9-C8   |
| 2   | G     | 1501 | DTP  | O4'-C1'-N9-C8   |

*Continued on next page...*

*Continued from previous page...*

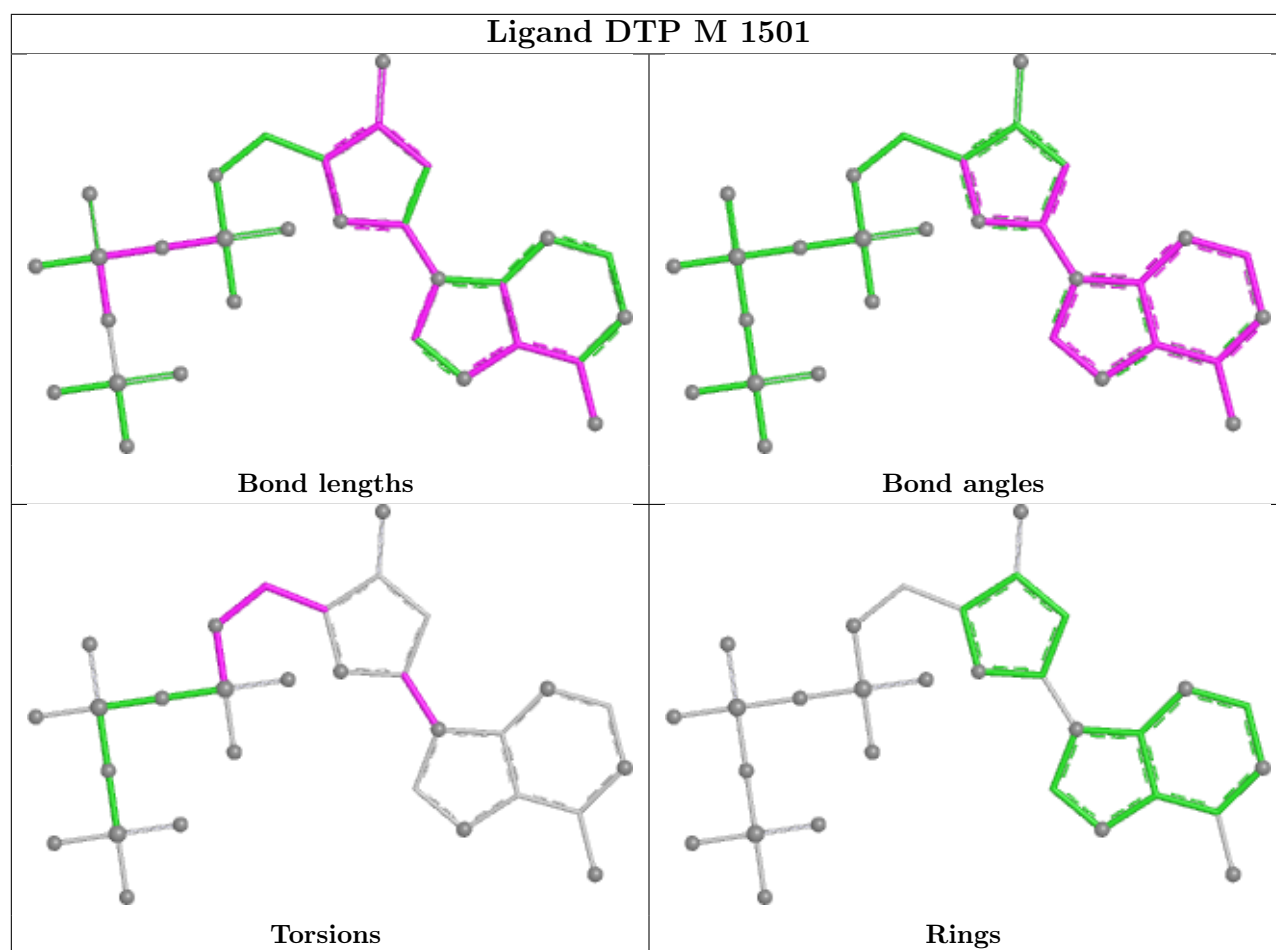
| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 2   | H     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | I     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | J     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | K     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | L     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | M     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | N     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | O     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | P     | 1501 | DTP  | O4'-C1'-N9-C8  |
| 2   | A     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | B     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | C     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | D     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | E     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | F     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | G     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | H     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | I     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | J     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | K     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | L     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | M     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | N     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | O     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | P     | 1501 | DTP  | C4'-C5'-O5'-PA |
| 2   | A     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | B     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | C     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | D     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | E     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | F     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | G     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | H     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | I     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | J     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | K     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | L     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | M     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | N     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | O     | 1501 | DTP  | O4'-C1'-N9-C4  |
| 2   | P     | 1501 | DTP  | O4'-C1'-N9-C4  |

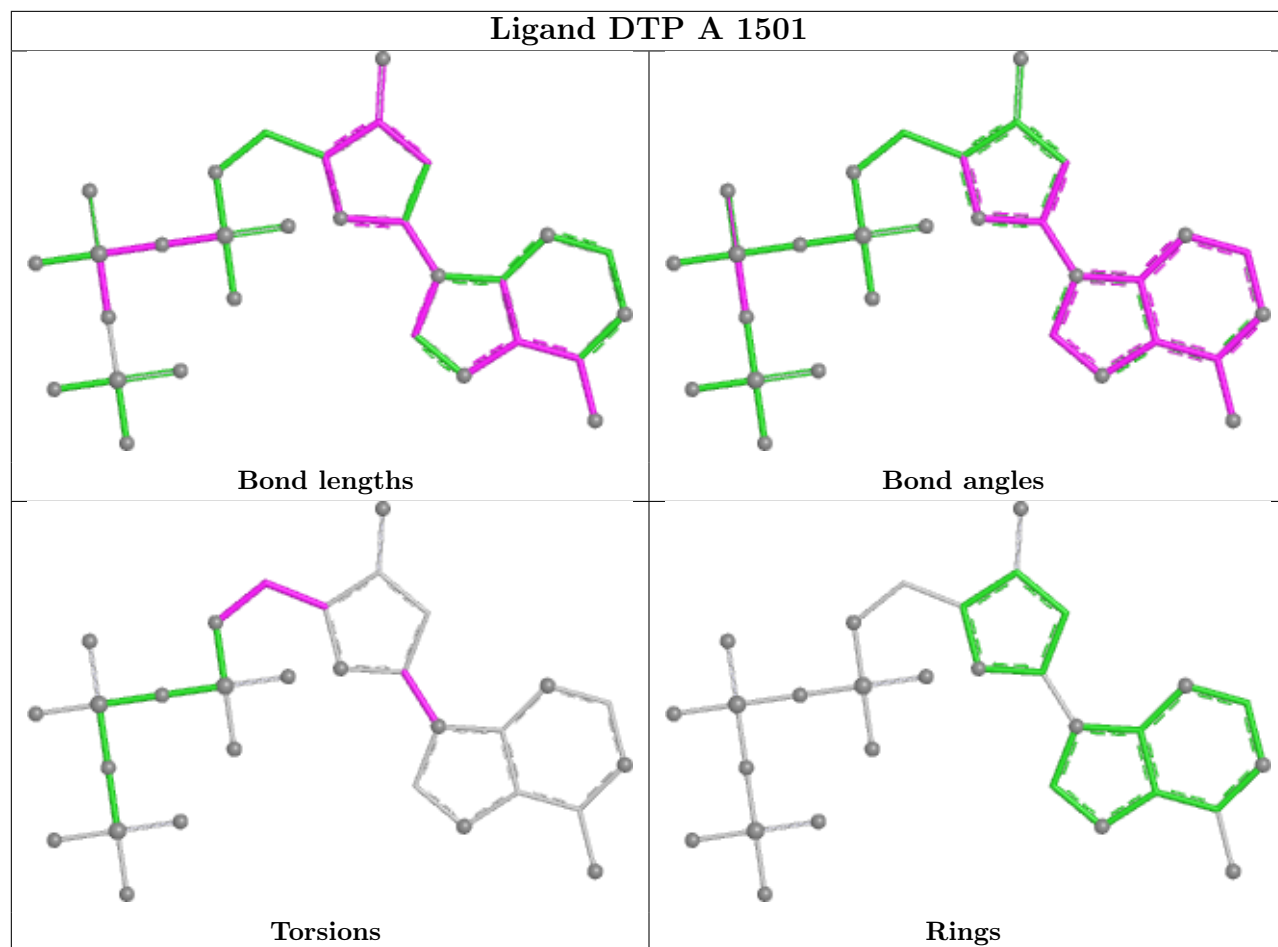
There are no ring outliers.

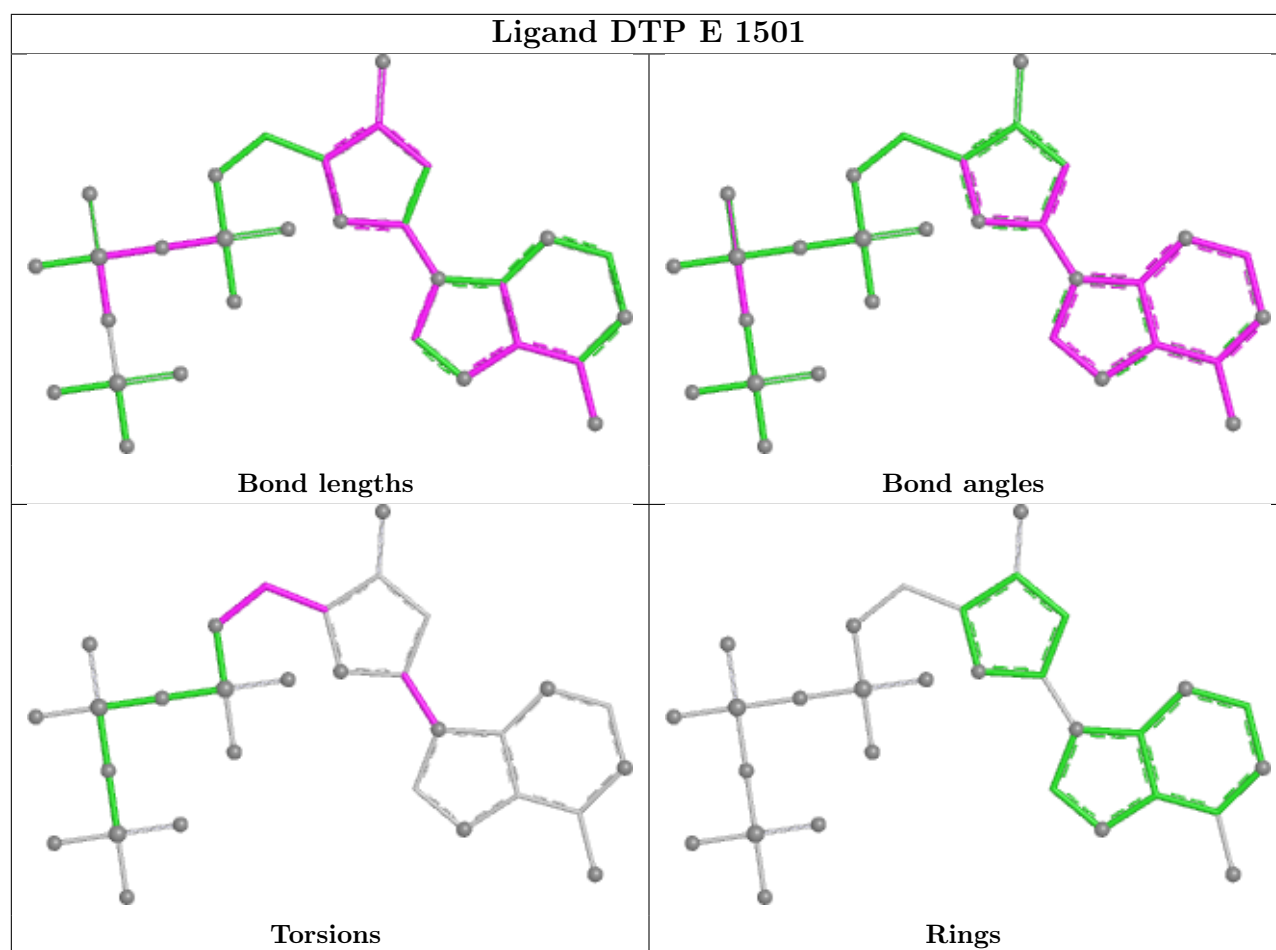
16 monomers are involved in 96 short contacts:

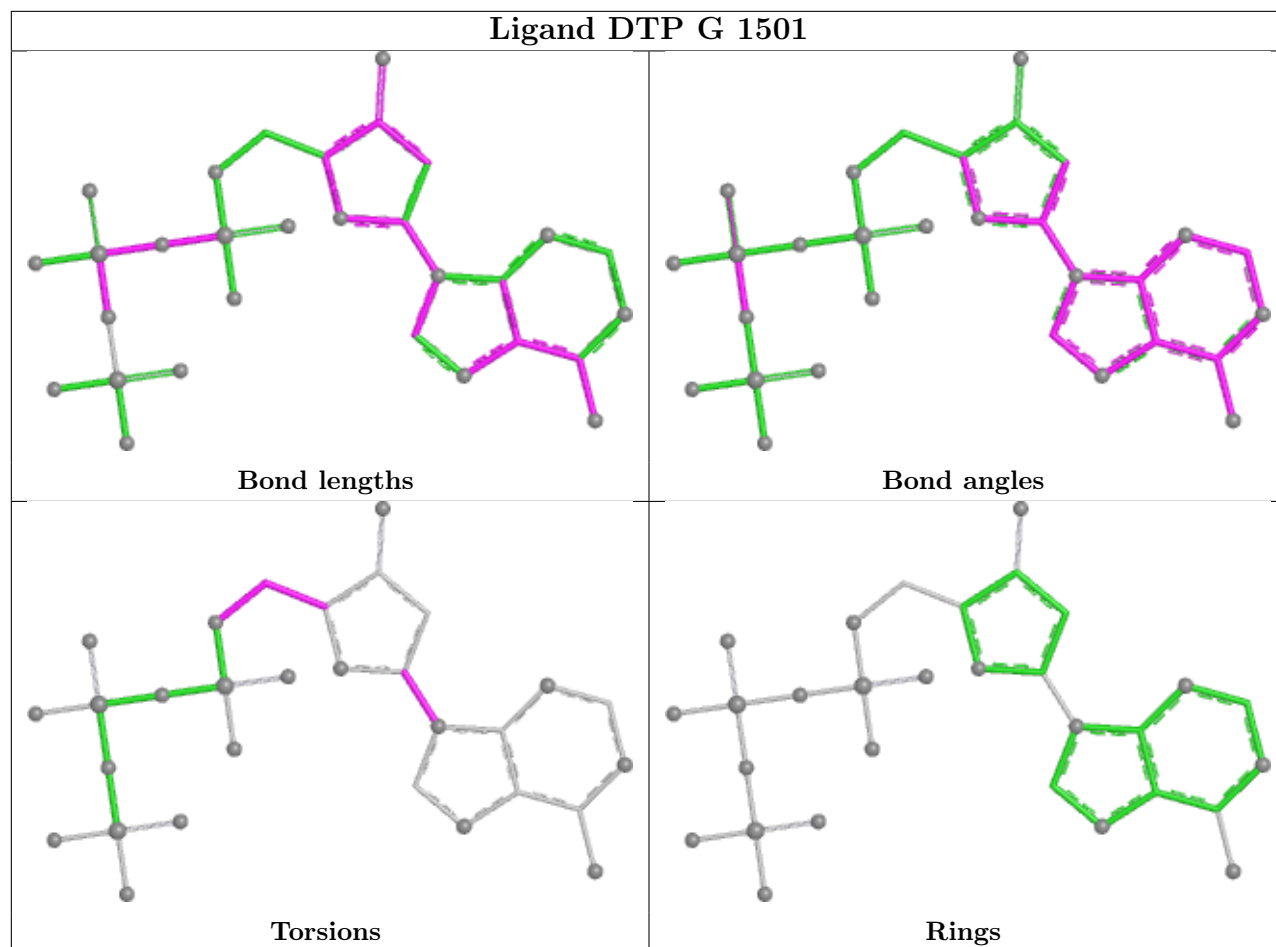
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | M     | 1501 | DTP  | 6       | 0            |
| 2   | A     | 1501 | DTP  | 6       | 0            |
| 2   | E     | 1501 | DTP  | 6       | 0            |
| 2   | G     | 1501 | DTP  | 6       | 0            |
| 2   | L     | 1501 | DTP  | 6       | 0            |
| 2   | O     | 1501 | DTP  | 6       | 0            |
| 2   | N     | 1501 | DTP  | 6       | 0            |
| 2   | P     | 1501 | DTP  | 6       | 0            |
| 2   | C     | 1501 | DTP  | 6       | 0            |
| 2   | F     | 1501 | DTP  | 6       | 0            |
| 2   | K     | 1501 | DTP  | 6       | 0            |
| 2   | I     | 1501 | DTP  | 6       | 0            |
| 2   | H     | 1501 | DTP  | 6       | 0            |
| 2   | D     | 1501 | DTP  | 6       | 0            |
| 2   | B     | 1501 | DTP  | 6       | 0            |
| 2   | J     | 1501 | DTP  | 6       | 0            |

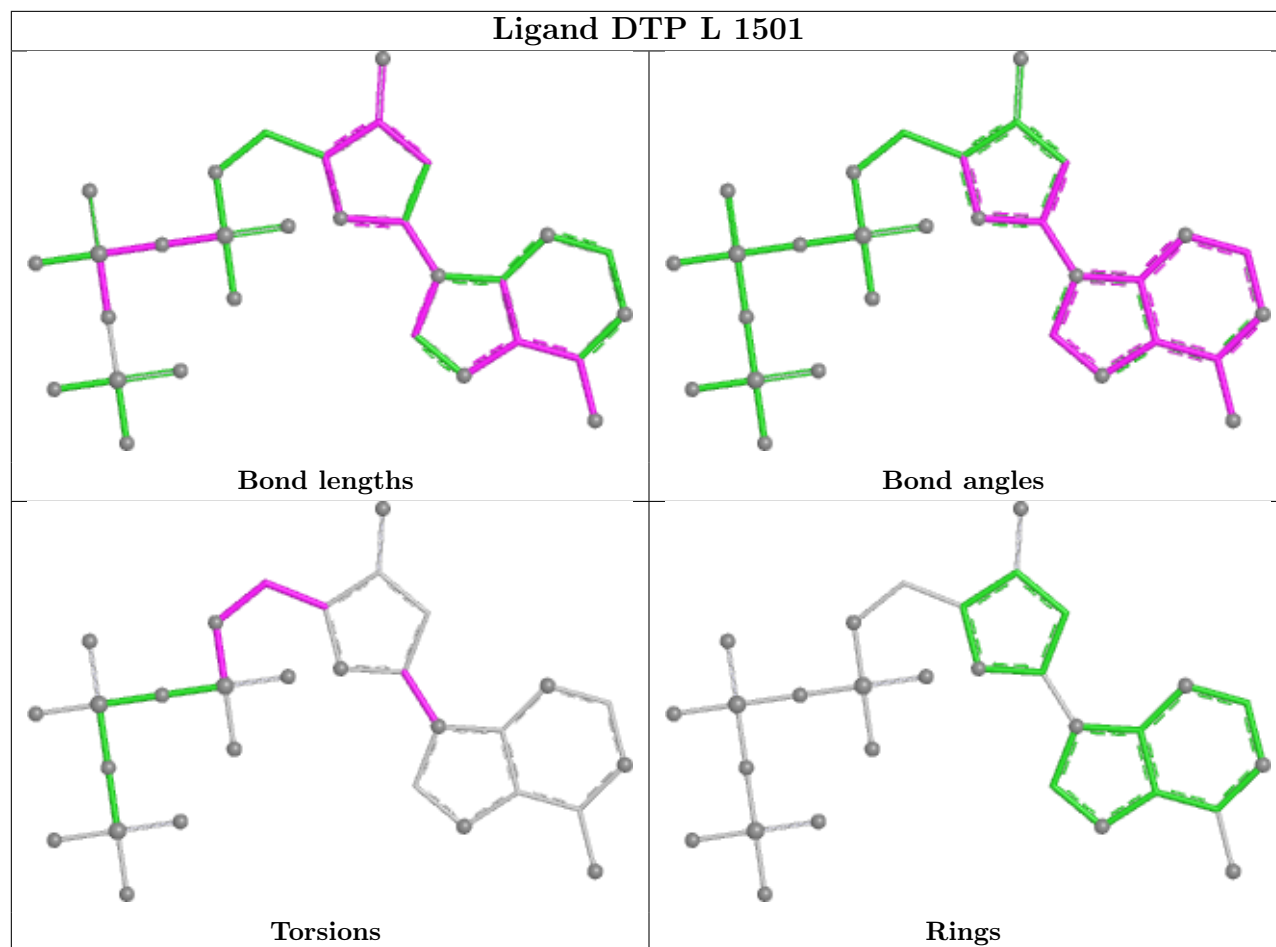
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

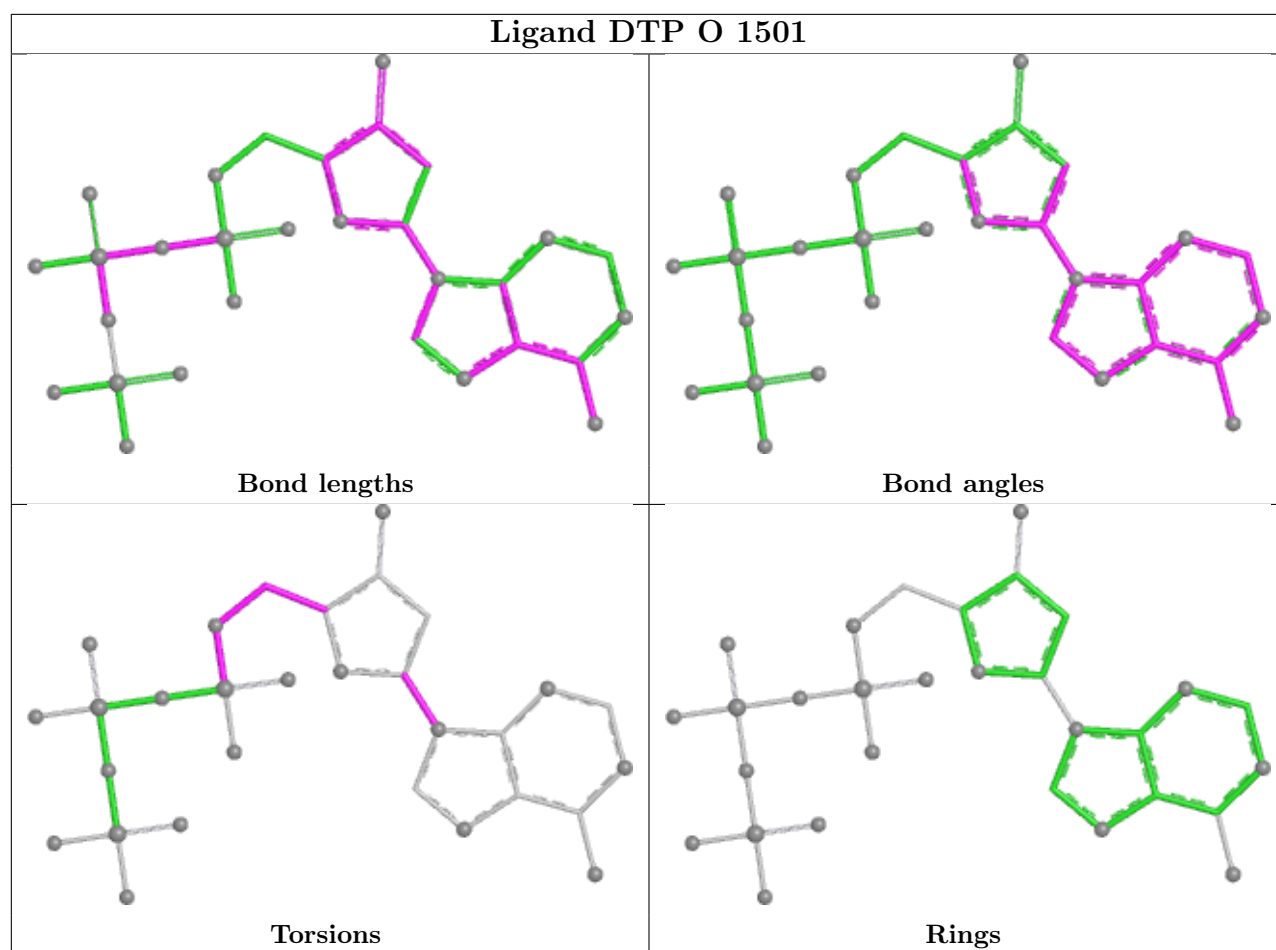


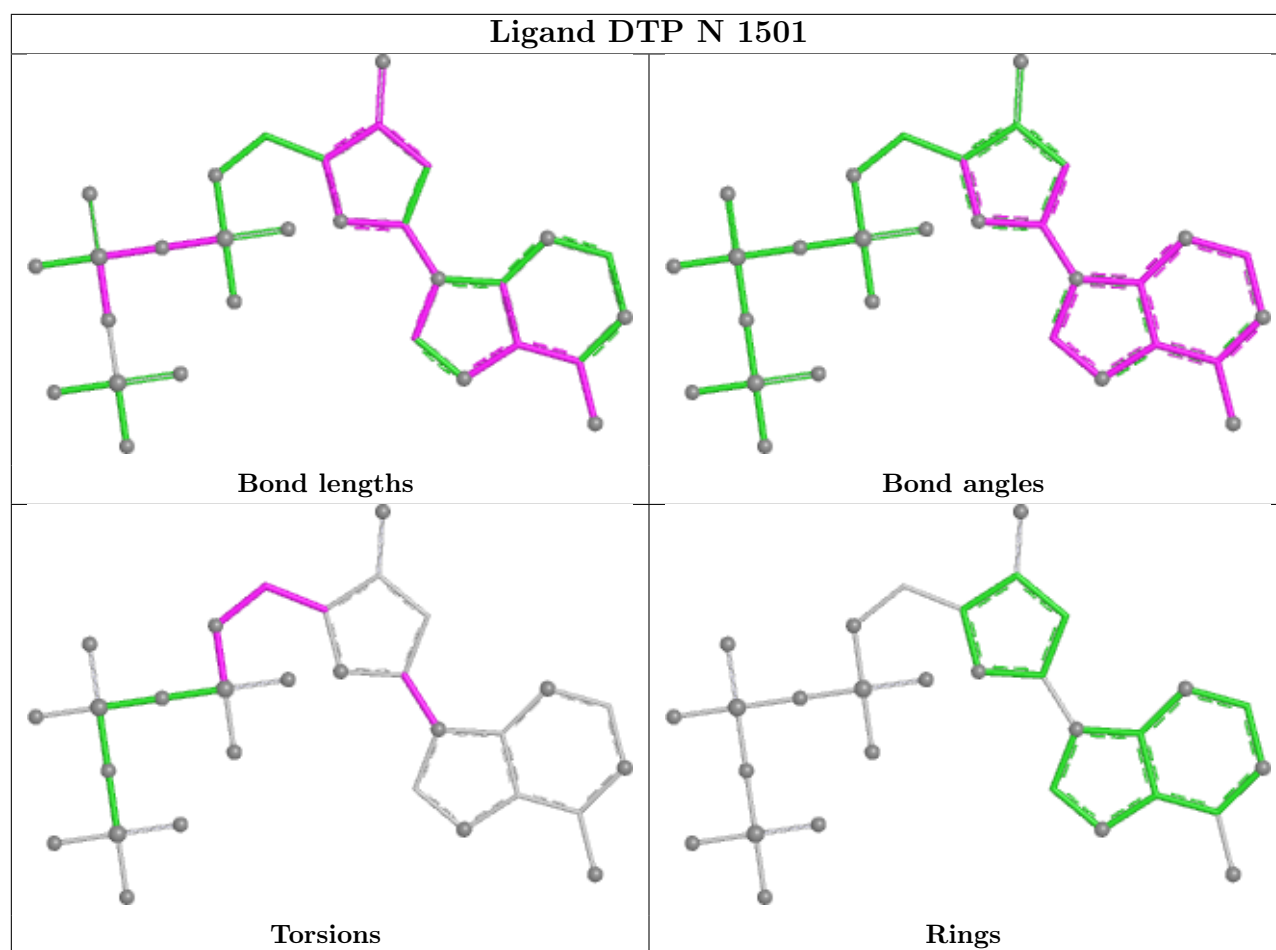


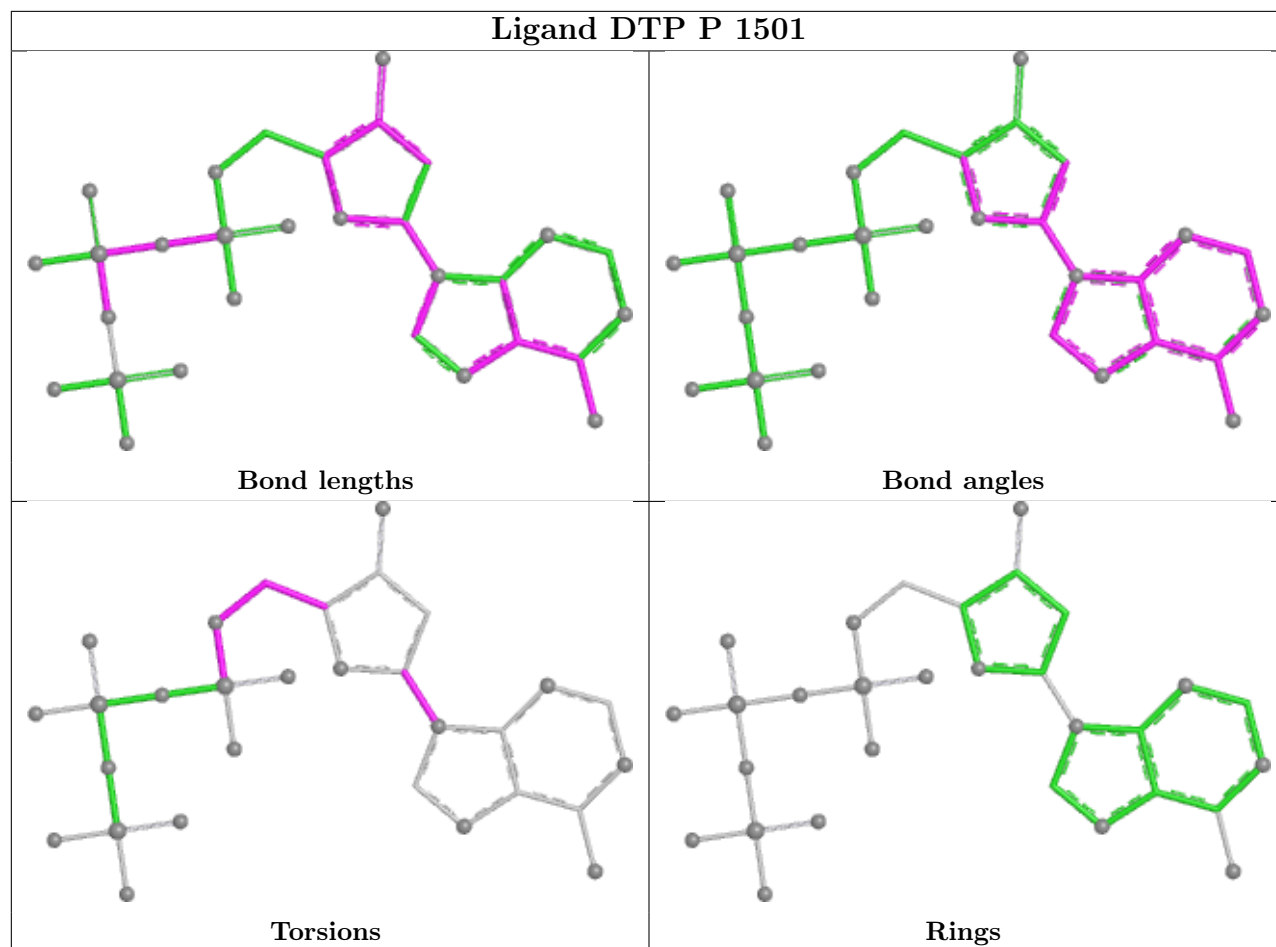


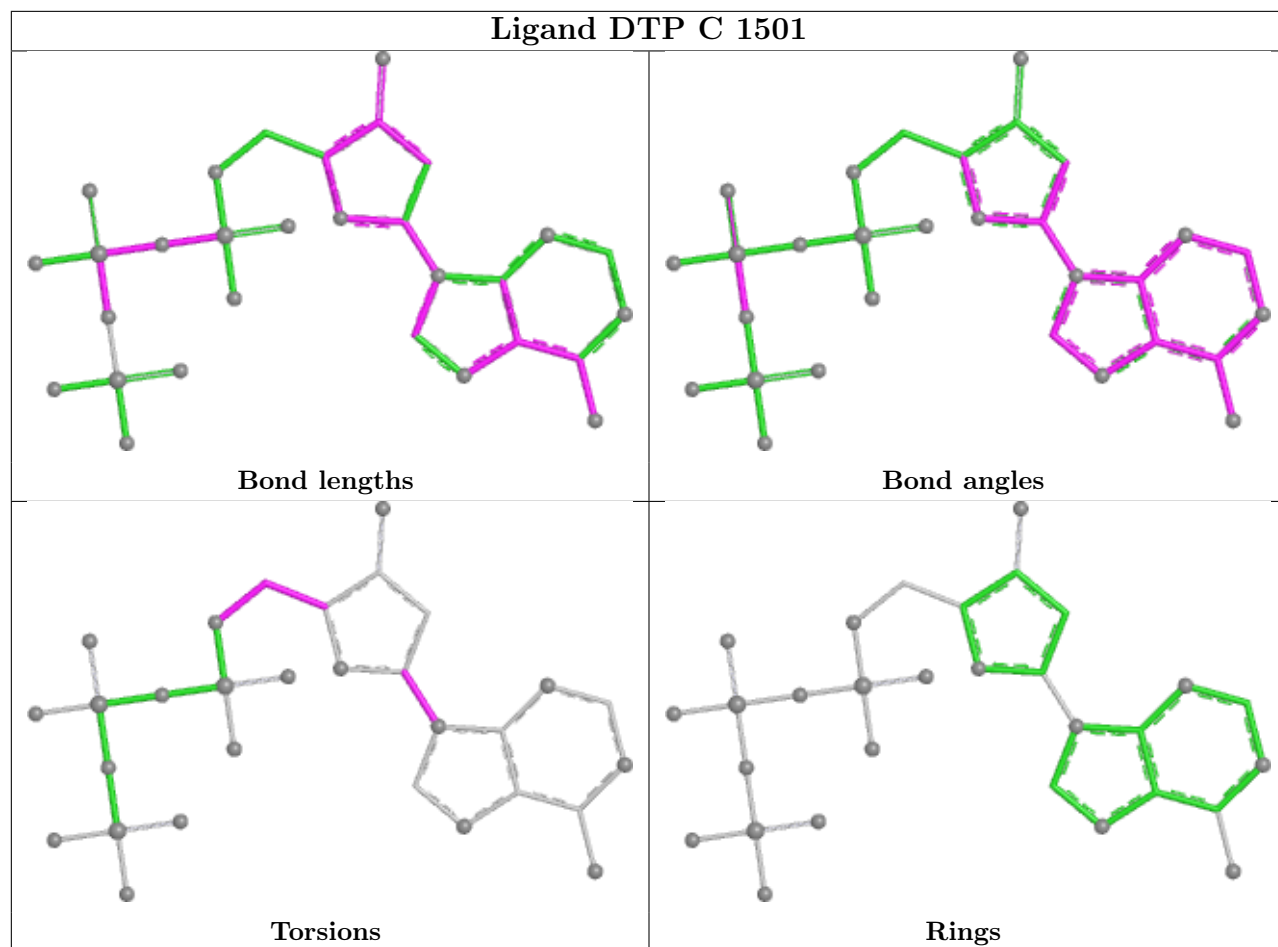


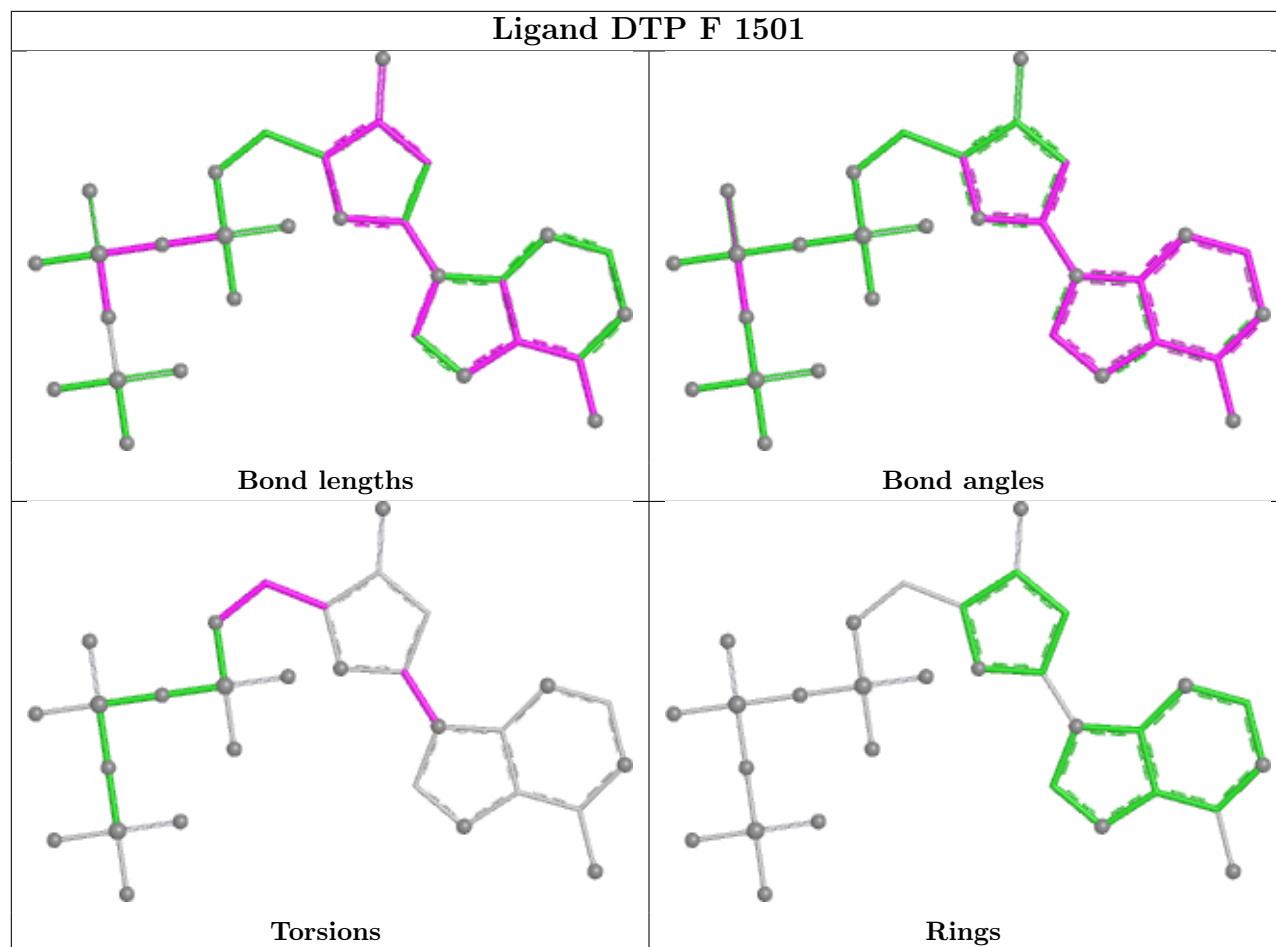


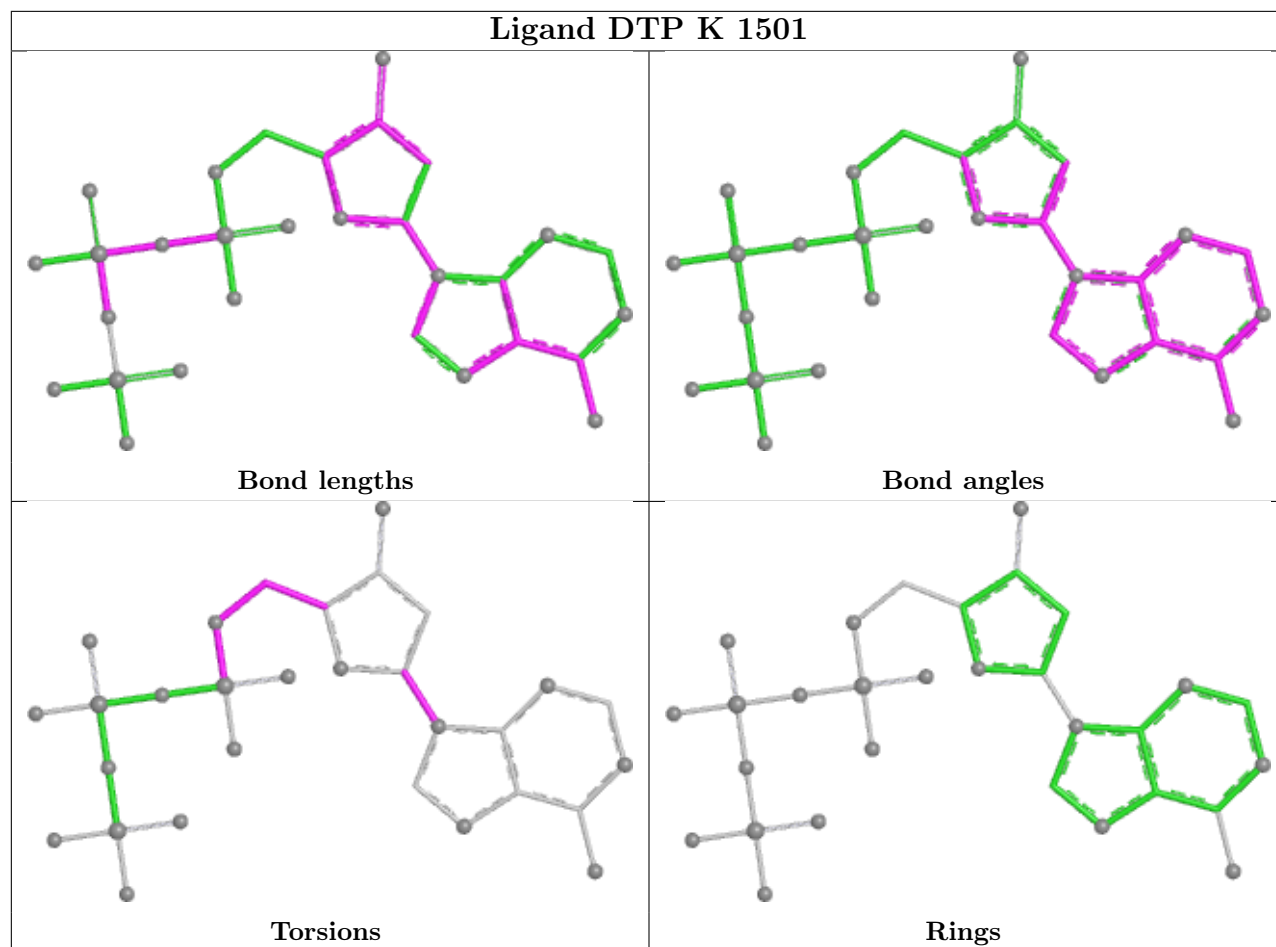


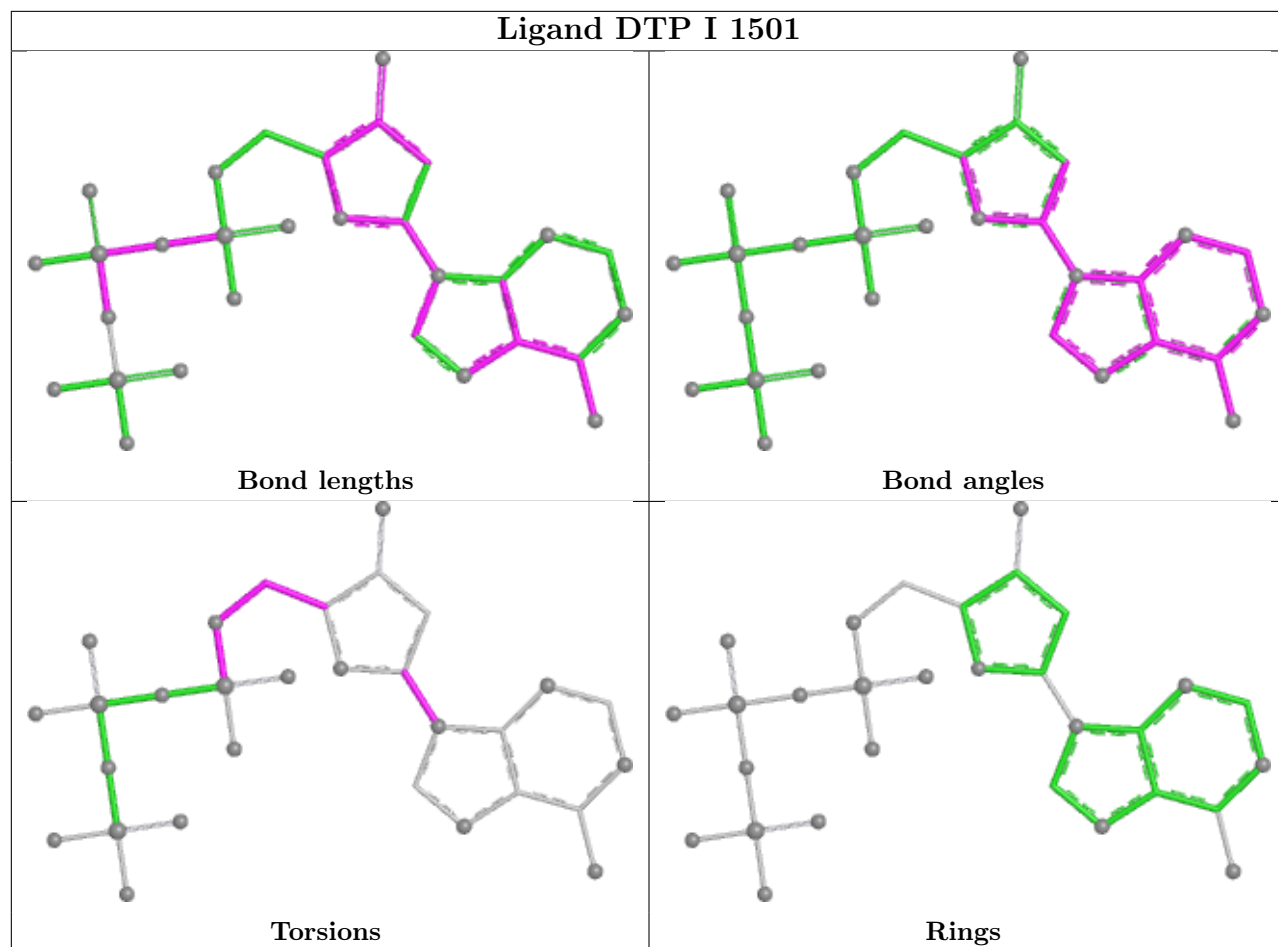


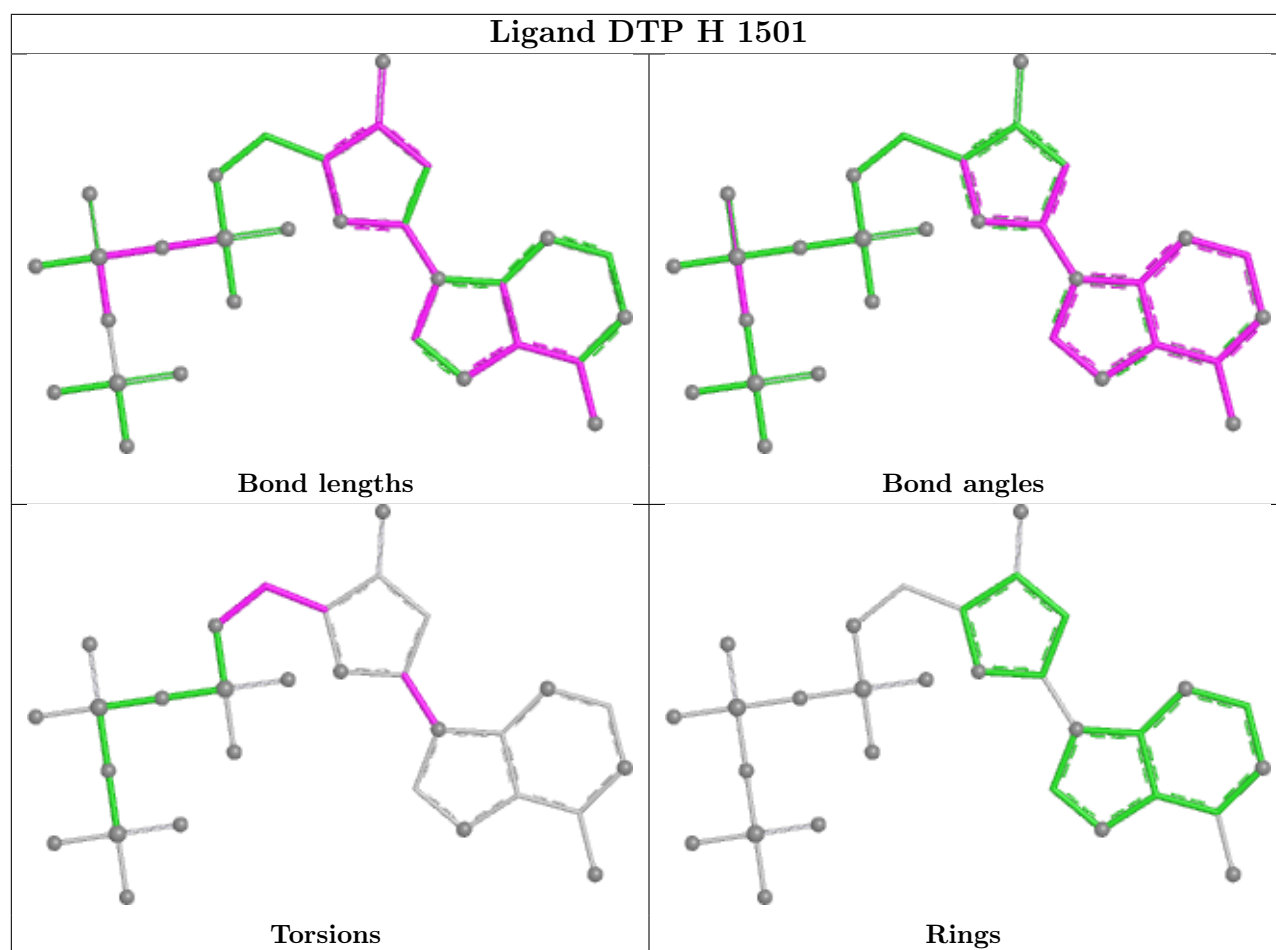


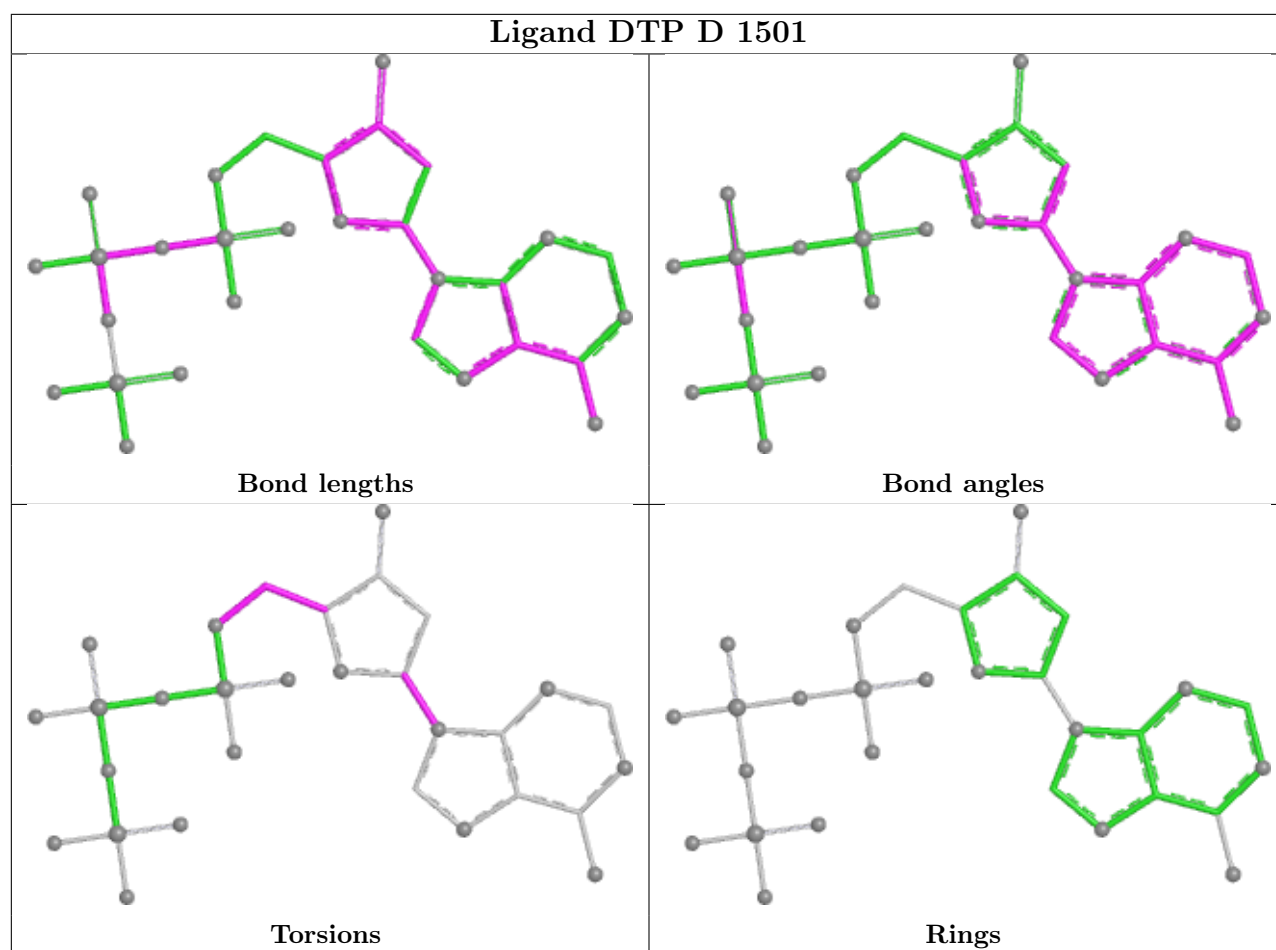


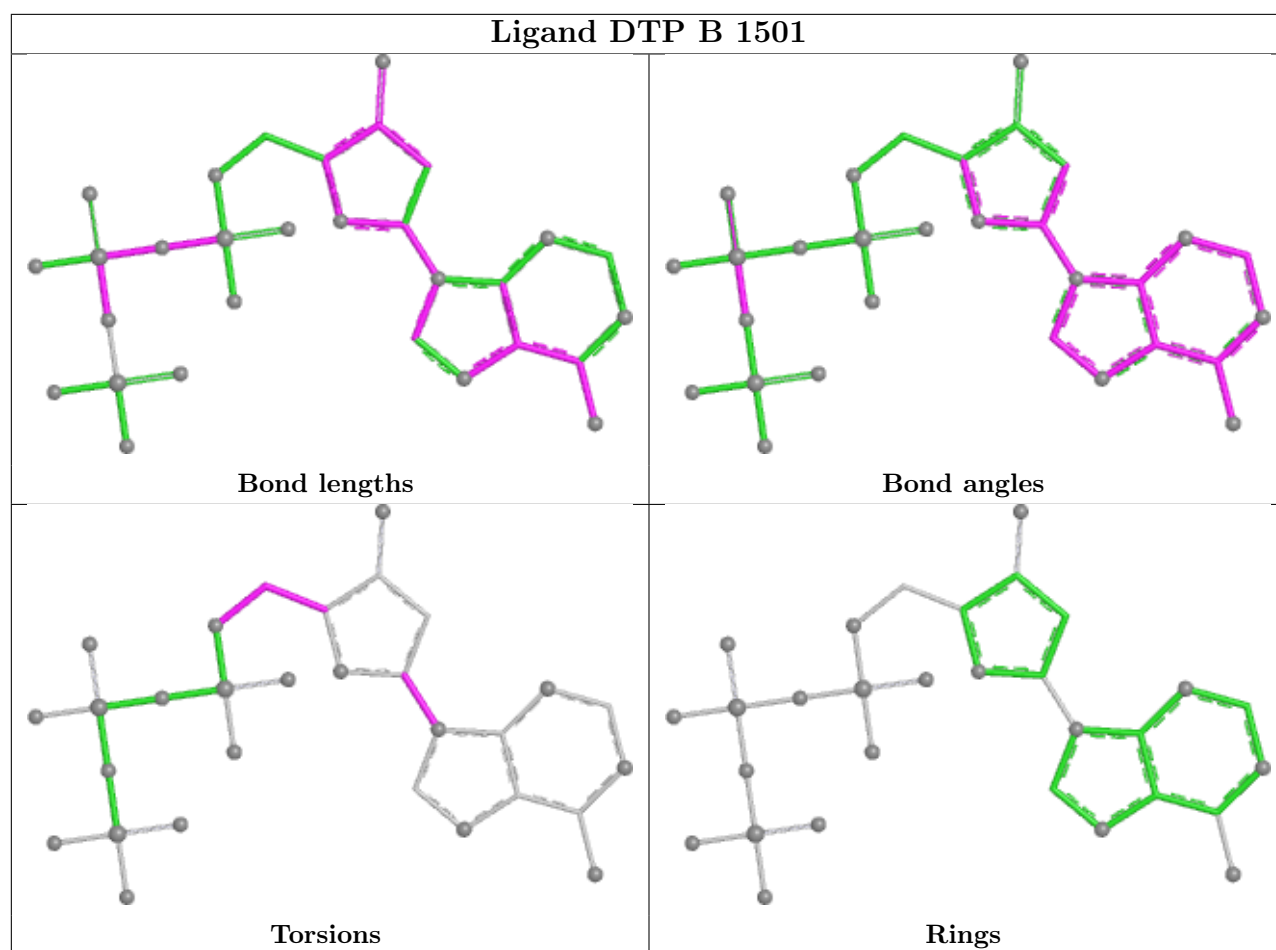


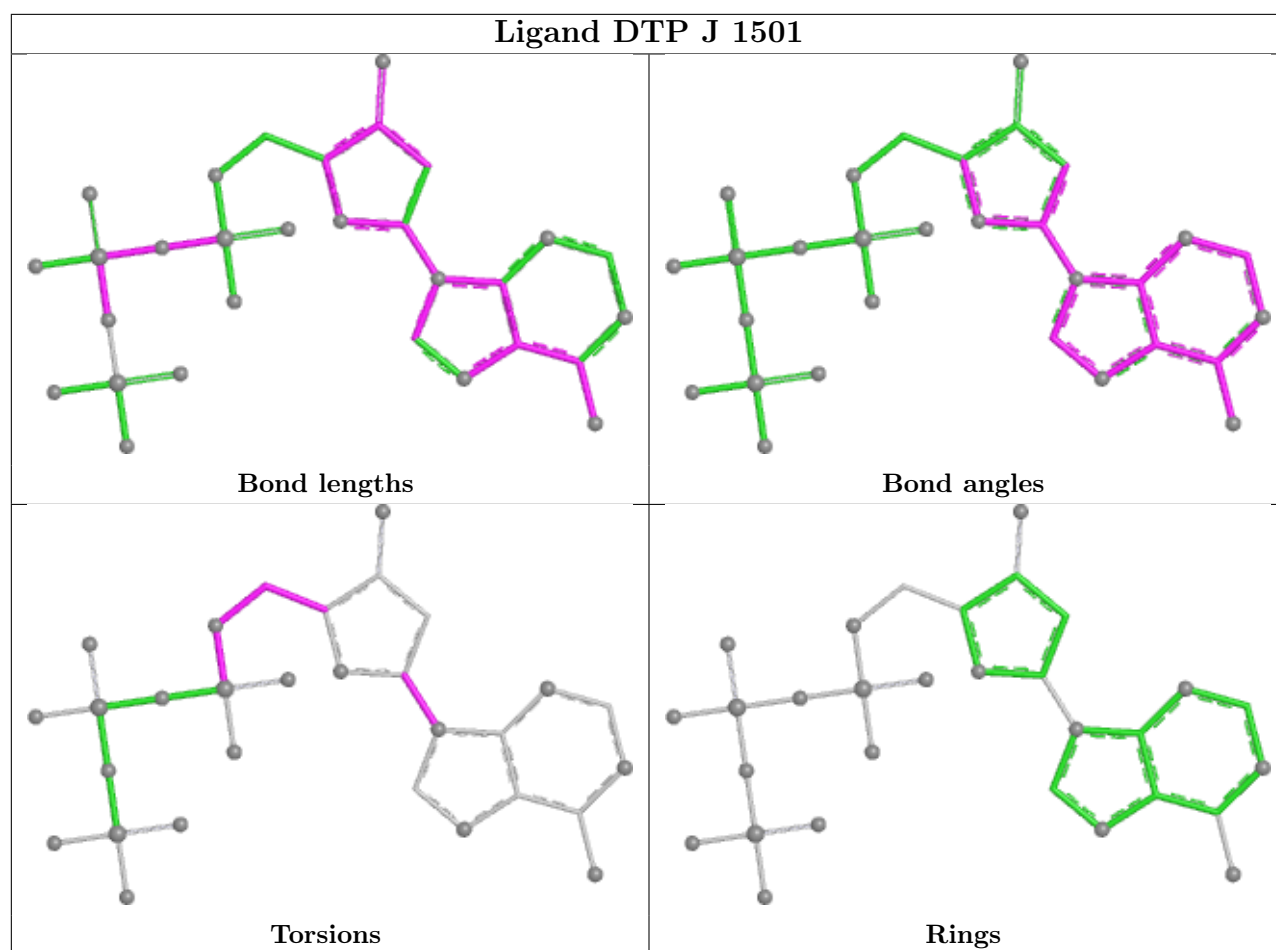












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

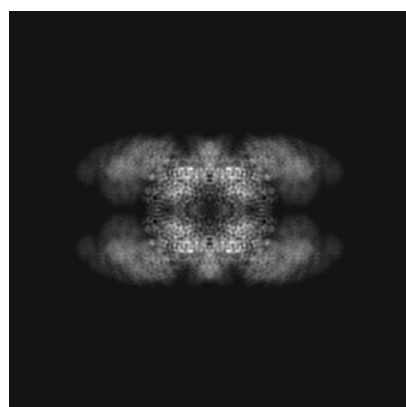
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8177. These allow visual inspection of the internal detail of the map and identification of artifacts.

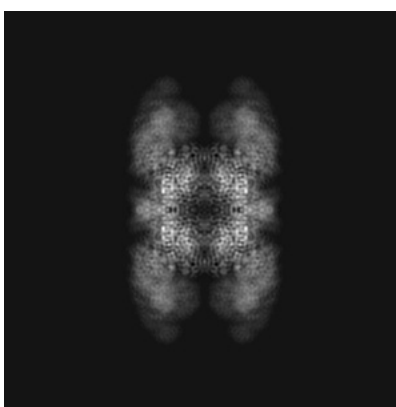
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

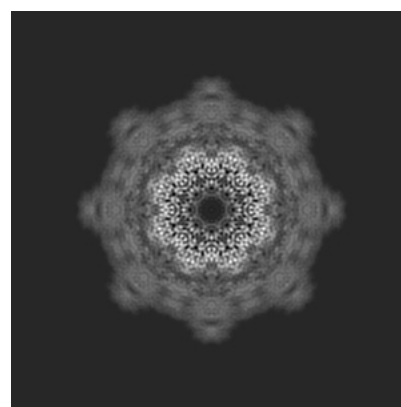
#### 6.1.1 Primary map



X



Y

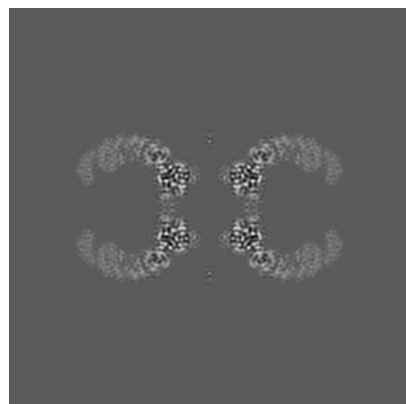


Z

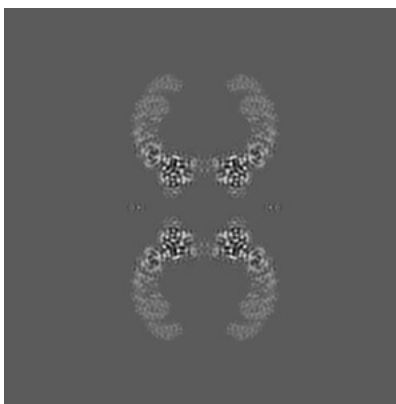
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 160



Y Index: 160

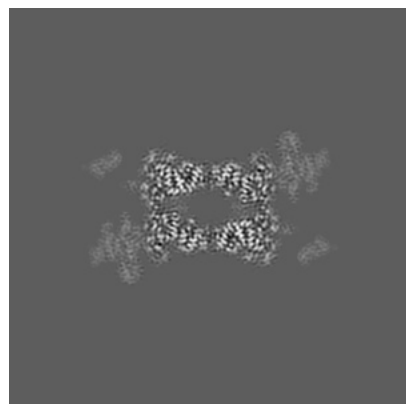


Z Index: 160

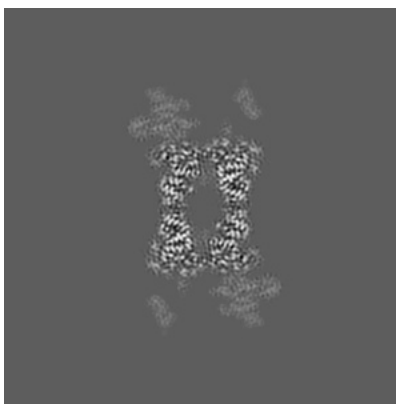
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

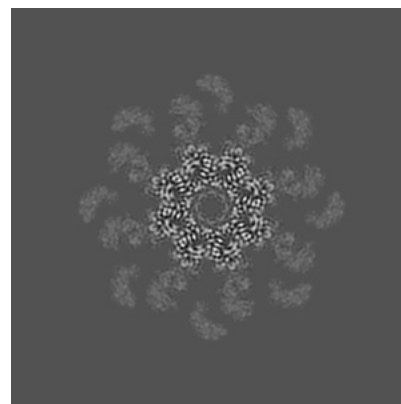
### 6.3.1 Primary map



X Index: 143



Y Index: 143

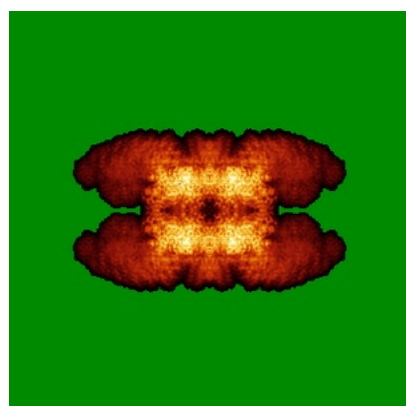


Z Index: 185

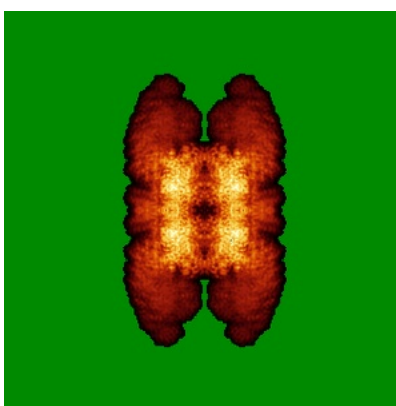
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

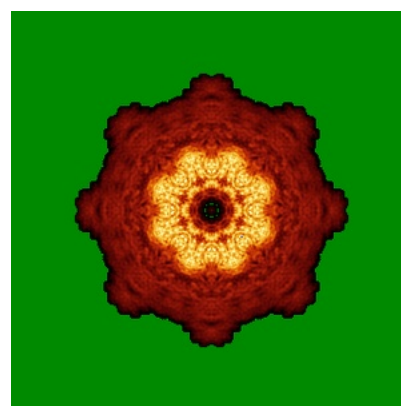
### 6.4.1 Primary map



X



Y

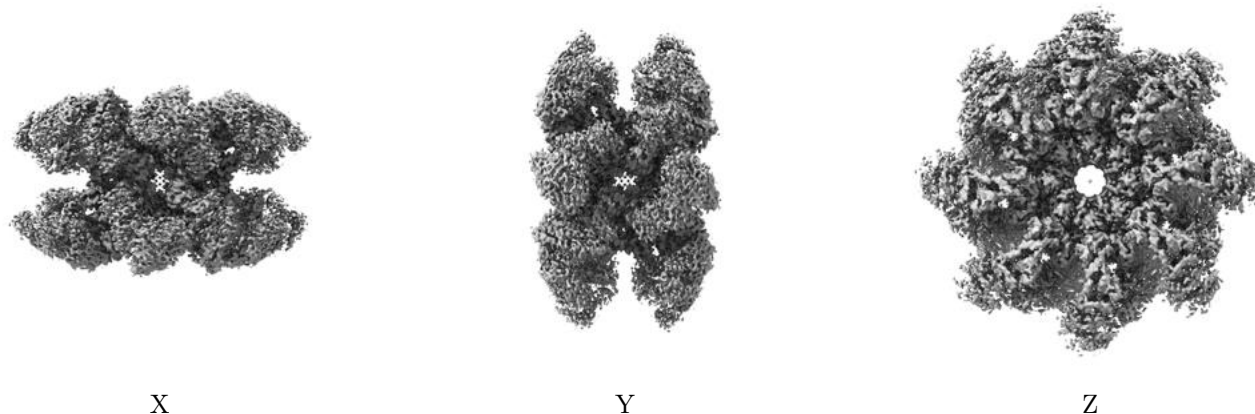


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

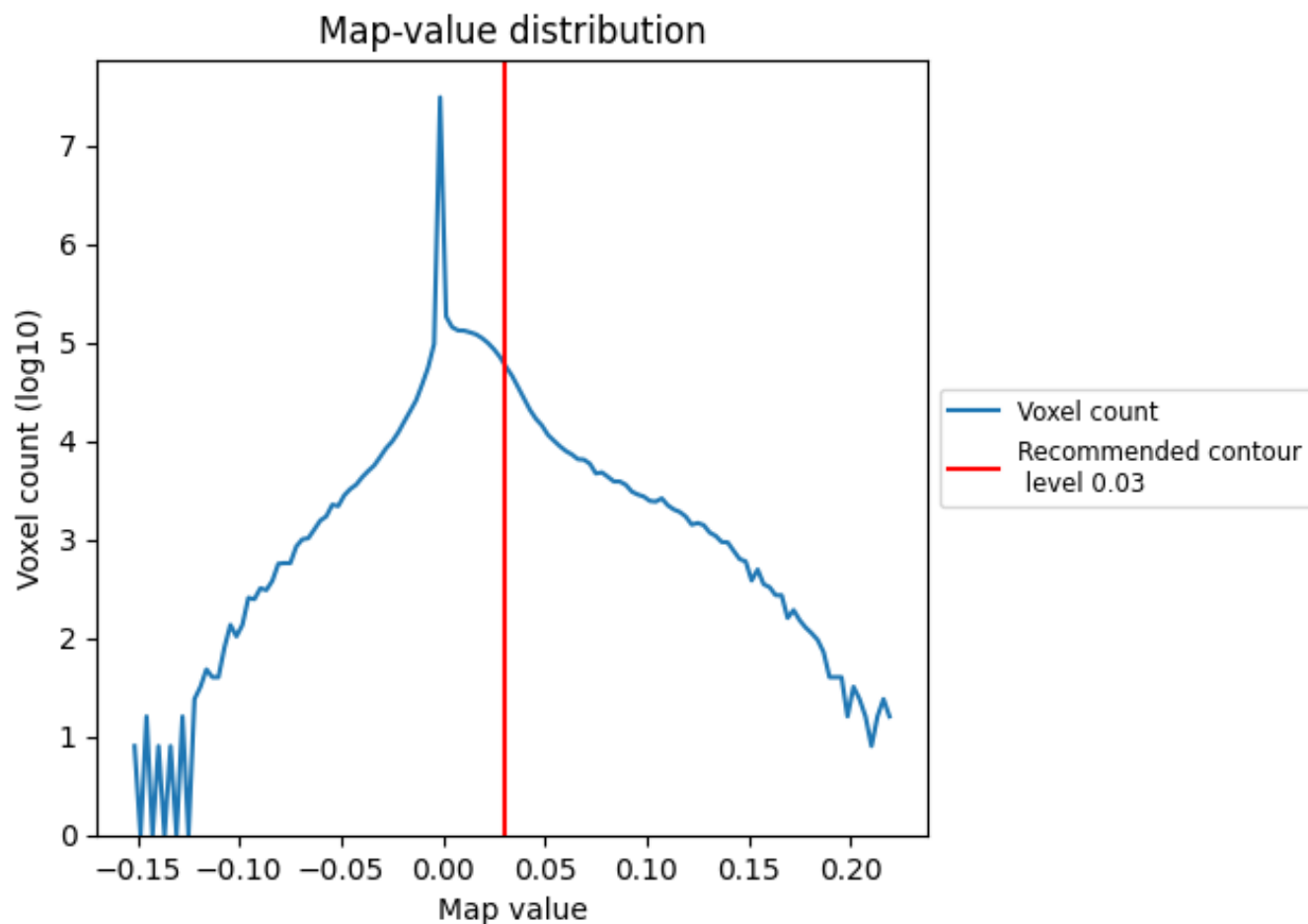
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

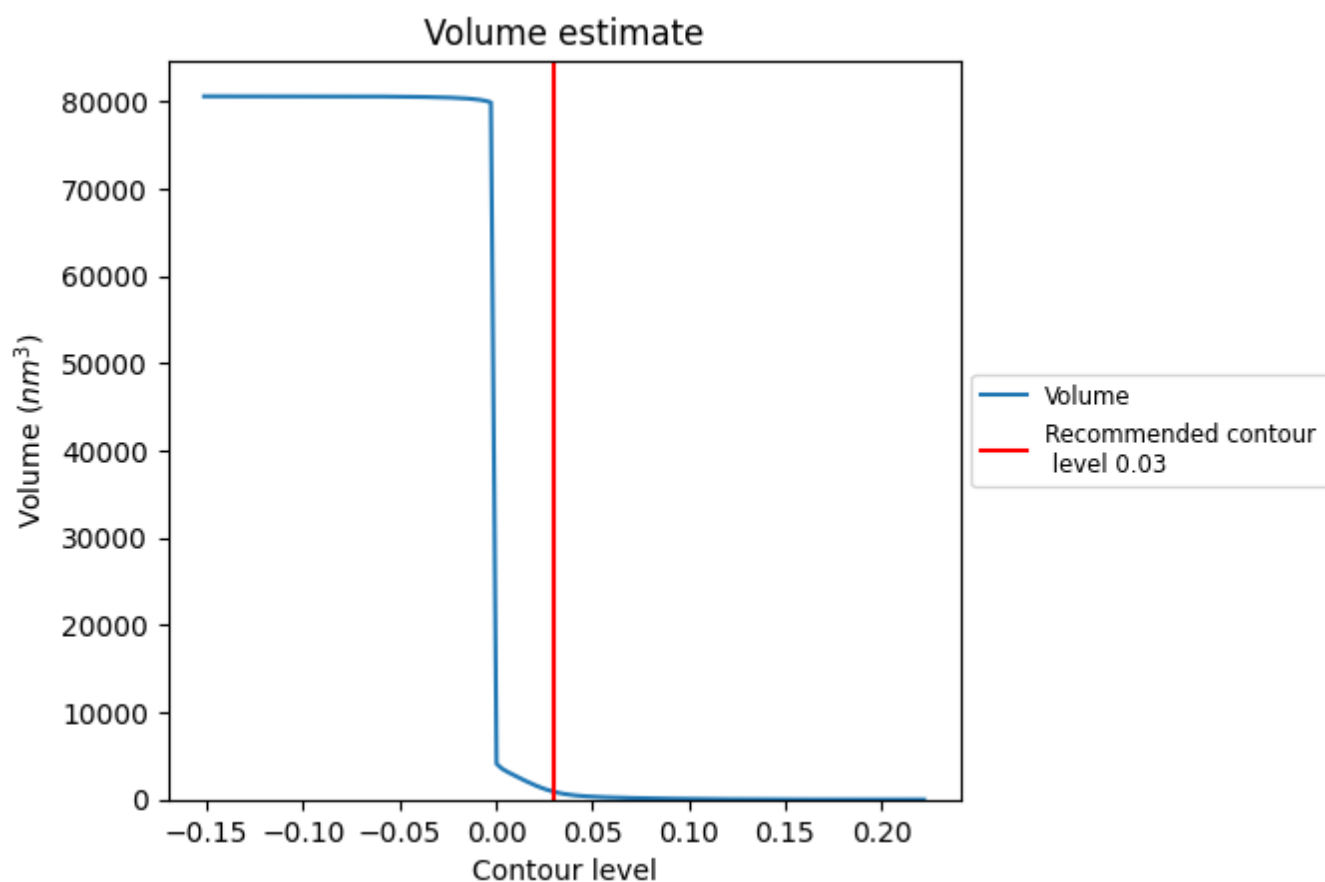
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

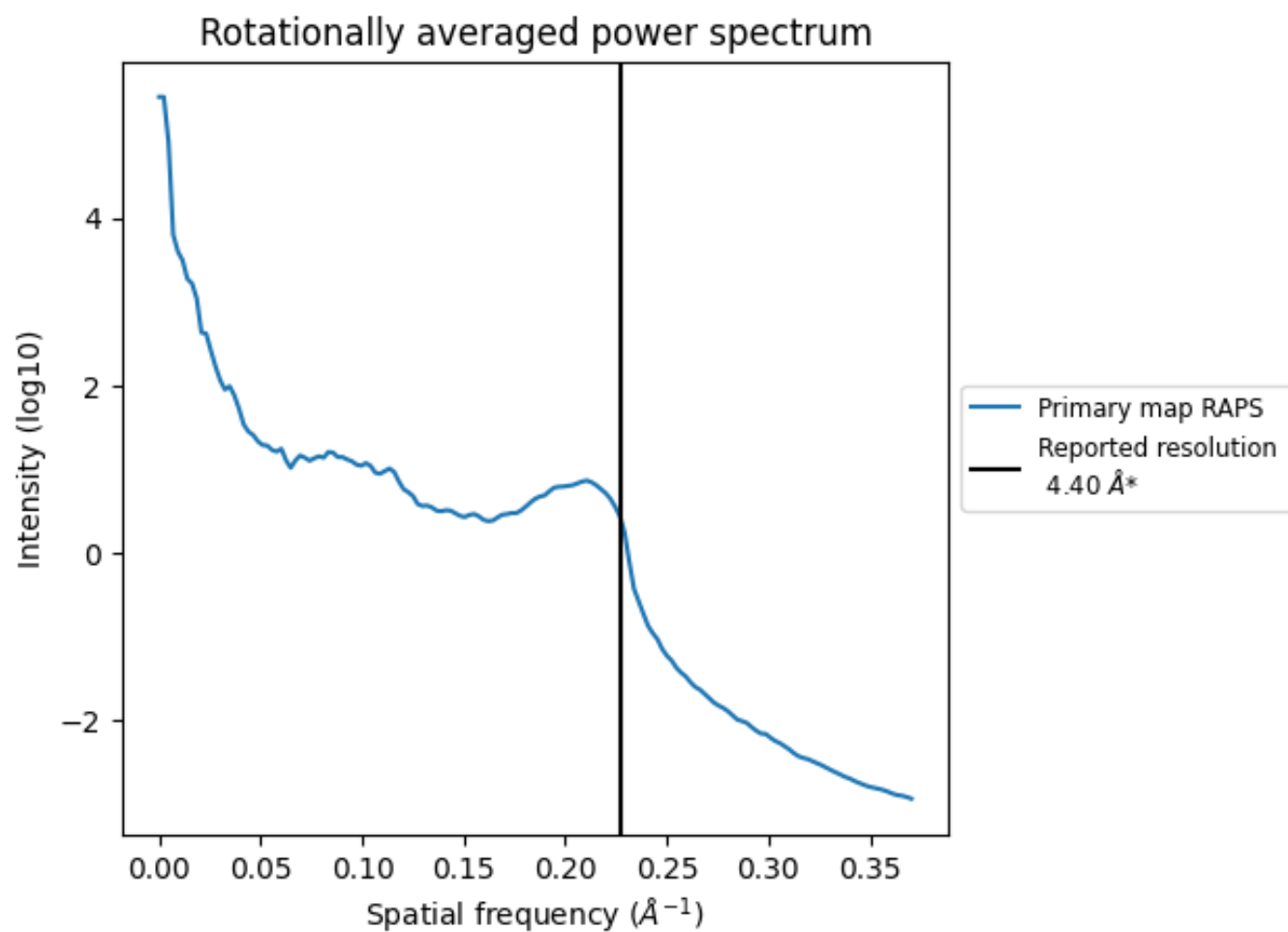
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 904 nm<sup>3</sup>; this corresponds to an approximate mass of 817 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

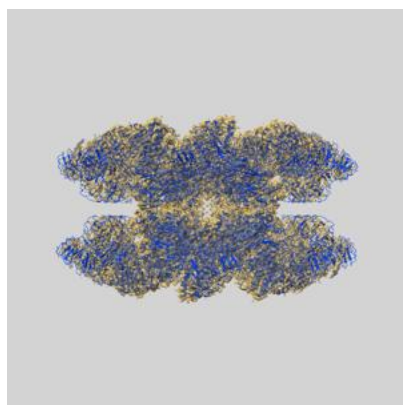
## 8 Fourier-Shell correlation

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

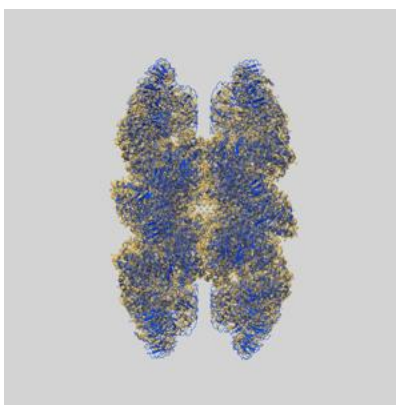
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8177 and PDB model 5JUL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

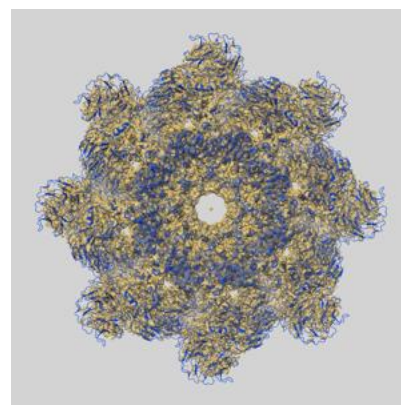
### 9.1 Map-model overlay [i](#)



X



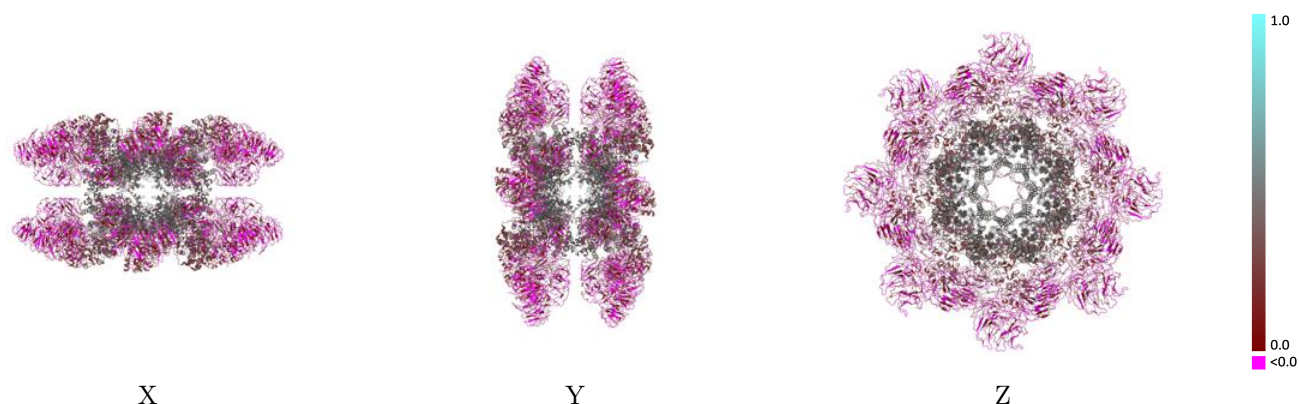
Y



Z

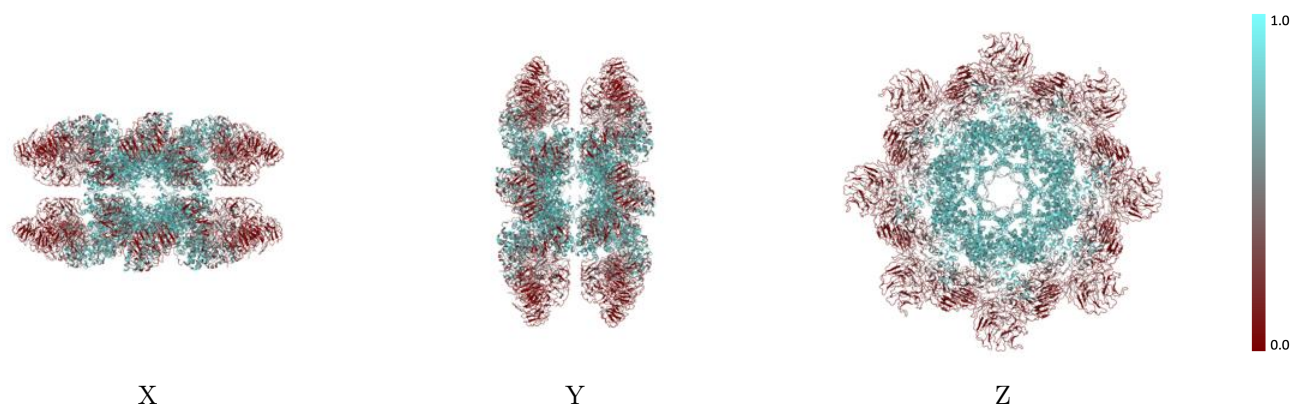
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



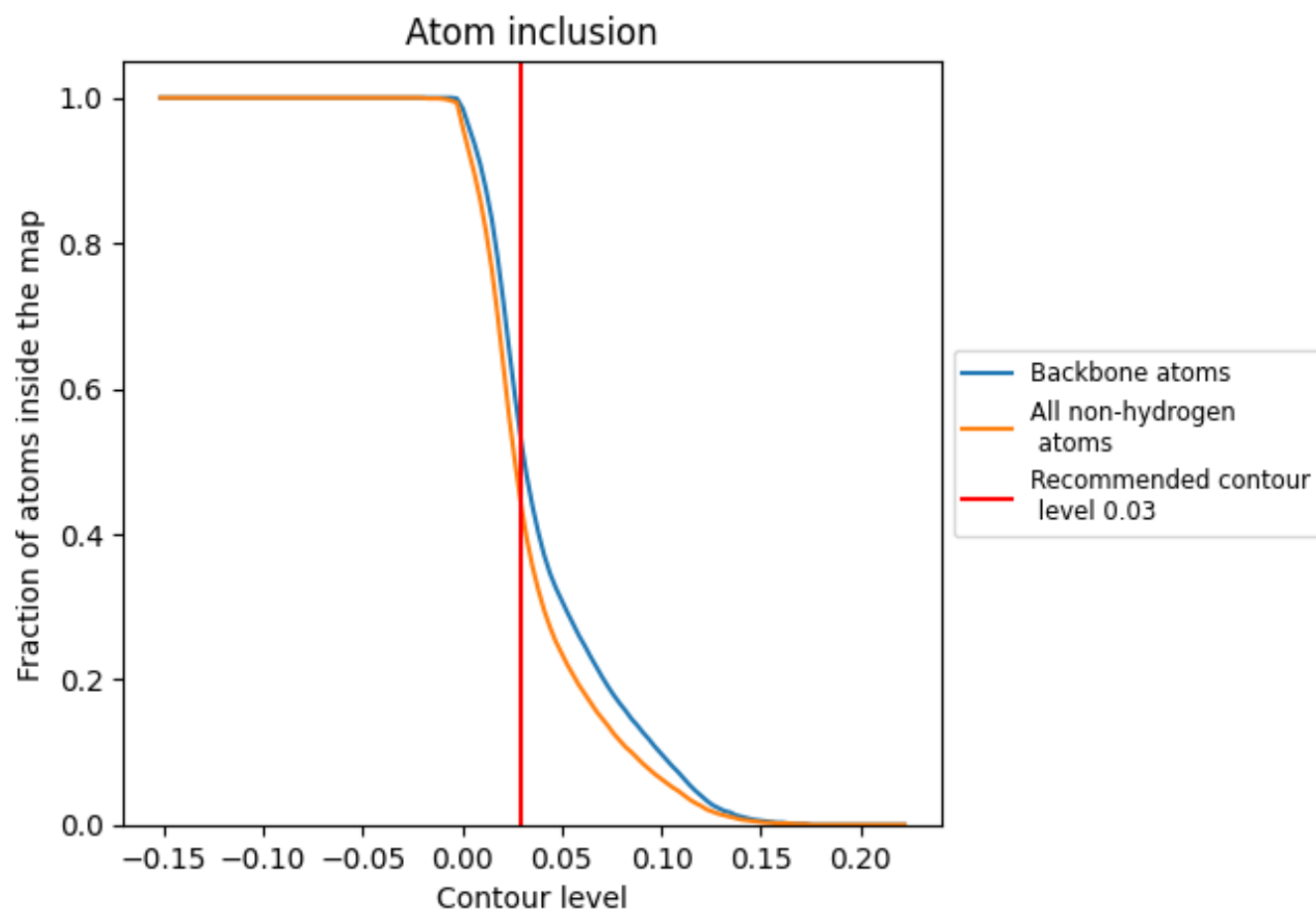
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.4340 | <div></div> 0.1940 |
| A     | <div></div> 0.4360 | <div></div> 0.1950 |
| B     | <div></div> 0.4300 | <div></div> 0.1890 |
| C     | <div></div> 0.4310 | <div></div> 0.1890 |
| D     | <div></div> 0.4330 | <div></div> 0.1960 |
| E     | <div></div> 0.4370 | <div></div> 0.1950 |
| F     | <div></div> 0.4280 | <div></div> 0.1900 |
| G     | <div></div> 0.4360 | <div></div> 0.1940 |
| H     | <div></div> 0.4360 | <div></div> 0.1950 |
| I     | <div></div> 0.4350 | <div></div> 0.1950 |
| J     | <div></div> 0.4370 | <div></div> 0.1950 |
| K     | <div></div> 0.4340 | <div></div> 0.1960 |
| L     | <div></div> 0.4280 | <div></div> 0.1880 |
| M     | <div></div> 0.4350 | <div></div> 0.1950 |
| N     | <div></div> 0.4370 | <div></div> 0.1950 |
| O     | <div></div> 0.4350 | <div></div> 0.1950 |
| P     | <div></div> 0.4330 | <div></div> 0.1960 |

