



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:30 AM UTC

PDB ID : 3PVM / pdb\_00003pvm  
Title : Structure of Complement C5 in Complex with CVF  
Authors : Laursen, N.S.; Andersen, K.R.; Braren, I.; Sottrup-Jensen, L.; Spillner, E.; Andersen, G.R.  
Deposited on : 2010-12-07  
Resolution : 4.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

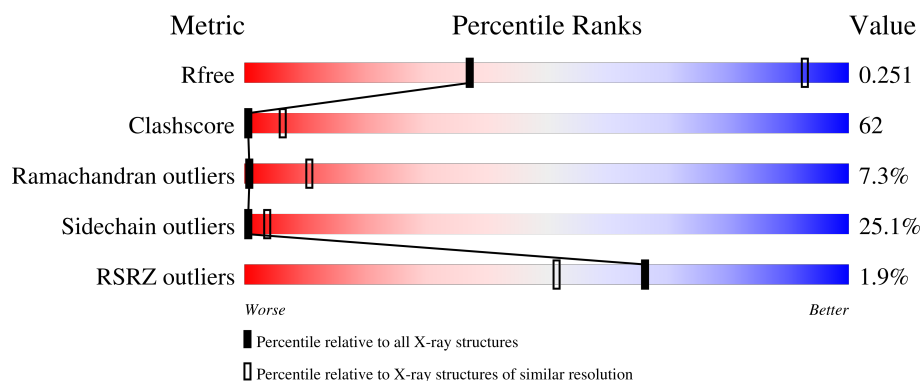
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1052 (4.70-3.90)                                      |
| Clashscore            | 190562                      | 1097 (4.70-3.90)                                      |
| Ramachandran outliers | 187476                      | 1001 (4.70-3.90)                                      |
| Sidechain outliers    | 187428                      | 1007 (4.72-3.88)                                      |
| RSRZ outliers         | 180081                      | 1049 (4.70-3.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                       |
|-----|-------|--------|--------------------------------------------------------|
| 1   | A     | 1676   | <div> <div>2%</div> <div>22% 50% 23% . .</div> </div>  |
| 1   | C     | 1676   | <div> <div>3%</div> <div>22% 50% 23% . .</div> </div>  |
| 2   | B     | 1642   | <div> <div>%</div> <div>21% 37% 15% . 25%</div> </div> |
| 2   | D     | 1642   | <div> <div>%</div> <div>20% 38% 15% . 25%</div> </div> |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45268 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

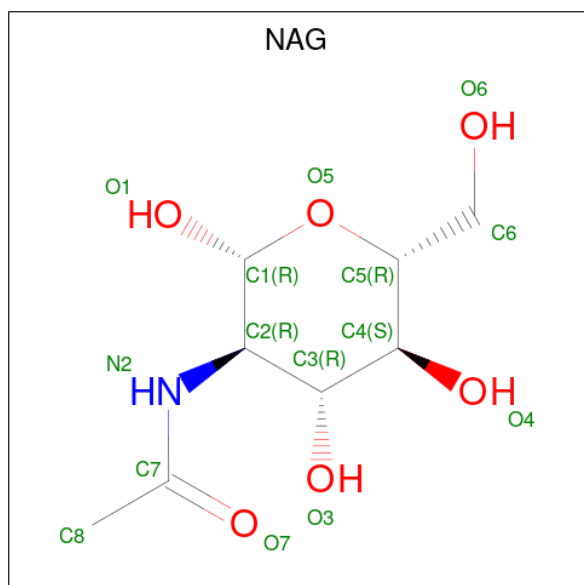
- Molecule 1 is a protein called Complement C5.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1627     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 12881 | 8246 | 2114 | 2469 | 52 |         |         |       |
| 1   | C     | 1627     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 12881 | 8246 | 2114 | 2469 | 52 |         |         |       |

- Molecule 2 is a protein called Cobra venom factor.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1225     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9711  | 6187 | 1633 | 1851 | 40 |         |         |       |
| 2   | D     | 1225     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9711  | 6187 | 1633 | 1851 | 40 |         |         |       |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

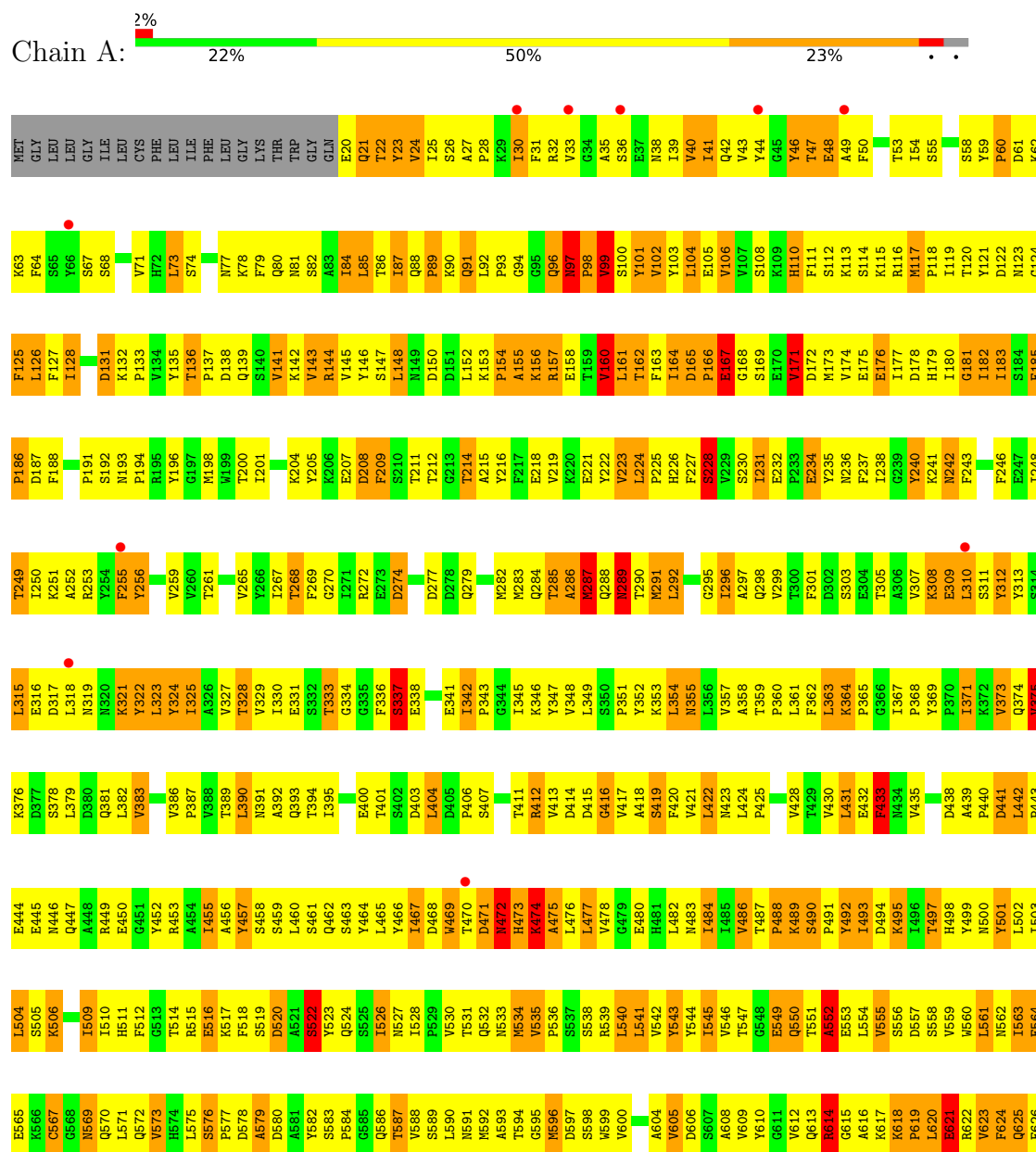


| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

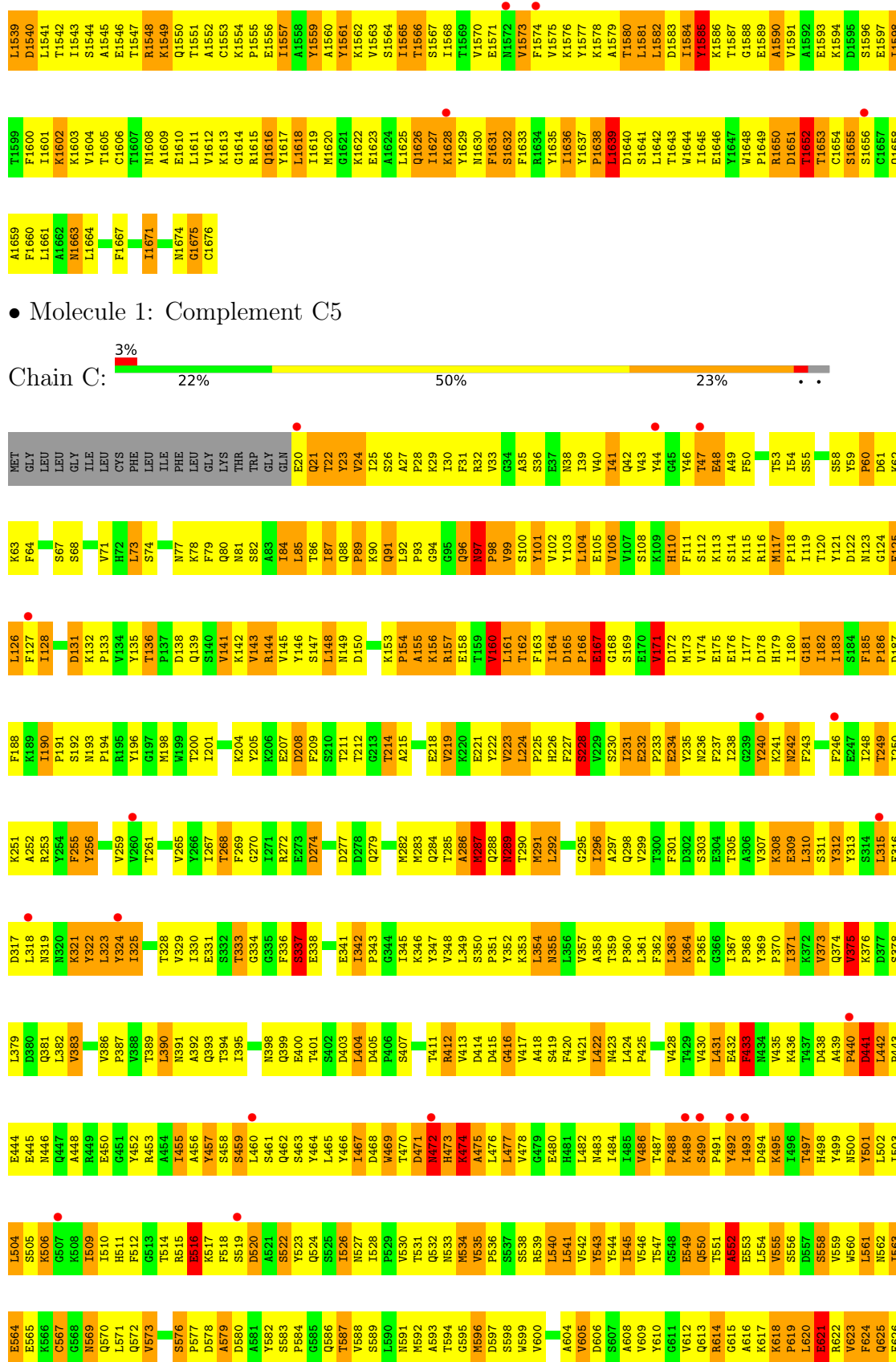
### 3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

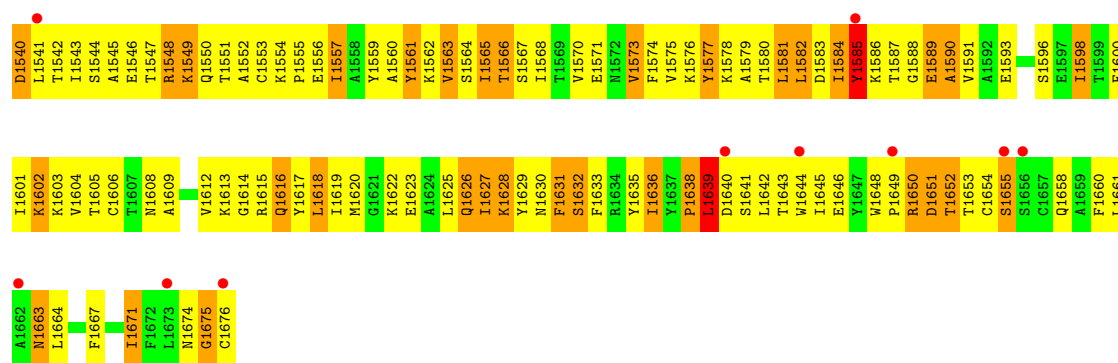
#### • Molecule 1: Complement C5



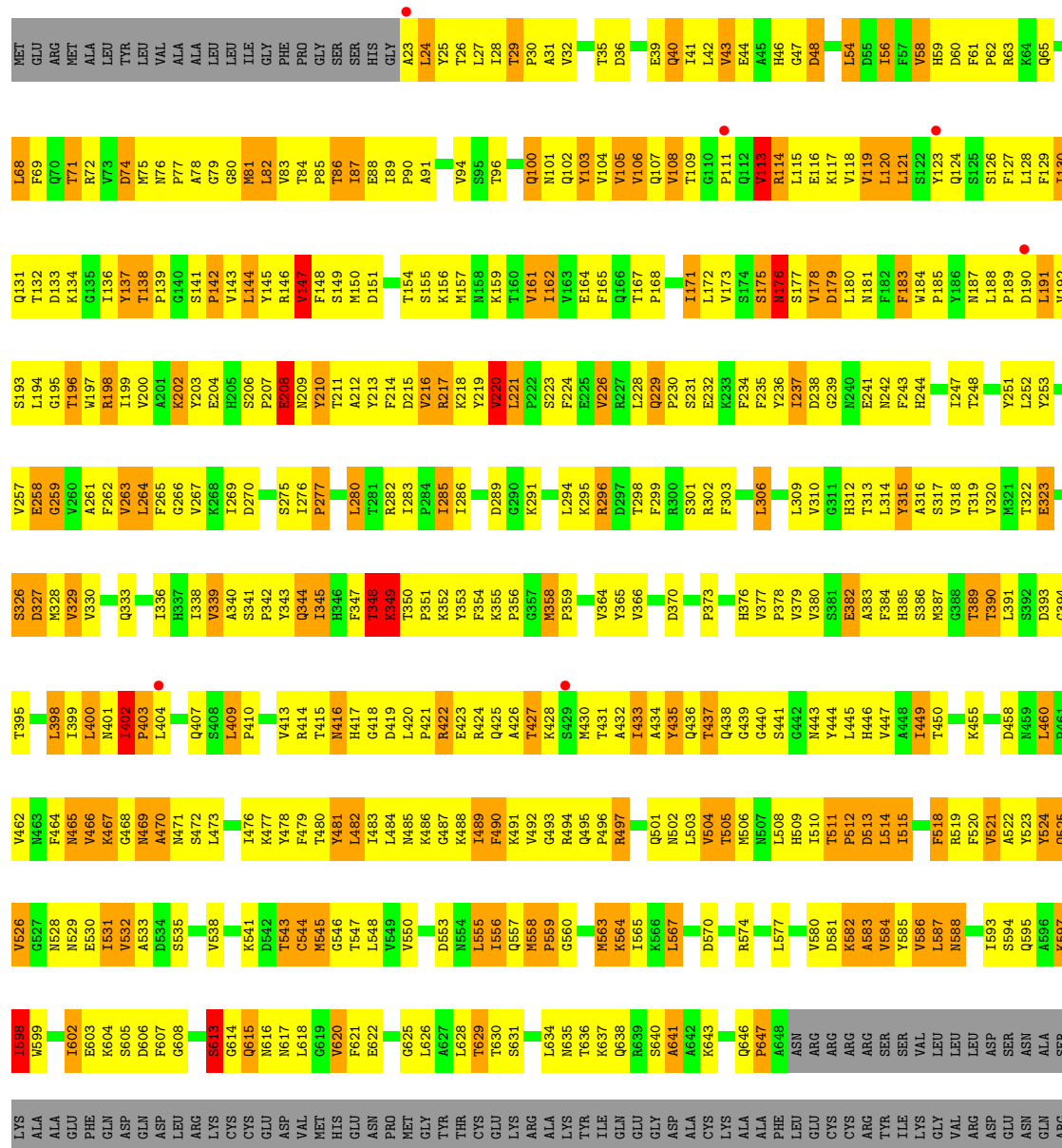
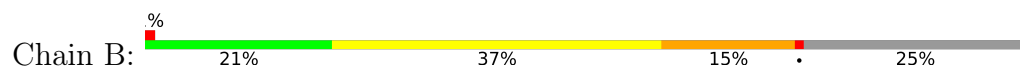
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |       |    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| F1477 | R1478 | L1479 | F1480 | L1481 | L1482 | F1483 | E1484 | V1485 | L1486 | F1487 | L1488 | S1489 | P1490 | A1491 | F1492 | T1493 | T1494 | V1495 | Y1496 | E1497 | L1498 | H1499 | R1500 | P1501 | D1502 | K1503 | Q1504 | C1505 | T1506 | M1507 | F1508 | Y1509 | S1510 | T1511 | S1512 | M1513 | L1514 | L1515 | L1516 | L1517 | L1518 | L1519 | L1520 | L1521 | L1522 | L1523 | L1524 | L1525 | L1526 | L1527 | L1528 | C1532 | G1533 | Q1534 | F1472 | M1535 | Q1536 | L1537 | E1538 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |       |    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| C1405 | A1406 | S1407 | Y1408 | L1409 | L1410 | L1411 | L1412 | L1413 | E1414 | S1420 | H1421 | A1422 | V1423 | L1424 | G1425 | L1426 | F1427 | L1428 | L1429 | T1430 | L1431 | L1432 | S1433 | L1434 | N1435 | E1436 | L1437 | L1438 | L1439 | K1440 | L1441 | L1442 | L1443 | L1444 | L1445 | L1446 | L1447 | L1448 | L1449 | F1450 | T1451 | D1452 | Q1453 | L1454 | L1455 | L1456 | D1457 | T1461 | L1462 | Q1463 | L1464 | N1465 | S1466 | T1467 | P1468 | S1469 | L1470 | D1471 | F1472 | L1473 | C1474 | V1475 | R1476 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |       |    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|       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |       |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |         |
| E1276 | E1277 | Q1278 | L1279 | Y1280 | L1281 | G1282 | G1283 | L1284 | Y1285 | L1286 | L1287 | L1288 | D1289 | L1290 | L1291 | L1292 | L1293 | L1294 | L1295 | E1299 | Y1300 | S1301 | L1302 | L1303 | V1304 | L1305 | Q1306 | L1307 | R1308 | L1309 | S1310 | M1311 | D1312 | L1313 | D1314 | L1315 | S1316 | Y1317 | K1320 | G1321 | L1322 | L1323 | H1324 | N1325 | L1326 | L1327 | M1328 | T1329 | D1330 | K1331 | L1332 | F1333 | L1334 | L1335 | L1336 | L1337 | L1338 | L1339 | L1402 | V1403 | L1404 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |       |    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|       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |       |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |         |
| G1151 | I1152 | K1153 | L1154 | L1155 | L1156 | L1157 | L1158 | L1159 | L1160 | L1161 | L1162 | L1163 | L1164 | L1165 | L1166 | L1167 | L1168 | L1169 | K1170 | A1171 | F1174 | L1175 | L1176 | E1177 | M1178 | L1179 | L1180 | F1181 | A1182 | Q1183 | S1184 | L1185 | L1186 | L1187 | L1188 | L1189 | A1190 | L1191 | L1192 | L1193 | L1194 | L1195 | L1196 | L1197 | L1198 | L1199 | L1200 | L1201 | L1202 | L1203 | L1204 | L1208 | L1209 | S1210 | A1211 | L1212 | K1213 | L1214 | F1215 | L1216 | L1217 | L1218 | L1219 | L1220 | L1221 | L1222 | L1223 | L1224 | L1225 | L1226 | L1227 | L1228 | L1229 | L1230 | L1231 | L1232 | L1233 | L1234 | L1235 | L1236 | L1237 | L1238 | L1239 | L1240 | L1241 | L1242 | L1243 | L1244 | L1245 | L1246 | L1247 | L1248 | L1249 | L1250 | L1251 | L1252 | L1253 | L1254 | L1255 | L1256 | L1257 | L1258 | L1259 | L1260 | L1261 | L1262 | L1263 | L1264 | L1265 | L1266 | L1267 | L1268 | L1269 | L1270 | L1271 | L1272 | L1273 | L1274 | L1275 |      |      |      |      |       |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |       |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |       |      |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       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| G1087 | Q1088 | Y1089 | N1090 | K1091 | Y1092 | L1093 | E1094 | Q1095 | D1096 | V1098 | P1099 | L1100 | D1037 | E972  | L973  | K974  | R975  | L976  | L977  | K1042 | S978  | K1043 | K1044 | K1045 | K1046 | K1047 | L982  | L983  | V984  | G985  | E986  | L988  | S989  | A990  | S993  | Q994  | E995  | G996  | S1007 | A1008 | E1009 | A1010 | L1011 | L1012 | F1081 | M1013 | S1014 | V1015 | V1016 | P1017 | V1018 | L1019 | Y1020 | F1021 | F1022 | H1023 | Y1024 | L1025 | E1026 | T1027 | W1031 | N1032 | V1033 | F1034 | D1037 | E972  | L973  | K974  | R975  | L976  | L977  | K1042 | S978  | K1043 | K1044 | K1045 | K1046 | K1047 | L982  | L983  | V984  | G985  | E986  | L988  | S989  | A990  | S993  | Q994  | E995  | G996  | S1007 | A1008 | E1009 | A1010 | L1011 | L1012 | F1081 | M1013 | S1014 | V1015 | V1016 | P1017 | V1018 | L1019 | Y1020 | F1021 | F1022 | H1023 | Y1024 | L1025 | E1026 | T1027 | W1031 | N1032 | V1033 | F1034 | D1037 | E972  | L973  | K974 | R975 | L976 | L977 | K1042 | 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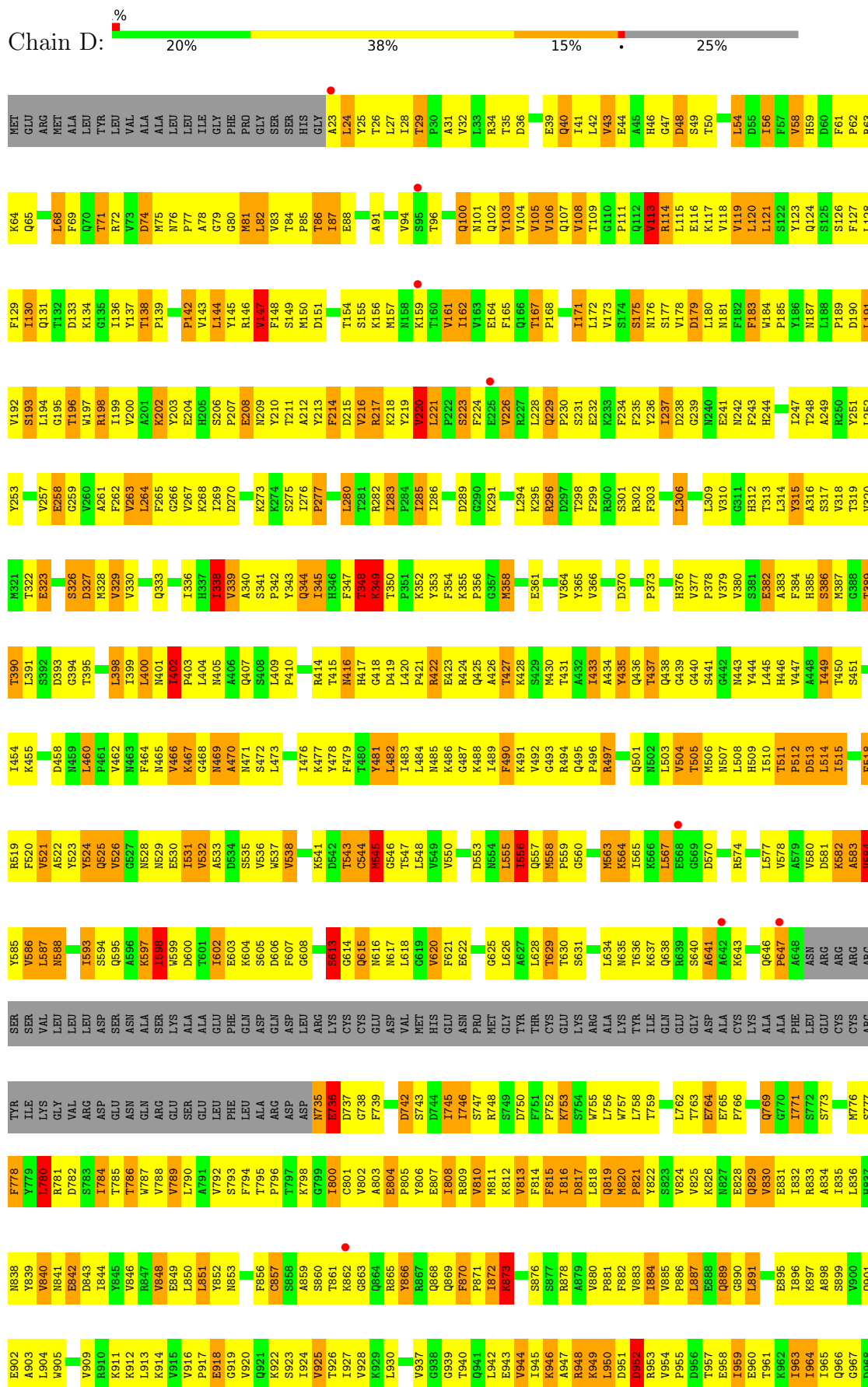
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| R1476 | A1404 | V1340 | Q1278 | R1214 | I1150 | G1087 | Y1020 | E958 | L895 | V828 |  |  | V695 | L627 |
|       | C1405 | L1341 | R1279 | E1215 | G1151 | Q1088 | V1021 | F959 | V896 | I829 |  |  | K696 | E628 |
| T1479 | A1406 | L1342 | Y1280 | A1216 | R1152 | Y1089 | F1022 | P960 | P330 | P830 |  |  | K697 | K629 |
| F1480 | S1407 | N1343 | G1281 | L1217 | R1153 | N1090 | H1023 | Y961 | F898 | Y831 |  |  | C698 | S630 |
| E1481 | Y1408 | D1344 | G1282 | K1218 | K1154 | K1091 | Y1024 | R962 | T899 | S832 |  |  | C699 | D631 |
| L1482 |       | D1345 | G1283 | K1219 | A1155 | Y1092 | L1025 | R963 | V900 | L632 |  |  | Y700 | L632 |
| F1483 | S1411 | L1346 | F1284 | G1220 |       | V1093 | E1026 | P964 | L901 | V833 |  |  | D701 | G633 |
| E1484 | R1412 | I1347 | Y1285 | N1221 | I1158 | E1094 | T1027 | L965 | P902 | V834 |  |  | G702 | C634 |
| L1485 | A1413 | F1348 | S1286 | R1222 | C1159 | P966  |       |      | L903 |      |  |  |      | G635 |
| E1414 | S1349 | S1349 | T1287 | F1160 | N1096 | L967  | W1031 | V968 | E904 | Q838 |  |  | W705 | A636 |
| F1487 | G1415 | T1350 | Q1288 | L1161 | N1097 | K974  | W1032 | K939 | I905 | I839 |  |  | W706 | G637 |
| L1488 | S1416 | G1351 | D1289 | V1162 | N1088 | P969  | I1033 | K970 | G906 | Q840 |  |  | N707 | G638 |
| S1489 |       | F1352 | T1290 | K1163 | S1099 | K971  | F1034 |      | L907 | W777 |  |  | W708 | G639 |
| F1490 | S1420 | G1353 | I1291 | L1164 | I1100 | T971  |       |      | H908 | L779 |  |  | E709 | L640 |
|       | H1421 | L1356 |       | D1165 | C1101 | E972  | D1037 |      | N909 | W780 |  |  | T710 | N641 |
| T1492 | A1422 | K1229 | I1294 | T1166 | N1102 | F973  | P1038 |      | I910 | P781 |  |  |      | N642 |
| F1493 | V1423 | E1295 | E1295 | L1167 | S1103 | K974  | L1039 |      | Y946 | W782 |  |  | Q713 | A643 |
| T1494 | T1358 | G1296 | G1296 | A1168 | L1104 | R975  | I1040 |      | F912 | R783 |  |  | R714 | N644 |
| Y1495 | V1359 | L1297 | N1231 | L1169 | L1105 | T976  | E1041 |      | S913 | K784 |  |  | A715 | V645 |
| L1496 | S1427 | Q1233 | K1232 | K1170 | W1106 | L977  | K1042 |      | L914 | Q785 |  |  |      |      |
| F1498 | L1428 | H1234 | H1234 | A1171 | L1107 | S978  | Q1043 |      | E915 | L786 |  |  | I718 | L651 |
| T1430 | T1430 | K1235 | K1235 |       | Y1108 | V979  | K1044 |      | T916 | Q787 |  |  | S719 | T652 |
| G1431 | G1431 | S1236 | E1236 | F1174 | E1109 | K980  | L1045 |      | W917 | F788 |  |  | L720 | F653 |
| L1432 | V1364 | S1237 | S1237 | L1175 | N1110 | G981  | K1046 |      | F918 | A789 |  |  | G721 | L654 |
| P1501 | L1302 | L1176 | L1176 | L1177 | Y1111 | L982  | K1047 |      | G919 | L790 |  |  | P722 | T655 |
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| A1434 | H1366 | P1240 | P1240 | T1178 | D1113 | V984  | L1049 |      | L923 | D792 |  |  | C724 | A657 |
|       | K1367 | Q1305 | K1305 | T1179 | G985  | E986  |       |      | V924 | S793 |  |  |      | M658 |
| E1436 | S1369 | L1307 | L1307 | F1180 | S1117 | L987  | M1053 |      | K925 | K858 |  |  | A727 | D661 |
| L1439 | T1370 | R1308 | R1308 | A1182 | F1118 | L988  | L1054 |      | S860 | F728 |  |  | F728 | S662 |
| K1440 | S1371 | L1309 | L1309 | Q1183 | K1119 | S889  | I1055 |      | A861 | W729 |  |  | W729 | Q663 |
| F1508 | E1372 | M1247 | S1310 | S1184 | E1120 | A990  | M1057 |      | V930 | C731 |  |  | C731 | E664 |
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| S1512 | D1314 | T1251 | T1251 | L1188 | Y1124 | F996  | N1061 |      | V934 | G803 |  |  |      | P668 |
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| T1514 | S1316 | Y1317 | Y1317 | I1190 | K1128 | N998  | D1063 |      | R936 | S805 |  |  | L736 | E671 |
| LYS   | A1380 |       |       | S1191 | L1129 | Y999  | Y1064 |      | E937 | N806 |  |  | R739 | L672 |
| ILE   | D1462 | L1254 | L1254 | A1192 | Q1130 | L1000 | S1065 |      | P871 | T807 |  |  |      | L673 |
| GLN   | Q1454 | L1256 | L1256 | Y1193 | Y1066 | L1000 | Y1066 |      | Y939 | V872 |  |  | I742 | ARG  |
| LYS   | T1455 | G1321 | G1321 | A1194 | S1067 | T1001 | S1067 |      | G941 | I809 |  |  | S743 | ARG  |
| VAL   | K1456 | S1257 | S1257 | L1195 | T1132 | H1002 | K1068 |      | D874 | C810 |  |  | HIS  | PRD  |
| CYS   | D1457 | L1259 | L1259 | S1196 | L1133 | L1003 | W1069 |      | V942 | V811 |  |  | LYS  | ARG  |
| GLU   | E1387 | N1260 | N1260 | L1197 | P1134 | P1004 | K1070 |      | Q876 | ASP  |  |  | ASP  | T678 |
| GLY   | ALA   | L1261 | L1261 | G1198 | V1135 |       |       |      | L944 | GLN  |  |  | MET  |      |
| ALA   | T1461 | Y1326 | Y1326 | D1199 | E1136 | S1007 | A1074 |      | D945 | K882 |  |  | LEU  | K681 |
| HIS   | SER   | M1327 | M1327 | K1200 | E1139 | A1008 | S1075 |      | P946 | C883 |  |  | GLY  | K682 |
| TYR   | L1462 | K1328 | K1328 | T1201 | E1140 | E1009 | T1076 |      | R947 | V884 |  |  |      | I683 |
| ARG   | Q1463 | T1329 | T1329 | H1202 | S1141 | A1010 | W1077 |      | G948 | R885 |  |  | R751 |      |
| GLY   | N1465 | D1330 | D1330 | Y1266 | L1142 | E1011 | L1078 |      | I949 | Q886 |  |  | L752 | T686 |
| TYR   | S1466 | K1331 | K1331 | Y1267 | Y1143 | L1012 | T1079 |      | Y950 | F820 |  |  | H753 | A687 |
| ASN   | P1468 | F1332 | F1332 | Q1204 | M1013 | M1013 | L1012 |      | K887 | K821 |  |  | W754 | A688 |
|       | S1469 | G1333 | G1333 |       | Y1144 | A1080 | G951  |      | G951 | F821 |  |  | T755 | K689 |
| S1470 | T1397 | L1334 | L1334 | I1208 | L1144 | F1081 | A1082 |      | T952 | D822 |  |  | K756 | Y690 |
| G1532 | D1398 | G1335 | G1335 | Y1209 | T1145 | A1082 | L1083 |      | S891 | K823 |  |  | T757 | K691 |
| G1533 | L1471 | R1336 | R1336 | S1210 | A1146 | L1084 | P1017 |      | R955 | F824 |  |  | L757 | H692 |
| Q1534 | F1472 | P1337 | P1337 | S1211 | T1147 | V1085 | R1084 |      | S892 | L825 |  |  | P758 | S693 |
| M1535 | L1473 | L1338 | L1338 | L1211 | F1148 | V1085 | V1085 |      | S893 | E826 |  |  | V760 | V694 |
|       | E1538 | C1474 | C1474 | K1213 | T1148 | L1211 | L1086 |      | H894 | M827 |  |  |      |      |
| L1539 |       |       |       |       |       |       |       |      |      |      |  |  |      |      |



## ● Molecule 2: Cobra venom factor



- Molecule 2: Cobra venom factor





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 176.52Å 179.20Å 389.69Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.47 – 4.30<br>49.47 – 4.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.2 (49.47-4.30)<br>94.2 (49.47-4.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.14                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.12 (at 4.29Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.6.4_486)                           | Depositor        |
| R, $R_{free}$                                                           | 0.233 , 0.262<br>0.228 , 0.251                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1734 reflections (2.17%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 135.2                                                       | Xtriage          |
| Anisotropy                                                              | 0.503                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 193.9                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.026 for k,h,-l                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 45268                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 192.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.74         | 0/13158        | 1.13        | 75/17851 (0.4%)  |
| 1   | C     | 0.74         | 2/13158 (0.0%) | 1.13        | 80/17851 (0.4%)  |
| 2   | B     | 0.71         | 1/9912 (0.0%)  | 1.12        | 57/13454 (0.4%)  |
| 2   | D     | 0.71         | 1/9912 (0.0%)  | 1.12        | 59/13454 (0.4%)  |
| All | All   | 0.73         | 4/46140 (0.0%) | 1.12        | 271/62610 (0.4%) |

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                   | 3                   |
| 1   | C     | 0                   | 3                   |
| 2   | B     | 0                   | 1                   |
| 2   | D     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | C     | 1563 | VAL  | CA-CB | -6.26 | 1.51        | 1.55     |
| 2   | B     | 584  | VAL  | C-O   | 5.80  | 1.30        | 1.24     |
| 2   | D     | 584  | VAL  | C-O   | 5.67  | 1.30        | 1.24     |
| 1   | C     | 686  | ILE  | CA-CB | 5.07  | 1.60        | 1.54     |

All (271) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 1346 | ASN  | CA-CB-CG | 12.98 | 125.58      | 112.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | D     | 1346 | ASN  | CA-CB-CG | 12.96 | 125.56      | 112.60   |
| 1   | C     | 930  | VAL  | CA-C-N   | 11.60 | 134.34      | 119.84   |
| 1   | C     | 930  | VAL  | C-N-CA   | 11.60 | 134.34      | 119.84   |
| 1   | A     | 930  | VAL  | CA-C-N   | 11.25 | 133.90      | 119.84   |
| 1   | A     | 930  | VAL  | C-N-CA   | 11.25 | 133.90      | 119.84   |
| 1   | C     | 117  | MET  | N-CA-C   | 10.94 | 117.98      | 108.13   |
| 1   | A     | 117  | MET  | N-CA-C   | 10.20 | 117.31      | 108.13   |
| 1   | C     | 290  | THR  | N-CA-C   | -9.09 | 102.31      | 113.50   |
| 1   | A     | 492  | TYR  | N-CA-C   | -8.78 | 101.68      | 111.07   |
| 1   | C     | 492  | TYR  | N-CA-C   | -8.77 | 101.69      | 111.07   |
| 2   | B     | 952  | ASP  | N-CA-C   | -8.71 | 102.67      | 113.20   |
| 1   | A     | 290  | THR  | N-CA-C   | -8.65 | 102.86      | 113.50   |
| 2   | D     | 952  | ASP  | N-CA-C   | -8.48 | 102.94      | 113.20   |
| 2   | D     | 587  | LEU  | CA-C-N   | -8.35 | 109.64      | 123.33   |
| 2   | D     | 587  | LEU  | C-N-CA   | -8.35 | 109.64      | 123.33   |
| 2   | B     | 587  | LEU  | CA-C-N   | -8.22 | 109.84      | 123.33   |
| 2   | B     | 587  | LEU  | C-N-CA   | -8.22 | 109.84      | 123.33   |
| 1   | A     | 564  | GLU  | N-CA-C   | 7.72  | 120.64      | 108.67   |
| 1   | A     | 1561 | TYR  | N-CA-C   | 7.46  | 119.93      | 108.07   |
| 2   | D     | 1432 | HIS  | N-CA-C   | -7.44 | 103.28      | 112.88   |
| 1   | C     | 1561 | TYR  | N-CA-C   | 7.25  | 119.59      | 108.07   |
| 1   | C     | 564  | GLU  | N-CA-C   | 7.24  | 119.89      | 108.67   |
| 1   | C     | 911  | ASN  | CA-C-N   | 7.22  | 133.03      | 122.41   |
| 1   | C     | 911  | ASN  | C-N-CA   | 7.22  | 133.03      | 122.41   |
| 1   | C     | 1563 | VAL  | CB-CA-C  | -7.22 | 104.95      | 111.74   |
| 1   | C     | 433  | PHE  | N-CA-C   | 7.21  | 120.40      | 109.23   |
| 1   | C     | 92   | LEU  | CA-C-N   | 7.12  | 128.74      | 119.84   |
| 1   | C     | 92   | LEU  | C-N-CA   | 7.12  | 128.74      | 119.84   |
| 1   | C     | 1474 | CYS  | N-CA-C   | 7.05  | 121.05      | 107.44   |
| 2   | D     | 402  | ILE  | CA-C-N   | 7.01  | 128.60      | 119.84   |
| 2   | D     | 402  | ILE  | C-N-CA   | 7.01  | 128.60      | 119.84   |
| 1   | A     | 342  | ILE  | CA-C-N   | 7.00  | 126.61      | 119.19   |
| 1   | A     | 342  | ILE  | C-N-CA   | 7.00  | 126.61      | 119.19   |
| 1   | A     | 92   | LEU  | CA-C-N   | 6.98  | 128.56      | 119.84   |
| 1   | A     | 92   | LEU  | C-N-CA   | 6.98  | 128.56      | 119.84   |
| 2   | B     | 815  | PHE  | N-CA-C   | 6.97  | 117.70      | 107.88   |
| 1   | A     | 473  | HIS  | N-CA-C   | -6.92 | 103.23      | 113.40   |
| 2   | B     | 402  | ILE  | N-CA-C   | 6.88  | 115.58      | 107.73   |
| 1   | C     | 473  | HIS  | N-CA-C   | -6.87 | 103.31      | 113.40   |
| 1   | A     | 1474 | CYS  | N-CA-C   | 6.84  | 120.64      | 107.44   |
| 2   | B     | 402  | ILE  | CA-C-N   | 6.83  | 128.37      | 119.84   |
| 2   | B     | 402  | ILE  | C-N-CA   | 6.83  | 128.37      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | C     | 629  | LYS  | N-CA-C   | -6.81 | 103.97      | 113.37   |
| 1   | A     | 769  | PHE  | CA-C-N   | 6.81  | 126.73      | 119.85   |
| 1   | A     | 769  | PHE  | C-N-CA   | 6.81  | 126.73      | 119.85   |
| 2   | D     | 1610 | TRP  | CA-C-N   | 6.80  | 128.34      | 119.84   |
| 2   | D     | 1610 | TRP  | C-N-CA   | 6.80  | 128.34      | 119.84   |
| 1   | A     | 556  | SER  | N-CA-C   | 6.78  | 117.19      | 108.24   |
| 2   | B     | 1432 | HIS  | N-CA-C   | -6.76 | 104.16      | 112.88   |
| 2   | D     | 588  | ASN  | N-CA-C   | 6.74  | 122.04      | 107.49   |
| 1   | A     | 98   | PRO  | CA-C-N   | -6.72 | 114.46      | 122.93   |
| 1   | A     | 98   | PRO  | C-N-CA   | -6.72 | 114.46      | 122.93   |
| 1   | A     | 433  | PHE  | N-CA-C   | 6.72  | 119.65      | 109.23   |
| 1   | C     | 556  | SER  | N-CA-C   | 6.70  | 117.09      | 108.24   |
| 2   | D     | 753  | LYS  | N-CA-C   | -6.69 | 106.06      | 114.56   |
| 1   | A     | 629  | LYS  | N-CA-C   | -6.69 | 104.14      | 113.37   |
| 2   | B     | 588  | ASN  | N-CA-C   | 6.67  | 121.90      | 107.49   |
| 2   | D     | 206  | SER  | CA-C-N   | 6.65  | 128.16      | 119.84   |
| 2   | D     | 206  | SER  | C-N-CA   | 6.65  | 128.16      | 119.84   |
| 1   | C     | 1224 | ILE  | CB-CA-C  | -6.64 | 105.14      | 111.05   |
| 1   | C     | 150  | ASP  | CA-CB-CG | -6.63 | 105.97      | 112.60   |
| 1   | C     | 342  | ILE  | CA-C-N   | 6.62  | 126.21      | 119.19   |
| 1   | C     | 342  | ILE  | C-N-CA   | 6.62  | 126.21      | 119.19   |
| 1   | C     | 165  | ASP  | CA-C-N   | 6.62  | 128.11      | 119.84   |
| 1   | C     | 165  | ASP  | C-N-CA   | 6.62  | 128.11      | 119.84   |
| 1   | A     | 150  | ASP  | CA-CB-CG | -6.55 | 106.05      | 112.60   |
| 1   | C     | 97   | ASN  | CA-C-N   | 6.54  | 127.79      | 120.66   |
| 1   | C     | 97   | ASN  | C-N-CA   | 6.54  | 127.79      | 120.66   |
| 2   | D     | 598  | ILE  | CB-CA-C  | -6.53 | 103.34      | 111.70   |
| 2   | B     | 598  | ILE  | CB-CA-C  | -6.51 | 103.37      | 111.70   |
| 1   | C     | 416  | GLY  | N-CA-C   | -6.50 | 103.69      | 114.48   |
| 2   | D     | 815  | PHE  | N-CA-C   | 6.45  | 116.97      | 107.88   |
| 2   | B     | 206  | SER  | CA-C-N   | 6.44  | 127.89      | 119.84   |
| 2   | B     | 206  | SER  | C-N-CA   | 6.44  | 127.89      | 119.84   |
| 2   | D     | 1350 | GLU  | N-CA-C   | 6.43  | 118.30      | 108.07   |
| 2   | B     | 1610 | TRP  | CA-C-N   | 6.37  | 127.80      | 119.84   |
| 2   | B     | 1610 | TRP  | C-N-CA   | 6.37  | 127.80      | 119.84   |
| 2   | B     | 1350 | GLU  | N-CA-C   | 6.36  | 118.18      | 108.07   |
| 2   | D     | 820  | MET  | CA-C-N   | 6.36  | 127.79      | 119.84   |
| 2   | D     | 820  | MET  | C-N-CA   | 6.36  | 127.79      | 119.84   |
| 1   | A     | 911  | ASN  | CA-C-N   | 6.34  | 131.73      | 122.41   |
| 1   | A     | 911  | ASN  | C-N-CA   | 6.34  | 131.73      | 122.41   |
| 1   | C     | 98   | PRO  | CA-C-N   | -6.29 | 113.92      | 122.91   |
| 1   | C     | 98   | PRO  | C-N-CA   | -6.29 | 113.92      | 122.91   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 901  | LEU  | CA-C-N   | 6.26  | 127.66      | 119.84   |
| 1   | A     | 901  | LEU  | C-N-CA   | 6.26  | 127.66      | 119.84   |
| 1   | C     | 769  | PHE  | CA-C-N   | 6.26  | 126.17      | 119.85   |
| 1   | C     | 769  | PHE  | C-N-CA   | 6.26  | 126.17      | 119.85   |
| 1   | C     | 718  | ILE  | N-CA-C   | 6.23  | 117.55      | 108.58   |
| 2   | B     | 1506 | ILE  | N-CA-C   | 6.22  | 116.82      | 107.80   |
| 2   | B     | 467  | LYS  | N-CA-C   | 6.21  | 118.57      | 108.76   |
| 2   | D     | 130  | ILE  | CB-CA-C  | -6.18 | 101.94      | 110.96   |
| 1   | A     | 165  | ASP  | CA-C-N   | 6.18  | 127.56      | 119.84   |
| 1   | A     | 165  | ASP  | C-N-CA   | 6.18  | 127.56      | 119.84   |
| 2   | B     | 1465 | ASP  | N-CA-C   | -6.18 | 104.91      | 112.88   |
| 1   | C     | 757  | LEU  | N-CA-C   | 6.17  | 119.08      | 109.52   |
| 2   | D     | 1547 | VAL  | CB-CA-C  | -6.16 | 102.69      | 111.31   |
| 1   | A     | 97   | ASN  | CA-C-N   | 6.16  | 127.37      | 120.66   |
| 1   | A     | 97   | ASN  | C-N-CA   | 6.16  | 127.37      | 120.66   |
| 1   | C     | 1374 | VAL  | N-CA-C   | 6.12  | 116.07      | 107.37   |
| 1   | C     | 193  | ASN  | CA-C-N   | 6.09  | 127.46      | 119.84   |
| 1   | C     | 193  | ASN  | C-N-CA   | 6.09  | 127.46      | 119.84   |
| 2   | D     | 195  | GLY  | N-CA-C   | 6.09  | 118.24      | 110.20   |
| 2   | B     | 1351 | ASN  | N-CA-C   | 6.03  | 119.01      | 110.50   |
| 1   | C     | 605  | VAL  | N-CA-C   | 6.01  | 118.88      | 108.90   |
| 2   | B     | 1344 | HIS  | N-CA-C   | -6.00 | 102.19      | 110.35   |
| 2   | D     | 1344 | HIS  | N-CA-C   | -5.98 | 102.22      | 110.35   |
| 2   | D     | 1351 | ASN  | N-CA-C   | 5.97  | 118.92      | 110.50   |
| 2   | B     | 138  | THR  | CA-C-N   | -5.97 | 113.80      | 119.89   |
| 2   | B     | 138  | THR  | C-N-CA   | -5.97 | 113.80      | 119.89   |
| 2   | B     | 830  | VAL  | N-CA-C   | 5.97  | 116.95      | 108.42   |
| 2   | D     | 113  | VAL  | N-CA-C   | 5.94  | 118.43      | 108.81   |
| 2   | B     | 208  | GLU  | N-CA-C   | -5.92 | 104.22      | 112.45   |
| 1   | C     | 667  | GLU  | N-CA-C   | 5.92  | 122.89      | 109.81   |
| 1   | C     | 228  | SER  | N-CA-C   | -5.91 | 98.78       | 108.41   |
| 1   | A     | 757  | LEU  | N-CA-C   | 5.90  | 118.67      | 109.52   |
| 2   | B     | 270  | ASP  | CB-CA-C  | -5.90 | 109.75      | 116.54   |
| 2   | D     | 270  | ASP  | CB-CA-C  | -5.89 | 109.77      | 116.54   |
| 1   | C     | 149  | ASN  | CA-CB-CG | 5.88  | 118.48      | 112.60   |
| 1   | A     | 667  | GLU  | N-CA-C   | 5.88  | 122.80      | 109.81   |
| 2   | D     | 1491 | ARG  | N-CA-C   | 5.86  | 116.29      | 108.38   |
| 1   | C     | 1653 | THR  | N-CA-C   | 5.86  | 117.61      | 110.41   |
| 2   | D     | 1421 | VAL  | N-CA-C   | -5.86 | 104.43      | 113.16   |
| 2   | B     | 113  | VAL  | N-CA-C   | 5.83  | 118.25      | 108.81   |
| 2   | D     | 1465 | ASP  | N-CA-C   | -5.82 | 105.37      | 112.88   |
| 1   | C     | 160  | VAL  | N-CA-C   | 5.82  | 116.38      | 107.77   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 193  | ASN  | CA-C-N  | 5.79  | 127.08      | 119.84   |
| 1   | A     | 193  | ASN  | C-N-CA  | 5.79  | 127.08      | 119.84   |
| 1   | C     | 910  | ILE  | CA-C-N  | 5.78  | 131.59      | 122.34   |
| 1   | C     | 910  | ILE  | C-N-CA  | 5.78  | 131.59      | 122.34   |
| 2   | B     | 130  | ILE  | CB-CA-C | -5.78 | 102.52      | 110.96   |
| 2   | B     | 1482 | ASN  | N-CA-C  | 5.77  | 118.63      | 110.50   |
| 1   | C     | 722  | PRO  | N-CA-C  | -5.76 | 106.35      | 113.84   |
| 1   | C     | 1180 | LEU  | N-CA-C  | 5.75  | 120.58      | 112.75   |
| 2   | D     | 138  | THR  | CA-C-N  | -5.74 | 114.04      | 119.89   |
| 2   | D     | 138  | THR  | C-N-CA  | -5.74 | 114.04      | 119.89   |
| 1   | C     | 932  | GLU  | N-CA-C  | 5.74  | 120.09      | 109.24   |
| 2   | D     | 1484 | ILE  | CB-CA-C | -5.74 | 102.07      | 110.62   |
| 2   | D     | 1482 | ASN  | N-CA-C  | 5.71  | 118.55      | 110.50   |
| 1   | A     | 605  | VAL  | N-CA-C  | 5.70  | 118.36      | 108.90   |
| 1   | A     | 1180 | LEU  | N-CA-C  | 5.70  | 120.50      | 112.75   |
| 1   | A     | 718  | ILE  | N-CA-C  | 5.70  | 116.78      | 108.58   |
| 1   | C     | 1650 | ARG  | N-CA-C  | 5.69  | 118.17      | 108.90   |
| 2   | B     | 195  | GLY  | N-CA-C  | 5.67  | 117.68      | 110.20   |
| 1   | C     | 117  | MET  | CA-C-N  | 5.67  | 126.46      | 120.11   |
| 1   | C     | 117  | MET  | C-N-CA  | 5.67  | 126.46      | 120.11   |
| 2   | B     | 366  | VAL  | N-CA-C  | 5.66  | 115.72      | 106.72   |
| 1   | A     | 722  | PRO  | N-CA-C  | -5.66 | 106.49      | 113.84   |
| 1   | C     | 1102 | ASN  | N-CA-C  | -5.65 | 104.33      | 111.11   |
| 1   | A     | 117  | MET  | CA-C-N  | 5.63  | 126.42      | 120.11   |
| 1   | A     | 117  | MET  | C-N-CA  | 5.63  | 126.42      | 120.11   |
| 1   | A     | 228  | SER  | N-CA-C  | -5.63 | 99.23       | 108.41   |
| 1   | A     | 1650 | ARG  | N-CA-C  | 5.61  | 118.05      | 108.90   |
| 2   | D     | 366  | VAL  | N-CA-C  | 5.61  | 115.64      | 106.72   |
| 2   | B     | 1421 | VAL  | N-CA-C  | -5.59 | 104.83      | 113.16   |
| 1   | A     | 160  | VAL  | CB-CA-C | -5.59 | 102.88      | 110.42   |
| 1   | A     | 181  | GLY  | N-CA-C  | 5.58  | 126.40      | 113.18   |
| 2   | D     | 848  | VAL  | CB-CA-C | -5.57 | 102.89      | 110.42   |
| 2   | D     | 1419 | GLN  | N-CA-C  | 5.57  | 118.88      | 112.97   |
| 2   | B     | 820  | MET  | CA-C-N  | 5.54  | 126.76      | 119.84   |
| 2   | B     | 820  | MET  | C-N-CA  | 5.54  | 126.76      | 119.84   |
| 2   | D     | 467  | LYS  | N-CA-C  | 5.51  | 117.46      | 108.76   |
| 2   | D     | 130  | ILE  | N-CA-C  | 5.50  | 115.78      | 107.80   |
| 1   | A     | 1331 | LYS  | N-CA-C  | -5.49 | 106.42      | 114.39   |
| 1   | A     | 1653 | THR  | N-CA-C  | 5.49  | 117.16      | 110.41   |
| 1   | A     | 932  | GLU  | N-CA-C  | 5.49  | 119.61      | 109.24   |
| 1   | A     | 160  | VAL  | N-CA-C  | 5.48  | 115.88      | 107.77   |
| 2   | D     | 402  | ILE  | N-CA-C  | 5.47  | 113.97      | 107.73   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 349  | LYS  | N-CA-C  | -5.47 | 99.15       | 110.80   |
| 1   | C     | 1422 | ALA  | N-CA-C  | 5.47  | 116.58      | 108.60   |
| 1   | C     | 901  | LEU  | CA-C-N  | 5.46  | 126.67      | 119.84   |
| 1   | C     | 901  | LEU  | C-N-CA  | 5.46  | 126.67      | 119.84   |
| 2   | D     | 283  | ILE  | CA-C-N  | 5.46  | 126.67      | 119.84   |
| 2   | D     | 283  | ILE  | C-N-CA  | 5.46  | 126.67      | 119.84   |
| 2   | D     | 349  | LYS  | N-CA-C  | -5.44 | 99.21       | 110.80   |
| 2   | B     | 1484 | ILE  | CB-CA-C | -5.43 | 102.53      | 110.62   |
| 2   | B     | 1491 | ARG  | N-CA-C  | 5.40  | 115.67      | 108.38   |
| 2   | B     | 229  | GLN  | CA-C-N  | 5.40  | 125.37      | 120.03   |
| 2   | B     | 229  | GLN  | C-N-CA  | 5.40  | 125.37      | 120.03   |
| 1   | C     | 1003 | LEU  | CA-C-N  | 5.38  | 126.57      | 119.84   |
| 1   | C     | 1003 | LEU  | C-N-CA  | 5.38  | 126.57      | 119.84   |
| 1   | C     | 160  | VAL  | CB-CA-C | -5.37 | 103.17      | 110.42   |
| 2   | D     | 147  | VAL  | N-CA-C  | 5.36  | 115.70      | 107.77   |
| 1   | A     | 1033 | ILE  | CB-CA-C | -5.35 | 102.52      | 111.29   |
| 2   | B     | 810  | VAL  | N-CA-C  | 5.34  | 115.65      | 108.17   |
| 1   | C     | 181  | GLY  | N-CA-C  | 5.34  | 125.83      | 113.18   |
| 1   | A     | 416  | GLY  | N-CA-C  | -5.33 | 106.05      | 114.10   |
| 1   | C     | 1197 | LEU  | N-CA-C  | 5.33  | 118.89      | 112.38   |
| 2   | D     | 229  | GLN  | CA-C-N  | 5.32  | 125.30      | 120.03   |
| 2   | D     | 229  | GLN  | C-N-CA  | 5.32  | 125.30      | 120.03   |
| 1   | A     | 1477 | PHE  | N-CA-C  | 5.32  | 116.61      | 108.52   |
| 2   | B     | 1419 | GLN  | N-CA-C  | 5.32  | 118.89      | 112.93   |
| 2   | D     | 451  | SER  | N-CA-C  | 5.32  | 116.79      | 110.19   |
| 2   | B     | 876  | SER  | N-CA-C  | 5.32  | 117.76      | 109.52   |
| 2   | D     | 556  | ILE  | N-CA-C  | 5.31  | 115.23      | 108.12   |
| 1   | A     | 143  | VAL  | N-CA-C  | 5.30  | 115.54      | 108.27   |
| 1   | C     | 1461 | ILE  | N-CA-C  | 5.30  | 116.01      | 107.73   |
| 1   | A     | 364  | LYS  | CA-C-N  | 5.30  | 126.13      | 119.98   |
| 1   | A     | 364  | LYS  | C-N-CA  | 5.30  | 126.13      | 119.98   |
| 1   | A     | 185  | PHE  | CA-C-N  | 5.30  | 126.47      | 119.84   |
| 1   | A     | 185  | PHE  | C-N-CA  | 5.30  | 126.47      | 119.84   |
| 1   | A     | 1189 | ALA  | N-CA-C  | 5.30  | 116.74      | 111.07   |
| 1   | A     | 614  | ARG  | N-CA-C  | 5.29  | 117.05      | 111.28   |
| 1   | A     | 1374 | VAL  | N-CA-C  | 5.29  | 115.24      | 107.15   |
| 1   | C     | 1331 | LYS  | N-CA-C  | -5.27 | 106.75      | 114.39   |
| 2   | B     | 413  | VAL  | N-CA-C  | 5.26  | 116.06      | 108.48   |
| 2   | B     | 24   | LEU  | N-CA-C  | 5.24  | 117.45      | 108.90   |
| 1   | A     | 1338 | VAL  | N-CA-C  | 5.24  | 116.85      | 108.89   |
| 1   | A     | 1224 | ILE  | CB-CA-C | -5.23 | 106.39      | 111.05   |
| 2   | B     | 147  | VAL  | N-CA-C  | 5.23  | 115.65      | 108.12   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 489  | ILE  | CB-CA-C  | -5.22 | 105.14      | 111.88   |
| 1   | C     | 1443 | VAL  | CB-CA-C  | -5.22 | 106.48      | 111.44   |
| 2   | D     | 899  | SER  | N-CA-C   | 5.22  | 117.00      | 109.07   |
| 2   | D     | 771  | ILE  | CB-CA-C  | -5.21 | 105.86      | 111.59   |
| 2   | B     | 850  | LEU  | N-CA-C   | -5.21 | 103.81      | 110.53   |
| 1   | C     | 516  | GLU  | N-CA-C   | -5.20 | 102.91      | 110.24   |
| 1   | C     | 143  | VAL  | N-CA-C   | 5.19  | 115.38      | 108.27   |
| 1   | C     | 1338 | VAL  | N-CA-C   | 5.19  | 116.78      | 108.89   |
| 1   | A     | 527  | ASN  | CA-C-N   | -5.19 | 117.62      | 123.02   |
| 1   | A     | 527  | ASN  | C-N-CA   | -5.19 | 117.62      | 123.02   |
| 2   | B     | 137  | TYR  | N-CA-C   | 5.18  | 117.86      | 108.69   |
| 2   | B     | 130  | ILE  | N-CA-C   | 5.17  | 115.30      | 107.80   |
| 2   | D     | 24   | LEU  | N-CA-C   | 5.16  | 117.31      | 108.90   |
| 2   | D     | 810  | VAL  | N-CA-C   | 5.15  | 115.39      | 108.17   |
| 2   | D     | 1391 | LEU  | CA-C-N   | 5.15  | 124.91      | 119.76   |
| 2   | D     | 1391 | LEU  | C-N-CA   | 5.15  | 124.91      | 119.76   |
| 2   | B     | 176  | ASN  | N-CA-C   | 5.15  | 116.63      | 108.96   |
| 1   | A     | 667  | GLU  | CA-C-N   | -5.14 | 114.44      | 119.99   |
| 1   | A     | 667  | GLU  | C-N-CA   | -5.14 | 114.44      | 119.99   |
| 2   | B     | 210  | TYR  | CA-CB-CG | -5.14 | 104.65      | 113.90   |
| 1   | A     | 892  | SER  | N-CA-C   | 5.14  | 114.40      | 108.49   |
| 1   | C     | 1180 | LEU  | CA-C-N   | -5.13 | 113.42      | 119.84   |
| 1   | C     | 1180 | LEU  | C-N-CA   | -5.13 | 113.42      | 119.84   |
| 2   | B     | 1363 | LEU  | N-CA-C   | 5.13  | 116.87      | 108.76   |
| 1   | A     | 1231 | ASN  | N-CA-C   | 5.13  | 120.92      | 114.31   |
| 1   | A     | 375  | VAL  | CB-CA-C  | -5.12 | 106.10      | 112.45   |
| 2   | D     | 1431 | SER  | N-CA-C   | 5.12  | 117.14      | 110.43   |
| 2   | D     | 338  | ILE  | N-CA-C   | 5.12  | 115.22      | 107.80   |
| 1   | C     | 1085 | VAL  | CB-CA-C  | -5.11 | 105.43      | 111.81   |
| 1   | A     | 46   | TYR  | N-CA-C   | 5.10  | 118.02      | 110.48   |
| 2   | D     | 50   | THR  | CA-C-N   | 5.10  | 126.21      | 119.84   |
| 2   | D     | 50   | THR  | C-N-CA   | 5.10  | 126.21      | 119.84   |
| 2   | B     | 178  | VAL  | N-CA-C   | 5.09  | 115.24      | 108.11   |
| 1   | A     | 99   | VAL  | N-CA-CB  | 5.09  | 117.10      | 110.99   |
| 1   | A     | 865  | ILE  | N-CA-C   | 5.09  | 115.24      | 108.11   |
| 1   | C     | 527  | ASN  | CA-C-N   | -5.08 | 117.73      | 123.02   |
| 1   | C     | 527  | ASN  | C-N-CA   | -5.08 | 117.73      | 123.02   |
| 2   | B     | 1391 | LEU  | CA-C-N   | 5.08  | 124.84      | 119.76   |
| 2   | B     | 1391 | LEU  | C-N-CA   | 5.08  | 124.84      | 119.76   |
| 1   | A     | 1197 | LEU  | N-CA-C   | 5.07  | 118.72      | 112.54   |
| 2   | D     | 876  | SER  | N-CA-C   | 5.06  | 117.36      | 109.52   |
| 1   | C     | 185  | PHE  | CA-C-N   | 5.05  | 126.15      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C     | 185  | PHE  | C-N-CA  | 5.05  | 126.15      | 119.84   |
| 1   | A     | 1443 | VAL  | CB-CA-C | -5.05 | 106.65      | 111.44   |
| 2   | B     | 1526 | THR  | N-CA-C  | 5.05  | 116.08      | 108.46   |
| 1   | A     | 810  | CYS  | N-CA-C  | 5.04  | 116.80      | 108.13   |
| 1   | A     | 1559 | TYR  | N-CA-C  | 5.04  | 116.62      | 108.41   |
| 1   | C     | 190  | ILE  | CA-C-N  | -5.04 | 115.38      | 120.21   |
| 1   | C     | 190  | ILE  | C-N-CA  | -5.04 | 115.38      | 120.21   |
| 1   | A     | 1461 | ILE  | N-CA-C  | 5.03  | 115.57      | 107.73   |
| 1   | C     | 1131 | GLY  | N-CA-C  | 5.03  | 118.09      | 110.75   |
| 1   | C     | 1231 | ASN  | N-CA-C  | 5.03  | 121.11      | 114.12   |
| 1   | C     | 375  | VAL  | CB-CA-C | -5.02 | 106.22      | 112.45   |
| 1   | C     | 667  | GLU  | CA-C-N  | -5.02 | 114.57      | 119.99   |
| 1   | C     | 667  | GLU  | C-N-CA  | -5.02 | 114.57      | 119.99   |
| 2   | B     | 259  | GLY  | N-CA-C  | 5.01  | 118.98      | 111.42   |
| 1   | C     | 364  | LYS  | CA-C-N  | 5.01  | 125.79      | 119.98   |
| 1   | C     | 364  | LYS  | C-N-CA  | 5.01  | 125.79      | 119.98   |
| 2   | D     | 1506 | ILE  | N-CA-C  | 5.01  | 115.06      | 107.80   |
| 2   | D     | 538  | VAL  | N-CA-C  | 5.00  | 114.96      | 108.35   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 472  | ASN  | Peptide |
| 1   | A     | 552  | ALA  | Peptide |
| 1   | A     | 667  | GLU  | Peptide |
| 2   | B     | 1351 | ASN  | Peptide |
| 1   | C     | 472  | ASN  | Peptide |
| 1   | C     | 552  | ALA  | Peptide |
| 1   | C     | 667  | GLU  | Peptide |
| 2   | D     | 1351 | ASN  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 12881 | 0        | 12821    | 1762    | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 12881 | 0        | 12821    | 1740    | 0            |
| 2   | B     | 9711  | 0        | 9702     | 1104    | 0            |
| 2   | D     | 9711  | 0        | 9702     | 1112    | 0            |
| 3   | A     | 14    | 0        | 13       | 2       | 0            |
| 3   | B     | 28    | 0        | 26       | 1       | 0            |
| 3   | C     | 14    | 0        | 13       | 2       | 0            |
| 3   | D     | 28    | 0        | 26       | 1       | 0            |
| All | All   | 45268 | 0        | 45124    | 5642    | 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 62.

All (5642) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:380:VAL:HG12 | 2:B:387:MET:HB3   | 1.24                     | 1.15              |
| 2:D:380:VAL:HG12 | 2:D:387:MET:HB3   | 1.26                     | 1.15              |
| 2:D:1609:ARG:HG2 | 2:D:1609:ARG:HH11 | 1.12                     | 1.13              |
| 1:A:386:VAL:H    | 1:A:411:THR:HG22  | 1.02                     | 1.12              |
| 1:C:386:VAL:H    | 1:C:411:THR:HG22  | 1.00                     | 1.11              |
| 2:D:261:ALA:HB2  | 2:D:320:VAL:HG23  | 1.30                     | 1.11              |
| 2:B:1609:ARG:HG2 | 2:B:1609:ARG:HH11 | 1.13                     | 1.10              |
| 1:A:1228:TRP:H   | 1:A:1251:THR:HG22 | 1.13                     | 1.10              |
| 1:C:979:VAL:HG21 | 1:C:1326:TYR:CE1  | 1.85                     | 1.10              |
| 1:A:59:TYR:CE2   | 1:A:99:VAL:HG21   | 1.85                     | 1.09              |
| 1:A:1278:GLN:OE1 | 1:A:1283:GLY:HA2  | 1.49                     | 1.09              |
| 1:A:1494:THR:HB  | 1:A:1506:THR:HG23 | 1.32                     | 1.07              |
| 1:C:1278:GLN:OE1 | 1:C:1283:GLY:HA2  | 1.53                     | 1.07              |
| 2:D:850:LEU:HB2  | 2:D:882:PHE:HE1   | 1.20                     | 1.07              |
| 1:C:1228:TRP:H   | 1:C:1251:THR:HG22 | 1.12                     | 1.06              |
| 2:B:261:ALA:HB2  | 2:B:320:VAL:HG23  | 1.36                     | 1.05              |
| 2:B:851:LEU:HD23 | 2:B:852:TYR:H     | 1.18                     | 1.05              |
| 1:A:979:VAL:HG21 | 1:A:1326:TYR:CE1  | 1.90                     | 1.05              |
| 2:B:344:GLN:HA   | 2:B:344:GLN:HE21  | 1.19                     | 1.04              |
| 1:C:1228:TRP:H   | 1:C:1251:THR:CG2  | 1.70                     | 1.03              |
| 2:D:526:VAL:HG23 | 2:D:530:GLU:HB3   | 1.37                     | 1.03              |
| 2:B:1473:HIS:CD2 | 2:B:1474:PRO:HD2  | 1.93                     | 1.03              |
| 1:C:492:TYR:CD2  | 1:C:493:ILE:N     | 2.27                     | 1.03              |
| 1:C:535:VAL:HG23 | 1:C:536:PRO:HD3   | 1.40                     | 1.03              |
| 1:A:492:TYR:CD2  | 1:A:493:ILE:N     | 2.27                     | 1.03              |
| 1:C:1494:THR:HB  | 1:C:1506:THR:HG23 | 1.39                     | 1.03              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:59:TYR:CE2    | 1:C:99:VAL:HG21   | 1.92                     | 1.03              |
| 1:C:1584:ILE:HG22 | 1:C:1585:TYR:H    | 1.24                     | 1.03              |
| 2:B:526:VAL:HG23  | 2:B:530:GLU:HB3   | 1.39                     | 1.02              |
| 2:B:1607:ILE:H    | 2:B:1607:ILE:HD12 | 1.22                     | 1.02              |
| 1:C:42:GLN:HB2    | 1:C:80:GLN:HE21   | 1.24                     | 1.02              |
| 1:A:535:VAL:HG23  | 1:A:536:PRO:HD3   | 1.40                     | 1.02              |
| 2:B:820:MET:HE2   | 2:B:832:ILE:HD13  | 1.42                     | 1.02              |
| 2:B:1590:LEU:HD23 | 2:B:1591:LEU:H    | 1.21                     | 1.02              |
| 1:A:42:GLN:HB2    | 1:A:80:GLN:HE21   | 1.25                     | 1.01              |
| 1:A:224:LEU:HD22  | 1:A:225:PRO:HD2   | 1.39                     | 1.01              |
| 1:C:24:VAL:CA     | 1:C:655:THR:HG21  | 1.88                     | 1.01              |
| 2:D:820:MET:HE2   | 2:D:832:ILE:HD13  | 1.40                     | 1.01              |
| 1:A:1228:TRP:H    | 1:A:1251:THR:CG2  | 1.73                     | 1.01              |
| 2:D:1473:HIS:CD2  | 2:D:1474:PRO:HD2  | 1.96                     | 1.01              |
| 2:D:344:GLN:HA    | 2:D:344:GLN:HE21  | 1.18                     | 1.01              |
| 2:D:1523:VAL:HG22 | 2:D:1584:TRP:HB2  | 1.39                     | 1.01              |
| 1:C:87:ILE:H      | 1:C:87:ILE:HD13   | 1.23                     | 1.00              |
| 1:C:222:TYR:HE1   | 1:C:768:TYR:HB2   | 1.25                     | 1.00              |
| 1:C:1008:ALA:HB3  | 1:C:1078:LEU:HD11 | 1.40                     | 1.00              |
| 1:A:87:ILE:HD13   | 1:A:87:ILE:H      | 1.21                     | 1.00              |
| 1:A:1584:ILE:HG22 | 1:A:1585:TYR:H    | 1.27                     | 1.00              |
| 1:C:24:VAL:HA     | 1:C:655:THR:CG2   | 1.89                     | 1.00              |
| 2:D:851:LEU:HD23  | 2:D:852:TYR:H     | 1.21                     | 1.00              |
| 1:A:44:TYR:HE1    | 1:A:497:THR:HG21  | 1.24                     | 1.00              |
| 2:B:850:LEU:HB2   | 2:B:882:PHE:HE1   | 1.25                     | 0.99              |
| 1:A:24:VAL:HA     | 1:A:655:THR:HG21  | 1.02                     | 0.99              |
| 1:A:24:VAL:HA     | 1:A:655:THR:CG2   | 1.91                     | 0.99              |
| 1:C:831:TYR:O     | 1:C:928:ARG:HD2   | 1.63                     | 0.99              |
| 1:A:24:VAL:CA     | 1:A:655:THR:HG21  | 1.91                     | 0.99              |
| 1:A:1056:ILE:HD11 | 1:A:1066:TYR:HE2  | 1.25                     | 0.99              |
| 2:B:548:LEU:HD22  | 2:B:793:SER:HB3   | 1.43                     | 0.99              |
| 1:A:222:TYR:HE1   | 1:A:768:TYR:HB2   | 1.28                     | 0.99              |
| 1:A:831:TYR:O     | 1:A:928:ARG:HD2   | 1.62                     | 0.99              |
| 2:D:548:LEU:HD22  | 2:D:793:SER:HB3   | 1.42                     | 0.99              |
| 1:A:576:SER:HB3   | 1:A:577:PRO:HD3   | 1.44                     | 0.98              |
| 2:D:1607:ILE:H    | 2:D:1607:ILE:HD12 | 1.28                     | 0.98              |
| 1:C:386:VAL:N     | 1:C:411:THR:HG22  | 1.76                     | 0.98              |
| 1:A:1008:ALA:HB3  | 1:A:1078:LEU:HD11 | 1.44                     | 0.97              |
| 1:C:111:PHE:HE2   | 1:C:113:LYS:HB2   | 1.26                     | 0.97              |
| 2:D:556:ILE:H     | 2:D:556:ILE:HD12  | 1.26                     | 0.97              |
| 1:C:224:LEU:HD22  | 1:C:225:PRO:HD2   | 1.42                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1068:VAL:HA   | 1:A:1078:LEU:HD12 | 1.47                     | 0.97              |
| 1:C:24:VAL:HA     | 1:C:655:THR:HG21  | 1.00                     | 0.97              |
| 1:C:1056:ILE:HD11 | 1:C:1066:TYR:HE2  | 1.27                     | 0.97              |
| 1:A:44:TYR:HB2    | 1:A:545:ILE:HD12  | 1.47                     | 0.97              |
| 2:B:531:ILE:HD11  | 2:B:634:LEU:HD23  | 1.42                     | 0.97              |
| 1:C:44:TYR:HB2    | 1:C:545:ILE:HD12  | 1.47                     | 0.97              |
| 1:A:386:VAL:N     | 1:A:411:THR:HG22  | 1.79                     | 0.96              |
| 2:D:1590:LEU:HD23 | 2:D:1591:LEU:H    | 1.27                     | 0.96              |
| 2:B:556:ILE:HD12  | 2:B:556:ILE:H     | 1.29                     | 0.96              |
| 2:B:1528:LEU:HD13 | 2:B:1542:MET:HE2  | 1.45                     | 0.96              |
| 1:C:576:SER:HB3   | 1:C:577:PRO:HD3   | 1.44                     | 0.96              |
| 1:A:111:PHE:HE2   | 1:A:113:LYS:HB2   | 1.27                     | 0.96              |
| 2:B:1523:VAL:HG22 | 2:B:1584:TRP:HB2  | 1.47                     | 0.96              |
| 1:A:421:VAL:HG11  | 2:B:505:THR:HG22  | 1.47                     | 0.96              |
| 1:C:386:VAL:H     | 1:C:411:THR:CG2   | 1.78                     | 0.96              |
| 2:D:531:ILE:HD11  | 2:D:634:LEU:HD23  | 1.46                     | 0.96              |
| 1:C:44:TYR:HE1    | 1:C:497:THR:HG21  | 1.28                     | 0.95              |
| 1:C:489:LYS:C     | 1:C:491:PRO:HD3   | 1.91                     | 0.95              |
| 1:C:236:ASN:HB2   | 1:C:379:LEU:HD21  | 1.48                     | 0.95              |
| 1:A:489:LYS:C     | 1:A:491:PRO:HD3   | 1.91                     | 0.95              |
| 2:D:954:VAL:HB    | 2:D:957:THR:HG21  | 1.47                     | 0.95              |
| 2:D:1528:LEU:HD13 | 2:D:1542:MET:HE2  | 1.48                     | 0.95              |
| 1:A:853:MET:O     | 1:A:888:VAL:HG12  | 1.66                     | 0.95              |
| 1:C:395:ILE:HG22  | 1:C:401:THR:HG22  | 1.49                     | 0.95              |
| 2:D:1284:ARG:CD   | 2:D:1285:GLU:H    | 1.80                     | 0.95              |
| 1:A:386:VAL:H     | 1:A:411:THR:CG2   | 1.79                     | 0.95              |
| 1:A:395:ILE:HG22  | 1:A:401:THR:HG22  | 1.49                     | 0.95              |
| 1:A:702:GLY:HA2   | 1:A:728:PHE:CE1   | 2.02                     | 0.94              |
| 1:C:330:ILE:HG22  | 1:C:337:SER:HB2   | 1.46                     | 0.94              |
| 1:C:1068:VAL:HA   | 1:C:1078:LEU:HD12 | 1.48                     | 0.94              |
| 1:C:1228:TRP:N    | 1:C:1251:THR:HG22 | 1.82                     | 0.94              |
| 2:B:1284:ARG:CD   | 2:B:1285:GLU:H    | 1.81                     | 0.94              |
| 1:C:111:PHE:CE2   | 1:C:113:LYS:HB2   | 2.02                     | 0.94              |
| 1:A:1012:LEU:HD22 | 1:A:1085:VAL:HG21 | 1.49                     | 0.94              |
| 1:A:236:ASN:HB2   | 1:A:379:LEU:HD21  | 1.47                     | 0.94              |
| 1:C:145:VAL:HB    | 1:C:183:ILE:HD12  | 1.49                     | 0.94              |
| 2:D:1450:PHE:HD1  | 2:D:1451:ILE:H    | 1.12                     | 0.94              |
| 2:B:120:LEU:HD12  | 2:B:121:LEU:H     | 1.30                     | 0.94              |
| 2:B:481:TYR:HB2   | 2:B:520:PHE:HE1   | 1.30                     | 0.94              |
| 2:B:1610:TRP:HA   | 2:B:1628:PHE:HE2  | 1.33                     | 0.94              |
| 2:D:787:TRP:HB2   | 2:D:808:ILE:HG22  | 1.49                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1610:TRP:HA   | 2:D:1628:PHE:HE2  | 1.33                     | 0.94              |
| 1:A:653:PHE:HD1   | 1:A:653:PHE:O     | 1.51                     | 0.94              |
| 1:A:1585:TYR:HD1  | 1:A:1671:ILE:HG12 | 1.33                     | 0.94              |
| 1:C:1585:TYR:HD1  | 1:C:1671:ILE:HG12 | 1.33                     | 0.94              |
| 1:A:1615:ARG:HH21 | 1:A:1650:ARG:HH22 | 1.09                     | 0.93              |
| 1:A:374:GLN:HA    | 1:A:416:GLY:O     | 1.68                     | 0.93              |
| 1:C:853:MET:O     | 1:C:888:VAL:HG12  | 1.67                     | 0.93              |
| 2:B:1273:LEU:HB2  | 2:B:1319:GLY:HA3  | 1.51                     | 0.93              |
| 2:B:1491:ARG:HG3  | 2:B:1492:CYS:H    | 1.33                     | 0.93              |
| 2:D:265:PHE:CD2   | 2:D:294:LEU:HB2   | 2.03                     | 0.93              |
| 1:A:682:LYS:NZ    | 1:A:686:ILE:HD11  | 1.84                     | 0.93              |
| 2:B:787:TRP:HB2   | 2:B:808:ILE:HG22  | 1.50                     | 0.93              |
| 2:B:285:ILE:H     | 2:B:285:ILE:HD12  | 1.32                     | 0.92              |
| 1:A:135:TYR:CZ    | 1:A:141:VAL:HG13  | 2.05                     | 0.92              |
| 1:A:1056:ILE:HD11 | 1:A:1066:TYR:CE2  | 2.04                     | 0.92              |
| 2:D:120:LEU:HD12  | 2:D:121:LEU:H     | 1.30                     | 0.92              |
| 2:B:510:ILE:HG23  | 2:B:514:LEU:HD12  | 1.52                     | 0.92              |
| 2:B:954:VAL:HB    | 2:B:957:THR:HG21  | 1.51                     | 0.92              |
| 2:B:1607:ILE:HD12 | 2:B:1607:ILE:N    | 1.85                     | 0.92              |
| 2:D:1273:LEU:HB2  | 2:D:1319:GLY:HA3  | 1.51                     | 0.92              |
| 1:A:869:GLU:C     | 1:A:871:PRO:HD3   | 1.95                     | 0.92              |
| 2:D:510:ILE:HG23  | 2:D:514:LEU:HD12  | 1.50                     | 0.92              |
| 1:C:1585:TYR:CD1  | 1:C:1671:ILE:HG12 | 2.05                     | 0.92              |
| 2:D:1491:ARG:HG3  | 2:D:1492:CYS:H    | 1.35                     | 0.92              |
| 1:A:371:ILE:HD11  | 1:A:433:PHE:CE2   | 2.04                     | 0.91              |
| 2:B:1386:MET:HE2  | 2:B:1386:MET:HA   | 1.52                     | 0.91              |
| 1:C:1615:ARG:HH21 | 1:C:1650:ARG:HH22 | 1.06                     | 0.91              |
| 2:D:285:ILE:HD12  | 2:D:285:ILE:H     | 1.33                     | 0.91              |
| 1:A:145:VAL:HB    | 1:A:183:ILE:HD12  | 1.51                     | 0.91              |
| 1:A:884:VAL:O     | 1:A:885:ARG:HB2   | 1.67                     | 0.91              |
| 1:C:135:TYR:CZ    | 1:C:141:VAL:HG13  | 2.06                     | 0.91              |
| 1:C:222:TYR:CE1   | 1:C:768:TYR:HB2   | 2.04                     | 0.91              |
| 1:C:869:GLU:C     | 1:C:871:PRO:HD3   | 1.95                     | 0.91              |
| 1:A:351:PRO:HG2   | 1:A:352:TYR:CD2   | 2.06                     | 0.91              |
| 2:B:1424:ILE:HD13 | 2:B:1424:ILE:H    | 1.34                     | 0.91              |
| 1:C:493:ILE:HG22  | 1:C:495:LYS:H     | 1.36                     | 0.91              |
| 2:D:197:TRP:HB2   | 2:D:214:PHE:CE1   | 2.05                     | 0.91              |
| 1:A:330:ILE:HG22  | 1:A:337:SER:HB2   | 1.51                     | 0.91              |
| 2:B:1450:PHE:HD1  | 2:B:1451:ILE:H    | 1.13                     | 0.91              |
| 1:A:111:PHE:CE2   | 1:A:113:LYS:HB2   | 2.06                     | 0.91              |
| 1:A:1404:ALA:HB1  | 1:A:1493:PHE:CE2  | 2.06                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:435:TYR:HD1   | 2:B:436:GLN:H     | 0.94                     | 0.91              |
| 1:C:371:ILE:HD11  | 1:C:433:PHE:CE2   | 2.06                     | 0.91              |
| 1:C:702:GLY:HA2   | 1:C:728:PHE:CE1   | 2.06                     | 0.91              |
| 2:D:42:LEU:HD11   | 2:D:82:LEU:HD12   | 1.52                     | 0.91              |
| 1:A:1228:TRP:N    | 1:A:1251:THR:HG22 | 1.85                     | 0.90              |
| 2:B:239:GLY:H     | 2:B:296:ARG:NH2   | 1.69                     | 0.90              |
| 1:C:682:LYS:NZ    | 1:C:686:ILE:HD11  | 1.85                     | 0.90              |
| 2:B:415:THR:HG1   | 2:B:425:GLN:HB3   | 1.35                     | 0.90              |
| 2:B:646:GLN:HB3   | 2:B:647:PRO:HD2   | 1.51                     | 0.90              |
| 2:D:239:GLY:H     | 2:D:296:ARG:NH2   | 1.69                     | 0.90              |
| 1:A:1585:TYR:CD1  | 1:A:1671:ILE:HG12 | 2.07                     | 0.90              |
| 2:B:481:TYR:O     | 2:B:481:TYR:HD2   | 1.54                     | 0.90              |
| 1:C:374:GLN:HA    | 1:C:416:GLY:O     | 1.72                     | 0.90              |
| 1:A:60:PRO:HD2    | 1:A:61:ASP:H      | 1.36                     | 0.90              |
| 1:A:222:TYR:CE1   | 1:A:768:TYR:HB2   | 2.06                     | 0.90              |
| 1:A:423:ASN:HB3   | 2:B:501:GLN:NE2   | 1.86                     | 0.90              |
| 1:A:702:GLY:HA2   | 1:A:728:PHE:HE1   | 1.37                     | 0.90              |
| 2:B:482:LEU:HB3   | 2:B:492:VAL:HG23  | 1.54                     | 0.90              |
| 2:B:1331:ALA:O    | 2:B:1332:GLN:HB3  | 1.70                     | 0.90              |
| 1:A:500:ASN:OD1   | 1:A:514:THR:HG23  | 1.71                     | 0.89              |
| 1:C:888:VAL:HG23  | 1:C:894:HIS:HB2   | 1.52                     | 0.89              |
| 2:D:481:TYR:HB2   | 2:D:520:PHE:HE1   | 1.36                     | 0.89              |
| 1:C:884:VAL:O     | 1:C:885:ARG:HB2   | 1.70                     | 0.89              |
| 2:D:435:TYR:HD1   | 2:D:436:GLN:H     | 0.94                     | 0.89              |
| 1:A:884:VAL:HG12  | 1:A:886:GLN:HG2   | 1.52                     | 0.89              |
| 1:A:849:ARG:HH11  | 1:A:849:ARG:HG3   | 1.37                     | 0.89              |
| 2:B:927:ILE:HG23  | 2:B:1324:THR:HG23 | 1.54                     | 0.89              |
| 1:A:493:ILE:HG22  | 1:A:495:LYS:H     | 1.36                     | 0.89              |
| 1:A:584:PRO:HB3   | 1:A:792:ASP:HA    | 1.54                     | 0.89              |
| 1:C:539:ARG:NH2   | 1:C:634:CYS:H     | 1.69                     | 0.89              |
| 2:D:1424:ILE:H    | 2:D:1424:ILE:HD13 | 1.36                     | 0.89              |
| 2:D:964:ILE:HG13  | 2:D:1302:THR:HG23 | 1.55                     | 0.89              |
| 1:C:584:PRO:HB3   | 1:C:792:ASP:HA    | 1.54                     | 0.89              |
| 1:C:1056:ILE:HD11 | 1:C:1066:TYR:CE2  | 2.07                     | 0.89              |
| 2:D:435:TYR:HD1   | 2:D:436:GLN:N     | 1.69                     | 0.89              |
| 2:D:850:LEU:HB2   | 2:D:882:PHE:CE1   | 2.08                     | 0.89              |
| 2:D:646:GLN:HB3   | 2:D:647:PRO:HD2   | 1.52                     | 0.89              |
| 2:B:42:LEU:HD11   | 2:B:82:LEU:HD12   | 1.51                     | 0.89              |
| 2:D:1607:ILE:HD12 | 2:D:1607:ILE:N    | 1.88                     | 0.89              |
| 2:B:265:PHE:CD2   | 2:B:294:LEU:HB2   | 2.08                     | 0.88              |
| 1:C:653:PHE:O     | 1:C:653:PHE:HD1   | 1.56                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:482:LEU:HB3   | 2:D:492:VAL:HG23  | 1.55                     | 0.88              |
| 1:A:490:SER:N     | 1:A:491:PRO:CD    | 2.36                     | 0.88              |
| 1:C:1086:LEU:HD12 | 1:C:1095:GLN:HG3  | 1.55                     | 0.88              |
| 1:C:470:THR:HG22  | 2:D:450:THR:HG22  | 1.55                     | 0.88              |
| 1:C:549:GLU:H     | 1:C:549:GLU:CD    | 1.80                     | 0.88              |
| 1:C:60:PRO:HD2    | 1:C:61:ASP:H      | 1.38                     | 0.88              |
| 1:C:849:ARG:HH11  | 1:C:849:ARG:HG3   | 1.37                     | 0.88              |
| 1:C:1315:VAL:HG12 | 1:C:1324:HIS:O    | 1.72                     | 0.88              |
| 2:D:161:VAL:HG21  | 2:D:180:LEU:HD21  | 1.55                     | 0.88              |
| 2:D:218:LYS:HB3   | 2:D:822:TYR:CD2   | 2.08                     | 0.88              |
| 2:D:221:LEU:HD11  | 2:D:753:LYS:HG2   | 1.55                     | 0.88              |
| 2:D:1386:MET:HE2  | 2:D:1386:MET:HA   | 1.56                     | 0.88              |
| 2:D:850:LEU:HG    | 2:D:851:LEU:N     | 1.89                     | 0.88              |
| 1:A:1102:ASN:HD21 | 1:C:1162:VAL:H    | 1.20                     | 0.88              |
| 2:B:435:TYR:HD1   | 2:B:436:GLN:N     | 1.70                     | 0.87              |
| 2:D:415:THR:HG1   | 2:D:425:GLN:HB3   | 1.39                     | 0.87              |
| 1:C:174:VAL:HG22  | 1:C:175:GLU:H     | 1.40                     | 0.87              |
| 1:C:351:PRO:HG2   | 1:C:352:TYR:CD2   | 2.10                     | 0.87              |
| 1:A:250:ILE:HD11  | 1:A:265:VAL:HG11  | 1.56                     | 0.87              |
| 1:C:1012:LEU:HD22 | 1:C:1085:VAL:HG21 | 1.57                     | 0.87              |
| 1:A:1162:VAL:HG22 | 1:C:1102:ASN:ND2  | 1.89                     | 0.87              |
| 2:D:481:TYR:HD2   | 2:D:481:TYR:O     | 1.57                     | 0.87              |
| 1:A:979:VAL:HG12  | 1:A:1359:VAL:HG22 | 1.55                     | 0.87              |
| 1:A:1162:VAL:H    | 1:C:1102:ASN:HD21 | 1.16                     | 0.87              |
| 1:A:1627:ILE:HD12 | 1:A:1629:TYR:HB3  | 1.57                     | 0.87              |
| 1:A:549:GLU:CD    | 1:A:549:GLU:H     | 1.81                     | 0.87              |
| 2:B:221:LEU:HD11  | 2:B:753:LYS:HG2   | 1.56                     | 0.87              |
| 1:C:127:PHE:HE2   | 1:C:623:VAL:HG13  | 1.39                     | 0.87              |
| 1:C:614:ARG:HD2   | 1:C:615:GLY:H     | 1.39                     | 0.87              |
| 2:D:1331:ALA:O    | 2:D:1332:GLN:HB3  | 1.70                     | 0.87              |
| 1:A:362:PHE:HE1   | 1:A:640:LEU:HD22  | 1.39                     | 0.86              |
| 1:A:614:ARG:HD2   | 1:A:615:GLY:H     | 1.41                     | 0.86              |
| 2:B:948:ARG:HH21  | 2:B:948:ARG:HB2   | 1.40                     | 0.86              |
| 2:B:192:VAL:HG22  | 2:B:193:SER:H     | 1.39                     | 0.86              |
| 1:C:884:VAL:HG12  | 1:C:886:GLN:HG2   | 1.55                     | 0.86              |
| 1:A:999:ILE:HG13  | 1:A:1000:LEU:H    | 1.41                     | 0.86              |
| 1:C:182:ILE:HG12  | 1:C:804:ILE:HD11  | 1.58                     | 0.86              |
| 1:C:490:SER:N     | 1:C:491:PRO:CD    | 2.38                     | 0.86              |
| 1:A:796:THR:HG23  | 1:A:818:LYS:HB3   | 1.55                     | 0.86              |
| 1:C:504:LEU:HD21  | 1:C:651:LEU:HG    | 1.57                     | 0.86              |
| 1:C:430:VAL:HG11  | 1:C:453:ARG:HH21  | 1.41                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:161:VAL:HG21  | 2:B:180:LEU:HD21  | 1.57                     | 0.86              |
| 1:A:162:THR:HG21  | 1:A:204:LYS:HE2   | 1.56                     | 0.86              |
| 1:A:1622:LYS:HZ2  | 1:A:1642:LEU:HB3  | 1.41                     | 0.86              |
| 1:A:1086:LEU:HD12 | 1:A:1095:GLN:HG3  | 1.57                     | 0.85              |
| 2:B:850:LEU:HG    | 2:B:851:LEU:N     | 1.91                     | 0.85              |
| 2:D:508:LEU:HD12  | 2:D:509:HIS:H     | 1.40                     | 0.85              |
| 1:A:504:LEU:HD21  | 1:A:651:LEU:HG    | 1.57                     | 0.85              |
| 1:C:1144:LEU:O    | 1:C:1148:THR:HG23 | 1.75                     | 0.85              |
| 1:A:1549:LYS:NZ   | 1:A:1667:PHE:HB3  | 1.90                     | 0.85              |
| 1:A:967:LEU:HD12  | 1:A:968:VAL:N     | 1.91                     | 0.85              |
| 2:D:44:GLU:HG2    | 2:D:82:LEU:HB2    | 1.58                     | 0.85              |
| 2:B:218:LYS:HB3   | 2:B:822:TYR:CD2   | 2.10                     | 0.85              |
| 1:C:250:ILE:HD11  | 1:C:265:VAL:HG11  | 1.58                     | 0.85              |
| 1:A:174:VAL:HG22  | 1:A:175:GLU:H     | 1.41                     | 0.85              |
| 1:A:979:VAL:HG21  | 1:A:1326:TYR:HE1  | 1.36                     | 0.85              |
| 1:A:539:ARG:NH2   | 1:A:634:CYS:H     | 1.72                     | 0.85              |
| 1:A:1278:GLN:OE1  | 1:A:1283:GLY:CA   | 2.25                     | 0.85              |
| 1:C:44:TYR:CE1    | 1:C:497:THR:HG21  | 2.12                     | 0.85              |
| 1:A:471:ASP:OD2   | 1:A:474:LYS:HB3   | 1.76                     | 0.85              |
| 2:B:44:GLU:HG2    | 2:B:82:LEU:HB2    | 1.57                     | 0.85              |
| 2:D:114:ARG:O     | 2:D:115:LEU:HD23  | 1.76                     | 0.85              |
| 1:A:470:THR:HG22  | 2:B:450:THR:HG22  | 1.57                     | 0.84              |
| 1:C:1490:PRO:HB3  | 1:C:1510:SER:HB2  | 1.58                     | 0.84              |
| 1:A:623:VAL:HG12  | 1:A:624:PHE:N     | 1.92                     | 0.84              |
| 1:A:1315:VAL:HG12 | 1:A:1324:HIS:O    | 1.77                     | 0.84              |
| 1:C:623:VAL:HG12  | 1:C:624:PHE:N     | 1.92                     | 0.84              |
| 1:C:982:LEU:H     | 1:C:982:LEU:HD12  | 1.41                     | 0.84              |
| 2:D:948:ARG:HH21  | 2:D:948:ARG:HB2   | 1.43                     | 0.84              |
| 2:D:1450:PHE:CD1  | 2:D:1451:ILE:N    | 2.45                     | 0.84              |
| 1:A:44:TYR:CE1    | 1:A:497:THR:HG21  | 2.10                     | 0.84              |
| 1:A:1109:GLU:HG2  | 1:C:1163:LYS:HZ1  | 1.41                     | 0.84              |
| 2:D:1561:HIS:CE1  | 2:D:1597:ILE:HD13 | 2.12                     | 0.84              |
| 1:A:888:VAL:HG23  | 1:A:894:HIS:HB2   | 1.57                     | 0.84              |
| 1:A:1576:LYS:HG2  | 1:A:1601:ILE:HG22 | 1.58                     | 0.84              |
| 1:C:471:ASP:OD2   | 1:C:474:LYS:HB3   | 1.77                     | 0.84              |
| 1:C:999:ILE:HG13  | 1:C:1000:LEU:H    | 1.42                     | 0.84              |
| 1:A:830:PRO:HG3   | 1:A:1483:PHE:CZ   | 2.13                     | 0.84              |
| 1:A:1490:PRO:HB3  | 1:A:1510:SER:HB2  | 1.58                     | 0.84              |
| 1:C:1068:VAL:HG21 | 1:C:1124:TYR:CD1  | 2.13                     | 0.84              |
| 1:A:113:LYS:HG2   | 1:A:114:SER:H     | 1.41                     | 0.84              |
| 1:C:979:VAL:HG21  | 1:C:1326:TYR:HE1  | 1.33                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:482:LEU:HD12  | 2:D:482:LEU:H     | 1.43                     | 0.84              |
| 1:A:87:ILE:HD13   | 1:A:87:ILE:N      | 1.91                     | 0.84              |
| 1:C:476:LEU:HD21  | 1:C:482:LEU:HD12  | 1.57                     | 0.84              |
| 1:C:1622:LYS:HZ2  | 1:C:1642:LEU:HB3  | 1.42                     | 0.84              |
| 1:C:796:THR:HG23  | 1:C:818:LYS:HB3   | 1.58                     | 0.84              |
| 2:D:1274:ASN:ND2  | 2:D:1293:ASN:HB3  | 1.93                     | 0.84              |
| 2:B:482:LEU:H     | 2:B:482:LEU:HD12  | 1.43                     | 0.83              |
| 1:A:546:VAL:O     | 1:A:553:GLU:HB3   | 1.78                     | 0.83              |
| 1:C:889:GLU:HB2   | 1:C:892:SER:HB2   | 1.59                     | 0.83              |
| 1:C:1383:THR:HG21 | 1:C:1511:THR:HG22 | 1.60                     | 0.83              |
| 1:A:127:PHE:HE2   | 1:A:623:VAL:HG13  | 1.42                     | 0.83              |
| 1:C:467:ILE:HG22  | 1:C:486:VAL:HG22  | 1.60                     | 0.83              |
| 1:C:1127:ILE:HD12 | 1:C:1127:ILE:H    | 1.44                     | 0.83              |
| 1:C:113:LYS:HG2   | 1:C:114:SER:H     | 1.44                     | 0.83              |
| 1:C:830:PRO:HG3   | 1:C:1483:PHE:CZ   | 2.12                     | 0.83              |
| 1:A:265:VAL:HG22  | 1:A:329:VAL:HG22  | 1.61                     | 0.83              |
| 2:B:964:ILE:HG13  | 2:B:1302:THR:HG23 | 1.60                     | 0.83              |
| 1:C:87:ILE:HD13   | 1:C:87:ILE:N      | 1.93                     | 0.83              |
| 1:C:1576:LYS:HG2  | 1:C:1601:ILE:HG22 | 1.60                     | 0.83              |
| 1:A:884:VAL:CG1   | 1:A:886:GLN:HG2   | 2.08                     | 0.83              |
| 2:B:83:VAL:C      | 2:B:85:PRO:HD3    | 2.03                     | 0.83              |
| 1:C:131:ASP:HB3   | 1:C:142:LYS:HB2   | 1.60                     | 0.83              |
| 1:C:1370:THR:HG23 | 1:C:1373:GLU:OE1  | 1.79                     | 0.83              |
| 1:A:42:GLN:HB2    | 1:A:80:GLN:NE2    | 1.93                     | 0.83              |
| 2:B:285:ILE:HD12  | 2:B:285:ILE:N     | 1.94                     | 0.83              |
| 2:B:1274:ASN:ND2  | 2:B:1293:ASN:HB3  | 1.94                     | 0.83              |
| 1:C:42:GLN:HB2    | 1:C:80:GLN:NE2    | 1.93                     | 0.83              |
| 2:B:508:LEU:HD12  | 2:B:509:HIS:H     | 1.44                     | 0.83              |
| 1:C:162:THR:HG21  | 1:C:204:LYS:HE2   | 1.58                     | 0.83              |
| 1:C:1320:LYS:HD2  | 1:C:1321:GLY:H    | 1.42                     | 0.83              |
| 1:C:1549:LYS:NZ   | 1:C:1667:PHE:HB3  | 1.93                     | 0.83              |
| 1:C:546:VAL:O     | 1:C:553:GLU:HB3   | 1.78                     | 0.83              |
| 1:A:491:PRO:HG2   | 1:A:494:ASP:HB3   | 1.60                     | 0.82              |
| 2:D:344:GLN:HA    | 2:D:344:GLN:NE2   | 1.93                     | 0.82              |
| 1:A:838:GLN:HA    | 1:A:901:LEU:HB2   | 1.59                     | 0.82              |
| 1:A:955:ARG:HG2   | 1:A:1350:THR:HG23 | 1.60                     | 0.82              |
| 1:A:1127:ILE:H    | 1:A:1127:ILE:HD12 | 1.44                     | 0.82              |
| 2:B:25:TYR:HB2    | 2:B:631:SER:HB3   | 1.60                     | 0.82              |
| 1:C:443:PRO:HD2   | 1:C:446:ASN:HB2   | 1.61                     | 0.82              |
| 1:A:905:ILE:HD12  | 1:A:931:PRO:HD3   | 1.61                     | 0.82              |
| 2:B:476:ILE:O     | 2:B:497:ARG:HG2   | 1.78                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:153:LYS:HB2   | 1:A:154:PRO:HD2   | 1.58                     | 0.82              |
| 1:C:153:LYS:HB2   | 1:C:154:PRO:HD2   | 1.60                     | 0.82              |
| 1:C:905:ILE:HD12  | 1:C:931:PRO:HD3   | 1.60                     | 0.82              |
| 1:A:1144:LEU:O    | 1:A:1148:THR:HG23 | 1.80                     | 0.82              |
| 2:B:1561:HIS:CE1  | 2:B:1597:ILE:HD13 | 2.14                     | 0.82              |
| 1:C:362:PHE:HE1   | 1:C:640:LEU:HD22  | 1.44                     | 0.82              |
| 1:C:967:LEU:HD12  | 1:C:968:VAL:N     | 1.94                     | 0.82              |
| 2:D:83:VAL:C      | 2:D:85:PRO:HD3    | 2.04                     | 0.82              |
| 1:C:743:SER:HB2   | 1:C:751:ARG:N     | 1.95                     | 0.82              |
| 1:A:238:ILE:HG23  | 1:A:242:ASN:HD22  | 1.41                     | 0.82              |
| 2:B:1450:PHE:CD1  | 2:B:1451:ILE:N    | 2.47                     | 0.82              |
| 1:A:1068:VAL:HG21 | 1:A:1124:TYR:CD1  | 2.13                     | 0.82              |
| 1:A:1320:LYS:HD2  | 1:A:1321:GLY:H    | 1.43                     | 0.82              |
| 1:C:1561:TYR:CD1  | 1:C:1581:LEU:HD21 | 2.14                     | 0.82              |
| 1:A:1561:TYR:CD1  | 1:A:1581:LEU:HD21 | 2.14                     | 0.82              |
| 1:C:979:VAL:HG12  | 1:C:1359:VAL:HG22 | 1.60                     | 0.82              |
| 1:A:857:VAL:HG23  | 1:A:884:VAL:HG21  | 1.59                     | 0.82              |
| 1:A:1626:GLN:HB2  | 1:A:1635:TYR:HD1  | 1.44                     | 0.82              |
| 1:C:1402:ILE:HG13 | 1:C:1479:ILE:HD12 | 1.59                     | 0.82              |
| 1:A:1533:GLY:O    | 1:A:1534:GLN:HB3  | 1.80                     | 0.81              |
| 1:C:35:ALA:O      | 1:C:86:THR:HG22   | 1.80                     | 0.81              |
| 1:C:491:PRO:HG2   | 1:C:494:ASP:HB3   | 1.60                     | 0.81              |
| 1:C:1278:GLN:OE1  | 1:C:1283:GLY:CA   | 2.28                     | 0.81              |
| 1:A:1383:THR:HG21 | 1:A:1511:THR:HG22 | 1.63                     | 0.81              |
| 2:B:339:VAL:HG23  | 2:B:341:SER:H     | 1.46                     | 0.81              |
| 1:C:160:VAL:HG22  | 1:C:175:GLU:HB3   | 1.61                     | 0.81              |
| 1:C:702:GLY:HA2   | 1:C:728:PHE:HE1   | 1.45                     | 0.81              |
| 1:C:857:VAL:HG23  | 1:C:884:VAL:HG21  | 1.62                     | 0.81              |
| 2:D:745:ILE:CG2   | 2:D:897:LYS:HD3   | 2.11                     | 0.81              |
| 2:D:1284:ARG:CG   | 2:D:1285:GLU:H    | 1.94                     | 0.81              |
| 1:A:375:VAL:O     | 1:A:383:VAL:HG13  | 1.80                     | 0.81              |
| 1:A:773:TRP:HZ3   | 1:A:788:PHE:CE1   | 1.98                     | 0.81              |
| 1:A:936:ARG:HG3   | 1:A:936:ARG:HH11  | 1.44                     | 0.81              |
| 1:A:944:LEU:HD12  | 1:A:1313:ILE:HD11 | 1.63                     | 0.81              |
| 1:A:982:LEU:HD12  | 1:A:982:LEU:H     | 1.44                     | 0.81              |
| 2:B:344:GLN:HA    | 2:B:344:GLN:NE2   | 1.94                     | 0.81              |
| 1:C:42:GLN:HG2    | 1:C:43:VAL:H      | 1.45                     | 0.81              |
| 2:D:339:VAL:HG23  | 2:D:341:SER:H     | 1.46                     | 0.81              |
| 1:A:182:ILE:HG12  | 1:A:804:ILE:HD11  | 1.62                     | 0.81              |
| 1:A:520:ASP:OD2   | 2:B:404:LEU:HB2   | 1.81                     | 0.81              |
| 1:A:113:LYS:HG2   | 1:A:114:SER:N     | 1.96                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:753:HIS:O     | 1:A:754:MET:HB3   | 1.81                     | 0.81              |
| 2:B:294:LEU:HD12  | 2:B:295:LYS:N     | 1.95                     | 0.81              |
| 1:C:1570:VAL:HA   | 1:C:1574:PHE:O    | 1.79                     | 0.81              |
| 2:D:422:ARG:H     | 2:D:422:ARG:HD3   | 1.45                     | 0.81              |
| 1:A:1590:ALA:HB1  | 1:A:1635:TYR:CE1  | 2.16                     | 0.81              |
| 2:B:850:LEU:HB2   | 2:B:882:PHE:CE1   | 2.14                     | 0.81              |
| 1:C:838:GLN:HA    | 1:C:901:LEU:HB2   | 1.62                     | 0.81              |
| 1:A:1370:THR:HG23 | 1:A:1373:GLU:OE1  | 1.81                     | 0.81              |
| 1:C:917:TRP:HB3   | 2:D:558:MET:SD    | 2.21                     | 0.81              |
| 1:C:1623:GLU:HB2  | 1:C:1638:PRO:HG2  | 1.63                     | 0.81              |
| 1:A:160:VAL:HG22  | 1:A:175:GLU:HB3   | 1.61                     | 0.81              |
| 1:A:309:GLU:HG2   | 1:A:310:LEU:H     | 1.44                     | 0.81              |
| 1:A:889:GLU:HB2   | 1:A:892:SER:HB2   | 1.62                     | 0.81              |
| 1:A:1549:LYS:HZ1  | 1:A:1667:PHE:HB3  | 1.44                     | 0.81              |
| 2:B:415:THR:OG1   | 2:B:425:GLN:HB3   | 1.81                     | 0.81              |
| 1:C:1176:LEU:HD21 | 1:C:1195:LEU:CD2  | 2.10                     | 0.81              |
| 1:C:309:GLU:HG2   | 1:C:310:LEU:H     | 1.43                     | 0.81              |
| 2:B:481:TYR:HE1   | 2:B:506:MET:SD    | 2.04                     | 0.80              |
| 1:C:1404:ALA:HB1  | 1:C:1493:PHE:CE2  | 2.16                     | 0.80              |
| 2:D:1347:VAL:HG22 | 2:D:1367:ILE:HG23 | 1.62                     | 0.80              |
| 1:A:131:ASP:HB3   | 1:A:142:LYS:HB2   | 1.62                     | 0.80              |
| 1:A:1620:MET:HB2  | 1:A:1644:TRP:HB3  | 1.64                     | 0.80              |
| 1:C:753:HIS:O     | 1:C:754:MET:HB3   | 1.78                     | 0.80              |
| 1:C:1615:ARG:HH21 | 1:C:1650:ARG:NH2  | 1.79                     | 0.80              |
| 2:D:415:THR:OG1   | 2:D:425:GLN:HB3   | 1.81                     | 0.80              |
| 1:A:596:MET:HA    | 1:A:782:ARG:HG2   | 1.62                     | 0.80              |
| 1:A:1570:VAL:HA   | 1:A:1574:PHE:O    | 1.80                     | 0.80              |
| 2:B:1284:ARG:HG3  | 2:B:1286:VAL:H    | 1.47                     | 0.80              |
| 1:A:924:VAL:HG21  | 3:A:2003:NAG:H82  | 1.64                     | 0.80              |
| 1:A:476:LEU:HD21  | 1:A:482:LEU:HD12  | 1.61                     | 0.80              |
| 1:C:837:GLU:O     | 1:C:901:LEU:HD12  | 1.81                     | 0.80              |
| 2:D:927:ILE:HG23  | 2:D:1324:THR:HG23 | 1.63                     | 0.80              |
| 2:B:1506:ILE:HD12 | 2:B:1627:ASP:HB2  | 1.64                     | 0.80              |
| 1:C:463:SER:HB3   | 1:C:491:PRO:HA    | 1.64                     | 0.80              |
| 1:C:470:THR:HG22  | 2:D:450:THR:CG2   | 2.11                     | 0.80              |
| 1:A:743:SER:HB2   | 1:A:751:ARG:N     | 1.96                     | 0.80              |
| 1:C:265:VAL:HG22  | 1:C:329:VAL:HG22  | 1.64                     | 0.80              |
| 1:C:500:ASN:CB    | 1:C:543:TYR:CE1   | 2.65                     | 0.80              |
| 1:C:969:PRO:HG3   | 1:C:1601:ILE:HD12 | 1.64                     | 0.80              |
| 1:A:35:ALA:O      | 1:A:86:THR:HG22   | 1.82                     | 0.80              |
| 1:A:1102:ASN:ND2  | 1:C:1162:VAL:H    | 1.79                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:484:LEU:HB2   | 2:B:519:ARG:HB2   | 1.63                     | 0.80              |
| 2:B:262:PHE:CE1   | 2:B:282:ARG:HG3   | 2.17                     | 0.80              |
| 1:A:443:PRO:HD2   | 1:A:446:ASN:HB2   | 1.63                     | 0.79              |
| 1:A:1152:ILE:HG21 | 1:A:1168:LEU:HD21 | 1.64                     | 0.79              |
| 1:C:238:ILE:HG23  | 1:C:242:ASN:HD22  | 1.44                     | 0.79              |
| 1:C:733:VAL:O     | 1:C:737:GLN:HG2   | 1.82                     | 0.79              |
| 2:D:25:TYR:HB2    | 2:D:631:SER:HB3   | 1.63                     | 0.79              |
| 1:A:1176:LEU:HD21 | 1:A:1195:LEU:CD2  | 2.12                     | 0.79              |
| 1:C:884:VAL:CG1   | 1:C:886:GLN:HG2   | 2.11                     | 0.79              |
| 2:D:563:MET:HG3   | 2:D:780:LEU:HD23  | 1.64                     | 0.79              |
| 1:A:500:ASN:HB3   | 1:A:543:TYR:HE1   | 1.47                     | 0.79              |
| 1:A:1244:THR:HG22 | 1:A:1247:MET:H    | 1.47                     | 0.79              |
| 2:B:563:MET:SD    | 2:B:808:ILE:HD11  | 2.21                     | 0.79              |
| 1:C:126:LEU:HD11  | 1:C:205:TYR:CE2   | 2.17                     | 0.79              |
| 1:C:773:TRP:HZ3   | 1:C:788:PHE:CE1   | 2.00                     | 0.79              |
| 2:D:164:GLU:HG2   | 2:D:175:SER:HB2   | 1.63                     | 0.79              |
| 1:A:315:LEU:HD13  | 1:A:317:ASP:HB2   | 1.62                     | 0.79              |
| 1:A:1309:LEU:HD11 | 1:A:1328:MET:HG3  | 1.64                     | 0.79              |
| 2:B:961:THR:HG22  | 2:B:1327:THR:HG23 | 1.64                     | 0.79              |
| 2:B:1393:ASP:HB2  | 2:B:1443:LEU:HD11 | 1.63                     | 0.79              |
| 1:A:500:ASN:CB    | 1:A:543:TYR:CE1   | 2.65                     | 0.79              |
| 2:B:422:ARG:H     | 2:B:422:ARG:HD3   | 1.46                     | 0.79              |
| 1:C:1590:ALA:HB1  | 1:C:1635:TYR:CE1  | 2.18                     | 0.79              |
| 2:D:285:ILE:HD12  | 2:D:285:ILE:N     | 1.96                     | 0.79              |
| 2:D:294:LEU:HD12  | 2:D:295:LYS:N     | 1.98                     | 0.79              |
| 1:C:1549:LYS:HZ1  | 1:C:1667:PHE:HB3  | 1.45                     | 0.79              |
| 2:D:262:PHE:CE1   | 2:D:282:ARG:HG3   | 2.17                     | 0.79              |
| 2:D:518:PHE:CE2   | 2:D:538:VAL:HB    | 2.18                     | 0.79              |
| 1:A:492:TYR:CG    | 1:A:493:ILE:N     | 2.50                     | 0.79              |
| 1:C:924:VAL:HG21  | 3:C:2003:NAG:H82  | 1.65                     | 0.79              |
| 1:C:1100:ILE:HG21 | 1:C:1158:ILE:HD12 | 1.65                     | 0.79              |
| 2:D:825:VAL:HB    | 2:D:828:GLU:CD    | 2.08                     | 0.79              |
| 1:C:596:MET:HA    | 1:C:782:ARG:HG2   | 1.64                     | 0.79              |
| 1:A:430:VAL:HG11  | 1:A:453:ARG:HH21  | 1.46                     | 0.78              |
| 2:D:476:ILE:O     | 2:D:497:ARG:HG2   | 1.82                     | 0.78              |
| 1:A:837:GLU:O     | 1:A:901:LEU:HD12  | 1.83                     | 0.78              |
| 1:A:1623:GLU:HB2  | 1:A:1638:PRO:HG2  | 1.66                     | 0.78              |
| 1:C:1620:MET:HB2  | 1:C:1644:TRP:HB3  | 1.65                     | 0.78              |
| 1:C:20:GLU:HG2    | 1:C:20:GLU:O      | 1.83                     | 0.78              |
| 1:A:489:LYS:NZ    | 2:B:502:ASN:H     | 1.82                     | 0.78              |
| 2:B:197:TRP:HB2   | 2:B:214:PHE:CE1   | 2.18                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:825:VAL:HB    | 2:B:828:GLU:CD    | 2.07                     | 0.78              |
| 1:C:576:SER:HB2   | 1:C:589:SER:H     | 1.48                     | 0.78              |
| 2:D:1482:ASN:HB2  | 2:D:1495:GLU:HG2  | 1.65                     | 0.78              |
| 2:B:1347:VAL:HG22 | 2:B:1367:ILE:HG23 | 1.63                     | 0.78              |
| 1:C:1186:PHE:HD1  | 1:C:1250:THR:HG22 | 1.49                     | 0.78              |
| 2:D:476:ILE:O     | 2:D:476:ILE:HG23  | 1.82                     | 0.78              |
| 2:D:563:MET:SD    | 2:D:808:ILE:HD11  | 2.24                     | 0.78              |
| 2:D:1444:LYS:HE2  | 2:D:1447:GLU:HA   | 1.64                     | 0.78              |
| 1:A:1411:SER:N    | 1:A:1414:GLU:HG3  | 1.99                     | 0.78              |
| 2:B:165:PHE:CZ    | 2:B:199:ILE:HD11  | 2.19                     | 0.78              |
| 1:C:91:GLN:OE1    | 1:C:91:GLN:HA     | 1.72                     | 0.78              |
| 1:C:500:ASN:HB2   | 1:C:543:TYR:CD1   | 2.19                     | 0.78              |
| 1:C:506:LYS:HD2   | 1:C:536:PRO:HD2   | 1.66                     | 0.78              |
| 2:D:127:PHE:HE2   | 2:D:602:ILE:HG23  | 1.49                     | 0.78              |
| 1:A:733:VAL:O     | 1:A:737:GLN:HG2   | 1.83                     | 0.78              |
| 2:B:244:HIS:HB3   | 2:B:291:LYS:HD2   | 1.64                     | 0.78              |
| 1:C:1244:THR:HG22 | 1:C:1247:MET:H    | 1.49                     | 0.78              |
| 1:C:1627:ILE:HD12 | 1:C:1629:TYR:HB3  | 1.65                     | 0.78              |
| 2:D:1614:ASP:O    | 2:D:1617:GLN:HG2  | 1.83                     | 0.78              |
| 1:A:1109:GLU:HG2  | 1:C:1163:LYS:NZ   | 1.98                     | 0.77              |
| 1:A:1153:ARG:HD2  | 1:A:1197:LEU:HB3  | 1.66                     | 0.77              |
| 1:C:500:ASN:OD1   | 1:C:514:THR:HG23  | 1.83                     | 0.77              |
| 2:D:563:MET:HB3   | 2:D:778:PHE:CE2   | 2.19                     | 0.77              |
| 1:A:126:LEU:HD11  | 1:A:205:TYR:CE2   | 2.19                     | 0.77              |
| 1:A:267:ILE:HD12  | 1:A:299:VAL:HG11  | 1.67                     | 0.77              |
| 1:A:682:LYS:HZ3   | 1:A:686:ILE:HD11  | 1.47                     | 0.77              |
| 2:B:1482:ASN:HB2  | 2:B:1495:GLU:HG2  | 1.66                     | 0.77              |
| 1:C:315:LEU:HD13  | 1:C:317:ASP:HB2   | 1.64                     | 0.77              |
| 1:C:1386:ILE:HG13 | 1:C:1387:GLU:H    | 1.50                     | 0.77              |
| 1:C:1533:GLY:O    | 1:C:1534:GLN:HB3  | 1.83                     | 0.77              |
| 2:D:484:LEU:HB2   | 2:D:519:ARG:HB2   | 1.66                     | 0.77              |
| 1:A:1615:ARG:HH21 | 1:A:1650:ARG:NH2  | 1.83                     | 0.77              |
| 2:B:1382:ILE:CD1  | 2:B:1458:VAL:HG22 | 2.14                     | 0.77              |
| 2:B:1444:LYS:HE2  | 2:B:1447:GLU:HA   | 1.65                     | 0.77              |
| 2:D:961:THR:HG22  | 2:D:1327:THR:HG23 | 1.67                     | 0.77              |
| 1:A:179:HIS:O     | 1:A:180:ILE:HG12  | 1.85                     | 0.77              |
| 1:A:514:THR:O     | 1:A:515:ARG:HD3   | 1.84                     | 0.77              |
| 2:B:518:PHE:CE2   | 2:B:538:VAL:HB    | 2.18                     | 0.77              |
| 1:A:465:LEU:HG    | 1:A:466:TYR:N     | 2.00                     | 0.77              |
| 1:A:1186:PHE:HD1  | 1:A:1250:THR:HG22 | 1.50                     | 0.77              |
| 2:B:1614:ASP:O    | 2:B:1617:GLN:HG2  | 1.84                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:365:PRO:HD2   | 1:C:464:TYR:CD2   | 2.19                     | 0.77              |
| 1:C:365:PRO:HG2   | 1:C:464:TYR:CE2   | 2.20                     | 0.77              |
| 1:C:465:LEU:HG    | 1:C:466:TYR:N     | 2.00                     | 0.77              |
| 1:C:500:ASN:HB3   | 1:C:543:TYR:HE1   | 1.49                     | 0.77              |
| 1:C:1176:LEU:HD21 | 1:C:1195:LEU:HD22 | 1.67                     | 0.77              |
| 1:A:126:LEU:HD11  | 1:A:205:TYR:CZ    | 2.20                     | 0.77              |
| 1:C:773:TRP:CE3   | 1:C:774:LEU:HB2   | 2.20                     | 0.77              |
| 1:C:1645:ILE:O    | 1:C:1646:GLU:HG3  | 1.83                     | 0.77              |
| 1:A:23:TYR:N      | 1:A:23:TYR:CD1    | 2.46                     | 0.77              |
| 1:A:362:PHE:CE1   | 1:A:640:LEU:HD22  | 2.19                     | 0.77              |
| 2:B:462:VAL:HG21  | 2:B:520:PHE:HE2   | 1.48                     | 0.77              |
| 2:D:194:LEU:CD1   | 2:D:217:ARG:HA    | 2.15                     | 0.77              |
| 1:A:488:PRO:HG3   | 1:A:499:TYR:OH    | 1.84                     | 0.77              |
| 1:C:135:TYR:CE1   | 1:C:141:VAL:HA    | 2.19                     | 0.77              |
| 1:C:1411:SER:N    | 1:C:1414:GLU:HG3  | 2.00                     | 0.77              |
| 1:A:576:SER:HB2   | 1:A:589:SER:H     | 1.49                     | 0.76              |
| 1:C:144:ARG:HD2   | 1:C:146:TYR:CE1   | 2.20                     | 0.76              |
| 1:C:1623:GLU:CB   | 1:C:1638:PRO:HG2  | 2.15                     | 0.76              |
| 2:D:221:LEU:CD1   | 2:D:753:LYS:HG2   | 2.15                     | 0.76              |
| 2:D:462:VAL:HG21  | 2:D:520:PHE:HE2   | 1.48                     | 0.76              |
| 1:A:1213:LYS:HG2  | 1:A:1266:TYR:HE2  | 1.49                     | 0.76              |
| 1:C:25:ILE:H      | 1:C:655:THR:CG2   | 1.97                     | 0.76              |
| 1:C:375:VAL:O     | 1:C:383:VAL:HG13  | 1.84                     | 0.76              |
| 1:C:1176:LEU:HB3  | 1:C:1204:GLN:HG2  | 1.68                     | 0.76              |
| 1:A:42:GLN:HG2    | 1:A:43:VAL:H      | 1.49                     | 0.76              |
| 1:A:1176:LEU:HD21 | 1:A:1195:LEU:HD22 | 1.67                     | 0.76              |
| 2:B:1284:ARG:CG   | 2:B:1285:GLU:H    | 1.98                     | 0.76              |
| 1:C:492:TYR:CG    | 1:C:493:ILE:N     | 2.50                     | 0.76              |
| 1:C:493:ILE:CG2   | 1:C:495:LYS:HB2   | 2.14                     | 0.76              |
| 2:D:518:PHE:HE2   | 2:D:538:VAL:HB    | 1.50                     | 0.76              |
| 1:A:773:TRP:CE3   | 1:A:774:LEU:HB2   | 2.20                     | 0.76              |
| 1:C:132:LYS:NZ    | 1:C:139:GLN:HE22  | 1.84                     | 0.76              |
| 2:D:922:LYS:HE3   | 2:D:1329:TYR:CZ   | 2.20                     | 0.76              |
| 1:A:104:LEU:HD12  | 1:A:105:GLU:H     | 1.50                     | 0.76              |
| 1:A:493:ILE:HG22  | 1:A:495:LYS:N     | 2.01                     | 0.76              |
| 1:A:618:LYS:N     | 1:A:619:PRO:HD2   | 2.01                     | 0.76              |
| 1:C:133:PRO:HD2   | 1:C:609:VAL:HG11  | 1.67                     | 0.76              |
| 1:C:470:THR:HG22  | 2:D:450:THR:CB    | 2.15                     | 0.76              |
| 1:C:1152:ILE:HG21 | 1:C:1168:LEU:HD21 | 1.68                     | 0.76              |
| 1:A:563:ILE:HG13  | 1:A:564:GLU:N     | 1.98                     | 0.76              |
| 1:A:1100:ILE:HG21 | 1:A:1158:ILE:HD12 | 1.68                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1320:LYS:CD   | 1:A:1321:GLY:H    | 1.98                     | 0.76              |
| 2:B:114:ARG:O     | 2:B:115:LEU:HD23  | 1.85                     | 0.76              |
| 1:C:628:GLU:C     | 1:C:630:SER:H     | 1.91                     | 0.76              |
| 1:C:666:ASP:O     | 1:C:668:PRO:HD2   | 1.84                     | 0.76              |
| 2:D:1393:ASP:HB2  | 2:D:1443:LEU:HD11 | 1.66                     | 0.76              |
| 1:A:493:ILE:CG2   | 1:A:495:LYS:HB2   | 2.14                     | 0.76              |
| 1:A:628:GLU:C     | 1:A:630:SER:H     | 1.92                     | 0.76              |
| 2:B:1387:LEU:HD21 | 2:B:1472:TYR:CE1  | 2.20                     | 0.76              |
| 1:C:412:ARG:HH22  | 1:C:472:ASN:ND2   | 1.83                     | 0.76              |
| 1:C:1244:THR:HB   | 1:C:1247:MET:HE3  | 1.66                     | 0.76              |
| 1:C:1626:GLN:HB2  | 1:C:1635:TYR:HD1  | 1.49                     | 0.76              |
| 2:D:137:TYR:HB2   | 2:D:216:VAL:HG23  | 1.68                     | 0.76              |
| 1:A:284:GLN:HG2   | 1:A:310:LEU:HD22  | 1.68                     | 0.76              |
| 1:A:322:TYR:N     | 1:A:322:TYR:HD2   | 1.84                     | 0.76              |
| 1:A:467:ILE:HG22  | 1:A:486:VAL:HG22  | 1.68                     | 0.76              |
| 1:C:59:TYR:CD1    | 1:C:60:PRO:HD3    | 2.21                     | 0.76              |
| 1:C:1365:VAL:HG22 | 1:C:1366:HIS:H    | 1.51                     | 0.76              |
| 1:A:132:LYS:NZ    | 1:A:139:GLN:HE22  | 1.84                     | 0.76              |
| 1:A:1227:PHE:C    | 1:A:1227:PHE:HD1  | 1.93                     | 0.76              |
| 1:A:1626:GLN:HB2  | 1:A:1635:TYR:CD1  | 2.20                     | 0.76              |
| 1:C:618:LYS:N     | 1:C:619:PRO:HD2   | 2.01                     | 0.76              |
| 1:C:944:LEU:HD12  | 1:C:1313:ILE:HD11 | 1.66                     | 0.76              |
| 1:C:1560:ALA:CB   | 1:C:1620:MET:HG2  | 2.16                     | 0.76              |
| 1:A:222:TYR:OH    | 1:A:224:LEU:HD23  | 1.86                     | 0.76              |
| 1:A:666:ASP:O     | 1:A:668:PRO:HD2   | 1.85                     | 0.76              |
| 2:B:476:ILE:O     | 2:B:476:ILE:HG23  | 1.83                     | 0.76              |
| 1:C:873:ILE:HD12  | 1:C:873:ILE:O     | 1.85                     | 0.76              |
| 1:A:690:TYR:HE1   | 1:A:696:LYS:HD2   | 1.51                     | 0.75              |
| 2:B:851:LEU:CD2   | 2:B:852:TYR:H     | 1.98                     | 0.75              |
| 2:B:1450:PHE:HD1  | 2:B:1451:ILE:N    | 1.82                     | 0.75              |
| 1:C:126:LEU:HD11  | 1:C:205:TYR:CZ    | 2.21                     | 0.75              |
| 1:C:936:ARG:HH11  | 1:C:936:ARG:HG3   | 1.50                     | 0.75              |
| 1:C:1056:ILE:HD13 | 1:C:1056:ILE:C    | 2.09                     | 0.75              |
| 1:C:1176:LEU:N    | 1:C:1176:LEU:HD23 | 2.00                     | 0.75              |
| 2:D:218:LYS:HD3   | 2:D:822:TYR:HE2   | 1.50                     | 0.75              |
| 1:A:77:ASN:ND2    | 1:A:81:ASN:HB2    | 2.01                     | 0.75              |
| 1:A:480:GLU:O     | 1:A:530:VAL:HG12  | 1.85                     | 0.75              |
| 1:C:267:ILE:HD12  | 1:C:299:VAL:HG11  | 1.68                     | 0.75              |
| 1:C:1320:LYS:CD   | 1:C:1321:GLY:H    | 1.97                     | 0.75              |
| 2:D:1450:PHE:HD1  | 2:D:1451:ILE:N    | 1.81                     | 0.75              |
| 2:D:1609:ARG:HH11 | 2:D:1609:ARG:CG   | 1.94                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:873:ILE:HD12  | 1:A:873:ILE:O     | 1.87                     | 0.75              |
| 1:A:1386:ILE:HG13 | 1:A:1387:GLU:H    | 1.52                     | 0.75              |
| 2:B:127:PHE:HE2   | 2:B:602:ILE:HG23  | 1.52                     | 0.75              |
| 2:B:235:PHE:HB3   | 2:B:338:ILE:HG22  | 1.68                     | 0.75              |
| 2:B:891:LEU:HB3   | 2:B:912:LYS:HD3   | 1.66                     | 0.75              |
| 1:C:77:ASN:ND2    | 1:C:81:ASN:HB2    | 2.01                     | 0.75              |
| 2:D:462:VAL:HG21  | 2:D:520:PHE:CE2   | 2.21                     | 0.75              |
| 1:A:1244:THR:HB   | 1:A:1247:MET:HE3  | 1.67                     | 0.75              |
| 1:C:284:GLN:HG2   | 1:C:310:LEU:HD22  | 1.67                     | 0.75              |
| 1:C:1244:THR:HG23 | 1:C:1502:ASP:OD2  | 1.87                     | 0.75              |
| 2:D:481:TYR:HE1   | 2:D:506:MET:SD    | 2.09                     | 0.75              |
| 2:D:1442:ILE:C    | 2:D:1443:LEU:HD12 | 2.11                     | 0.75              |
| 1:A:268:THR:HG21  | 1:A:282:MET:HE3   | 1.68                     | 0.75              |
| 1:A:1159:CYS:SG   | 1:A:1161:LEU:HD23 | 2.27                     | 0.75              |
| 2:B:410:PRO:HA    | 2:B:431:THR:HG22  | 1.68                     | 0.75              |
| 2:B:469:ASN:OD1   | 2:B:472:SER:HB2   | 1.85                     | 0.75              |
| 2:B:563:MET:HB3   | 2:B:778:PHE:CE2   | 2.21                     | 0.75              |
| 2:D:1506:ILE:HD12 | 2:D:1627:ASP:HB2  | 1.68                     | 0.75              |
| 1:A:91:GLN:OE1    | 1:A:91:GLN:HA     | 1.77                     | 0.75              |
| 2:B:221:LEU:CD1   | 2:B:753:LYS:HG2   | 2.17                     | 0.75              |
| 2:B:1583:ILE:HG23 | 2:B:1607:ILE:HG23 | 1.67                     | 0.75              |
| 1:C:243:PHE:CE1   | 1:C:316:GLU:HB3   | 2.22                     | 0.75              |
| 2:B:494:ARG:HG3   | 2:B:494:ARG:HH11  | 1.51                     | 0.75              |
| 1:C:1085:VAL:O    | 1:C:1089:VAL:HG23 | 1.86                     | 0.75              |
| 2:D:960:GLU:OE1   | 2:D:1306:LYS:HE2  | 1.87                     | 0.75              |
| 1:A:765:ILE:HD12  | 1:A:765:ILE:O     | 1.87                     | 0.75              |
| 2:B:299:PHE:HE1   | 2:B:303:PHE:HD2   | 1.35                     | 0.75              |
| 1:C:493:ILE:HG22  | 1:C:495:LYS:N     | 2.01                     | 0.75              |
| 1:C:563:ILE:HG13  | 1:C:564:GLU:N     | 1.98                     | 0.75              |
| 2:D:1284:ARG:HG3  | 2:D:1286:VAL:H    | 1.51                     | 0.75              |
| 1:A:975:ARG:NH2   | 1:A:1346:LEU:HD22 | 2.02                     | 0.74              |
| 1:A:1053:MET:HE1  | 1:A:1085:VAL:HG12 | 1.69                     | 0.74              |
| 1:C:111:PHE:HE2   | 1:C:113:LYS:CB    | 2.00                     | 0.74              |
| 1:C:955:ARG:HG2   | 1:C:1350:THR:HG23 | 1.69                     | 0.74              |
| 2:D:244:HIS:HB3   | 2:D:291:LYS:HD2   | 1.68                     | 0.74              |
| 2:B:462:VAL:HG21  | 2:B:520:PHE:CE2   | 2.22                     | 0.74              |
| 2:B:745:ILE:CG2   | 2:B:897:LYS:HD3   | 2.17                     | 0.74              |
| 2:B:948:ARG:HB2   | 2:B:948:ARG:NH2   | 2.02                     | 0.74              |
| 2:D:296:ARG:HH11  | 2:D:296:ARG:HG3   | 1.53                     | 0.74              |
| 1:A:20:GLU:O      | 1:A:20:GLU:HG2    | 1.85                     | 0.74              |
| 1:A:500:ASN:HB2   | 1:A:543:TYR:CD1   | 2.22                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:506:LYS:HD2   | 1:A:536:PRO:HD2   | 1.69                     | 0.74              |
| 2:B:518:PHE:HE2   | 2:B:538:VAL:HB    | 1.52                     | 0.74              |
| 1:C:690:TYR:HE1   | 1:C:696:LYS:HD2   | 1.52                     | 0.74              |
| 1:C:1227:PHE:C    | 1:C:1227:PHE:HD1  | 1.95                     | 0.74              |
| 2:D:1457:LYS:HG2  | 2:D:1469:THR:OG1  | 1.87                     | 0.74              |
| 1:A:322:TYR:N     | 1:A:322:TYR:CD2   | 2.55                     | 0.74              |
| 1:A:829:ILE:HG12  | 1:A:925:LYS:HG2   | 1.69                     | 0.74              |
| 1:C:620:LEU:O     | 1:C:622:ARG:N     | 2.21                     | 0.74              |
| 1:A:120:THR:HG22  | 1:A:122:ASP:H     | 1.52                     | 0.74              |
| 1:A:423:ASN:OD1   | 2:B:504:VAL:HG22  | 1.87                     | 0.74              |
| 1:A:809:ILE:HG12  | 1:A:810:CYS:N     | 2.03                     | 0.74              |
| 1:A:849:ARG:NH1   | 2:B:555:LEU:HD13  | 2.02                     | 0.74              |
| 1:C:113:LYS:HG2   | 1:C:114:SER:N     | 1.99                     | 0.74              |
| 1:C:1033:ILE:HG22 | 1:C:1034:PHE:CD1  | 2.22                     | 0.74              |
| 1:C:1309:LEU:HD11 | 1:C:1328:MET:HG3  | 1.69                     | 0.74              |
| 1:A:412:ARG:HH22  | 1:A:472:ASN:ND2   | 1.86                     | 0.74              |
| 2:B:481:TYR:HB2   | 2:B:520:PHE:CE1   | 2.20                     | 0.74              |
| 1:C:222:TYR:OH    | 1:C:224:LEU:HD23  | 1.87                     | 0.74              |
| 1:C:682:LYS:HZ2   | 1:C:686:ILE:HD11  | 1.51                     | 0.74              |
| 1:C:1584:ILE:HG22 | 1:C:1585:TYR:N    | 2.02                     | 0.74              |
| 2:D:192:VAL:HG22  | 2:D:193:SER:H     | 1.51                     | 0.74              |
| 1:A:59:TYR:CD1    | 1:A:60:PRO:HD3    | 2.23                     | 0.74              |
| 1:A:88:GLN:O      | 1:A:90:LYS:HD3    | 1.88                     | 0.74              |
| 1:A:969:PRO:HG3   | 1:A:1601:ILE:HD12 | 1.70                     | 0.74              |
| 1:C:132:LYS:O     | 1:C:135:TYR:HE2   | 1.70                     | 0.74              |
| 1:C:809:ILE:HG12  | 1:C:810:CYS:N     | 2.03                     | 0.74              |
| 2:D:168:PRO:HG3   | 2:D:196:THR:C     | 2.12                     | 0.74              |
| 2:B:952:ASP:OD1   | 2:B:952:ASP:N     | 2.21                     | 0.73              |
| 1:C:834:VAL:HB    | 1:C:837:GLU:CD    | 2.13                     | 0.73              |
| 2:D:435:TYR:CD1   | 2:D:436:GLN:N     | 2.49                     | 0.73              |
| 2:D:1520:VAL:HG11 | 2:D:1584:TRP:CD1  | 2.23                     | 0.73              |
| 1:C:473:HIS:CE1   | 2:D:455:LYS:HZ1   | 2.05                     | 0.73              |
| 1:C:937:GLU:O     | 1:C:1363:THR:HG23 | 1.88                     | 0.73              |
| 2:D:353:TYR:HB2   | 2:D:613:SER:OG    | 1.88                     | 0.73              |
| 2:D:1387:LEU:HD21 | 2:D:1472:TYR:CE1  | 2.23                     | 0.73              |
| 1:A:25:ILE:H      | 1:A:655:THR:CG2   | 2.00                     | 0.73              |
| 1:A:830:PRO:HG3   | 1:A:1483:PHE:CE2  | 2.23                     | 0.73              |
| 2:B:380:VAL:CG1   | 2:B:387:MET:HB3   | 2.13                     | 0.73              |
| 1:C:182:ILE:HG12  | 1:C:804:ILE:CD1   | 2.18                     | 0.73              |
| 1:C:1053:MET:HE2  | 1:C:1086:LEU:HD13 | 1.69                     | 0.73              |
| 2:D:848:VAL:HG22  | 2:D:898:ALA:HB2   | 1.70                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:682:LYS:HZ3   | 1:C:686:ILE:HD11  | 1.53                     | 0.73              |
| 1:C:871:PRO:HB3   | 1:C:882:LYS:HG3   | 1.70                     | 0.73              |
| 1:C:1627:ILE:HG13 | 1:C:1627:ILE:O    | 1.88                     | 0.73              |
| 2:D:1514:LYS:O    | 2:D:1517:GLU:HB2  | 1.89                     | 0.73              |
| 1:A:1402:ILE:HG13 | 1:A:1479:ILE:HD12 | 1.70                     | 0.73              |
| 1:C:135:TYR:HE1   | 1:C:141:VAL:HA    | 1.54                     | 0.73              |
| 1:A:60:PRO:CD     | 1:A:61:ASP:H      | 2.00                     | 0.73              |
| 1:A:538:SER:O     | 1:A:561:LEU:HB2   | 1.88                     | 0.73              |
| 2:B:1457:LYS:HG2  | 2:B:1469:THR:OG1  | 1.88                     | 0.73              |
| 2:B:1609:ARG:HH11 | 2:B:1609:ARG:CG   | 1.95                     | 0.73              |
| 1:C:538:SER:O     | 1:C:561:LEU:HB2   | 1.88                     | 0.73              |
| 1:C:907:LEU:HD12  | 1:C:908:HIS:H     | 1.52                     | 0.73              |
| 2:D:548:LEU:CD2   | 2:D:793:SER:HB3   | 2.16                     | 0.73              |
| 1:A:977:LEU:HD22  | 1:A:978:SER:N     | 2.04                     | 0.73              |
| 1:A:1560:ALA:CB   | 1:A:1620:MET:HG2  | 2.19                     | 0.73              |
| 1:A:1623:GLU:CB   | 1:A:1638:PRO:HG2  | 2.19                     | 0.73              |
| 2:D:961:THR:CG2   | 2:D:1327:THR:HG23 | 2.19                     | 0.73              |
| 2:D:1520:VAL:HG11 | 2:D:1584:TRP:HD1  | 1.52                     | 0.73              |
| 1:A:1244:THR:HG23 | 1:A:1502:ASP:OD2  | 1.89                     | 0.73              |
| 1:A:1323:LEU:HD12 | 1:A:1324:HIS:H    | 1.54                     | 0.73              |
| 1:C:154:PRO:O     | 1:C:155:ALA:CB    | 2.37                     | 0.73              |
| 2:D:320:VAL:HG12  | 2:D:329:VAL:HG22  | 1.71                     | 0.73              |
| 1:A:871:PRO:HB3   | 1:A:882:LYS:HG3   | 1.70                     | 0.73              |
| 1:A:1019:PHE:C    | 1:A:1019:PHE:CD2  | 2.67                     | 0.73              |
| 2:B:750:ASP:O     | 2:B:782:ASP:HB2   | 1.88                     | 0.73              |
| 2:B:1408:ILE:HD11 | 2:B:1425:ILE:HG12 | 1.71                     | 0.73              |
| 1:C:268:THR:HG21  | 1:C:282:MET:HE3   | 1.69                     | 0.73              |
| 1:C:393:GLN:HG2   | 1:C:403:ASP:OD1   | 1.89                     | 0.73              |
| 1:C:977:LEU:HD22  | 1:C:978:SER:N     | 2.03                     | 0.73              |
| 2:D:811:MET:HE1   | 2:D:839:TYR:HD2   | 1.54                     | 0.73              |
| 1:A:182:ILE:HG12  | 1:A:804:ILE:CD1   | 2.19                     | 0.73              |
| 1:A:1176:LEU:N    | 1:A:1176:LEU:HD23 | 2.02                     | 0.73              |
| 1:A:1627:ILE:CD1  | 1:A:1629:TYR:HB3  | 2.17                     | 0.73              |
| 2:B:435:TYR:CD1   | 2:B:436:GLN:N     | 2.50                     | 0.73              |
| 2:B:960:GLU:OE1   | 2:B:1306:LYS:HE2  | 1.89                     | 0.73              |
| 1:C:830:PRO:HG3   | 1:C:1483:PHE:CE2  | 2.22                     | 0.73              |
| 1:C:1333:PHE:O    | 1:C:1334:LEU:HB2  | 1.88                     | 0.73              |
| 1:A:104:LEU:HD12  | 1:A:105:GLU:N     | 2.03                     | 0.72              |
| 1:A:144:ARG:HD2   | 1:A:146:TYR:CE1   | 2.24                     | 0.72              |
| 1:C:20:GLU:HB2    | 1:C:551:THR:HA    | 1.70                     | 0.72              |
| 1:C:480:GLU:O     | 1:C:530:VAL:HG12  | 1.89                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1159:CYS:SG   | 1:C:1161:LEU:HD23 | 2.29                     | 0.72              |
| 2:D:137:TYR:CZ    | 2:D:143:VAL:HG22  | 2.24                     | 0.72              |
| 1:A:500:ASN:HB3   | 1:A:543:TYR:CE1   | 2.24                     | 0.72              |
| 1:A:1090:ASN:O    | 1:A:1092:TYR:N    | 2.22                     | 0.72              |
| 1:A:1549:LYS:HZ2  | 1:A:1667:PHE:HD1  | 1.35                     | 0.72              |
| 2:B:104:VAL:HG22  | 2:B:105:VAL:H     | 1.54                     | 0.72              |
| 2:B:961:THR:CG2   | 2:B:1327:THR:HG23 | 2.19                     | 0.72              |
| 1:C:88:GLN:O      | 1:C:90:LYS:HD3    | 1.89                     | 0.72              |
| 1:C:975:ARG:NH1   | 1:C:1340:VAL:HG11 | 2.05                     | 0.72              |
| 1:C:1323:LEU:HD12 | 1:C:1324:HIS:H    | 1.54                     | 0.72              |
| 2:D:165:PHE:CZ    | 2:D:199:ILE:HD11  | 2.24                     | 0.72              |
| 1:A:1083:LEU:HD22 | 1:A:1104:LEU:HD21 | 1.70                     | 0.72              |
| 2:B:618:LEU:HD22  | 2:B:636:THR:HA    | 1.70                     | 0.72              |
| 2:B:1473:HIS:HD2  | 2:B:1474:PRO:HD2  | 1.54                     | 0.72              |
| 1:C:362:PHE:CE1   | 1:C:640:LEU:HD22  | 2.23                     | 0.72              |
| 1:A:720:LEU:HD13  | 1:A:724:CYS:HB3   | 1.72                     | 0.72              |
| 1:A:938:SER:C     | 1:A:940:SER:H     | 1.97                     | 0.72              |
| 2:B:1613:GLU:O    | 2:B:1616:CYS:HB2  | 1.89                     | 0.72              |
| 1:C:60:PRO:CD     | 1:C:61:ASP:H      | 2.01                     | 0.72              |
| 1:C:371:ILE:HG22  | 1:C:420:PHE:HB2   | 1.70                     | 0.72              |
| 1:C:934:VAL:HG22  | 1:C:1366:HIS:CD2  | 2.23                     | 0.72              |
| 1:A:62:LYS:HD3    | 1:A:103:TYR:CD2   | 2.24                     | 0.72              |
| 1:A:1227:PHE:C    | 1:A:1227:PHE:CD1  | 2.67                     | 0.72              |
| 2:B:120:LEU:HD12  | 2:B:121:LEU:N     | 2.03                     | 0.72              |
| 2:B:164:GLU:HG2   | 2:B:175:SER:HB2   | 1.70                     | 0.72              |
| 2:B:262:PHE:HE1   | 2:B:282:ARG:HG3   | 1.54                     | 0.72              |
| 1:C:516:GLU:H     | 1:C:516:GLU:CD    | 1.97                     | 0.72              |
| 1:A:786:LEU:HD23  | 1:A:786:LEU:H     | 1.54                     | 0.72              |
| 1:A:796:THR:HG23  | 1:A:818:LYS:CB    | 2.18                     | 0.72              |
| 1:A:934:VAL:HG22  | 1:A:1366:HIS:CD2  | 2.23                     | 0.72              |
| 1:A:1573:VAL:O    | 1:A:1603:LYS:HD2  | 1.88                     | 0.72              |
| 1:C:489:LYS:HG2   | 1:C:490:SER:N     | 2.04                     | 0.72              |
| 1:C:1431:GLY:C    | 1:C:1432:ILE:HD13 | 2.13                     | 0.72              |
| 1:C:1549:LYS:HZ2  | 1:C:1667:PHE:HD1  | 1.35                     | 0.72              |
| 1:C:1568:ILE:HG23 | 1:C:1577:TYR:HE1  | 1.54                     | 0.72              |
| 2:D:104:VAL:HG22  | 2:D:105:VAL:H     | 1.54                     | 0.72              |
| 2:D:127:PHE:CE2   | 2:D:602:ILE:HG23  | 2.23                     | 0.72              |
| 1:A:1645:ILE:O    | 1:A:1646:GLU:HG3  | 1.89                     | 0.72              |
| 2:B:1442:ILE:C    | 2:B:1443:LEU:HD12 | 2.14                     | 0.72              |
| 1:C:720:LEU:HD13  | 1:C:724:CYS:HB3   | 1.72                     | 0.72              |
| 1:C:1365:VAL:HG22 | 1:C:1366:HIS:N    | 2.05                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:120:LEU:HD12  | 2:D:121:LEU:N     | 2.04                     | 0.72              |
| 2:D:829:GLN:HE22  | 2:D:883:VAL:HG13  | 1.53                     | 0.72              |
| 2:D:948:ARG:HB2   | 2:D:948:ARG:NH2   | 2.04                     | 0.72              |
| 2:D:1382:ILE:CD1  | 2:D:1458:VAL:HG22 | 2.19                     | 0.72              |
| 2:B:922:LYS:HE3   | 2:B:1329:TYR:CZ   | 2.24                     | 0.72              |
| 1:C:614:ARG:HD2   | 1:C:615:GLY:N     | 2.04                     | 0.72              |
| 1:C:697:LYS:O     | 1:C:700:TYR:HB3   | 1.90                     | 0.72              |
| 1:C:1083:LEU:HD22 | 1:C:1104:LEU:HD21 | 1.69                     | 0.72              |
| 1:A:620:LEU:O     | 1:A:622:ARG:N     | 2.23                     | 0.72              |
| 2:B:851:LEU:HD23  | 2:B:852:TYR:N     | 2.01                     | 0.72              |
| 1:C:1153:ARG:HD2  | 1:C:1197:LEU:HB3  | 1.71                     | 0.72              |
| 1:A:30:ILE:HG23   | 1:A:118:PRO:HB2   | 1.71                     | 0.72              |
| 1:C:1660:PHE:HE2  | 1:C:1664:LEU:HD12 | 1.54                     | 0.72              |
| 2:B:1514:LYS:O    | 2:B:1517:GLU:HB2  | 1.90                     | 0.71              |
| 1:C:786:LEU:H     | 1:C:786:LEU:HD23  | 1.53                     | 0.71              |
| 1:C:1271:ILE:HD13 | 1:C:1300:TYR:CE1  | 2.24                     | 0.71              |
| 2:D:422:ARG:H     | 2:D:422:ARG:CD    | 2.02                     | 0.71              |
| 2:D:449:ILE:HD13  | 2:D:462:VAL:HG23  | 1.71                     | 0.71              |
| 2:D:925:VAL:HG13  | 2:D:1326:LEU:HD23 | 1.71                     | 0.71              |
| 2:B:296:ARG:HH11  | 2:B:296:ARG:HG3   | 1.54                     | 0.71              |
| 2:B:824:VAL:HG21  | 2:B:830:VAL:HG11  | 1.70                     | 0.71              |
| 2:B:1391:LEU:HB2  | 2:B:1417:MET:HE2  | 1.72                     | 0.71              |
| 1:C:115:LYS:HB2   | 1:C:654:LEU:HD11  | 1.71                     | 0.71              |
| 1:C:461:SER:HB2   | 1:C:553:GLU:OE2   | 1.90                     | 0.71              |
| 1:C:554:LEU:HB3   | 1:C:642:ASN:OD1   | 1.90                     | 0.71              |
| 2:D:745:ILE:HG21  | 2:D:897:LYS:HD3   | 1.72                     | 0.71              |
| 1:A:1132:THR:HG22 | 1:A:1133:LEU:H    | 1.55                     | 0.71              |
| 1:A:1333:PHE:O    | 1:A:1334:LEU:HB2  | 1.88                     | 0.71              |
| 2:B:194:LEU:CD1   | 2:B:217:ARG:HA    | 2.20                     | 0.71              |
| 2:B:548:LEU:CD2   | 2:B:793:SER:HB3   | 2.18                     | 0.71              |
| 1:C:148:LEU:HD12  | 1:C:154:PRO:O     | 1.91                     | 0.71              |
| 1:C:154:PRO:O     | 1:C:155:ALA:HB3   | 1.89                     | 0.71              |
| 1:A:115:LYS:HB2   | 1:A:654:LEU:HD11  | 1.71                     | 0.71              |
| 1:A:365:PRO:HD2   | 1:A:464:TYR:CD2   | 2.25                     | 0.71              |
| 1:A:393:GLN:HG2   | 1:A:403:ASP:OD1   | 1.90                     | 0.71              |
| 2:B:137:TYR:CZ    | 2:B:143:VAL:HG22  | 2.26                     | 0.71              |
| 1:C:765:ILE:HD12  | 1:C:765:ILE:O     | 1.91                     | 0.71              |
| 1:A:20:GLU:HB2    | 1:A:551:THR:HA    | 1.71                     | 0.71              |
| 1:A:135:TYR:CE1   | 1:A:141:VAL:HA    | 2.25                     | 0.71              |
| 1:A:1098:ASN:OD1  | 1:C:1160:PRO:HG2  | 1.90                     | 0.71              |
| 2:B:208:GLU:OE1   | 2:B:210:TYR:HB2   | 1.91                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1305:THR:HG23 | 2:B:1307:LEU:H    | 1.54                     | 0.71              |
| 2:B:1610:TRP:HA   | 2:B:1628:PHE:CE2  | 2.23                     | 0.71              |
| 1:C:322:TYR:HD2   | 1:C:322:TYR:N     | 1.89                     | 0.71              |
| 2:D:106:VAL:HG23  | 2:D:117:LYS:O     | 1.89                     | 0.71              |
| 1:A:133:PRO:HD2   | 1:A:609:VAL:HG11  | 1.71                     | 0.71              |
| 1:A:638:GLY:HA2   | 1:A:645:VAL:HG22  | 1.73                     | 0.71              |
| 2:B:106:VAL:HG23  | 2:B:117:LYS:O     | 1.89                     | 0.71              |
| 2:B:811:MET:HE1   | 2:B:839:TYR:HD2   | 1.55                     | 0.71              |
| 1:C:489:LYS:C     | 1:C:491:PRO:CD    | 2.63                     | 0.71              |
| 1:C:638:GLY:HA2   | 1:C:645:VAL:HG22  | 1.72                     | 0.71              |
| 1:C:1136:GLU:O    | 1:C:1139:GLU:HB2  | 1.91                     | 0.71              |
| 2:D:1613:GLU:O    | 2:D:1616:CYS:HB2  | 1.91                     | 0.71              |
| 1:A:614:ARG:HD2   | 1:A:615:GLY:N     | 2.05                     | 0.71              |
| 1:A:1365:VAL:HG22 | 1:A:1366:HIS:H    | 1.55                     | 0.71              |
| 2:B:320:VAL:HG12  | 2:B:329:VAL:HG22  | 1.73                     | 0.71              |
| 1:C:156:LYS:O     | 1:C:157:ARG:HG2   | 1.91                     | 0.71              |
| 1:C:1227:PHE:C    | 1:C:1227:PHE:CD1  | 2.68                     | 0.71              |
| 1:C:1626:GLN:HB2  | 1:C:1635:TYR:CD1  | 2.25                     | 0.71              |
| 2:D:494:ARG:HH11  | 2:D:494:ARG:HG3   | 1.55                     | 0.71              |
| 2:D:824:VAL:HG21  | 2:D:830:VAL:HG11  | 1.71                     | 0.71              |
| 2:B:848:VAL:HG22  | 2:B:898:ALA:HB2   | 1.72                     | 0.71              |
| 1:C:754:MET:HE3   | 1:C:756:THR:OG1   | 1.91                     | 0.71              |
| 1:C:796:THR:HG23  | 1:C:818:LYS:CB    | 2.20                     | 0.71              |
| 1:C:1650:ARG:H    | 1:C:1650:ARG:HD2  | 1.56                     | 0.71              |
| 1:A:489:LYS:HG2   | 1:A:490:SER:N     | 2.04                     | 0.71              |
| 1:A:682:LYS:HZ2   | 1:A:686:ILE:HD11  | 1.55                     | 0.71              |
| 1:A:1012:LEU:HD13 | 1:A:1081:PHE:HD2  | 1.54                     | 0.71              |
| 1:A:506:LYS:HE2   | 1:A:533:ASN:O     | 1.90                     | 0.71              |
| 1:A:595:GLY:HA2   | 1:A:782:ARG:HH11  | 1.56                     | 0.71              |
| 1:A:907:LEU:HD12  | 1:A:908:HIS:H     | 1.55                     | 0.71              |
| 1:A:1176:LEU:HB3  | 1:A:1204:GLN:HG2  | 1.73                     | 0.71              |
| 1:C:322:TYR:N     | 1:C:322:TYR:CD2   | 2.59                     | 0.71              |
| 1:C:1581:LEU:CD1  | 1:C:1598:ILE:HD11 | 2.21                     | 0.71              |
| 2:D:1288:ILE:HD12 | 2:D:1303:VAL:HG21 | 1.71                     | 0.71              |
| 2:D:1391:LEU:HB2  | 2:D:1417:MET:HE2  | 1.71                     | 0.71              |
| 2:D:1610:TRP:HA   | 2:D:1628:PHE:CE2  | 2.24                     | 0.71              |
| 1:A:576:SER:CB    | 1:A:577:PRO:HD3   | 2.19                     | 0.70              |
| 1:A:1479:ILE:HD13 | 1:A:1479:ILE:N    | 2.06                     | 0.70              |
| 2:B:294:LEU:HD12  | 2:B:295:LYS:H     | 1.56                     | 0.70              |
| 1:C:989:SER:O     | 1:C:993:SER:HB2   | 1.91                     | 0.70              |
| 2:D:262:PHE:HE1   | 2:D:282:ARG:HG3   | 1.54                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1341:ASN:ND2  | 2:D:1342:LYS:HG2  | 2.06                     | 0.70              |
| 1:A:365:PRO:HG2   | 1:A:464:TYR:CE2   | 2.26                     | 0.70              |
| 1:A:371:ILE:HG22  | 1:A:420:PHE:HB2   | 1.72                     | 0.70              |
| 1:C:983:LEU:HD21  | 1:C:1271:ILE:HD12 | 1.74                     | 0.70              |
| 2:D:218:LYS:HD3   | 2:D:822:TYR:CE2   | 2.25                     | 0.70              |
| 2:D:299:PHE:HE1   | 2:D:303:PHE:HD2   | 1.39                     | 0.70              |
| 2:D:380:VAL:CG1   | 2:D:387:MET:HB3   | 2.16                     | 0.70              |
| 1:A:1056:ILE:HD13 | 1:A:1056:ILE:C    | 2.15                     | 0.70              |
| 2:B:1288:ILE:HD12 | 2:B:1303:VAL:HG21 | 1.71                     | 0.70              |
| 2:B:1590:LEU:HD23 | 2:B:1591:LEU:N    | 2.02                     | 0.70              |
| 1:A:625:GLN:HG2   | 1:A:626:PHE:N     | 2.06                     | 0.70              |
| 1:A:1085:VAL:O    | 1:A:1089:VAL:HG23 | 1.91                     | 0.70              |
| 1:A:1627:ILE:O    | 1:A:1627:ILE:HG13 | 1.88                     | 0.70              |
| 2:B:353:TYR:HB2   | 2:B:613:SER:OG    | 1.92                     | 0.70              |
| 2:B:449:ILE:HD13  | 2:B:462:VAL:HG23  | 1.72                     | 0.70              |
| 2:B:1382:ILE:HD12 | 2:B:1458:VAL:HG22 | 1.72                     | 0.70              |
| 1:C:595:GLY:HA2   | 1:C:782:ARG:HH11  | 1.56                     | 0.70              |
| 1:C:849:ARG:HG3   | 1:C:849:ARG:NH1   | 2.06                     | 0.70              |
| 2:D:216:VAL:O     | 2:D:216:VAL:HG12  | 1.90                     | 0.70              |
| 2:D:829:GLN:HA    | 2:D:885:VAL:HG12  | 1.72                     | 0.70              |
| 2:D:1305:THR:HG23 | 2:D:1307:LEU:H    | 1.55                     | 0.70              |
| 1:A:983:LEU:HD21  | 1:A:1271:ILE:HD12 | 1.73                     | 0.70              |
| 2:B:422:ARG:H     | 2:B:422:ARG:CD    | 2.04                     | 0.70              |
| 1:C:123:ASN:C     | 1:C:123:ASN:OD1   | 2.33                     | 0.70              |
| 1:A:1584:ILE:HG22 | 1:A:1585:TYR:N    | 2.04                     | 0.70              |
| 1:C:1145:THR:O    | 1:C:1149:VAL:HG23 | 1.92                     | 0.70              |
| 2:D:1408:ILE:HD11 | 2:D:1425:ILE:HG12 | 1.73                     | 0.70              |
| 1:A:516:GLU:CD    | 1:A:516:GLU:H     | 1.99                     | 0.70              |
| 1:A:1033:ILE:HG22 | 1:A:1034:PHE:CD1  | 2.26                     | 0.70              |
| 1:C:640:LEU:H     | 1:C:644:ASN:HB3   | 1.57                     | 0.70              |
| 1:C:1450:PHE:HZ   | 1:C:1475:VAL:HB   | 1.57                     | 0.70              |
| 1:C:1534:GLN:HG3  | 1:C:1534:GLN:O    | 1.91                     | 0.70              |
| 1:A:1427:SER:HB3  | 1:A:1492:THR:HG23 | 1.74                     | 0.70              |
| 2:D:481:TYR:HB2   | 2:D:520:PHE:CE1   | 2.25                     | 0.70              |
| 1:A:148:LEU:HD12  | 1:A:154:PRO:O     | 1.92                     | 0.70              |
| 1:A:554:LEU:HB3   | 1:A:642:ASN:OD1   | 1.91                     | 0.70              |
| 1:A:1145:THR:O    | 1:A:1149:VAL:HG23 | 1.92                     | 0.70              |
| 1:A:1271:ILE:HD13 | 1:A:1300:TYR:CE1  | 2.26                     | 0.70              |
| 1:C:506:LYS:HE2   | 1:C:533:ASN:O     | 1.92                     | 0.70              |
| 1:A:495:LYS:HE2   | 1:A:495:LYS:HA    | 1.72                     | 0.70              |
| 1:A:1013:MET:O    | 1:A:1016:VAL:HG23 | 1.91                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:127:PHE:CE2   | 2:B:602:ILE:HG23  | 2.26                     | 0.70              |
| 2:B:525:GLN:HA    | 2:B:530:GLU:O     | 1.91                     | 0.70              |
| 2:B:1341:ASN:ND2  | 2:B:1342:LYS:HG2  | 2.07                     | 0.70              |
| 1:C:1226:ARG:CZ   | 1:C:1266:TYR:HE1  | 2.05                     | 0.70              |
| 2:D:834:ALA:O     | 2:D:835:ILE:HD13  | 1.91                     | 0.70              |
| 2:D:1275:LEU:HD21 | 2:D:1319:GLY:O    | 1.91                     | 0.70              |
| 1:A:931:PRO:HB2   | 1:A:1366:HIS:CD2  | 2.27                     | 0.69              |
| 1:A:955:ARG:HG2   | 1:A:1350:THR:CG2  | 2.22                     | 0.69              |
| 2:B:239:GLY:H     | 2:B:296:ARG:HH22  | 1.37                     | 0.69              |
| 2:B:1275:LEU:HD21 | 2:B:1319:GLY:O    | 1.92                     | 0.69              |
| 1:C:23:TYR:N      | 1:C:23:TYR:CD1    | 2.54                     | 0.69              |
| 1:C:33:VAL:HG21   | 1:C:121:TYR:CD1   | 2.26                     | 0.69              |
| 1:C:104:LEU:HD12  | 1:C:105:GLU:H     | 1.56                     | 0.69              |
| 1:C:180:ILE:O     | 1:C:182:ILE:N     | 2.24                     | 0.69              |
| 1:C:576:SER:CB    | 1:C:577:PRO:HD3   | 2.18                     | 0.69              |
| 1:C:1090:ASN:O    | 1:C:1092:TYR:N    | 2.25                     | 0.69              |
| 2:D:1383:ASP:O    | 2:D:1456:VAL:HA   | 1.92                     | 0.69              |
| 1:A:687:ALA:O     | 1:A:690:TYR:HB3   | 1.92                     | 0.69              |
| 1:A:1581:LEU:CD1  | 1:A:1598:ILE:HD11 | 2.23                     | 0.69              |
| 2:B:481:TYR:O     | 2:B:481:TYR:CD2   | 2.42                     | 0.69              |
| 2:B:1500:LEU:C    | 2:B:1500:LEU:HD12 | 2.17                     | 0.69              |
| 1:C:495:LYS:HA    | 1:C:495:LYS:HE2   | 1.73                     | 0.69              |
| 1:C:625:GLN:HG2   | 1:C:626:PHE:N     | 2.06                     | 0.69              |
| 1:A:154:PRO:O     | 1:A:155:ALA:CB    | 2.40                     | 0.69              |
| 1:A:361:LEU:HD12  | 1:A:361:LEU:N     | 2.08                     | 0.69              |
| 2:B:818:LEU:HD23  | 2:B:911:LYS:HD2   | 1.73                     | 0.69              |
| 1:C:463:SER:CB    | 1:C:491:PRO:HA    | 2.23                     | 0.69              |
| 1:C:975:ARG:NH2   | 1:C:1346:LEU:HD22 | 2.07                     | 0.69              |
| 1:C:1213:LYS:HG2  | 1:C:1266:TYR:HE2  | 1.56                     | 0.69              |
| 1:A:123:ASN:C     | 1:A:123:ASN:OD1   | 2.35                     | 0.69              |
| 2:B:168:PRO:HG3   | 2:B:196:THR:C     | 2.16                     | 0.69              |
| 2:B:524:TYR:CE1   | 2:B:532:VAL:HG12  | 2.27                     | 0.69              |
| 2:D:218:LYS:HB3   | 2:D:822:TYR:HD2   | 1.56                     | 0.69              |
| 2:D:618:LEU:HD22  | 2:D:636:THR:HA    | 1.73                     | 0.69              |
| 1:A:1108:VAL:HG11 | 1:A:1164:ILE:HG22 | 1.74                     | 0.69              |
| 1:C:62:LYS:HD3    | 1:C:103:TYR:CD2   | 2.27                     | 0.69              |
| 1:C:269:PHE:HB2   | 1:C:283:MET:HE3   | 1.74                     | 0.69              |
| 1:C:1244:THR:O    | 1:C:1247:MET:HB3  | 1.93                     | 0.69              |
| 2:D:750:ASP:O     | 2:D:782:ASP:HB2   | 1.91                     | 0.69              |
| 1:A:955:ARG:NH1   | 1:A:1352:PHE:HA   | 2.06                     | 0.69              |
| 1:A:1162:VAL:H    | 1:C:1102:ASN:ND2  | 1.88                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:953:ARG:CG    | 2:B:954:VAL:H     | 2.05                     | 0.69              |
| 2:B:1590:LEU:CD2  | 2:B:1591:LEU:H    | 2.03                     | 0.69              |
| 1:C:495:LYS:HA    | 1:C:495:LYS:CE    | 2.21                     | 0.69              |
| 2:D:563:MET:HE2   | 2:D:563:MET:HA    | 1.73                     | 0.69              |
| 2:D:891:LEU:HB3   | 2:D:912:LYS:HD3   | 1.73                     | 0.69              |
| 1:A:493:ILE:HG22  | 1:A:495:LYS:HB2   | 1.73                     | 0.69              |
| 1:A:1136:GLU:O    | 1:A:1139:GLU:HB2  | 1.92                     | 0.69              |
| 2:B:137:TYR:HB2   | 2:B:216:VAL:HG23  | 1.75                     | 0.69              |
| 2:B:603:GLU:O     | 2:B:605:SER:N     | 2.25                     | 0.69              |
| 1:C:120:THR:HG22  | 1:C:122:ASP:H     | 1.57                     | 0.69              |
| 1:C:1450:PHE:CZ   | 1:C:1475:VAL:HB   | 2.28                     | 0.69              |
| 2:D:598:ILE:CD1   | 2:D:800:ILE:HG21  | 2.22                     | 0.69              |
| 1:A:269:PHE:HB2   | 1:A:283:MET:HE3   | 1.74                     | 0.69              |
| 1:A:697:LYS:O     | 1:A:700:TYR:HB3   | 1.93                     | 0.69              |
| 1:A:824:PHE:H     | 1:A:824:PHE:HD2   | 1.39                     | 0.69              |
| 1:A:1244:THR:O    | 1:A:1247:MET:HB3  | 1.91                     | 0.69              |
| 2:B:312:HIS:O     | 2:B:338:ILE:HG12  | 1.92                     | 0.69              |
| 2:B:1273:LEU:CB   | 2:B:1319:GLY:HA3  | 2.22                     | 0.69              |
| 1:C:196:TYR:CE1   | 1:C:221:GLU:HB2   | 2.28                     | 0.69              |
| 1:C:234:GLU:HG3   | 1:C:235:TYR:CD2   | 2.27                     | 0.69              |
| 1:C:363:LEU:O     | 1:C:363:LEU:HD12  | 1.93                     | 0.69              |
| 1:C:654:LEU:O     | 1:C:655:THR:HG23  | 1.92                     | 0.69              |
| 1:C:752:LEU:HD12  | 1:C:753:HIS:N     | 2.06                     | 0.69              |
| 1:C:906:GLY:O     | 1:C:908:HIS:CE1   | 2.46                     | 0.69              |
| 1:C:938:SER:C     | 1:C:940:SER:H     | 2.00                     | 0.69              |
| 1:C:1013:MET:O    | 1:C:1016:VAL:HG23 | 1.92                     | 0.69              |
| 1:C:1019:PHE:C    | 1:C:1019:PHE:CD2  | 2.70                     | 0.69              |
| 1:C:1068:VAL:HG13 | 1:C:1069:TRP:H    | 1.58                     | 0.69              |
| 1:C:1575:VAL:HB   | 1:C:1602:LYS:O    | 1.93                     | 0.69              |
| 2:D:235:PHE:HB3   | 2:D:338:ILE:HG22  | 1.74                     | 0.69              |
| 1:A:1084:ARG:HD2  | 1:A:1154:LYS:HG3  | 1.75                     | 0.69              |
| 2:B:1383:ASP:O    | 2:B:1456:VAL:HA   | 1.92                     | 0.69              |
| 1:C:1211:ALA:HA   | 1:C:1214:ARG:HH11 | 1.57                     | 0.69              |
| 2:D:469:ASN:OD1   | 2:D:472:SER:HB2   | 1.93                     | 0.69              |
| 1:A:421:VAL:HG11  | 2:B:505:THR:CG2   | 2.20                     | 0.69              |
| 1:C:145:VAL:HB    | 1:C:183:ILE:CD1   | 2.22                     | 0.69              |
| 1:C:931:PRO:HB2   | 1:C:1366:HIS:CD2  | 2.27                     | 0.69              |
| 1:C:982:LEU:HD12  | 1:C:982:LEU:N     | 2.08                     | 0.69              |
| 2:D:194:LEU:HD12  | 2:D:217:ARG:HA    | 1.73                     | 0.69              |
| 2:D:269:ILE:HA    | 2:D:312:HIS:CD2   | 2.27                     | 0.69              |
| 2:D:603:GLU:O     | 2:D:605:SER:N     | 2.26                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:925:VAL:HG13  | 2:B:1326:LEU:HD23 | 1.72                     | 0.68              |
| 1:C:500:ASN:HB2   | 1:C:543:TYR:CE1   | 2.27                     | 0.68              |
| 2:D:1284:ARG:CG   | 2:D:1285:GLU:N    | 2.55                     | 0.68              |
| 1:A:1211:ALA:HA   | 1:A:1214:ARG:HH11 | 1.57                     | 0.68              |
| 1:A:1421:HIS:HD2  | 1:A:1422:ALA:N    | 1.91                     | 0.68              |
| 1:A:1534:GLN:HG3  | 1:A:1534:GLN:O    | 1.93                     | 0.68              |
| 1:C:514:THR:O     | 1:C:515:ARG:HD3   | 1.93                     | 0.68              |
| 1:C:1573:VAL:O    | 1:C:1603:LYS:HD2  | 1.93                     | 0.68              |
| 2:D:76:ASN:HB2    | 2:D:77:PRO:HD2    | 1.75                     | 0.68              |
| 2:D:513:ASP:OD2   | 2:D:513:ASP:N     | 2.25                     | 0.68              |
| 2:D:1583:ILE:HG23 | 2:D:1607:ILE:HG23 | 1.75                     | 0.68              |
| 1:A:1660:PHE:HE2  | 1:A:1664:LEU:HD12 | 1.57                     | 0.68              |
| 1:C:493:ILE:HG22  | 1:C:495:LYS:HB2   | 1.73                     | 0.68              |
| 1:C:1279:ARG:HD3  | 1:C:1280:TYR:N    | 2.08                     | 0.68              |
| 2:B:24:LEU:HB3    | 2:B:46:HIS:HB2    | 1.76                     | 0.68              |
| 2:B:844:ILE:HG13  | 2:B:872:ILE:HG12  | 1.76                     | 0.68              |
| 1:C:360:PRO:HB3   | 1:C:636:ALA:HB3   | 1.75                     | 0.68              |
| 2:D:481:TYR:O     | 2:D:481:TYR:CD2   | 2.45                     | 0.68              |
| 1:A:154:PRO:O     | 1:A:155:ALA:HB3   | 1.92                     | 0.68              |
| 1:A:243:PHE:CE1   | 1:A:316:GLU:HB3   | 2.28                     | 0.68              |
| 1:A:654:LEU:O     | 1:A:655:THR:HG23  | 1.93                     | 0.68              |
| 2:B:513:ASP:OD2   | 2:B:513:ASP:N     | 2.26                     | 0.68              |
| 1:C:222:TYR:CD2   | 1:C:223:VAL:N     | 2.62                     | 0.68              |
| 1:C:1024:TYR:HA   | 1:C:1302:LEU:HD21 | 1.75                     | 0.68              |
| 1:C:1487:PHE:N    | 1:C:1487:PHE:CD2  | 2.61                     | 0.68              |
| 1:A:156:LYS:O     | 1:A:157:ARG:HG2   | 1.94                     | 0.68              |
| 1:A:1450:PHE:HZ   | 1:A:1475:VAL:HB   | 1.59                     | 0.68              |
| 1:C:500:ASN:HB3   | 1:C:543:TYR:CE1   | 2.29                     | 0.68              |
| 2:D:208:GLU:OE1   | 2:D:210:TYR:HB2   | 1.94                     | 0.68              |
| 2:D:622:GLU:OE2   | 2:D:637:LYS:HD3   | 1.93                     | 0.68              |
| 1:A:224:LEU:HD22  | 1:A:225:PRO:CD    | 2.21                     | 0.68              |
| 1:A:439:ALA:HB3   | 1:A:442:LEU:HD12  | 1.76                     | 0.68              |
| 1:A:1219:LYS:HE2  | 1:A:1239:VAL:HG21 | 1.76                     | 0.68              |
| 2:B:194:LEU:HD12  | 2:B:217:ARG:HA    | 1.75                     | 0.68              |
| 1:C:1008:ALA:CB   | 1:C:1078:LEU:HD11 | 2.22                     | 0.68              |
| 1:C:1024:TYR:HD2  | 1:C:1025:LEU:N    | 1.92                     | 0.68              |
| 2:D:548:LEU:HD22  | 2:D:793:SER:CB    | 2.20                     | 0.68              |
| 2:D:818:LEU:HD23  | 2:D:911:LYS:HD2   | 1.75                     | 0.68              |
| 1:A:936:ARG:HG3   | 1:A:936:ARG:NH1   | 2.09                     | 0.68              |
| 2:B:128:LEU:O     | 2:B:129:PHE:CD1   | 2.47                     | 0.68              |
| 1:A:145:VAL:HB    | 1:A:183:ILE:CD1   | 2.24                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:961:TYR:OH    | 1:A:1343:ASN:CG   | 2.37                     | 0.68              |
| 1:A:977:LEU:HD23  | 1:A:1361:VAL:HG13 | 1.76                     | 0.68              |
| 2:B:218:LYS:HB3   | 2:B:822:TYR:HD2   | 1.57                     | 0.68              |
| 1:A:1561:TYR:HD1  | 1:A:1581:LEU:HD21 | 1.57                     | 0.68              |
| 1:C:42:GLN:HG2    | 1:C:43:VAL:N      | 2.09                     | 0.68              |
| 2:D:916:VAL:HG23  | 2:D:917:PRO:HD2   | 1.76                     | 0.68              |
| 1:A:594:THR:O     | 1:A:782:ARG:HD3   | 1.94                     | 0.67              |
| 1:A:906:GLY:O     | 1:A:908:HIS:CE1   | 2.47                     | 0.67              |
| 1:A:1365:VAL:HG22 | 1:A:1366:HIS:N    | 2.08                     | 0.67              |
| 2:B:168:PRO:HD3   | 2:B:197:TRP:CD1   | 2.29                     | 0.67              |
| 2:B:189:PRO:C     | 2:B:191:LEU:H     | 2.02                     | 0.67              |
| 1:C:269:PHE:HE1   | 1:C:287:MET:HB3   | 1.58                     | 0.67              |
| 1:C:1053:MET:HE1  | 1:C:1085:VAL:HG12 | 1.77                     | 0.67              |
| 1:C:1644:TRP:NE1  | 1:C:1646:GLU:OE1  | 2.26                     | 0.67              |
| 2:D:312:HIS:O     | 2:D:338:ILE:HG12  | 1.93                     | 0.67              |
| 2:D:1323:MET:HE3  | 2:D:1325:ILE:HD11 | 1.76                     | 0.67              |
| 2:D:1501:ASN:HD22 | 2:D:1501:ASN:H    | 1.40                     | 0.67              |
| 1:C:179:HIS:O     | 1:C:180:ILE:HG12  | 1.95                     | 0.67              |
| 1:C:1108:VAL:HG11 | 1:C:1164:ILE:HG22 | 1.76                     | 0.67              |
| 1:C:1128:LYS:C    | 1:C:1129:LEU:HD23 | 2.19                     | 0.67              |
| 1:C:1174:PHE:O    | 1:C:1178:ASN:HB2  | 1.95                     | 0.67              |
| 2:D:214:PHE:O     | 2:D:214:PHE:CD1   | 2.47                     | 0.67              |
| 2:D:482:LEU:HD12  | 2:D:482:LEU:N     | 2.09                     | 0.67              |
| 2:D:1474:PRO:HG2  | 2:D:1475:ASP:OD1  | 1.93                     | 0.67              |
| 1:A:222:TYR:CD2   | 1:A:223:VAL:N     | 2.63                     | 0.67              |
| 1:A:539:ARG:HE    | 1:A:633:GLY:HA3   | 1.59                     | 0.67              |
| 1:A:1450:PHE:CZ   | 1:A:1475:VAL:HB   | 2.29                     | 0.67              |
| 1:C:128:ILE:HD11  | 1:C:214:THR:C     | 2.19                     | 0.67              |
| 2:D:511:THR:O     | 2:D:514:LEU:HG    | 1.93                     | 0.67              |
| 1:A:269:PHE:HE1   | 1:A:287:MET:HB3   | 1.57                     | 0.67              |
| 1:A:937:GLU:O     | 1:A:1363:THR:HG23 | 1.94                     | 0.67              |
| 2:B:829:GLN:HE22  | 2:B:883:VAL:HG13  | 1.59                     | 0.67              |
| 2:D:129:PHE:CE2   | 2:D:598:ILE:HG23  | 2.30                     | 0.67              |
| 2:D:168:PRO:HD3   | 2:D:197:TRP:CD1   | 2.30                     | 0.67              |
| 2:D:1382:ILE:HD12 | 2:D:1458:VAL:HG22 | 1.75                     | 0.67              |
| 1:A:33:VAL:HG21   | 1:A:121:TYR:CD1   | 2.29                     | 0.67              |
| 1:A:132:LYS:O     | 1:A:135:TYR:HE2   | 1.77                     | 0.67              |
| 1:A:432:GLU:HG2   | 1:A:453:ARG:HB3   | 1.76                     | 0.67              |
| 1:A:1097:GLN:O    | 1:A:1098:ASN:C    | 2.37                     | 0.67              |
| 2:B:521:VAL:HG13  | 2:B:535:SER:HB3   | 1.76                     | 0.67              |
| 1:C:576:SER:HB3   | 1:C:577:PRO:CD    | 2.22                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:24:LEU:HB3    | 2:D:46:HIS:HB2    | 1.77                     | 0.67              |
| 2:D:239:GLY:H     | 2:D:296:ARG:HH22  | 1.39                     | 0.67              |
| 1:A:162:THR:HB    | 1:A:173:MET:HE2   | 1.76                     | 0.67              |
| 1:A:228:SER:O     | 1:A:252:ALA:HA    | 1.95                     | 0.67              |
| 1:A:425:PRO:O     | 1:A:428:VAL:HG12  | 1.94                     | 0.67              |
| 1:A:576:SER:HB3   | 1:A:577:PRO:CD    | 2.23                     | 0.67              |
| 1:A:591:ASN:HB3   | 1:A:785:GLN:HE21  | 1.59                     | 0.67              |
| 1:A:642:ASN:HD22  | 1:A:642:ASN:C     | 2.03                     | 0.67              |
| 1:A:791:PRO:CG    | 1:A:797:TRP:HE1   | 2.06                     | 0.67              |
| 1:A:975:ARG:NH1   | 1:A:1340:VAL:HG11 | 2.10                     | 0.67              |
| 1:A:1102:ASN:ND2  | 1:C:1162:VAL:HG22 | 2.10                     | 0.67              |
| 1:A:1650:ARG:H    | 1:A:1650:ARG:HD2  | 1.60                     | 0.67              |
| 2:B:76:ASN:HB2    | 2:B:77:PRO:HD2    | 1.75                     | 0.67              |
| 2:B:192:VAL:HG22  | 2:B:193:SER:N     | 2.09                     | 0.67              |
| 1:C:174:VAL:HG22  | 1:C:175:GLU:N     | 2.09                     | 0.67              |
| 1:C:489:LYS:CG    | 1:C:490:SER:N     | 2.58                     | 0.67              |
| 1:C:500:ASN:CB    | 1:C:543:TYR:HE1   | 2.06                     | 0.67              |
| 1:C:623:VAL:O     | 1:C:624:PHE:C     | 2.38                     | 0.67              |
| 1:C:941:GLY:O     | 1:C:942:VAL:HG13  | 1.94                     | 0.67              |
| 1:C:1003:LEU:HD11 | 1:C:1286:SER:HA   | 1.75                     | 0.67              |
| 1:C:1560:ALA:HB1  | 1:C:1620:MET:HG2  | 1.77                     | 0.67              |
| 1:A:234:GLU:HG3   | 1:A:235:TYR:CD2   | 2.29                     | 0.67              |
| 1:A:834:VAL:HB    | 1:A:837:GLU:CD    | 2.20                     | 0.67              |
| 1:A:1008:ALA:O    | 1:A:1009:GLU:C    | 2.38                     | 0.67              |
| 2:B:563:MET:HG3   | 2:B:780:LEU:HD23  | 1.76                     | 0.67              |
| 2:B:829:GLN:HA    | 2:B:885:VAL:HG12  | 1.76                     | 0.67              |
| 2:B:1284:ARG:CG   | 2:B:1285:GLU:N    | 2.58                     | 0.67              |
| 2:B:1520:VAL:HG11 | 2:B:1584:TRP:CD1  | 2.30                     | 0.67              |
| 1:C:1127:ILE:HG13 | 1:C:1143:TYR:HE2  | 1.60                     | 0.67              |
| 2:D:1273:LEU:CB   | 2:D:1319:GLY:HA3  | 2.24                     | 0.67              |
| 1:A:475:ALA:HB1   | 1:A:477:LEU:HD21  | 1.76                     | 0.67              |
| 1:A:765:ILE:HD13  | 1:A:767:SER:O     | 1.94                     | 0.67              |
| 2:B:482:LEU:HD12  | 2:B:482:LEU:N     | 2.10                     | 0.67              |
| 2:B:548:LEU:HD22  | 2:B:793:SER:CB    | 2.21                     | 0.67              |
| 1:A:174:VAL:HG22  | 1:A:175:GLU:N     | 2.09                     | 0.67              |
| 1:A:415:ASP:HB2   | 1:A:417:VAL:HB    | 1.77                     | 0.67              |
| 2:B:29:THR:HB     | 2:B:41:ILE:HG22   | 1.77                     | 0.67              |
| 1:C:551:THR:O     | 1:C:552:ALA:HB2   | 1.93                     | 0.67              |
| 1:C:591:ASN:HB3   | 1:C:785:GLN:HE21  | 1.60                     | 0.67              |
| 2:D:265:PHE:CE2   | 2:D:294:LEU:HB2   | 2.30                     | 0.67              |
| 2:D:563:MET:HB3   | 2:D:778:PHE:HE2   | 1.57                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:218:LYS:HD3   | 2:B:822:TYR:HE2   | 1.59                     | 0.67              |
| 1:C:39:ILE:HD11   | 1:C:104:LEU:HD21  | 1.78                     | 0.67              |
| 1:C:90:LYS:O      | 1:C:91:GLN:NE2    | 2.28                     | 0.67              |
| 1:C:710:THR:HG23  | 1:C:713:GLN:NE2   | 2.10                     | 0.67              |
| 2:D:183:PHE:CD2   | 2:D:183:PHE:N     | 2.62                     | 0.67              |
| 2:D:508:LEU:HD12  | 2:D:509:HIS:N     | 2.10                     | 0.67              |
| 1:A:500:ASN:HB2   | 1:A:543:TYR:CE1   | 2.30                     | 0.66              |
| 1:A:504:LEU:HD21  | 1:A:651:LEU:CG    | 2.26                     | 0.66              |
| 1:A:1199:ASP:CG   | 1:A:1199:ASP:O    | 2.37                     | 0.66              |
| 1:A:1431:GLY:C    | 1:A:1432:ILE:HD13 | 2.19                     | 0.66              |
| 1:C:180:ILE:HG21  | 1:C:599:TRP:CE3   | 2.30                     | 0.66              |
| 1:C:473:HIS:CE1   | 2:D:455:LYS:NZ    | 2.63                     | 0.66              |
| 1:C:1561:TYR:HD1  | 1:C:1581:LEU:HD21 | 1.57                     | 0.66              |
| 1:A:490:SER:N     | 1:A:491:PRO:HD2   | 2.09                     | 0.66              |
| 1:A:640:LEU:H     | 1:A:644:ASN:HB3   | 1.60                     | 0.66              |
| 1:A:1053:MET:HE1  | 1:A:1085:VAL:CG1  | 2.25                     | 0.66              |
| 2:B:511:THR:O     | 2:B:514:LEU:HG    | 1.95                     | 0.66              |
| 1:C:791:PRO:CG    | 1:C:797:TRP:HE1   | 2.08                     | 0.66              |
| 1:C:1199:ASP:O    | 1:C:1199:ASP:CG   | 2.37                     | 0.66              |
| 2:D:214:PHE:O     | 2:D:214:PHE:HD1   | 1.78                     | 0.66              |
| 1:A:101:TYR:HE1   | 1:A:116:ARG:CZ    | 2.07                     | 0.66              |
| 1:A:153:LYS:HB2   | 1:A:154:PRO:CD    | 2.25                     | 0.66              |
| 1:A:423:ASN:CG    | 2:B:504:VAL:HG22  | 2.20                     | 0.66              |
| 1:A:982:LEU:HD12  | 1:A:982:LEU:N     | 2.10                     | 0.66              |
| 1:A:1539:LEU:O    | 1:A:1540:ASP:HB3  | 1.94                     | 0.66              |
| 1:A:1560:ALA:HB3  | 1:A:1585:TYR:CE2  | 2.31                     | 0.66              |
| 2:B:531:ILE:HD11  | 2:B:634:LEU:CD2   | 2.24                     | 0.66              |
| 1:C:1127:ILE:CG1  | 1:C:1143:TYR:CE2  | 2.79                     | 0.66              |
| 1:C:1563:VAL:HG21 | 1:C:1619:ILE:HD12 | 1.77                     | 0.66              |
| 2:D:147:VAL:H     | 2:D:183:PHE:HZ    | 1.42                     | 0.66              |
| 2:D:410:PRO:HA    | 2:D:431:THR:HG22  | 1.77                     | 0.66              |
| 2:D:844:ILE:HG13  | 2:D:872:ILE:HG12  | 1.77                     | 0.66              |
| 2:D:889:GLN:HE21  | 2:D:890:GLY:N     | 1.93                     | 0.66              |
| 1:A:160:VAL:HG12  | 1:A:160:VAL:O     | 1.94                     | 0.66              |
| 2:B:524:TYR:HE1   | 2:B:532:VAL:HG12  | 1.61                     | 0.66              |
| 1:C:1012:LEU:HD13 | 1:C:1081:PHE:HD2  | 1.59                     | 0.66              |
| 1:C:1132:THR:HG22 | 1:C:1133:LEU:H    | 1.61                     | 0.66              |
| 1:C:1493:PHE:HD1  | 1:C:1494:THR:N    | 1.92                     | 0.66              |
| 2:D:851:LEU:HD23  | 2:D:852:TYR:N     | 2.05                     | 0.66              |
| 2:D:1606:TRP:CD1  | 2:D:1606:TRP:C    | 2.73                     | 0.66              |
| 1:A:495:LYS:HA    | 1:A:495:LYS:CE    | 2.21                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1381:ILE:HD12 | 1:A:1493:PHE:CD2  | 2.30                     | 0.66              |
| 1:A:1568:ILE:HG23 | 1:A:1577:TYR:HE1  | 1.60                     | 0.66              |
| 1:A:1573:VAL:HG12 | 1:A:1603:LYS:HB3  | 1.76                     | 0.66              |
| 2:B:563:MET:HE2   | 2:B:563:MET:HA    | 1.77                     | 0.66              |
| 1:C:30:ILE:HG23   | 1:C:118:PRO:HB2   | 1.77                     | 0.66              |
| 1:C:439:ALA:HB3   | 1:C:442:LEU:HD12  | 1.78                     | 0.66              |
| 1:C:1016:VAL:HG11 | 1:C:1291:ILE:HG13 | 1.76                     | 0.66              |
| 1:C:1186:PHE:CD1  | 1:C:1250:THR:HG22 | 2.30                     | 0.66              |
| 2:D:29:THR:HB     | 2:D:41:ILE:HG22   | 1.76                     | 0.66              |
| 1:A:551:THR:O     | 1:A:552:ALA:HB2   | 1.94                     | 0.66              |
| 1:A:1226:ARG:CZ   | 1:A:1266:TYR:HE1  | 2.09                     | 0.66              |
| 1:C:365:PRO:HG2   | 1:C:464:TYR:HE2   | 1.57                     | 0.66              |
| 1:C:373:VAL:HG23  | 1:C:418:ALA:HB3   | 1.78                     | 0.66              |
| 1:C:475:ALA:HB1   | 1:C:477:LEU:HD21  | 1.76                     | 0.66              |
| 1:C:792:ASP:O     | 1:C:793:SER:HB3   | 1.94                     | 0.66              |
| 1:C:1479:ILE:HD13 | 1:C:1479:ILE:N    | 2.11                     | 0.66              |
| 2:D:1443:LEU:HD12 | 2:D:1443:LEU:N    | 2.10                     | 0.66              |
| 1:A:111:PHE:HE2   | 1:A:113:LYS:CB    | 2.05                     | 0.66              |
| 2:B:183:PHE:CD2   | 2:B:183:PHE:N     | 2.63                     | 0.66              |
| 2:D:347:PHE:O     | 2:D:349:LYS:N     | 2.29                     | 0.66              |
| 2:D:769:GLN:HB3   | 2:D:771:ILE:HG12  | 1.77                     | 0.66              |
| 1:A:22:THR:HG21   | 1:A:656:ASN:O     | 1.96                     | 0.66              |
| 1:A:90:LYS:O      | 1:A:91:GLN:NE2    | 2.29                     | 0.66              |
| 2:B:266:GLY:HA2   | 2:B:276:ILE:HG13  | 1.76                     | 0.66              |
| 1:C:642:ASN:C     | 1:C:642:ASN:HD22  | 2.04                     | 0.66              |
| 1:A:47:THR:O      | 1:A:48:GLU:HB2    | 1.94                     | 0.66              |
| 1:A:1239:VAL:O    | 1:A:1239:VAL:HG12 | 1.96                     | 0.66              |
| 2:B:613:SER:HA    | 2:B:620:VAL:HG22  | 1.78                     | 0.66              |
| 1:C:104:LEU:HD12  | 1:C:105:GLU:N     | 2.10                     | 0.66              |
| 1:C:361:LEU:N     | 1:C:361:LEU:HD12  | 2.11                     | 0.66              |
| 1:C:470:THR:CG2   | 2:D:450:THR:HG22  | 2.25                     | 0.66              |
| 1:C:576:SER:HB2   | 1:C:589:SER:HB2   | 1.78                     | 0.66              |
| 1:C:1053:MET:CE   | 1:C:1086:LEU:HD22 | 2.25                     | 0.66              |
| 1:C:1627:ILE:CD1  | 1:C:1629:TYR:HB3  | 2.25                     | 0.66              |
| 2:D:525:GLN:HA    | 2:D:530:GLU:O     | 1.95                     | 0.66              |
| 2:D:953:ARG:CG    | 2:D:954:VAL:H     | 2.07                     | 0.66              |
| 1:A:128:ILE:HG22  | 1:A:145:VAL:HG22  | 1.77                     | 0.66              |
| 1:A:135:TYR:HE1   | 1:A:141:VAL:HA    | 1.61                     | 0.66              |
| 1:C:228:SER:O     | 1:C:252:ALA:HA    | 1.96                     | 0.66              |
| 1:C:474:LYS:HD3   | 1:C:474:LYS:H     | 1.61                     | 0.66              |
| 2:D:1590:LEU:HD23 | 2:D:1591:LEU:N    | 2.07                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:412:ARG:HD2   | 2:B:458:ASP:OD1   | 1.96                     | 0.65              |
| 1:A:535:VAL:O     | 1:A:563:ILE:HG12  | 1.96                     | 0.65              |
| 1:A:887:LYS:H     | 1:A:887:LYS:HD2   | 1.61                     | 0.65              |
| 1:A:989:SER:O     | 1:A:993:SER:HB2   | 1.96                     | 0.65              |
| 1:A:1068:VAL:HG13 | 1:A:1069:TRP:H    | 1.61                     | 0.65              |
| 1:A:1127:ILE:HG13 | 1:A:1143:TYR:HE2  | 1.62                     | 0.65              |
| 2:B:615:GLN:HB2   | 2:B:616:ASN:HD22  | 1.60                     | 0.65              |
| 1:C:492:TYR:HD2   | 1:C:493:ILE:H     | 1.33                     | 0.65              |
| 1:C:829:ILE:HG12  | 1:C:925:LYS:HG2   | 1.77                     | 0.65              |
| 2:D:417:HIS:O     | 2:D:419:ASP:N     | 2.28                     | 0.65              |
| 1:A:653:PHE:O     | 1:A:653:PHE:CD1   | 2.43                     | 0.65              |
| 2:B:144:LEU:HD23  | 2:B:144:LEU:H     | 1.62                     | 0.65              |
| 2:B:769:GLN:HB3   | 2:B:771:ILE:HG12  | 1.78                     | 0.65              |
| 2:B:1323:MET:HE3  | 2:B:1325:ILE:HD11 | 1.79                     | 0.65              |
| 1:C:594:THR:O     | 1:C:782:ARG:HD3   | 1.96                     | 0.65              |
| 1:C:681:LYS:HD2   | 1:C:738:LEU:HD21  | 1.77                     | 0.65              |
| 1:C:781:PRO:O     | 1:C:782:ARG:HB2   | 1.96                     | 0.65              |
| 2:D:476:ILE:HG12  | 2:D:524:TYR:CD2   | 2.31                     | 0.65              |
| 2:D:1563:TYR:HB3  | 2:D:1601:ILE:HD11 | 1.76                     | 0.65              |
| 1:A:576:SER:HB2   | 1:A:589:SER:HB2   | 1.78                     | 0.65              |
| 2:B:54:LEU:HD21   | 2:B:75:MET:HE2    | 1.77                     | 0.65              |
| 2:B:963:ILE:HD11  | 2:B:1311:ILE:HG12 | 1.77                     | 0.65              |
| 2:B:1474:PRO:HG2  | 2:B:1475:ASP:OD1  | 1.96                     | 0.65              |
| 2:B:1601:ILE:N    | 2:B:1601:ILE:HD12 | 2.12                     | 0.65              |
| 1:C:171:VAL:HG12  | 1:C:172:ASP:N     | 2.11                     | 0.65              |
| 1:C:1180:LEU:O    | 1:C:1182:ALA:N    | 2.30                     | 0.65              |
| 1:A:489:LYS:HZ3   | 2:B:502:ASN:H     | 1.44                     | 0.65              |
| 1:A:1024:TYR:HD2  | 1:A:1025:LEU:N    | 1.94                     | 0.65              |
| 2:B:269:ILE:HA    | 2:B:312:HIS:CD2   | 2.31                     | 0.65              |
| 2:B:800:ILE:HG23  | 2:B:801:CYS:N     | 2.10                     | 0.65              |
| 2:B:1458:VAL:O    | 2:B:1466:GLU:HG2  | 1.97                     | 0.65              |
| 1:C:955:ARG:NH1   | 1:C:1352:PHE:HA   | 2.12                     | 0.65              |
| 1:C:955:ARG:O     | 1:C:1349:SER:HA   | 1.96                     | 0.65              |
| 1:C:1381:ILE:O    | 1:C:1382:ASP:HB3  | 1.96                     | 0.65              |
| 1:C:1539:LEU:O    | 1:C:1540:ASP:HB3  | 1.95                     | 0.65              |
| 2:D:1429:LYS:N    | 2:D:1429:LYS:HE3  | 2.12                     | 0.65              |
| 1:A:474:LYS:HD3   | 1:A:474:LYS:H     | 1.61                     | 0.65              |
| 1:A:752:LEU:HD12  | 1:A:753:HIS:N     | 2.12                     | 0.65              |
| 1:A:1219:LYS:CE   | 1:A:1239:VAL:HG21 | 2.27                     | 0.65              |
| 2:B:958:GLU:OE1   | 2:B:958:GLU:HA    | 1.95                     | 0.65              |
| 1:C:160:VAL:O     | 1:C:160:VAL:HG12  | 1.97                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:539:ARG:HE    | 1:C:633:GLY:HA3   | 1.61                     | 0.65              |
| 1:C:687:ALA:O     | 1:C:690:TYR:HB3   | 1.97                     | 0.65              |
| 1:C:1031:TRP:CZ3  | 1:C:1042:LYS:HA   | 2.30                     | 0.65              |
| 2:D:565:ILE:HD11  | 2:D:776:MET:HE3   | 1.78                     | 0.65              |
| 2:D:919:GLY:HA2   | 2:D:1332:GLN:HB3  | 1.79                     | 0.65              |
| 2:D:1473:HIS:HD2  | 2:D:1474:PRO:HD2  | 1.59                     | 0.65              |
| 1:A:849:ARG:HH12  | 2:B:555:LEU:HD13  | 1.59                     | 0.65              |
| 1:A:1024:TYR:HA   | 1:A:1302:LEU:HD21 | 1.77                     | 0.65              |
| 2:B:237:ILE:O     | 2:B:306:LEU:HD11  | 1.95                     | 0.65              |
| 2:B:951:ASP:C     | 2:B:953:ARG:H     | 2.02                     | 0.65              |
| 1:C:506:LYS:HD2   | 1:C:536:PRO:CD    | 2.26                     | 0.65              |
| 1:C:961:TYR:OH    | 1:C:1343:ASN:CG   | 2.40                     | 0.65              |
| 1:C:1016:VAL:N    | 1:C:1017:PRO:CD   | 2.60                     | 0.65              |
| 2:D:40:GLN:HG3    | 2:D:86:THR:HG23   | 1.78                     | 0.65              |
| 2:D:218:LYS:HB3   | 2:D:822:TYR:CE2   | 2.32                     | 0.65              |
| 2:D:476:ILE:O     | 2:D:476:ILE:CG2   | 2.44                     | 0.65              |
| 1:A:1053:MET:HE2  | 1:A:1086:LEU:HD13 | 1.76                     | 0.65              |
| 2:B:172:LEU:HD12  | 2:B:173:VAL:H     | 1.62                     | 0.65              |
| 2:B:1408:ILE:CD1  | 2:B:1425:ILE:HG12 | 2.27                     | 0.65              |
| 1:C:490:SER:N     | 1:C:491:PRO:HD2   | 2.11                     | 0.65              |
| 1:C:1024:TYR:CD2  | 1:C:1025:LEU:N    | 2.64                     | 0.65              |
| 1:C:1219:LYS:HE2  | 1:C:1239:VAL:HG21 | 1.79                     | 0.65              |
| 1:C:1226:ARG:CZ   | 1:C:1266:TYR:CE1  | 2.80                     | 0.65              |
| 1:C:1584:ILE:CG2  | 1:C:1585:TYR:H    | 2.02                     | 0.65              |
| 1:A:99:VAL:HG22   | 1:A:100:SER:O     | 1.97                     | 0.65              |
| 2:B:115:LEU:HD13  | 2:B:629:THR:HG22  | 1.79                     | 0.65              |
| 2:B:172:LEU:HD12  | 2:B:173:VAL:N     | 2.11                     | 0.65              |
| 2:B:417:HIS:O     | 2:B:419:ASP:N     | 2.30                     | 0.65              |
| 1:C:797:TRP:HA    | 1:C:797:TRP:CE3   | 2.32                     | 0.65              |
| 2:D:136:ILE:HA    | 2:D:215:ASP:O     | 1.95                     | 0.65              |
| 2:D:236:TYR:C     | 2:D:238:ASP:H     | 2.05                     | 0.65              |
| 2:D:563:MET:HE2   | 2:D:564:LYS:H     | 1.60                     | 0.65              |
| 1:A:196:TYR:CE1   | 1:A:221:GLU:HB2   | 2.32                     | 0.65              |
| 1:A:976:ILE:HB    | 1:A:1362:THR:HG22 | 1.78                     | 0.65              |
| 1:A:1562:LYS:HD2  | 1:A:1648:TRP:HZ2  | 1.61                     | 0.65              |
| 2:B:241:GLU:O     | 2:B:296:ARG:HD3   | 1.97                     | 0.65              |
| 2:B:1446:PHE:HD2  | 2:B:1448:VAL:HG22 | 1.62                     | 0.65              |
| 1:C:127:PHE:CE2   | 1:C:623:VAL:HG13  | 2.29                     | 0.65              |
| 1:C:425:PRO:O     | 1:C:428:VAL:HG12  | 1.96                     | 0.65              |
| 1:C:1113:LEU:HD23 | 1:C:1114:ASP:H    | 1.61                     | 0.65              |
| 1:C:1581:LEU:HD12 | 1:C:1598:ILE:HD11 | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:189:PRO:C     | 2:D:191:LEU:H     | 2.05                     | 0.65              |
| 2:D:613:SER:HA    | 2:D:620:VAL:HG22  | 1.79                     | 0.65              |
| 1:A:128:ILE:HD11  | 1:A:214:THR:C     | 2.22                     | 0.65              |
| 1:A:1113:LEU:HD23 | 1:A:1114:ASP:H    | 1.61                     | 0.65              |
| 1:A:1575:VAL:HB   | 1:A:1602:LYS:O    | 1.97                     | 0.65              |
| 2:B:622:GLU:OE2   | 2:B:637:LYS:HD3   | 1.97                     | 0.65              |
| 2:B:889:GLN:HE21  | 2:B:890:GLY:N     | 1.95                     | 0.65              |
| 1:C:1124:TYR:HA   | 1:C:1465:ASN:OD1  | 1.96                     | 0.65              |
| 1:C:1431:GLY:O    | 1:C:1432:ILE:HD13 | 1.97                     | 0.65              |
| 2:D:1277:ILE:CG2  | 2:D:1290:TYR:HB2  | 2.27                     | 0.65              |
| 1:A:180:ILE:O     | 1:A:182:ILE:N     | 2.30                     | 0.64              |
| 1:A:864:GLY:HA3   | 1:A:907:LEU:CD2   | 2.27                     | 0.64              |
| 1:C:442:LEU:HD23  | 1:C:443:PRO:HD2   | 1.79                     | 0.64              |
| 2:D:1408:ILE:CD1  | 2:D:1425:ILE:HG12 | 2.27                     | 0.64              |
| 1:A:1186:PHE:CD1  | 1:A:1250:THR:HG22 | 2.31                     | 0.64              |
| 1:A:1487:PHE:CD2  | 1:A:1487:PHE:N    | 2.64                     | 0.64              |
| 2:B:919:GLY:HA2   | 2:B:1332:GLN:HB3  | 1.79                     | 0.64              |
| 1:C:238:ILE:HG12  | 1:C:246:PHE:CE1   | 2.32                     | 0.64              |
| 1:C:432:GLU:HG2   | 1:C:453:ARG:HB3   | 1.78                     | 0.64              |
| 1:C:824:PHE:H     | 1:C:824:PHE:HD2   | 1.43                     | 0.64              |
| 1:C:871:PRO:CB    | 1:C:882:LYS:HG3   | 2.27                     | 0.64              |
| 2:D:1274:ASN:HD21 | 2:D:1293:ASN:HB3  | 1.62                     | 0.64              |
| 1:A:830:PRO:HG3   | 1:A:1483:PHE:HZ   | 1.60                     | 0.64              |
| 1:A:849:ARG:HG3   | 1:A:849:ARG:NH1   | 2.08                     | 0.64              |
| 1:A:1493:PHE:HD1  | 1:A:1494:THR:N    | 1.94                     | 0.64              |
| 2:B:1501:ASN:H    | 2:B:1501:ASN:HD22 | 1.45                     | 0.64              |
| 1:C:415:ASP:HB2   | 1:C:417:VAL:HB    | 1.80                     | 0.64              |
| 1:C:773:TRP:HZ2   | 1:C:797:TRP:CD1   | 2.16                     | 0.64              |
| 1:C:969:PRO:O     | 1:C:971:THR:HG23  | 1.98                     | 0.64              |
| 1:C:1239:VAL:HG12 | 1:C:1239:VAL:O    | 1.96                     | 0.64              |
| 1:A:681:LYS:HD2   | 1:A:738:LEU:HD21  | 1.79                     | 0.64              |
| 2:B:547:THR:HG22  | 2:B:548:LEU:H     | 1.63                     | 0.64              |
| 2:B:1424:ILE:HD13 | 2:B:1424:ILE:N    | 2.10                     | 0.64              |
| 2:B:1591:LEU:C    | 2:B:1591:LEU:HD23 | 2.22                     | 0.64              |
| 2:D:294:LEU:HD12  | 2:D:295:LYS:H     | 1.62                     | 0.64              |
| 2:D:951:ASP:C     | 2:D:953:ARG:H     | 2.02                     | 0.64              |
| 1:A:811:VAL:O     | 1:A:811:VAL:HG12  | 1.97                     | 0.64              |
| 1:A:1124:TYR:HA   | 1:A:1465:ASN:OD1  | 1.97                     | 0.64              |
| 1:A:1127:ILE:CG1  | 1:A:1143:TYR:CE2  | 2.81                     | 0.64              |
| 1:A:1174:PHE:O    | 1:A:1178:ASN:HB2  | 1.97                     | 0.64              |
| 1:A:1279:ARG:HD3  | 1:A:1280:TYR:N    | 2.11                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1587:THR:HB   | 1:A:1591:VAL:HG22 | 1.80                     | 0.64              |
| 2:B:1285:GLU:O    | 2:B:1287:PRO:HD3  | 1.98                     | 0.64              |
| 1:C:1084:ARG:HD2  | 1:C:1154:LYS:HG3  | 1.80                     | 0.64              |
| 1:C:1427:SER:HB3  | 1:C:1492:THR:HG23 | 1.79                     | 0.64              |
| 2:D:531:ILE:HD11  | 2:D:634:LEU:CD2   | 2.26                     | 0.64              |
| 1:A:977:LEU:HA    | 1:A:1361:VAL:CG1  | 2.27                     | 0.64              |
| 2:B:285:ILE:H     | 2:B:285:ILE:CD1   | 2.08                     | 0.64              |
| 2:B:316:ALA:HB3   | 2:B:333:GLN:HB3   | 1.79                     | 0.64              |
| 2:B:481:TYR:HE2   | 2:B:493:GLY:CA    | 2.11                     | 0.64              |
| 2:B:481:TYR:CB    | 2:B:520:PHE:HE1   | 2.10                     | 0.64              |
| 2:B:598:ILE:CD1   | 2:B:800:ILE:HG21  | 2.27                     | 0.64              |
| 2:B:762:LEU:N     | 2:B:762:LEU:HD12  | 2.12                     | 0.64              |
| 2:D:316:ALA:HB3   | 2:D:333:GLN:HB3   | 1.78                     | 0.64              |
| 2:D:735:ASN:HB3   | 2:D:869:GLN:HE22  | 1.63                     | 0.64              |
| 2:D:967:GLY:HA2   | 2:D:1321:ALA:HA   | 1.80                     | 0.64              |
| 1:A:44:TYR:CB     | 1:A:545:ILE:HD12  | 2.26                     | 0.64              |
| 1:A:146:TYR:CD1   | 1:A:182:ILE:HG23  | 2.32                     | 0.64              |
| 1:A:363:LEU:HD12  | 1:A:363:LEU:O     | 1.97                     | 0.64              |
| 1:A:375:VAL:HG11  | 1:A:386:VAL:HG11  | 1.79                     | 0.64              |
| 1:A:492:TYR:HD2   | 1:A:493:ILE:H     | 1.33                     | 0.64              |
| 1:A:1581:LEU:HD12 | 1:A:1598:ILE:HD11 | 1.80                     | 0.64              |
| 1:C:307:VAL:HG13  | 1:C:313:TYR:HB2   | 1.79                     | 0.64              |
| 1:C:905:ILE:HD12  | 1:C:931:PRO:CD    | 2.27                     | 0.64              |
| 1:C:1573:VAL:HG12 | 1:C:1603:LYS:HB3  | 1.79                     | 0.64              |
| 2:D:482:LEU:HD11  | 2:D:521:VAL:HB    | 1.79                     | 0.64              |
| 2:D:1429:LYS:HE3  | 2:D:1429:LYS:H    | 1.63                     | 0.64              |
| 1:A:1204:GLN:O    | 1:A:1208:ILE:HG13 | 1.98                     | 0.64              |
| 2:B:1365:LEU:HD12 | 2:B:1366:LYS:H    | 1.62                     | 0.64              |
| 1:C:85:LEU:HD22   | 1:C:85:LEU:N      | 2.12                     | 0.64              |
| 1:C:1008:ALA:O    | 1:C:1009:GLU:C    | 2.41                     | 0.64              |
| 1:C:1013:MET:HE3  | 1:C:1287:THR:HB   | 1.78                     | 0.64              |
| 1:C:1584:ILE:O    | 1:C:1585:TYR:HB3  | 1.97                     | 0.64              |
| 2:D:1591:LEU:HD23 | 2:D:1591:LEU:C    | 2.22                     | 0.64              |
| 1:A:353:LYS:HE3   | 1:A:378:SER:HA    | 1.80                     | 0.64              |
| 1:A:871:PRO:CB    | 1:A:882:LYS:HG3   | 2.28                     | 0.64              |
| 2:B:234:PHE:CD1   | 2:B:234:PHE:C     | 2.76                     | 0.64              |
| 2:B:236:TYR:C     | 2:B:238:ASP:H     | 2.06                     | 0.64              |
| 2:B:476:ILE:HG12  | 2:B:524:TYR:CD2   | 2.33                     | 0.64              |
| 1:C:146:TYR:CD1   | 1:C:182:ILE:HG23  | 2.33                     | 0.64              |
| 1:C:243:PHE:CZ    | 1:C:316:GLU:HB3   | 2.33                     | 0.64              |
| 1:C:1562:LYS:HD2  | 1:C:1648:TRP:HZ2  | 1.63                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1417:MET:HG2  | 2:D:1443:LEU:HD22 | 1.80                     | 0.64              |
| 2:D:1500:LEU:C    | 2:D:1500:LEU:HD12 | 2.23                     | 0.64              |
| 1:A:476:LEU:HB3   | 1:A:563:ILE:HA    | 1.80                     | 0.64              |
| 1:A:1381:ILE:O    | 1:A:1382:ASP:HB3  | 1.98                     | 0.64              |
| 2:B:476:ILE:O     | 2:B:476:ILE:CG2   | 2.46                     | 0.64              |
| 2:B:1274:ASN:HD21 | 2:B:1293:ASN:HB3  | 1.63                     | 0.64              |
| 2:B:1417:MET:HG2  | 2:B:1443:LEU:HD22 | 1.80                     | 0.64              |
| 1:C:24:VAL:HG11   | 1:C:543:TYR:CE2   | 2.33                     | 0.64              |
| 1:C:1554:LYS:HG3  | 1:C:1555:PRO:HD2  | 1.80                     | 0.64              |
| 2:D:521:VAL:HG13  | 2:D:535:SER:HB3   | 1.78                     | 0.64              |
| 1:A:33:VAL:HG21   | 1:A:121:TYR:CE1   | 2.32                     | 0.63              |
| 1:A:315:LEU:HD12  | 1:A:318:LEU:HG    | 1.79                     | 0.63              |
| 1:A:710:THR:HG23  | 1:A:713:GLN:NE2   | 2.12                     | 0.63              |
| 1:A:1644:TRP:NE1  | 1:A:1646:GLU:OE1  | 2.31                     | 0.63              |
| 1:C:830:PRO:HG3   | 1:C:1483:PHE:HZ   | 1.60                     | 0.63              |
| 1:C:984:VAL:HG22  | 1:C:987:ILE:HD12  | 1.79                     | 0.63              |
| 1:C:1421:HIS:HD2  | 1:C:1422:ALA:N    | 1.95                     | 0.63              |
| 2:D:115:LEU:HD13  | 2:D:629:THR:HG22  | 1.81                     | 0.63              |
| 1:A:788:PHE:HD2   | 1:A:788:PHE:N     | 1.96                     | 0.63              |
| 1:A:797:TRP:HA    | 1:A:797:TRP:CE3   | 2.32                     | 0.63              |
| 1:A:1082:ALA:O    | 1:A:1086:LEU:HD23 | 1.99                     | 0.63              |
| 1:A:1421:HIS:C    | 1:A:1421:HIS:CD2  | 2.75                     | 0.63              |
| 1:A:1560:ALA:HB1  | 1:A:1620:MET:HG2  | 1.81                     | 0.63              |
| 1:A:1627:ILE:O    | 1:A:1627:ILE:CG1  | 2.45                     | 0.63              |
| 2:B:154:THR:OG1   | 2:B:157:MET:HE3   | 1.97                     | 0.63              |
| 2:B:563:MET:HB3   | 2:B:778:PHE:HE2   | 1.63                     | 0.63              |
| 1:C:38:ASN:HA     | 1:C:84:ILE:HG22   | 1.79                     | 0.63              |
| 1:C:705:VAL:HA    | 1:C:739:ARG:NH1   | 2.13                     | 0.63              |
| 2:D:738:GLY:O     | 2:D:901:GLN:HA    | 1.99                     | 0.63              |
| 2:D:1365:LEU:HD12 | 2:D:1366:LYS:H    | 1.61                     | 0.63              |
| 1:A:44:TYR:HB2    | 1:A:545:ILE:CD1   | 2.27                     | 0.63              |
| 1:A:623:VAL:O     | 1:A:624:PHE:C     | 2.39                     | 0.63              |
| 1:A:781:PRO:O     | 1:A:782:ARG:HB2   | 1.97                     | 0.63              |
| 1:A:1128:LYS:C    | 1:A:1129:LEU:HD23 | 2.23                     | 0.63              |
| 2:B:416:ASN:HA    | 2:B:425:GLN:HE22  | 1.63                     | 0.63              |
| 2:B:464:PHE:HB2   | 2:B:504:VAL:O     | 1.97                     | 0.63              |
| 2:B:1427:LEU:HD13 | 2:B:1427:LEU:N    | 2.14                     | 0.63              |
| 1:C:219:VAL:O     | 1:C:219:VAL:HG12  | 1.98                     | 0.63              |
| 1:C:535:VAL:O     | 1:C:563:ILE:HG12  | 1.99                     | 0.63              |
| 1:C:1315:VAL:HG23 | 1:C:1348:VAL:HG22 | 1.81                     | 0.63              |
| 1:A:1234:HIS:HD2  | 1:A:1236:ASP:H    | 1.46                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:137:TYR:CE2   | 2:B:143:VAL:HG22  | 2.34                     | 0.63              |
| 2:B:745:ILE:HG21  | 2:B:897:LYS:HD3   | 1.80                     | 0.63              |
| 2:B:1609:ARG:HG2  | 2:B:1609:ARG:NH1  | 1.94                     | 0.63              |
| 1:C:753:HIS:O     | 1:C:754:MET:CB    | 2.46                     | 0.63              |
| 1:C:765:ILE:HD13  | 1:C:767:SER:O     | 1.98                     | 0.63              |
| 1:C:1033:ILE:HG22 | 1:C:1034:PHE:N    | 2.12                     | 0.63              |
| 2:D:175:SER:H     | 2:D:1300:ALA:HB2  | 1.63                     | 0.63              |
| 2:D:416:ASN:HA    | 2:D:425:GLN:HE22  | 1.64                     | 0.63              |
| 1:A:392:ALA:HB2   | 1:A:433:PHE:HB3   | 1.79                     | 0.63              |
| 1:A:1031:TRP:CZ3  | 1:A:1042:LYS:HA   | 2.33                     | 0.63              |
| 1:A:1431:GLY:HA3  | 1:A:1483:PHE:CE1  | 2.34                     | 0.63              |
| 2:B:565:ILE:HD11  | 2:B:776:MET:HE3   | 1.78                     | 0.63              |
| 1:C:307:VAL:CG1   | 1:C:313:TYR:HB2   | 2.28                     | 0.63              |
| 1:C:491:PRO:CG    | 1:C:494:ASP:HB3   | 2.29                     | 0.63              |
| 1:C:572:GLN:HB2   | 1:C:593:ALA:HB3   | 1.80                     | 0.63              |
| 2:D:851:LEU:CD2   | 2:D:852:TYR:H     | 2.02                     | 0.63              |
| 1:A:599:TRP:NE1   | 1:A:779:LEU:HA    | 2.14                     | 0.63              |
| 1:A:1431:GLY:CA   | 1:A:1483:PHE:CE1  | 2.81                     | 0.63              |
| 2:B:967:GLY:HA2   | 2:B:1321:ALA:HA   | 1.81                     | 0.63              |
| 2:B:1284:ARG:HD2  | 2:B:1285:GLU:H    | 1.62                     | 0.63              |
| 1:C:47:THR:O      | 1:C:48:GLU:HB2    | 1.96                     | 0.63              |
| 1:C:820:PHE:O     | 1:C:821:LYS:HG2   | 1.98                     | 0.63              |
| 1:C:887:LYS:HD2   | 1:C:887:LYS:H     | 1.62                     | 0.63              |
| 1:C:1133:LEU:HB2  | 1:C:1134:PRO:HD3  | 1.81                     | 0.63              |
| 1:C:1255:LEU:O    | 1:C:1255:LEU:HD12 | 1.98                     | 0.63              |
| 2:D:26:THR:HG22   | 2:D:630:THR:HG22  | 1.79                     | 0.63              |
| 2:D:524:TYR:CE1   | 2:D:532:VAL:HG12  | 2.33                     | 0.63              |
| 2:D:1458:VAL:O    | 2:D:1466:GLU:HG2  | 1.98                     | 0.63              |
| 1:A:422:LEU:H     | 1:A:422:LEU:HD12  | 1.63                     | 0.63              |
| 1:A:523:TYR:CZ    | 2:B:359:PRO:HD2   | 2.34                     | 0.63              |
| 1:A:955:ARG:O     | 1:A:1349:SER:HA   | 1.98                     | 0.63              |
| 1:A:1008:ALA:CB   | 1:A:1078:LEU:HD11 | 2.26                     | 0.63              |
| 2:B:1491:ARG:HG3  | 2:B:1492:CYS:N    | 2.11                     | 0.63              |
| 1:C:33:VAL:HG21   | 1:C:121:TYR:CE1   | 2.33                     | 0.63              |
| 1:C:932:GLU:OE1   | 1:C:932:GLU:N     | 2.32                     | 0.63              |
| 2:D:144:LEU:HD23  | 2:D:144:LEU:H     | 1.64                     | 0.63              |
| 2:D:1289:ARG:O    | 2:D:1290:TYR:HD1  | 1.81                     | 0.63              |
| 1:A:171:VAL:HG12  | 1:A:172:ASP:N     | 2.13                     | 0.63              |
| 1:A:373:VAL:HG23  | 1:A:418:ALA:HB3   | 1.81                     | 0.63              |
| 1:A:987:ILE:HD11  | 1:A:1294:ILE:HG23 | 1.80                     | 0.63              |
| 2:B:129:PHE:CE2   | 2:B:598:ILE:HG23  | 2.34                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1606:TRP:CD1  | 2:B:1606:TRP:C    | 2.76                     | 0.63              |
| 2:D:82:LEU:HG     | 2:D:83:VAL:N      | 2.12                     | 0.63              |
| 2:D:762:LEU:HD12  | 2:D:762:LEU:N     | 2.13                     | 0.63              |
| 1:A:360:PRO:HB3   | 1:A:636:ALA:HB3   | 1.80                     | 0.63              |
| 1:A:627:LEU:O     | 1:A:627:LEU:HD13  | 1.99                     | 0.63              |
| 1:A:1305:LYS:O    | 1:A:1307:LEU:HD13 | 1.99                     | 0.63              |
| 1:A:1641:SER:C    | 1:A:1643:THR:H    | 2.06                     | 0.63              |
| 1:C:44:TYR:HB2    | 1:C:545:ILE:CD1   | 2.28                     | 0.63              |
| 1:C:101:TYR:HE1   | 1:C:116:ARG:CZ    | 2.12                     | 0.63              |
| 1:C:628:GLU:C     | 1:C:630:SER:N     | 2.56                     | 0.63              |
| 1:C:907:LEU:HD12  | 1:C:908:HIS:N     | 2.14                     | 0.63              |
| 2:D:216:VAL:O     | 2:D:216:VAL:CG1   | 2.46                     | 0.63              |
| 2:D:856:PHE:CD1   | 2:D:884:ILE:HD11  | 2.33                     | 0.63              |
| 1:A:503:ILE:HB    | 1:A:511:HIS:HB2   | 1.81                     | 0.62              |
| 1:A:1226:ARG:CZ   | 1:A:1266:TYR:CE1  | 2.82                     | 0.62              |
| 1:A:1304:VAL:HG12 | 1:A:1305:LYS:N    | 2.13                     | 0.62              |
| 2:B:595:GLN:O     | 2:B:598:ILE:HB    | 1.99                     | 0.62              |
| 2:B:1528:LEU:HD21 | 2:B:1531:ILE:HD11 | 1.81                     | 0.62              |
| 1:C:392:ALA:HB2   | 1:C:433:PHE:HB3   | 1.80                     | 0.62              |
| 1:C:1219:LYS:CE   | 1:C:1239:VAL:HG21 | 2.28                     | 0.62              |
| 2:D:481:TYR:HE2   | 2:D:493:GLY:CA    | 2.12                     | 0.62              |
| 2:D:595:GLN:O     | 2:D:598:ILE:HB    | 1.99                     | 0.62              |
| 2:D:872:ILE:HG22  | 2:D:878:ARG:HG3   | 1.81                     | 0.62              |
| 2:D:1387:LEU:HB2  | 2:D:1390:PHE:CD2  | 2.34                     | 0.62              |
| 2:D:1446:PHE:HD2  | 2:D:1448:VAL:HG22 | 1.64                     | 0.62              |
| 1:A:491:PRO:CG    | 1:A:494:ASP:HB3   | 2.29                     | 0.62              |
| 1:A:754:MET:HE3   | 1:A:756:THR:OG1   | 1.99                     | 0.62              |
| 1:A:941:GLY:O     | 1:A:942:VAL:HG13  | 1.99                     | 0.62              |
| 1:A:969:PRO:O     | 1:A:971:THR:HG23  | 1.99                     | 0.62              |
| 2:B:326:SER:HB2   | 2:B:819:GLN:HG3   | 1.81                     | 0.62              |
| 2:B:1602:THR:C    | 2:B:1604:ASN:H    | 2.05                     | 0.62              |
| 1:C:854:GLN:H     | 1:C:854:GLN:CD    | 2.07                     | 0.62              |
| 2:D:128:LEU:O     | 2:D:129:PHE:CD1   | 2.52                     | 0.62              |
| 2:D:326:SER:HB2   | 2:D:819:GLN:HG3   | 1.81                     | 0.62              |
| 2:D:1623:LYS:HZ2  | 2:D:1623:LYS:HB3  | 1.64                     | 0.62              |
| 1:A:489:LYS:C     | 1:A:491:PRO:CD    | 2.63                     | 0.62              |
| 1:A:981:GLY:CA    | 1:A:1333:PHE:HB2  | 2.29                     | 0.62              |
| 1:A:985:GLY:O     | 1:A:986:GLU:C     | 2.42                     | 0.62              |
| 1:A:1180:LEU:O    | 1:A:1182:ALA:N    | 2.32                     | 0.62              |
| 1:A:1213:LYS:HG2  | 1:A:1266:TYR:CE2  | 2.32                     | 0.62              |
| 1:A:1671:ILE:O    | 1:A:1671:ILE:HG13 | 1.98                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:175:SER:H     | 2:B:1300:ALA:HB2  | 1.64                     | 0.62              |
| 2:B:1443:LEU:HD12 | 2:B:1443:LEU:N    | 2.13                     | 0.62              |
| 1:C:162:THR:HB    | 1:C:173:MET:HE2   | 1.81                     | 0.62              |
| 1:C:627:LEU:O     | 1:C:627:LEU:HD13  | 1.99                     | 0.62              |
| 1:C:986:GLU:HG2   | 1:C:987:ILE:N     | 2.13                     | 0.62              |
| 1:C:1304:VAL:HG12 | 1:C:1305:LYS:N    | 2.14                     | 0.62              |
| 1:C:1560:ALA:HB3  | 1:C:1585:TYR:CE2  | 2.34                     | 0.62              |
| 2:D:237:ILE:O     | 2:D:306:LEU:HD11  | 1.97                     | 0.62              |
| 2:D:247:ILE:HD11  | 2:D:318:VAL:HG21  | 1.81                     | 0.62              |
| 2:D:407:GLN:NE2   | 2:D:407:GLN:HA    | 2.15                     | 0.62              |
| 2:D:1609:ARG:HG2  | 2:D:1609:ARG:NH1  | 1.93                     | 0.62              |
| 1:A:38:ASN:HA     | 1:A:84:ILE:HG22   | 1.81                     | 0.62              |
| 1:A:42:GLN:HG2    | 1:A:43:VAL:N      | 2.15                     | 0.62              |
| 1:A:292:LEU:HA    | 1:A:297:ALA:HB2   | 1.80                     | 0.62              |
| 1:A:1593:GLU:HB2  | 1:A:1596:SER:OG   | 1.99                     | 0.62              |
| 2:B:563:MET:HE2   | 2:B:564:LYS:H     | 1.64                     | 0.62              |
| 1:C:838:GLN:OE1   | 1:C:1528:VAL:HG12 | 2.00                     | 0.62              |
| 1:C:1053:MET:HE1  | 1:C:1085:VAL:CG1  | 2.29                     | 0.62              |
| 1:C:1097:GLN:O    | 1:C:1098:ASN:C    | 2.41                     | 0.62              |
| 1:C:1127:ILE:CG1  | 1:C:1143:TYR:HE2  | 2.12                     | 0.62              |
| 2:D:464:PHE:HB2   | 2:D:504:VAL:O     | 1.99                     | 0.62              |
| 2:D:565:ILE:CD1   | 2:D:776:MET:HE3   | 2.29                     | 0.62              |
| 1:A:376:LYS:HA    | 1:A:381:GLN:O     | 2.00                     | 0.62              |
| 1:A:461:SER:HB2   | 1:A:553:GLU:OE2   | 1.99                     | 0.62              |
| 1:A:968:VAL:HG13  | 1:A:1366:HIS:O    | 2.00                     | 0.62              |
| 1:A:1133:LEU:HB2  | 1:A:1134:PRO:HD3  | 1.81                     | 0.62              |
| 2:B:216:VAL:O     | 2:B:216:VAL:HG12  | 1.97                     | 0.62              |
| 1:C:788:PHE:N     | 1:C:788:PHE:HD2   | 1.97                     | 0.62              |
| 1:C:804:ILE:HG22  | 1:C:809:ILE:HG13  | 1.79                     | 0.62              |
| 1:C:909:ASN:O     | 1:C:910:ILE:HG12  | 1.99                     | 0.62              |
| 1:C:936:ARG:HG3   | 1:C:936:ARG:NH1   | 2.14                     | 0.62              |
| 2:D:54:LEU:HD21   | 2:D:75:MET:HE2    | 1.81                     | 0.62              |
| 2:D:137:TYR:CE2   | 2:D:143:VAL:HG22  | 2.34                     | 0.62              |
| 2:D:154:THR:OG1   | 2:D:157:MET:HE3   | 1.98                     | 0.62              |
| 2:D:234:PHE:C     | 2:D:234:PHE:CD1   | 2.77                     | 0.62              |
| 2:D:958:GLU:OE1   | 2:D:958:GLU:HA    | 1.97                     | 0.62              |
| 1:A:457:TYR:C     | 1:A:457:TYR:CD2   | 2.78                     | 0.62              |
| 1:A:504:LEU:HD12  | 1:A:509:ILE:HA    | 1.81                     | 0.62              |
| 1:A:506:LYS:HD2   | 1:A:536:PRO:CD    | 2.29                     | 0.62              |
| 1:A:596:MET:CA    | 1:A:782:ARG:HG2   | 2.29                     | 0.62              |
| 1:A:849:ARG:NH2   | 2:B:555:LEU:HB2   | 2.15                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1024:TYR:CD2  | 1:A:1025:LEU:N    | 2.67                     | 0.62              |
| 1:A:1068:VAL:HA   | 1:A:1078:LEU:CD1  | 2.27                     | 0.62              |
| 1:A:1255:LEU:HD12 | 1:A:1255:LEU:O    | 1.99                     | 0.62              |
| 2:B:200:VAL:HG23  | 2:B:200:VAL:O     | 1.99                     | 0.62              |
| 2:B:218:LYS:HD3   | 2:B:822:TYR:CE2   | 2.34                     | 0.62              |
| 2:B:950:LEU:HD22  | 2:B:1329:TYR:CE1  | 2.34                     | 0.62              |
| 1:C:371:ILE:CD1   | 1:C:433:PHE:CE2   | 2.82                     | 0.62              |
| 1:C:476:LEU:HB3   | 1:C:563:ILE:HA    | 1.82                     | 0.62              |
| 1:C:981:GLY:CA    | 1:C:1333:PHE:HB2  | 2.29                     | 0.62              |
| 2:D:131:GLN:OE1   | 2:D:146:ARG:NH1   | 2.32                     | 0.62              |
| 2:D:1284:ARG:HG3  | 2:D:1285:GLU:N    | 2.15                     | 0.62              |
| 2:D:1427:LEU:HD13 | 2:D:1427:LEU:N    | 2.15                     | 0.62              |
| 2:B:40:GLN:HG3    | 2:B:86:THR:HG23   | 1.81                     | 0.62              |
| 2:B:315:TYR:CD1   | 2:B:315:TYR:C     | 2.77                     | 0.62              |
| 1:C:308:LYS:HG3   | 1:C:309:GLU:N     | 2.15                     | 0.62              |
| 1:C:1143:TYR:CE1  | 1:C:1147:PHE:HB2  | 2.34                     | 0.62              |
| 1:C:1560:ALA:HB2  | 1:C:1620:MET:HG2  | 1.81                     | 0.62              |
| 2:D:285:ILE:H     | 2:D:285:ILE:CD1   | 2.10                     | 0.62              |
| 2:D:944:VAL:HG22  | 2:D:1312:THR:OG1  | 1.99                     | 0.62              |
| 1:A:39:ILE:HD11   | 1:A:104:LEU:HD21  | 1.82                     | 0.62              |
| 1:A:970:LYS:HD3   | 1:A:1640:ASP:OD2  | 1.99                     | 0.62              |
| 1:A:1570:VAL:HG22 | 1:A:1575:VAL:HG22 | 1.81                     | 0.62              |
| 2:B:955:PRO:O     | 2:B:957:THR:HG23  | 2.00                     | 0.62              |
| 1:C:132:LYS:O     | 1:C:135:TYR:CE2   | 2.53                     | 0.62              |
| 1:C:353:LYS:HE3   | 1:C:378:SER:HA    | 1.82                     | 0.62              |
| 1:C:773:TRP:HE1   | 1:C:797:TRP:NE1   | 1.97                     | 0.62              |
| 1:C:1221:ASN:HA   | 1:C:1222:PRO:C    | 2.25                     | 0.62              |
| 1:C:1431:GLY:CA   | 1:C:1483:PHE:CE1  | 2.82                     | 0.62              |
| 2:D:390:THR:HG22  | 2:D:394:GLY:C     | 2.24                     | 0.62              |
| 1:A:489:LYS:CG    | 1:A:490:SER:N     | 2.61                     | 0.62              |
| 1:A:788:PHE:N     | 1:A:788:PHE:CD2   | 2.67                     | 0.62              |
| 1:A:792:ASP:O     | 1:A:793:SER:HB3   | 1.99                     | 0.62              |
| 1:A:999:ILE:HG13  | 1:A:1000:LEU:N    | 2.13                     | 0.62              |
| 1:A:1431:GLY:HA3  | 1:A:1483:PHE:HE1  | 1.64                     | 0.62              |
| 2:B:494:ARG:HG3   | 2:B:494:ARG:NH1   | 2.13                     | 0.62              |
| 1:C:128:ILE:HG22  | 1:C:145:VAL:HG22  | 1.81                     | 0.62              |
| 1:C:571:LEU:HA    | 1:C:593:ALA:O     | 2.00                     | 0.62              |
| 1:C:1271:ILE:HD13 | 1:C:1300:TYR:CZ   | 2.35                     | 0.62              |
| 1:C:1429:PRO:HB2  | 1:C:1432:ILE:HG13 | 1.81                     | 0.62              |
| 2:D:241:GLU:O     | 2:D:296:ARG:HD3   | 2.00                     | 0.62              |
| 1:A:85:LEU:N      | 1:A:85:LEU:HD22   | 2.14                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1227:PHE:HD2  | 1:A:1273:TRP:CE2  | 2.17                     | 0.62              |
| 1:A:1315:VAL:HG23 | 1:A:1348:VAL:HG22 | 1.82                     | 0.62              |
| 2:B:82:LEU:HG     | 2:B:83:VAL:N      | 2.14                     | 0.62              |
| 2:B:179:ASP:OD1   | 2:B:181:ASN:HB2   | 2.00                     | 0.62              |
| 2:B:218:LYS:HB3   | 2:B:822:TYR:CE2   | 2.35                     | 0.62              |
| 2:B:482:LEU:HD11  | 2:B:521:VAL:HB    | 1.80                     | 0.62              |
| 2:B:953:ARG:CZ    | 2:B:959:ILE:HD11  | 2.30                     | 0.62              |
| 1:C:977:LEU:HD23  | 1:C:1361:VAL:HG13 | 1.81                     | 0.62              |
| 1:C:1234:HIS:HD2  | 1:C:1236:ASP:H    | 1.46                     | 0.62              |
| 1:C:1587:THR:HB   | 1:C:1591:VAL:HG22 | 1.82                     | 0.62              |
| 2:D:1284:ARG:CD   | 2:D:1285:GLU:N    | 2.58                     | 0.62              |
| 1:A:540:LEU:C     | 1:A:540:LEU:HD12  | 2.25                     | 0.61              |
| 1:A:773:TRP:HZ2   | 1:A:797:TRP:CD1   | 2.18                     | 0.61              |
| 1:A:905:ILE:HD12  | 1:A:931:PRO:CD    | 2.29                     | 0.61              |
| 1:A:979:VAL:C     | 1:A:980:LYS:HG2   | 2.24                     | 0.61              |
| 1:A:1221:ASN:HA   | 1:A:1222:PRO:C    | 2.24                     | 0.61              |
| 1:C:696:LYS:NZ    | 1:C:759:PRO:HG2   | 2.15                     | 0.61              |
| 1:C:797:TRP:HA    | 1:C:797:TRP:HE3   | 1.63                     | 0.61              |
| 1:C:895:LEU:HD12  | 1:C:896:VAL:N     | 2.15                     | 0.61              |
| 1:C:977:LEU:HD13  | 1:C:977:LEU:C     | 2.24                     | 0.61              |
| 1:C:1012:LEU:O    | 1:C:1015:VAL:HG12 | 2.00                     | 0.61              |
| 1:C:1127:ILE:HD11 | 1:C:1143:TYR:CD2  | 2.35                     | 0.61              |
| 1:C:1188:LEU:HD23 | 1:C:1212:LEU:HD22 | 1.81                     | 0.61              |
| 2:D:1602:THR:C    | 2:D:1604:ASN:H    | 2.07                     | 0.61              |
| 1:A:81:ASN:CG     | 1:A:82:SER:H      | 2.09                     | 0.61              |
| 1:A:754:MET:SD    | 1:A:755:LYS:N     | 2.73                     | 0.61              |
| 2:B:147:VAL:H     | 2:B:183:PHE:HZ    | 1.45                     | 0.61              |
| 2:B:247:ILE:HD11  | 2:B:318:VAL:HG21  | 1.82                     | 0.61              |
| 2:B:615:GLN:HB2   | 2:B:616:ASN:ND2   | 2.14                     | 0.61              |
| 1:C:811:VAL:O     | 1:C:811:VAL:HG12  | 1.99                     | 0.61              |
| 1:C:1083:LEU:CD2  | 1:C:1104:LEU:HD21 | 2.30                     | 0.61              |
| 2:D:31:ALA:O      | 2:D:119:VAL:HG12  | 2.00                     | 0.61              |
| 2:D:137:TYR:HB2   | 2:D:216:VAL:CG2   | 2.30                     | 0.61              |
| 2:D:172:LEU:HD12  | 2:D:173:VAL:N     | 2.15                     | 0.61              |
| 2:D:1601:ILE:HD12 | 2:D:1601:ILE:N    | 2.15                     | 0.61              |
| 1:A:457:TYR:C     | 1:A:457:TYR:HD2   | 2.08                     | 0.61              |
| 1:A:551:THR:O     | 1:A:552:ALA:CB    | 2.47                     | 0.61              |
| 1:A:977:LEU:HA    | 1:A:1361:VAL:HG13 | 1.80                     | 0.61              |
| 1:A:1271:ILE:HD13 | 1:A:1300:TYR:CZ   | 2.36                     | 0.61              |
| 1:A:1554:LYS:HG3  | 1:A:1555:PRO:HD2  | 1.83                     | 0.61              |
| 2:B:214:PHE:O     | 2:B:214:PHE:CD1   | 2.53                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:945:ILE:HD13  | 2:B:1311:ILE:HB   | 1.82                     | 0.61              |
| 1:C:25:ILE:H      | 1:C:655:THR:HG23  | 1.63                     | 0.61              |
| 1:C:985:GLY:O     | 1:C:986:GLU:C     | 2.42                     | 0.61              |
| 2:D:423:GLU:N     | 2:D:423:GLU:OE2   | 2.33                     | 0.61              |
| 2:D:838:ASN:OD1   | 2:D:840:VAL:HG23  | 1.99                     | 0.61              |
| 2:D:1610:TRP:CA   | 2:D:1628:PHE:HE2  | 2.11                     | 0.61              |
| 1:A:160:VAL:CG2   | 1:A:175:GLU:HB3   | 2.30                     | 0.61              |
| 1:A:284:GLN:CG    | 1:A:310:LEU:HD22  | 2.30                     | 0.61              |
| 1:A:1127:ILE:HD11 | 1:A:1143:TYR:CD2  | 2.35                     | 0.61              |
| 2:B:322:THR:HG21  | 2:B:326:SER:OG    | 2.01                     | 0.61              |
| 2:B:1520:VAL:HG11 | 2:B:1584:TRP:HD1  | 1.63                     | 0.61              |
| 1:C:1451:THR:O    | 1:C:1452:ASP:CB   | 2.49                     | 0.61              |
| 1:A:311:SER:O     | 1:A:313:TYR:N     | 2.33                     | 0.61              |
| 1:A:655:THR:O     | 1:A:657:ALA:N     | 2.33                     | 0.61              |
| 1:A:696:LYS:NZ    | 1:A:759:PRO:HG2   | 2.16                     | 0.61              |
| 1:A:932:GLU:OE1   | 1:A:932:GLU:N     | 2.34                     | 0.61              |
| 1:A:986:GLU:HG2   | 1:A:987:ILE:N     | 2.14                     | 0.61              |
| 1:A:1166:THR:O    | 1:A:1170:LYS:HG2  | 2.01                     | 0.61              |
| 1:C:520:ASP:OD2   | 2:D:404:LEU:HB2   | 2.00                     | 0.61              |
| 1:C:754:MET:SD    | 1:C:755:LYS:N     | 2.74                     | 0.61              |
| 1:C:949:ILE:O     | 1:C:950:TYR:CD1   | 2.54                     | 0.61              |
| 1:C:1082:ALA:O    | 1:C:1086:LEU:HD23 | 2.01                     | 0.61              |
| 2:D:266:GLY:HA2   | 2:D:276:ILE:HG13  | 1.81                     | 0.61              |
| 2:D:1517:GLU:OE1  | 2:D:1517:GLU:HA   | 1.98                     | 0.61              |
| 1:A:371:ILE:CD1   | 1:A:433:PHE:CE2   | 2.83                     | 0.61              |
| 1:A:572:GLN:HB2   | 1:A:593:ALA:HB3   | 1.81                     | 0.61              |
| 1:A:702:GLY:CA    | 1:A:728:PHE:CE1   | 2.80                     | 0.61              |
| 2:B:407:GLN:NE2   | 2:B:407:GLN:HA    | 2.14                     | 0.61              |
| 2:B:501:GLN:HG2   | 2:B:504:VAL:HG23  | 1.81                     | 0.61              |
| 1:C:551:THR:O     | 1:C:552:ALA:CB    | 2.48                     | 0.61              |
| 1:C:970:LYS:HD3   | 1:C:1640:ASP:OD2  | 2.00                     | 0.61              |
| 1:C:1229:LYS:NZ   | 1:C:1240:PRO:HD2  | 2.15                     | 0.61              |
| 1:C:1420:SER:O    | 1:C:1421:HIS:C    | 2.44                     | 0.61              |
| 1:C:1570:VAL:O    | 1:C:1571:GLU:HG3  | 2.01                     | 0.61              |
| 1:A:165:ASP:C     | 1:A:165:ASP:OD2   | 2.44                     | 0.61              |
| 1:A:532:GLN:HE21  | 1:A:807:THR:HB    | 1.66                     | 0.61              |
| 1:A:1117:SER:HB3  | 1:A:1174:PHE:CE2  | 2.36                     | 0.61              |
| 1:A:1188:LEU:HD23 | 1:A:1212:LEU:HD22 | 1.82                     | 0.61              |
| 2:B:28:ILE:HD12   | 2:B:42:LEU:HD23   | 1.82                     | 0.61              |
| 1:C:292:LEU:HA    | 1:C:297:ALA:HB2   | 1.81                     | 0.61              |
| 1:C:690:TYR:CE1   | 1:C:696:LYS:HD2   | 2.35                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:990:ALA:HB1   | 1:C:1000:LEU:HD11 | 1.82                     | 0.61              |
| 2:D:523:TYR:C     | 2:D:523:TYR:CD1   | 2.79                     | 0.61              |
| 1:A:231:ILE:O     | 1:A:231:ILE:HG12  | 1.99                     | 0.61              |
| 1:A:251:LYS:HG2   | 1:A:296:ILE:HD11  | 1.82                     | 0.61              |
| 1:A:373:VAL:O     | 1:A:417:VAL:HA    | 2.01                     | 0.61              |
| 1:A:653:PHE:HD1   | 1:A:653:PHE:C     | 2.08                     | 0.61              |
| 1:A:820:PHE:O     | 1:A:821:LYS:HG2   | 2.00                     | 0.61              |
| 1:A:847:ASN:HD22  | 1:A:888:VAL:HG13  | 1.66                     | 0.61              |
| 1:A:895:LEU:HD12  | 1:A:896:VAL:N     | 2.16                     | 0.61              |
| 1:A:1034:PHE:CE2  | 1:A:1041:GLU:HG2  | 2.36                     | 0.61              |
| 1:C:23:TYR:HA     | 1:C:43:VAL:HA     | 1.81                     | 0.61              |
| 1:C:976:ILE:HB    | 1:C:1362:THR:HG22 | 1.82                     | 0.61              |
| 1:C:1068:VAL:HA   | 1:C:1078:LEU:CD1  | 2.28                     | 0.61              |
| 1:C:1283:GLY:HA3  | 1:C:1290:THR:HG23 | 1.82                     | 0.61              |
| 1:C:1381:ILE:HG12 | 1:C:1382:ASP:N    | 2.14                     | 0.61              |
| 2:D:1284:ARG:HG3  | 2:D:1285:GLU:H    | 1.64                     | 0.61              |
| 1:A:265:VAL:O     | 1:A:289:ASN:HA    | 2.01                     | 0.61              |
| 1:A:838:GLN:OE1   | 1:A:1528:VAL:HG12 | 2.01                     | 0.61              |
| 1:A:1431:GLY:O    | 1:A:1432:ILE:HD13 | 2.01                     | 0.61              |
| 2:B:508:LEU:HD12  | 2:B:509:HIS:N     | 2.14                     | 0.61              |
| 2:B:735:ASN:HB3   | 2:B:869:GLN:HE22  | 1.65                     | 0.61              |
| 2:B:1429:LYS:N    | 2:B:1429:LYS:HE3  | 2.14                     | 0.61              |
| 2:B:1517:GLU:OE1  | 2:B:1517:GLU:HA   | 2.00                     | 0.61              |
| 1:C:455:ILE:HG22  | 1:C:456:ALA:H     | 1.66                     | 0.61              |
| 1:C:1641:SER:C    | 1:C:1643:THR:H    | 2.07                     | 0.61              |
| 2:D:261:ALA:N     | 2:D:285:ILE:HD11  | 2.15                     | 0.61              |
| 2:D:800:ILE:HG23  | 2:D:801:CYS:N     | 2.14                     | 0.61              |
| 2:D:1399:ARG:HG2  | 2:D:1399:ARG:HH11 | 1.66                     | 0.61              |
| 1:A:1003:LEU:HD11 | 1:A:1286:SER:HA   | 1.82                     | 0.61              |
| 1:A:1033:ILE:HG22 | 1:A:1034:PHE:N    | 2.14                     | 0.61              |
| 2:B:365:TYR:HD1   | 2:B:395:THR:HG22  | 1.66                     | 0.61              |
| 2:B:816:ILE:HD13  | 2:B:896:ILE:HG22  | 1.83                     | 0.61              |
| 2:B:1534:GLN:HB2  | 2:B:1539:ILE:HD11 | 1.83                     | 0.61              |
| 1:C:161:LEU:HD11  | 1:C:185:PHE:CD1   | 2.36                     | 0.61              |
| 2:D:524:TYR:HE1   | 2:D:532:VAL:HG12  | 1.66                     | 0.61              |
| 2:D:1285:GLU:O    | 2:D:1287:PRO:HD3  | 2.01                     | 0.61              |
| 1:A:238:ILE:HG12  | 1:A:246:PHE:CE1   | 2.35                     | 0.60              |
| 1:A:270:GLY:HA3   | 1:A:282:MET:HG3   | 1.82                     | 0.60              |
| 1:A:690:TYR:CE1   | 1:A:696:LYS:HD2   | 2.35                     | 0.60              |
| 1:A:797:TRP:HA    | 1:A:797:TRP:HE3   | 1.64                     | 0.60              |
| 1:A:804:ILE:HG22  | 1:A:809:ILE:HG13  | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:265:PHE:CE2   | 2:B:294:LEU:HB2   | 2.36                     | 0.60              |
| 1:A:180:ILE:HG21  | 1:A:599:TRP:CE3   | 2.36                     | 0.60              |
| 1:A:653:PHE:CD1   | 1:A:653:PHE:C     | 2.79                     | 0.60              |
| 1:A:1226:ARG:NH1  | 1:A:1266:TYR:HE1  | 1.99                     | 0.60              |
| 2:B:565:ILE:CD1   | 2:B:776:MET:HE3   | 2.30                     | 0.60              |
| 2:B:603:GLU:C     | 2:B:605:SER:H     | 2.09                     | 0.60              |
| 2:B:916:VAL:HG23  | 2:B:917:PRO:HD2   | 1.82                     | 0.60              |
| 1:C:532:GLN:HE21  | 1:C:807:THR:HB    | 1.67                     | 0.60              |
| 1:C:540:LEU:C     | 1:C:540:LEU:HD12  | 2.26                     | 0.60              |
| 1:C:591:ASN:HB3   | 1:C:785:GLN:HG3   | 1.82                     | 0.60              |
| 1:C:1176:LEU:HD21 | 1:C:1195:LEU:HD21 | 1.82                     | 0.60              |
| 2:D:963:ILE:HD11  | 2:D:1311:ILE:HG12 | 1.81                     | 0.60              |
| 2:B:423:GLU:N     | 2:B:423:GLU:OE2   | 2.33                     | 0.60              |
| 1:C:160:VAL:CG2   | 1:C:175:GLU:HB3   | 2.31                     | 0.60              |
| 1:C:640:LEU:H     | 1:C:644:ASN:CB    | 2.14                     | 0.60              |
| 1:C:742:ILE:O     | 1:C:742:ILE:HG13  | 2.01                     | 0.60              |
| 1:C:950:TYR:OH    | 1:C:1307:LEU:HD21 | 2.02                     | 0.60              |
| 1:C:1625:LEU:HB3  | 1:C:1636:ILE:HG22 | 1.83                     | 0.60              |
| 2:D:251:TYR:CE2   | 2:D:257:VAL:HG22  | 2.36                     | 0.60              |
| 1:A:84:ILE:O      | 1:A:84:ILE:HD12   | 2.01                     | 0.60              |
| 1:A:307:VAL:CG1   | 1:A:313:TYR:HB2   | 2.31                     | 0.60              |
| 1:A:1000:LEU:O    | 1:A:1001:THR:HG23 | 2.01                     | 0.60              |
| 1:A:1016:VAL:N    | 1:A:1017:PRO:CD   | 2.64                     | 0.60              |
| 1:A:1016:VAL:HG11 | 1:A:1291:ILE:HG13 | 1.82                     | 0.60              |
| 1:A:1127:ILE:CG1  | 1:A:1143:TYR:HE2  | 2.14                     | 0.60              |
| 1:A:1423:VAL:HG11 | 1:A:1496:TYR:CZ   | 2.36                     | 0.60              |
| 1:A:1479:ILE:HD13 | 1:A:1479:ILE:H    | 1.65                     | 0.60              |
| 2:B:165:PHE:CE2   | 2:B:199:ILE:HD11  | 2.35                     | 0.60              |
| 2:B:1429:LYS:HE3  | 2:B:1429:LYS:H    | 1.66                     | 0.60              |
| 1:C:1593:GLU:HB2  | 1:C:1596:SER:OG   | 2.01                     | 0.60              |
| 2:D:263:VAL:HG23  | 2:D:283:ILE:HD13  | 1.83                     | 0.60              |
| 2:D:870:PHE:HB2   | 2:D:871:PRO:HD2   | 1.82                     | 0.60              |
| 1:A:930:VAL:HG22  | 1:A:931:PRO:HD2   | 1.84                     | 0.60              |
| 1:A:1112:GLN:HB2  | 1:A:1118:PHE:HE1  | 1.66                     | 0.60              |
| 1:C:39:ILE:CD1    | 1:C:104:LEU:HD21  | 2.31                     | 0.60              |
| 1:C:596:MET:CA    | 1:C:782:ARG:HG2   | 2.32                     | 0.60              |
| 2:D:322:THR:HG21  | 2:D:326:SER:OG    | 2.01                     | 0.60              |
| 1:A:502:LEU:HD22  | 1:A:509:ILE:HG21  | 1.83                     | 0.60              |
| 1:A:990:ALA:HB1   | 1:A:1000:LEU:HD11 | 1.82                     | 0.60              |
| 2:B:1387:LEU:HB2  | 2:B:1390:PHE:CD2  | 2.37                     | 0.60              |
| 1:C:1191:SER:O    | 1:C:1194:ALA:HB3  | 2.02                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1568:ILE:HG23 | 1:C:1577:TYR:CE1  | 2.36                     | 0.60              |
| 2:D:28:ILE:HD12   | 2:D:42:LEU:HD23   | 1.83                     | 0.60              |
| 2:D:315:TYR:CD1   | 2:D:315:TYR:C     | 2.78                     | 0.60              |
| 2:D:547:THR:HG22  | 2:D:548:LEU:H     | 1.67                     | 0.60              |
| 2:D:955:PRO:O     | 2:D:957:THR:HG23  | 2.00                     | 0.60              |
| 2:D:1273:LEU:C    | 2:D:1273:LEU:HD12 | 2.27                     | 0.60              |
| 1:A:355:ASN:HD22  | 1:A:355:ASN:N     | 2.00                     | 0.60              |
| 2:B:785:THR:OG1   | 2:B:786:THR:N     | 2.29                     | 0.60              |
| 1:C:311:SER:O     | 1:C:313:TYR:N     | 2.34                     | 0.60              |
| 1:C:457:TYR:C     | 1:C:457:TYR:CD2   | 2.79                     | 0.60              |
| 1:C:653:PHE:HD1   | 1:C:653:PHE:C     | 2.09                     | 0.60              |
| 1:A:1560:ALA:HB2  | 1:A:1620:MET:HG2  | 1.82                     | 0.60              |
| 2:B:469:ASN:ND2   | 2:B:469:ASN:C     | 2.57                     | 0.60              |
| 2:B:1611:PRO:HD2  | 2:B:1628:PHE:CE2  | 2.37                     | 0.60              |
| 1:C:653:PHE:C     | 1:C:653:PHE:CD1   | 2.80                     | 0.60              |
| 1:C:830:PRO:CG    | 1:C:1483:PHE:HZ   | 2.14                     | 0.60              |
| 1:C:1562:LYS:C    | 1:C:1563:VAL:HG13 | 2.26                     | 0.60              |
| 2:D:148:PHE:CE2   | 2:D:792:VAL:HG11  | 2.36                     | 0.60              |
| 1:A:455:ILE:HG22  | 1:A:456:ALA:H     | 1.67                     | 0.60              |
| 1:A:907:LEU:HD12  | 1:A:908:HIS:N     | 2.16                     | 0.60              |
| 1:C:308:LYS:HG3   | 1:C:309:GLU:H     | 1.66                     | 0.60              |
| 1:C:599:TRP:NE1   | 1:C:779:LEU:HA    | 2.16                     | 0.60              |
| 1:C:788:PHE:N     | 1:C:788:PHE:CD2   | 2.68                     | 0.60              |
| 1:C:844:THR:HG22  | 1:C:895:LEU:HB2   | 1.83                     | 0.60              |
| 1:C:1431:GLY:HA3  | 1:C:1483:PHE:CE1  | 2.37                     | 0.60              |
| 2:D:88:GLU:CD     | 2:D:155:SER:HB2   | 2.27                     | 0.60              |
| 2:D:603:GLU:C     | 2:D:605:SER:H     | 2.10                     | 0.60              |
| 2:D:615:GLN:HB2   | 2:D:616:ASN:HD22  | 1.66                     | 0.60              |
| 2:D:745:ILE:HG22  | 2:D:745:ILE:O     | 2.00                     | 0.60              |
| 1:A:1132:THR:H    | 1:A:1135:VAL:HB   | 1.66                     | 0.60              |
| 1:A:1563:VAL:HG21 | 1:A:1619:ILE:HD12 | 1.84                     | 0.60              |
| 2:B:31:ALA:O      | 2:B:119:VAL:HG12  | 2.02                     | 0.60              |
| 2:B:148:PHE:CE2   | 2:B:792:VAL:HG11  | 2.36                     | 0.60              |
| 1:C:44:TYR:CB     | 1:C:545:ILE:HD12  | 2.27                     | 0.60              |
| 1:C:177:ILE:HG22  | 1:C:178:ASP:H     | 1.67                     | 0.60              |
| 1:C:655:THR:O     | 1:C:657:ALA:N     | 2.35                     | 0.60              |
| 1:C:752:LEU:HD12  | 1:C:752:LEU:C     | 2.25                     | 0.60              |
| 1:C:875:HIS:HB2   | 2:D:901:GLN:NE2   | 2.17                     | 0.60              |
| 1:C:955:ARG:HG2   | 1:C:1350:THR:CG2  | 2.31                     | 0.60              |
| 1:C:1317:TYR:HD2  | 1:C:1344:ASP:HB3  | 1.67                     | 0.60              |
| 1:C:1431:GLY:CA   | 1:C:1483:PHE:HE1  | 2.15                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1483:PHE:O   | 1:C:1483:PHE:HD1  | 1.85                     | 0.60              |
| 1:A:492:TYR:CE2  | 1:A:493:ILE:HB    | 2.37                     | 0.59              |
| 1:A:1420:SER:O   | 1:A:1421:HIS:C    | 2.45                     | 0.59              |
| 1:A:1625:LEU:HB3 | 1:A:1636:ILE:HG22 | 1.84                     | 0.59              |
| 2:B:261:ALA:N    | 2:B:285:ILE:HD11  | 2.17                     | 0.59              |
| 2:B:745:ILE:O    | 2:B:745:ILE:HG22  | 2.01                     | 0.59              |
| 1:C:22:THR:HG21  | 1:C:656:ASN:O     | 2.02                     | 0.59              |
| 1:C:315:LEU:HD12 | 1:C:318:LEU:HG    | 1.83                     | 0.59              |
| 1:C:830:PRO:CG   | 1:C:1483:PHE:CZ   | 2.84                     | 0.59              |
| 1:C:934:VAL:CG2  | 1:C:1366:HIS:CD2  | 2.85                     | 0.59              |
| 1:C:999:ILE:HG13 | 1:C:1000:LEU:N    | 2.14                     | 0.59              |
| 2:D:494:ARG:HG3  | 2:D:494:ARG:NH1   | 2.14                     | 0.59              |
| 2:D:785:THR:OG1  | 2:D:786:THR:N     | 2.34                     | 0.59              |
| 2:D:1442:ILE:CA  | 2:D:1443:LEU:HD12 | 2.32                     | 0.59              |
| 1:A:864:GLY:HA3  | 1:A:907:LEU:HD23  | 1.84                     | 0.59              |
| 1:A:993:SER:C    | 1:A:995:GLU:H     | 2.10                     | 0.59              |
| 2:B:478:TYR:O    | 2:B:478:TYR:CD1   | 2.55                     | 0.59              |
| 2:B:838:ASN:OD1  | 2:B:840:VAL:HG23  | 2.03                     | 0.59              |
| 1:C:470:THR:HG22 | 2:D:450:THR:HB    | 1.84                     | 0.59              |
| 1:C:1421:HIS:C   | 1:C:1421:HIS:CD2  | 2.78                     | 0.59              |
| 2:D:958:GLU:O    | 2:D:959:ILE:HG13  | 2.02                     | 0.59              |
| 1:A:128:ILE:HD11 | 1:A:215:ALA:N     | 2.17                     | 0.59              |
| 1:A:219:VAL:O    | 1:A:219:VAL:HG12  | 2.00                     | 0.59              |
| 1:A:243:PHE:O    | 1:A:303:SER:HB2   | 2.02                     | 0.59              |
| 1:A:1252:ALA:O   | 1:A:1253:TYR:C    | 2.46                     | 0.59              |
| 1:A:1377:PHE:CE1 | 1:A:1408:TYR:HD1  | 2.21                     | 0.59              |
| 1:A:1434:ALA:HA  | 1:A:1479:ILE:HG22 | 1.83                     | 0.59              |
| 2:B:315:TYR:CD1  | 2:B:315:TYR:O     | 2.55                     | 0.59              |
| 1:C:628:GLU:HA   | 1:C:630:SER:OG    | 2.01                     | 0.59              |
| 1:C:790:LEU:HD12 | 1:C:790:LEU:H     | 1.66                     | 0.59              |
| 1:C:968:VAL:HG23 | 1:C:971:THR:HG21  | 1.83                     | 0.59              |
| 1:C:1090:ASN:C   | 1:C:1092:TYR:H    | 2.11                     | 0.59              |
| 1:A:367:ILE:HD13 | 1:A:466:TYR:CD2   | 2.38                     | 0.59              |
| 1:A:430:VAL:HG22 | 1:A:455:ILE:HG23  | 1.83                     | 0.59              |
| 1:A:977:LEU:HD13 | 1:A:977:LEU:C     | 2.27                     | 0.59              |
| 1:A:1013:MET:SD  | 1:A:1016:VAL:HG21 | 2.42                     | 0.59              |
| 1:A:1090:ASN:C   | 1:A:1092:TYR:H    | 2.11                     | 0.59              |
| 2:B:138:THR:O    | 2:B:139:PRO:C     | 2.44                     | 0.59              |
| 1:C:133:PRO:HD2  | 1:C:609:VAL:CG1   | 2.33                     | 0.59              |
| 1:C:373:VAL:O    | 1:C:417:VAL:HA    | 2.03                     | 0.59              |
| 1:C:457:TYR:C    | 1:C:457:TYR:HD2   | 2.09                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:492:TYR:CE2  | 1:C:493:ILE:HB    | 2.37                     | 0.59              |
| 1:C:987:ILE:HD11 | 1:C:1294:ILE:HG23 | 1.83                     | 0.59              |
| 1:C:1133:LEU:H   | 1:C:1133:LEU:HD12 | 1.67                     | 0.59              |
| 1:C:1431:GLY:HA3 | 1:C:1483:PHE:HE1  | 1.67                     | 0.59              |
| 2:D:133:ASP:HA   | 2:D:757:TRP:HZ3   | 1.67                     | 0.59              |
| 2:D:582:LYS:O    | 2:D:583:ALA:C     | 2.45                     | 0.59              |
| 2:D:1456:VAL:O   | 2:D:1456:VAL:HG12 | 2.01                     | 0.59              |
| 1:A:101:TYR:CZ   | 1:C:1305:LYS:HG3  | 2.38                     | 0.59              |
| 1:A:442:LEU:HD23 | 1:A:443:PRO:HD2   | 1.83                     | 0.59              |
| 1:A:968:VAL:HG23 | 1:A:971:THR:HG21  | 1.83                     | 0.59              |
| 1:A:974:LYS:O    | 1:A:1364:VAL:HG12 | 2.03                     | 0.59              |
| 2:B:857:CYS:H    | 2:B:887:LEU:HD21  | 1.67                     | 0.59              |
| 1:C:25:ILE:HB    | 1:C:654:LEU:O     | 2.03                     | 0.59              |
| 1:C:689:LYS:HG2  | 1:C:699:CYS:SG    | 2.41                     | 0.59              |
| 1:C:979:VAL:C    | 1:C:980:LYS:HG2   | 2.28                     | 0.59              |
| 1:C:1084:ARG:HD2 | 1:C:1154:LYS:HE3  | 1.83                     | 0.59              |
| 1:C:1186:PHE:HA  | 1:C:1250:THR:HG22 | 1.84                     | 0.59              |
| 2:D:355:LYS:N    | 2:D:355:LYS:HD2   | 2.17                     | 0.59              |
| 2:D:803:ALA:O    | 2:D:805:PRO:HD3   | 2.02                     | 0.59              |
| 2:D:857:CYS:H    | 2:D:887:LEU:HD21  | 1.67                     | 0.59              |
| 1:A:128:ILE:HG13 | 1:A:215:ALA:HB2   | 1.84                     | 0.59              |
| 1:A:595:GLY:HA2  | 1:A:782:ARG:NH1   | 2.18                     | 0.59              |
| 1:A:640:LEU:HB2  | 1:A:644:ASN:OD1   | 2.03                     | 0.59              |
| 1:A:1045:LEU:O   | 1:A:1046:LYS:C    | 2.45                     | 0.59              |
| 2:B:28:ILE:HG12  | 2:B:628:LEU:HD13  | 1.83                     | 0.59              |
| 2:B:529:ASN:O    | 2:B:529:ASN:OD1   | 2.21                     | 0.59              |
| 2:B:1277:ILE:CG2 | 2:B:1290:TYR:HB2  | 2.32                     | 0.59              |
| 1:C:132:LYS:HZ1  | 1:C:139:GLN:HE22  | 1.50                     | 0.59              |
| 1:C:284:GLN:CG   | 1:C:310:LEU:HD22  | 2.32                     | 0.59              |
| 1:C:382:LEU:HD22 | 1:C:416:GLY:HA3   | 1.85                     | 0.59              |
| 1:C:504:LEU:HD21 | 1:C:651:LEU:CG    | 2.32                     | 0.59              |
| 1:C:993:SER:C    | 1:C:995:GLU:H     | 2.11                     | 0.59              |
| 1:C:1623:GLU:HB2 | 1:C:1638:PRO:CG   | 2.33                     | 0.59              |
| 2:D:159:LYS:HD3  | 2:D:180:LEU:HD12  | 1.85                     | 0.59              |
| 2:D:202:LYS:HG3  | 2:D:203:TYR:N     | 2.18                     | 0.59              |
| 2:D:257:VAL:CG1  | 2:D:258:GLU:N     | 2.65                     | 0.59              |
| 2:D:786:THR:OG1  | 2:D:809:ARG:HG3   | 2.03                     | 0.59              |
| 2:D:1534:GLN:HB2 | 2:D:1539:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:23:TYR:O     | 1:A:23:TYR:HD1    | 1.84                     | 0.59              |
| 1:A:591:ASN:HB3  | 1:A:785:GLN:HG3   | 1.83                     | 0.59              |
| 1:A:1429:PRO:HB2 | 1:A:1432:ILE:HG13 | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1423:VAL:HG11 | 1:C:1496:TYR:CZ   | 2.36                     | 0.59              |
| 2:D:376:HIS:O     | 2:D:378:PRO:HD3   | 2.02                     | 0.59              |
| 1:A:1431:GLY:CA   | 1:A:1483:PHE:HE1  | 2.16                     | 0.59              |
| 2:B:856:PHE:CD1   | 2:B:884:ILE:HD11  | 2.37                     | 0.59              |
| 2:B:965:ILE:HG13  | 2:B:1301:ARG:HB2  | 1.85                     | 0.59              |
| 2:B:1610:TRP:CA   | 2:B:1628:PHE:HE2  | 2.12                     | 0.59              |
| 1:C:156:LYS:HD2   | 1:C:156:LYS:C     | 2.27                     | 0.59              |
| 1:C:265:VAL:O     | 1:C:289:ASN:HA    | 2.03                     | 0.59              |
| 1:C:488:PRO:HG3   | 1:C:499:TYR:OH    | 2.02                     | 0.59              |
| 1:C:1627:ILE:O    | 1:C:1627:ILE:CG1  | 2.50                     | 0.59              |
| 1:A:1012:LEU:HD13 | 1:A:1081:PHE:CD2  | 2.37                     | 0.59              |
| 1:A:1083:LEU:CD2  | 1:A:1104:LEU:HD21 | 2.33                     | 0.59              |
| 1:A:1229:LYS:NZ   | 1:A:1240:PRO:HD2  | 2.16                     | 0.59              |
| 2:B:347:PHE:O     | 2:B:349:LYS:N     | 2.36                     | 0.59              |
| 2:B:485:ASN:OD1   | 2:B:486:LYS:HD2   | 2.03                     | 0.59              |
| 1:C:430:VAL:HG11  | 1:C:453:ARG:NH2   | 2.16                     | 0.59              |
| 1:C:465:LEU:HD12  | 1:C:488:PRO:HA    | 1.85                     | 0.59              |
| 1:C:632:LEU:HD23  | 1:C:632:LEU:N     | 2.17                     | 0.59              |
| 2:D:54:LEU:N      | 2:D:54:LEU:HD23   | 2.17                     | 0.59              |
| 2:D:243:PHE:CD1   | 2:D:314:LEU:HD23  | 2.38                     | 0.59              |
| 2:D:1284:ARG:HD2  | 2:D:1285:GLU:H    | 1.65                     | 0.59              |
| 1:A:25:ILE:H      | 1:A:655:THR:HG23  | 1.67                     | 0.59              |
| 1:A:39:ILE:CD1    | 1:A:104:LEU:HD21  | 2.32                     | 0.59              |
| 1:A:505:SER:OG    | 1:A:506:LYS:HD3   | 2.03                     | 0.59              |
| 1:A:753:HIS:O     | 1:A:754:MET:CB    | 2.49                     | 0.59              |
| 1:A:799:ILE:HG22  | 1:A:815:VAL:O     | 2.01                     | 0.59              |
| 1:A:1307:LEU:HD22 | 1:A:1307:LEU:H    | 1.68                     | 0.59              |
| 1:A:1451:THR:O    | 1:A:1452:ASP:CB   | 2.51                     | 0.59              |
| 1:A:1576:LYS:HG2  | 1:A:1601:ILE:CG2  | 2.32                     | 0.59              |
| 2:B:26:THR:HG22   | 2:B:630:THR:HG22  | 1.85                     | 0.59              |
| 1:C:99:VAL:HG22   | 1:C:100:SER:O     | 2.02                     | 0.59              |
| 1:C:270:GLY:HA3   | 1:C:282:MET:HG3   | 1.84                     | 0.59              |
| 1:C:286:ALA:O     | 1:C:287:MET:C     | 2.46                     | 0.59              |
| 1:C:505:SER:OG    | 1:C:506:LYS:HD3   | 2.02                     | 0.59              |
| 1:C:653:PHE:O     | 1:C:653:PHE:CD1   | 2.48                     | 0.59              |
| 1:C:949:ILE:O     | 1:C:949:ILE:HG22  | 2.03                     | 0.59              |
| 2:D:104:VAL:HG22  | 2:D:105:VAL:N     | 2.17                     | 0.59              |
| 1:A:571:LEU:HA    | 1:A:593:ALA:O     | 2.04                     | 0.58              |
| 1:A:790:LEU:H     | 1:A:790:LEU:HD12  | 1.67                     | 0.58              |
| 1:A:833:VAL:O     | 1:A:929:VAL:HA    | 2.02                     | 0.58              |
| 1:A:1139:GLU:O    | 1:A:1140:ASN:C    | 2.45                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:247:ILE:CD1   | 2:B:318:VAL:HG21  | 2.33                     | 0.58              |
| 2:B:299:PHE:HE1   | 2:B:303:PHE:CD2   | 2.20                     | 0.58              |
| 2:B:401:ASN:C     | 2:B:402:ILE:HD13  | 2.28                     | 0.58              |
| 1:C:23:TYR:O      | 1:C:23:TYR:HD1    | 1.86                     | 0.58              |
| 1:C:502:LEU:HD22  | 1:C:509:ILE:HG21  | 1.85                     | 0.58              |
| 1:C:1226:ARG:NH1  | 1:C:1266:TYR:HE1  | 2.00                     | 0.58              |
| 1:C:1446:VAL:O    | 1:C:1446:VAL:HG12 | 2.01                     | 0.58              |
| 2:D:35:THR:HB     | 2:D:91:ALA:HB2    | 1.84                     | 0.58              |
| 2:D:39:GLU:O      | 2:D:87:ILE:HD12   | 2.03                     | 0.58              |
| 2:D:47:GLY:O      | 2:D:48:ASP:HB2    | 2.02                     | 0.58              |
| 2:D:745:ILE:CG2   | 2:D:745:ILE:O     | 2.51                     | 0.58              |
| 1:A:87:ILE:N      | 1:A:87:ILE:CD1    | 2.63                     | 0.58              |
| 1:A:125:PHE:CD1   | 1:A:627:LEU:HD21  | 2.38                     | 0.58              |
| 1:A:628:GLU:C     | 1:A:630:SER:N     | 2.57                     | 0.58              |
| 1:A:1180:LEU:CD2  | 1:A:1208:ILE:HG12 | 2.33                     | 0.58              |
| 1:A:1232:LEU:O    | 1:A:1233:GLN:HB3  | 2.02                     | 0.58              |
| 1:A:1381:ILE:HG12 | 1:A:1382:ASP:N    | 2.16                     | 0.58              |
| 1:A:1560:ALA:O    | 1:A:1585:TYR:HD2  | 1.86                     | 0.58              |
| 2:B:137:TYR:HB2   | 2:B:216:VAL:CG2   | 2.33                     | 0.58              |
| 2:B:844:ILE:O     | 2:B:871:PRO:HA    | 2.04                     | 0.58              |
| 1:C:128:ILE:HD11  | 1:C:215:ALA:N     | 2.18                     | 0.58              |
| 1:C:503:ILE:HB    | 1:C:511:HIS:HB2   | 1.85                     | 0.58              |
| 1:C:1204:GLN:O    | 1:C:1208:ILE:HG13 | 2.03                     | 0.58              |
| 1:C:1305:LYS:O    | 1:C:1307:LEU:HD13 | 2.02                     | 0.58              |
| 2:D:266:GLY:O     | 2:D:314:LEU:HD12  | 2.03                     | 0.58              |
| 2:D:478:TYR:O     | 2:D:478:TYR:CD1   | 2.56                     | 0.58              |
| 2:D:950:LEU:HD22  | 2:D:1329:TYR:CE1  | 2.37                     | 0.58              |
| 2:D:1620:GLU:HG2  | 2:D:1621:PHE:CE2  | 2.38                     | 0.58              |
| 1:A:625:GLN:HG2   | 1:A:626:PHE:H     | 1.68                     | 0.58              |
| 2:B:266:GLY:O     | 2:B:314:LEU:HD12  | 2.02                     | 0.58              |
| 2:B:748:ARG:HH12  | 2:B:784:ILE:HG12  | 1.68                     | 0.58              |
| 2:B:891:LEU:CB    | 2:B:912:LYS:HD3   | 2.31                     | 0.58              |
| 1:C:171:VAL:HG13  | 1:C:1054:LEU:HD21 | 1.84                     | 0.58              |
| 1:C:355:ASN:HD22  | 1:C:355:ASN:N     | 2.02                     | 0.58              |
| 1:C:833:VAL:O     | 1:C:929:VAL:HA    | 2.02                     | 0.58              |
| 1:C:1164:ILE:O    | 1:C:1165:ASP:C    | 2.41                     | 0.58              |
| 2:D:384:PHE:CD1   | 2:D:400:LEU:HG    | 2.38                     | 0.58              |
| 2:D:1527:LYS:HE2  | 2:D:1578:ASN:OD1  | 2.03                     | 0.58              |
| 1:A:573:VAL:HG12  | 1:A:592:MET:HG2   | 1.84                     | 0.58              |
| 1:A:689:LYS:HG2   | 1:A:699:CYS:SG    | 2.43                     | 0.58              |
| 1:A:734:VAL:O     | 1:A:737:GLN:HB2   | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:830:PRO:CG    | 1:A:1483:PHE:CZ   | 2.86                     | 0.58              |
| 1:A:1573:VAL:C    | 1:A:1603:LYS:HD2  | 2.27                     | 0.58              |
| 2:B:39:GLU:O      | 2:B:87:ILE:HD12   | 2.03                     | 0.58              |
| 2:B:69:PHE:CG     | 2:B:87:ILE:HG22   | 2.38                     | 0.58              |
| 2:B:133:ASP:HA    | 2:B:757:TRP:HZ3   | 1.68                     | 0.58              |
| 2:B:476:ILE:HD11  | 2:B:524:TYR:HB2   | 1.86                     | 0.58              |
| 2:B:870:PHE:HB2   | 2:B:871:PRO:HD2   | 1.85                     | 0.58              |
| 2:B:953:ARG:CG    | 2:B:954:VAL:N     | 2.67                     | 0.58              |
| 2:B:1273:LEU:HD12 | 2:B:1273:LEU:C    | 2.29                     | 0.58              |
| 2:B:1442:ILE:CA   | 2:B:1443:LEU:HD12 | 2.34                     | 0.58              |
| 2:B:1475:ASP:OD1  | 2:B:1475:ASP:N    | 2.27                     | 0.58              |
| 1:C:375:VAL:HG11  | 1:C:386:VAL:HG11  | 1.85                     | 0.58              |
| 1:C:862:VAL:HB    | 1:C:865:ILE:HD11  | 1.86                     | 0.58              |
| 1:C:980:LYS:HD3   | 1:C:986:GLU:HA    | 1.86                     | 0.58              |
| 1:C:1493:PHE:CD1  | 1:C:1493:PHE:C    | 2.79                     | 0.58              |
| 2:D:172:LEU:HD12  | 2:D:173:VAL:H     | 1.67                     | 0.58              |
| 2:D:1371:TYR:CG   | 2:D:1377:SER:HB3  | 2.38                     | 0.58              |
| 1:A:117:MET:HB2   | 1:A:118:PRO:CD    | 2.33                     | 0.58              |
| 1:A:292:LEU:HD13  | 1:A:296:ILE:O     | 2.03                     | 0.58              |
| 1:A:308:LYS:HG3   | 1:A:309:GLU:N     | 2.19                     | 0.58              |
| 1:A:469:TRP:N     | 1:A:469:TRP:HE3   | 2.01                     | 0.58              |
| 1:A:1493:PHE:C    | 1:A:1493:PHE:CD1  | 2.79                     | 0.58              |
| 2:B:606:ASP:OD1   | 2:B:606:ASP:O     | 2.21                     | 0.58              |
| 2:B:885:VAL:O     | 2:B:885:VAL:HG23  | 2.01                     | 0.58              |
| 1:C:23:TYR:CD1    | 1:C:655:THR:HB    | 2.38                     | 0.58              |
| 1:C:84:ILE:HD12   | 1:C:84:ILE:O      | 2.03                     | 0.58              |
| 1:C:640:LEU:HB2   | 1:C:644:ASN:OD1   | 2.04                     | 0.58              |
| 1:C:977:LEU:HA    | 1:C:1361:VAL:CG1  | 2.34                     | 0.58              |
| 1:C:1000:LEU:O    | 1:C:1001:THR:HG23 | 2.03                     | 0.58              |
| 2:D:138:THR:O     | 2:D:139:PRO:C     | 2.43                     | 0.58              |
| 2:D:261:ALA:CB    | 2:D:285:ILE:HD11  | 2.33                     | 0.58              |
| 2:D:476:ILE:HD11  | 2:D:524:TYR:CG    | 2.38                     | 0.58              |
| 2:D:628:LEU:HD12  | 2:D:629:THR:H     | 1.69                     | 0.58              |
| 1:A:640:LEU:H     | 1:A:644:ASN:CB    | 2.16                     | 0.58              |
| 1:A:698:CYS:C     | 1:A:700:TYR:H     | 2.12                     | 0.58              |
| 1:A:854:GLN:H     | 1:A:854:GLN:CD    | 2.11                     | 0.58              |
| 2:B:100:GLN:HG3   | 2:B:101:ASN:N     | 2.19                     | 0.58              |
| 2:B:263:VAL:HG13  | 2:B:318:VAL:HG23  | 1.85                     | 0.58              |
| 2:B:953:ARG:HA    | 2:B:1330:ASN:O    | 2.03                     | 0.58              |
| 2:B:1620:GLU:HG2  | 2:B:1621:PHE:CE2  | 2.39                     | 0.58              |
| 1:C:502:LEU:HB2   | 1:C:541:LEU:HD23  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:550:GLN:O     | 1:C:550:GLN:HG2   | 2.03                     | 0.58              |
| 1:C:576:SER:HB2   | 1:C:589:SER:CB    | 2.33                     | 0.58              |
| 1:C:799:ILE:HG22  | 1:C:815:VAL:O     | 2.04                     | 0.58              |
| 1:C:1381:ILE:HD12 | 1:C:1493:PHE:CD2  | 2.38                     | 0.58              |
| 1:C:1576:LYS:HG2  | 1:C:1601:ILE:CG2  | 2.33                     | 0.58              |
| 2:D:69:PHE:CG     | 2:D:87:ILE:HG22   | 2.38                     | 0.58              |
| 2:D:243:PHE:HD1   | 2:D:314:LEU:HD23  | 1.67                     | 0.58              |
| 2:D:866:TYR:CD2   | 2:D:866:TYR:C     | 2.82                     | 0.58              |
| 2:D:1611:PRO:HD2  | 2:D:1628:PHE:CE2  | 2.39                     | 0.58              |
| 1:A:1012:LEU:O    | 1:A:1015:VAL:HG12 | 2.04                     | 0.58              |
| 1:A:1147:PHE:O    | 1:A:1150:ILE:HB   | 2.04                     | 0.58              |
| 2:B:243:PHE:CD1   | 2:B:314:LEU:HD23  | 2.38                     | 0.58              |
| 2:B:806:TYR:CD1   | 2:B:806:TYR:C     | 2.81                     | 0.58              |
| 1:C:243:PHE:O     | 1:C:303:SER:HB2   | 2.04                     | 0.58              |
| 1:C:469:TRP:N     | 1:C:469:TRP:HE3   | 2.01                     | 0.58              |
| 1:C:493:ILE:HG21  | 1:C:495:LYS:HB2   | 1.85                     | 0.58              |
| 1:C:1628:LYS:HB3  | 1:C:1633:PHE:CD1  | 2.38                     | 0.58              |
| 1:C:1671:ILE:HG13 | 1:C:1671:ILE:O    | 2.02                     | 0.58              |
| 2:D:628:LEU:HD12  | 2:D:629:THR:N     | 2.19                     | 0.58              |
| 1:A:77:ASN:HD22   | 1:A:81:ASN:HB2    | 1.68                     | 0.58              |
| 1:A:113:LYS:CG    | 1:A:114:SER:H     | 2.14                     | 0.58              |
| 1:A:357:VAL:O     | 1:A:359:THR:HG22  | 2.04                     | 0.58              |
| 1:A:705:VAL:HA    | 1:A:739:ARG:NH1   | 2.18                     | 0.58              |
| 1:A:857:VAL:CG2   | 1:A:884:VAL:HG21  | 2.31                     | 0.58              |
| 1:A:970:LYS:C     | 1:A:971:THR:HG23  | 2.29                     | 0.58              |
| 1:A:1176:LEU:HD21 | 1:A:1195:LEU:HD21 | 1.84                     | 0.58              |
| 2:B:263:VAL:HG23  | 2:B:283:ILE:HD13  | 1.84                     | 0.58              |
| 1:C:177:ILE:HG22  | 1:C:178:ASP:N     | 2.19                     | 0.58              |
| 1:C:367:ILE:HD13  | 1:C:466:TYR:CD2   | 2.39                     | 0.58              |
| 1:C:625:GLN:HG2   | 1:C:626:PHE:H     | 1.68                     | 0.58              |
| 1:C:1474:CYS:HB3  | 1:C:1476:ARG:HH12 | 1.67                     | 0.58              |
| 2:D:221:LEU:HD11  | 2:D:753:LYS:CG    | 2.29                     | 0.58              |
| 2:D:476:ILE:HG12  | 2:D:524:TYR:HD2   | 1.66                     | 0.58              |
| 2:D:963:ILE:HG12  | 2:D:1325:ILE:HG12 | 1.86                     | 0.58              |
| 1:A:23:TYR:HA     | 1:A:43:VAL:HA     | 1.84                     | 0.58              |
| 1:A:243:PHE:CZ    | 1:A:316:GLU:HB3   | 2.39                     | 0.58              |
| 1:A:382:LEU:HD22  | 1:A:416:GLY:HA3   | 1.86                     | 0.58              |
| 1:A:1143:TYR:CE1  | 1:A:1147:PHE:HB2  | 2.38                     | 0.58              |
| 2:B:107:GLN:HG3   | 2:B:116:GLU:HG3   | 1.86                     | 0.58              |
| 2:B:628:LEU:HD12  | 2:B:629:THR:H     | 1.69                     | 0.58              |
| 2:B:738:GLY:O     | 2:B:901:GLN:HA    | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1284:ARG:CD   | 2:B:1285:GLU:N    | 2.60                     | 0.58              |
| 2:B:1365:LEU:HD12 | 2:B:1366:LYS:N    | 2.18                     | 0.58              |
| 1:C:31:PHE:HB2    | 1:C:119:ILE:HG22  | 1.86                     | 0.58              |
| 2:D:179:ASP:OD1   | 2:D:181:ASN:HB2   | 2.03                     | 0.58              |
| 1:A:307:VAL:HG13  | 1:A:313:TYR:HB2   | 1.84                     | 0.58              |
| 1:A:1084:ARG:HD2  | 1:A:1154:LYS:HE3  | 1.85                     | 0.58              |
| 1:A:1568:ILE:HG12 | 1:A:1577:TYR:CE1  | 2.39                     | 0.58              |
| 2:B:130:ILE:HB    | 2:B:212:ALA:HB2   | 1.86                     | 0.58              |
| 2:B:315:TYR:C     | 2:B:315:TYR:HD1   | 2.12                     | 0.58              |
| 2:B:339:VAL:HG23  | 2:B:341:SER:N     | 2.18                     | 0.58              |
| 2:B:628:LEU:HD12  | 2:B:629:THR:N     | 2.19                     | 0.58              |
| 1:C:1033:ILE:CG2  | 1:C:1034:PHE:CD1  | 2.87                     | 0.58              |
| 1:C:1570:VAL:HG22 | 1:C:1575:VAL:HG22 | 1.85                     | 0.58              |
| 2:D:247:ILE:CD1   | 2:D:318:VAL:HG21  | 2.34                     | 0.58              |
| 2:D:342:PRO:HG2   | 2:D:420:LEU:HD13  | 1.84                     | 0.58              |
| 2:D:1371:TYR:CD1  | 2:D:1377:SER:HB3  | 2.39                     | 0.58              |
| 1:A:224:LEU:CD2   | 1:A:225:PRO:HD2   | 2.24                     | 0.57              |
| 1:A:395:ILE:HD12  | 1:A:395:ILE:O     | 2.04                     | 0.57              |
| 2:B:88:GLU:CD     | 2:B:155:SER:HB2   | 2.29                     | 0.57              |
| 2:B:476:ILE:HD11  | 2:B:524:TYR:CG    | 2.39                     | 0.57              |
| 2:B:1621:PHE:O    | 2:B:1622:GLN:C    | 2.47                     | 0.57              |
| 1:C:251:LYS:HG2   | 1:C:296:ILE:HD11  | 1.86                     | 0.57              |
| 1:C:1300:TYR:C    | 1:C:1300:TYR:CD2  | 2.82                     | 0.57              |
| 2:D:789:VAL:C     | 2:D:790:LEU:HD12  | 2.28                     | 0.57              |
| 2:D:825:VAL:HB    | 2:D:828:GLU:OE2   | 2.04                     | 0.57              |
| 2:D:861:THR:O     | 2:D:863:GLY:N     | 2.37                     | 0.57              |
| 2:D:1365:LEU:HD12 | 2:D:1366:LYS:N    | 2.18                     | 0.57              |
| 1:A:576:SER:HB2   | 1:A:589:SER:CB    | 2.34                     | 0.57              |
| 1:A:1033:ILE:HD13 | 1:A:1333:PHE:HZ   | 1.69                     | 0.57              |
| 1:A:1574:PHE:HA   | 1:A:1603:LYS:CD   | 2.35                     | 0.57              |
| 1:A:1584:ILE:O    | 1:A:1585:TYR:HB3  | 2.02                     | 0.57              |
| 2:B:243:PHE:HD1   | 2:B:314:LEU:HD23  | 1.68                     | 0.57              |
| 1:C:117:MET:HB2   | 1:C:118:PRO:CD    | 2.34                     | 0.57              |
| 1:C:128:ILE:HG13  | 1:C:215:ALA:HB2   | 1.84                     | 0.57              |
| 1:C:316:GLU:O     | 1:C:349:LEU:HD21  | 2.04                     | 0.57              |
| 1:C:862:VAL:HB    | 1:C:865:ILE:CD1   | 2.34                     | 0.57              |
| 1:C:903:LEU:HD22  | 1:C:903:LEU:N     | 2.19                     | 0.57              |
| 1:C:969:PRO:HG3   | 1:C:1601:ILE:CD1  | 2.32                     | 0.57              |
| 1:C:1573:VAL:C    | 1:C:1603:LYS:HD2  | 2.29                     | 0.57              |
| 2:D:100:GLN:HG3   | 2:D:101:ASN:N     | 2.18                     | 0.57              |
| 1:A:24:VAL:HG11   | 1:A:543:TYR:CE2   | 2.39                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:101:TYR:CE1   | 1:A:116:ARG:NH2   | 2.73                     | 0.57              |
| 1:A:161:LEU:HD11  | 1:A:185:PHE:CD1   | 2.40                     | 0.57              |
| 1:A:502:LEU:HB2   | 1:A:541:LEU:HD23  | 1.86                     | 0.57              |
| 1:A:1227:PHE:HD2  | 1:A:1273:TRP:NE1  | 2.02                     | 0.57              |
| 2:B:352:LYS:HG3   | 2:B:430:MET:HE1   | 1.86                     | 0.57              |
| 2:B:953:ARG:HG2   | 2:B:954:VAL:H     | 1.69                     | 0.57              |
| 1:C:469:TRP:N     | 1:C:469:TRP:CE3   | 2.72                     | 0.57              |
| 1:C:696:LYS:HZ3   | 1:C:759:PRO:HG2   | 1.69                     | 0.57              |
| 1:C:1147:PHE:O    | 1:C:1150:ILE:HB   | 2.05                     | 0.57              |
| 2:D:23:ALA:HB3    | 2:D:528:ASN:HD22  | 1.67                     | 0.57              |
| 2:D:841:ASN:O     | 2:D:842:GLU:C     | 2.47                     | 0.57              |
| 2:D:1573:LEU:HB3  | 2:D:1575:LEU:HD23 | 1.86                     | 0.57              |
| 1:A:614:ARG:H     | 1:A:614:ARG:NE    | 2.01                     | 0.57              |
| 1:A:1019:PHE:HD2  | 1:A:1020:TYR:N    | 2.03                     | 0.57              |
| 2:B:885:VAL:HG23  | 2:B:887:LEU:HD21  | 1.86                     | 0.57              |
| 2:B:961:THR:HG22  | 2:B:1327:THR:CG2  | 2.34                     | 0.57              |
| 1:C:249:THR:HG23  | 1:C:298:GLN:HE21  | 1.69                     | 0.57              |
| 1:C:855:PHE:C     | 1:C:855:PHE:CD1   | 2.83                     | 0.57              |
| 1:C:1132:THR:H    | 1:C:1135:VAL:HB   | 1.69                     | 0.57              |
| 1:C:1227:PHE:HD2  | 1:C:1273:TRP:NE1  | 2.02                     | 0.57              |
| 1:A:59:TYR:CZ     | 1:A:99:VAL:HG21   | 2.39                     | 0.57              |
| 1:A:238:ILE:HG23  | 1:A:242:ASN:ND2   | 2.15                     | 0.57              |
| 1:A:250:ILE:HD11  | 1:A:265:VAL:CG1   | 2.32                     | 0.57              |
| 1:A:365:PRO:HG2   | 1:A:464:TYR:HE2   | 1.66                     | 0.57              |
| 1:A:692:HIS:HA    | 1:A:696:LYS:HD3   | 1.85                     | 0.57              |
| 1:A:844:THR:HG22  | 1:A:895:LEU:HB2   | 1.85                     | 0.57              |
| 1:A:1562:LYS:HD3  | 1:A:1664:LEU:HD21 | 1.87                     | 0.57              |
| 2:B:1426:TYR:N    | 2:B:1426:TYR:CD2  | 2.72                     | 0.57              |
| 1:C:231:ILE:O     | 1:C:231:ILE:HG12  | 2.02                     | 0.57              |
| 1:C:292:LEU:HD13  | 1:C:296:ILE:O     | 2.05                     | 0.57              |
| 1:C:734:VAL:O     | 1:C:737:GLN:HB2   | 2.05                     | 0.57              |
| 1:C:938:SER:C     | 1:C:940:SER:N     | 2.60                     | 0.57              |
| 1:C:1227:PHE:HB2  | 1:C:1251:THR:HG21 | 1.86                     | 0.57              |
| 1:C:1568:ILE:HG12 | 1:C:1577:TYR:CE1  | 2.39                     | 0.57              |
| 2:D:315:TYR:CD1   | 2:D:315:TYR:O     | 2.58                     | 0.57              |
| 1:A:156:LYS:HD2   | 1:A:156:LYS:C     | 2.29                     | 0.57              |
| 1:A:1507:MET:HG3  | 1:A:1508:PHE:O    | 2.04                     | 0.57              |
| 2:B:257:VAL:CG1   | 2:B:258:GLU:N     | 2.67                     | 0.57              |
| 2:B:944:VAL:HG22  | 2:B:1312:THR:OG1  | 2.04                     | 0.57              |
| 2:B:1563:TYR:HB3  | 2:B:1601:ILE:HD11 | 1.85                     | 0.57              |
| 1:C:395:ILE:HD12  | 1:C:395:ILE:O     | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:461:SER:O     | 1:C:462:GLN:HB2   | 2.02                     | 0.57              |
| 1:C:595:GLY:HA2   | 1:C:782:ARG:NH1   | 2.20                     | 0.57              |
| 2:D:384:PHE:CE1   | 2:D:400:LEU:HG    | 2.39                     | 0.57              |
| 2:D:953:ARG:CG    | 2:D:954:VAL:N     | 2.68                     | 0.57              |
| 1:A:308:LYS:HG3   | 1:A:309:GLU:H     | 1.69                     | 0.57              |
| 1:A:315:LEU:CD1   | 1:A:318:LEU:HG    | 2.34                     | 0.57              |
| 1:A:493:ILE:HG21  | 1:A:495:LYS:HB2   | 1.85                     | 0.57              |
| 1:A:742:ILE:O     | 1:A:742:ILE:HG13  | 2.04                     | 0.57              |
| 1:A:938:SER:C     | 1:A:940:SER:N     | 2.57                     | 0.57              |
| 1:A:980:LYS:HD3   | 1:A:986:GLU:HA    | 1.87                     | 0.57              |
| 1:A:1562:LYS:C    | 1:A:1563:VAL:HG13 | 2.28                     | 0.57              |
| 2:B:582:LYS:O     | 2:B:583:ALA:C     | 2.46                     | 0.57              |
| 2:B:640:SER:O     | 2:B:641:ALA:HB2   | 2.04                     | 0.57              |
| 2:B:841:ASN:O     | 2:B:842:GLU:C     | 2.48                     | 0.57              |
| 1:C:161:LEU:HD11  | 1:C:185:PHE:CG    | 2.39                     | 0.57              |
| 1:C:1333:PHE:O    | 1:C:1334:LEU:CB   | 2.52                     | 0.57              |
| 2:D:226:VAL:HG21  | 2:D:320:VAL:HG11  | 1.87                     | 0.57              |
| 2:D:953:ARG:CZ    | 2:D:959:ILE:HD11  | 2.35                     | 0.57              |
| 2:D:1424:ILE:HD13 | 2:D:1424:ILE:N    | 2.12                     | 0.57              |
| 1:A:470:THR:HG22  | 2:B:450:THR:CG2   | 2.30                     | 0.57              |
| 1:A:1127:ILE:HD11 | 1:A:1143:TYR:HD2  | 1.70                     | 0.57              |
| 1:A:1323:LEU:HD12 | 1:A:1324:HIS:N    | 2.18                     | 0.57              |
| 1:A:1570:VAL:O    | 1:A:1571:GLU:HG3  | 2.05                     | 0.57              |
| 2:B:462:VAL:CG1   | 2:B:506:MET:HE3   | 2.35                     | 0.57              |
| 2:B:793:SER:OG    | 2:B:801:CYS:HB3   | 2.04                     | 0.57              |
| 2:B:958:GLU:O     | 2:B:959:ILE:HG13  | 2.04                     | 0.57              |
| 2:B:963:ILE:HG12  | 2:B:1325:ILE:HG12 | 1.86                     | 0.57              |
| 1:C:422:LEU:HD12  | 1:C:422:LEU:H     | 1.67                     | 0.57              |
| 1:C:709:GLU:HB3   | 1:C:713:GLN:OE1   | 2.05                     | 0.57              |
| 1:C:1034:PHE:CE2  | 1:C:1041:GLU:HG2  | 2.40                     | 0.57              |
| 1:C:1450:PHE:HB3  | 1:C:1463:GLN:O    | 2.04                     | 0.57              |
| 2:D:197:TRP:CB    | 2:D:214:PHE:CE1   | 2.85                     | 0.57              |
| 2:D:200:VAL:O     | 2:D:200:VAL:HG23  | 2.04                     | 0.57              |
| 1:A:182:ILE:CG1   | 1:A:804:ILE:HD11  | 2.34                     | 0.57              |
| 1:A:469:TRP:N     | 1:A:469:TRP:CE3   | 2.73                     | 0.57              |
| 1:A:599:TRP:HE1   | 1:A:779:LEU:HD13  | 1.69                     | 0.57              |
| 1:A:830:PRO:CG    | 1:A:1483:PHE:HZ   | 2.16                     | 0.57              |
| 1:A:944:LEU:HD12  | 1:A:1313:ILE:CD1  | 2.33                     | 0.57              |
| 2:B:209:ASN:CG    | 3:B:2001:NAG:C7   | 2.78                     | 0.57              |
| 2:B:221:LEU:HD11  | 2:B:753:LYS:CG    | 2.31                     | 0.57              |
| 2:B:251:TYR:CE2   | 2:B:257:VAL:HG22  | 2.39                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:39:ILE:HG21   | 1:C:54:ILE:HD13   | 1.87                     | 0.57              |
| 1:C:516:GLU:OE1   | 1:C:516:GLU:N     | 2.38                     | 0.57              |
| 1:C:1053:MET:HE3  | 1:C:1086:LEU:HD22 | 1.86                     | 0.57              |
| 1:C:1084:ARG:CD   | 1:C:1154:LYS:HE3  | 2.35                     | 0.57              |
| 1:C:1352:PHE:CD2  | 1:C:1353:GLY:N    | 2.73                     | 0.57              |
| 1:C:1617:TYR:HA   | 1:C:1646:GLU:O    | 2.04                     | 0.57              |
| 2:D:263:VAL:HG13  | 2:D:318:VAL:HG23  | 1.85                     | 0.57              |
| 2:D:806:TYR:CD1   | 2:D:806:TYR:C     | 2.83                     | 0.57              |
| 2:D:953:ARG:HA    | 2:D:1330:ASN:O    | 2.04                     | 0.57              |
| 2:D:965:ILE:HG13  | 2:D:1301:ARG:HB2  | 1.87                     | 0.57              |
| 1:A:957:LYS:HD2   | 1:A:958:GLU:H     | 1.70                     | 0.57              |
| 1:A:1300:TYR:C    | 1:A:1300:TYR:CD2  | 2.83                     | 0.57              |
| 1:A:1421:HIS:CD2  | 1:A:1422:ALA:N    | 2.72                     | 0.57              |
| 1:A:1560:ALA:HB3  | 1:A:1585:TYR:HE2  | 1.68                     | 0.57              |
| 2:B:202:LYS:HG3   | 2:B:203:TYR:N     | 2.20                     | 0.57              |
| 2:B:766:PRO:HA    | 2:B:771:ILE:O     | 2.05                     | 0.57              |
| 2:B:825:VAL:HB    | 2:B:828:GLU:OE2   | 2.05                     | 0.57              |
| 2:B:872:ILE:HG22  | 2:B:878:ARG:HG3   | 1.87                     | 0.57              |
| 1:C:165:ASP:C     | 1:C:165:ASP:OD2   | 2.47                     | 0.57              |
| 1:C:957:LYS:HD2   | 1:C:958:GLU:H     | 1.69                     | 0.57              |
| 1:C:1166:THR:O    | 1:C:1170:LYS:HG2  | 2.05                     | 0.57              |
| 1:C:1488:LEU:HD12 | 1:C:1488:LEU:O    | 2.05                     | 0.57              |
| 2:D:756:LEU:HD22  | 2:D:778:PHE:CE1   | 2.40                     | 0.57              |
| 1:A:617:LYS:C     | 1:A:619:PRO:HD2   | 2.30                     | 0.56              |
| 1:A:632:LEU:N     | 1:A:632:LEU:HD23  | 2.19                     | 0.56              |
| 1:A:934:VAL:CG2   | 1:A:1366:HIS:CD2  | 2.88                     | 0.56              |
| 1:A:967:LEU:HD12  | 1:A:968:VAL:H     | 1.70                     | 0.56              |
| 2:B:1399:ARG:HG2  | 2:B:1399:ARG:HH11 | 1.70                     | 0.56              |
| 1:C:442:LEU:HD23  | 1:C:443:PRO:CD    | 2.35                     | 0.56              |
| 1:C:779:LEU:O     | 1:C:781:PRO:HD3   | 2.05                     | 0.56              |
| 1:C:869:GLU:O     | 1:C:871:PRO:HD3   | 2.05                     | 0.56              |
| 1:C:1551:THR:O    | 1:C:1557:ILE:HG13 | 2.05                     | 0.56              |
| 1:A:269:PHE:CG    | 1:A:301:PHE:CE1   | 2.92                     | 0.56              |
| 1:A:501:TYR:O     | 1:A:501:TYR:HD1   | 1.88                     | 0.56              |
| 1:A:949:ILE:O     | 1:A:950:TYR:CD1   | 2.58                     | 0.56              |
| 1:A:1081:PHE:O    | 1:A:1084:ARG:N    | 2.38                     | 0.56              |
| 2:B:745:ILE:CG2   | 2:B:745:ILE:O     | 2.53                     | 0.56              |
| 2:B:1512:ILE:O    | 2:B:1516:CYS:HB2  | 2.06                     | 0.56              |
| 1:C:224:LEU:HD22  | 1:C:225:PRO:CD    | 2.25                     | 0.56              |
| 1:C:539:ARG:NE    | 1:C:633:GLY:HA3   | 2.19                     | 0.56              |
| 1:C:1232:LEU:O    | 1:C:1233:GLN:HB3  | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1377:PHE:CE1  | 1:C:1408:TYR:HD1  | 2.23                     | 0.56              |
| 2:D:495:GLN:NE2   | 2:D:496:PRO:HD2   | 2.20                     | 0.56              |
| 2:D:1426:TYR:CD2  | 2:D:1426:TYR:N    | 2.73                     | 0.56              |
| 2:D:1621:PHE:O    | 2:D:1622:GLN:C    | 2.48                     | 0.56              |
| 1:A:39:ILE:HG21   | 1:A:54:ILE:HD13   | 1.87                     | 0.56              |
| 1:A:361:LEU:HD12  | 1:A:361:LEU:H     | 1.71                     | 0.56              |
| 1:A:696:LYS:HZ3   | 1:A:759:PRO:HG2   | 1.71                     | 0.56              |
| 1:A:869:GLU:O     | 1:A:871:PRO:HD3   | 2.05                     | 0.56              |
| 1:A:1227:PHE:CD2  | 1:A:1273:TRP:CE2  | 2.93                     | 0.56              |
| 2:B:23:ALA:HB3    | 2:B:528:ASN:HD22  | 1.70                     | 0.56              |
| 2:B:239:GLY:N     | 2:B:296:ARG:NH2   | 2.48                     | 0.56              |
| 2:B:556:ILE:H     | 2:B:556:ILE:CD1   | 1.99                     | 0.56              |
| 2:B:557:GLN:HE21  | 2:B:563:MET:HE3   | 1.70                     | 0.56              |
| 1:C:77:ASN:HD22   | 1:C:81:ASN:HB2    | 1.68                     | 0.56              |
| 1:C:87:ILE:N      | 1:C:87:ILE:CD1    | 2.64                     | 0.56              |
| 1:C:153:LYS:HB2   | 1:C:154:PRO:CD    | 2.31                     | 0.56              |
| 1:C:443:PRO:HD2   | 1:C:446:ASN:CB    | 2.33                     | 0.56              |
| 1:C:614:ARG:H     | 1:C:614:ARG:NE    | 2.03                     | 0.56              |
| 1:C:654:LEU:O     | 1:C:655:THR:CG2   | 2.53                     | 0.56              |
| 1:C:870:SER:C     | 1:C:872:VAL:H     | 2.13                     | 0.56              |
| 1:C:970:LYS:C     | 1:C:971:THR:HG23  | 2.30                     | 0.56              |
| 1:C:1150:ILE:HG22 | 1:C:1151:GLY:N    | 2.20                     | 0.56              |
| 1:C:1431:GLY:HA2  | 1:C:1483:PHE:CE1  | 2.39                     | 0.56              |
| 1:C:1561:TYR:CE1  | 1:C:1581:LEU:HD21 | 2.40                     | 0.56              |
| 2:D:165:PHE:CE2   | 2:D:199:ILE:HD11  | 2.39                     | 0.56              |
| 2:D:191:LEU:HD13  | 2:D:960:GLU:HB3   | 1.87                     | 0.56              |
| 2:D:237:ILE:HD11  | 2:D:309:LEU:CB    | 2.34                     | 0.56              |
| 2:D:804:GLU:OE1   | 2:D:805:PRO:HD2   | 2.05                     | 0.56              |
| 2:D:961:THR:HG22  | 2:D:1327:THR:CG2  | 2.35                     | 0.56              |
| 2:D:1346:ASN:O    | 2:D:1368:CYS:HB2  | 2.05                     | 0.56              |
| 2:B:376:HIS:O     | 2:B:378:PRO:HD3   | 2.06                     | 0.56              |
| 2:B:476:ILE:HG12  | 2:B:524:TYR:HD2   | 1.69                     | 0.56              |
| 2:B:803:ALA:O     | 2:B:805:PRO:HD3   | 2.05                     | 0.56              |
| 2:B:1573:LEU:HB3  | 2:B:1575:LEU:HD23 | 1.87                     | 0.56              |
| 1:C:73:LEU:HD23   | 1:C:73:LEU:H      | 1.71                     | 0.56              |
| 1:C:81:ASN:CG     | 1:C:82:SER:H      | 2.13                     | 0.56              |
| 1:C:565:GLU:HG3   | 1:C:624:PHE:CB    | 2.35                     | 0.56              |
| 1:C:803:GLY:O     | 1:C:810:CYS:CB    | 2.53                     | 0.56              |
| 1:C:1479:ILE:HD13 | 1:C:1479:ILE:H    | 1.70                     | 0.56              |
| 2:D:130:ILE:HB    | 2:D:212:ALA:HB2   | 1.88                     | 0.56              |
| 2:D:477:LYS:HD3   | 2:D:477:LYS:N     | 2.20                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:563:MET:HG3   | 2:D:780:LEU:CD2   | 2.35                     | 0.56              |
| 2:D:615:GLN:HB2   | 2:D:616:ASN:ND2   | 2.20                     | 0.56              |
| 2:D:885:VAL:HG23  | 2:D:885:VAL:O     | 2.05                     | 0.56              |
| 2:D:1491:ARG:HG3  | 2:D:1492:CYS:N    | 2.13                     | 0.56              |
| 2:D:1607:ILE:H    | 2:D:1607:ILE:CD1  | 2.11                     | 0.56              |
| 1:A:101:TYR:HE1   | 1:A:116:ARG:NH2   | 2.03                     | 0.56              |
| 1:A:116:ARG:HH21  | 1:C:1305:LYS:CB   | 2.17                     | 0.56              |
| 1:A:171:VAL:HG13  | 1:A:1054:LEU:HD21 | 1.86                     | 0.56              |
| 1:A:249:THR:HG23  | 1:A:298:GLN:HE21  | 1.71                     | 0.56              |
| 1:A:1049:LEU:HD11 | 1:A:1089:VAL:HG13 | 1.88                     | 0.56              |
| 1:A:1474:CYS:HB3  | 1:A:1476:ARG:HH12 | 1.69                     | 0.56              |
| 2:B:54:LEU:HD23   | 2:B:54:LEU:N      | 2.19                     | 0.56              |
| 2:B:234:PHE:C     | 2:B:234:PHE:HD1   | 2.14                     | 0.56              |
| 2:B:1387:LEU:HD12 | 2:B:1442:ILE:HD11 | 1.88                     | 0.56              |
| 1:C:539:ARG:NH2   | 1:C:634:CYS:N     | 2.49                     | 0.56              |
| 2:D:228:LEU:HD22  | 2:D:247:ILE:HG12  | 1.87                     | 0.56              |
| 2:D:299:PHE:HE1   | 2:D:303:PHE:CD2   | 2.23                     | 0.56              |
| 1:A:23:TYR:CD1    | 1:A:655:THR:HB    | 2.40                     | 0.56              |
| 1:A:1053:MET:CE   | 1:A:1086:LEU:HD22 | 2.34                     | 0.56              |
| 1:A:1403:VAL:HG22 | 1:A:1476:ARG:HB3  | 1.88                     | 0.56              |
| 1:A:1483:PHE:O    | 1:A:1483:PHE:HD1  | 1.88                     | 0.56              |
| 2:B:127:PHE:O     | 2:B:149:SER:HA    | 2.06                     | 0.56              |
| 1:C:535:VAL:HG23  | 1:C:536:PRO:CD    | 2.27                     | 0.56              |
| 1:C:641:ASN:O     | 1:C:642:ASN:C     | 2.49                     | 0.56              |
| 1:C:698:CYS:C     | 1:C:700:TYR:H     | 2.13                     | 0.56              |
| 1:C:1024:TYR:CD2  | 1:C:1024:TYR:C    | 2.83                     | 0.56              |
| 1:C:1560:ALA:O    | 1:C:1585:TYR:HD2  | 1.89                     | 0.56              |
| 2:D:192:VAL:HG22  | 2:D:193:SER:N     | 2.19                     | 0.56              |
| 2:D:236:TYR:O     | 2:D:238:ASP:N     | 2.38                     | 0.56              |
| 2:D:582:LYS:O     | 2:D:583:ALA:O     | 2.23                     | 0.56              |
| 2:D:1624:LEU:O    | 2:D:1625:CYS:C    | 2.49                     | 0.56              |
| 1:A:455:ILE:HG22  | 1:A:456:ALA:N     | 2.21                     | 0.56              |
| 1:A:628:GLU:HA    | 1:A:630:SER:OG    | 2.05                     | 0.56              |
| 1:A:634:CYS:HA    | 1:A:671:GLU:OE2   | 2.06                     | 0.56              |
| 1:A:690:TYR:HE1   | 1:A:696:LYS:CD    | 2.19                     | 0.56              |
| 1:A:752:LEU:HD12  | 1:A:752:LEU:C     | 2.29                     | 0.56              |
| 1:A:870:SER:C     | 1:A:872:VAL:H     | 2.14                     | 0.56              |
| 2:B:235:PHE:CE2   | 2:B:299:PHE:CE2   | 2.93                     | 0.56              |
| 2:B:518:PHE:HE2   | 2:B:538:VAL:CB    | 2.19                     | 0.56              |
| 1:C:267:ILE:HG22  | 1:C:268:THR:N     | 2.20                     | 0.56              |
| 1:C:576:SER:CB    | 1:C:589:SER:H     | 2.18                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1033:ILE:HD13 | 1:C:1333:PHE:HZ   | 1.70                     | 0.56              |
| 1:C:1112:GLN:NE2  | 1:C:1171:ALA:HB2  | 2.20                     | 0.56              |
| 1:C:1224:ILE:HG22 | 1:C:1225:TYR:CD2  | 2.41                     | 0.56              |
| 1:C:1451:THR:O    | 1:C:1452:ASP:HB2  | 2.06                     | 0.56              |
| 2:D:352:LYS:HG3   | 2:D:430:MET:HE1   | 1.87                     | 0.56              |
| 2:D:541:LYS:O     | 2:D:543:THR:HG23  | 2.05                     | 0.56              |
| 2:D:1367:ILE:HD13 | 2:D:1456:VAL:HG21 | 1.88                     | 0.56              |
| 1:A:132:LYS:O     | 1:A:135:TYR:CE2   | 2.59                     | 0.56              |
| 1:A:286:ALA:O     | 1:A:287:MET:C     | 2.48                     | 0.56              |
| 1:A:1016:VAL:HG21 | 1:A:1291:ILE:HD12 | 1.88                     | 0.56              |
| 1:A:1446:VAL:O    | 1:A:1446:VAL:HG12 | 2.05                     | 0.56              |
| 1:A:1450:PHE:HB3  | 1:A:1463:GLN:O    | 2.05                     | 0.56              |
| 1:A:1617:TYR:HA   | 1:A:1646:GLU:O    | 2.05                     | 0.56              |
| 2:B:136:ILE:HA    | 2:B:215:ASP:O     | 2.04                     | 0.56              |
| 2:B:214:PHE:O     | 2:B:214:PHE:HD1   | 1.88                     | 0.56              |
| 2:B:541:LYS:O     | 2:B:543:THR:HG23  | 2.05                     | 0.56              |
| 2:B:861:THR:O     | 2:B:863:GLY:N     | 2.38                     | 0.56              |
| 2:B:1305:THR:CG2  | 2:B:1307:LEU:H    | 2.17                     | 0.56              |
| 1:C:827:MET:SD    | 1:C:843:GLY:HA3   | 2.46                     | 0.56              |
| 1:C:1045:LEU:O    | 1:C:1046:LYS:C    | 2.47                     | 0.56              |
| 1:C:1139:GLU:OE1  | 1:C:1184:SER:HB3  | 2.05                     | 0.56              |
| 2:D:501:GLN:HG2   | 2:D:504:VAL:HG23  | 1.88                     | 0.56              |
| 2:D:1387:LEU:HD12 | 2:D:1442:ILE:HD11 | 1.88                     | 0.56              |
| 1:A:96:GLN:HG3    | 1:A:97:ASN:ND2    | 2.20                     | 0.56              |
| 1:A:231:ILE:HA    | 1:A:250:ILE:HG22  | 1.88                     | 0.56              |
| 1:A:889:GLU:O     | 1:A:890:GLY:O     | 2.24                     | 0.56              |
| 1:A:1139:GLU:O    | 1:A:1142:LEU:N    | 2.38                     | 0.56              |
| 1:A:1333:PHE:O    | 1:A:1334:LEU:CB   | 2.52                     | 0.56              |
| 1:A:1618:LEU:O    | 1:A:1618:LEU:HD13 | 2.06                     | 0.56              |
| 1:A:1623:GLU:HB2  | 1:A:1638:PRO:CG   | 2.35                     | 0.56              |
| 2:B:104:VAL:HG22  | 2:B:105:VAL:N     | 2.18                     | 0.56              |
| 2:B:547:THR:HG22  | 2:B:548:LEU:N     | 2.21                     | 0.56              |
| 2:B:842:GLU:O     | 2:B:843:ASP:C     | 2.48                     | 0.56              |
| 2:B:959:ILE:HG22  | 2:B:959:ILE:O     | 2.05                     | 0.56              |
| 2:B:1284:ARG:HG3  | 2:B:1285:GLU:N    | 2.20                     | 0.56              |
| 2:B:1548:ILE:HD13 | 2:B:1548:ILE:N    | 2.21                     | 0.56              |
| 1:C:455:ILE:HG22  | 1:C:456:ALA:N     | 2.21                     | 0.56              |
| 1:C:1117:SER:HB3  | 1:C:1174:PHE:CE2  | 2.41                     | 0.56              |
| 2:D:347:PHE:O     | 2:D:348:THR:C     | 2.49                     | 0.56              |
| 1:A:373:VAL:HG11  | 1:A:435:VAL:HG11  | 1.87                     | 0.56              |
| 1:A:950:TYR:OH    | 1:A:1307:LEU:HD21 | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1554:LYS:HE3  | 1:A:1556:GLU:OE1  | 2.06                     | 0.56              |
| 1:A:1564:SER:HB2  | 1:A:1616:GLN:HG3  | 1.88                     | 0.56              |
| 2:B:236:TYR:O     | 2:B:238:ASP:N     | 2.39                     | 0.56              |
| 2:B:342:PRO:HG2   | 2:B:420:LEU:HD13  | 1.86                     | 0.56              |
| 2:B:786:THR:OG1   | 2:B:809:ARG:HG3   | 2.06                     | 0.56              |
| 2:B:829:GLN:HB3   | 2:B:1471:PHE:HE2  | 1.71                     | 0.56              |
| 2:B:866:TYR:C     | 2:B:866:TYR:CD2   | 2.84                     | 0.56              |
| 1:C:182:ILE:CG1   | 1:C:804:ILE:HD11  | 2.33                     | 0.56              |
| 1:C:968:VAL:HG13  | 1:C:1366:HIS:O    | 2.06                     | 0.56              |
| 2:D:409:LEU:C     | 2:D:409:LEU:HD12  | 2.30                     | 0.56              |
| 2:D:963:ILE:CG1   | 2:D:1325:ILE:HG12 | 2.36                     | 0.56              |
| 1:A:161:LEU:HD11  | 1:A:185:PHE:CG    | 2.42                     | 0.55              |
| 1:A:267:ILE:CD1   | 1:A:299:VAL:HG11  | 2.34                     | 0.55              |
| 1:A:709:GLU:HB3   | 1:A:713:GLN:OE1   | 2.06                     | 0.55              |
| 1:A:1264:ILE:O    | 1:A:1267:VAL:HB   | 2.06                     | 0.55              |
| 1:A:1628:LYS:HB3  | 1:A:1633:PHE:CD1  | 2.41                     | 0.55              |
| 2:B:482:LEU:CD1   | 2:B:521:VAL:HB    | 2.34                     | 0.55              |
| 2:B:756:LEU:HD22  | 2:B:778:PHE:CE1   | 2.41                     | 0.55              |
| 2:B:757:TRP:O     | 2:B:758:LEU:HD23  | 2.06                     | 0.55              |
| 1:C:125:PHE:CD1   | 1:C:627:LEU:HD21  | 2.41                     | 0.55              |
| 1:C:906:GLY:O     | 1:C:908:HIS:NE2   | 2.39                     | 0.55              |
| 1:C:930:VAL:HG22  | 1:C:931:PRO:HD2   | 1.88                     | 0.55              |
| 1:C:1127:ILE:HD11 | 1:C:1143:TYR:HD2  | 1.70                     | 0.55              |
| 1:C:1562:LYS:HD3  | 1:C:1664:LEU:HD21 | 1.89                     | 0.55              |
| 1:C:1574:PHE:HA   | 1:C:1603:LYS:CD   | 2.36                     | 0.55              |
| 2:D:518:PHE:HE2   | 2:D:538:VAL:CB    | 2.19                     | 0.55              |
| 2:D:756:LEU:HD12  | 2:D:758:LEU:HG    | 1.88                     | 0.55              |
| 2:D:885:VAL:HG23  | 2:D:887:LEU:HD21  | 1.87                     | 0.55              |
| 1:A:862:VAL:HB    | 1:A:865:ILE:CD1   | 2.36                     | 0.55              |
| 2:B:78:ALA:C      | 2:B:80:GLY:H      | 2.14                     | 0.55              |
| 2:B:191:LEU:HD13  | 2:B:960:GLU:HB3   | 1.88                     | 0.55              |
| 2:B:355:LYS:N     | 2:B:355:LYS:HD2   | 2.21                     | 0.55              |
| 2:B:523:TYR:CD1   | 2:B:523:TYR:C     | 2.83                     | 0.55              |
| 1:C:599:TRP:HE1   | 1:C:779:LEU:HD13  | 1.71                     | 0.55              |
| 1:C:944:LEU:HD12  | 1:C:1313:ILE:CD1  | 2.35                     | 0.55              |
| 1:C:977:LEU:HA    | 1:C:1361:VAL:HG13 | 1.86                     | 0.55              |
| 1:C:1377:PHE:CD2  | 1:C:1495:VAL:HG22 | 2.41                     | 0.55              |
| 1:C:1577:TYR:HB2  | 1:C:1600:PHE:O    | 2.06                     | 0.55              |
| 2:D:315:TYR:C     | 2:D:315:TYR:HD1   | 2.13                     | 0.55              |
| 2:D:322:THR:HG22  | 2:D:327:ASP:O     | 2.06                     | 0.55              |
| 2:D:485:ASN:OD1   | 2:D:486:LYS:HD2   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:870:PHE:HB2   | 2:D:871:PRO:CD    | 2.36                     | 0.55              |
| 2:D:1443:LEU:N    | 2:D:1443:LEU:CD1  | 2.69                     | 0.55              |
| 2:D:1623:LYS:HZ3  | 2:D:1623:LYS:HA   | 1.71                     | 0.55              |
| 1:A:267:ILE:HG22  | 1:A:268:THR:N     | 2.21                     | 0.55              |
| 1:A:422:LEU:HD12  | 1:A:422:LEU:N     | 2.20                     | 0.55              |
| 1:A:654:LEU:O     | 1:A:655:THR:CG2   | 2.53                     | 0.55              |
| 1:A:981:GLY:HA3   | 1:A:1333:PHE:HB2  | 1.87                     | 0.55              |
| 1:A:1118:PHE:HD2  | 1:A:1148:THR:HG1  | 1.52                     | 0.55              |
| 1:A:1159:CYS:O    | 1:A:1161:LEU:N    | 2.32                     | 0.55              |
| 1:A:1549:LYS:NZ   | 1:A:1667:PHE:CB   | 2.67                     | 0.55              |
| 2:B:199:ILE:O     | 2:B:199:ILE:HG22  | 2.05                     | 0.55              |
| 2:B:322:THR:HG22  | 2:B:327:ASP:O     | 2.06                     | 0.55              |
| 2:B:345:ILE:HD11  | 2:B:427:THR:C     | 2.31                     | 0.55              |
| 2:B:523:TYR:HB3   | 2:B:533:ALA:HB2   | 1.88                     | 0.55              |
| 2:B:750:ASP:OD1   | 2:B:752:PRO:HD3   | 2.06                     | 0.55              |
| 2:B:1624:LEU:O    | 2:B:1625:CYS:C    | 2.49                     | 0.55              |
| 1:C:59:TYR:CG     | 1:C:60:PRO:HD3    | 2.41                     | 0.55              |
| 1:C:221:GLU:HG2   | 1:C:222:TYR:O     | 2.07                     | 0.55              |
| 1:C:250:ILE:HD11  | 1:C:265:VAL:CG1   | 2.31                     | 0.55              |
| 1:C:371:ILE:HG22  | 1:C:371:ILE:O     | 2.07                     | 0.55              |
| 1:C:1139:GLU:O    | 1:C:1142:LEU:N    | 2.40                     | 0.55              |
| 1:C:1487:PHE:N    | 1:C:1487:PHE:HD2  | 2.04                     | 0.55              |
| 1:C:1562:LYS:HD2  | 1:C:1582:LEU:HD11 | 1.88                     | 0.55              |
| 1:A:25:ILE:HB     | 1:A:654:LEU:O     | 2.06                     | 0.55              |
| 1:A:936:ARG:HH11  | 1:A:936:ARG:CG    | 2.17                     | 0.55              |
| 1:A:942:VAL:HG11  | 1:A:957:LYS:CB    | 2.36                     | 0.55              |
| 1:A:1186:PHE:HA   | 1:A:1250:THR:HG22 | 1.87                     | 0.55              |
| 2:B:415:THR:O     | 2:B:425:GLN:CD    | 2.49                     | 0.55              |
| 2:B:850:LEU:HD13  | 2:B:882:PHE:CD1   | 2.42                     | 0.55              |
| 2:B:1447:GLU:HG3  | 2:B:1447:GLU:O    | 2.06                     | 0.55              |
| 1:C:560:TRP:CH2   | 1:C:562:ASN:HB2   | 2.42                     | 0.55              |
| 1:C:919:GLY:HA2   | 2:D:813:VAL:HG11  | 1.88                     | 0.55              |
| 1:C:1129:LEU:HD23 | 1:C:1129:LEU:N    | 2.18                     | 0.55              |
| 1:C:1139:GLU:O    | 1:C:1140:ASN:C    | 2.49                     | 0.55              |
| 1:C:1323:LEU:HD12 | 1:C:1324:HIS:N    | 2.19                     | 0.55              |
| 2:D:234:PHE:C     | 2:D:234:PHE:HD1   | 2.15                     | 0.55              |
| 2:D:529:ASN:OD1   | 2:D:529:ASN:O     | 2.24                     | 0.55              |
| 1:A:599:TRP:CD1   | 1:A:779:LEU:HA    | 2.42                     | 0.55              |
| 1:A:949:ILE:O     | 1:A:949:ILE:HG22  | 2.06                     | 0.55              |
| 1:A:976:ILE:HB    | 1:A:1362:THR:CG2  | 2.36                     | 0.55              |
| 1:A:1133:LEU:H    | 1:A:1133:LEU:HD12 | 1.72                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:189:PRO:C     | 2:B:191:LEU:N     | 2.65                     | 0.55              |
| 2:B:219:TYR:O     | 2:B:220:VAL:HG13  | 2.07                     | 0.55              |
| 2:B:756:LEU:HD12  | 2:B:758:LEU:HG    | 1.89                     | 0.55              |
| 2:B:918:GLU:N     | 2:B:918:GLU:OE2   | 2.39                     | 0.55              |
| 1:C:634:CYS:HA    | 1:C:671:GLU:OE2   | 2.05                     | 0.55              |
| 1:C:690:TYR:HE1   | 1:C:696:LYS:CD    | 2.20                     | 0.55              |
| 2:D:339:VAL:HG23  | 2:D:341:SER:N     | 2.20                     | 0.55              |
| 1:A:73:LEU:HD23   | 1:A:73:LEU:H      | 1.71                     | 0.55              |
| 1:A:283:MET:HE1   | 1:A:301:PHE:HZ    | 1.69                     | 0.55              |
| 1:A:560:TRP:CE3   | 1:A:673:LEU:HD22  | 2.42                     | 0.55              |
| 1:A:691:LYS:C     | 1:A:693:SER:H     | 2.15                     | 0.55              |
| 1:A:984:VAL:HG22  | 1:A:987:ILE:HD12  | 1.88                     | 0.55              |
| 1:A:1019:PHE:CD2  | 1:A:1020:TYR:N    | 2.75                     | 0.55              |
| 1:A:1488:LEU:HD12 | 1:A:1488:LEU:O    | 2.07                     | 0.55              |
| 2:B:384:PHE:CE1   | 2:B:400:LEU:HG    | 2.41                     | 0.55              |
| 2:B:518:PHE:O     | 2:B:518:PHE:HD2   | 1.90                     | 0.55              |
| 1:C:144:ARG:HD2   | 1:C:146:TYR:HE1   | 1.67                     | 0.55              |
| 1:C:376:LYS:HA    | 1:C:381:GLN:O     | 2.05                     | 0.55              |
| 1:C:1227:PHE:HD2  | 1:C:1273:TRP:CE2  | 2.24                     | 0.55              |
| 1:C:1403:VAL:HG22 | 1:C:1476:ARG:HB3  | 1.89                     | 0.55              |
| 1:C:1500:ARG:C    | 1:C:1502:ASP:H    | 2.15                     | 0.55              |
| 1:A:54:ILE:HG12   | 1:A:106:VAL:HG13  | 1.88                     | 0.55              |
| 1:A:127:PHE:CE2   | 1:A:623:VAL:HG13  | 2.32                     | 0.55              |
| 1:A:855:PHE:CD1   | 1:A:855:PHE:C     | 2.84                     | 0.55              |
| 1:A:1317:TYR:HD2  | 1:A:1344:ASP:HB3  | 1.72                     | 0.55              |
| 2:B:35:THR:HB     | 2:B:91:ALA:HB2    | 1.87                     | 0.55              |
| 2:B:173:VAL:O     | 2:B:173:VAL:HG12  | 2.06                     | 0.55              |
| 2:B:315:TYR:O     | 2:B:315:TYR:HD1   | 1.89                     | 0.55              |
| 1:C:430:VAL:HG22  | 1:C:455:ILE:HG23  | 1.88                     | 0.55              |
| 1:C:791:PRO:HG3   | 1:C:797:TRP:HE1   | 1.71                     | 0.55              |
| 1:C:1507:MET:HG3  | 1:C:1508:PHE:O    | 2.07                     | 0.55              |
| 2:D:219:TYR:O     | 2:D:220:VAL:HG13  | 2.07                     | 0.55              |
| 2:D:322:THR:HG21  | 2:D:326:SER:HG    | 1.72                     | 0.55              |
| 2:D:482:LEU:CD1   | 2:D:521:VAL:HB    | 2.36                     | 0.55              |
| 2:D:850:LEU:HD13  | 2:D:882:PHE:CD1   | 2.42                     | 0.55              |
| 2:D:953:ARG:HG2   | 2:D:954:VAL:H     | 1.71                     | 0.55              |
| 2:D:1528:LEU:HD21 | 2:D:1531:ILE:HD11 | 1.89                     | 0.55              |
| 1:A:523:TYR:CE1   | 2:B:359:PRO:HG2   | 2.41                     | 0.55              |
| 1:A:539:ARG:NE    | 1:A:633:GLY:HA3   | 2.21                     | 0.55              |
| 1:A:550:GLN:O     | 1:A:550:GLN:HG2   | 2.05                     | 0.55              |
| 1:A:862:VAL:HB    | 1:A:865:ILE:HD11  | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1549:LYS:HZ2  | 1:A:1667:PHE:HB3  | 1.72                     | 0.55              |
| 2:B:347:PHE:O     | 2:B:348:THR:C     | 2.49                     | 0.55              |
| 2:B:963:ILE:CG1   | 2:B:1325:ILE:HG12 | 2.37                     | 0.55              |
| 1:C:700:TYR:HD2   | 1:C:701:ASP:N     | 2.05                     | 0.55              |
| 1:C:1003:LEU:N    | 1:C:1003:LEU:HD23 | 2.22                     | 0.55              |
| 1:C:1044:LYS:O    | 1:C:1047:LYS:HB3  | 2.07                     | 0.55              |
| 2:D:235:PHE:CE2   | 2:D:299:PHE:CE2   | 2.94                     | 0.55              |
| 2:D:296:ARG:HG3   | 2:D:296:ARG:NH1   | 2.21                     | 0.55              |
| 2:D:793:SER:OG    | 2:D:801:CYS:HB3   | 2.05                     | 0.55              |
| 1:A:803:GLY:O     | 1:A:810:CYS:CB    | 2.55                     | 0.55              |
| 1:A:1162:VAL:HG22 | 1:C:1102:ASN:HD22 | 1.67                     | 0.55              |
| 1:A:1431:GLY:HA2  | 1:A:1483:PHE:CE1  | 2.41                     | 0.55              |
| 2:B:384:PHE:CD1   | 2:B:400:LEU:HG    | 2.41                     | 0.55              |
| 2:B:518:PHE:C     | 2:B:518:PHE:CD2   | 2.83                     | 0.55              |
| 1:C:115:LYS:CE    | 1:C:654:LEU:HD11  | 2.37                     | 0.55              |
| 1:C:296:ILE:HG23  | 1:C:297:ALA:N     | 2.21                     | 0.55              |
| 1:C:433:PHE:CE1   | 1:C:452:TYR:HB2   | 2.42                     | 0.55              |
| 1:C:489:LYS:CG    | 1:C:490:SER:H     | 2.20                     | 0.55              |
| 1:C:599:TRP:CD1   | 1:C:779:LEU:HA    | 2.42                     | 0.55              |
| 2:D:345:ILE:HD11  | 2:D:427:THR:C     | 2.32                     | 0.55              |
| 2:D:476:ILE:HD11  | 2:D:524:TYR:HB2   | 1.89                     | 0.55              |
| 2:D:1600:ILE:O    | 2:D:1602:THR:HG23 | 2.05                     | 0.55              |
| 1:A:331:GLU:HG2   | 1:A:333:THR:HG23  | 1.88                     | 0.55              |
| 1:A:471:ASP:OD2   | 1:A:474:LYS:HD2   | 2.07                     | 0.55              |
| 1:A:700:TYR:HD2   | 1:A:701:ASP:N     | 2.06                     | 0.55              |
| 1:A:1003:LEU:HD23 | 1:A:1003:LEU:N    | 2.22                     | 0.55              |
| 2:B:216:VAL:O     | 2:B:216:VAL:CG1   | 2.54                     | 0.55              |
| 1:C:272:ARG:O     | 1:C:321:LYS:HB2   | 2.07                     | 0.55              |
| 1:C:975:ARG:HG3   | 1:C:1340:VAL:HB   | 1.89                     | 0.55              |
| 1:C:1180:LEU:CD2  | 1:C:1208:ILE:HG12 | 2.37                     | 0.55              |
| 1:C:1268:ASN:N    | 1:C:1269:PRO:CD   | 2.70                     | 0.55              |
| 2:D:209:ASN:CG    | 3:D:2001:NAG:C7   | 2.80                     | 0.55              |
| 2:D:469:ASN:ND2   | 2:D:469:ASN:C     | 2.65                     | 0.55              |
| 2:D:748:ARG:HH12  | 2:D:784:ILE:HG12  | 1.72                     | 0.55              |
| 2:D:750:ASP:OD1   | 2:D:752:PRO:HD3   | 2.07                     | 0.55              |
| 2:D:945:ILE:HD13  | 2:D:1311:ILE:HB   | 1.89                     | 0.55              |
| 2:D:1447:GLU:HG3  | 2:D:1447:GLU:O    | 2.07                     | 0.55              |
| 1:A:221:GLU:HG2   | 1:A:222:TYR:O     | 2.07                     | 0.54              |
| 1:A:433:PHE:N     | 1:A:433:PHE:HD1   | 2.05                     | 0.54              |
| 1:A:499:TYR:HE2   | 1:A:517:LYS:HG3   | 1.72                     | 0.54              |
| 1:A:706:ASN:ND2   | 1:A:709:GLU:H     | 2.05                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1429:PRO:HB2  | 1:A:1432:ILE:CG1  | 2.37                     | 0.54              |
| 2:B:762:LEU:HD12  | 2:B:762:LEU:H     | 1.71                     | 0.54              |
| 2:B:834:ALA:O     | 2:B:835:ILE:HD13  | 2.07                     | 0.54              |
| 1:C:136:THR:O     | 1:C:139:GLN:HB2   | 2.08                     | 0.54              |
| 1:C:238:ILE:HG23  | 1:C:242:ASN:ND2   | 2.18                     | 0.54              |
| 1:C:1164:ILE:O    | 1:C:1167:ALA:N    | 2.40                     | 0.54              |
| 2:D:239:GLY:N     | 2:D:296:ARG:NH2   | 2.48                     | 0.54              |
| 2:D:574:ARG:HG2   | 2:D:794:PHE:HB3   | 1.88                     | 0.54              |
| 2:D:849:GLU:OE2   | 2:D:865:ARG:HD2   | 2.06                     | 0.54              |
| 2:D:891:LEU:CB    | 2:D:912:LYS:HD3   | 2.36                     | 0.54              |
| 1:A:59:TYR:CG     | 1:A:60:PRO:HD3    | 2.42                     | 0.54              |
| 1:A:523:TYR:OH    | 2:B:359:PRO:HD2   | 2.06                     | 0.54              |
| 1:A:791:PRO:HG3   | 1:A:797:TRP:HE1   | 1.71                     | 0.54              |
| 1:A:805:SER:O     | 1:A:807:THR:N     | 2.40                     | 0.54              |
| 1:A:1013:MET:HE3  | 1:A:1287:THR:HB   | 1.87                     | 0.54              |
| 1:A:1049:LEU:HD11 | 1:A:1089:VAL:CG1  | 2.37                     | 0.54              |
| 1:A:1304:VAL:CG1  | 1:A:1305:LYS:N    | 2.70                     | 0.54              |
| 1:A:1560:ALA:O    | 1:A:1585:TYR:CD2  | 2.61                     | 0.54              |
| 1:A:1561:TYR:CE1  | 1:A:1581:LEU:HD21 | 2.41                     | 0.54              |
| 1:C:331:GLU:HG2   | 1:C:333:THR:HG23  | 1.88                     | 0.54              |
| 1:C:573:VAL:HG12  | 1:C:592:MET:HG2   | 1.88                     | 0.54              |
| 1:C:692:HIS:HA    | 1:C:696:LYS:HD3   | 1.88                     | 0.54              |
| 1:C:1019:PHE:HD2  | 1:C:1020:TYR:N    | 2.05                     | 0.54              |
| 2:D:28:ILE:HG12   | 2:D:628:LEU:HD13  | 1.88                     | 0.54              |
| 2:D:850:LEU:CG    | 2:D:851:LEU:N     | 2.69                     | 0.54              |
| 2:D:916:VAL:HG22  | 2:D:917:PRO:N     | 2.21                     | 0.54              |
| 2:D:1288:ILE:CD1  | 2:D:1303:VAL:HG21 | 2.37                     | 0.54              |
| 2:D:1623:LYS:HB3  | 2:D:1623:LYS:NZ   | 2.22                     | 0.54              |
| 1:A:60:PRO:CD     | 1:A:61:ASP:N      | 2.66                     | 0.54              |
| 1:A:177:ILE:HG22  | 1:A:178:ASP:H     | 1.72                     | 0.54              |
| 1:A:970:LYS:O     | 1:A:971:THR:CG2   | 2.56                     | 0.54              |
| 1:A:1190:ILE:HG12 | 1:A:1253:TYR:CE1  | 2.42                     | 0.54              |
| 1:A:1440:LYS:HD3  | 1:A:1453:TYR:OH   | 2.07                     | 0.54              |
| 2:B:302:ARG:HG3   | 2:B:303:PHE:CD1   | 2.42                     | 0.54              |
| 2:B:1371:TYR:CG   | 2:B:1377:SER:HB3  | 2.42                     | 0.54              |
| 1:C:864:GLY:HA3   | 1:C:907:LEU:CD2   | 2.36                     | 0.54              |
| 1:C:888:VAL:CG2   | 1:C:894:HIS:HB2   | 2.33                     | 0.54              |
| 1:C:1454:GLN:C    | 1:C:1455:ILE:HD12 | 2.33                     | 0.54              |
| 2:D:816:ILE:HD13  | 2:D:896:ILE:HG22  | 1.89                     | 0.54              |
| 2:D:1390:PHE:O    | 2:D:1391:LEU:HD23 | 2.07                     | 0.54              |
| 1:A:1024:TYR:CD2  | 1:A:1024:TYR:C    | 2.84                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:50:PHE:CD1    | 1:C:50:PHE:C      | 2.85                     | 0.54              |
| 1:C:371:ILE:CG2   | 1:C:420:PHE:HB2   | 2.37                     | 0.54              |
| 1:C:961:TYR:CE2   | 1:C:1343:ASN:HA   | 2.43                     | 0.54              |
| 1:C:1049:LEU:HD11 | 1:C:1089:VAL:HG13 | 1.89                     | 0.54              |
| 1:A:50:PHE:CD1    | 1:A:50:PHE:C      | 2.86                     | 0.54              |
| 1:A:565:GLU:HG3   | 1:A:624:PHE:CB    | 2.37                     | 0.54              |
| 1:A:1084:ARG:CD   | 1:A:1154:LYS:HE3  | 2.38                     | 0.54              |
| 1:A:1164:ILE:O    | 1:A:1165:ASP:C    | 2.47                     | 0.54              |
| 1:A:1451:THR:O    | 1:A:1452:ASP:HB2  | 2.08                     | 0.54              |
| 2:B:88:GLU:OE1    | 2:B:155:SER:HB2   | 2.07                     | 0.54              |
| 2:B:481:TYR:CE1   | 2:B:506:MET:SD    | 2.94                     | 0.54              |
| 1:C:691:LYS:C     | 1:C:693:SER:H     | 2.15                     | 0.54              |
| 2:D:173:VAL:HG12  | 2:D:173:VAL:O     | 2.06                     | 0.54              |
| 2:D:598:ILE:HD11  | 2:D:800:ILE:HG21  | 1.90                     | 0.54              |
| 2:D:1475:ASP:OD1  | 2:D:1475:ASP:N    | 2.25                     | 0.54              |
| 1:A:309:GLU:O     | 1:A:312:TYR:N     | 2.39                     | 0.54              |
| 1:A:443:PRO:HD2   | 1:A:446:ASN:CB    | 2.36                     | 0.54              |
| 1:A:1106:TRP:HE3  | 1:A:1107:LEU:HD13 | 1.73                     | 0.54              |
| 2:B:1288:ILE:CD1  | 2:B:1303:VAL:HG21 | 2.38                     | 0.54              |
| 2:B:1390:PHE:O    | 2:B:1391:LEU:HD23 | 2.08                     | 0.54              |
| 2:B:1482:ASN:HB3  | 2:B:1493:ALA:HB3  | 1.89                     | 0.54              |
| 1:C:947:ARG:O     | 1:C:949:ILE:HG12  | 2.07                     | 0.54              |
| 1:C:1023:HIS:CE1  | 1:C:1302:LEU:HD11 | 2.43                     | 0.54              |
| 1:C:1127:ILE:HD12 | 1:C:1127:ILE:N    | 2.14                     | 0.54              |
| 1:A:174:VAL:CG2   | 1:A:175:GLU:H     | 2.17                     | 0.54              |
| 1:A:955:ARG:CG    | 1:A:1350:THR:HG23 | 2.35                     | 0.54              |
| 1:A:1227:PHE:HB2  | 1:A:1251:THR:HG21 | 1.90                     | 0.54              |
| 1:A:1283:GLY:HA3  | 1:A:1290:THR:HG23 | 1.88                     | 0.54              |
| 1:A:1487:PHE:O    | 1:A:1488:LEU:C    | 2.50                     | 0.54              |
| 1:A:1582:LEU:HD12 | 1:A:1583:ASP:H    | 1.72                     | 0.54              |
| 2:B:481:TYR:CE2   | 2:B:493:GLY:CA    | 2.89                     | 0.54              |
| 1:C:617:LYS:C     | 1:C:619:PRO:HD2   | 2.33                     | 0.54              |
| 1:C:967:LEU:HD12  | 1:C:968:VAL:H     | 1.72                     | 0.54              |
| 1:C:981:GLY:HA3   | 1:C:1333:PHE:HB2  | 1.89                     | 0.54              |
| 1:C:1534:GLN:HA   | 1:C:1608:ASN:HD22 | 1.73                     | 0.54              |
| 1:C:1554:LYS:HE3  | 1:C:1556:GLU:OE1  | 2.08                     | 0.54              |
| 1:A:133:PRO:HD2   | 1:A:609:VAL:CG1   | 2.37                     | 0.54              |
| 1:A:639:GLY:H     | 1:A:645:VAL:HG22  | 1.73                     | 0.54              |
| 1:A:1093:VAL:O    | 1:A:1093:VAL:HG12 | 2.08                     | 0.54              |
| 2:B:965:ILE:HG22  | 2:B:1323:MET:HB2  | 1.90                     | 0.54              |
| 1:C:174:VAL:CG2   | 1:C:175:GLU:H     | 2.16                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1093:VAL:HG12 | 1:C:1093:VAL:O    | 2.07                     | 0.54              |
| 1:C:1317:TYR:CD2  | 1:C:1344:ASP:HB3  | 2.43                     | 0.54              |
| 2:D:88:GLU:OE1    | 2:D:155:SER:HB2   | 2.07                     | 0.54              |
| 2:D:142:PRO:HB3   | 2:D:187:ASN:ND2   | 2.23                     | 0.54              |
| 2:D:145:TYR:CD1   | 2:D:145:TYR:C     | 2.86                     | 0.54              |
| 1:A:371:ILE:HD13  | 1:A:390:LEU:HD21  | 1.90                     | 0.54              |
| 1:A:483:ASN:ND2   | 2:B:399:ILE:HB    | 2.22                     | 0.54              |
| 1:A:495:LYS:HE2   | 1:A:495:LYS:CA    | 2.38                     | 0.54              |
| 1:A:576:SER:CB    | 1:A:589:SER:H     | 2.20                     | 0.54              |
| 1:A:1033:ILE:CG2  | 1:A:1034:PHE:CD1  | 2.91                     | 0.54              |
| 1:A:1163:LYS:NZ   | 1:C:1109:GLU:HG2  | 2.23                     | 0.54              |
| 1:A:1562:LYS:HD2  | 1:A:1582:LEU:HD11 | 1.89                     | 0.54              |
| 2:B:495:GLN:NE2   | 2:B:496:PRO:HD2   | 2.23                     | 0.54              |
| 2:B:581:ASP:O     | 2:B:582:LYS:C     | 2.51                     | 0.54              |
| 2:B:1284:ARG:HD2  | 2:B:1285:GLU:N    | 2.22                     | 0.54              |
| 2:B:1623:LYS:NZ   | 2:B:1623:LYS:HB3  | 2.23                     | 0.54              |
| 1:C:365:PRO:HD2   | 1:C:464:TYR:CE2   | 2.42                     | 0.54              |
| 1:C:373:VAL:HG11  | 1:C:435:VAL:HG11  | 1.88                     | 0.54              |
| 1:C:974:LYS:O     | 1:C:1364:VAL:HG12 | 2.08                     | 0.54              |
| 1:C:1213:LYS:HG2  | 1:C:1266:TYR:CE2  | 2.41                     | 0.54              |
| 1:C:1252:ALA:O    | 1:C:1253:TYR:C    | 2.50                     | 0.54              |
| 1:C:1265:ASN:C    | 1:C:1267:VAL:H    | 2.16                     | 0.54              |
| 1:C:1429:PRO:HB2  | 1:C:1432:ILE:CG1  | 2.37                     | 0.54              |
| 1:C:1560:ALA:HB3  | 1:C:1585:TYR:HE2  | 1.72                     | 0.54              |
| 2:D:69:PHE:C      | 2:D:69:PHE:CD2    | 2.86                     | 0.54              |
| 2:D:129:PHE:HE2   | 2:D:598:ILE:HG23  | 1.70                     | 0.54              |
| 2:D:519:ARG:NH1   | 2:D:606:ASP:OD2   | 2.40                     | 0.54              |
| 1:A:678:THR:HG21  | 1:A:742:ILE:HB    | 1.90                     | 0.54              |
| 1:A:773:TRP:HE1   | 1:A:797:TRP:NE1   | 2.06                     | 0.54              |
| 1:A:934:VAL:CG1   | 1:A:935:LYS:N     | 2.71                     | 0.54              |
| 1:A:1066:TYR:N    | 1:A:1066:TYR:CD1  | 2.74                     | 0.54              |
| 1:A:1164:ILE:O    | 1:A:1167:ALA:N    | 2.41                     | 0.54              |
| 2:B:501:GLN:CG    | 2:B:504:VAL:HG23  | 2.38                     | 0.54              |
| 2:B:814:PHE:CZ    | 2:B:846:VAL:HG21  | 2.43                     | 0.54              |
| 2:B:829:GLN:CG    | 2:B:1480:LEU:HD13 | 2.38                     | 0.54              |
| 1:C:576:SER:HB2   | 1:C:589:SER:N     | 2.21                     | 0.54              |
| 1:C:1008:ALA:O    | 1:C:1011:GLU:N    | 2.40                     | 0.54              |
| 1:C:1013:MET:SD   | 1:C:1016:VAL:HG21 | 2.48                     | 0.54              |
| 1:C:1068:VAL:HG13 | 1:C:1069:TRP:N    | 2.23                     | 0.54              |
| 2:D:353:TYR:HA    | 2:D:433:ILE:O     | 2.07                     | 0.54              |
| 2:D:415:THR:O     | 2:D:425:GLN:CD    | 2.51                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1284:ARG:HD2  | 2:D:1285:GLU:N    | 2.22                     | 0.54              |
| 2:D:1623:LYS:NZ   | 2:D:1623:LYS:CB   | 2.71                     | 0.54              |
| 1:A:24:VAL:O      | 1:A:24:VAL:HG12   | 2.08                     | 0.53              |
| 1:A:115:LYS:CE    | 1:A:654:LEU:HD11  | 2.38                     | 0.53              |
| 1:A:162:THR:CB    | 1:A:173:MET:HE2   | 2.38                     | 0.53              |
| 1:A:228:SER:HB3   | 1:A:253:ARG:HG2   | 1.90                     | 0.53              |
| 1:A:582:TYR:CE2   | 1:A:817:ALA:HB1   | 2.43                     | 0.53              |
| 1:A:961:TYR:CE2   | 1:A:1343:ASN:HA   | 2.43                     | 0.53              |
| 1:A:1629:TYR:O    | 1:A:1630:ASN:HB2  | 2.07                     | 0.53              |
| 2:B:296:ARG:HG3   | 2:B:296:ARG:NH1   | 2.24                     | 0.53              |
| 2:B:481:TYR:CD2   | 2:B:481:TYR:C     | 2.85                     | 0.53              |
| 1:C:222:TYR:HD2   | 1:C:223:VAL:N     | 2.05                     | 0.53              |
| 1:C:1565:ILE:HB   | 1:C:1614:GLY:H    | 1.73                     | 0.53              |
| 1:C:1582:LEU:HD12 | 1:C:1583:ASP:H    | 1.72                     | 0.53              |
| 2:D:27:LEU:HD13   | 2:D:43:VAL:HG23   | 1.90                     | 0.53              |
| 2:D:262:PHE:CD1   | 2:D:282:ARG:HG3   | 2.43                     | 0.53              |
| 1:A:825:LEU:HD12  | 1:A:844:THR:O     | 2.08                     | 0.53              |
| 1:A:1008:ALA:O    | 1:A:1011:GLU:N    | 2.40                     | 0.53              |
| 1:A:1110:ASN:O    | 1:A:1111:TYR:CG   | 2.62                     | 0.53              |
| 1:A:1268:ASN:H    | 1:A:1268:ASN:ND2  | 2.05                     | 0.53              |
| 1:A:1268:ASN:N    | 1:A:1269:PRO:CD   | 2.71                     | 0.53              |
| 1:A:1565:ILE:HB   | 1:A:1614:GLY:H    | 1.72                     | 0.53              |
| 1:C:371:ILE:HD13  | 1:C:390:LEU:HD21  | 1.90                     | 0.53              |
| 1:C:502:LEU:HB2   | 1:C:541:LEU:CD2   | 2.39                     | 0.53              |
| 1:C:606:ASP:O     | 1:C:609:VAL:HG23  | 2.08                     | 0.53              |
| 1:C:823:VAL:HG23  | 1:C:846:TYR:O     | 2.08                     | 0.53              |
| 1:C:875:HIS:CB    | 2:D:901:GLN:NE2   | 2.72                     | 0.53              |
| 1:C:1024:TYR:O    | 1:C:1025:LEU:C    | 2.51                     | 0.53              |
| 2:D:829:GLN:CG    | 2:D:1480:LEU:HD13 | 2.38                     | 0.53              |
| 2:D:829:GLN:HB3   | 2:D:1471:PHE:HE2  | 1.74                     | 0.53              |
| 1:A:177:ILE:HG22  | 1:A:178:ASP:N     | 2.22                     | 0.53              |
| 1:A:827:MET:SD    | 1:A:843:GLY:HA3   | 2.48                     | 0.53              |
| 1:A:969:PRO:HG3   | 1:A:1601:ILE:CD1  | 2.37                     | 0.53              |
| 1:A:1352:PHE:CD2  | 1:A:1353:GLY:N    | 2.76                     | 0.53              |
| 1:A:1619:ILE:HG12 | 1:A:1645:ILE:CD1  | 2.38                     | 0.53              |
| 2:B:322:THR:HG21  | 2:B:326:SER:HG    | 1.74                     | 0.53              |
| 2:B:438:GLN:CD    | 2:B:530:GLU:HG3   | 2.34                     | 0.53              |
| 2:B:481:TYR:CE2   | 2:B:493:GLY:C     | 2.86                     | 0.53              |
| 2:B:850:LEU:CG    | 2:B:851:LEU:N     | 2.70                     | 0.53              |
| 1:C:422:LEU:HD12  | 1:C:422:LEU:N     | 2.22                     | 0.53              |
| 1:C:471:ASP:OD2   | 1:C:474:LYS:HD2   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:483:ASN:ND2   | 2:D:399:ILE:HB    | 2.24                     | 0.53              |
| 1:C:1106:TRP:HE3  | 1:C:1107:LEU:HD13 | 1.72                     | 0.53              |
| 1:C:1475:VAL:CG2  | 1:C:1476:ARG:N    | 2.71                     | 0.53              |
| 2:D:184:TRP:HB2   | 2:D:185:PRO:CD    | 2.39                     | 0.53              |
| 2:D:556:ILE:H     | 2:D:556:ILE:CD1   | 1.98                     | 0.53              |
| 2:D:1292:ILE:HD11 | 2:D:1301:ARG:HE   | 1.74                     | 0.53              |
| 1:A:371:ILE:HD11  | 1:A:433:PHE:CD2   | 2.44                     | 0.53              |
| 1:A:672:ILE:C     | 1:A:673:LEU:HG    | 2.33                     | 0.53              |
| 1:A:906:GLY:O     | 1:A:908:HIS:NE2   | 2.41                     | 0.53              |
| 1:A:1024:TYR:O    | 1:A:1025:LEU:C    | 2.51                     | 0.53              |
| 1:A:1244:THR:HG22 | 1:A:1246:ARG:N    | 2.23                     | 0.53              |
| 1:A:1548:ARG:HH21 | 1:A:1550:GLN:HE22 | 1.56                     | 0.53              |
| 2:B:742:ASP:C     | 2:B:742:ASP:OD1   | 2.52                     | 0.53              |
| 1:C:889:GLU:O     | 1:C:890:GLY:O     | 2.27                     | 0.53              |
| 1:C:961:TYR:HD1   | 1:C:961:TYR:O     | 1.92                     | 0.53              |
| 1:C:1548:ARG:HH21 | 1:C:1550:GLN:HE22 | 1.56                     | 0.53              |
| 2:D:547:THR:HG22  | 2:D:548:LEU:N     | 2.24                     | 0.53              |
| 2:D:563:MET:HA    | 2:D:563:MET:CE    | 2.38                     | 0.53              |
| 1:A:931:PRO:CB    | 1:A:1366:HIS:CD2  | 2.91                     | 0.53              |
| 1:A:1500:ARG:C    | 1:A:1502:ASP:H    | 2.17                     | 0.53              |
| 2:B:130:ILE:HA    | 2:B:147:VAL:HG23  | 1.91                     | 0.53              |
| 2:B:261:ALA:CB    | 2:B:285:ILE:HD11  | 2.39                     | 0.53              |
| 2:B:342:PRO:HB2   | 2:B:343:TYR:CD1   | 2.43                     | 0.53              |
| 2:B:574:ARG:HG2   | 2:B:794:PHE:HB3   | 1.89                     | 0.53              |
| 1:C:494:ASP:CG    | 1:C:494:ASP:O     | 2.52                     | 0.53              |
| 1:C:942:VAL:HG11  | 1:C:957:LYS:CB    | 2.38                     | 0.53              |
| 1:C:1304:VAL:CG1  | 1:C:1305:LYS:N    | 2.71                     | 0.53              |
| 1:C:1565:ILE:HG22 | 1:C:1566:THR:H    | 1.72                     | 0.53              |
| 2:D:25:TYR:CE2    | 2:D:113:VAL:HG22  | 2.43                     | 0.53              |
| 2:D:401:ASN:C     | 2:D:402:ILE:HD13  | 2.33                     | 0.53              |
| 2:D:557:GLN:HE21  | 2:D:563:MET:HE3   | 1.73                     | 0.53              |
| 2:D:646:GLN:CB    | 2:D:647:PRO:HD2   | 2.32                     | 0.53              |
| 1:A:433:PHE:N     | 1:A:433:PHE:CD1   | 2.75                     | 0.53              |
| 1:A:442:LEU:HD23  | 1:A:443:PRO:CD    | 2.39                     | 0.53              |
| 1:A:678:THR:CG2   | 1:A:742:ILE:HB    | 2.39                     | 0.53              |
| 1:A:1226:ARG:O    | 1:A:1270:VAL:HG22 | 2.09                     | 0.53              |
| 1:A:1577:TYR:HB2  | 1:A:1600:PHE:O    | 2.09                     | 0.53              |
| 2:B:1273:LEU:HD12 | 2:B:1273:LEU:O    | 2.09                     | 0.53              |
| 2:B:1330:ASN:N    | 2:B:1330:ASN:ND2  | 2.56                     | 0.53              |
| 2:B:1371:TYR:CD1  | 2:B:1377:SER:HB3  | 2.43                     | 0.53              |
| 2:B:1482:ASN:H    | 2:B:1495:GLU:HG2  | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1609:ARG:CG   | 2:B:1609:ARG:NH1  | 2.63                     | 0.53              |
| 1:C:185:PHE:HD1   | 1:C:186:PRO:HD2   | 1.74                     | 0.53              |
| 1:C:433:PHE:N     | 1:C:433:PHE:HD1   | 2.07                     | 0.53              |
| 1:C:857:VAL:CG2   | 1:C:884:VAL:HG21  | 2.37                     | 0.53              |
| 1:C:1081:PHE:O    | 1:C:1084:ARG:N    | 2.42                     | 0.53              |
| 1:C:1533:GLY:O    | 1:C:1534:GLN:CB   | 2.56                     | 0.53              |
| 1:C:1563:VAL:HG22 | 1:C:1617:TYR:O    | 2.08                     | 0.53              |
| 2:D:315:TYR:O     | 2:D:315:TYR:HD1   | 1.91                     | 0.53              |
| 2:D:481:TYR:CE2   | 2:D:493:GLY:CA    | 2.90                     | 0.53              |
| 1:A:115:LYS:HB2   | 1:A:654:LEU:CD1   | 2.38                     | 0.53              |
| 2:B:819:GLN:HA    | 2:B:819:GLN:HE21  | 1.74                     | 0.53              |
| 2:B:1284:ARG:HG3  | 2:B:1286:VAL:N    | 2.21                     | 0.53              |
| 1:C:473:HIS:HE1   | 2:D:455:LYS:NZ    | 2.07                     | 0.53              |
| 1:C:1112:GLN:HB2  | 1:C:1118:PHE:HE1  | 1.73                     | 0.53              |
| 1:C:1244:THR:HG22 | 1:C:1246:ARG:N    | 2.23                     | 0.53              |
| 1:C:1279:ARG:NH1  | 1:C:1280:TYR:CE2  | 2.77                     | 0.53              |
| 1:C:1629:TYR:O    | 1:C:1630:ASN:HB2  | 2.09                     | 0.53              |
| 1:A:191:PRO:O     | 1:A:194:PRO:HD3   | 2.08                     | 0.53              |
| 1:A:1053:MET:CE   | 1:A:1089:VAL:HG21 | 2.38                     | 0.53              |
| 2:B:69:PHE:C      | 2:B:69:PHE:CD2    | 2.87                     | 0.53              |
| 2:B:105:VAL:HG12  | 2:B:118:VAL:HA    | 1.91                     | 0.53              |
| 2:B:224:PHE:CZ    | 2:B:329:VAL:HG13  | 2.44                     | 0.53              |
| 2:B:415:THR:O     | 2:B:425:GLN:NE2   | 2.42                     | 0.53              |
| 2:B:1446:PHE:CD2  | 2:B:1448:VAL:HG22 | 2.44                     | 0.53              |
| 1:C:25:ILE:HD13   | 1:C:41:ILE:HB     | 1.90                     | 0.53              |
| 1:C:847:ASN:HD22  | 1:C:888:VAL:HG13  | 1.72                     | 0.53              |
| 1:C:1628:LYS:HB3  | 1:C:1633:PHE:HD1  | 1.74                     | 0.53              |
| 2:D:523:TYR:HB3   | 2:D:533:ALA:HB2   | 1.91                     | 0.53              |
| 2:D:742:ASP:C     | 2:D:742:ASP:OD1   | 2.52                     | 0.53              |
| 2:D:819:GLN:HE21  | 2:D:819:GLN:HA    | 1.72                     | 0.53              |
| 2:D:1301:ARG:HB3  | 2:D:1301:ARG:HH11 | 1.74                     | 0.53              |
| 2:D:1590:LEU:CD2  | 2:D:1591:LEU:H    | 2.09                     | 0.53              |
| 1:A:125:PHE:CE1   | 1:A:627:LEU:HD21  | 2.43                     | 0.53              |
| 1:A:423:ASN:HB3   | 2:B:501:GLN:HE22  | 1.73                     | 0.53              |
| 1:A:461:SER:O     | 1:A:462:GLN:HB2   | 2.07                     | 0.53              |
| 1:A:463:SER:HB3   | 1:A:491:PRO:HA    | 1.91                     | 0.53              |
| 1:A:1411:SER:H    | 1:A:1414:GLU:HG3  | 1.73                     | 0.53              |
| 2:B:224:PHE:CE2   | 2:B:329:VAL:HG13  | 2.44                     | 0.53              |
| 1:C:495:LYS:HE2   | 1:C:495:LYS:CA    | 2.38                     | 0.53              |
| 1:C:1053:MET:CE   | 1:C:1089:VAL:HG21 | 2.39                     | 0.53              |
| 2:D:189:PRO:C     | 2:D:191:LEU:N     | 2.67                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:214:PHE:CD1   | 2:D:214:PHE:C     | 2.86                     | 0.53              |
| 2:D:342:PRO:HB2   | 2:D:343:TYR:CD1   | 2.43                     | 0.53              |
| 2:D:1305:THR:CG2  | 2:D:1307:LEU:H    | 2.20                     | 0.53              |
| 1:A:371:ILE:CG2   | 1:A:420:PHE:HB2   | 2.39                     | 0.53              |
| 1:A:520:ASP:N     | 1:A:520:ASP:OD1   | 2.41                     | 0.53              |
| 1:A:573:VAL:CG1   | 1:A:592:MET:HG2   | 2.39                     | 0.53              |
| 1:A:576:SER:HB2   | 1:A:589:SER:N     | 2.22                     | 0.53              |
| 1:A:641:ASN:O     | 1:A:642:ASN:C     | 2.50                     | 0.53              |
| 1:A:1139:GLU:OE1  | 1:A:1184:SER:HB3  | 2.09                     | 0.53              |
| 1:A:1143:TYR:O    | 1:A:1144:LEU:C    | 2.52                     | 0.53              |
| 1:A:1190:ILE:HG12 | 1:A:1253:TYR:CD1  | 2.44                     | 0.53              |
| 2:B:248:THR:HG22  | 2:B:289:ASP:OD1   | 2.09                     | 0.53              |
| 2:B:646:GLN:CB    | 2:B:647:PRO:HD2   | 2.30                     | 0.53              |
| 2:B:1456:VAL:O    | 2:B:1456:VAL:HG12 | 2.09                     | 0.53              |
| 1:C:433:PHE:N     | 1:C:433:PHE:CD1   | 2.77                     | 0.53              |
| 1:C:824:PHE:CE2   | 1:C:846:TYR:HD1   | 2.27                     | 0.53              |
| 1:C:1183:GLN:NE2  | 1:C:1232:LEU:HD22 | 2.23                     | 0.53              |
| 1:C:1264:ILE:O    | 1:C:1267:VAL:HB   | 2.09                     | 0.53              |
| 2:D:1284:ARG:NE   | 2:D:1285:GLU:H    | 2.07                     | 0.53              |
| 1:A:516:GLU:N     | 1:A:516:GLU:OE1   | 2.42                     | 0.52              |
| 1:A:598:SER:O     | 1:A:599:TRP:HD1   | 1.91                     | 0.52              |
| 1:A:706:ASN:HB2   | 1:A:714:ARG:NH1   | 2.24                     | 0.52              |
| 1:A:779:LEU:O     | 1:A:781:PRO:HD3   | 2.09                     | 0.52              |
| 1:A:1191:SER:O    | 1:A:1194:ALA:HB3  | 2.08                     | 0.52              |
| 1:A:1307:LEU:HD22 | 1:A:1307:LEU:N    | 2.24                     | 0.52              |
| 1:A:1551:THR:O    | 1:A:1557:ILE:HG13 | 2.08                     | 0.52              |
| 2:B:131:GLN:OE1   | 2:B:146:ARG:NH1   | 2.41                     | 0.52              |
| 2:B:159:LYS:HD3   | 2:B:180:LEU:HD12  | 1.91                     | 0.52              |
| 2:B:228:LEU:HD22  | 2:B:247:ILE:HG12  | 1.91                     | 0.52              |
| 2:B:276:ILE:O     | 2:B:277:PRO:C     | 2.52                     | 0.52              |
| 2:B:1391:LEU:HD12 | 2:B:1417:MET:HE2  | 1.90                     | 0.52              |
| 1:C:23:TYR:CE1    | 1:C:655:THR:HB    | 2.43                     | 0.52              |
| 1:C:224:LEU:CD2   | 1:C:225:PRO:HD2   | 2.28                     | 0.52              |
| 1:C:308:LYS:HB3   | 1:C:309:GLU:OE1   | 2.09                     | 0.52              |
| 1:C:309:GLU:O     | 1:C:312:TYR:N     | 2.41                     | 0.52              |
| 1:C:549:GLU:CD    | 1:C:549:GLU:N     | 2.56                     | 0.52              |
| 1:C:678:THR:HG21  | 1:C:742:ILE:HB    | 1.91                     | 0.52              |
| 1:C:825:LEU:HD12  | 1:C:844:THR:O     | 2.08                     | 0.52              |
| 1:C:1066:TYR:N    | 1:C:1066:TYR:CD1  | 2.75                     | 0.52              |
| 2:D:107:GLN:HG3   | 2:D:116:GLU:HG3   | 1.91                     | 0.52              |
| 2:D:844:ILE:O     | 2:D:871:PRO:HA    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:23:TYR:CE1    | 1:A:655:THR:HB   | 2.43                     | 0.52              |
| 1:A:54:ILE:O      | 1:A:68:SER:HA    | 2.09                     | 0.52              |
| 1:A:185:PHE:HD1   | 1:A:186:PRO:HD2  | 1.73                     | 0.52              |
| 1:A:268:THR:CG2   | 1:A:282:MET:HE3  | 2.37                     | 0.52              |
| 1:A:371:ILE:HG22  | 1:A:371:ILE:O    | 2.08                     | 0.52              |
| 1:A:433:PHE:CE1   | 1:A:452:TYR:HB2  | 2.45                     | 0.52              |
| 1:A:535:VAL:HG23  | 1:A:536:PRO:CD   | 2.28                     | 0.52              |
| 1:A:903:LEU:HD22  | 1:A:903:LEU:N    | 2.24                     | 0.52              |
| 1:A:998:ASN:HB3   | 1:A:1000:LEU:HG  | 1.89                     | 0.52              |
| 1:A:1022:PHE:O    | 1:A:1024:TYR:N   | 2.42                     | 0.52              |
| 1:A:1159:CYS:N    | 1:A:1160:PRO:CD  | 2.73                     | 0.52              |
| 1:A:1562:LYS:HD3  | 1:A:1648:TRP:HE1 | 1.74                     | 0.52              |
| 2:B:598:ILE:HD11  | 2:B:800:ILE:HG21 | 1.91                     | 0.52              |
| 2:B:804:GLU:OE1   | 2:B:805:PRO:HD2  | 2.10                     | 0.52              |
| 2:B:1443:LEU:N    | 2:B:1443:LEU:CD1 | 2.72                     | 0.52              |
| 1:C:501:TYR:O     | 1:C:501:TYR:HD1  | 1.91                     | 0.52              |
| 1:C:970:LYS:O     | 1:C:971:THR:CG2  | 2.57                     | 0.52              |
| 1:C:1268:ASN:HB2  | 1:C:1269:PRO:HD3 | 1.91                     | 0.52              |
| 1:C:1411:SER:H    | 1:C:1414:GLU:HG3 | 1.73                     | 0.52              |
| 1:C:1571:GLU:O    | 1:C:1574:PHE:CD2 | 2.62                     | 0.52              |
| 2:D:353:TYR:CD2   | 2:D:614:GLY:C    | 2.87                     | 0.52              |
| 2:D:438:GLN:CD    | 2:D:530:GLU:HG3  | 2.35                     | 0.52              |
| 2:D:813:VAL:HG12  | 2:D:839:TYR:O    | 2.09                     | 0.52              |
| 2:D:1457:LYS:HG2  | 2:D:1469:THR:HG1 | 1.73                     | 0.52              |
| 1:A:165:ASP:HB2   | 1:A:166:PRO:HD2  | 1.91                     | 0.52              |
| 1:A:491:PRO:CG    | 1:A:494:ASP:CB   | 2.88                     | 0.52              |
| 1:A:494:ASP:CG    | 1:A:494:ASP:O    | 2.52                     | 0.52              |
| 1:A:824:PHE:CE2   | 1:A:846:TYR:HD1  | 2.28                     | 0.52              |
| 1:A:837:GLU:C     | 1:A:901:LEU:HD12 | 2.34                     | 0.52              |
| 1:A:840:GLN:NE2   | 1:A:897:THR:HG21 | 2.24                     | 0.52              |
| 1:A:938:SER:O     | 1:A:940:SER:N    | 2.43                     | 0.52              |
| 1:A:1068:VAL:HG21 | 1:A:1124:TYR:HD1 | 1.73                     | 0.52              |
| 2:B:145:TYR:C     | 2:B:145:TYR:CD1  | 2.88                     | 0.52              |
| 2:B:262:PHE:CD1   | 2:B:282:ARG:HG3  | 2.44                     | 0.52              |
| 2:B:813:VAL:HG12  | 2:B:839:TYR:O    | 2.08                     | 0.52              |
| 2:B:1527:LYS:HE2  | 2:B:1578:ASN:OD1 | 2.09                     | 0.52              |
| 1:C:307:VAL:O     | 1:C:308:LYS:O    | 2.27                     | 0.52              |
| 1:C:961:TYR:HB2   | 1:C:1345:ASP:OD2 | 2.10                     | 0.52              |
| 1:C:1493:PHE:CD1  | 1:C:1494:THR:N   | 2.76                     | 0.52              |
| 2:D:762:LEU:HD12  | 2:D:762:LEU:H    | 1.74                     | 0.52              |
| 1:A:560:TRP:CH2   | 1:A:562:ASN:HB2  | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:606:ASP:O     | 1:A:609:VAL:HG23  | 2.09                     | 0.52              |
| 1:A:702:GLY:CA    | 1:A:728:PHE:CD1   | 2.93                     | 0.52              |
| 1:A:1565:ILE:HG22 | 1:A:1566:THR:H    | 1.74                     | 0.52              |
| 2:B:353:TYR:HA    | 2:B:433:ILE:O     | 2.09                     | 0.52              |
| 2:B:829:GLN:HE21  | 2:B:830:VAL:N     | 2.07                     | 0.52              |
| 2:B:840:VAL:HG12  | 2:B:841:ASN:H     | 1.74                     | 0.52              |
| 2:B:881:PRO:O     | 2:B:882:PHE:CD2   | 2.63                     | 0.52              |
| 2:B:1445:HIS:CG   | 2:B:1446:PHE:N    | 2.77                     | 0.52              |
| 1:C:269:PHE:CG    | 1:C:301:PHE:CE1   | 2.97                     | 0.52              |
| 1:C:924:VAL:HG21  | 3:C:2003:NAG:C8   | 2.38                     | 0.52              |
| 1:C:1012:LEU:HD13 | 1:C:1081:PHE:CD2  | 2.44                     | 0.52              |
| 1:C:1161:LEU:O    | 1:C:1164:ILE:HG12 | 2.09                     | 0.52              |
| 2:D:766:PRO:HA    | 2:D:771:ILE:O     | 2.09                     | 0.52              |
| 2:D:842:GLU:O     | 2:D:843:ASP:C     | 2.53                     | 0.52              |
| 2:D:1529:LEU:O    | 2:D:1577:VAL:HG13 | 2.08                     | 0.52              |
| 1:A:1129:LEU:HD23 | 1:A:1129:LEU:N    | 2.22                     | 0.52              |
| 1:A:1224:ILE:HG22 | 1:A:1225:TYR:CD2  | 2.45                     | 0.52              |
| 2:B:1326:LEU:HD11 | 2:B:1328:PHE:CE2  | 2.44                     | 0.52              |
| 1:C:96:GLN:HG3    | 1:C:97:ASN:ND2    | 2.24                     | 0.52              |
| 1:C:191:PRO:HD2   | 1:C:194:PRO:HB3   | 1.92                     | 0.52              |
| 1:C:560:TRP:CE3   | 1:C:673:LEU:HD22  | 2.44                     | 0.52              |
| 1:C:1421:HIS:CD2  | 1:C:1422:ALA:N    | 2.76                     | 0.52              |
| 2:D:415:THR:O     | 2:D:425:GLN:NE2   | 2.43                     | 0.52              |
| 2:D:581:ASP:O     | 2:D:582:LYS:C     | 2.50                     | 0.52              |
| 2:D:1277:ILE:HG22 | 2:D:1290:TYR:HB2  | 1.91                     | 0.52              |
| 2:D:1289:ARG:C    | 2:D:1290:TYR:HD1  | 2.18                     | 0.52              |
| 1:A:132:LYS:HZ1   | 1:A:139:GLN:HE22  | 1.52                     | 0.52              |
| 1:A:163:PHE:HE2   | 1:A:201:ILE:HD13  | 1.74                     | 0.52              |
| 1:A:694:VAL:O     | 1:A:697:LYS:HE3   | 2.10                     | 0.52              |
| 1:A:862:VAL:HB    | 1:A:865:ILE:HG13  | 1.92                     | 0.52              |
| 1:A:924:VAL:HG21  | 3:A:2003:NAG:C8   | 2.38                     | 0.52              |
| 1:A:1022:PHE:O    | 1:A:1023:HIS:C    | 2.51                     | 0.52              |
| 1:A:1423:VAL:HG11 | 1:A:1496:TYR:CE1  | 2.45                     | 0.52              |
| 1:A:1590:ALA:HB1  | 1:A:1635:TYR:CD1  | 2.44                     | 0.52              |
| 2:B:235:PHE:HE2   | 2:B:299:PHE:CE2   | 2.28                     | 0.52              |
| 2:B:746:ILE:H     | 2:B:746:ILE:HD13  | 1.74                     | 0.52              |
| 1:C:228:SER:HB3   | 1:C:253:ARG:HG2   | 1.92                     | 0.52              |
| 1:C:238:ILE:HD12  | 1:C:347:TYR:CE1   | 2.44                     | 0.52              |
| 1:C:998:ASN:HB3   | 1:C:1000:LEU:HG   | 1.90                     | 0.52              |
| 1:C:1031:TRP:CH2  | 1:C:1042:LYS:HG3  | 2.45                     | 0.52              |
| 1:C:1268:ASN:ND2  | 1:C:1268:ASN:H    | 2.06                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1487:PHE:O    | 1:C:1488:LEU:C    | 2.53                     | 0.52              |
| 2:D:1504:GLU:OE2  | 2:D:1505:ARG:N    | 2.43                     | 0.52              |
| 1:A:1475:VAL:CG2  | 1:A:1476:ARG:N    | 2.72                     | 0.52              |
| 2:B:755:TRP:O     | 2:B:756:LEU:HB3   | 2.10                     | 0.52              |
| 2:B:1290:TYR:CE2  | 2:B:1301:ARG:HB3  | 2.45                     | 0.52              |
| 1:C:153:LYS:O     | 1:C:154:PRO:C     | 2.53                     | 0.52              |
| 1:C:1023:HIS:O    | 1:C:1027:THR:HB   | 2.10                     | 0.52              |
| 2:D:44:GLU:HG2    | 2:D:82:LEU:CB     | 2.36                     | 0.52              |
| 2:D:127:PHE:O     | 2:D:149:SER:HA    | 2.10                     | 0.52              |
| 2:D:203:TYR:O     | 2:D:204:GLU:C     | 2.53                     | 0.52              |
| 2:D:860:SER:OG    | 2:D:866:TYR:N     | 2.42                     | 0.52              |
| 2:D:1354:LEU:O    | 2:D:1354:LEU:HD23 | 2.09                     | 0.52              |
| 1:A:1454:GLN:C    | 1:A:1455:ILE:HD12 | 2.35                     | 0.52              |
| 2:B:436:GLN:O     | 2:B:437:THR:C     | 2.53                     | 0.52              |
| 2:B:822:TYR:O     | 2:B:914:LYS:HB3   | 2.10                     | 0.52              |
| 2:B:1341:ASN:HD22 | 2:B:1342:LYS:HG2  | 1.73                     | 0.52              |
| 2:B:1480:LEU:HD21 | 2:B:1483:LYS:NZ   | 2.25                     | 0.52              |
| 2:B:1525:LYS:HD2  | 2:B:1610:TRP:CH2  | 2.45                     | 0.52              |
| 1:C:267:ILE:CD1   | 1:C:299:VAL:HG11  | 2.39                     | 0.52              |
| 1:C:365:PRO:CG    | 1:C:464:TYR:CE2   | 2.91                     | 0.52              |
| 1:C:582:TYR:CE2   | 1:C:817:ALA:HB1   | 2.45                     | 0.52              |
| 1:C:678:THR:CG2   | 1:C:742:ILE:HB    | 2.40                     | 0.52              |
| 1:C:730:GLU:O     | 1:C:734:VAL:HG23  | 2.10                     | 0.52              |
| 1:C:840:GLN:NE2   | 1:C:897:THR:HG21  | 2.24                     | 0.52              |
| 1:C:1016:VAL:HG21 | 1:C:1291:ILE:HD12 | 1.92                     | 0.52              |
| 1:C:1559:TYR:HE1  | 1:C:1587:THR:HA   | 1.75                     | 0.52              |
| 2:D:27:LEU:O      | 2:D:628:LEU:HD12  | 2.10                     | 0.52              |
| 2:D:59:HIS:HA     | 2:D:68:LEU:HD22   | 1.91                     | 0.52              |
| 2:D:952:ASP:OD1   | 2:D:952:ASP:N     | 2.43                     | 0.52              |
| 2:D:1556:PRO:O    | 2:D:1558:ALA:N    | 2.43                     | 0.52              |
| 1:A:111:PHE:CD2   | 1:A:112:SER:N     | 2.76                     | 0.52              |
| 1:A:316:GLU:O     | 1:A:349:LEU:HD21  | 2.10                     | 0.52              |
| 1:A:430:VAL:HG11  | 1:A:453:ARG:NH2   | 2.20                     | 0.52              |
| 1:A:489:LYS:CG    | 1:A:490:SER:H     | 2.22                     | 0.52              |
| 1:A:1053:MET:HE3  | 1:A:1086:LEU:HD22 | 1.91                     | 0.52              |
| 1:A:1488:LEU:HD12 | 1:A:1488:LEU:C    | 2.35                     | 0.52              |
| 2:B:109:THR:HG22  | 2:B:114:ARG:HB3   | 1.91                     | 0.52              |
| 2:B:236:TYR:C     | 2:B:238:ASP:N     | 2.68                     | 0.52              |
| 2:B:1327:THR:HG22 | 2:B:1328:PHE:N    | 2.25                     | 0.52              |
| 1:C:101:TYR:CE1   | 1:C:116:ARG:NH2   | 2.78                     | 0.52              |
| 1:C:113:LYS:CG    | 1:C:114:SER:H     | 2.19                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:371:ILE:HD11  | 1:C:433:PHE:CD2   | 2.44                     | 0.52              |
| 1:C:837:GLU:C     | 1:C:901:LEU:HD12  | 2.34                     | 0.52              |
| 1:C:1190:ILE:HG12 | 1:C:1253:TYR:CD1  | 2.45                     | 0.52              |
| 1:C:1279:ARG:HB2  | 1:C:1284:PHE:HB2  | 1.92                     | 0.52              |
| 1:C:1488:LEU:HD12 | 1:C:1488:LEU:C    | 2.35                     | 0.52              |
| 1:C:1560:ALA:O    | 1:C:1585:TYR:CD2  | 2.63                     | 0.52              |
| 2:D:365:TYR:HD1   | 2:D:395:THR:HG22  | 1.75                     | 0.52              |
| 2:D:481:TYR:CD2   | 2:D:481:TYR:C     | 2.87                     | 0.52              |
| 2:D:916:VAL:HG22  | 2:D:917:PRO:O     | 2.10                     | 0.52              |
| 1:A:23:TYR:CD1    | 1:A:23:TYR:C      | 2.88                     | 0.52              |
| 2:B:25:TYR:CE2    | 2:B:113:VAL:HG22  | 2.44                     | 0.52              |
| 2:B:44:GLU:HG2    | 2:B:82:LEU:CB     | 2.37                     | 0.52              |
| 2:B:553:ASP:CG    | 2:B:555:LEU:HD11  | 2.34                     | 0.52              |
| 2:B:1556:PRO:O    | 2:B:1558:ALA:N    | 2.43                     | 0.52              |
| 1:C:238:ILE:HB    | 1:C:347:TYR:CD1   | 2.45                     | 0.52              |
| 1:C:706:ASN:ND2   | 1:C:709:GLU:H     | 2.07                     | 0.52              |
| 1:C:947:ARG:NH1   | 1:C:1352:PHE:CE2  | 2.78                     | 0.52              |
| 1:C:1128:LYS:HD3  | 1:C:1414:GLU:OE1  | 2.10                     | 0.52              |
| 1:C:1440:LYS:HD3  | 1:C:1453:TYR:OH   | 2.09                     | 0.52              |
| 2:D:235:PHE:HE2   | 2:D:299:PHE:CE2   | 2.28                     | 0.52              |
| 2:D:302:ARG:HG3   | 2:D:303:PHE:CD1   | 2.45                     | 0.52              |
| 2:D:319:THR:HG23  | 2:D:330:VAL:HG12  | 1.92                     | 0.52              |
| 2:D:348:THR:O     | 2:D:348:THR:OG1   | 2.23                     | 0.52              |
| 2:D:829:GLN:HG3   | 2:D:1480:LEU:HD13 | 1.92                     | 0.52              |
| 2:D:829:GLN:HE21  | 2:D:830:VAL:N     | 2.08                     | 0.52              |
| 2:D:1296:ASN:O    | 2:D:1297:ALA:C    | 2.53                     | 0.52              |
| 2:D:1525:LYS:HD2  | 2:D:1610:TRP:CH2  | 2.45                     | 0.52              |
| 1:A:144:ARG:HD2   | 1:A:146:TYR:HE1   | 1.74                     | 0.51              |
| 1:A:549:GLU:CD    | 1:A:549:GLU:N     | 2.57                     | 0.51              |
| 1:A:1020:TYR:CE1  | 1:A:1295:GLU:HG3  | 2.45                     | 0.51              |
| 2:B:69:PHE:CD2    | 2:B:87:ILE:HG22   | 2.45                     | 0.51              |
| 2:B:945:ILE:HD12  | 2:B:945:ILE:N     | 2.26                     | 0.51              |
| 1:C:1096:ASN:O    | 1:C:1099:SER:HB3  | 2.09                     | 0.51              |
| 1:C:1190:ILE:HG12 | 1:C:1253:TYR:CE1  | 2.45                     | 0.51              |
| 1:C:1311:MET:HG2  | 1:C:1313:ILE:HG12 | 1.91                     | 0.51              |
| 1:C:1564:SER:HB2  | 1:C:1616:GLN:HG3  | 1.92                     | 0.51              |
| 1:A:307:VAL:O     | 1:A:308:LYS:O     | 2.27                     | 0.51              |
| 1:A:702:GLY:HA3   | 1:A:728:PHE:CD1   | 2.45                     | 0.51              |
| 1:A:947:ARG:O     | 1:A:949:ILE:HG12  | 2.09                     | 0.51              |
| 1:A:1227:PHE:CD2  | 1:A:1273:TRP:NE1  | 2.78                     | 0.51              |
| 2:B:69:PHE:CE2    | 2:B:71:THR:HB     | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:640:SER:O     | 2:B:641:ALA:CB    | 2.57                     | 0.51              |
| 2:B:849:GLU:OE2   | 2:B:865:ARG:HD2   | 2.10                     | 0.51              |
| 1:C:42:GLN:CG     | 1:C:43:VAL:N      | 2.71                     | 0.51              |
| 1:C:138:ASP:OD1   | 1:C:192:SER:HA    | 2.10                     | 0.51              |
| 1:C:178:ASP:OD2   | 1:C:179:HIS:N     | 2.43                     | 0.51              |
| 1:C:478:VAL:HG21  | 1:C:532:GLN:OE1   | 2.10                     | 0.51              |
| 1:C:956:ARG:HG2   | 1:C:1349:SER:HB3  | 1.92                     | 0.51              |
| 1:C:1040:ILE:O    | 1:C:1043:GLN:HB2  | 2.10                     | 0.51              |
| 1:C:1077:TRP:O    | 1:C:1080:ALA:HB3  | 2.10                     | 0.51              |
| 1:C:1423:VAL:HG11 | 1:C:1496:TYR:CE1  | 2.45                     | 0.51              |
| 2:D:155:SER:O     | 2:D:156:LYS:HG2   | 2.10                     | 0.51              |
| 2:D:443:ASN:OD1   | 2:D:469:ASN:HB3   | 2.10                     | 0.51              |
| 2:D:462:VAL:CG1   | 2:D:506:MET:HE3   | 2.40                     | 0.51              |
| 2:D:481:TYR:HE2   | 2:D:493:GLY:HA3   | 1.74                     | 0.51              |
| 2:D:481:TYR:CB    | 2:D:520:PHE:HE1   | 2.16                     | 0.51              |
| 2:D:640:SER:O     | 2:D:641:ALA:HB2   | 2.08                     | 0.51              |
| 2:D:843:ASP:HA    | 2:D:873:LYS:O     | 2.10                     | 0.51              |
| 2:D:853:ASN:C     | 2:D:853:ASN:OD1   | 2.53                     | 0.51              |
| 2:D:918:GLU:N     | 2:D:918:GLU:OE2   | 2.43                     | 0.51              |
| 2:D:944:VAL:HG22  | 2:D:1312:THR:HG1  | 1.74                     | 0.51              |
| 2:D:1273:LEU:HD12 | 2:D:1273:LEU:O    | 2.09                     | 0.51              |
| 2:D:1330:ASN:N    | 2:D:1330:ASN:ND2  | 2.59                     | 0.51              |
| 1:A:31:PHE:HB2    | 1:A:119:ILE:HG22  | 1.92                     | 0.51              |
| 1:A:165:ASP:OD2   | 1:A:165:ASP:O     | 2.28                     | 0.51              |
| 1:A:191:PRO:HD2   | 1:A:194:PRO:HB3   | 1.91                     | 0.51              |
| 2:B:952:ASP:O     | 2:B:1331:ALA:HA   | 2.10                     | 0.51              |
| 2:B:1292:ILE:HD11 | 2:B:1301:ARG:HE   | 1.76                     | 0.51              |
| 2:B:1367:ILE:HD13 | 2:B:1456:VAL:HG21 | 1.92                     | 0.51              |
| 1:C:315:LEU:CD1   | 1:C:318:LEU:HG    | 2.40                     | 0.51              |
| 1:C:491:PRO:CG    | 1:C:494:ASP:CB    | 2.88                     | 0.51              |
| 1:C:694:VAL:O     | 1:C:697:LYS:HE3   | 2.10                     | 0.51              |
| 1:C:1031:TRP:CZ2  | 1:C:1042:LYS:HG3  | 2.45                     | 0.51              |
| 1:C:1229:LYS:HZ3  | 1:C:1240:PRO:HD2  | 1.75                     | 0.51              |
| 2:D:130:ILE:HA    | 2:D:147:VAL:HG23  | 1.92                     | 0.51              |
| 2:D:518:PHE:C     | 2:D:518:PHE:CD2   | 2.88                     | 0.51              |
| 2:D:1445:HIS:CG   | 2:D:1446:PHE:N    | 2.79                     | 0.51              |
| 1:A:369:TYR:HB3   | 1:A:422:LEU:CD1   | 2.41                     | 0.51              |
| 2:B:47:GLY:O      | 2:B:48:ASP:HB2    | 2.09                     | 0.51              |
| 2:B:252:LEU:HD22  | 2:B:582:LYS:HB3   | 1.92                     | 0.51              |
| 2:B:814:PHE:HZ    | 2:B:846:VAL:HG21  | 1.75                     | 0.51              |
| 2:B:1623:LYS:NZ   | 2:B:1623:LYS:CB   | 2.74                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:594:THR:OG1   | 1:C:782:ARG:HA    | 2.11                     | 0.51              |
| 1:C:633:GLY:O     | 1:C:634:CYS:HB2   | 2.11                     | 0.51              |
| 1:C:874:ASP:O     | 1:C:875:HIS:CG    | 2.63                     | 0.51              |
| 1:C:984:VAL:O     | 1:C:984:VAL:HG13  | 2.10                     | 0.51              |
| 1:C:1110:ASN:N    | 1:C:1110:ASN:OD1  | 2.44                     | 0.51              |
| 1:C:1146:ALA:O    | 1:C:1147:PHE:C    | 2.53                     | 0.51              |
| 1:C:1618:LEU:O    | 1:C:1618:LEU:HD13 | 2.11                     | 0.51              |
| 2:D:161:VAL:CG2   | 2:D:180:LEU:HD21  | 2.36                     | 0.51              |
| 2:D:467:LYS:HG2   | 2:D:468:GLY:N     | 2.25                     | 0.51              |
| 2:D:961:THR:HG22  | 2:D:1327:THR:CB   | 2.41                     | 0.51              |
| 2:D:1301:ARG:HB3  | 2:D:1301:ARG:NH1  | 2.25                     | 0.51              |
| 2:D:1480:LEU:HD21 | 2:D:1483:LYS:NZ   | 2.25                     | 0.51              |
| 2:D:1628:PHE:O    | 2:D:1629:ALA:C    | 2.52                     | 0.51              |
| 1:A:96:GLN:O      | 1:A:97:ASN:O      | 2.29                     | 0.51              |
| 1:A:478:VAL:HG21  | 1:A:532:GLN:OE1   | 2.11                     | 0.51              |
| 1:A:486:VAL:HG11  | 1:A:499:TYR:CE1   | 2.45                     | 0.51              |
| 1:A:594:THR:OG1   | 1:A:782:ARG:HA    | 2.10                     | 0.51              |
| 1:A:730:GLU:O     | 1:A:734:VAL:HG23  | 2.10                     | 0.51              |
| 1:A:1279:ARG:NH1  | 1:A:1280:TYR:CE2  | 2.79                     | 0.51              |
| 1:A:1618:LEU:HD22 | 1:A:1618:LEU:C    | 2.35                     | 0.51              |
| 2:B:27:LEU:HD13   | 2:B:43:VAL:HG23   | 1.91                     | 0.51              |
| 2:B:214:PHE:CD1   | 2:B:214:PHE:C     | 2.88                     | 0.51              |
| 2:B:242:ASN:OD1   | 2:B:295:LYS:HD2   | 2.10                     | 0.51              |
| 2:B:353:TYR:CD2   | 2:B:614:GLY:O     | 2.64                     | 0.51              |
| 2:B:481:TYR:HE2   | 2:B:493:GLY:HA3   | 1.74                     | 0.51              |
| 2:B:523:TYR:CB    | 2:B:533:ALA:HB2   | 2.41                     | 0.51              |
| 1:C:101:TYR:HE1   | 1:C:116:ARG:NH2   | 2.08                     | 0.51              |
| 1:C:145:VAL:CB    | 1:C:183:ILE:HD12  | 2.33                     | 0.51              |
| 1:C:1016:VAL:HG11 | 1:C:1291:ILE:CG1  | 2.41                     | 0.51              |
| 1:C:1139:GLU:OE2  | 1:C:1187:THR:OG1  | 2.26                     | 0.51              |
| 1:C:1590:ALA:HB1  | 1:C:1635:TYR:CD1  | 2.44                     | 0.51              |
| 2:D:69:PHE:CE2    | 2:D:71:THR:HB     | 2.45                     | 0.51              |
| 2:D:210:TYR:CG    | 2:D:211:THR:N     | 2.79                     | 0.51              |
| 2:D:218:LYS:CD    | 2:D:822:TYR:HE2   | 2.23                     | 0.51              |
| 2:D:840:VAL:HG12  | 2:D:841:ASN:H     | 1.75                     | 0.51              |
| 2:D:881:PRO:O     | 2:D:882:PHE:CD2   | 2.64                     | 0.51              |
| 2:D:1548:ILE:HD12 | 2:D:1636:THR:OG1  | 2.10                     | 0.51              |
| 1:A:1110:ASN:OD1  | 1:A:1110:ASN:N    | 2.43                     | 0.51              |
| 1:A:1265:ASN:C    | 1:A:1267:VAL:H    | 2.17                     | 0.51              |
| 1:A:1279:ARG:HH21 | 1:A:1362:THR:HG21 | 1.75                     | 0.51              |
| 1:A:1533:GLY:O    | 1:A:1534:GLN:CB   | 2.54                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1296:ASN:O    | 2:B:1297:ALA:C    | 2.53                     | 0.51              |
| 2:B:1635:LEU:O    | 2:B:1636:THR:C    | 2.53                     | 0.51              |
| 1:C:268:THR:CG2   | 1:C:282:MET:HE3   | 2.39                     | 0.51              |
| 1:C:706:ASN:HB2   | 1:C:714:ARG:NH1   | 2.25                     | 0.51              |
| 1:C:961:TYR:O     | 1:C:961:TYR:CD1   | 2.64                     | 0.51              |
| 1:C:987:ILE:HG22  | 1:C:1021:VAL:HG23 | 1.92                     | 0.51              |
| 2:D:78:ALA:C      | 2:D:80:GLY:H      | 2.18                     | 0.51              |
| 2:D:257:VAL:HG12  | 2:D:258:GLU:N     | 2.25                     | 0.51              |
| 2:D:390:THR:HG22  | 2:D:395:THR:N     | 2.26                     | 0.51              |
| 1:A:138:ASP:OD1   | 1:A:192:SER:HA    | 2.10                     | 0.51              |
| 1:A:1377:PHE:CD2  | 1:A:1495:VAL:HG22 | 2.45                     | 0.51              |
| 1:A:1381:ILE:HD12 | 1:A:1493:PHE:HD2  | 1.76                     | 0.51              |
| 1:A:1568:ILE:HG23 | 1:A:1577:TYR:CE1  | 2.41                     | 0.51              |
| 2:B:263:VAL:HG22  | 2:B:318:VAL:HG23  | 1.92                     | 0.51              |
| 2:B:345:ILE:HG13  | 2:B:428:LYS:CB    | 2.40                     | 0.51              |
| 2:B:390:THR:HG22  | 2:B:394:GLY:C     | 2.35                     | 0.51              |
| 2:B:518:PHE:O     | 2:B:518:PHE:CD2   | 2.63                     | 0.51              |
| 2:B:1278:THR:HB   | 2:B:1314:THR:HB   | 1.92                     | 0.51              |
| 1:C:33:VAL:HG23   | 1:C:120:THR:O     | 2.10                     | 0.51              |
| 1:C:862:VAL:HB    | 1:C:865:ILE:HG13  | 1.92                     | 0.51              |
| 1:C:947:ARG:O     | 1:C:949:ILE:N     | 2.44                     | 0.51              |
| 1:C:1563:VAL:HG12 | 1:C:1581:LEU:HD23 | 1.91                     | 0.51              |
| 2:D:198:ARG:HB3   | 2:D:213:TYR:CE1   | 2.46                     | 0.51              |
| 2:D:251:TYR:CD2   | 2:D:257:VAL:HG22  | 2.45                     | 0.51              |
| 2:D:922:LYS:HE3   | 2:D:1329:TYR:OH   | 2.10                     | 0.51              |
| 2:D:1591:LEU:C    | 2:D:1591:LEU:CD2  | 2.84                     | 0.51              |
| 1:A:115:LYS:HE2   | 1:A:654:LEU:HD11  | 1.93                     | 0.51              |
| 1:A:288:GLN:O     | 1:A:289:ASN:C     | 2.54                     | 0.51              |
| 1:A:351:PRO:HG2   | 1:A:352:TYR:HD2   | 1.67                     | 0.51              |
| 1:A:1188:LEU:HD23 | 1:A:1212:LEU:HA   | 1.93                     | 0.51              |
| 1:A:1421:HIS:CE1  | 1:A:1498:TYR:CD1  | 2.98                     | 0.51              |
| 1:A:1612:VAL:HB   | 1:A:1615:ARG:HB3  | 1.93                     | 0.51              |
| 1:A:1628:LYS:HB3  | 1:A:1633:PHE:HD1  | 1.76                     | 0.51              |
| 2:B:59:HIS:HA     | 2:B:68:LEU:HD22   | 1.92                     | 0.51              |
| 2:B:283:ILE:N     | 2:B:283:ILE:HD12  | 2.25                     | 0.51              |
| 2:B:469:ASN:CG    | 2:B:472:SER:HB2   | 2.35                     | 0.51              |
| 2:B:853:ASN:C     | 2:B:853:ASN:OD1   | 2.54                     | 0.51              |
| 1:C:902:PRO:C     | 1:C:903:LEU:HD22  | 2.36                     | 0.51              |
| 1:C:1132:THR:HB   | 1:C:1134:PRO:HD2  | 1.93                     | 0.51              |
| 1:C:1483:PHE:O    | 1:C:1485:VAL:HG13 | 2.11                     | 0.51              |
| 1:C:1554:LYS:CG   | 1:C:1555:PRO:HD2  | 2.41                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1560:ALA:HB1  | 1:C:1620:MET:CG   | 2.40                     | 0.51              |
| 1:C:1616:GLN:NE2  | 1:C:1648:TRP:CZ3  | 2.79                     | 0.51              |
| 2:D:197:TRP:HB2   | 2:D:214:PHE:CD1   | 2.46                     | 0.51              |
| 2:D:248:THR:HG22  | 2:D:289:ASP:OD1   | 2.10                     | 0.51              |
| 2:D:830:VAL:CG2   | 2:D:831:GLU:N     | 2.71                     | 0.51              |
| 1:A:146:TYR:HD1   | 1:A:182:ILE:HG23  | 1.73                     | 0.51              |
| 1:A:365:PRO:HD2   | 1:A:464:TYR:CE2   | 2.45                     | 0.51              |
| 1:A:884:VAL:O     | 1:A:885:ARG:CB    | 2.49                     | 0.51              |
| 1:A:1150:ILE:HG22 | 1:A:1151:GLY:N    | 2.25                     | 0.51              |
| 2:B:319:THR:HG23  | 2:B:330:VAL:HG12  | 1.93                     | 0.51              |
| 2:B:746:ILE:HD13  | 2:B:746:ILE:N     | 2.26                     | 0.51              |
| 1:C:240:TYR:HA    | 1:C:243:PHE:HB2   | 1.91                     | 0.51              |
| 1:C:283:MET:HE1   | 1:C:301:PHE:HZ    | 1.75                     | 0.51              |
| 1:C:357:VAL:O     | 1:C:359:THR:HG22  | 2.11                     | 0.51              |
| 1:C:369:TYR:HB3   | 1:C:422:LEU:CD1   | 2.41                     | 0.51              |
| 1:C:477:LEU:HD22  | 1:C:477:LEU:N     | 2.26                     | 0.51              |
| 1:C:618:LYS:N     | 1:C:619:PRO:CD    | 2.73                     | 0.51              |
| 1:C:825:LEU:HB2   | 1:C:845:VAL:HG23  | 1.92                     | 0.51              |
| 1:C:1188:LEU:HD23 | 1:C:1212:LEU:HA   | 1.93                     | 0.51              |
| 2:D:44:GLU:OE2    | 2:D:523:TYR:OH    | 2.28                     | 0.51              |
| 2:D:464:PHE:O     | 2:D:503:LEU:HA    | 2.10                     | 0.51              |
| 2:D:629:THR:HA    | 2:D:635:ASN:OD1   | 2.10                     | 0.51              |
| 2:D:945:ILE:HD12  | 2:D:945:ILE:N     | 2.26                     | 0.51              |
| 2:D:1635:LEU:O    | 2:D:1636:THR:C    | 2.53                     | 0.51              |
| 1:A:25:ILE:HD13   | 1:A:41:ILE:HB     | 1.91                     | 0.51              |
| 1:A:391:ASN:O     | 1:A:392:ALA:HB2   | 2.11                     | 0.51              |
| 1:A:501:TYR:CD1   | 1:A:501:TYR:C     | 2.89                     | 0.51              |
| 1:A:961:TYR:O     | 1:A:961:TYR:HD1   | 1.94                     | 0.51              |
| 1:A:1088:GLN:C    | 1:A:1090:ASN:H    | 2.19                     | 0.51              |
| 1:A:1534:GLN:HA   | 1:A:1608:ASN:HD22 | 1.75                     | 0.51              |
| 2:B:142:PRO:HB3   | 2:B:187:ASN:HD21  | 1.76                     | 0.51              |
| 2:B:161:VAL:CG2   | 2:B:180:LEU:HD21  | 2.37                     | 0.51              |
| 2:B:164:GLU:HB2   | 2:B:200:VAL:HG23  | 1.93                     | 0.51              |
| 2:B:353:TYR:CD2   | 2:B:614:GLY:C     | 2.89                     | 0.51              |
| 2:B:485:ASN:C     | 2:B:487:GLY:H     | 2.18                     | 0.51              |
| 2:B:1354:LEU:HD23 | 2:B:1354:LEU:O    | 2.11                     | 0.51              |
| 2:B:1480:LEU:HD21 | 2:B:1483:LYS:HZ2  | 1.76                     | 0.51              |
| 1:C:672:ILE:C     | 1:C:673:LEU:HG    | 2.36                     | 0.51              |
| 1:C:820:PHE:CG    | 1:C:821:LYS:N     | 2.79                     | 0.51              |
| 1:C:976:ILE:HB    | 1:C:1362:THR:CG2  | 2.40                     | 0.51              |
| 1:C:1094:GLU:H    | 1:C:1094:GLU:CD   | 2.19                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1279:ARG:NH1  | 1:C:1280:TYR:CD2  | 2.79                     | 0.51              |
| 2:D:242:ASN:OD1   | 2:D:295:LYS:HD2   | 2.10                     | 0.51              |
| 2:D:358:MET:CE    | 2:D:467:LYS:HD2   | 2.41                     | 0.51              |
| 2:D:481:TYR:CE2   | 2:D:493:GLY:C     | 2.88                     | 0.51              |
| 2:D:503:LEU:HD23  | 2:D:503:LEU:C     | 2.36                     | 0.51              |
| 2:D:924:ILE:HG22  | 2:D:924:ILE:O     | 2.11                     | 0.51              |
| 1:A:518:PHE:O     | 1:A:520:ASP:N     | 2.39                     | 0.50              |
| 1:A:587:THR:HG22  | 1:A:789:ALA:HB2   | 1.92                     | 0.50              |
| 1:A:1112:GLN:NE2  | 1:A:1171:ALA:HB2  | 2.25                     | 0.50              |
| 2:B:1591:LEU:C    | 2:B:1591:LEU:CD2  | 2.84                     | 0.50              |
| 1:C:111:PHE:CD2   | 1:C:112:SER:N     | 2.76                     | 0.50              |
| 1:C:1019:PHE:CD2  | 1:C:1020:TYR:N    | 2.78                     | 0.50              |
| 1:C:1279:ARG:HH21 | 1:C:1362:THR:HG21 | 1.75                     | 0.50              |
| 2:D:130:ILE:HG23  | 2:D:147:VAL:HG23  | 1.93                     | 0.50              |
| 2:D:232:GLU:C     | 2:D:234:PHE:H     | 2.19                     | 0.50              |
| 2:D:866:TYR:OH    | 2:D:1388:THR:HG21 | 2.10                     | 0.50              |
| 2:D:959:ILE:HG22  | 2:D:959:ILE:O     | 2.11                     | 0.50              |
| 2:D:961:THR:HG22  | 2:D:1327:THR:HA   | 1.93                     | 0.50              |
| 2:D:964:ILE:HG13  | 2:D:1302:THR:CG2  | 2.34                     | 0.50              |
| 1:A:153:LYS:O     | 1:A:154:PRO:C     | 2.54                     | 0.50              |
| 1:A:489:LYS:HZ1   | 2:B:502:ASN:H     | 1.57                     | 0.50              |
| 1:A:1007:SER:OG   | 1:A:1008:ALA:N    | 2.39                     | 0.50              |
| 1:A:1161:LEU:O    | 1:A:1164:ILE:HG12 | 2.12                     | 0.50              |
| 1:A:1183:GLN:NE2  | 1:A:1232:LEU:HD22 | 2.26                     | 0.50              |
| 2:B:356:PRO:HD2   | 2:B:444:TYR:CE2   | 2.46                     | 0.50              |
| 2:B:843:ASP:HA    | 2:B:873:LYS:O     | 2.11                     | 0.50              |
| 2:B:1623:LYS:HZ3  | 2:B:1623:LYS:HA   | 1.76                     | 0.50              |
| 1:C:584:PRO:HD3   | 1:C:820:PHE:HB2   | 1.93                     | 0.50              |
| 1:C:1110:ASN:O    | 1:C:1111:TYR:CG   | 2.63                     | 0.50              |
| 1:C:1314:ASP:HA   | 1:C:1325:ASN:HB2  | 1.93                     | 0.50              |
| 1:C:1429:PRO:O    | 1:C:1432:ILE:HG12 | 2.11                     | 0.50              |
| 2:D:1482:ASN:H    | 2:D:1495:GLU:HG2  | 1.76                     | 0.50              |
| 1:A:136:THR:O     | 1:A:139:GLN:HB2   | 2.11                     | 0.50              |
| 1:A:238:ILE:HB    | 1:A:347:TYR:CD1   | 2.46                     | 0.50              |
| 1:A:1559:TYR:HE1  | 1:A:1587:THR:HA   | 1.77                     | 0.50              |
| 2:B:130:ILE:HG23  | 2:B:147:VAL:HG23  | 1.93                     | 0.50              |
| 2:B:275:SER:C     | 2:B:277:PRO:HD3   | 2.36                     | 0.50              |
| 2:B:515:ILE:HG21  | 2:B:599:TRP:CZ2   | 2.46                     | 0.50              |
| 2:B:949:LYS:O     | 2:B:950:LEU:HG    | 2.12                     | 0.50              |
| 2:B:1380:THR:HG22 | 2:B:1381:ILE:H    | 1.76                     | 0.50              |
| 2:B:1628:PHE:O    | 2:B:1629:ALA:C    | 2.54                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:23:TYR:O     | 1:C:655:THR:HG21  | 2.09                     | 0.50              |
| 1:C:146:TYR:CE1  | 1:C:182:ILE:HG23  | 2.46                     | 0.50              |
| 1:C:504:LEU:HD12 | 1:C:509:ILE:HA    | 1.92                     | 0.50              |
| 1:C:552:ALA:HB3  | 1:C:658:ASN:HB3   | 1.93                     | 0.50              |
| 1:C:819:VAL:O    | 1:C:820:PHE:O     | 2.29                     | 0.50              |
| 1:C:931:PRO:CB   | 1:C:1366:HIS:CD2  | 2.95                     | 0.50              |
| 2:D:228:LEU:CD2  | 2:D:247:ILE:HG12  | 2.41                     | 0.50              |
| 2:D:952:ASP:O    | 2:D:1331:ALA:HA   | 2.11                     | 0.50              |
| 2:D:965:ILE:HG22 | 2:D:1323:MET:HB2  | 1.94                     | 0.50              |
| 2:D:1529:LEU:N   | 2:D:1529:LEU:HD12 | 2.27                     | 0.50              |
| 1:A:23:TYR:HD1   | 1:A:23:TYR:C      | 2.18                     | 0.50              |
| 1:A:222:TYR:HD2  | 1:A:223:VAL:N     | 2.06                     | 0.50              |
| 1:A:820:PHE:CG   | 1:A:821:LYS:N     | 2.79                     | 0.50              |
| 1:A:1421:HIS:NE2 | 1:A:1498:TYR:CD1  | 2.80                     | 0.50              |
| 2:B:235:PHE:HB3  | 2:B:338:ILE:CG2   | 2.39                     | 0.50              |
| 2:B:421:PRO:HD2  | 2:B:424:ARG:HG3   | 1.93                     | 0.50              |
| 2:B:519:ARG:CZ   | 2:B:608:GLY:HA3   | 2.41                     | 0.50              |
| 2:B:1346:ASN:O   | 2:B:1368:CYS:HB2  | 2.11                     | 0.50              |
| 2:B:1429:LYS:O   | 2:B:1430:VAL:HG23 | 2.11                     | 0.50              |
| 1:C:191:PRO:O    | 1:C:194:PRO:HD3   | 2.11                     | 0.50              |
| 1:C:308:LYS:CG   | 1:C:309:GLU:H     | 2.22                     | 0.50              |
| 1:C:488:PRO:O    | 1:C:489:LYS:O     | 2.29                     | 0.50              |
| 1:C:790:LEU:HB3  | 1:C:791:PRO:CD    | 2.42                     | 0.50              |
| 1:C:831:TYR:CZ   | 1:C:1457:ASP:HB3  | 2.46                     | 0.50              |
| 1:C:1151:GLY:O   | 1:C:1152:ILE:C    | 2.54                     | 0.50              |
| 2:D:253:TYR:HE1  | 2:D:839:TYR:HE2   | 1.59                     | 0.50              |
| 2:D:345:ILE:HG13 | 2:D:428:LYS:CB    | 2.41                     | 0.50              |
| 1:A:178:ASP:OD2  | 1:A:179:HIS:N     | 2.45                     | 0.50              |
| 1:A:531:THR:HG23 | 1:A:533:ASN:H     | 1.77                     | 0.50              |
| 1:A:633:GLY:O    | 1:A:634:CYS:HB2   | 2.12                     | 0.50              |
| 1:A:773:TRP:CZ3  | 1:A:788:PHE:CE1   | 2.90                     | 0.50              |
| 1:A:859:MET:HE2  | 1:A:912:PHE:CZ    | 2.47                     | 0.50              |
| 1:A:947:ARG:O    | 1:A:949:ILE:N     | 2.45                     | 0.50              |
| 1:A:975:ARG:HG3  | 1:A:1340:VAL:HB   | 1.94                     | 0.50              |
| 1:A:1162:VAL:N   | 1:C:1102:ASN:HD21 | 1.97                     | 0.50              |
| 2:B:27:LEU:O     | 2:B:628:LEU:HD12  | 2.11                     | 0.50              |
| 2:B:259:GLY:HA2  | 2:B:323:GLU:HB3   | 1.92                     | 0.50              |
| 2:B:961:THR:HG22 | 2:B:1327:THR:CB   | 2.42                     | 0.50              |
| 2:B:1602:THR:H   | 2:B:1605:THR:HB   | 1.76                     | 0.50              |
| 1:C:60:PRO:CD    | 1:C:61:ASP:N      | 2.68                     | 0.50              |
| 1:C:1434:ALA:HA  | 1:C:1479:ILE:HG22 | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:103:TYR:CD2   | 2:D:103:TYR:N     | 2.77                     | 0.50              |
| 2:D:356:PRO:HD2   | 2:D:444:TYR:CE2   | 2.46                     | 0.50              |
| 2:D:421:PRO:HD2   | 2:D:424:ARG:HG3   | 1.93                     | 0.50              |
| 2:D:512:PRO:O     | 2:D:515:ILE:HD12  | 2.11                     | 0.50              |
| 2:D:553:ASP:CG    | 2:D:555:LEU:HD11  | 2.36                     | 0.50              |
| 2:D:1326:LEU:HD11 | 2:D:1328:PHE:CE2  | 2.46                     | 0.50              |
| 1:A:20:GLU:HA     | 1:A:551:THR:HG22  | 1.94                     | 0.50              |
| 1:A:23:TYR:O      | 1:A:655:THR:HG21  | 2.11                     | 0.50              |
| 1:A:269:PHE:O     | 1:A:282:MET:HG2   | 2.11                     | 0.50              |
| 1:A:1099:SER:O    | 1:A:1100:ILE:C    | 2.55                     | 0.50              |
| 1:A:1571:GLU:O    | 1:A:1574:PHE:CD2  | 2.64                     | 0.50              |
| 2:B:481:TYR:CD2   | 2:B:493:GLY:O     | 2.64                     | 0.50              |
| 2:B:582:LYS:O     | 2:B:583:ALA:O     | 2.30                     | 0.50              |
| 2:B:1482:ASN:HB3  | 2:B:1493:ALA:CB   | 2.41                     | 0.50              |
| 1:C:96:GLN:O      | 1:C:97:ASN:O      | 2.30                     | 0.50              |
| 1:C:573:VAL:CG1   | 1:C:592:MET:HG2   | 2.42                     | 0.50              |
| 1:C:1266:TYR:O    | 1:C:1266:TYR:CD1  | 2.64                     | 0.50              |
| 1:C:1268:ASN:N    | 1:C:1269:PRO:HD2  | 2.27                     | 0.50              |
| 2:D:485:ASN:C     | 2:D:487:GLY:H     | 2.19                     | 0.50              |
| 2:D:523:TYR:CB    | 2:D:533:ALA:HB2   | 2.42                     | 0.50              |
| 2:D:599:TRP:HA    | 2:D:599:TRP:CE3   | 2.45                     | 0.50              |
| 2:D:778:PHE:N     | 2:D:778:PHE:CD2   | 2.80                     | 0.50              |
| 2:D:1520:VAL:CG1  | 2:D:1584:TRP:HD1  | 2.24                     | 0.50              |
| 1:A:499:TYR:CE2   | 1:A:517:LYS:HG3   | 2.47                     | 0.50              |
| 1:A:706:ASN:HB2   | 1:A:714:ARG:HH11  | 1.77                     | 0.50              |
| 1:A:902:PRO:C     | 1:A:903:LEU:HD22  | 2.37                     | 0.50              |
| 1:A:1088:GLN:C    | 1:A:1090:ASN:N    | 2.69                     | 0.50              |
| 1:A:1279:ARG:NH1  | 1:A:1280:TYR:CD2  | 2.80                     | 0.50              |
| 1:A:1311:MET:HG2  | 1:A:1313:ILE:HG12 | 1.93                     | 0.50              |
| 1:A:1378:TYR:O    | 1:A:1406:ALA:HA   | 2.12                     | 0.50              |
| 1:A:1552:ALA:HB2  | 1:A:1620:MET:HE3  | 1.93                     | 0.50              |
| 2:B:203:TYR:O     | 2:B:204:GLU:C     | 2.55                     | 0.50              |
| 2:B:467:LYS:HG2   | 2:B:468:GLY:N     | 2.26                     | 0.50              |
| 2:B:784:ILE:HD12  | 2:B:817:ASP:OD1   | 2.11                     | 0.50              |
| 2:B:824:VAL:HG22  | 2:B:825:VAL:H     | 1.76                     | 0.50              |
| 2:B:947:ALA:HB2   | 2:B:1309:GLN:HA   | 1.93                     | 0.50              |
| 2:B:954:VAL:CG1   | 2:B:955:PRO:HD2   | 2.42                     | 0.50              |
| 2:B:1607:ILE:H    | 2:B:1607:ILE:CD1  | 2.05                     | 0.50              |
| 1:C:115:LYS:HE2   | 1:C:654:LEU:HD11  | 1.93                     | 0.50              |
| 1:C:163:PHE:HE2   | 1:C:201:ILE:HD13  | 1.75                     | 0.50              |
| 1:C:774:LEU:HG    | 1:C:788:PHE:CE1   | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:934:VAL:CG1   | 1:C:935:LYS:N     | 2.74                     | 0.50              |
| 1:C:1049:LEU:HD11 | 1:C:1089:VAL:CG1  | 2.41                     | 0.50              |
| 2:D:105:VAL:HG12  | 2:D:118:VAL:HA    | 1.93                     | 0.50              |
| 2:D:237:ILE:HD11  | 2:D:309:LEU:HB2   | 1.92                     | 0.50              |
| 2:D:481:TYR:CE1   | 2:D:506:MET:SD    | 2.98                     | 0.50              |
| 2:D:778:PHE:N     | 2:D:778:PHE:HD2   | 2.10                     | 0.50              |
| 2:D:1382:ILE:HB   | 2:D:1425:ILE:HB   | 1.94                     | 0.50              |
| 1:A:477:LEU:HD22  | 1:A:477:LEU:N     | 2.27                     | 0.50              |
| 1:A:917:TRP:HB3   | 2:B:558:MET:SD    | 2.51                     | 0.50              |
| 1:A:987:ILE:CD1   | 1:A:1294:ILE:HG23 | 2.42                     | 0.50              |
| 1:A:1023:HIS:CE1  | 1:A:1302:LEU:HD11 | 2.47                     | 0.50              |
| 1:A:1031:TRP:CH2  | 1:A:1042:LYS:HG3  | 2.47                     | 0.50              |
| 1:A:1487:PHE:N    | 1:A:1487:PHE:HD2  | 2.05                     | 0.50              |
| 1:A:1562:LYS:CD   | 1:A:1648:TRP:HZ2  | 2.24                     | 0.50              |
| 2:B:546:GLY:HA3   | 2:B:570:ASP:OD1   | 2.10                     | 0.50              |
| 2:B:550:VAL:HG22  | 2:B:567:LEU:HD21  | 1.93                     | 0.50              |
| 2:B:563:MET:O     | 2:B:777:SER:HA    | 2.12                     | 0.50              |
| 2:B:922:LYS:HE3   | 2:B:1329:TYR:OH   | 2.11                     | 0.50              |
| 1:C:115:LYS:HG3   | 1:C:116:ARG:O     | 2.12                     | 0.50              |
| 1:C:237:PHE:HA    | 1:C:345:ILE:HG23  | 1.94                     | 0.50              |
| 1:C:463:SER:O     | 1:C:555:VAL:HG21  | 2.11                     | 0.50              |
| 1:C:856:CYS:HB2   | 2:D:904:LEU:HD21  | 1.94                     | 0.50              |
| 1:C:1619:ILE:HG12 | 1:C:1645:ILE:CD1  | 2.42                     | 0.50              |
| 2:D:142:PRO:HB3   | 2:D:187:ASN:HD21  | 1.76                     | 0.50              |
| 2:D:415:THR:HG23  | 2:D:426:ALA:O     | 2.12                     | 0.50              |
| 2:D:445:LEU:HD12  | 2:D:446:HIS:N     | 2.27                     | 0.50              |
| 2:D:928:VAL:HG23  | 2:D:1323:MET:HB3  | 1.93                     | 0.50              |
| 2:D:949:LYS:O     | 2:D:950:LEU:HG    | 2.11                     | 0.50              |
| 1:A:296:ILE:HG23  | 1:A:297:ALA:N     | 2.26                     | 0.50              |
| 1:A:1031:TRP:CZ2  | 1:A:1042:LYS:HG3  | 2.46                     | 0.50              |
| 1:A:1559:TYR:CE1  | 1:A:1587:THR:HA   | 2.47                     | 0.50              |
| 2:B:142:PRO:HB3   | 2:B:187:ASN:ND2   | 2.27                     | 0.50              |
| 2:B:870:PHE:HB2   | 2:B:871:PRO:CD    | 2.42                     | 0.50              |
| 2:B:1284:ARG:NE   | 2:B:1285:GLU:H    | 2.09                     | 0.50              |
| 2:B:1331:ALA:O    | 2:B:1332:GLN:CB   | 2.49                     | 0.50              |
| 2:B:1500:LEU:C    | 2:B:1500:LEU:CD1  | 2.84                     | 0.50              |
| 2:B:1632:SER:O    | 2:B:1636:THR:HB   | 2.12                     | 0.50              |
| 1:C:115:LYS:HB2   | 1:C:654:LEU:CD1   | 2.40                     | 0.50              |
| 1:C:323:LEU:O     | 1:C:323:LEU:HD13  | 2.12                     | 0.50              |
| 1:C:936:ARG:HH11  | 1:C:936:ARG:CG    | 2.21                     | 0.50              |
| 1:C:955:ARG:CG    | 1:C:1350:THR:HG23 | 2.40                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1019:PHE:CE1  | 1:C:1088:GLN:HB3  | 2.47                     | 0.50              |
| 1:C:1019:PHE:CZ   | 1:C:1088:GLN:HB3  | 2.47                     | 0.50              |
| 1:C:1127:ILE:HD13 | 1:C:1129:LEU:HD21 | 1.94                     | 0.50              |
| 1:C:1227:PHE:CD2  | 1:C:1273:TRP:CE2  | 3.00                     | 0.50              |
| 1:C:1562:LYS:HD3  | 1:C:1648:TRP:HE1  | 1.75                     | 0.50              |
| 2:D:204:GLU:O     | 2:D:204:GLU:HG3   | 2.12                     | 0.50              |
| 2:D:586:VAL:HG12  | 2:D:587:LEU:N     | 2.26                     | 0.50              |
| 2:D:950:LEU:O     | 2:D:951:ASP:HB2   | 2.12                     | 0.50              |
| 1:A:42:GLN:CG     | 1:A:43:VAL:N      | 2.75                     | 0.49              |
| 1:A:101:TYR:CE1   | 1:A:116:ARG:CZ    | 2.93                     | 0.49              |
| 1:A:146:TYR:CE1   | 1:A:182:ILE:HG23  | 2.46                     | 0.49              |
| 1:A:855:PHE:CZ    | 1:A:886:GLN:HB2   | 2.47                     | 0.49              |
| 1:A:1020:TYR:O    | 1:A:1021:VAL:C    | 2.54                     | 0.49              |
| 1:A:1271:ILE:HD13 | 1:A:1300:TYR:CD1  | 2.47                     | 0.49              |
| 2:B:162:ILE:CG2   | 2:B:202:LYS:HG2   | 2.42                     | 0.49              |
| 2:B:358:MET:CE    | 2:B:467:LYS:HD2   | 2.41                     | 0.49              |
| 2:B:460:LEU:HD23  | 2:B:460:LEU:O     | 2.11                     | 0.49              |
| 1:C:325:ILE:O     | 1:C:341:GLU:HB2   | 2.13                     | 0.49              |
| 1:C:824:PHE:O     | 1:C:845:VAL:HG22  | 2.12                     | 0.49              |
| 1:C:834:VAL:HB    | 1:C:837:GLU:OE2   | 2.12                     | 0.49              |
| 1:C:1007:SER:OG   | 1:C:1008:ALA:N    | 2.40                     | 0.49              |
| 1:C:1421:HIS:CE1  | 1:C:1498:TYR:CD1  | 2.99                     | 0.49              |
| 2:D:825:VAL:O     | 2:D:826:LYS:C     | 2.55                     | 0.49              |
| 2:D:1331:ALA:O    | 2:D:1332:GLN:CB   | 2.49                     | 0.49              |
| 1:A:809:ILE:CG1   | 1:A:810:CYS:N     | 2.75                     | 0.49              |
| 1:A:854:GLN:OE1   | 1:A:854:GLN:O     | 2.30                     | 0.49              |
| 1:A:1007:SER:HA   | 1:A:1069:TRP:HD1  | 1.77                     | 0.49              |
| 1:A:1279:ARG:HB2  | 1:A:1284:PHE:HB2  | 1.94                     | 0.49              |
| 1:A:1299:GLU:O    | 1:A:1303:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:1543:ILE:O    | 1:A:1547:THR:HG23 | 2.12                     | 0.49              |
| 1:A:1570:VAL:CG2  | 1:A:1575:VAL:HG22 | 2.42                     | 0.49              |
| 2:B:184:TRP:HB2   | 2:B:185:PRO:CD    | 2.42                     | 0.49              |
| 2:B:519:ARG:NH1   | 2:B:606:ASP:OD2   | 2.45                     | 0.49              |
| 2:B:522:ALA:O     | 2:B:533:ALA:HB1   | 2.12                     | 0.49              |
| 2:B:965:ILE:CD1   | 2:B:1277:ILE:HD13 | 2.42                     | 0.49              |
| 2:B:1282:PRO:HD2  | 2:B:1309:GLN:CD   | 2.37                     | 0.49              |
| 2:B:1508:VAL:HB   | 2:B:1509:PRO:HD3  | 1.93                     | 0.49              |
| 1:C:54:ILE:O      | 1:C:68:SER:HA     | 2.13                     | 0.49              |
| 1:C:231:ILE:HA    | 1:C:250:ILE:HG22  | 1.94                     | 0.49              |
| 1:C:805:SER:O     | 1:C:807:THR:N     | 2.45                     | 0.49              |
| 1:C:1190:ILE:O    | 1:C:1191:SER:C    | 2.55                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1562:LYS:O    | 1:C:1563:VAL:CG1  | 2.60                     | 0.49              |
| 1:C:1585:TYR:CE2  | 1:C:1586:LYS:HB3  | 2.47                     | 0.49              |
| 2:D:541:LYS:HG3   | 2:D:543:THR:HG22  | 1.94                     | 0.49              |
| 2:D:546:GLY:HA3   | 2:D:570:ASP:OD1   | 2.11                     | 0.49              |
| 2:D:1341:ASN:HD22 | 2:D:1342:LYS:HG2  | 1.75                     | 0.49              |
| 2:D:1482:ASN:HB3  | 2:D:1493:ALA:HB3  | 1.94                     | 0.49              |
| 1:A:33:VAL:HA     | 1:A:87:ILE:HG12   | 1.95                     | 0.49              |
| 1:A:165:ASP:C     | 1:A:167:GLU:H     | 2.20                     | 0.49              |
| 1:A:185:PHE:CD1   | 1:A:186:PRO:HD2   | 2.48                     | 0.49              |
| 1:A:520:ASP:HB2   | 2:B:404:LEU:HD13  | 1.94                     | 0.49              |
| 1:A:540:LEU:HD12  | 1:A:541:LEU:N     | 2.27                     | 0.49              |
| 1:A:639:GLY:H     | 1:A:645:VAL:CG2   | 2.25                     | 0.49              |
| 1:A:823:VAL:HG23  | 1:A:846:TYR:O     | 2.12                     | 0.49              |
| 1:A:825:LEU:HB2   | 1:A:845:VAL:HG23  | 1.93                     | 0.49              |
| 1:A:984:VAL:HG13  | 1:A:984:VAL:O     | 2.12                     | 0.49              |
| 1:A:1102:ASN:HD22 | 1:C:1162:VAL:HG22 | 1.75                     | 0.49              |
| 1:A:1213:LYS:CG   | 1:A:1266:TYR:HE2  | 2.23                     | 0.49              |
| 1:A:1317:TYR:CD2  | 1:A:1344:ASP:HB3  | 2.47                     | 0.49              |
| 2:B:400:LEU:HB3   | 2:B:402:ILE:HD11  | 1.94                     | 0.49              |
| 2:B:484:LEU:HD11  | 2:B:626:LEU:HD11  | 1.94                     | 0.49              |
| 2:B:1391:LEU:CB   | 2:B:1417:MET:HE2  | 2.42                     | 0.49              |
| 2:B:1540:TYR:HE1  | 2:B:1575:LEU:HB2  | 1.78                     | 0.49              |
| 1:C:331:GLU:CG    | 1:C:333:THR:HG23  | 2.41                     | 0.49              |
| 1:C:361:LEU:HD12  | 1:C:361:LEU:H     | 1.77                     | 0.49              |
| 1:C:987:ILE:CD1   | 1:C:1294:ILE:HG23 | 2.42                     | 0.49              |
| 1:C:1213:LYS:C    | 1:C:1215:GLU:H    | 2.20                     | 0.49              |
| 1:C:1499:HIS:C    | 1:C:1500:ARG:HG3  | 2.36                     | 0.49              |
| 2:D:226:VAL:O     | 2:D:226:VAL:HG12  | 2.11                     | 0.49              |
| 2:D:550:VAL:HG22  | 2:D:567:LEU:HD21  | 1.93                     | 0.49              |
| 2:D:563:MET:CB    | 2:D:778:PHE:CE2   | 2.94                     | 0.49              |
| 2:D:824:VAL:HG12  | 2:D:913:LEU:HD21  | 1.94                     | 0.49              |
| 2:D:1327:THR:HG22 | 2:D:1328:PHE:N    | 2.27                     | 0.49              |
| 2:D:1420:LYS:HB3  | 2:D:1422:ALA:O    | 2.12                     | 0.49              |
| 1:A:116:ARG:O     | 1:A:117:MET:HB3   | 2.12                     | 0.49              |
| 1:A:126:LEU:HD12  | 1:A:147:SER:HB2   | 1.93                     | 0.49              |
| 1:A:1268:ASN:H    | 1:A:1268:ASN:HD22 | 1.60                     | 0.49              |
| 2:B:323:GLU:C     | 2:B:323:GLU:OE1   | 2.55                     | 0.49              |
| 2:B:435:TYR:CE1   | 2:B:616:ASN:HA    | 2.47                     | 0.49              |
| 2:B:524:TYR:HE1   | 2:B:532:VAL:CG1   | 2.25                     | 0.49              |
| 2:B:586:VAL:HG12  | 2:B:587:LEU:N     | 2.27                     | 0.49              |
| 2:B:825:VAL:HG22  | 2:B:916:VAL:HG13  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1301:ARG:HB3  | 2:B:1301:ARG:NH1  | 2.27                     | 0.49              |
| 2:B:1382:ILE:HB   | 2:B:1425:ILE:HB   | 1.94                     | 0.49              |
| 2:B:1529:LEU:N    | 2:B:1529:LEU:HD12 | 2.27                     | 0.49              |
| 1:C:59:TYR:CZ     | 1:C:99:VAL:HG21   | 2.44                     | 0.49              |
| 1:C:820:PHE:O     | 1:C:821:LYS:CG    | 2.60                     | 0.49              |
| 1:C:834:VAL:HA    | 1:C:930:VAL:O     | 2.12                     | 0.49              |
| 1:C:864:GLY:HA3   | 1:C:907:LEU:HD23  | 1.94                     | 0.49              |
| 1:C:1549:LYS:HZ2  | 1:C:1667:PHE:HB3  | 1.76                     | 0.49              |
| 1:C:1648:TRP:NE1  | 1:C:1664:LEU:HD22 | 2.28                     | 0.49              |
| 2:D:162:ILE:CG2   | 2:D:202:LYS:HG2   | 2.43                     | 0.49              |
| 2:D:350:THR:HG23  | 2:D:350:THR:O     | 2.11                     | 0.49              |
| 2:D:518:PHE:HD2   | 2:D:518:PHE:O     | 1.96                     | 0.49              |
| 2:D:755:TRP:O     | 2:D:756:LEU:HB3   | 2.12                     | 0.49              |
| 2:D:1278:THR:HB   | 2:D:1314:THR:HB   | 1.94                     | 0.49              |
| 2:D:1523:VAL:HG22 | 2:D:1584:TRP:CB   | 2.28                     | 0.49              |
| 1:A:100:SER:HB2   | 1:A:101:TYR:HD2   | 1.78                     | 0.49              |
| 1:A:475:ALA:HB1   | 1:A:477:LEU:CD2   | 2.42                     | 0.49              |
| 1:A:1104:LEU:O    | 1:A:1108:VAL:HG12 | 2.11                     | 0.49              |
| 2:B:482:LEU:N     | 2:B:482:LEU:CD1   | 2.76                     | 0.49              |
| 2:B:930:LEU:HB2   | 2:B:1321:ALA:HB3  | 1.93                     | 0.49              |
| 2:B:1330:ASN:HD22 | 2:B:1330:ASN:H    | 1.60                     | 0.49              |
| 2:B:1412:GLU:HB2  | 2:B:1419:GLN:CG   | 2.42                     | 0.49              |
| 1:C:100:SER:CB    | 1:C:101:TYR:HD2   | 2.25                     | 0.49              |
| 1:C:162:THR:CB    | 1:C:173:MET:HE2   | 2.43                     | 0.49              |
| 1:C:792:ASP:O     | 1:C:793:SER:CB    | 2.60                     | 0.49              |
| 1:C:1549:LYS:NZ   | 1:C:1667:PHE:CB   | 2.70                     | 0.49              |
| 1:C:1559:TYR:CE1  | 1:C:1587:THR:HA   | 2.46                     | 0.49              |
| 2:D:224:PHE:CZ    | 2:D:329:VAL:HG13  | 2.47                     | 0.49              |
| 2:D:309:LEU:O     | 2:D:310:VAL:C     | 2.54                     | 0.49              |
| 2:D:469:ASN:CG    | 2:D:472:SER:HB2   | 2.36                     | 0.49              |
| 2:D:825:VAL:HG22  | 2:D:916:VAL:HG13  | 1.95                     | 0.49              |
| 2:D:1278:THR:O    | 2:D:1313:VAL:HA   | 2.12                     | 0.49              |
| 2:D:1345:LEU:O    | 2:D:1345:LEU:HG   | 2.13                     | 0.49              |
| 2:D:1512:ILE:O    | 2:D:1516:CYS:HB2  | 2.12                     | 0.49              |
| 1:A:240:TYR:HA    | 1:A:243:PHE:HB2   | 1.93                     | 0.49              |
| 1:A:1185:THR:OG1  | 1:A:1231:ASN:HB3  | 2.12                     | 0.49              |
| 1:A:1560:ALA:HB1  | 1:A:1620:MET:CG   | 2.42                     | 0.49              |
| 2:B:778:PHE:CD2   | 2:B:778:PHE:N     | 2.81                     | 0.49              |
| 1:C:21:GLN:HE22   | 1:C:46:TYR:HD2    | 1.61                     | 0.49              |
| 1:C:23:TYR:HD1    | 1:C:23:TYR:C      | 2.20                     | 0.49              |
| 1:C:357:VAL:HG12  | 1:C:358:ALA:N     | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:431:LEU:O     | 1:C:431:LEU:HD13  | 2.11                     | 0.49              |
| 1:C:531:THR:HG23  | 1:C:533:ASN:H     | 1.78                     | 0.49              |
| 1:C:598:SER:O     | 1:C:599:TRP:HD1   | 1.95                     | 0.49              |
| 1:C:702:GLY:CA    | 1:C:728:PHE:CD1   | 2.95                     | 0.49              |
| 1:C:1004:PRO:HG3  | 1:C:1461:ILE:HD13 | 1.95                     | 0.49              |
| 1:C:1068:VAL:HG21 | 1:C:1124:TYR:HD1  | 1.72                     | 0.49              |
| 1:C:1543:ILE:O    | 1:C:1547:THR:HG23 | 2.13                     | 0.49              |
| 2:D:1429:LYS:O    | 2:D:1430:VAL:HG23 | 2.13                     | 0.49              |
| 2:D:1507:ASP:OD1  | 2:D:1509:PRO:HD2  | 2.12                     | 0.49              |
| 1:A:681:LYS:HB2   | 1:A:738:LEU:HD11  | 1.95                     | 0.49              |
| 1:A:690:TYR:C     | 1:A:692:HIS:H     | 2.19                     | 0.49              |
| 1:A:827:MET:HB3   | 1:A:829:ILE:CD1   | 2.42                     | 0.49              |
| 1:A:946:PRO:HB3   | 1:A:1352:PHE:O    | 2.12                     | 0.49              |
| 1:A:1016:VAL:HG11 | 1:A:1291:ILE:CG1  | 2.43                     | 0.49              |
| 1:A:1023:HIS:O    | 1:A:1027:THR:HB   | 2.12                     | 0.49              |
| 1:A:1584:ILE:CG2  | 1:A:1585:TYR:H    | 2.04                     | 0.49              |
| 2:B:40:GLN:O      | 2:B:489:ILE:HD12  | 2.12                     | 0.49              |
| 2:B:61:PHE:CG     | 2:B:62:PRO:HA     | 2.47                     | 0.49              |
| 2:B:806:TYR:CE1   | 2:B:807:GLU:O     | 2.66                     | 0.49              |
| 2:B:961:THR:HG22  | 2:B:1327:THR:HA   | 1.95                     | 0.49              |
| 1:C:23:TYR:CD1    | 1:C:23:TYR:C      | 2.90                     | 0.49              |
| 1:C:1088:GLN:C    | 1:C:1090:ASN:N    | 2.71                     | 0.49              |
| 2:D:84:THR:N      | 2:D:85:PRO:HD3    | 2.27                     | 0.49              |
| 2:D:353:TYR:CD2   | 2:D:614:GLY:O     | 2.66                     | 0.49              |
| 2:D:954:VAL:HB    | 2:D:957:THR:CG2   | 2.31                     | 0.49              |
| 2:D:1392:PRO:HB2  | 2:D:1397:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:166:PRO:HB3   | 1:A:198:MET:H     | 1.77                     | 0.49              |
| 1:A:238:ILE:HD12  | 1:A:347:TYR:CE1   | 2.48                     | 0.49              |
| 1:A:367:ILE:CD1   | 1:A:466:TYR:HB3   | 2.43                     | 0.49              |
| 1:A:565:GLU:H     | 1:A:565:GLU:CD    | 2.20                     | 0.49              |
| 1:A:874:ASP:O     | 1:A:875:HIS:CG    | 2.66                     | 0.49              |
| 2:B:409:LEU:C     | 2:B:409:LEU:HD12  | 2.36                     | 0.49              |
| 2:B:482:LEU:H     | 2:B:482:LEU:CD1   | 2.21                     | 0.49              |
| 2:B:795:THR:HG22  | 2:B:796:PRO:HD2   | 1.95                     | 0.49              |
| 2:B:829:GLN:HG3   | 2:B:1480:LEU:HD13 | 1.95                     | 0.49              |
| 2:B:1349:VAL:HA   | 2:B:1364:MET:O    | 2.10                     | 0.49              |
| 1:C:108:SER:HG    | 1:C:111:PHE:C     | 2.20                     | 0.49              |
| 1:C:128:ILE:HD11  | 1:C:214:THR:CA    | 2.43                     | 0.49              |
| 1:C:207:GLU:O     | 1:C:209:PHE:N     | 2.45                     | 0.49              |
| 1:C:773:TRP:HZ3   | 1:C:788:PHE:HE1   | 1.56                     | 0.49              |
| 1:C:946:PRO:HB3   | 1:C:1352:PHE:O    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:989:SER:O    | 1:C:993:SER:CB    | 2.60                     | 0.49              |
| 1:C:1562:LYS:C   | 1:C:1563:VAL:CG1  | 2.85                     | 0.49              |
| 1:C:1658:GLN:NE2 | 1:C:1661:LEU:HD12 | 2.28                     | 0.49              |
| 2:D:61:PHE:CG    | 2:D:62:PRO:HA     | 2.47                     | 0.49              |
| 2:D:137:TYR:CE1  | 2:D:143:VAL:HG22  | 2.47                     | 0.49              |
| 2:D:597:LYS:NZ   | 2:D:597:LYS:HB3   | 2.27                     | 0.49              |
| 2:D:735:ASN:CB   | 2:D:869:GLN:HE22  | 2.25                     | 0.49              |
| 2:D:784:ILE:HD12 | 2:D:817:ASP:OD1   | 2.13                     | 0.49              |
| 2:D:814:PHE:CZ   | 2:D:846:VAL:HG21  | 2.48                     | 0.49              |
| 2:D:965:ILE:CD1  | 2:D:1277:ILE:HD13 | 2.42                     | 0.49              |
| 1:A:27:ALA:HB1   | 1:A:28:PRO:CD     | 2.43                     | 0.49              |
| 1:A:970:LYS:C    | 1:A:971:THR:CG2   | 2.86                     | 0.49              |
| 1:A:1109:GLU:HB3 | 1:A:1110:ASN:OD1  | 2.11                     | 0.49              |
| 1:A:1564:SER:O   | 1:A:1579:ALA:HB1  | 2.13                     | 0.49              |
| 1:A:1648:TRP:NE1 | 1:A:1664:LEU:HD22 | 2.28                     | 0.49              |
| 2:B:155:SER:O    | 2:B:156:LYS:HG2   | 2.13                     | 0.49              |
| 2:B:204:GLU:HG3  | 2:B:204:GLU:O     | 2.13                     | 0.49              |
| 2:B:417:HIS:N    | 2:B:425:GLN:OE1   | 2.45                     | 0.49              |
| 2:B:437:THR:HG21 | 2:B:443:ASN:N     | 2.27                     | 0.49              |
| 2:B:924:ILE:O    | 2:B:924:ILE:HG22  | 2.12                     | 0.49              |
| 1:C:20:GLU:HA    | 1:C:551:THR:HG22  | 1.93                     | 0.49              |
| 1:C:111:PHE:CG   | 1:C:112:SER:N     | 2.81                     | 0.49              |
| 1:C:222:TYR:HE1  | 1:C:768:TYR:CB    | 2.10                     | 0.49              |
| 1:C:639:GLY:H    | 1:C:645:VAL:HG22  | 1.78                     | 0.49              |
| 1:C:792:ASP:OD1  | 1:C:792:ASP:N     | 2.45                     | 0.49              |
| 1:C:1008:ALA:O   | 1:C:1010:ALA:N    | 2.45                     | 0.49              |
| 1:C:1099:SER:O   | 1:C:1100:ILE:C    | 2.53                     | 0.49              |
| 2:D:109:THR:HG22 | 2:D:114:ARG:HB3   | 1.94                     | 0.49              |
| 1:A:120:THR:CG2  | 1:A:122:ASP:H     | 2.24                     | 0.49              |
| 1:A:331:GLU:CG   | 1:A:333:THR:HG23  | 2.42                     | 0.49              |
| 1:A:618:LYS:O    | 1:A:619:PRO:O     | 2.31                     | 0.49              |
| 1:A:631:ASP:C    | 1:A:633:GLY:H     | 2.21                     | 0.49              |
| 1:A:773:TRP:HZ3  | 1:A:788:PHE:HE1   | 1.55                     | 0.49              |
| 1:A:1088:GLN:O   | 1:A:1090:ASN:N    | 2.46                     | 0.49              |
| 1:A:1101:CYS:O   | 1:A:1105:LEU:HD12 | 2.13                     | 0.49              |
| 1:A:1132:THR:HB  | 1:A:1134:PRO:HD2  | 1.94                     | 0.49              |
| 1:A:1140:ASN:O   | 1:A:1143:TYR:HB3  | 2.12                     | 0.49              |
| 1:A:1152:ILE:CG2 | 1:A:1168:LEU:HD21 | 2.40                     | 0.49              |
| 1:A:1268:ASN:HB2 | 1:A:1269:PRO:HD3  | 1.95                     | 0.49              |
| 2:B:103:TYR:CD2  | 2:B:103:TYR:N     | 2.79                     | 0.49              |
| 1:C:916:THR:C    | 1:C:918:PHE:N     | 2.71                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1003:LEU:HA   | 1:C:1004:PRO:HD2  | 1.64                     | 0.49              |
| 1:C:1271:ILE:HD13 | 1:C:1300:TYR:CD1  | 2.47                     | 0.49              |
| 1:C:1279:ARG:NH2  | 1:C:1362:THR:HG21 | 2.28                     | 0.49              |
| 1:C:1324:HIS:CD2  | 1:C:1336:ARG:NH2  | 2.81                     | 0.49              |
| 1:C:1365:VAL:CG2  | 1:C:1366:HIS:H    | 2.23                     | 0.49              |
| 1:C:1455:ILE:HD12 | 1:C:1455:ILE:N    | 2.27                     | 0.49              |
| 2:D:422:ARG:HD3   | 2:D:422:ARG:N     | 2.22                     | 0.49              |
| 2:D:447:VAL:HG13  | 2:D:447:VAL:O     | 2.12                     | 0.49              |
| 1:A:471:ASP:O     | 1:A:472:ASN:HB3   | 2.13                     | 0.48              |
| 1:A:618:LYS:N     | 1:A:619:PRO:CD    | 2.72                     | 0.48              |
| 1:A:834:VAL:HB    | 1:A:837:GLU:OE2   | 2.13                     | 0.48              |
| 1:A:961:TYR:HB2   | 1:A:1345:ASP:OD2  | 2.13                     | 0.48              |
| 1:A:1563:VAL:HG12 | 1:A:1581:LEU:HD23 | 1.94                     | 0.48              |
| 2:B:421:PRO:O     | 2:B:424:ARG:HB2   | 2.13                     | 0.48              |
| 2:B:1301:ARG:HB3  | 2:B:1301:ARG:HH11 | 1.78                     | 0.48              |
| 2:B:1600:ILE:O    | 2:B:1602:THR:HG23 | 2.12                     | 0.48              |
| 1:C:126:LEU:HD12  | 1:C:147:SER:HB2   | 1.94                     | 0.48              |
| 1:C:161:LEU:HD11  | 1:C:185:PHE:CE1   | 2.47                     | 0.48              |
| 1:C:516:GLU:CD    | 1:C:516:GLU:N     | 2.70                     | 0.48              |
| 1:C:1226:ARG:O    | 1:C:1270:VAL:HG22 | 2.13                     | 0.48              |
| 1:C:1480:PHE:N    | 1:C:1480:PHE:CD1  | 2.81                     | 0.48              |
| 2:D:58:VAL:HG12   | 2:D:104:VAL:HG22  | 1.94                     | 0.48              |
| 1:A:142:LYS:HA    | 1:A:187:ASP:OD1   | 2.12                     | 0.48              |
| 1:A:283:MET:HE1   | 1:A:301:PHE:CZ    | 2.48                     | 0.48              |
| 1:A:599:TRP:HE1   | 1:A:779:LEU:CD1   | 2.26                     | 0.48              |
| 1:A:819:VAL:O     | 1:A:820:PHE:O     | 2.30                     | 0.48              |
| 1:A:1493:PHE:CD1  | 1:A:1494:THR:N    | 2.79                     | 0.48              |
| 1:A:1563:VAL:HG22 | 1:A:1617:TYR:O    | 2.14                     | 0.48              |
| 2:B:378:PRO:HA    | 2:B:389:THR:HA    | 1.94                     | 0.48              |
| 2:B:1345:LEU:O    | 2:B:1345:LEU:HG   | 2.13                     | 0.48              |
| 1:C:706:ASN:HB2   | 1:C:714:ARG:HH11  | 1.77                     | 0.48              |
| 1:C:875:HIS:CB    | 2:D:901:GLN:HE22  | 2.25                     | 0.48              |
| 2:D:795:THR:HG22  | 2:D:796:PRO:HD2   | 1.95                     | 0.48              |
| 2:D:850:LEU:HG    | 2:D:851:LEU:O     | 2.13                     | 0.48              |
| 2:D:913:LEU:HD23  | 2:D:914:LYS:N     | 2.28                     | 0.48              |
| 2:D:1480:LEU:C    | 2:D:1480:LEU:HD12 | 2.39                     | 0.48              |
| 1:A:21:GLN:HE22   | 1:A:46:TYR:HD2    | 1.61                     | 0.48              |
| 1:A:135:TYR:OH    | 1:A:141:VAL:HG13  | 2.13                     | 0.48              |
| 1:A:324:TYR:C     | 1:A:324:TYR:CD2   | 2.91                     | 0.48              |
| 1:A:790:LEU:HB3   | 1:A:791:PRO:CD    | 2.44                     | 0.48              |
| 1:A:1077:TRP:O    | 1:A:1080:ALA:HB3  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1151:GLY:O    | 1:A:1152:ILE:C    | 2.53                     | 0.48              |
| 1:A:1247:MET:O    | 1:A:1248:VAL:C    | 2.56                     | 0.48              |
| 2:B:44:GLU:OE2    | 2:B:523:TYR:OH    | 2.30                     | 0.48              |
| 2:B:309:LEU:O     | 2:B:310:VAL:C     | 2.57                     | 0.48              |
| 2:B:354:PHE:CD1   | 2:B:354:PHE:C     | 2.91                     | 0.48              |
| 2:B:964:ILE:HG13  | 2:B:1302:THR:CG2  | 2.38                     | 0.48              |
| 1:C:24:VAL:O      | 1:C:24:VAL:HG12   | 2.13                     | 0.48              |
| 1:C:113:LYS:CG    | 1:C:114:SER:N     | 2.74                     | 0.48              |
| 1:C:309:GLU:N     | 1:C:309:GLU:OE1   | 2.46                     | 0.48              |
| 1:C:367:ILE:CD1   | 1:C:466:TYR:HB3   | 2.43                     | 0.48              |
| 1:C:690:TYR:C     | 1:C:692:HIS:H     | 2.19                     | 0.48              |
| 1:C:956:ARG:HA    | 1:C:1348:VAL:O    | 2.12                     | 0.48              |
| 1:C:968:VAL:CG2   | 1:C:971:THR:HG21  | 2.43                     | 0.48              |
| 1:C:1381:ILE:O    | 1:C:1382:ASP:CB   | 2.59                     | 0.48              |
| 1:C:1535:MET:HG2  | 1:C:1608:ASN:O    | 2.14                     | 0.48              |
| 2:D:223:SER:O     | 2:D:252:LEU:HG    | 2.13                     | 0.48              |
| 2:D:283:ILE:N     | 2:D:283:ILE:HD12  | 2.29                     | 0.48              |
| 2:D:1391:LEU:HD12 | 2:D:1417:MET:HE2  | 1.94                     | 0.48              |
| 2:D:1446:PHE:CD2  | 2:D:1448:VAL:HG22 | 2.45                     | 0.48              |
| 1:A:591:ASN:C     | 1:A:592:MET:HG3   | 2.38                     | 0.48              |
| 1:A:968:VAL:CG2   | 1:A:971:THR:HG21  | 2.44                     | 0.48              |
| 1:A:1008:ALA:O    | 1:A:1010:ALA:N    | 2.46                     | 0.48              |
| 1:A:1069:TRP:CZ3  | 1:A:1451:THR:HG21 | 2.48                     | 0.48              |
| 1:A:1132:THR:HG22 | 1:A:1133:LEU:N    | 2.27                     | 0.48              |
| 1:A:1450:PHE:HA   | 1:A:1464:LEU:HB3  | 1.96                     | 0.48              |
| 2:B:58:VAL:HG12   | 2:B:104:VAL:HG22  | 1.94                     | 0.48              |
| 2:B:226:VAL:O     | 2:B:226:VAL:HG12  | 2.12                     | 0.48              |
| 2:B:350:THR:HG23  | 2:B:350:THR:O     | 2.12                     | 0.48              |
| 2:B:512:PRO:O     | 2:B:515:ILE:HD12  | 2.13                     | 0.48              |
| 2:B:842:GLU:O     | 2:B:844:ILE:HG23  | 2.14                     | 0.48              |
| 2:B:1424:ILE:N    | 2:B:1424:ILE:CD1  | 2.74                     | 0.48              |
| 2:B:1602:THR:C    | 2:B:1604:ASN:N    | 2.69                     | 0.48              |
| 1:C:146:TYR:HD1   | 1:C:182:ILE:HG23  | 1.75                     | 0.48              |
| 1:C:540:LEU:HD12  | 1:C:541:LEU:N     | 2.28                     | 0.48              |
| 1:C:944:LEU:HD23  | 1:C:944:LEU:N     | 2.28                     | 0.48              |
| 1:C:1022:PHE:O    | 1:C:1024:TYR:N    | 2.47                     | 0.48              |
| 1:C:1127:ILE:HG12 | 1:C:1143:TYR:CE2  | 2.48                     | 0.48              |
| 1:C:1560:ALA:O    | 1:C:1561:TYR:HB3  | 2.13                     | 0.48              |
| 2:D:69:PHE:CD2    | 2:D:87:ILE:HG22   | 2.49                     | 0.48              |
| 2:D:470:ALA:C     | 2:D:472:SER:H     | 2.20                     | 0.48              |
| 2:D:825:VAL:N     | 2:D:828:GLU:OE1   | 2.39                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1619:GLU:HA   | 2:D:1622:GLN:NE2  | 2.27                     | 0.48              |
| 1:A:961:TYR:O     | 1:A:961:TYR:CD1   | 2.66                     | 0.48              |
| 1:A:1279:ARG:NH2  | 1:A:1362:THR:HG21 | 2.28                     | 0.48              |
| 1:A:1562:LYS:O    | 1:A:1563:VAL:CG1  | 2.62                     | 0.48              |
| 1:A:1585:TYR:CE2  | 1:A:1586:LYS:HB3  | 2.48                     | 0.48              |
| 2:B:235:PHE:CE2   | 2:B:299:PHE:HE2   | 2.31                     | 0.48              |
| 2:B:816:ILE:CD1   | 2:B:896:ILE:HG22  | 2.44                     | 0.48              |
| 2:B:830:VAL:CG2   | 2:B:831:GLU:N     | 2.72                     | 0.48              |
| 2:B:1562:GLN:CB   | 2:B:1598:SER:HB3  | 2.43                     | 0.48              |
| 1:C:185:PHE:CD1   | 1:C:186:PRO:HD2   | 2.48                     | 0.48              |
| 1:C:227:PHE:HB2   | 1:C:338:GLU:HG3   | 1.94                     | 0.48              |
| 1:C:494:ASP:OD1   | 1:C:494:ASP:C     | 2.57                     | 0.48              |
| 1:C:979:VAL:HG21  | 1:C:1326:TYR:CZ   | 2.43                     | 0.48              |
| 1:C:1033:ILE:HG22 | 1:C:1034:PHE:HD1  | 1.77                     | 0.48              |
| 1:C:1061:ASN:HB3  | 1:C:1062:ALA:H    | 1.54                     | 0.48              |
| 1:C:1109:GLU:HB3  | 1:C:1110:ASN:OD1  | 2.13                     | 0.48              |
| 1:C:1224:ILE:HG22 | 1:C:1225:TYR:HD2  | 1.78                     | 0.48              |
| 1:C:1227:PHE:CD2  | 1:C:1273:TRP:NE1  | 2.80                     | 0.48              |
| 1:C:1439:LEU:O    | 1:C:1440:LYS:C    | 2.57                     | 0.48              |
| 2:D:91:ALA:HA     | 2:D:94:VAL:HG23   | 1.96                     | 0.48              |
| 2:D:558:MET:HE3   | 2:D:559:PRO:HD2   | 1.95                     | 0.48              |
| 1:A:308:LYS:HB3   | 1:A:309:GLU:OE1   | 2.13                     | 0.48              |
| 1:A:463:SER:O     | 1:A:555:VAL:HG21  | 2.14                     | 0.48              |
| 1:A:1146:ALA:O    | 1:A:1147:PHE:C    | 2.57                     | 0.48              |
| 1:A:1314:ASP:HA   | 1:A:1325:ASN:HB2  | 1.95                     | 0.48              |
| 2:B:83:VAL:HB     | 2:B:85:PRO:HD3    | 1.95                     | 0.48              |
| 2:B:129:PHE:HE2   | 2:B:598:ILE:HG23  | 1.75                     | 0.48              |
| 2:B:422:ARG:HD3   | 2:B:422:ARG:N     | 2.23                     | 0.48              |
| 2:B:541:LYS:HG3   | 2:B:543:THR:HG22  | 1.95                     | 0.48              |
| 2:B:1482:ASN:C    | 2:B:1493:ALA:HB3  | 2.38                     | 0.48              |
| 1:C:125:PHE:CE1   | 1:C:627:LEU:HD21  | 2.47                     | 0.48              |
| 1:C:544:TYR:HE2   | 1:C:546:VAL:CG2   | 2.26                     | 0.48              |
| 1:C:950:TYR:HD1   | 1:C:1268:ASN:OD1  | 1.95                     | 0.48              |
| 1:C:1622:LYS:NZ   | 1:C:1642:LEU:HB3  | 2.21                     | 0.48              |
| 2:D:511:THR:H     | 2:D:514:LEU:CD1   | 2.26                     | 0.48              |
| 2:D:746:ILE:H     | 2:D:746:ILE:HD13  | 1.77                     | 0.48              |
| 2:D:947:ALA:HB2   | 2:D:1309:GLN:HA   | 1.95                     | 0.48              |
| 1:A:251:LYS:HG2   | 1:A:296:ILE:CD1   | 2.43                     | 0.48              |
| 1:A:444:GLU:O     | 1:A:445:GLU:C     | 2.57                     | 0.48              |
| 1:A:794:LEU:HD12  | 1:A:794:LEU:N     | 2.28                     | 0.48              |
| 1:A:831:TYR:CZ    | 1:A:1457:ASP:HB3  | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1323:LEU:CD1  | 1:A:1324:HIS:H    | 2.26                     | 0.48              |
| 1:A:1562:LYS:C    | 1:A:1563:VAL:CG1  | 2.86                     | 0.48              |
| 2:B:162:ILE:HG21  | 2:B:202:LYS:HG2   | 1.94                     | 0.48              |
| 2:B:778:PHE:N     | 2:B:778:PHE:HD2   | 2.11                     | 0.48              |
| 1:C:391:ASN:O     | 1:C:392:ALA:HB2   | 2.12                     | 0.48              |
| 1:C:631:ASP:C     | 1:C:633:GLY:H     | 2.22                     | 0.48              |
| 1:C:809:ILE:CG1   | 1:C:810:CYS:N     | 2.76                     | 0.48              |
| 1:C:855:PHE:CZ    | 1:C:886:GLN:HB2   | 2.48                     | 0.48              |
| 1:C:916:THR:C     | 1:C:918:PHE:H     | 2.20                     | 0.48              |
| 1:C:1185:THR:OG1  | 1:C:1231:ASN:HB3  | 2.13                     | 0.48              |
| 1:C:1279:ARG:O    | 1:C:1280:TYR:C    | 2.57                     | 0.48              |
| 1:C:1500:ARG:C    | 1:C:1502:ASP:N    | 2.72                     | 0.48              |
| 1:C:1612:VAL:HB   | 1:C:1615:ARG:HB3  | 1.96                     | 0.48              |
| 1:C:1675:GLY:O    | 1:C:1676:CYS:OXT  | 2.32                     | 0.48              |
| 2:D:71:THR:HG23   | 2:D:72:ARG:N      | 2.29                     | 0.48              |
| 2:D:640:SER:O     | 2:D:641:ALA:CB    | 2.61                     | 0.48              |
| 2:D:916:VAL:CG2   | 2:D:917:PRO:HD2   | 2.43                     | 0.48              |
| 1:A:115:LYS:HG3   | 1:A:116:ARG:O     | 2.14                     | 0.48              |
| 1:A:120:THR:HG22  | 1:A:121:TYR:N     | 2.29                     | 0.48              |
| 1:A:534:MET:HB3   | 1:A:538:SER:OG    | 2.14                     | 0.48              |
| 1:A:1565:ILE:O    | 1:A:1566:THR:HG22 | 2.14                     | 0.48              |
| 2:B:84:THR:N      | 2:B:85:PRO:HD3    | 2.28                     | 0.48              |
| 2:B:299:PHE:CE1   | 2:B:303:PHE:HD2   | 2.24                     | 0.48              |
| 2:B:356:PRO:HD2   | 2:B:444:TYR:CZ    | 2.48                     | 0.48              |
| 2:B:477:LYS:N     | 2:B:477:LYS:HD3   | 2.29                     | 0.48              |
| 2:B:860:SER:OG    | 2:B:866:TYR:N     | 2.46                     | 0.48              |
| 2:B:1300:ALA:O    | 2:B:1301:ARG:HD2  | 2.13                     | 0.48              |
| 1:C:135:TYR:OH    | 1:C:141:VAL:HG13  | 2.14                     | 0.48              |
| 1:C:618:LYS:O     | 1:C:619:PRO:O     | 2.32                     | 0.48              |
| 1:C:1020:TYR:CE1  | 1:C:1295:GLU:HG3  | 2.48                     | 0.48              |
| 1:C:1140:ASN:O    | 1:C:1143:TYR:HB3  | 2.14                     | 0.48              |
| 1:C:1313:ILE:HD13 | 1:C:1313:ILE:HA   | 1.68                     | 0.48              |
| 1:C:1563:VAL:HG12 | 1:C:1581:LEU:CD2  | 2.44                     | 0.48              |
| 2:D:378:PRO:HA    | 2:D:389:THR:HA    | 1.95                     | 0.48              |
| 2:D:436:GLN:O     | 2:D:437:THR:C     | 2.56                     | 0.48              |
| 1:A:325:ILE:O     | 1:A:341:GLU:HB2   | 2.14                     | 0.48              |
| 1:A:583:SER:O     | 1:A:586:GLN:HB3   | 2.14                     | 0.48              |
| 1:A:642:ASN:C     | 1:A:642:ASN:ND2   | 2.72                     | 0.48              |
| 1:A:700:TYR:OH    | 1:A:757:LEU:HD22  | 2.14                     | 0.48              |
| 1:A:1483:PHE:O    | 1:A:1485:VAL:HG13 | 2.14                     | 0.48              |
| 2:B:91:ALA:HA     | 2:B:94:VAL:HG23   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:365:TYR:HA    | 2:B:394:GLY:O     | 2.14                     | 0.48              |
| 2:B:455:LYS:O     | 2:B:458:ASP:HB2   | 2.14                     | 0.48              |
| 2:B:850:LEU:HG    | 2:B:851:LEU:O     | 2.14                     | 0.48              |
| 2:B:916:VAL:HG22  | 2:B:917:PRO:O     | 2.14                     | 0.48              |
| 2:B:966:GLN:HG3   | 2:B:966:GLN:O     | 2.14                     | 0.48              |
| 1:C:25:ILE:N      | 1:C:655:THR:CG2   | 2.73                     | 0.48              |
| 1:C:166:PRO:HB3   | 1:C:198:MET:H     | 1.78                     | 0.48              |
| 1:C:700:TYR:OH    | 1:C:757:LEU:HD22  | 2.13                     | 0.48              |
| 1:C:935:LYS:HD3   | 1:C:1373:GLU:OE2  | 2.14                     | 0.48              |
| 2:D:421:PRO:O     | 2:D:424:ARG:HB2   | 2.14                     | 0.48              |
| 2:D:951:ASP:C     | 2:D:953:ARG:N     | 2.68                     | 0.48              |
| 1:A:248:ILE:HD13  | 1:A:325:ILE:CD1   | 2.44                     | 0.48              |
| 1:A:354:LEU:HD23  | 1:A:450:GLU:HG3   | 1.96                     | 0.48              |
| 1:A:1247:MET:HE3  | 1:A:1247:MET:HB2  | 1.63                     | 0.48              |
| 1:A:1268:ASN:N    | 1:A:1269:PRO:HD2  | 2.29                     | 0.48              |
| 1:A:1381:ILE:O    | 1:A:1382:ASP:CB   | 2.62                     | 0.48              |
| 1:A:1554:LYS:CG   | 1:A:1555:PRO:HD2  | 2.43                     | 0.48              |
| 1:A:1567:SER:HB3  | 1:A:1578:LYS:HB2  | 1.96                     | 0.48              |
| 2:B:928:VAL:HG23  | 2:B:1323:MET:HB3  | 1.96                     | 0.48              |
| 1:C:1076:THR:HG22 | 1:C:1144:LEU:HD11 | 1.95                     | 0.48              |
| 1:C:1474:CYS:HB3  | 1:C:1476:ARG:NH1  | 2.29                     | 0.48              |
| 1:C:1567:SER:HB3  | 1:C:1578:LYS:HB2  | 1.96                     | 0.48              |
| 2:D:482:LEU:N     | 2:D:482:LEU:CD1   | 2.75                     | 0.48              |
| 2:D:746:ILE:HD13  | 2:D:746:ILE:N     | 2.29                     | 0.48              |
| 2:D:1632:SER:O    | 2:D:1636:THR:HB   | 2.13                     | 0.48              |
| 1:A:367:ILE:O     | 1:A:368:PRO:C     | 2.57                     | 0.47              |
| 1:A:494:ASP:OD1   | 1:A:494:ASP:C     | 2.57                     | 0.47              |
| 1:A:811:VAL:O     | 1:A:811:VAL:CG1   | 2.62                     | 0.47              |
| 1:A:934:VAL:O     | 1:A:935:LYS:HG3   | 2.13                     | 0.47              |
| 1:A:1075:SER:HB2  | 1:A:1120:GLU:OE1  | 2.14                     | 0.47              |
| 1:A:1128:LYS:HD3  | 1:A:1414:GLU:OE1  | 2.14                     | 0.47              |
| 1:A:1143:TYR:O    | 1:A:1146:ALA:N    | 2.47                     | 0.47              |
| 1:A:1229:LYS:HZ3  | 1:A:1240:PRO:HD2  | 1.79                     | 0.47              |
| 1:A:1532:CYS:SG   | 1:A:1533:GLY:N    | 2.87                     | 0.47              |
| 1:A:1559:TYR:OH   | 1:A:1591:VAL:HA   | 2.14                     | 0.47              |
| 2:B:198:ARG:HB3   | 2:B:213:TYR:CE1   | 2.49                     | 0.47              |
| 2:B:251:TYR:CD2   | 2:B:257:VAL:HG22  | 2.49                     | 0.47              |
| 2:B:345:ILE:HG13  | 2:B:428:LYS:HB2   | 1.94                     | 0.47              |
| 2:B:415:THR:HG23  | 2:B:426:ALA:O     | 2.13                     | 0.47              |
| 2:B:555:LEU:H     | 2:B:555:LEU:HG    | 1.49                     | 0.47              |
| 2:B:795:THR:CG2   | 2:B:796:PRO:HD2   | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:100:SER:HB2   | 1:C:101:TYR:HD2   | 1.78                     | 0.47              |
| 1:C:346:LYS:HE3   | 1:C:348:VAL:HG22  | 1.96                     | 0.47              |
| 1:C:471:ASP:O     | 1:C:472:ASN:HB3   | 2.14                     | 0.47              |
| 1:C:854:GLN:OE1   | 1:C:854:GLN:O     | 2.32                     | 0.47              |
| 1:C:963:ILE:HG23  | 1:C:967:LEU:HD23  | 1.95                     | 0.47              |
| 1:C:1143:TYR:O    | 1:C:1146:ALA:N    | 2.47                     | 0.47              |
| 2:D:338:ILE:C     | 2:D:339:VAL:CG1   | 2.87                     | 0.47              |
| 2:D:358:MET:HB2   | 2:D:358:MET:HE3   | 1.70                     | 0.47              |
| 2:D:795:THR:CG2   | 2:D:796:PRO:HD2   | 2.44                     | 0.47              |
| 2:D:1517:GLU:OE2  | 2:D:1518:THR:HG22 | 2.13                     | 0.47              |
| 1:A:100:SER:CB    | 1:A:101:TYR:HD2   | 2.27                     | 0.47              |
| 1:A:163:PHE:HE1   | 1:A:188:PHE:CB    | 2.26                     | 0.47              |
| 1:A:270:GLY:HA3   | 1:A:282:MET:CG    | 2.43                     | 0.47              |
| 1:A:968:VAL:HG23  | 1:A:971:THR:CG2   | 2.44                     | 0.47              |
| 1:A:1148:THR:O    | 1:A:1149:VAL:C    | 2.57                     | 0.47              |
| 2:B:443:ASN:OD1   | 2:B:469:ASN:HB3   | 2.14                     | 0.47              |
| 2:B:449:ILE:HG23  | 2:B:449:ILE:O     | 2.14                     | 0.47              |
| 2:B:646:GLN:O     | 2:B:647:PRO:C     | 2.57                     | 0.47              |
| 2:B:844:ILE:CD1   | 2:B:872:ILE:HD11  | 2.44                     | 0.47              |
| 2:B:1278:THR:O    | 2:B:1313:VAL:HA   | 2.13                     | 0.47              |
| 2:B:1420:LYS:HB3  | 2:B:1422:ALA:O    | 2.14                     | 0.47              |
| 1:C:156:LYS:C     | 1:C:156:LYS:CD    | 2.87                     | 0.47              |
| 1:C:289:ASN:OD1   | 1:C:289:ASN:N     | 2.46                     | 0.47              |
| 1:C:330:ILE:HG22  | 1:C:337:SER:CB    | 2.31                     | 0.47              |
| 1:C:351:PRO:HG2   | 1:C:352:TYR:HD2   | 1.71                     | 0.47              |
| 1:C:475:ALA:HB1   | 1:C:477:LEU:CD2   | 2.44                     | 0.47              |
| 1:C:971:THR:O     | 1:C:972:GLU:C     | 2.57                     | 0.47              |
| 1:C:1022:PHE:O    | 1:C:1023:HIS:C    | 2.57                     | 0.47              |
| 1:C:1041:GLU:O    | 1:C:1045:LEU:HG   | 2.14                     | 0.47              |
| 1:C:1299:GLU:O    | 1:C:1303:LEU:HB2  | 2.13                     | 0.47              |
| 1:C:1561:TYR:CE1  | 1:C:1581:LEU:HD11 | 2.49                     | 0.47              |
| 2:D:235:PHE:CE2   | 2:D:299:PHE:HE2   | 2.32                     | 0.47              |
| 2:D:259:GLY:HA2   | 2:D:323:GLU:HB3   | 1.94                     | 0.47              |
| 2:D:276:ILE:O     | 2:D:277:PRO:C     | 2.57                     | 0.47              |
| 2:D:449:ILE:O     | 2:D:449:ILE:HG23  | 2.14                     | 0.47              |
| 2:D:628:LEU:HB3   | 2:D:636:THR:HG23  | 1.96                     | 0.47              |
| 2:D:1382:ILE:HG12 | 2:D:1427:LEU:HD11 | 1.95                     | 0.47              |
| 1:A:600:VAL:CG2   | 1:A:780:VAL:HG21  | 2.45                     | 0.47              |
| 1:A:1246:ARG:O    | 1:A:1250:THR:HG23 | 2.15                     | 0.47              |
| 1:A:1271:ILE:CD1  | 1:A:1300:TYR:CZ   | 2.97                     | 0.47              |
| 1:A:1289:ASP:O    | 1:A:1290:THR:C    | 2.55                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1561:TYR:CE1  | 1:A:1581:LEU:HD11 | 2.50                     | 0.47              |
| 2:B:951:ASP:C     | 2:B:953:ARG:N     | 2.68                     | 0.47              |
| 2:B:1476:LYS:HE3  | 2:B:1476:LYS:HB3  | 1.60                     | 0.47              |
| 2:B:1623:LYS:HB3  | 2:B:1623:LYS:HZ2  | 1.80                     | 0.47              |
| 1:C:560:TRP:CZ3   | 1:C:562:ASN:HB2   | 2.49                     | 0.47              |
| 1:C:774:LEU:HD12  | 1:C:799:ILE:HD11  | 1.97                     | 0.47              |
| 1:C:990:ALA:HB1   | 1:C:1000:LEU:CD1  | 2.44                     | 0.47              |
| 1:C:1279:ARG:C    | 1:C:1279:ARG:CD   | 2.87                     | 0.47              |
| 1:C:1307:LEU:HD22 | 1:C:1307:LEU:H    | 1.79                     | 0.47              |
| 1:C:1344:ASP:OD1  | 1:C:1345:ASP:N    | 2.47                     | 0.47              |
| 2:D:126:SER:OG    | 2:D:127:PHE:N     | 2.47                     | 0.47              |
| 2:D:139:PRO:HG2   | 2:D:218:LYS:HE2   | 1.96                     | 0.47              |
| 2:D:217:ARG:HG2   | 2:D:218:LYS:N     | 2.29                     | 0.47              |
| 2:D:437:THR:HG21  | 2:D:443:ASN:N     | 2.30                     | 0.47              |
| 2:D:501:GLN:CG    | 2:D:504:VAL:HG23  | 2.43                     | 0.47              |
| 2:D:543:THR:OG1   | 2:D:544:CYS:N     | 2.43                     | 0.47              |
| 2:D:953:ARG:HG2   | 2:D:954:VAL:N     | 2.29                     | 0.47              |
| 2:D:1384:ILE:HB   | 2:D:1423:VAL:HG12 | 1.96                     | 0.47              |
| 2:D:1484:ILE:HG22 | 2:D:1485:CYS:N    | 2.29                     | 0.47              |
| 2:D:1613:GLU:O    | 2:D:1616:CYS:CB   | 2.61                     | 0.47              |
| 1:A:237:PHE:HA    | 1:A:345:ILE:HG23  | 1.97                     | 0.47              |
| 1:A:308:LYS:CG    | 1:A:309:GLU:H     | 2.25                     | 0.47              |
| 1:A:516:GLU:CD    | 1:A:516:GLU:N     | 2.71                     | 0.47              |
| 1:A:820:PHE:CE2   | 1:A:821:LYS:O     | 2.67                     | 0.47              |
| 1:A:864:GLY:HA3   | 1:A:907:LEU:HD22  | 1.96                     | 0.47              |
| 1:A:1139:GLU:OE2  | 1:A:1187:THR:OG1  | 2.24                     | 0.47              |
| 2:B:26:THR:OG1    | 2:B:44:GLU:HB2    | 2.15                     | 0.47              |
| 2:B:953:ARG:HG2   | 2:B:954:VAL:N     | 2.29                     | 0.47              |
| 2:B:1427:LEU:HD23 | 2:B:1430:VAL:HG23 | 1.96                     | 0.47              |
| 1:C:333:THR:OG1   | 1:C:334:GLY:N     | 2.48                     | 0.47              |
| 1:C:520:ASP:OD1   | 1:C:520:ASP:N     | 2.47                     | 0.47              |
| 1:C:705:VAL:HA    | 1:C:739:ARG:HH12  | 1.77                     | 0.47              |
| 1:C:975:ARG:HH22  | 1:C:1346:LEU:HD22 | 1.79                     | 0.47              |
| 1:C:1104:LEU:O    | 1:C:1108:VAL:HG12 | 2.13                     | 0.47              |
| 2:D:40:GLN:O      | 2:D:489:ILE:HD12  | 2.14                     | 0.47              |
| 2:D:199:ILE:O     | 2:D:199:ILE:HG22  | 2.12                     | 0.47              |
| 2:D:224:PHE:CE2   | 2:D:329:VAL:HG13  | 2.49                     | 0.47              |
| 2:D:481:TYR:CD2   | 2:D:493:GLY:O     | 2.67                     | 0.47              |
| 2:D:581:ASP:OD2   | 2:D:785:THR:HG21  | 2.12                     | 0.47              |
| 2:D:940:THR:HG22  | 2:D:942:LEU:HD22  | 1.96                     | 0.47              |
| 1:A:908:HIS:O     | 1:A:909:ASN:CB    | 2.61                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1016:VAL:HG11 | 1:A:1291:ILE:CD1  | 2.45                     | 0.47              |
| 1:A:1090:ASN:C    | 1:A:1092:TYR:N    | 2.72                     | 0.47              |
| 1:A:1279:ARG:O    | 1:A:1280:TYR:C    | 2.56                     | 0.47              |
| 2:B:192:VAL:CG2   | 2:B:193:SER:H     | 2.17                     | 0.47              |
| 2:B:584:VAL:HG12  | 2:B:585:TYR:N     | 2.29                     | 0.47              |
| 2:B:599:TRP:HA    | 2:B:599:TRP:CE3   | 2.48                     | 0.47              |
| 2:B:825:VAL:N     | 2:B:828:GLU:OE1   | 2.39                     | 0.47              |
| 2:B:940:THR:HG22  | 2:B:942:LEU:HD22  | 1.97                     | 0.47              |
| 2:B:1517:GLU:OE2  | 2:B:1518:THR:HG22 | 2.14                     | 0.47              |
| 1:C:163:PHE:CD2   | 1:C:201:ILE:HG12  | 2.49                     | 0.47              |
| 1:C:373:VAL:CG2   | 1:C:418:ALA:HB3   | 2.43                     | 0.47              |
| 1:C:531:THR:O     | 1:C:534:MET:HG3   | 2.15                     | 0.47              |
| 1:C:706:ASN:HD21  | 1:C:709:GLU:HB2   | 1.79                     | 0.47              |
| 1:C:1143:TYR:O    | 1:C:1144:LEU:C    | 2.56                     | 0.47              |
| 1:C:1183:GLN:HE22 | 1:C:1232:LEU:HD22 | 1.80                     | 0.47              |
| 1:C:1217:LEU:HD13 | 1:C:1237:SER:HA   | 1.95                     | 0.47              |
| 1:C:1255:LEU:HD12 | 1:C:1255:LEU:C    | 2.40                     | 0.47              |
| 2:D:275:SER:C     | 2:D:277:PRO:HD3   | 2.39                     | 0.47              |
| 2:D:382:GLU:C     | 2:D:384:PHE:N     | 2.71                     | 0.47              |
| 2:D:781:ARG:HD3   | 2:D:781:ARG:HA    | 1.58                     | 0.47              |
| 2:D:842:GLU:O     | 2:D:844:ILE:HG23  | 2.15                     | 0.47              |
| 1:A:117:MET:HB2   | 1:A:118:PRO:HD2   | 1.97                     | 0.47              |
| 1:A:502:LEU:HB2   | 1:A:541:LEU:CD2   | 2.45                     | 0.47              |
| 1:A:889:GLU:HB2   | 1:A:892:SER:CB    | 2.39                     | 0.47              |
| 1:A:930:VAL:HA    | 1:A:931:PRO:HD3   | 1.78                     | 0.47              |
| 1:A:1040:ILE:O    | 1:A:1043:GLN:HB2  | 2.14                     | 0.47              |
| 1:A:1086:LEU:O    | 1:A:1087:GLY:C    | 2.57                     | 0.47              |
| 1:A:1102:ASN:HD21 | 1:C:1162:VAL:N    | 1.99                     | 0.47              |
| 2:B:416:ASN:HA    | 2:B:425:GLN:NE2   | 2.29                     | 0.47              |
| 2:B:735:ASN:CB    | 2:B:869:GLN:HE22  | 2.27                     | 0.47              |
| 1:C:174:VAL:CG2   | 1:C:175:GLU:N     | 2.77                     | 0.47              |
| 1:C:500:ASN:O     | 1:C:542:VAL:HA    | 2.15                     | 0.47              |
| 1:C:958:GLU:HA    | 1:C:1346:LEU:O    | 2.14                     | 0.47              |
| 1:C:1549:LYS:HZ3  | 1:C:1549:LYS:HG3  | 1.57                     | 0.47              |
| 1:C:1641:SER:C    | 1:C:1643:THR:N    | 2.73                     | 0.47              |
| 2:D:102:GLN:C     | 2:D:103:TYR:HD2   | 2.22                     | 0.47              |
| 2:D:557:GLN:OE1   | 2:D:557:GLN:HA    | 2.15                     | 0.47              |
| 2:D:1480:LEU:HD21 | 2:D:1483:LYS:HZ2  | 1.80                     | 0.47              |
| 2:D:1581:TYR:HA   | 2:D:1608:GLU:O    | 2.15                     | 0.47              |
| 1:A:571:LEU:CD2   | 1:A:812:ALA:HB2   | 2.44                     | 0.47              |
| 1:A:641:ASN:OD1   | 1:A:644:ASN:HB2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:820:PHE:O     | 1:A:821:LYS:CG    | 2.62                     | 0.47              |
| 1:A:834:VAL:HA    | 1:A:930:VAL:O     | 2.15                     | 0.47              |
| 1:A:950:TYR:HD1   | 1:A:1268:ASN:OD1  | 1.98                     | 0.47              |
| 1:A:1004:PRO:HG3  | 1:A:1461:ILE:HD13 | 1.97                     | 0.47              |
| 1:A:1044:LYS:O    | 1:A:1047:LYS:HB3  | 2.15                     | 0.47              |
| 1:A:1054:LEU:HD22 | 1:A:1057:MET:CE   | 2.45                     | 0.47              |
| 1:A:1094:GLU:CD   | 1:A:1094:GLU:H    | 2.22                     | 0.47              |
| 1:A:1190:ILE:HD11 | 1:A:1253:TYR:CZ   | 2.50                     | 0.47              |
| 1:A:1482:LEU:HD23 | 1:A:1482:LEU:O    | 2.15                     | 0.47              |
| 2:B:148:PHE:CB    | 2:B:800:ILE:HD11  | 2.45                     | 0.47              |
| 2:B:232:GLU:C     | 2:B:234:PHE:H     | 2.22                     | 0.47              |
| 2:B:478:TYR:O     | 2:B:478:TYR:HD1   | 1.98                     | 0.47              |
| 2:B:558:MET:HE3   | 2:B:559:PRO:HD2   | 1.96                     | 0.47              |
| 2:B:964:ILE:O     | 2:B:964:ILE:HG22  | 2.15                     | 0.47              |
| 2:B:1270:HIS:O    | 2:B:1270:HIS:CG   | 2.68                     | 0.47              |
| 2:B:1370:ARG:HG2  | 2:B:1371:TYR:O    | 2.14                     | 0.47              |
| 1:C:54:ILE:HG12   | 1:C:106:VAL:HG13  | 1.95                     | 0.47              |
| 1:C:59:TYR:CD1    | 1:C:60:PRO:CD     | 2.97                     | 0.47              |
| 1:C:444:GLU:O     | 1:C:445:GLU:C     | 2.57                     | 0.47              |
| 1:C:624:PHE:CD1   | 1:C:625:GLN:N     | 2.83                     | 0.47              |
| 1:C:1088:GLN:C    | 1:C:1090:ASN:H    | 2.22                     | 0.47              |
| 1:C:1320:LYS:HD2  | 1:C:1321:GLY:N    | 2.22                     | 0.47              |
| 1:C:1421:HIS:NE2  | 1:C:1498:TYR:CD1  | 2.82                     | 0.47              |
| 1:C:1548:ARG:HD3  | 1:C:1548:ARG:H    | 1.79                     | 0.47              |
| 1:C:1559:TYR:OH   | 1:C:1591:VAL:HA   | 2.14                     | 0.47              |
| 1:C:1565:ILE:O    | 1:C:1566:THR:HG22 | 2.14                     | 0.47              |
| 2:D:63:ARG:HB2    | 2:D:65:GLN:HG3    | 1.97                     | 0.47              |
| 2:D:150:MET:HE1   | 2:D:545:MET:HE3   | 1.97                     | 0.47              |
| 2:D:354:PHE:CE2   | 2:D:409:LEU:HB2   | 2.50                     | 0.47              |
| 2:D:435:TYR:CE1   | 2:D:616:ASN:HA    | 2.50                     | 0.47              |
| 2:D:545:MET:HG3   | 2:D:798:LYS:O     | 2.15                     | 0.47              |
| 2:D:621:PHE:H     | 2:D:621:PHE:HD2   | 1.62                     | 0.47              |
| 2:D:818:LEU:HG    | 2:D:818:LEU:O     | 2.15                     | 0.47              |
| 2:D:916:VAL:CG2   | 2:D:917:PRO:N     | 2.78                     | 0.47              |
| 2:D:1380:THR:HG22 | 2:D:1381:ILE:H    | 1.79                     | 0.47              |
| 2:D:1509:PRO:O    | 2:D:1512:ILE:HG13 | 2.14                     | 0.47              |
| 1:A:265:VAL:HG23  | 1:A:292:LEU:H     | 1.79                     | 0.47              |
| 1:A:501:TYR:HD1   | 1:A:501:TYR:C     | 2.21                     | 0.47              |
| 1:A:987:ILE:HG22  | 1:A:1021:VAL:HG23 | 1.96                     | 0.47              |
| 1:A:1076:THR:HG22 | 1:A:1144:LEU:HD11 | 1.97                     | 0.47              |
| 2:B:646:GLN:HB3   | 2:B:647:PRO:CD    | 2.35                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:866:TYR:OH    | 2:B:1388:THR:HG21 | 2.15                     | 0.47              |
| 1:C:165:ASP:HB2   | 1:C:166:PRO:HD2   | 1.97                     | 0.47              |
| 1:C:354:LEU:HA    | 1:C:374:GLN:O     | 2.15                     | 0.47              |
| 1:C:364:LYS:HE2   | 1:C:465:LEU:O     | 2.14                     | 0.47              |
| 1:C:599:TRP:HE1   | 1:C:779:LEU:CD1   | 2.27                     | 0.47              |
| 1:C:794:LEU:HD12  | 1:C:794:LEU:N     | 2.30                     | 0.47              |
| 1:C:1159:CYS:N    | 1:C:1160:PRO:CD   | 2.77                     | 0.47              |
| 1:C:1209:VAL:HG12 | 1:C:1210:SER:N    | 2.30                     | 0.47              |
| 1:C:1450:PHE:HA   | 1:C:1464:LEU:HB3  | 1.97                     | 0.47              |
| 1:C:1475:VAL:HG22 | 1:C:1476:ARG:N    | 2.30                     | 0.47              |
| 2:D:59:HIS:O      | 2:D:104:VAL:HG23  | 2.14                     | 0.47              |
| 2:D:252:LEU:HD22  | 2:D:582:LYS:HB3   | 1.97                     | 0.47              |
| 2:D:1349:VAL:HA   | 2:D:1364:MET:O    | 2.14                     | 0.47              |
| 2:D:1402:LYS:HD3  | 2:D:1402:LYS:HA   | 1.52                     | 0.47              |
| 2:D:1412:GLU:HB2  | 2:D:1419:GLN:CG   | 2.45                     | 0.47              |
| 2:D:1438:LEU:C    | 2:D:1438:LEU:HD22 | 2.39                     | 0.47              |
| 1:A:365:PRO:CG    | 1:A:464:TYR:CE2   | 2.97                     | 0.47              |
| 1:A:500:ASN:O     | 1:A:542:VAL:HA    | 2.15                     | 0.47              |
| 1:A:1255:LEU:HD12 | 1:A:1255:LEU:C    | 2.39                     | 0.47              |
| 1:A:1370:THR:O    | 1:A:1371:SER:C    | 2.56                     | 0.47              |
| 1:A:1548:ARG:H    | 1:A:1548:ARG:HD3  | 1.80                     | 0.47              |
| 2:B:490:PHE:CD1   | 2:B:490:PHE:C     | 2.91                     | 0.47              |
| 2:B:525:GLN:NE2   | 2:B:528:ASN:H     | 2.13                     | 0.47              |
| 2:B:563:MET:HG3   | 2:B:780:LEU:CD2   | 2.43                     | 0.47              |
| 2:B:1330:ASN:N    | 2:B:1330:ASN:HD22 | 2.12                     | 0.47              |
| 2:B:1599:TYR:N    | 2:B:1599:TYR:HD1  | 2.13                     | 0.47              |
| 1:C:25:ILE:HD13   | 1:C:41:ILE:HG13   | 1.96                     | 0.47              |
| 1:C:238:ILE:HG12  | 1:C:246:PHE:HE1   | 1.80                     | 0.47              |
| 1:C:968:VAL:HG23  | 1:C:971:THR:CG2   | 2.44                     | 0.47              |
| 1:C:970:LYS:C     | 1:C:971:THR:CG2   | 2.87                     | 0.47              |
| 1:C:1000:LEU:HD22 | 1:C:1281:GLY:CA   | 2.45                     | 0.47              |
| 1:C:1188:LEU:HD23 | 1:C:1212:LEU:CD2  | 2.45                     | 0.47              |
| 1:C:1304:VAL:CG1  | 1:C:1305:LYS:H    | 2.27                     | 0.47              |
| 1:C:1323:LEU:CD1  | 1:C:1324:HIS:H    | 2.27                     | 0.47              |
| 1:C:1618:LEU:C    | 1:C:1618:LEU:HD22 | 2.40                     | 0.47              |
| 2:D:555:LEU:H     | 2:D:555:LEU:HG    | 1.48                     | 0.47              |
| 2:D:584:VAL:HG12  | 2:D:585:TYR:N     | 2.29                     | 0.47              |
| 2:D:745:ILE:HG22  | 2:D:897:LYS:HD3   | 1.93                     | 0.47              |
| 2:D:1506:ILE:HD11 | 2:D:1628:PHE:CE1  | 2.50                     | 0.47              |
| 1:A:36:SER:HA     | 1:A:86:THR:CG2    | 2.45                     | 0.47              |
| 1:A:81:ASN:CG     | 1:A:82:SER:N      | 2.72                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:136:THR:HG21  | 1:A:222:TYR:HB2   | 1.96                     | 0.47              |
| 1:A:1113:LEU:HD23 | 1:A:1114:ASP:N    | 2.29                     | 0.47              |
| 1:A:1344:ASP:OD1  | 1:A:1345:ASP:N    | 2.47                     | 0.47              |
| 2:B:137:TYR:CE1   | 2:B:143:VAL:HG22  | 2.49                     | 0.47              |
| 2:B:524:TYR:O     | 2:B:524:TYR:HD1   | 1.98                     | 0.47              |
| 1:C:165:ASP:OD2   | 1:C:165:ASP:O     | 2.32                     | 0.47              |
| 1:C:558:SER:HB3   | 1:C:645:VAL:HG13  | 1.97                     | 0.47              |
| 1:C:1084:ARG:NE   | 1:C:1154:LYS:HE3  | 2.30                     | 0.47              |
| 1:C:1090:ASN:OD1  | 1:C:1094:GLU:HA   | 2.15                     | 0.47              |
| 1:C:1268:ASN:H    | 1:C:1268:ASN:HD22 | 1.62                     | 0.47              |
| 1:C:1584:ILE:HG22 | 1:C:1586:LYS:H    | 1.80                     | 0.47              |
| 2:D:433:ILE:HG22  | 2:D:434:ALA:N     | 2.30                     | 0.47              |
| 2:D:478:TYR:O     | 2:D:478:TYR:HD1   | 1.98                     | 0.47              |
| 2:D:515:ILE:HG21  | 2:D:599:TRP:CZ2   | 2.50                     | 0.47              |
| 2:D:1391:LEU:CB   | 2:D:1417:MET:HE2  | 2.41                     | 0.47              |
| 2:D:1522:TYR:OH   | 2:D:1563:TYR:OH   | 2.33                     | 0.47              |
| 1:A:163:PHE:CD2   | 1:A:201:ILE:HG12  | 2.50                     | 0.46              |
| 1:A:367:ILE:HD13  | 1:A:466:TYR:HD2   | 1.80                     | 0.46              |
| 1:A:604:ALA:HB3   | 1:A:773:TRP:O     | 2.14                     | 0.46              |
| 1:A:944:LEU:N     | 1:A:944:LEU:HD23  | 2.31                     | 0.46              |
| 1:A:960:PRO:HB2   | 1:A:961:TYR:H     | 1.59                     | 0.46              |
| 1:A:1026:GLU:HA   | 1:A:1031:TRP:HE1  | 1.79                     | 0.46              |
| 1:A:1358:THR:HB   | 1:A:1360:HIS:CE1  | 2.51                     | 0.46              |
| 1:A:1480:PHE:N    | 1:A:1480:PHE:CD1  | 2.83                     | 0.46              |
| 2:B:102:GLN:C     | 2:B:103:TYR:HD2   | 2.23                     | 0.46              |
| 2:B:253:TYR:HE1   | 2:B:839:TYR:HE2   | 1.62                     | 0.46              |
| 2:B:1392:PRO:HB2  | 2:B:1397:LEU:HD22 | 1.96                     | 0.46              |
| 1:C:36:SER:HA     | 1:C:86:THR:CG2    | 2.45                     | 0.46              |
| 1:C:136:THR:HG21  | 1:C:222:TYR:HB2   | 1.96                     | 0.46              |
| 1:C:938:SER:O     | 1:C:940:SER:N     | 2.48                     | 0.46              |
| 1:C:949:ILE:C     | 1:C:950:TYR:CG    | 2.93                     | 0.46              |
| 1:C:985:GLY:O     | 1:C:987:ILE:N     | 2.48                     | 0.46              |
| 1:C:1020:TYR:O    | 1:C:1021:VAL:C    | 2.59                     | 0.46              |
| 1:C:1552:ALA:HB2  | 1:C:1620:MET:HE3  | 1.96                     | 0.46              |
| 1:C:1562:LYS:CD   | 1:C:1648:TRP:HZ2  | 2.27                     | 0.46              |
| 2:D:58:VAL:HG12   | 2:D:104:VAL:CG2   | 2.45                     | 0.46              |
| 2:D:196:THR:HG23  | 2:D:215:ASP:OD1   | 2.16                     | 0.46              |
| 2:D:230:PRO:HG3   | 2:D:333:GLN:HG2   | 1.97                     | 0.46              |
| 2:D:398:LEU:HD23  | 2:D:398:LEU:HA    | 1.67                     | 0.46              |
| 2:D:522:ALA:O     | 2:D:533:ALA:HB1   | 2.15                     | 0.46              |
| 2:D:919:GLY:HA2   | 2:D:1331:ALA:O    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:930:LEU:HB2   | 2:D:1321:ALA:HB3  | 1.96                     | 0.46              |
| 2:D:954:VAL:O     | 2:D:957:THR:HG23  | 2.16                     | 0.46              |
| 2:D:1275:LEU:HA   | 2:D:1317:GLY:HA3  | 1.97                     | 0.46              |
| 2:D:1378:THR:O    | 2:D:1379:MET:C    | 2.58                     | 0.46              |
| 1:A:124:GLY:C     | 1:A:125:PHE:CG    | 2.93                     | 0.46              |
| 1:A:392:ALA:HB2   | 1:A:433:PHE:CB    | 2.45                     | 0.46              |
| 1:A:888:VAL:CG2   | 1:A:894:HIS:HB2   | 2.38                     | 0.46              |
| 1:A:977:LEU:HA    | 1:A:1361:VAL:HG12 | 1.97                     | 0.46              |
| 1:A:1037:ASP:HA   | 1:A:1038:PRO:HD3  | 1.81                     | 0.46              |
| 1:A:1180:LEU:HD21 | 1:A:1208:ILE:HG12 | 1.95                     | 0.46              |
| 2:B:133:ASP:HB3   | 2:B:757:TRP:CZ3   | 2.51                     | 0.46              |
| 2:B:464:PHE:O     | 2:B:503:LEU:HA    | 2.14                     | 0.46              |
| 2:B:919:GLY:HA2   | 2:B:1331:ALA:O    | 2.16                     | 0.46              |
| 2:B:1386:MET:HA   | 2:B:1386:MET:CE   | 2.34                     | 0.46              |
| 2:B:1606:TRP:O    | 2:B:1606:TRP:HD1  | 1.98                     | 0.46              |
| 2:B:1635:LEU:O    | 2:B:1637:GLU:N    | 2.48                     | 0.46              |
| 1:C:145:VAL:O     | 1:C:183:ILE:HD12  | 2.15                     | 0.46              |
| 1:C:222:TYR:CD2   | 1:C:222:TYR:C     | 2.93                     | 0.46              |
| 1:C:421:VAL:HG11  | 2:D:505:THR:HG22  | 1.97                     | 0.46              |
| 1:C:600:VAL:CG2   | 1:C:780:VAL:HG21  | 2.45                     | 0.46              |
| 1:C:623:VAL:O     | 1:C:625:GLN:N     | 2.49                     | 0.46              |
| 1:C:692:HIS:O     | 1:C:692:HIS:CD2   | 2.68                     | 0.46              |
| 1:C:1563:VAL:CG2  | 1:C:1619:ILE:HD12 | 2.43                     | 0.46              |
| 2:D:162:ILE:CG2   | 2:D:162:ILE:O     | 2.63                     | 0.46              |
| 2:D:268:LYS:HG3   | 2:D:273:LYS:HG2   | 1.97                     | 0.46              |
| 2:D:356:PRO:HD2   | 2:D:444:TYR:CZ    | 2.50                     | 0.46              |
| 2:D:519:ARG:CZ    | 2:D:608:GLY:HA3   | 2.44                     | 0.46              |
| 2:D:857:CYS:HB3   | 2:D:885:VAL:CG2   | 2.46                     | 0.46              |
| 2:D:1300:ALA:O    | 2:D:1301:ARG:HD2  | 2.15                     | 0.46              |
| 1:A:222:TYR:CD2   | 1:A:222:TYR:C     | 2.94                     | 0.46              |
| 1:A:346:LYS:HE3   | 1:A:348:VAL:HG22  | 1.97                     | 0.46              |
| 1:A:654:LEU:C     | 1:A:655:THR:HG23  | 2.40                     | 0.46              |
| 1:A:774:LEU:HG    | 1:A:788:PHE:CE1   | 2.50                     | 0.46              |
| 1:A:909:ASN:O     | 1:A:910:ILE:HG12  | 2.15                     | 0.46              |
| 1:A:1067:SER:HA   | 1:A:1074:ALA:HA   | 1.98                     | 0.46              |
| 1:A:1556:GLU:HB2  | 1:A:1622:LYS:HE2  | 1.96                     | 0.46              |
| 1:A:1584:ILE:CG2  | 1:A:1585:TYR:N    | 2.72                     | 0.46              |
| 2:B:433:ILE:HG22  | 2:B:434:ALA:N     | 2.30                     | 0.46              |
| 2:B:1289:ARG:O    | 2:B:1290:TYR:HD1  | 1.96                     | 0.46              |
| 2:B:1292:ILE:HD12 | 2:B:1296:ASN:OD1  | 2.16                     | 0.46              |
| 2:B:1312:THR:HG22 | 2:B:1312:THR:O    | 2.14                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:683:ILE:O     | 1:C:687:ALA:HB3   | 2.15                     | 0.46              |
| 1:C:1290:THR:O    | 1:C:1294:ILE:CG1  | 2.63                     | 0.46              |
| 1:C:1413:GLU:OE2  | 1:C:1413:GLU:HA   | 2.15                     | 0.46              |
| 1:C:1435:ASN:O    | 1:C:1436:GLU:C    | 2.58                     | 0.46              |
| 1:C:1648:TRP:HE1  | 1:C:1664:LEU:HD22 | 1.81                     | 0.46              |
| 2:D:162:ILE:HG21  | 2:D:202:LYS:HG2   | 1.97                     | 0.46              |
| 2:D:646:GLN:O     | 2:D:647:PRO:C     | 2.59                     | 0.46              |
| 2:D:757:TRP:O     | 2:D:758:LEU:HD23  | 2.16                     | 0.46              |
| 1:A:240:TYR:C     | 1:A:240:TYR:CD2   | 2.89                     | 0.46              |
| 1:A:353:LYS:CE    | 1:A:378:SER:HA    | 2.46                     | 0.46              |
| 1:A:971:THR:O     | 1:A:972:GLU:C     | 2.58                     | 0.46              |
| 1:A:977:LEU:CD2   | 1:A:1361:VAL:HG13 | 2.45                     | 0.46              |
| 1:A:1000:LEU:HD22 | 1:A:1281:GLY:CA   | 2.45                     | 0.46              |
| 1:A:1041:GLU:O    | 1:A:1045:LEU:HG   | 2.16                     | 0.46              |
| 1:A:1068:VAL:HG13 | 1:A:1069:TRP:N    | 2.27                     | 0.46              |
| 1:A:1479:ILE:N    | 1:A:1479:ILE:CD1  | 2.78                     | 0.46              |
| 1:A:1500:ARG:C    | 1:A:1502:ASP:N    | 2.73                     | 0.46              |
| 1:A:1587:THR:HB   | 1:A:1591:VAL:HG13 | 1.97                     | 0.46              |
| 2:B:237:ILE:HD11  | 2:B:309:LEU:CB    | 2.44                     | 0.46              |
| 2:B:629:THR:HA    | 2:B:635:ASN:OD1   | 2.15                     | 0.46              |
| 1:C:466:TYR:CZ    | 1:C:468:ASP:HB2   | 2.50                     | 0.46              |
| 1:C:591:ASN:C     | 1:C:592:MET:HG3   | 2.40                     | 0.46              |
| 1:C:700:TYR:CD2   | 1:C:701:ASP:N     | 2.83                     | 0.46              |
| 1:C:803:GLY:O     | 1:C:810:CYS:HB2   | 2.16                     | 0.46              |
| 1:C:1271:ILE:CD1  | 1:C:1300:TYR:CZ   | 2.98                     | 0.46              |
| 1:C:1602:LYS:HB3  | 1:C:1639:LEU:CB   | 2.45                     | 0.46              |
| 2:D:214:PHE:HD1   | 2:D:214:PHE:C     | 2.22                     | 0.46              |
| 2:D:345:ILE:HG13  | 2:D:428:LYS:HB2   | 1.95                     | 0.46              |
| 2:D:806:TYR:CE1   | 2:D:807:GLU:O     | 2.68                     | 0.46              |
| 2:D:824:VAL:HG22  | 2:D:825:VAL:H     | 1.79                     | 0.46              |
| 2:D:1466:GLU:CD   | 2:D:1468:CYS:HB2  | 2.41                     | 0.46              |
| 2:D:1606:TRP:C    | 2:D:1606:TRP:HD1  | 2.22                     | 0.46              |
| 1:A:488:PRO:O     | 1:A:489:LYS:O     | 2.33                     | 0.46              |
| 1:A:584:PRO:HD3   | 1:A:820:PHE:HB2   | 1.97                     | 0.46              |
| 1:A:792:ASP:OD1   | 1:A:792:ASP:N     | 2.47                     | 0.46              |
| 1:A:975:ARG:HH22  | 1:A:1346:LEU:HD22 | 1.74                     | 0.46              |
| 1:A:1086:LEU:CD1  | 1:A:1095:GLN:HG3  | 2.39                     | 0.46              |
| 1:A:1160:PRO:HG2  | 1:C:1098:ASN:OD1  | 2.15                     | 0.46              |
| 1:A:1188:LEU:HD23 | 1:A:1212:LEU:CD2  | 2.45                     | 0.46              |
| 1:A:1266:TYR:O    | 1:A:1266:TYR:CD1  | 2.69                     | 0.46              |
| 1:A:1565:ILE:HD13 | 1:A:1565:ILE:N    | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1658:GLN:NE2  | 1:A:1661:LEU:HD12 | 2.31                     | 0.46              |
| 2:B:445:LEU:HD12  | 2:B:446:HIS:N     | 2.31                     | 0.46              |
| 2:B:885:VAL:HA    | 2:B:886:PRO:HD3   | 1.76                     | 0.46              |
| 1:C:267:ILE:CG2   | 1:C:268:THR:N     | 2.78                     | 0.46              |
| 2:D:162:ILE:O     | 2:D:162:ILE:HG23  | 2.16                     | 0.46              |
| 2:D:820:MET:HA    | 2:D:821:PRO:HD3   | 1.78                     | 0.46              |
| 2:D:923:SER:C     | 2:D:924:ILE:HD12  | 2.41                     | 0.46              |
| 2:D:1275:LEU:HD21 | 2:D:1319:GLY:C    | 2.39                     | 0.46              |
| 2:D:1407:TYR:C    | 2:D:1407:TYR:CD2  | 2.92                     | 0.46              |
| 2:D:1522:TYR:HB2  | 2:D:1524:TYR:CE1  | 2.50                     | 0.46              |
| 2:D:1540:TYR:HE1  | 2:D:1575:LEU:HB2  | 1.80                     | 0.46              |
| 1:A:955:ARG:HD3   | 1:A:1351:GLY:O    | 2.16                     | 0.46              |
| 1:A:958:GLU:HA    | 1:A:1346:LEU:O    | 2.16                     | 0.46              |
| 1:A:1175:LEU:HB3  | 1:A:1195:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:1474:CYS:HB3  | 1:A:1476:ARG:NH1  | 2.31                     | 0.46              |
| 1:A:1616:GLN:NE2  | 1:A:1648:TRP:CZ3  | 2.84                     | 0.46              |
| 2:B:210:TYR:CG    | 2:B:211:THR:N     | 2.83                     | 0.46              |
| 2:B:383:ALA:C     | 2:B:384:PHE:CD2   | 2.94                     | 0.46              |
| 2:B:848:VAL:HG22  | 2:B:898:ALA:CB    | 2.43                     | 0.46              |
| 2:B:916:VAL:HG22  | 2:B:917:PRO:N     | 2.30                     | 0.46              |
| 1:C:251:LYS:HG2   | 1:C:296:ILE:CD1   | 2.45                     | 0.46              |
| 1:C:286:ALA:O     | 1:C:287:MET:O     | 2.33                     | 0.46              |
| 1:C:501:TYR:CD1   | 1:C:501:TYR:C     | 2.93                     | 0.46              |
| 1:C:565:GLU:CD    | 1:C:565:GLU:H     | 2.22                     | 0.46              |
| 1:C:702:GLY:HA2   | 1:C:728:PHE:CD1   | 2.48                     | 0.46              |
| 1:C:820:PHE:CE2   | 1:C:821:LYS:O     | 2.69                     | 0.46              |
| 1:C:969:PRO:HD3   | 1:C:1603:LYS:HZ1  | 1.81                     | 0.46              |
| 1:C:1043:GLN:O    | 1:C:1044:LYS:C    | 2.58                     | 0.46              |
| 1:C:1556:GLU:HB2  | 1:C:1622:LYS:HE2  | 1.97                     | 0.46              |
| 1:C:1622:LYS:HD2  | 1:C:1642:LEU:HB2  | 1.97                     | 0.46              |
| 1:C:1623:GLU:CB   | 1:C:1638:PRO:CG   | 2.91                     | 0.46              |
| 2:D:531:ILE:O     | 2:D:617:ASN:ND2   | 2.48                     | 0.46              |
| 2:D:822:TYR:O     | 2:D:914:LYS:HB3   | 2.15                     | 0.46              |
| 2:D:1480:LEU:HD12 | 2:D:1481:LEU:N    | 2.31                     | 0.46              |
| 2:D:1527:LYS:H    | 2:D:1545:LEU:HD13 | 1.81                     | 0.46              |
| 1:A:59:TYR:CD1    | 1:A:60:PRO:CD     | 2.97                     | 0.46              |
| 1:A:259:VAL:HB    | 1:A:295:GLY:HA2   | 1.97                     | 0.46              |
| 1:A:642:ASN:HD21  | 1:A:646:PHE:HE1   | 1.63                     | 0.46              |
| 1:A:990:ALA:HB1   | 1:A:1000:LEU:CD1  | 2.46                     | 0.46              |
| 1:A:1327:LYS:C    | 1:A:1328:MET:HE2  | 2.41                     | 0.46              |
| 2:B:63:ARG:HB2    | 2:B:65:GLN:HG3    | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:563:MET:HA    | 2:B:563:MET:CE    | 2.45                     | 0.46              |
| 1:C:100:SER:O     | 1:C:101:TYR:HB2   | 2.15                     | 0.46              |
| 1:C:288:GLN:O     | 1:C:289:ASN:C     | 2.57                     | 0.46              |
| 1:C:352:TYR:HE1   | 1:C:383:VAL:HG21  | 1.80                     | 0.46              |
| 1:C:392:ALA:HB2   | 1:C:433:PHE:CB    | 2.45                     | 0.46              |
| 1:C:587:THR:HG22  | 1:C:789:ALA:HB2   | 1.97                     | 0.46              |
| 1:C:654:LEU:C     | 1:C:655:THR:HG23  | 2.40                     | 0.46              |
| 1:C:1159:CYS:O    | 1:C:1164:ILE:HD11 | 2.15                     | 0.46              |
| 2:D:133:ASP:OD2   | 2:D:134:LYS:HG2   | 2.15                     | 0.46              |
| 2:D:263:VAL:HG22  | 2:D:318:VAL:HG23  | 1.98                     | 0.46              |
| 2:D:844:ILE:CD1   | 2:D:872:ILE:HD11  | 2.46                     | 0.46              |
| 2:D:1282:PRO:HD2  | 2:D:1309:GLN:CD   | 2.40                     | 0.46              |
| 2:D:1607:ILE:N    | 2:D:1607:ILE:CD1  | 2.59                     | 0.46              |
| 1:A:612:VAL:O     | 1:A:612:VAL:HG12  | 2.16                     | 0.46              |
| 1:A:692:HIS:CD2   | 1:A:692:HIS:O     | 2.69                     | 0.46              |
| 1:A:694:VAL:HG12  | 1:A:697:LYS:HE3   | 1.98                     | 0.46              |
| 1:A:956:ARG:HG2   | 1:A:1349:SER:HB3  | 1.98                     | 0.46              |
| 1:A:985:GLY:O     | 1:A:987:ILE:N     | 2.49                     | 0.46              |
| 1:A:1117:SER:HB3  | 1:A:1174:PHE:CD2  | 2.49                     | 0.46              |
| 1:A:1323:LEU:O    | 1:A:1324:HIS:O    | 2.33                     | 0.46              |
| 1:A:1618:LEU:HD22 | 1:A:1619:ILE:N    | 2.31                     | 0.46              |
| 1:A:1675:GLY:O    | 1:A:1676:CYS:OXT  | 2.34                     | 0.46              |
| 2:B:829:GLN:HE21  | 2:B:829:GLN:C     | 2.23                     | 0.46              |
| 1:C:431:LEU:HD22  | 1:C:432:GLU:N     | 2.30                     | 0.46              |
| 1:C:486:VAL:O     | 1:C:486:VAL:HG12  | 2.15                     | 0.46              |
| 1:C:501:TYR:CE1   | 1:C:512:PHE:C     | 2.94                     | 0.46              |
| 1:C:968:VAL:HG12  | 1:C:1368:THR:CG2  | 2.45                     | 0.46              |
| 1:C:1013:MET:O    | 1:C:1017:PRO:HD3  | 2.16                     | 0.46              |
| 1:C:1075:SER:HB2  | 1:C:1120:GLU:OE1  | 2.16                     | 0.46              |
| 1:C:1142:LEU:HD13 | 1:C:1187:THR:CG2  | 2.46                     | 0.46              |
| 1:C:1616:GLN:CD   | 1:C:1648:TRP:CZ3  | 2.94                     | 0.46              |
| 1:C:1631:PHE:N    | 1:C:1631:PHE:CD2  | 2.82                     | 0.46              |
| 2:D:378:PRO:HG3   | 2:D:389:THR:HG23  | 1.97                     | 0.46              |
| 2:D:383:ALA:C     | 2:D:384:PHE:CD2   | 2.94                     | 0.46              |
| 2:D:466:VAL:HG12  | 2:D:524:TYR:CE2   | 2.50                     | 0.46              |
| 2:D:482:LEU:O     | 2:D:482:LEU:HD13  | 2.16                     | 0.46              |
| 2:D:814:PHE:HZ    | 2:D:846:VAL:HG21  | 1.81                     | 0.46              |
| 2:D:1330:ASN:H    | 2:D:1330:ASN:HD22 | 1.64                     | 0.46              |
| 1:A:42:GLN:OE1    | 1:A:500:ASN:ND2   | 2.49                     | 0.46              |
| 1:A:96:GLN:HG3    | 1:A:97:ASN:H      | 1.80                     | 0.46              |
| 1:A:383:VAL:O     | 1:A:383:VAL:HG22  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:552:ALA:HB3   | 1:A:658:ASN:HB3   | 1.98                     | 0.46              |
| 1:A:849:ARG:NH1   | 1:A:849:ARG:CG    | 2.76                     | 0.46              |
| 1:A:875:HIS:HB3   | 2:B:901:GLN:HE22  | 1.81                     | 0.46              |
| 1:A:947:ARG:CZ    | 1:A:1354:SER:HB3  | 2.46                     | 0.46              |
| 1:A:1631:PHE:CD2  | 1:A:1631:PHE:N    | 2.80                     | 0.46              |
| 2:B:625:GLY:O     | 2:B:626:LEU:HG    | 2.16                     | 0.46              |
| 1:C:487:THR:HG22  | 1:C:523:TYR:HB2   | 1.98                     | 0.46              |
| 1:C:681:LYS:HB2   | 1:C:738:LEU:HD11  | 1.96                     | 0.46              |
| 1:C:691:LYS:O     | 1:C:693:SER:N     | 2.49                     | 0.46              |
| 1:C:859:MET:HE3   | 1:C:898:PHE:CG    | 2.51                     | 0.46              |
| 1:C:1570:VAL:CG2  | 1:C:1575:VAL:HG22 | 2.46                     | 0.46              |
| 2:D:966:GLN:O     | 2:D:966:GLN:HG3   | 2.15                     | 0.46              |
| 2:D:1610:TRP:HA   | 2:D:1611:PRO:HD2  | 1.74                     | 0.46              |
| 1:A:33:VAL:HG23   | 1:A:120:THR:O     | 2.14                     | 0.46              |
| 1:A:145:VAL:O     | 1:A:183:ILE:HD12  | 2.15                     | 0.46              |
| 1:A:179:HIS:C     | 1:A:180:ILE:HG12  | 2.40                     | 0.46              |
| 1:A:596:MET:SD    | 1:A:782:ARG:HG3   | 2.56                     | 0.46              |
| 1:A:709:GLU:OE1   | 1:A:709:GLU:HA    | 2.16                     | 0.46              |
| 1:A:756:THR:O     | 1:A:757:LEU:HD23  | 2.16                     | 0.46              |
| 1:A:1081:PHE:HD1  | 1:A:1147:PHE:HZ   | 1.63                     | 0.46              |
| 1:A:1183:GLN:HE22 | 1:A:1232:LEU:HD22 | 1.81                     | 0.46              |
| 1:A:1320:LYS:HD2  | 1:A:1321:GLY:N    | 2.23                     | 0.46              |
| 1:A:1563:VAL:HG12 | 1:A:1581:LEU:CD2  | 2.46                     | 0.46              |
| 1:A:1612:VAL:HB   | 1:A:1615:ARG:CB   | 2.46                     | 0.46              |
| 2:B:382:GLU:C     | 2:B:384:PHE:N     | 2.72                     | 0.46              |
| 2:B:757:TRP:C     | 2:B:758:LEU:HD23  | 2.41                     | 0.46              |
| 2:B:950:LEU:O     | 2:B:951:ASP:HB2   | 2.16                     | 0.46              |
| 2:B:1407:TYR:O    | 2:B:1408:ILE:HD13 | 2.16                     | 0.46              |
| 2:B:1448:VAL:O    | 2:B:1449:GLY:O    | 2.34                     | 0.46              |
| 2:B:1590:LEU:CD2  | 2:B:1591:LEU:N    | 2.72                     | 0.46              |
| 2:B:1599:TYR:N    | 2:B:1599:TYR:CD1  | 2.84                     | 0.46              |
| 1:C:398:ASN:O     | 1:C:399:GLN:HB2   | 2.16                     | 0.46              |
| 1:C:565:GLU:HG3   | 1:C:624:PHE:CG    | 2.51                     | 0.46              |
| 1:C:604:ALA:HB3   | 1:C:773:TRP:O     | 2.14                     | 0.46              |
| 1:C:1026:GLU:HA   | 1:C:1031:TRP:HE1  | 1.80                     | 0.46              |
| 2:D:164:GLU:HB2   | 2:D:200:VAL:HG23  | 1.97                     | 0.46              |
| 2:D:338:ILE:C     | 2:D:339:VAL:HG13  | 2.41                     | 0.46              |
| 2:D:361:GLU:HB3   | 2:D:399:ILE:CD1   | 2.46                     | 0.46              |
| 2:D:365:TYR:HA    | 2:D:394:GLY:O     | 2.16                     | 0.46              |
| 2:D:438:GLN:O     | 2:D:439:GLY:C     | 2.59                     | 0.46              |
| 2:D:833:ARG:HE    | 2:D:833:ARG:HB2   | 1.56                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:156:LYS:O     | 1:A:156:LYS:HG3   | 2.16                     | 0.45              |
| 1:A:487:THR:HG22  | 1:A:523:TYR:HB2   | 1.98                     | 0.45              |
| 1:A:824:PHE:O     | 1:A:845:VAL:HG22  | 2.17                     | 0.45              |
| 1:A:1037:ASP:O    | 1:A:1040:ILE:HB   | 2.15                     | 0.45              |
| 1:A:1304:VAL:CG1  | 1:A:1305:LYS:H    | 2.28                     | 0.45              |
| 1:A:1365:VAL:CG2  | 1:A:1366:HIS:H    | 2.25                     | 0.45              |
| 1:A:1365:VAL:CG2  | 1:A:1366:HIS:N    | 2.77                     | 0.45              |
| 1:A:1570:VAL:HG22 | 1:A:1575:VAL:HG13 | 1.97                     | 0.45              |
| 2:B:257:VAL:HG12  | 2:B:258:GLU:N     | 2.30                     | 0.45              |
| 2:B:263:VAL:HG13  | 2:B:318:VAL:HA    | 1.97                     | 0.45              |
| 2:B:415:THR:O     | 2:B:425:GLN:HB3   | 2.16                     | 0.45              |
| 2:B:438:GLN:O     | 2:B:439:GLY:C     | 2.58                     | 0.45              |
| 2:B:511:THR:H     | 2:B:514:LEU:CD1   | 2.29                     | 0.45              |
| 2:B:825:VAL:O     | 2:B:826:LYS:C     | 2.58                     | 0.45              |
| 2:B:916:VAL:CG2   | 2:B:917:PRO:HD2   | 2.45                     | 0.45              |
| 2:B:1382:ILE:HG12 | 2:B:1427:LEU:HD11 | 1.96                     | 0.45              |
| 2:B:1512:ILE:HG22 | 2:B:1631:PHE:CE1  | 2.51                     | 0.45              |
| 1:C:270:GLY:HA3   | 1:C:282:MET:CG    | 2.46                     | 0.45              |
| 1:C:690:TYR:CZ    | 1:C:692:HIS:HB2   | 2.51                     | 0.45              |
| 1:C:1106:TRP:CE3  | 1:C:1107:LEU:HD13 | 2.51                     | 0.45              |
| 1:C:1189:ALA:O    | 1:C:1192:ALA:HB3  | 2.15                     | 0.45              |
| 1:C:1271:ILE:HG21 | 1:C:1300:TYR:CD1  | 2.51                     | 0.45              |
| 1:C:1532:CYS:SG   | 1:C:1533:GLY:N    | 2.89                     | 0.45              |
| 1:C:1638:PRO:O    | 1:C:1639:LEU:HD23 | 2.16                     | 0.45              |
| 2:D:813:VAL:HG12  | 2:D:840:VAL:HG22  | 1.98                     | 0.45              |
| 2:D:1292:ILE:HD12 | 2:D:1296:ASN:OD1  | 2.16                     | 0.45              |
| 1:A:120:THR:HG22  | 1:A:122:ASP:N     | 2.27                     | 0.45              |
| 1:A:123:ASN:HB3   | 1:A:209:PHE:CD2   | 2.51                     | 0.45              |
| 1:A:309:GLU:N     | 1:A:309:GLU:OE1   | 2.50                     | 0.45              |
| 1:A:626:PHE:C     | 1:A:628:GLU:H     | 2.23                     | 0.45              |
| 1:A:706:ASN:HD21  | 1:A:709:GLU:HB2   | 1.81                     | 0.45              |
| 1:A:721:GLY:C     | 1:A:723:ARG:N     | 2.73                     | 0.45              |
| 1:A:956:ARG:HA    | 1:A:1348:VAL:O    | 2.16                     | 0.45              |
| 2:B:56:ILE:HG12   | 2:B:71:THR:O      | 2.16                     | 0.45              |
| 2:B:59:HIS:O      | 2:B:104:VAL:HG23  | 2.16                     | 0.45              |
| 2:B:96:THR:HB     | 2:B:123:TYR:OH    | 2.15                     | 0.45              |
| 2:B:108:VAL:O     | 2:B:114:ARG:HA    | 2.16                     | 0.45              |
| 2:B:226:VAL:HG21  | 2:B:320:VAL:HG11  | 1.98                     | 0.45              |
| 2:B:440:GLY:O     | 2:B:441:SER:C     | 2.60                     | 0.45              |
| 2:B:543:THR:OG1   | 2:B:544:CYS:N     | 2.42                     | 0.45              |
| 2:B:884:ILE:CG1   | 2:B:885:VAL:N     | 2.79                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:924:ILE:HD13  | 2:B:1329:TYR:HE2  | 1.82                     | 0.45              |
| 1:C:161:LEU:HD11  | 1:C:185:PHE:CD2   | 2.51                     | 0.45              |
| 1:C:232:GLU:HA    | 1:C:233:PRO:HD3   | 1.77                     | 0.45              |
| 1:C:248:ILE:HD13  | 1:C:325:ILE:CD1   | 2.46                     | 0.45              |
| 1:C:367:ILE:O     | 1:C:368:PRO:C     | 2.58                     | 0.45              |
| 1:C:639:GLY:H     | 1:C:645:VAL:CG2   | 2.29                     | 0.45              |
| 1:C:702:GLY:CA    | 1:C:728:PHE:CE1   | 2.88                     | 0.45              |
| 2:D:130:ILE:HD13  | 2:D:199:ILE:HG22  | 1.98                     | 0.45              |
| 2:D:1407:TYR:O    | 2:D:1408:ILE:HD13 | 2.16                     | 0.45              |
| 2:D:1480:LEU:HD12 | 2:D:1481:LEU:O    | 2.17                     | 0.45              |
| 2:D:1602:THR:C    | 2:D:1604:ASN:N    | 2.70                     | 0.45              |
| 1:A:161:LEU:HD11  | 1:A:185:PHE:CE1   | 2.51                     | 0.45              |
| 1:A:163:PHE:HE1   | 1:A:188:PHE:HB2   | 1.81                     | 0.45              |
| 1:A:227:PHE:HB2   | 1:A:338:GLU:HG3   | 1.98                     | 0.45              |
| 1:A:333:THR:OG1   | 1:A:334:GLY:N     | 2.49                     | 0.45              |
| 1:A:560:TRP:CZ3   | 1:A:562:ASN:HB2   | 2.51                     | 0.45              |
| 1:A:803:GLY:O     | 1:A:810:CYS:HB3   | 2.15                     | 0.45              |
| 1:A:899:THR:C     | 1:A:900:VAL:HG13  | 2.41                     | 0.45              |
| 1:A:1061:ASN:HB3  | 1:A:1062:ALA:H    | 1.52                     | 0.45              |
| 1:A:1103:SER:O    | 1:A:1106:TRP:N    | 2.48                     | 0.45              |
| 1:A:1404:ALA:HB1  | 1:A:1493:PHE:HE2  | 1.74                     | 0.45              |
| 1:A:1538:GLU:O    | 1:A:1539:LEU:C    | 2.59                     | 0.45              |
| 2:B:164:GLU:HB2   | 2:B:200:VAL:CG2   | 2.47                     | 0.45              |
| 2:B:466:VAL:HG12  | 2:B:524:TYR:CE2   | 2.51                     | 0.45              |
| 2:B:490:PHE:CG    | 2:B:491:LYS:N     | 2.83                     | 0.45              |
| 2:B:824:VAL:HG22  | 2:B:825:VAL:N     | 2.32                     | 0.45              |
| 2:B:954:VAL:HG12  | 2:B:955:PRO:HD2   | 1.99                     | 0.45              |
| 2:B:1284:ARG:HG3  | 2:B:1285:GLU:H    | 1.71                     | 0.45              |
| 2:B:1407:TYR:C    | 2:B:1407:TYR:CD2  | 2.94                     | 0.45              |
| 2:B:1504:GLU:OE2  | 2:B:1505:ARG:N    | 2.49                     | 0.45              |
| 2:B:1509:PRO:O    | 2:B:1512:ILE:HG13 | 2.15                     | 0.45              |
| 2:B:1556:PRO:C    | 2:B:1558:ALA:N    | 2.72                     | 0.45              |
| 1:C:101:TYR:CE1   | 1:C:116:ARG:CZ    | 2.97                     | 0.45              |
| 1:C:120:THR:CG2   | 1:C:122:ASP:H     | 2.27                     | 0.45              |
| 1:C:265:VAL:HG23  | 1:C:292:LEU:H     | 1.80                     | 0.45              |
| 1:C:641:ASN:OD1   | 1:C:644:ASN:HB2   | 2.15                     | 0.45              |
| 1:C:1088:GLN:O    | 1:C:1090:ASN:N    | 2.49                     | 0.45              |
| 1:C:1277:GLU:O    | 1:C:1278:GLN:C    | 2.58                     | 0.45              |
| 1:C:1290:THR:O    | 1:C:1294:ILE:HG12 | 2.16                     | 0.45              |
| 1:C:1320:LYS:CG   | 1:C:1321:GLY:N    | 2.79                     | 0.45              |
| 2:D:198:ARG:HB3   | 2:D:213:TYR:HE1   | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:228:LEU:HD12  | 2:D:333:GLN:HB2   | 1.97                     | 0.45              |
| 2:D:484:LEU:HD11  | 2:D:626:LEU:HD11  | 1.98                     | 0.45              |
| 2:D:563:MET:O     | 2:D:777:SER:HA    | 2.16                     | 0.45              |
| 2:D:1289:ARG:C    | 2:D:1290:TYR:CD1  | 2.94                     | 0.45              |
| 2:D:1292:ILE:HD11 | 2:D:1301:ARG:NE   | 2.30                     | 0.45              |
| 2:D:1444:LYS:CE   | 2:D:1447:GLU:HA   | 2.43                     | 0.45              |
| 2:D:1466:GLU:OE2  | 2:D:1468:CYS:HB2  | 2.16                     | 0.45              |
| 2:D:1526:THR:CG2  | 2:D:1583:ILE:HG13 | 2.46                     | 0.45              |
| 1:A:152:LEU:HD12  | 1:A:152:LEU:HA    | 1.81                     | 0.45              |
| 1:A:226:HIS:ND1   | 1:A:336:PHE:CE2   | 2.85                     | 0.45              |
| 1:A:267:ILE:CG2   | 1:A:268:THR:N     | 2.79                     | 0.45              |
| 1:A:791:PRO:CD    | 1:A:797:TRP:HE1   | 2.28                     | 0.45              |
| 1:A:1066:TYR:N    | 1:A:1066:TYR:HD1  | 2.13                     | 0.45              |
| 1:A:1233:GLN:O    | 1:A:1234:HIS:HB3  | 2.17                     | 0.45              |
| 1:A:1439:LEU:O    | 1:A:1440:LYS:C    | 2.60                     | 0.45              |
| 1:A:1560:ALA:O    | 1:A:1561:TYR:HB3  | 2.16                     | 0.45              |
| 1:A:1584:ILE:HG22 | 1:A:1586:LYS:H    | 1.82                     | 0.45              |
| 1:A:1610:GLU:C    | 1:A:1611:LEU:HD23 | 2.41                     | 0.45              |
| 2:B:196:THR:HG23  | 2:B:215:ASP:OD1   | 2.16                     | 0.45              |
| 2:B:345:ILE:HD11  | 2:B:427:THR:N     | 2.31                     | 0.45              |
| 2:B:470:ALA:C     | 2:B:472:SER:H     | 2.23                     | 0.45              |
| 2:B:789:VAL:C     | 2:B:790:LEU:HD12  | 2.41                     | 0.45              |
| 2:B:963:ILE:CD1   | 2:B:1311:ILE:HG12 | 2.45                     | 0.45              |
| 2:B:1414:ASP:O    | 2:B:1415:ASN:C    | 2.58                     | 0.45              |
| 2:B:1623:LYS:HZ3  | 2:B:1623:LYS:CA   | 2.30                     | 0.45              |
| 1:C:124:GLY:C     | 1:C:125:PHE:CG    | 2.94                     | 0.45              |
| 1:C:296:ILE:CG2   | 1:C:297:ALA:N     | 2.78                     | 0.45              |
| 1:C:330:ILE:O     | 1:C:330:ILE:HG13  | 2.16                     | 0.45              |
| 1:C:934:VAL:O     | 1:C:935:LYS:HG3   | 2.16                     | 0.45              |
| 1:C:942:VAL:CG2   | 1:C:1359:VAL:HB   | 2.47                     | 0.45              |
| 1:C:1090:ASN:C    | 1:C:1092:TYR:N    | 2.71                     | 0.45              |
| 1:C:1152:ILE:CG2  | 1:C:1168:LEU:HD21 | 2.41                     | 0.45              |
| 1:C:1570:VAL:C    | 1:C:1571:GLU:HG3  | 2.42                     | 0.45              |
| 2:D:83:VAL:HB     | 2:D:85:PRO:HD3    | 1.98                     | 0.45              |
| 2:D:183:PHE:N     | 2:D:183:PHE:HD2   | 2.13                     | 0.45              |
| 2:D:267:VAL:HG13  | 2:D:313:THR:O     | 2.16                     | 0.45              |
| 2:D:416:ASN:HA    | 2:D:425:GLN:NE2   | 2.30                     | 0.45              |
| 2:D:445:LEU:HD12  | 2:D:465:ASN:O     | 2.17                     | 0.45              |
| 2:D:464:PHE:HB3   | 2:D:479:PHE:CE2   | 2.51                     | 0.45              |
| 2:D:889:GLN:HE21  | 2:D:889:GLN:C     | 2.24                     | 0.45              |
| 2:D:964:ILE:O     | 2:D:964:ILE:HG22  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1506:ILE:CD1  | 2:D:1628:PHE:CD1  | 2.99                     | 0.45              |
| 1:A:363:LEU:HD12  | 1:A:456:ALA:HA    | 1.98                     | 0.45              |
| 1:A:672:ILE:O     | 1:A:673:LEU:HG    | 2.15                     | 0.45              |
| 1:A:691:LYS:O     | 1:A:693:SER:N     | 2.50                     | 0.45              |
| 1:A:820:PHE:CZ    | 1:A:822:ASP:HB2   | 2.51                     | 0.45              |
| 1:A:916:THR:C     | 1:A:918:PHE:H     | 2.25                     | 0.45              |
| 1:A:1096:ASN:O    | 1:A:1099:SER:HB3  | 2.16                     | 0.45              |
| 1:A:1277:GLU:O    | 1:A:1278:GLN:C    | 2.58                     | 0.45              |
| 2:B:402:ILE:HA    | 2:B:403:PRO:HD2   | 1.76                     | 0.45              |
| 2:B:829:GLN:HG2   | 2:B:1480:LEU:HD13 | 1.99                     | 0.45              |
| 2:B:944:VAL:HG22  | 2:B:1312:THR:HG1  | 1.82                     | 0.45              |
| 2:B:1527:LYS:O    | 2:B:1529:LEU:HD12 | 2.16                     | 0.45              |
| 1:C:23:TYR:C      | 1:C:655:THR:HG21  | 2.40                     | 0.45              |
| 1:C:365:PRO:CG    | 1:C:464:TYR:HE2   | 2.28                     | 0.45              |
| 1:C:640:LEU:N     | 1:C:644:ASN:HB3   | 2.28                     | 0.45              |
| 1:C:856:CYS:HB2   | 2:D:904:LEU:HD11  | 1.97                     | 0.45              |
| 1:C:908:HIS:O     | 1:C:909:ASN:CB    | 2.64                     | 0.45              |
| 1:C:917:TRP:O     | 2:D:813:VAL:CG2   | 2.65                     | 0.45              |
| 1:C:1037:ASP:HA   | 1:C:1038:PRO:HD3  | 1.79                     | 0.45              |
| 1:C:1054:LEU:HD22 | 1:C:1057:MET:CE   | 2.46                     | 0.45              |
| 1:C:1079:THR:HG21 | 1:C:1107:LEU:CD1  | 2.46                     | 0.45              |
| 1:C:1212:LEU:O    | 1:C:1212:LEU:HD13 | 2.17                     | 0.45              |
| 1:C:1289:ASP:O    | 1:C:1290:THR:C    | 2.60                     | 0.45              |
| 2:D:354:PHE:CD1   | 2:D:354:PHE:C     | 2.93                     | 0.45              |
| 2:D:1448:VAL:O    | 2:D:1449:GLY:O    | 2.34                     | 0.45              |
| 2:D:1502:HIS:O    | 2:D:1503:GLN:HB2  | 2.16                     | 0.45              |
| 1:A:357:VAL:HG12  | 1:A:358:ALA:N     | 2.31                     | 0.45              |
| 1:A:706:ASN:HD22  | 1:A:709:GLU:H     | 1.65                     | 0.45              |
| 1:A:792:ASP:O     | 1:A:793:SER:CB    | 2.63                     | 0.45              |
| 1:A:829:ILE:CG1   | 1:A:925:LYS:HG2   | 2.41                     | 0.45              |
| 1:A:1020:TYR:HE1  | 1:A:1295:GLU:HG3  | 1.80                     | 0.45              |
| 1:A:1043:GLN:O    | 1:A:1044:LYS:C    | 2.59                     | 0.45              |
| 1:A:1112:GLN:HB2  | 1:A:1118:PHE:CE1  | 2.49                     | 0.45              |
| 1:A:1364:VAL:O    | 1:A:1364:VAL:HG13 | 2.16                     | 0.45              |
| 1:A:1404:ALA:HB1  | 1:A:1493:PHE:CZ   | 2.49                     | 0.45              |
| 1:A:1455:ILE:HD12 | 1:A:1455:ILE:N    | 2.29                     | 0.45              |
| 1:A:1549:LYS:HZ3  | 1:A:1549:LYS:HG3  | 1.59                     | 0.45              |
| 1:A:1627:ILE:O    | 1:A:1629:TYR:N    | 2.50                     | 0.45              |
| 2:B:824:VAL:HG12  | 2:B:913:LEU:HD21  | 1.99                     | 0.45              |
| 2:B:942:LEU:HD13  | 2:B:1314:THR:HG23 | 1.98                     | 0.45              |
| 2:B:1393:ASP:CB   | 2:B:1443:LEU:HD11 | 2.42                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:32:ARG:HB2    | 1:C:35:ALA:HB2    | 1.98                     | 0.45              |
| 1:C:116:ARG:O     | 1:C:117:MET:HB3   | 2.15                     | 0.45              |
| 1:C:165:ASP:C     | 1:C:167:GLU:H     | 2.24                     | 0.45              |
| 1:C:672:ILE:O     | 1:C:673:LEU:HG    | 2.16                     | 0.45              |
| 1:C:709:GLU:OE1   | 1:C:709:GLU:HA    | 2.16                     | 0.45              |
| 1:C:773:TRP:NE1   | 1:C:797:TRP:NE1   | 2.64                     | 0.45              |
| 1:C:856:CYS:SG    | 2:D:904:LEU:HD21  | 2.57                     | 0.45              |
| 1:C:1552:ALA:HB2  | 1:C:1620:MET:CE   | 2.47                     | 0.45              |
| 1:C:1581:LEU:HD11 | 1:C:1598:ILE:HD11 | 1.96                     | 0.45              |
| 1:C:1602:LYS:HB3  | 1:C:1639:LEU:HB2  | 1.99                     | 0.45              |
| 1:C:1627:ILE:O    | 1:C:1629:TYR:N    | 2.50                     | 0.45              |
| 2:D:243:PHE:CE1   | 2:D:336:ILE:HG21  | 2.52                     | 0.45              |
| 2:D:323:GLU:C     | 2:D:323:GLU:OE1   | 2.59                     | 0.45              |
| 2:D:525:GLN:NE2   | 2:D:528:ASN:H     | 2.14                     | 0.45              |
| 2:D:1270:HIS:CG   | 2:D:1270:HIS:O    | 2.70                     | 0.45              |
| 2:D:1332:GLN:C    | 2:D:1332:GLN:CD   | 2.84                     | 0.45              |
| 2:D:1508:VAL:HB   | 2:D:1509:PRO:HD3  | 1.98                     | 0.45              |
| 1:A:156:LYS:C     | 1:A:156:LYS:CD    | 2.89                     | 0.45              |
| 1:A:272:ARG:O     | 1:A:321:LYS:HB2   | 2.17                     | 0.45              |
| 1:A:364:LYS:HE2   | 1:A:465:LEU:O     | 2.16                     | 0.45              |
| 1:A:531:THR:O     | 1:A:534:MET:HG3   | 2.16                     | 0.45              |
| 1:A:700:TYR:CD2   | 1:A:701:ASP:N     | 2.83                     | 0.45              |
| 1:A:784:LYS:HG2   | 1:A:785:GLN:N     | 2.30                     | 0.45              |
| 1:A:1079:THR:HG22 | 1:A:1107:LEU:HD21 | 1.99                     | 0.45              |
| 1:A:1213:LYS:C    | 1:A:1215:GLU:H    | 2.25                     | 0.45              |
| 1:A:1290:THR:O    | 1:A:1294:ILE:CG1  | 2.65                     | 0.45              |
| 1:A:1381:ILE:HD13 | 1:A:1509:TYR:CG   | 2.52                     | 0.45              |
| 2:B:954:VAL:HB    | 2:B:957:THR:CG2   | 2.35                     | 0.45              |
| 2:B:1569:CYS:O    | 2:B:1570:GLN:C    | 2.59                     | 0.45              |
| 1:C:721:GLY:C     | 1:C:723:ARG:N     | 2.73                     | 0.45              |
| 1:C:915:GLU:OE2   | 2:D:903:ALA:HA    | 2.17                     | 0.45              |
| 2:D:111:PRO:O     | 2:D:113:VAL:HG23  | 2.17                     | 0.45              |
| 2:D:848:VAL:HG22  | 2:D:898:ALA:CB    | 2.43                     | 0.45              |
| 2:D:1523:VAL:O    | 2:D:1548:ILE:HB   | 2.17                     | 0.45              |
| 1:A:78:LYS:HD2    | 1:A:498:HIS:NE2   | 2.32                     | 0.45              |
| 1:A:945:ASP:OD1   | 1:A:945:ASP:C     | 2.59                     | 0.45              |
| 1:A:1190:ILE:O    | 1:A:1191:SER:C    | 2.58                     | 0.45              |
| 2:B:150:MET:HE1   | 2:B:545:MET:HE3   | 1.98                     | 0.45              |
| 2:B:151:ASP:HB2   | 2:B:794:PHE:HZ    | 1.82                     | 0.45              |
| 2:B:172:LEU:HD23  | 2:B:966:GLN:NE2   | 2.31                     | 0.45              |
| 2:B:183:PHE:N     | 2:B:183:PHE:HD2   | 2.15                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:553:ASP:O     | 2:B:555:LEU:HG   | 2.17                     | 0.45              |
| 2:B:1290:TYR:CD2  | 2:B:1301:ARG:HB3 | 2.51                     | 0.45              |
| 2:B:1326:LEU:HD11 | 2:B:1328:PHE:HE2 | 1.82                     | 0.45              |
| 2:B:1601:ILE:N    | 2:B:1601:ILE:CD1 | 2.77                     | 0.45              |
| 2:B:1601:ILE:HD12 | 2:B:1601:ILE:H   | 1.82                     | 0.45              |
| 1:C:142:LYS:HA    | 1:C:187:ASP:OD1  | 2.17                     | 0.45              |
| 1:C:156:LYS:O     | 1:C:156:LYS:HG3  | 2.16                     | 0.45              |
| 1:C:240:TYR:CD2   | 1:C:240:TYR:C    | 2.92                     | 0.45              |
| 1:C:324:TYR:CD2   | 1:C:324:TYR:C    | 2.95                     | 0.45              |
| 1:C:371:ILE:HG21  | 1:C:390:LEU:CD2  | 2.47                     | 0.45              |
| 1:C:803:GLY:O     | 1:C:810:CYS:HB3  | 2.16                     | 0.45              |
| 1:C:889:GLU:HB2   | 1:C:892:SER:CB   | 2.38                     | 0.45              |
| 1:C:1130:GLN:NE2  | 1:C:1230:ASP:HB3 | 2.32                     | 0.45              |
| 1:C:1323:LEU:O    | 1:C:1324:HIS:O   | 2.35                     | 0.45              |
| 1:C:1538:GLU:O    | 1:C:1539:LEU:C   | 2.60                     | 0.45              |
| 1:C:1565:ILE:HD13 | 1:C:1565:ILE:N   | 2.32                     | 0.45              |
| 2:D:370:ASP:OD1   | 2:D:370:ASP:N    | 2.50                     | 0.45              |
| 2:D:417:HIS:N     | 2:D:425:GLN:OE1  | 2.48                     | 0.45              |
| 2:D:1273:LEU:HB2  | 2:D:1319:GLY:CA  | 2.36                     | 0.45              |
| 1:A:23:TYR:C      | 1:A:655:THR:HG21 | 2.41                     | 0.45              |
| 1:A:163:PHE:CE1   | 1:A:188:PHE:CG   | 3.04                     | 0.45              |
| 1:A:164:ILE:O     | 1:A:164:ILE:HG22 | 2.15                     | 0.45              |
| 1:A:522:SER:HB2   | 1:A:523:TYR:H    | 1.60                     | 0.45              |
| 1:A:690:TYR:CZ    | 1:A:692:HIS:HB2  | 2.52                     | 0.45              |
| 1:A:963:ILE:HG23  | 1:A:967:LEU:HD23 | 1.97                     | 0.45              |
| 1:A:1127:ILE:HG12 | 1:A:1143:TYR:CE2 | 2.51                     | 0.45              |
| 1:A:1141:SER:O    | 1:A:1142:LEU:C   | 2.60                     | 0.45              |
| 1:A:1324:HIS:CD2  | 1:A:1336:ARG:NH2 | 2.85                     | 0.45              |
| 1:A:1562:LYS:HD2  | 1:A:1648:TRP:CZ2 | 2.46                     | 0.45              |
| 2:B:228:LEU:CD2   | 2:B:247:ILE:HG12 | 2.47                     | 0.45              |
| 2:B:390:THR:HG22  | 2:B:395:THR:N    | 2.32                     | 0.45              |
| 2:B:545:MET:HG3   | 2:B:798:LYS:O    | 2.16                     | 0.45              |
| 2:B:1294:TYR:O    | 2:B:1294:TYR:HD2 | 1.99                     | 0.45              |
| 2:B:1540:TYR:CE1  | 2:B:1575:LEU:HB2 | 2.51                     | 0.45              |
| 1:C:683:ILE:O     | 1:C:687:ALA:CB   | 2.65                     | 0.45              |
| 1:C:773:TRP:CZ2   | 1:C:797:TRP:CD1  | 3.02                     | 0.45              |
| 1:C:829:ILE:CG1   | 1:C:925:LYS:HG2  | 2.47                     | 0.45              |
| 1:C:859:MET:HE2   | 1:C:912:PHE:CZ   | 2.52                     | 0.45              |
| 1:C:862:VAL:HB    | 1:C:865:ILE:CG1  | 2.45                     | 0.45              |
| 1:C:916:THR:O     | 1:C:918:PHE:N    | 2.50                     | 0.45              |
| 1:C:1086:LEU:O    | 1:C:1087:GLY:C   | 2.60                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1184:SER:O    | 1:C:1187:THR:HB   | 2.17                     | 0.45              |
| 1:C:1568:ILE:CG2  | 1:C:1577:TYR:HE1  | 2.26                     | 0.45              |
| 2:D:61:PHE:CE2    | 2:D:62:PRO:HB3    | 2.51                     | 0.45              |
| 2:D:172:LEU:HD23  | 2:D:966:GLN:NE2   | 2.31                     | 0.45              |
| 2:D:455:LYS:O     | 2:D:458:ASP:HB2   | 2.17                     | 0.45              |
| 2:D:518:PHE:CD2   | 2:D:518:PHE:O     | 2.69                     | 0.45              |
| 2:D:954:VAL:CG1   | 2:D:955:PRO:HD2   | 2.47                     | 0.45              |
| 2:D:1556:PRO:C    | 2:D:1558:ALA:N    | 2.73                     | 0.45              |
| 1:A:32:ARG:HB2    | 1:A:35:ALA:HB2    | 1.99                     | 0.45              |
| 1:A:161:LEU:HD11  | 1:A:185:PHE:CD2   | 2.52                     | 0.45              |
| 1:A:554:LEU:HD23  | 1:A:554:LEU:HA    | 1.67                     | 0.45              |
| 1:A:829:ILE:N     | 1:A:829:ILE:HD12  | 2.32                     | 0.45              |
| 1:A:862:VAL:HG12  | 1:A:907:LEU:HD21  | 1.99                     | 0.45              |
| 1:A:1184:SER:O    | 1:A:1187:THR:HB   | 2.17                     | 0.45              |
| 1:A:1245:ALA:HB2  | 1:A:1285:TYR:HB3  | 1.98                     | 0.45              |
| 1:A:1623:GLU:CB   | 1:A:1638:PRO:CG   | 2.93                     | 0.45              |
| 2:B:78:ALA:O      | 2:B:80:GLY:N      | 2.49                     | 0.45              |
| 2:B:148:PHE:HB2   | 2:B:800:ILE:HD11  | 1.99                     | 0.45              |
| 2:B:265:PHE:O     | 2:B:276:ILE:HG13  | 2.17                     | 0.45              |
| 2:B:348:THR:O     | 2:B:348:THR:OG1   | 2.27                     | 0.45              |
| 2:B:373:PRO:HB3   | 2:B:393:ASP:O     | 2.17                     | 0.45              |
| 2:B:1275:LEU:HD21 | 2:B:1319:GLY:C    | 2.41                     | 0.45              |
| 2:B:1466:GLU:CD   | 2:B:1468:CYS:HB2  | 2.42                     | 0.45              |
| 1:C:87:ILE:O      | 1:C:87:ILE:HG12   | 2.16                     | 0.45              |
| 1:C:259:VAL:HB    | 1:C:295:GLY:HA2   | 1.98                     | 0.45              |
| 1:C:532:GLN:O     | 1:C:535:VAL:HG22  | 2.17                     | 0.45              |
| 1:C:694:VAL:HG12  | 1:C:697:LYS:HE3   | 1.99                     | 0.45              |
| 1:C:1243:GLY:O    | 1:C:1285:TYR:CE2  | 2.69                     | 0.45              |
| 1:C:1245:ALA:O    | 1:C:1246:ARG:C    | 2.59                     | 0.45              |
| 1:C:1525:CYS:N    | 1:C:1528:VAL:HG13 | 2.32                     | 0.45              |
| 2:D:80:GLY:O      | 2:D:81:MET:HB2    | 2.17                     | 0.45              |
| 2:D:103:TYR:N     | 2:D:103:TYR:HD2   | 2.15                     | 0.45              |
| 2:D:151:ASP:HB2   | 2:D:794:PHE:HZ    | 1.82                     | 0.45              |
| 2:D:236:TYR:C     | 2:D:238:ASP:N     | 2.67                     | 0.45              |
| 2:D:490:PHE:CG    | 2:D:491:LYS:N     | 2.85                     | 0.45              |
| 1:A:500:ASN:CB    | 1:A:543:TYR:HE1   | 2.10                     | 0.44              |
| 1:A:501:TYR:O     | 1:A:501:TYR:CD1   | 2.69                     | 0.44              |
| 1:A:839:ILE:CD1   | 1:A:1485:VAL:HG12 | 2.48                     | 0.44              |
| 1:A:947:ARG:NH1   | 1:A:1352:PHE:CE2  | 2.84                     | 0.44              |
| 1:A:968:VAL:HG12  | 1:A:1368:THR:CG2  | 2.47                     | 0.44              |
| 1:A:1638:PRO:O    | 1:A:1639:LEU:HD23 | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:484:LEU:HD11  | 2:B:626:LEU:CD1   | 2.47                     | 0.44              |
| 2:B:628:LEU:HB3   | 2:B:636:THR:HG23  | 1.98                     | 0.44              |
| 2:B:829:GLN:HE21  | 2:B:829:GLN:CA    | 2.30                     | 0.44              |
| 2:B:923:SER:C     | 2:B:924:ILE:HD12  | 2.43                     | 0.44              |
| 2:B:1594:LYS:HA   | 2:B:1594:LYS:HE2  | 1.97                     | 0.44              |
| 1:C:120:THR:HG22  | 1:C:121:TYR:N     | 2.32                     | 0.44              |
| 1:C:185:PHE:CB    | 1:C:186:PRO:HD2   | 2.47                     | 0.44              |
| 1:C:701:ASP:N     | 1:C:701:ASP:OD1   | 2.50                     | 0.44              |
| 1:C:1037:ASP:C    | 1:C:1037:ASP:OD1  | 2.60                     | 0.44              |
| 1:C:1061:ASN:HB2  | 1:C:1065:SER:O    | 2.17                     | 0.44              |
| 1:C:1175:LEU:HB3  | 1:C:1195:LEU:HD11 | 1.98                     | 0.44              |
| 1:C:1320:LYS:HG2  | 1:C:1342:LEU:HD12 | 1.99                     | 0.44              |
| 1:C:1564:SER:O    | 1:C:1579:ALA:HB1  | 2.17                     | 0.44              |
| 2:D:884:ILE:CG1   | 2:D:885:VAL:N     | 2.79                     | 0.44              |
| 2:D:1312:THR:O    | 2:D:1312:THR:HG22 | 2.16                     | 0.44              |
| 2:D:1387:LEU:O    | 2:D:1390:PHE:HB2  | 2.17                     | 0.44              |
| 1:A:161:LEU:H     | 1:A:161:LEU:HD12  | 1.82                     | 0.44              |
| 1:A:534:MET:HG3   | 1:A:534:MET:H     | 1.56                     | 0.44              |
| 1:A:916:THR:C     | 1:A:918:PHE:N     | 2.75                     | 0.44              |
| 1:A:935:LYS:HD3   | 1:A:1373:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:1084:ARG:NE   | 1:A:1154:LYS:HE3  | 2.33                     | 0.44              |
| 1:A:1313:ILE:HD13 | 1:A:1350:THR:HB   | 1.99                     | 0.44              |
| 1:A:1320:LYS:CG   | 1:A:1321:GLY:N    | 2.79                     | 0.44              |
| 1:A:1329:THR:OG1  | 1:A:1331:LYS:HG2  | 2.18                     | 0.44              |
| 1:A:1648:TRP:HE1  | 1:A:1664:LEU:HD22 | 1.82                     | 0.44              |
| 2:B:71:THR:HG23   | 2:B:72:ARG:N      | 2.32                     | 0.44              |
| 2:B:1529:LEU:O    | 2:B:1577:VAL:HG13 | 2.16                     | 0.44              |
| 2:B:1613:GLU:O    | 2:B:1616:CYS:CB   | 2.63                     | 0.44              |
| 1:C:115:LYS:HE3   | 1:C:654:LEU:HD11  | 1.99                     | 0.44              |
| 1:C:180:ILE:CG2   | 1:C:599:TRP:CE3   | 3.00                     | 0.44              |
| 1:C:1069:TRP:HH2  | 1:C:1465:ASN:CG   | 2.26                     | 0.44              |
| 1:C:1311:MET:HB2  | 1:C:1311:MET:HE3  | 1.64                     | 0.44              |
| 2:D:400:LEU:HB3   | 2:D:402:ILE:HD11  | 1.99                     | 0.44              |
| 1:A:539:ARG:NH2   | 1:A:634:CYS:N     | 2.52                     | 0.44              |
| 1:A:875:HIS:HB3   | 2:B:901:GLN:NE2   | 2.32                     | 0.44              |
| 1:A:961:TYR:HE1   | 1:A:963:ILE:HG12  | 1.83                     | 0.44              |
| 1:A:1209:VAL:HG12 | 1:A:1210:SER:N    | 2.32                     | 0.44              |
| 1:A:1217:LEU:HD13 | 1:A:1237:SER:HA   | 1.99                     | 0.44              |
| 1:A:1231:ASN:O    | 1:A:1234:HIS:O    | 2.35                     | 0.44              |
| 1:A:1271:ILE:O    | 1:A:1272:LYS:C    | 2.57                     | 0.44              |
| 1:A:1328:MET:HE2  | 1:A:1328:MET:CA   | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1377:PHE:CD1  | 1:A:1408:TYR:HA   | 2.53                     | 0.44              |
| 2:B:130:ILE:HD13  | 2:B:199:ILE:HG22  | 1.99                     | 0.44              |
| 2:B:262:PHE:HE1   | 2:B:282:ARG:CG    | 2.28                     | 0.44              |
| 2:B:1332:GLN:CD   | 2:B:1332:GLN:C    | 2.85                     | 0.44              |
| 2:B:1442:ILE:HA   | 2:B:1443:LEU:HD12 | 1.99                     | 0.44              |
| 1:C:283:MET:HE1   | 1:C:301:PHE:CZ    | 2.52                     | 0.44              |
| 1:C:571:LEU:CD2   | 1:C:812:ALA:HB2   | 2.47                     | 0.44              |
| 1:C:577:PRO:CD    | 1:C:588:VAL:HG23  | 2.48                     | 0.44              |
| 1:C:695:VAL:HG12  | 1:C:727:ALA:CB    | 2.47                     | 0.44              |
| 1:C:753:HIS:HB3   | 1:C:754:MET:H     | 1.43                     | 0.44              |
| 1:C:1271:ILE:O    | 1:C:1272:LYS:C    | 2.60                     | 0.44              |
| 1:C:1346:LEU:HD12 | 1:C:1346:LEU:HA   | 1.45                     | 0.44              |
| 1:C:1366:HIS:N    | 1:C:1366:HIS:ND1  | 2.66                     | 0.44              |
| 1:C:1381:ILE:HD13 | 1:C:1509:TYR:CG   | 2.53                     | 0.44              |
| 1:C:1559:TYR:CE1  | 1:C:1586:LYS:O    | 2.70                     | 0.44              |
| 1:C:1618:LEU:HD22 | 1:C:1619:ILE:N    | 2.33                     | 0.44              |
| 2:D:32:VAL:HB     | 2:D:607:PHE:CZ    | 2.53                     | 0.44              |
| 2:D:226:VAL:CG2   | 2:D:320:VAL:HG11  | 2.47                     | 0.44              |
| 2:D:756:LEU:HD22  | 2:D:778:PHE:CD1   | 2.52                     | 0.44              |
| 2:D:1442:ILE:HA   | 2:D:1443:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:207:GLU:O     | 1:A:209:PHE:N     | 2.50                     | 0.44              |
| 1:A:255:PHE:O     | 1:A:255:PHE:HD1   | 2.00                     | 0.44              |
| 1:A:623:VAL:O     | 1:A:625:GLN:N     | 2.51                     | 0.44              |
| 1:A:930:VAL:HG13  | 1:A:931:PRO:N     | 2.33                     | 0.44              |
| 1:A:1194:ALA:O    | 1:A:1195:LEU:C    | 2.60                     | 0.44              |
| 1:A:1274:LEU:O    | 1:A:1277:GLU:N    | 2.49                     | 0.44              |
| 1:A:1279:ARG:CD   | 1:A:1279:ARG:C    | 2.91                     | 0.44              |
| 1:A:1455:ILE:O    | 1:A:1455:ILE:HG22 | 2.16                     | 0.44              |
| 2:B:462:VAL:HG11  | 2:B:506:MET:HE3   | 1.98                     | 0.44              |
| 2:B:597:LYS:HB3   | 2:B:597:LYS:NZ    | 2.33                     | 0.44              |
| 2:B:775:THR:HG22  | 2:B:776:MET:N     | 2.32                     | 0.44              |
| 2:B:1484:ILE:HG22 | 2:B:1485:CYS:N    | 2.31                     | 0.44              |
| 2:B:1527:LYS:H    | 2:B:1545:LEU:HD13 | 1.82                     | 0.44              |
| 1:C:196:TYR:CD2   | 1:C:196:TYR:N     | 2.82                     | 0.44              |
| 1:C:412:ARG:HG3   | 1:C:413:VAL:N     | 2.32                     | 0.44              |
| 1:C:534:MET:HG3   | 1:C:534:MET:H     | 1.56                     | 0.44              |
| 1:C:693:SER:C     | 1:C:695:VAL:N     | 2.75                     | 0.44              |
| 1:C:931:PRO:C     | 1:C:932:GLU:OE1   | 2.60                     | 0.44              |
| 1:C:961:TYR:HE1   | 1:C:963:ILE:HG12  | 1.82                     | 0.44              |
| 1:C:1086:LEU:CD1  | 1:C:1095:GLN:HG3  | 2.37                     | 0.44              |
| 1:C:1113:LEU:HD23 | 1:C:1114:ASP:N    | 2.31                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1179:THR:HG22 | 1:C:1180:LEU:HD23 | 2.00                     | 0.44              |
| 1:C:1638:PRO:HB2  | 1:C:1639:LEU:H    | 1.48                     | 0.44              |
| 2:D:319:THR:HG23  | 2:D:330:VAL:CG1   | 2.47                     | 0.44              |
| 2:D:567:LEU:HD11  | 2:D:577:LEU:HD21  | 1.99                     | 0.44              |
| 2:D:1501:ASN:H    | 2:D:1501:ASN:ND2  | 2.12                     | 0.44              |
| 2:D:1626:ASP:O    | 2:D:1627:ASP:C    | 2.60                     | 0.44              |
| 1:A:108:SER:HG    | 1:A:111:PHE:C     | 2.26                     | 0.44              |
| 1:A:532:GLN:O     | 1:A:535:VAL:HG13  | 2.17                     | 0.44              |
| 1:A:961:TYR:HE2   | 1:A:1343:ASN:HA   | 1.82                     | 0.44              |
| 1:A:1019:PHE:CE1  | 1:A:1088:GLN:HB3  | 2.53                     | 0.44              |
| 1:A:1366:HIS:N    | 1:A:1366:HIS:ND1  | 2.65                     | 0.44              |
| 2:B:126:SER:OG    | 2:B:127:PHE:N     | 2.49                     | 0.44              |
| 2:B:347:PHE:CE1   | 2:B:430:MET:HG2   | 2.53                     | 0.44              |
| 2:B:355:LYS:O     | 2:B:358:MET:HB2   | 2.17                     | 0.44              |
| 2:B:430:MET:HE3   | 2:B:430:MET:HB2   | 1.74                     | 0.44              |
| 1:C:234:GLU:HG3   | 1:C:235:TYR:CE2   | 2.52                     | 0.44              |
| 1:C:255:PHE:O     | 1:C:255:PHE:HD1   | 2.00                     | 0.44              |
| 1:C:412:ARG:HH12  | 1:C:472:ASN:HD21  | 1.64                     | 0.44              |
| 1:C:443:PRO:CD    | 1:C:446:ASN:HB2   | 2.38                     | 0.44              |
| 1:C:518:PHE:O     | 1:C:520:ASP:N     | 2.43                     | 0.44              |
| 1:C:977:LEU:HD22  | 1:C:977:LEU:C     | 2.43                     | 0.44              |
| 2:D:235:PHE:HB3   | 2:D:338:ILE:CG2   | 2.46                     | 0.44              |
| 2:D:299:PHE:CE1   | 2:D:303:PHE:HD2   | 2.27                     | 0.44              |
| 2:D:460:LEU:O     | 2:D:460:LEU:HD23  | 2.17                     | 0.44              |
| 2:D:558:MET:HE2   | 2:D:558:MET:HB3   | 1.55                     | 0.44              |
| 2:D:1623:LYS:HZ3  | 2:D:1623:LYS:CA   | 2.30                     | 0.44              |
| 1:A:32:ARG:O      | 1:A:33:VAL:C      | 2.61                     | 0.44              |
| 1:A:77:ASN:C      | 1:A:79:PHE:N      | 2.73                     | 0.44              |
| 1:A:97:ASN:HA     | 1:A:98:PRO:HD3    | 1.83                     | 0.44              |
| 1:A:286:ALA:O     | 1:A:287:MET:O     | 2.35                     | 0.44              |
| 1:A:323:LEU:O     | 1:A:323:LEU:HD13  | 2.18                     | 0.44              |
| 1:A:352:TYR:HE1   | 1:A:383:VAL:HG21  | 1.81                     | 0.44              |
| 1:A:431:LEU:HD13  | 1:A:431:LEU:O     | 2.17                     | 0.44              |
| 1:A:466:TYR:CZ    | 1:A:468:ASP:HB2   | 2.53                     | 0.44              |
| 1:A:754:MET:SD    | 1:A:754:MET:C     | 3.00                     | 0.44              |
| 1:A:949:ILE:C     | 1:A:950:TYR:CG    | 2.95                     | 0.44              |
| 1:A:1494:THR:CB   | 1:A:1506:THR:HG23 | 2.24                     | 0.44              |
| 1:A:1566:THR:O    | 1:A:1613:LYS:HE3  | 2.18                     | 0.44              |
| 2:B:61:PHE:CE2    | 2:B:62:PRO:HB3    | 2.52                     | 0.44              |
| 2:B:266:GLY:HA3   | 2:B:315:TYR:CE1   | 2.53                     | 0.44              |
| 2:B:447:VAL:O     | 2:B:447:VAL:HG13  | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:602:ILE:O     | 2:B:603:GLU:C     | 2.60                     | 0.44              |
| 2:B:913:LEU:HD23  | 2:B:913:LEU:C     | 2.43                     | 0.44              |
| 2:B:913:LEU:HD23  | 2:B:914:LYS:N     | 2.33                     | 0.44              |
| 2:B:1526:THR:CG2  | 2:B:1583:ILE:HG13 | 2.47                     | 0.44              |
| 2:B:1626:ASP:O    | 2:B:1627:ASP:C    | 2.59                     | 0.44              |
| 1:C:180:ILE:HB    | 1:C:599:TRP:CZ3   | 2.52                     | 0.44              |
| 1:C:274:ASP:OD1   | 1:C:277:ASP:CG    | 2.61                     | 0.44              |
| 1:C:392:ALA:HB1   | 1:C:432:GLU:O     | 2.18                     | 0.44              |
| 1:C:501:TYR:HE1   | 1:C:512:PHE:C     | 2.25                     | 0.44              |
| 1:C:950:TYR:C     | 1:C:952:THR:H     | 2.25                     | 0.44              |
| 1:C:1085:VAL:O    | 1:C:1089:VAL:CG2  | 2.63                     | 0.44              |
| 1:C:1117:SER:HB3  | 1:C:1174:PHE:CD2  | 2.51                     | 0.44              |
| 1:C:1379:LEU:HD12 | 1:C:1505:CYS:SG   | 2.58                     | 0.44              |
| 1:C:1455:ILE:O    | 1:C:1455:ILE:HG22 | 2.18                     | 0.44              |
| 1:C:1482:LEU:O    | 1:C:1482:LEU:HD23 | 2.17                     | 0.44              |
| 1:C:1562:LYS:NZ   | 1:C:1664:LEU:HD23 | 2.32                     | 0.44              |
| 2:D:113:VAL:HG12  | 2:D:114:ARG:N     | 2.33                     | 0.44              |
| 2:D:133:ASP:HB3   | 2:D:757:TRP:CZ3   | 2.53                     | 0.44              |
| 2:D:1482:ASN:C    | 2:D:1493:ALA:HB3  | 2.43                     | 0.44              |
| 2:D:1594:LYS:HE2  | 2:D:1594:LYS:HA   | 1.99                     | 0.44              |
| 1:A:171:VAL:CG1   | 1:A:172:ASP:N     | 2.81                     | 0.44              |
| 1:A:256:TYR:HE2   | 1:A:826:GLU:OE2   | 2.00                     | 0.44              |
| 1:A:274:ASP:OD1   | 1:A:277:ASP:CG    | 2.61                     | 0.44              |
| 1:A:695:VAL:HG12  | 1:A:727:ALA:CB    | 2.47                     | 0.44              |
| 1:A:859:MET:HE3   | 1:A:898:PHE:CG    | 2.53                     | 0.44              |
| 1:A:1013:MET:C    | 1:A:1016:VAL:HG23 | 2.43                     | 0.44              |
| 1:A:1079:THR:HG21 | 1:A:1107:LEU:CD1  | 2.47                     | 0.44              |
| 1:A:1106:TRP:CE3  | 1:A:1107:LEU:HD13 | 2.52                     | 0.44              |
| 1:A:1309:LEU:HD22 | 1:A:1309:LEU:HA   | 1.77                     | 0.44              |
| 1:A:1364:VAL:HG22 | 1:A:1365:VAL:N    | 2.32                     | 0.44              |
| 2:B:58:VAL:HG12   | 2:B:104:VAL:CG2   | 2.48                     | 0.44              |
| 2:B:134:LYS:HB2   | 2:B:584:VAL:HG11  | 2.00                     | 0.44              |
| 2:B:138:THR:HB    | 2:B:141:SER:OG    | 2.18                     | 0.44              |
| 2:B:243:PHE:C     | 2:B:243:PHE:CD2   | 2.96                     | 0.44              |
| 2:B:319:THR:HG23  | 2:B:330:VAL:CG1   | 2.48                     | 0.44              |
| 2:B:364:VAL:O     | 2:B:395:THR:HA    | 2.18                     | 0.44              |
| 2:B:1438:LEU:C    | 2:B:1438:LEU:HD22 | 2.43                     | 0.44              |
| 2:B:1466:GLU:HG3  | 2:B:1468:CYS:H    | 1.83                     | 0.44              |
| 1:C:33:VAL:HA     | 1:C:87:ILE:HG12   | 2.00                     | 0.44              |
| 1:C:77:ASN:C      | 1:C:79:PHE:N      | 2.73                     | 0.44              |
| 1:C:91:GLN:OE1    | 1:C:91:GLN:CA     | 2.54                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:123:ASN:HB3   | 1:C:209:PHE:CD2  | 2.53                     | 0.44              |
| 1:C:148:LEU:HD12  | 1:C:148:LEU:HA   | 1.79                     | 0.44              |
| 1:C:820:PHE:CZ    | 1:C:822:ASP:HB2  | 2.53                     | 0.44              |
| 1:C:1066:TYR:O    | 1:C:1074:ALA:HB1 | 2.17                     | 0.44              |
| 1:C:1148:THR:O    | 1:C:1149:VAL:C   | 2.56                     | 0.44              |
| 1:C:1386:ILE:HG13 | 1:C:1387:GLU:N   | 2.28                     | 0.44              |
| 2:D:306:LEU:HD12  | 2:D:306:LEU:HA   | 1.82                     | 0.44              |
| 2:D:345:ILE:HD11  | 2:D:427:THR:N    | 2.32                     | 0.44              |
| 2:D:476:ILE:CG1   | 2:D:524:TYR:CD2  | 3.01                     | 0.44              |
| 2:D:1553:ASP:C    | 2:D:1555:ASN:N   | 2.76                     | 0.44              |
| 1:A:27:ALA:HB2    | 1:A:39:ILE:HG12  | 1.99                     | 0.44              |
| 1:A:87:ILE:HG12   | 1:A:87:ILE:O     | 2.18                     | 0.44              |
| 1:A:373:VAL:CG2   | 1:A:418:ALA:HB3  | 2.47                     | 0.44              |
| 1:A:475:ALA:O     | 1:A:476:LEU:HB2  | 2.17                     | 0.44              |
| 1:A:515:ARG:HG3   | 1:A:526:ILE:HG23 | 2.00                     | 0.44              |
| 1:A:640:LEU:N     | 1:A:644:ASN:HB3  | 2.30                     | 0.44              |
| 1:A:1084:ARG:HB2  | 1:A:1151:GLY:HA2 | 1.99                     | 0.44              |
| 1:A:1406:ALA:O    | 1:A:1472:PHE:HA  | 2.18                     | 0.44              |
| 1:A:1475:VAL:HG22 | 1:A:1476:ARG:N   | 2.32                     | 0.44              |
| 1:A:1562:LYS:HD3  | 1:A:1664:LEU:CD2 | 2.46                     | 0.44              |
| 1:A:1622:LYS:HD2  | 1:A:1642:LEU:HB2 | 1.98                     | 0.44              |
| 1:A:1641:SER:C    | 1:A:1643:THR:N   | 2.71                     | 0.44              |
| 2:B:889:GLN:HE21  | 2:B:889:GLN:C    | 2.26                     | 0.44              |
| 2:B:1275:LEU:HA   | 2:B:1317:GLY:HA3 | 1.99                     | 0.44              |
| 2:B:1279:ILE:O    | 2:B:1287:PRO:HB2 | 2.18                     | 0.44              |
| 2:B:1522:TYR:OH   | 2:B:1563:TYR:OH  | 2.31                     | 0.44              |
| 2:B:1610:TRP:CD1  | 2:B:1628:PHE:HD2 | 2.36                     | 0.44              |
| 1:C:117:MET:HB2   | 1:C:118:PRO:HD2  | 1.99                     | 0.44              |
| 1:C:269:PHE:O     | 1:C:282:MET:HG2  | 2.17                     | 0.44              |
| 1:C:491:PRO:HB2   | 1:C:493:ILE:C    | 2.43                     | 0.44              |
| 1:C:914:LEU:HD12  | 1:C:915:GLU:N    | 2.32                     | 0.44              |
| 1:C:1257:THR:O    | 1:C:1261:LEU:HG  | 2.18                     | 0.44              |
| 2:D:347:PHE:CE1   | 2:D:430:MET:HG2  | 2.53                     | 0.44              |
| 2:D:382:GLU:CD    | 2:D:382:GLU:H    | 2.25                     | 0.44              |
| 2:D:415:THR:O     | 2:D:425:GLN:HB3  | 2.18                     | 0.44              |
| 2:D:625:GLY:O     | 2:D:626:LEU:HG   | 2.17                     | 0.44              |
| 2:D:856:PHE:CG    | 2:D:884:ILE:HD11 | 2.53                     | 0.44              |
| 2:D:924:ILE:HD13  | 2:D:1329:TYR:HE2 | 1.83                     | 0.44              |
| 2:D:1279:ILE:O    | 2:D:1287:PRO:HB2 | 2.18                     | 0.44              |
| 2:D:1466:GLU:HG3  | 2:D:1468:CYS:H   | 1.83                     | 0.44              |
| 1:A:96:GLN:HG3    | 1:A:97:ASN:N     | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:110:HIS:ND1   | 1:A:110:HIS:N     | 2.65                     | 0.44              |
| 1:A:476:LEU:HD12  | 1:A:562:ASN:O     | 2.18                     | 0.44              |
| 1:A:530:VAL:HA    | 1:A:534:MET:SD    | 2.58                     | 0.44              |
| 1:A:1183:GLN:NE2  | 1:A:1183:GLN:O    | 2.50                     | 0.44              |
| 1:A:1285:TYR:O    | 1:A:1286:SER:O    | 2.36                     | 0.44              |
| 1:A:1499:HIS:C    | 1:A:1500:ARG:HG3  | 2.42                     | 0.44              |
| 1:A:1559:TYR:CE1  | 1:A:1586:LYS:O    | 2.70                     | 0.44              |
| 2:B:228:LEU:HD12  | 2:B:333:GLN:HB2   | 1.99                     | 0.44              |
| 2:B:349:LYS:HE2   | 2:B:365:TYR:CD1   | 2.53                     | 0.44              |
| 2:B:594:SER:O     | 2:B:595:GLN:C     | 2.60                     | 0.44              |
| 1:C:96:GLN:HG3    | 1:C:97:ASN:H      | 1.81                     | 0.44              |
| 1:C:164:ILE:O     | 1:C:164:ILE:HG22  | 2.16                     | 0.44              |
| 1:C:412:ARG:HG3   | 1:C:413:VAL:H     | 1.82                     | 0.44              |
| 1:C:476:LEU:HD12  | 1:C:562:ASN:O     | 2.17                     | 0.44              |
| 1:C:1066:TYR:N    | 1:C:1066:TYR:HD1  | 2.15                     | 0.44              |
| 1:C:1079:THR:HG22 | 1:C:1107:LEU:HD21 | 2.00                     | 0.44              |
| 1:C:1213:LYS:C    | 1:C:1215:GLU:N    | 2.73                     | 0.44              |
| 1:C:1632:SER:C    | 1:C:1633:PHE:CG   | 2.96                     | 0.44              |
| 2:D:263:VAL:HG13  | 2:D:318:VAL:HA    | 1.99                     | 0.44              |
| 2:D:1427:LEU:HD23 | 2:D:1430:VAL:HG23 | 1.99                     | 0.44              |
| 2:D:1599:TYR:N    | 2:D:1599:TYR:CD1  | 2.86                     | 0.44              |
| 1:A:284:GLN:O     | 1:A:285:THR:CB    | 2.66                     | 0.43              |
| 1:A:491:PRO:HB2   | 1:A:493:ILE:C     | 2.43                     | 0.43              |
| 1:A:720:LEU:HB2   | 1:A:721:GLY:H     | 1.72                     | 0.43              |
| 1:A:1435:ASN:O    | 1:A:1436:GLU:C    | 2.61                     | 0.43              |
| 1:A:1552:ALA:HB2  | 1:A:1620:MET:CE   | 2.48                     | 0.43              |
| 1:A:1562:LYS:NZ   | 1:A:1664:LEU:HD23 | 2.32                     | 0.43              |
| 1:A:1648:TRP:HE1  | 1:A:1664:LEU:CD2  | 2.31                     | 0.43              |
| 2:B:387:MET:O     | 2:B:398:LEU:HD21  | 2.18                     | 0.43              |
| 2:B:581:ASP:OD2   | 2:B:785:THR:HG21  | 2.17                     | 0.43              |
| 2:B:1286:VAL:O    | 2:B:1286:VAL:HG12 | 2.18                     | 0.43              |
| 2:B:1383:ASP:HB3  | 2:B:1457:LYS:HB2  | 2.00                     | 0.43              |
| 1:C:423:ASN:HB3   | 2:D:501:GLN:NE2   | 2.33                     | 0.43              |
| 1:C:504:LEU:N     | 1:C:504:LEU:CD1   | 2.80                     | 0.43              |
| 1:C:695:VAL:HG13  | 1:C:724:CYS:HA    | 2.00                     | 0.43              |
| 2:D:226:VAL:HG22  | 2:D:249:ALA:HB2   | 1.99                     | 0.43              |
| 2:D:580:VAL:HG12  | 2:D:581:ASP:N     | 2.32                     | 0.43              |
| 2:D:902:GLU:HG3   | 2:D:902:GLU:O     | 2.18                     | 0.43              |
| 2:D:916:VAL:CG2   | 2:D:917:PRO:CD    | 2.95                     | 0.43              |
| 2:D:1414:ASP:O    | 2:D:1415:ASN:C    | 2.60                     | 0.43              |
| 2:D:1438:LEU:HD13 | 2:D:1438:LEU:N    | 2.32                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1482:ASN:HB3  | 2:D:1493:ALA:CB   | 2.47                     | 0.43              |
| 2:D:1512:ILE:HG23 | 2:D:1631:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:127:PHE:CD1   | 1:A:127:PHE:N     | 2.84                     | 0.43              |
| 1:A:154:PRO:HB2   | 1:A:155:ALA:H     | 1.57                     | 0.43              |
| 1:A:578:ASP:O     | 1:A:579:ALA:O     | 2.35                     | 0.43              |
| 1:A:642:ASN:ND2   | 1:A:646:PHE:CD1   | 2.86                     | 0.43              |
| 1:A:862:VAL:HB    | 1:A:865:ILE:CG1   | 2.47                     | 0.43              |
| 1:A:917:TRP:O     | 2:B:813:VAL:HG22  | 2.18                     | 0.43              |
| 1:A:942:VAL:HA    | 1:A:1276:GLU:CD   | 2.43                     | 0.43              |
| 1:A:977:LEU:HD22  | 1:A:977:LEU:C     | 2.39                     | 0.43              |
| 1:A:1118:PHE:CD2  | 1:A:1148:THR:OG1  | 2.67                     | 0.43              |
| 1:A:1142:LEU:O    | 1:A:1143:TYR:O    | 2.36                     | 0.43              |
| 1:A:1224:ILE:HG22 | 1:A:1225:TYR:HD2  | 1.83                     | 0.43              |
| 1:A:1267:VAL:O    | 1:A:1270:VAL:HB   | 2.17                     | 0.43              |
| 1:A:1546:GLU:HG2  | 1:A:1663:ASN:OD1  | 2.18                     | 0.43              |
| 1:A:1602:LYS:HB3  | 1:A:1639:LEU:CB   | 2.48                     | 0.43              |
| 2:B:171:ILE:H     | 2:B:171:ILE:HG13  | 1.60                     | 0.43              |
| 2:B:229:GLN:HA    | 2:B:230:PRO:HD3   | 1.81                     | 0.43              |
| 2:B:237:ILE:HD11  | 2:B:309:LEU:HB2   | 2.00                     | 0.43              |
| 2:B:338:ILE:C     | 2:B:339:VAL:CG1   | 2.90                     | 0.43              |
| 2:B:410:PRO:CA    | 2:B:431:THR:HG22  | 2.44                     | 0.43              |
| 2:B:857:CYS:HB3   | 2:B:885:VAL:CG2   | 2.48                     | 0.43              |
| 2:B:1296:ASN:HB2  | 2:B:1299:LEU:HD22 | 2.00                     | 0.43              |
| 2:B:1384:ILE:HB   | 2:B:1423:VAL:HG12 | 1.99                     | 0.43              |
| 2:B:1520:VAL:CG1  | 2:B:1584:TRP:HD1  | 2.29                     | 0.43              |
| 1:C:439:ALA:O     | 1:C:441:ASP:N     | 2.47                     | 0.43              |
| 1:C:612:VAL:O     | 1:C:612:VAL:HG12  | 2.17                     | 0.43              |
| 1:C:702:GLY:HA3   | 1:C:728:PHE:CD1   | 2.53                     | 0.43              |
| 1:C:1158:ILE:O    | 1:C:1158:ILE:HG22 | 2.17                     | 0.43              |
| 2:D:221:LEU:HD11  | 2:D:753:LYS:CD    | 2.48                     | 0.43              |
| 2:D:243:PHE:C     | 2:D:243:PHE:CD2   | 2.96                     | 0.43              |
| 2:D:789:VAL:HG23  | 2:D:806:TYR:O     | 2.18                     | 0.43              |
| 2:D:1562:GLN:CB   | 2:D:1598:SER:HB3  | 2.48                     | 0.43              |
| 1:A:111:PHE:CG    | 1:A:112:SER:N     | 2.82                     | 0.43              |
| 1:A:223:VAL:O     | 1:A:225:PRO:HD3   | 2.18                     | 0.43              |
| 1:A:415:ASP:CB    | 1:A:417:VAL:HB    | 2.48                     | 0.43              |
| 1:A:701:ASP:O     | 1:A:704:CYS:HB2   | 2.18                     | 0.43              |
| 1:A:847:ASN:HD21  | 1:A:853:MET:HB2   | 1.83                     | 0.43              |
| 1:A:984:VAL:O     | 1:A:987:ILE:HB    | 2.18                     | 0.43              |
| 1:A:1127:ILE:HD13 | 1:A:1129:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:1320:LYS:HG2  | 1:A:1342:LEU:HD12 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1493:PHE:HD1  | 1:A:1493:PHE:C    | 2.21                     | 0.43              |
| 1:A:1549:LYS:NZ   | 1:A:1667:PHE:CD1  | 2.84                     | 0.43              |
| 1:A:1549:LYS:H    | 1:A:1549:LYS:HG2  | 1.49                     | 0.43              |
| 2:B:35:THR:O      | 2:B:36:ASP:C      | 2.61                     | 0.43              |
| 2:B:198:ARG:HB3   | 2:B:213:TYR:HE1   | 1.82                     | 0.43              |
| 2:B:446:HIS:O     | 2:B:465:ASN:HB2   | 2.18                     | 0.43              |
| 2:B:567:LEU:HD11  | 2:B:577:LEU:HD21  | 1.99                     | 0.43              |
| 2:B:856:PHE:CG    | 2:B:884:ILE:HD11  | 2.54                     | 0.43              |
| 1:C:322:TYR:HA    | 1:C:346:LYS:HA    | 2.00                     | 0.43              |
| 1:C:439:ALA:HA    | 1:C:440:PRO:HD3   | 1.79                     | 0.43              |
| 1:C:506:LYS:CE    | 1:C:533:ASN:O     | 2.65                     | 0.43              |
| 1:C:691:LYS:C     | 1:C:693:SER:N     | 2.76                     | 0.43              |
| 1:C:1016:VAL:CG1  | 1:C:1291:ILE:HG13 | 2.45                     | 0.43              |
| 1:C:1213:LYS:CG   | 1:C:1266:TYR:HE2  | 2.29                     | 0.43              |
| 1:C:1231:ASN:O    | 1:C:1234:HIS:O    | 2.37                     | 0.43              |
| 1:C:1237:SER:C    | 1:C:1238:SER:O    | 2.62                     | 0.43              |
| 1:C:1378:TYR:O    | 1:C:1406:ALA:HA   | 2.17                     | 0.43              |
| 1:C:1548:ARG:C    | 1:C:1550:GLN:H    | 2.26                     | 0.43              |
| 1:C:1562:LYS:HD3  | 1:C:1664:LEU:CD2  | 2.47                     | 0.43              |
| 2:D:145:TYR:HE2   | 2:D:165:PHE:CE1   | 2.35                     | 0.43              |
| 2:D:229:GLN:HA    | 2:D:230:PRO:HD3   | 1.83                     | 0.43              |
| 2:D:261:ALA:HB3   | 2:D:285:ILE:HD11  | 1.99                     | 0.43              |
| 2:D:466:VAL:CG1   | 2:D:524:TYR:HE2   | 2.31                     | 0.43              |
| 2:D:1284:ARG:HG3  | 2:D:1286:VAL:N    | 2.24                     | 0.43              |
| 2:D:1527:LYS:O    | 2:D:1529:LEU:HD12 | 2.18                     | 0.43              |
| 2:D:1601:ILE:N    | 2:D:1601:ILE:CD1  | 2.81                     | 0.43              |
| 2:D:1609:ARG:CG   | 2:D:1609:ARG:NH1  | 2.61                     | 0.43              |
| 1:A:234:GLU:HG3   | 1:A:235:TYR:CE2   | 2.54                     | 0.43              |
| 1:A:269:PHE:CE1   | 1:A:287:MET:HB3   | 2.46                     | 0.43              |
| 1:A:424:LEU:N     | 1:A:424:LEU:HD23  | 2.32                     | 0.43              |
| 1:A:700:TYR:CD2   | 1:A:700:TYR:C     | 2.96                     | 0.43              |
| 1:A:989:SER:O     | 1:A:993:SER:CB    | 2.64                     | 0.43              |
| 1:A:1033:ILE:HG22 | 1:A:1034:PHE:HD1  | 1.81                     | 0.43              |
| 2:B:148:PHE:CZ    | 2:B:792:VAL:HG11  | 2.53                     | 0.43              |
| 2:B:238:ASP:OD1   | 2:B:238:ASP:O     | 2.36                     | 0.43              |
| 2:B:352:LYS:O     | 2:B:432:ALA:HB1   | 2.19                     | 0.43              |
| 2:B:919:GLY:CA    | 2:B:1331:ALA:O    | 2.66                     | 0.43              |
| 1:C:431:LEU:HD13  | 1:C:431:LEU:C     | 2.44                     | 0.43              |
| 1:C:467:ILE:HG22  | 1:C:486:VAL:CG2   | 2.38                     | 0.43              |
| 1:C:476:LEU:HD23  | 1:C:476:LEU:HA    | 1.81                     | 0.43              |
| 1:C:610:TYR:N     | 1:C:610:TYR:CD1   | 2.86                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:949:ILE:O    | 1:C:949:ILE:CG2   | 2.67                     | 0.43              |
| 1:C:1013:MET:C   | 1:C:1016:VAL:HG23 | 2.43                     | 0.43              |
| 1:C:1081:PHE:O   | 1:C:1082:ALA:C    | 2.61                     | 0.43              |
| 1:C:1358:THR:HB  | 1:C:1360:HIS:CE1  | 2.54                     | 0.43              |
| 2:D:266:GLY:HA3  | 2:D:315:TYR:CE1   | 2.54                     | 0.43              |
| 2:D:511:THR:H    | 2:D:514:LEU:HD11  | 1.83                     | 0.43              |
| 2:D:574:ARG:HH21 | 2:D:759:THR:HG21  | 1.83                     | 0.43              |
| 2:D:735:ASN:OD1  | 2:D:735:ASN:N     | 2.52                     | 0.43              |
| 2:D:825:VAL:HA   | 2:D:916:VAL:O     | 2.19                     | 0.43              |
| 2:D:1599:TYR:N   | 2:D:1599:TYR:HD1  | 2.16                     | 0.43              |
| 1:A:165:ASP:O    | 1:A:167:GLU:N     | 2.48                     | 0.43              |
| 1:A:371:ILE:HG21 | 1:A:390:LEU:CD2   | 2.49                     | 0.43              |
| 1:A:565:GLU:HG3  | 1:A:624:PHE:CG    | 2.53                     | 0.43              |
| 1:A:565:GLU:HG2  | 1:A:565:GLU:O     | 2.18                     | 0.43              |
| 1:A:571:LEU:HG   | 1:A:812:ALA:HB2   | 2.00                     | 0.43              |
| 1:A:705:VAL:HA   | 1:A:739:ARG:HH12  | 1.83                     | 0.43              |
| 1:A:970:LYS:O    | 1:A:971:THR:HG22  | 2.19                     | 0.43              |
| 1:A:1068:VAL:CG2 | 1:A:1124:TYR:CD1  | 2.95                     | 0.43              |
| 1:A:1257:THR:O   | 1:A:1261:LEU:HG   | 2.18                     | 0.43              |
| 2:B:80:GLY:O     | 2:B:81:MET:HB2    | 2.17                     | 0.43              |
| 2:B:464:PHE:HB3  | 2:B:479:PHE:CE2   | 2.54                     | 0.43              |
| 2:B:800:ILE:CG2  | 2:B:801:CYS:N     | 2.69                     | 0.43              |
| 1:C:190:ILE:CG2  | 1:C:194:PRO:HG3   | 2.48                     | 0.43              |
| 1:C:395:ILE:HD12 | 1:C:395:ILE:C     | 2.43                     | 0.43              |
| 1:C:520:ASP:HB2  | 2:D:404:LEU:HD13  | 2.01                     | 0.43              |
| 1:C:561:LEU:HD23 | 1:C:561:LEU:HA    | 1.80                     | 0.43              |
| 1:C:955:ARG:HG2  | 1:C:1350:THR:O    | 2.18                     | 0.43              |
| 1:C:1233:GLN:O   | 1:C:1234:HIS:HB3  | 2.18                     | 0.43              |
| 1:C:1377:PHE:CD1 | 1:C:1408:TYR:HA   | 2.53                     | 0.43              |
| 1:C:1546:GLU:HG2 | 1:C:1663:ASN:OD1  | 2.18                     | 0.43              |
| 1:C:1562:LYS:HD2 | 1:C:1648:TRP:CZ2  | 2.48                     | 0.43              |
| 1:C:1601:ILE:O   | 1:C:1638:PRO:O    | 2.36                     | 0.43              |
| 1:C:1660:PHE:HE2 | 1:C:1664:LEU:CD1  | 2.26                     | 0.43              |
| 2:D:1500:LEU:C   | 2:D:1500:LEU:CD1  | 2.90                     | 0.43              |
| 1:A:443:PRO:CD   | 1:A:446:ASN:HB2   | 2.41                     | 0.43              |
| 1:A:1022:PHE:C   | 1:A:1024:TYR:N    | 2.76                     | 0.43              |
| 1:A:1081:PHE:O   | 1:A:1082:ALA:C    | 2.61                     | 0.43              |
| 1:A:1202:HIS:CG  | 1:A:1203:PRO:HD2  | 2.53                     | 0.43              |
| 1:A:1245:ALA:O   | 1:A:1246:ARG:C    | 2.62                     | 0.43              |
| 1:A:1264:ILE:H   | 1:A:1264:ILE:HG13 | 1.39                     | 0.43              |
| 2:B:103:TYR:N    | 2:B:103:TYR:HD2   | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:230:PRO:HG3   | 2:B:333:GLN:HG2   | 2.01                     | 0.43              |
| 2:B:621:PHE:H     | 2:B:621:PHE:HD2   | 1.66                     | 0.43              |
| 2:B:735:ASN:OD1   | 2:B:735:ASN:N     | 2.51                     | 0.43              |
| 2:B:1378:THR:O    | 2:B:1379:MET:C    | 2.60                     | 0.43              |
| 2:B:1502:HIS:O    | 2:B:1503:GLN:HB2  | 2.18                     | 0.43              |
| 2:B:1548:ILE:CG2  | 2:B:1635:LEU:HB3  | 2.48                     | 0.43              |
| 1:C:369:TYR:HA    | 1:C:370:PRO:HD3   | 1.88                     | 0.43              |
| 1:C:500:ASN:ND2   | 1:C:543:TYR:CE1   | 2.86                     | 0.43              |
| 1:C:532:GLN:O     | 1:C:535:VAL:HG13  | 2.18                     | 0.43              |
| 1:C:583:SER:O     | 1:C:586:GLN:HB3   | 2.18                     | 0.43              |
| 1:C:754:MET:SD    | 1:C:754:MET:C     | 3.02                     | 0.43              |
| 1:C:1243:GLY:O    | 1:C:1285:TYR:CZ   | 2.71                     | 0.43              |
| 1:C:1644:TRP:CD1  | 1:C:1646:GLU:OE1  | 2.71                     | 0.43              |
| 2:D:939:GLY:O     | 2:D:1316:SER:HA   | 2.18                     | 0.43              |
| 2:D:946:LYS:HA    | 2:D:1310:ASP:OD1  | 2.18                     | 0.43              |
| 2:D:1512:ILE:HG22 | 2:D:1631:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:608:ALA:O     | 1:A:609:VAL:C     | 2.61                     | 0.43              |
| 1:A:651:LEU:HD23  | 1:A:651:LEU:HA    | 1.74                     | 0.43              |
| 1:A:809:ILE:HG12  | 1:A:810:CYS:H     | 1.82                     | 0.43              |
| 1:A:1243:GLY:O    | 1:A:1285:TYR:CE2  | 2.72                     | 0.43              |
| 1:A:1381:ILE:HB   | 1:A:1493:PHE:CE2  | 2.54                     | 0.43              |
| 1:A:1622:LYS:HB2  | 1:A:1643:THR:HG22 | 1.99                     | 0.43              |
| 1:A:1656:SER:O    | 1:A:1659:ALA:HB3  | 2.19                     | 0.43              |
| 2:B:129:PHE:CE2   | 2:B:598:ILE:HD13  | 2.53                     | 0.43              |
| 2:B:820:MET:HA    | 2:B:821:PRO:HD3   | 1.79                     | 0.43              |
| 2:B:1402:LYS:HD3  | 2:B:1402:LYS:HA   | 1.53                     | 0.43              |
| 1:C:486:VAL:HG11  | 1:C:499:TYR:CE1   | 2.54                     | 0.43              |
| 1:C:567:CYS:HB3   | 1:C:570:GLN:HB3   | 2.01                     | 0.43              |
| 1:C:824:PHE:CD2   | 1:C:824:PHE:N     | 2.85                     | 0.43              |
| 1:C:827:MET:HB3   | 1:C:829:ILE:CD1   | 2.47                     | 0.43              |
| 1:C:1589:GLU:HB2  | 1:C:1590:ALA:H    | 1.46                     | 0.43              |
| 2:D:358:MET:HE2   | 2:D:467:LYS:HD2   | 2.00                     | 0.43              |
| 2:D:373:PRO:HB3   | 2:D:393:ASP:O     | 2.19                     | 0.43              |
| 2:D:387:MET:O     | 2:D:398:LEU:HD21  | 2.18                     | 0.43              |
| 2:D:859:ALA:O     | 2:D:866:TYR:HB2   | 2.19                     | 0.43              |
| 2:D:861:THR:C     | 2:D:863:GLY:N     | 2.77                     | 0.43              |
| 2:D:866:TYR:OH    | 2:D:1388:THR:CG2  | 2.67                     | 0.43              |
| 2:D:1330:ASN:N    | 2:D:1330:ASN:HD22 | 2.16                     | 0.43              |
| 1:A:163:PHE:CE1   | 1:A:188:PHE:CD1   | 3.06                     | 0.43              |
| 1:A:342:ILE:HA    | 1:A:343:PRO:HD3   | 1.74                     | 0.43              |
| 1:A:884:VAL:CG1   | 1:A:886:GLN:CG    | 2.90                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1013:MET:O    | 1:A:1017:PRO:HD3  | 2.18                     | 0.43              |
| 1:A:1037:ASP:OD1  | 1:A:1037:ASP:C    | 2.62                     | 0.43              |
| 1:A:1212:LEU:O    | 1:A:1215:GLU:HB2  | 2.18                     | 0.43              |
| 1:A:1265:ASN:C    | 1:A:1267:VAL:N    | 2.77                     | 0.43              |
| 1:A:1637:TYR:HA   | 1:A:1638:PRO:HD3  | 1.86                     | 0.43              |
| 2:B:445:LEU:HD12  | 2:B:465:ASN:O     | 2.19                     | 0.43              |
| 2:B:481:TYR:CD1   | 2:B:506:MET:HE1   | 2.54                     | 0.43              |
| 2:B:885:VAL:HG23  | 2:B:887:LEU:CD2   | 2.48                     | 0.43              |
| 2:B:1387:LEU:O    | 2:B:1390:PHE:HB2  | 2.18                     | 0.43              |
| 2:B:1390:PHE:CD1  | 2:B:1442:ILE:HG13 | 2.54                     | 0.43              |
| 1:C:27:ALA:HB2    | 1:C:39:ILE:HG12   | 2.01                     | 0.43              |
| 1:C:226:HIS:ND1   | 1:C:336:PHE:CE2   | 2.86                     | 0.43              |
| 1:C:317:ASP:C     | 1:C:319:ASN:H     | 2.27                     | 0.43              |
| 1:C:354:LEU:HD23  | 1:C:450:GLU:HG3   | 2.01                     | 0.43              |
| 1:C:383:VAL:O     | 1:C:383:VAL:HG22  | 2.18                     | 0.43              |
| 1:C:599:TRP:HE1   | 1:C:779:LEU:CB    | 2.32                     | 0.43              |
| 1:C:867:THR:O     | 1:C:868:SER:HB3   | 2.19                     | 0.43              |
| 1:C:1067:SER:HA   | 1:C:1074:ALA:HA   | 2.01                     | 0.43              |
| 1:C:1120:GLU:OE2  | 1:C:1121:ASN:N    | 2.52                     | 0.43              |
| 1:C:1127:ILE:HG13 | 1:C:1143:TYR:CE2  | 2.44                     | 0.43              |
| 1:C:1142:LEU:O    | 1:C:1143:TYR:O    | 2.37                     | 0.43              |
| 1:C:1159:CYS:O    | 1:C:1161:LEU:N    | 2.42                     | 0.43              |
| 1:C:1168:LEU:N    | 1:C:1168:LEU:HD23 | 2.32                     | 0.43              |
| 1:C:1527:CYS:O    | 1:C:1528:VAL:C    | 2.61                     | 0.43              |
| 2:D:261:ALA:N     | 2:D:285:ILE:CD1   | 2.82                     | 0.43              |
| 2:D:481:TYR:CD1   | 2:D:506:MET:HE1   | 2.53                     | 0.43              |
| 2:D:829:GLN:HE21  | 2:D:829:GLN:CA    | 2.31                     | 0.43              |
| 2:D:963:ILE:CD1   | 2:D:1311:ILE:HG12 | 2.49                     | 0.43              |
| 2:D:1296:ASN:HB2  | 2:D:1299:LEU:HD22 | 2.01                     | 0.43              |
| 1:A:128:ILE:HD11  | 1:A:214:THR:CA    | 2.49                     | 0.43              |
| 1:A:222:TYR:HE1   | 1:A:768:TYR:CB    | 2.13                     | 0.43              |
| 1:A:624:PHE:CD1   | 1:A:625:GLN:N     | 2.85                     | 0.43              |
| 1:A:867:THR:O     | 1:A:868:SER:HB3   | 2.18                     | 0.43              |
| 1:A:1650:ARG:HD2  | 1:A:1650:ARG:N    | 2.27                     | 0.43              |
| 2:B:32:VAL:HB     | 2:B:607:PHE:CZ    | 2.54                     | 0.43              |
| 2:B:145:TYR:HE2   | 2:B:165:PHE:CE1   | 2.37                     | 0.43              |
| 2:B:378:PRO:HG3   | 2:B:389:THR:HG23  | 2.00                     | 0.43              |
| 2:B:511:THR:O     | 2:B:513:ASP:N     | 2.52                     | 0.43              |
| 2:B:745:ILE:HG22  | 2:B:897:LYS:HD3   | 1.97                     | 0.43              |
| 2:B:755:TRP:O     | 2:B:756:LEU:CB    | 2.66                     | 0.43              |
| 2:B:847:ARG:CZ    | 2:B:867:ARG:NH1   | 2.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:902:GLU:O     | 2:B:903:ALA:HB2   | 2.19                     | 0.43              |
| 2:B:946:LYS:HA    | 2:B:1310:ASP:OD1  | 2.18                     | 0.43              |
| 2:B:1391:LEU:HD12 | 2:B:1417:MET:CE   | 2.49                     | 0.43              |
| 2:B:1481:LEU:C    | 2:B:1481:LEU:CD1  | 2.92                     | 0.43              |
| 1:C:223:VAL:O     | 1:C:225:PRO:HD3   | 2.19                     | 0.43              |
| 1:C:421:VAL:HG23  | 2:D:507:ASN:ND2   | 2.33                     | 0.43              |
| 1:C:516:GLU:C     | 1:C:517:LYS:O     | 2.62                     | 0.43              |
| 1:C:552:ALA:O     | 1:C:658:ASN:ND2   | 2.52                     | 0.43              |
| 1:C:593:ALA:O     | 1:C:594:THR:HG23  | 2.17                     | 0.43              |
| 1:C:700:TYR:CD2   | 1:C:700:TYR:C     | 2.97                     | 0.43              |
| 1:C:756:THR:O     | 1:C:757:LEU:HD23  | 2.19                     | 0.43              |
| 1:C:804:ILE:HG13  | 1:C:804:ILE:O     | 2.19                     | 0.43              |
| 1:C:1132:THR:HG22 | 1:C:1133:LEU:N    | 2.31                     | 0.43              |
| 1:C:1193:TYR:O    | 1:C:1194:ALA:C    | 2.62                     | 0.43              |
| 1:C:1279:ARG:HD3  | 1:C:1279:ARG:C    | 2.43                     | 0.43              |
| 2:D:430:MET:HE3   | 2:D:430:MET:HB2   | 1.74                     | 0.43              |
| 2:D:523:TYR:C     | 2:D:523:TYR:HD1   | 2.25                     | 0.43              |
| 2:D:578:VAL:O     | 2:D:578:VAL:HG13  | 2.18                     | 0.43              |
| 2:D:923:SER:O     | 2:D:924:ILE:HD12  | 2.18                     | 0.43              |
| 2:D:946:LYS:HD3   | 2:D:946:LYS:N     | 2.34                     | 0.43              |
| 2:D:1326:LEU:HD11 | 2:D:1328:PHE:HE2  | 1.84                     | 0.43              |
| 2:D:1556:PRO:C    | 2:D:1558:ALA:H    | 2.25                     | 0.43              |
| 1:A:101:TYR:CD2   | 1:A:101:TYR:N     | 2.87                     | 0.43              |
| 1:A:317:ASP:C     | 1:A:319:ASN:H     | 2.27                     | 0.43              |
| 1:A:354:LEU:HA    | 1:A:374:GLN:O     | 2.19                     | 0.43              |
| 1:A:395:ILE:HD12  | 1:A:395:ILE:C     | 2.43                     | 0.43              |
| 1:A:412:ARG:HG3   | 1:A:413:VAL:N     | 2.34                     | 0.43              |
| 1:A:495:LYS:HA    | 1:A:495:LYS:HD3   | 1.59                     | 0.43              |
| 1:A:504:LEU:HD12  | 1:A:509:ILE:CA    | 2.48                     | 0.43              |
| 1:A:1057:MET:O    | 1:A:1058:SER:C    | 2.59                     | 0.43              |
| 1:A:1153:ARG:NH2  | 1:A:1168:LEU:HD13 | 2.34                     | 0.43              |
| 1:A:1162:VAL:HG11 | 1:C:1064:TYR:HE2  | 1.83                     | 0.43              |
| 1:A:1638:PRO:O    | 1:A:1639:LEU:HB2  | 2.19                     | 0.43              |
| 1:A:1638:PRO:HB2  | 1:A:1639:LEU:H    | 1.48                     | 0.43              |
| 2:B:355:LYS:HA    | 2:B:356:PRO:HD3   | 1.91                     | 0.43              |
| 2:B:466:VAL:CG1   | 2:B:524:TYR:HE2   | 2.32                     | 0.43              |
| 2:B:756:LEU:HD22  | 2:B:778:PHE:CD1   | 2.53                     | 0.43              |
| 2:B:788:VAL:HG22  | 2:B:807:GLU:HG2   | 2.01                     | 0.43              |
| 1:C:25:ILE:HD13   | 1:C:41:ILE:CG1    | 2.49                     | 0.43              |
| 1:C:74:SER:HA     | 1:C:79:PHE:HE1    | 1.84                     | 0.43              |
| 1:C:101:TYR:N     | 1:C:101:TYR:CD2   | 2.87                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:553:GLU:OE1   | 1:C:553:GLU:HA    | 2.19                     | 0.43              |
| 1:C:606:ASP:C     | 1:C:608:ALA:N     | 2.77                     | 0.43              |
| 1:C:773:TRP:CZ3   | 1:C:788:PHE:CE1   | 2.92                     | 0.43              |
| 1:C:1134:PRO:O    | 1:C:1135:VAL:C    | 2.61                     | 0.43              |
| 1:C:1155:ALA:O    | 1:C:1158:ILE:HG13 | 2.19                     | 0.43              |
| 1:C:1298:THR:O    | 1:C:1301:SER:N    | 2.52                     | 0.43              |
| 1:C:1365:VAL:CG2  | 1:C:1366:HIS:N    | 2.75                     | 0.43              |
| 1:C:1455:ILE:N    | 1:C:1455:ILE:CD1  | 2.82                     | 0.43              |
| 1:C:1664:LEU:HD23 | 1:C:1664:LEU:O    | 2.19                     | 0.43              |
| 2:D:74:ASP:OD1    | 2:D:74:ASP:N      | 2.52                     | 0.43              |
| 2:D:96:THR:HB     | 2:D:123:TYR:OH    | 2.18                     | 0.43              |
| 2:D:202:LYS:CG    | 2:D:203:TYR:N     | 2.82                     | 0.43              |
| 2:D:262:PHE:HE1   | 2:D:282:ARG:CG    | 2.29                     | 0.43              |
| 2:D:646:GLN:HB3   | 2:D:647:PRO:CD    | 2.37                     | 0.43              |
| 2:D:1525:LYS:HD2  | 2:D:1610:TRP:CZ2  | 2.53                     | 0.43              |
| 1:A:27:ALA:HB1    | 1:A:28:PRO:HD2    | 2.00                     | 0.42              |
| 1:A:33:VAL:HA     | 1:A:87:ILE:CG1    | 2.49                     | 0.42              |
| 1:A:196:TYR:CD2   | 1:A:196:TYR:N     | 2.85                     | 0.42              |
| 1:A:412:ARG:HG3   | 1:A:413:VAL:H     | 1.84                     | 0.42              |
| 1:A:587:THR:CG2   | 1:A:789:ALA:HB2   | 2.49                     | 0.42              |
| 1:A:916:THR:O     | 1:A:918:PHE:N     | 2.52                     | 0.42              |
| 1:A:967:LEU:HD12  | 1:A:967:LEU:C     | 2.41                     | 0.42              |
| 2:B:531:ILE:O     | 2:B:617:ASN:ND2   | 2.51                     | 0.42              |
| 2:B:748:ARG:NH1   | 2:B:784:ILE:HG12  | 2.33                     | 0.42              |
| 2:B:1466:GLU:OE2  | 2:B:1468:CYS:HB2  | 2.19                     | 0.42              |
| 2:B:1505:ARG:NH1  | 2:B:1627:ASP:OD1  | 2.51                     | 0.42              |
| 2:B:1562:GLN:HB2  | 2:B:1598:SER:HB3  | 2.00                     | 0.42              |
| 1:C:49:ALA:HB2    | 1:C:74:SER:HB2    | 2.01                     | 0.42              |
| 1:C:186:PRO:O     | 1:C:187:ASP:C     | 2.62                     | 0.42              |
| 1:C:348:VAL:HG12  | 1:C:350:SER:H     | 1.84                     | 0.42              |
| 1:C:473:HIS:HE1   | 2:D:455:LYS:HZ3   | 1.67                     | 0.42              |
| 1:C:501:TYR:HD1   | 1:C:501:TYR:C     | 2.26                     | 0.42              |
| 1:C:503:ILE:HD11  | 1:C:528:ILE:HG21  | 2.01                     | 0.42              |
| 1:C:554:LEU:HA    | 1:C:554:LEU:HD23  | 1.60                     | 0.42              |
| 1:C:1007:SER:HA   | 1:C:1069:TRP:HD1  | 1.83                     | 0.42              |
| 1:C:1053:MET:HE3  | 1:C:1086:LEU:CD2  | 2.48                     | 0.42              |
| 1:C:1103:SER:O    | 1:C:1104:LEU:C    | 2.62                     | 0.42              |
| 1:C:1213:LYS:HE2  | 1:C:1266:TYR:CE2  | 2.54                     | 0.42              |
| 1:C:1648:TRP:HE1  | 1:C:1664:LEU:CD2  | 2.32                     | 0.42              |
| 2:D:449:ILE:HD13  | 2:D:462:VAL:CG2   | 2.45                     | 0.42              |
| 2:D:490:PHE:C     | 2:D:490:PHE:CD1   | 2.96                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:567:LEU:HD23  | 2:D:567:LEU:HA    | 1.55                     | 0.42              |
| 2:D:580:VAL:CG1   | 2:D:581:ASP:N     | 2.81                     | 0.42              |
| 2:D:824:VAL:HG22  | 2:D:825:VAL:N     | 2.34                     | 0.42              |
| 2:D:952:ASP:O     | 2:D:1331:ALA:HB1  | 2.19                     | 0.42              |
| 2:D:1387:LEU:O    | 2:D:1388:THR:C    | 2.61                     | 0.42              |
| 2:D:1614:ASP:C    | 2:D:1616:CYS:N    | 2.76                     | 0.42              |
| 1:A:153:LYS:O     | 1:A:154:PRO:O     | 2.37                     | 0.42              |
| 1:A:171:VAL:HG22  | 1:A:1057:MET:CE   | 2.49                     | 0.42              |
| 1:A:847:ASN:ND2   | 1:A:853:MET:HB2   | 2.34                     | 0.42              |
| 1:A:969:PRO:HD3   | 1:A:1603:LYS:HZ1  | 1.84                     | 0.42              |
| 1:A:1022:PHE:O    | 1:A:1025:LEU:N    | 2.52                     | 0.42              |
| 1:A:1060:ARG:CG   | 1:A:1061:ASN:N    | 2.82                     | 0.42              |
| 1:A:1226:ARG:HD3  | 1:A:1266:TYR:CE1  | 2.54                     | 0.42              |
| 1:A:1413:GLU:OE2  | 1:A:1413:GLU:HA   | 2.19                     | 0.42              |
| 2:B:350:THR:HA    | 2:B:351:PRO:HD3   | 1.88                     | 0.42              |
| 2:B:511:THR:OG1   | 2:B:512:PRO:HD2   | 2.18                     | 0.42              |
| 2:B:946:LYS:HD3   | 2:B:946:LYS:N     | 2.34                     | 0.42              |
| 2:B:949:LYS:C     | 2:B:950:LEU:HG    | 2.44                     | 0.42              |
| 2:B:1391:LEU:CG   | 2:B:1417:MET:HE2  | 2.48                     | 0.42              |
| 1:C:110:HIS:ND1   | 1:C:110:HIS:N     | 2.66                     | 0.42              |
| 1:C:363:LEU:HD12  | 1:C:456:ALA:HA    | 2.00                     | 0.42              |
| 1:C:620:LEU:H     | 1:C:620:LEU:HG    | 1.60                     | 0.42              |
| 1:C:784:LYS:HG2   | 1:C:785:GLN:N     | 2.33                     | 0.42              |
| 1:C:862:VAL:HG12  | 1:C:907:LEU:HD21  | 2.01                     | 0.42              |
| 1:C:961:TYR:HE2   | 1:C:1343:ASN:HA   | 1.83                     | 0.42              |
| 1:C:1118:PHE:HE2  | 1:C:1148:THR:HG1  | 1.57                     | 0.42              |
| 1:C:1324:HIS:CG   | 1:C:1336:ARG:NH2  | 2.87                     | 0.42              |
| 1:C:1467:ILE:HA   | 1:C:1468:PRO:HD3  | 1.78                     | 0.42              |
| 1:C:1570:VAL:HG22 | 1:C:1575:VAL:HG13 | 2.00                     | 0.42              |
| 2:D:129:PHE:CE2   | 2:D:598:ILE:HD13  | 2.54                     | 0.42              |
| 2:D:553:ASP:O     | 2:D:555:LEU:HG    | 2.19                     | 0.42              |
| 2:D:811:MET:HG3   | 2:D:812:LYS:N     | 2.34                     | 0.42              |
| 2:D:919:GLY:CA    | 2:D:1331:ALA:O    | 2.67                     | 0.42              |
| 2:D:942:LEU:HD13  | 2:D:1314:THR:HG23 | 2.01                     | 0.42              |
| 2:D:943:GLU:HB2   | 2:D:1313:VAL:HG23 | 2.01                     | 0.42              |
| 2:D:949:LYS:C     | 2:D:950:LEU:HG    | 2.44                     | 0.42              |
| 2:D:1481:LEU:C    | 2:D:1481:LEU:CD1  | 2.93                     | 0.42              |
| 1:A:693:SER:C     | 1:A:695:VAL:N     | 2.77                     | 0.42              |
| 1:A:832:SER:HA    | 1:A:928:ARG:HB3   | 2.02                     | 0.42              |
| 1:A:847:ASN:ND2   | 1:A:853:MET:CB    | 2.83                     | 0.42              |
| 1:A:914:LEU:HD12  | 1:A:915:GLU:N     | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1179:THR:HG22 | 1:A:1180:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:1189:ALA:O    | 1:A:1192:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:1226:ARG:HD2  | 1:A:1270:VAL:CG2  | 2.50                     | 0.42              |
| 1:A:1464:LEU:C    | 1:A:1464:LEU:HD22 | 2.44                     | 0.42              |
| 2:B:111:PRO:O     | 2:B:113:VAL:HG23  | 2.19                     | 0.42              |
| 2:B:113:VAL:HG12  | 2:B:114:ARG:N     | 2.34                     | 0.42              |
| 2:B:218:LYS:CD    | 2:B:822:TYR:HE2   | 2.31                     | 0.42              |
| 2:B:336:ILE:HD13  | 2:B:336:ILE:HA    | 1.78                     | 0.42              |
| 2:B:775:THR:HG22  | 2:B:776:MET:H     | 1.84                     | 0.42              |
| 2:B:1273:LEU:HB2  | 2:B:1319:GLY:CA   | 2.36                     | 0.42              |
| 2:B:1506:ILE:HD11 | 2:B:1628:PHE:CE1  | 2.54                     | 0.42              |
| 2:B:1548:ILE:HD12 | 2:B:1636:THR:OG1  | 2.18                     | 0.42              |
| 1:C:144:ARG:HD2   | 1:C:146:TYR:CZ    | 2.54                     | 0.42              |
| 1:C:499:TYR:HE2   | 1:C:517:LYS:HG3   | 1.84                     | 0.42              |
| 1:C:534:MET:HB3   | 1:C:538:SER:OG    | 2.19                     | 0.42              |
| 1:C:584:PRO:CB    | 1:C:792:ASP:HA    | 2.37                     | 0.42              |
| 1:C:626:PHE:C     | 1:C:628:GLU:H     | 2.26                     | 0.42              |
| 1:C:827:MET:HB3   | 1:C:829:ILE:HD13  | 2.01                     | 0.42              |
| 1:C:870:SER:N     | 1:C:871:PRO:HD3   | 2.33                     | 0.42              |
| 1:C:1020:TYR:HE1  | 1:C:1295:GLU:HG3  | 1.84                     | 0.42              |
| 1:C:1068:VAL:CG2  | 1:C:1124:TYR:CD1  | 2.94                     | 0.42              |
| 1:C:1165:ASP:C    | 1:C:1165:ASP:OD2  | 2.61                     | 0.42              |
| 1:C:1381:ILE:CG1  | 1:C:1382:ASP:N    | 2.81                     | 0.42              |
| 1:C:1658:GLN:HA   | 1:C:1661:LEU:HB2  | 2.01                     | 0.42              |
| 2:D:64:LYS:HG3    | 2:D:64:LYS:O      | 2.20                     | 0.42              |
| 2:D:69:PHE:HE2    | 2:D:71:THR:HB     | 1.84                     | 0.42              |
| 2:D:138:THR:HG22  | 2:D:139:PRO:O     | 2.18                     | 0.42              |
| 2:D:477:LYS:HD3   | 2:D:477:LYS:H     | 1.84                     | 0.42              |
| 2:D:788:VAL:HG22  | 2:D:807:GLU:HG2   | 2.01                     | 0.42              |
| 2:D:1305:THR:HG23 | 2:D:1307:LEU:N    | 2.30                     | 0.42              |
| 1:A:54:ILE:CG1    | 1:A:106:VAL:HG13  | 2.49                     | 0.42              |
| 1:A:482:LEU:HD23  | 1:A:482:LEU:C     | 2.44                     | 0.42              |
| 1:A:774:LEU:HD12  | 1:A:799:ILE:HD11  | 2.02                     | 0.42              |
| 1:A:1013:MET:HA   | 1:A:1016:VAL:HG23 | 2.00                     | 0.42              |
| 1:A:1027:THR:HG21 | 1:A:1302:LEU:HD13 | 2.02                     | 0.42              |
| 1:A:1664:LEU:HD23 | 1:A:1664:LEU:O    | 2.19                     | 0.42              |
| 2:B:338:ILE:C     | 2:B:339:VAL:HG13  | 2.44                     | 0.42              |
| 2:B:449:ILE:HD13  | 2:B:462:VAL:CG2   | 2.46                     | 0.42              |
| 2:B:491:LYS:HE2   | 2:B:491:LYS:HB3   | 1.71                     | 0.42              |
| 2:B:830:VAL:HG23  | 2:B:831:GLU:N     | 2.34                     | 0.42              |
| 2:B:933:ARG:HH11  | 2:B:933:ARG:HG3   | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1305:THR:HG23 | 2:B:1306:LYS:N    | 2.34                     | 0.42              |
| 2:B:1525:LYS:HD2  | 2:B:1610:TRP:CZ2  | 2.54                     | 0.42              |
| 2:B:1556:PRO:C    | 2:B:1558:ALA:H    | 2.25                     | 0.42              |
| 1:C:27:ALA:HB1    | 1:C:28:PRO:CD     | 2.50                     | 0.42              |
| 1:C:395:ILE:CG1   | 1:C:430:VAL:HB    | 2.50                     | 0.42              |
| 1:C:424:LEU:N     | 1:C:424:LEU:HD23  | 2.34                     | 0.42              |
| 1:C:706:ASN:HD22  | 1:C:709:GLU:C     | 2.26                     | 0.42              |
| 1:C:774:LEU:HG    | 1:C:788:PHE:HE1   | 1.84                     | 0.42              |
| 1:C:780:VAL:HA    | 1:C:781:PRO:HD3   | 1.85                     | 0.42              |
| 1:C:1027:THR:HG21 | 1:C:1302:LEU:HD13 | 2.01                     | 0.42              |
| 1:C:1247:MET:O    | 1:C:1248:VAL:C    | 2.62                     | 0.42              |
| 1:C:1280:TYR:O    | 1:C:1280:TYR:CG   | 2.72                     | 0.42              |
| 1:C:1307:LEU:HD22 | 1:C:1307:LEU:N    | 2.33                     | 0.42              |
| 1:C:1439:LEU:HD23 | 1:C:1439:LEU:HA   | 1.61                     | 0.42              |
| 1:C:1545:ALA:HB2  | 1:C:1660:PHE:CE1  | 2.54                     | 0.42              |
| 1:C:1585:TYR:CE1  | 1:C:1671:ILE:HG12 | 2.51                     | 0.42              |
| 2:D:415:THR:OG1   | 2:D:415:THR:O     | 2.34                     | 0.42              |
| 2:D:829:GLN:HG2   | 2:D:1480:LEU:HD13 | 2.01                     | 0.42              |
| 2:D:1370:ARG:HG2  | 2:D:1371:TYR:O    | 2.19                     | 0.42              |
| 1:A:443:PRO:O     | 1:A:444:GLU:C     | 2.63                     | 0.42              |
| 1:A:532:GLN:O     | 1:A:535:VAL:HG22  | 2.20                     | 0.42              |
| 1:A:610:TYR:N     | 1:A:610:TYR:CD1   | 2.86                     | 0.42              |
| 1:A:1016:VAL:CG2  | 1:A:1291:ILE:HD12 | 2.49                     | 0.42              |
| 1:A:1091:LYS:H    | 1:A:1091:LYS:HG3  | 1.39                     | 0.42              |
| 1:A:1237:SER:C    | 1:A:1238:SER:O    | 2.62                     | 0.42              |
| 2:B:354:PHE:O     | 2:B:434:ALA:HA    | 2.19                     | 0.42              |
| 2:B:485:ASN:C     | 2:B:487:GLY:N     | 2.77                     | 0.42              |
| 2:B:485:ASN:O     | 2:B:486:LYS:HB2   | 2.18                     | 0.42              |
| 2:B:567:LEU:HD23  | 2:B:567:LEU:HA    | 1.52                     | 0.42              |
| 2:B:780:LEU:HA    | 2:B:780:LEU:HD22  | 1.83                     | 0.42              |
| 2:B:1292:ILE:HD11 | 2:B:1301:ARG:NE   | 2.32                     | 0.42              |
| 2:B:1506:ILE:CD1  | 2:B:1628:PHE:CD1  | 3.03                     | 0.42              |
| 2:B:1525:LYS:HD2  | 2:B:1610:TRP:CZ3  | 2.54                     | 0.42              |
| 1:C:85:LEU:N      | 1:C:85:LEU:CD2    | 2.79                     | 0.42              |
| 1:C:196:TYR:H     | 1:C:196:TYR:HD2   | 1.64                     | 0.42              |
| 1:C:256:TYR:HE2   | 1:C:826:GLU:OE2   | 2.02                     | 0.42              |
| 1:C:1083:LEU:CD1  | 1:C:1104:LEU:HD23 | 2.49                     | 0.42              |
| 1:C:1101:CYS:O    | 1:C:1105:LEU:HD12 | 2.20                     | 0.42              |
| 1:C:1142:LEU:O    | 1:C:1143:TYR:C    | 2.62                     | 0.42              |
| 1:C:1183:GLN:NE2  | 1:C:1183:GLN:O    | 2.53                     | 0.42              |
| 2:D:108:VAL:O     | 2:D:114:ARG:HA    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:382:GLU:C     | 2:D:384:PHE:H     | 2.27                     | 0.42              |
| 2:D:524:TYR:HE1   | 2:D:532:VAL:CG1   | 2.29                     | 0.42              |
| 2:D:822:TYR:C     | 2:D:822:TYR:CD1   | 2.96                     | 0.42              |
| 2:D:859:ALA:HB1   | 2:D:866:TYR:CD1   | 2.55                     | 0.42              |
| 2:D:1385:SER:OG   | 2:D:1455:SER:N    | 2.47                     | 0.42              |
| 2:D:1606:TRP:HD1  | 2:D:1606:TRP:O    | 2.03                     | 0.42              |
| 2:D:1635:LEU:O    | 2:D:1637:GLU:N    | 2.52                     | 0.42              |
| 1:A:185:PHE:CB    | 1:A:186:PRO:HD2   | 2.49                     | 0.42              |
| 1:A:438:ASP:HA    | 1:A:447:GLN:NE2   | 2.35                     | 0.42              |
| 1:A:626:PHE:O     | 1:A:628:GLU:N     | 2.52                     | 0.42              |
| 1:A:689:LYS:O     | 1:A:691:LYS:N     | 2.52                     | 0.42              |
| 1:A:1018:VAL:O    | 1:A:1019:PHE:C    | 2.63                     | 0.42              |
| 1:A:1142:LEU:O    | 1:A:1143:TYR:C    | 2.61                     | 0.42              |
| 1:A:1165:ASP:C    | 1:A:1165:ASP:OD2  | 2.62                     | 0.42              |
| 1:A:1213:LYS:C    | 1:A:1215:GLU:N    | 2.77                     | 0.42              |
| 1:A:1581:LEU:HD11 | 1:A:1598:ILE:HD11 | 1.99                     | 0.42              |
| 2:B:503:LEU:HD23  | 2:B:503:LEU:C     | 2.45                     | 0.42              |
| 2:B:581:ASP:CG    | 2:B:785:THR:HG21  | 2.44                     | 0.42              |
| 1:C:309:GLU:N     | 1:C:309:GLU:CD    | 2.77                     | 0.42              |
| 1:C:487:THR:HA    | 1:C:488:PRO:HD3   | 1.81                     | 0.42              |
| 1:C:715:ALA:O     | 1:C:718:ILE:HG13  | 2.20                     | 0.42              |
| 1:C:829:ILE:HA    | 1:C:830:PRO:HD3   | 1.84                     | 0.42              |
| 1:C:839:ILE:CD1   | 1:C:1485:VAL:HG12 | 2.50                     | 0.42              |
| 1:C:849:ARG:NH2   | 2:D:556:ILE:O     | 2.52                     | 0.42              |
| 1:C:946:PRO:HB2   | 1:C:947:ARG:H     | 1.52                     | 0.42              |
| 1:C:1037:ASP:O    | 1:C:1040:ILE:HB   | 2.19                     | 0.42              |
| 2:D:263:VAL:HG23  | 2:D:283:ILE:CD1   | 2.48                     | 0.42              |
| 2:D:1367:ILE:HD13 | 2:D:1456:VAL:CG2  | 2.49                     | 0.42              |
| 2:D:1540:TYR:CE1  | 2:D:1575:LEU:HB2  | 2.54                     | 0.42              |
| 1:A:501:TYR:CE1   | 1:A:512:PHE:C     | 2.98                     | 0.42              |
| 1:A:950:TYR:C     | 1:A:952:THR:H     | 2.28                     | 0.42              |
| 1:A:1025:LEU:HD23 | 1:A:1025:LEU:HA   | 1.72                     | 0.42              |
| 1:A:1046:LYS:O    | 1:A:1047:LYS:C    | 2.61                     | 0.42              |
| 1:A:1208:ILE:O    | 1:A:1208:ILE:HG22 | 2.19                     | 0.42              |
| 1:A:1279:ARG:HD3  | 1:A:1279:ARG:C    | 2.44                     | 0.42              |
| 1:A:1504:GLN:HG3  | 1:A:1505:CYS:N    | 2.35                     | 0.42              |
| 1:A:1602:LYS:HB3  | 1:A:1639:LEU:HB2  | 2.02                     | 0.42              |
| 1:A:1652:THR:HB   | 1:A:1653:THR:H    | 1.73                     | 0.42              |
| 2:B:29:THR:CB     | 2:B:30:PRO:CD     | 2.97                     | 0.42              |
| 2:B:219:TYR:CD1   | 2:B:220:VAL:N     | 2.86                     | 0.42              |
| 2:B:229:GLN:HA    | 2:B:229:GLN:OE1   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:236:TYR:CZ    | 2:B:424:ARG:HD2   | 2.54                     | 0.42              |
| 2:B:263:VAL:CG1   | 2:B:318:VAL:HG23  | 2.50                     | 0.42              |
| 2:B:480:THR:OG1   | 2:B:494:ARG:NE    | 2.51                     | 0.42              |
| 2:B:861:THR:C     | 2:B:863:GLY:N     | 2.77                     | 0.42              |
| 1:C:117:MET:HB3   | 1:C:117:MET:HE2   | 1.57                     | 0.42              |
| 1:C:269:PHE:CE1   | 1:C:287:MET:HB3   | 2.47                     | 0.42              |
| 1:C:365:PRO:CD    | 1:C:464:TYR:CE2   | 3.03                     | 0.42              |
| 1:C:864:GLY:HA3   | 1:C:907:LEU:HD22  | 2.01                     | 0.42              |
| 1:C:1364:VAL:HG22 | 1:C:1365:VAL:N    | 2.35                     | 0.42              |
| 1:C:1549:LYS:NZ   | 1:C:1667:PHE:CD1  | 2.85                     | 0.42              |
| 1:C:1549:LYS:H    | 1:C:1549:LYS:HG2  | 1.51                     | 0.42              |
| 1:C:1658:GLN:N    | 1:C:1658:GLN:HE21 | 2.17                     | 0.42              |
| 2:D:35:THR:O      | 2:D:36:ASP:C      | 2.62                     | 0.42              |
| 2:D:524:TYR:HD1   | 2:D:524:TYR:O     | 2.03                     | 0.42              |
| 2:D:916:VAL:HG23  | 2:D:917:PRO:CD    | 2.48                     | 0.42              |
| 1:A:25:ILE:HD13   | 1:A:41:ILE:HG13   | 2.01                     | 0.42              |
| 1:A:162:THR:HG21  | 1:A:204:LYS:CE    | 2.40                     | 0.42              |
| 1:A:386:VAL:HA    | 1:A:387:PRO:HD3   | 1.89                     | 0.42              |
| 1:A:391:ASN:HD21  | 1:A:406:PRO:HG3   | 1.84                     | 0.42              |
| 1:A:517:LYS:HG2   | 1:A:518:PHE:H     | 1.85                     | 0.42              |
| 1:A:544:TYR:HE2   | 1:A:546:VAL:CG2   | 2.33                     | 0.42              |
| 1:A:594:THR:OG1   | 1:A:782:ARG:CA    | 2.67                     | 0.42              |
| 1:A:786:LEU:HD23  | 1:A:786:LEU:N     | 2.30                     | 0.42              |
| 1:A:1047:LYS:O    | 1:A:1048:LYS:C    | 2.63                     | 0.42              |
| 2:B:69:PHE:HE2    | 2:B:71:THR:HB     | 1.85                     | 0.42              |
| 2:B:214:PHE:HD1   | 2:B:214:PHE:C     | 2.27                     | 0.42              |
| 2:B:350:THR:O     | 2:B:350:THR:CG2   | 2.68                     | 0.42              |
| 2:B:398:LEU:HD23  | 2:B:398:LEU:HA    | 1.68                     | 0.42              |
| 2:B:438:GLN:HB2   | 2:B:617:ASN:HD21  | 1.83                     | 0.42              |
| 2:B:476:ILE:HD11  | 2:B:524:TYR:CB    | 2.49                     | 0.42              |
| 2:B:603:GLU:C     | 2:B:605:SER:N     | 2.73                     | 0.42              |
| 2:B:742:ASP:OD1   | 2:B:743:SER:N     | 2.53                     | 0.42              |
| 2:B:842:GLU:C     | 2:B:843:ASP:O     | 2.62                     | 0.42              |
| 2:B:847:ARG:HG3   | 2:B:869:GLN:CG    | 2.50                     | 0.42              |
| 2:B:954:VAL:O     | 2:B:957:THR:HG23  | 2.20                     | 0.42              |
| 2:B:1623:LYS:N    | 2:B:1623:LYS:HD2  | 2.31                     | 0.42              |
| 1:C:31:PHE:O      | 1:C:119:ILE:HA    | 2.19                     | 0.42              |
| 1:C:42:GLN:HE21   | 1:C:43:VAL:C      | 2.28                     | 0.42              |
| 1:C:482:LEU:C     | 1:C:482:LEU:HD23  | 2.44                     | 0.42              |
| 1:C:571:LEU:HD22  | 1:C:803:GLY:HA3   | 2.02                     | 0.42              |
| 1:C:639:GLY:H     | 1:C:645:VAL:HA    | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:874:ASP:C     | 1:C:875:HIS:CG    | 2.98                     | 0.42              |
| 1:C:1056:ILE:HD13 | 1:C:1056:ILE:O    | 2.17                     | 0.42              |
| 1:C:1103:SER:O    | 1:C:1106:TRP:N    | 2.50                     | 0.42              |
| 1:C:1381:ILE:HB   | 1:C:1493:PHE:CE2  | 2.55                     | 0.42              |
| 1:C:1587:THR:HB   | 1:C:1591:VAL:HG13 | 2.01                     | 0.42              |
| 2:D:146:ARG:HA    | 2:D:183:PHE:CE2   | 2.54                     | 0.42              |
| 2:D:164:GLU:HB2   | 2:D:200:VAL:CG2   | 2.50                     | 0.42              |
| 2:D:264:LEU:HB2   | 2:D:280:LEU:HB2   | 2.02                     | 0.42              |
| 2:D:354:PHE:O     | 2:D:434:ALA:HA    | 2.19                     | 0.42              |
| 2:D:440:GLY:O     | 2:D:441:SER:C     | 2.61                     | 0.42              |
| 2:D:819:GLN:CA    | 2:D:819:GLN:NE2   | 2.82                     | 0.42              |
| 2:D:1286:VAL:O    | 2:D:1286:VAL:HG12 | 2.20                     | 0.42              |
| 2:D:1371:TYR:HB2  | 2:D:1377:SER:HB3  | 2.02                     | 0.42              |
| 2:D:1584:TRP:CD1  | 2:D:1584:TRP:C    | 2.97                     | 0.42              |
| 1:A:431:LEU:HD13  | 1:A:431:LEU:C     | 2.45                     | 0.42              |
| 1:A:606:ASP:C     | 1:A:608:ALA:N     | 2.77                     | 0.42              |
| 1:A:831:TYR:O     | 1:A:928:ARG:CB    | 2.67                     | 0.42              |
| 1:A:870:SER:N     | 1:A:871:PRO:HD3   | 2.33                     | 0.42              |
| 1:A:1069:TRP:HH2  | 1:A:1465:ASN:CG   | 2.28                     | 0.42              |
| 1:A:1243:GLY:O    | 1:A:1285:TYR:CZ   | 2.73                     | 0.42              |
| 1:A:1545:ALA:HB2  | 1:A:1660:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:1548:ARG:C    | 1:A:1550:GLN:H    | 2.27                     | 0.42              |
| 1:A:1587:THR:HB   | 1:A:1591:VAL:CG2  | 2.48                     | 0.42              |
| 2:B:370:ASP:OD1   | 2:B:370:ASP:N     | 2.52                     | 0.42              |
| 2:B:382:GLU:CD    | 2:B:382:GLU:H     | 2.24                     | 0.42              |
| 2:B:511:THR:O     | 2:B:512:PRO:C     | 2.62                     | 0.42              |
| 2:B:818:LEU:HD23  | 2:B:911:LYS:CD    | 2.44                     | 0.42              |
| 2:B:838:ASN:OD1   | 2:B:838:ASN:C     | 2.61                     | 0.42              |
| 2:B:963:ILE:O     | 2:B:963:ILE:HG22  | 2.20                     | 0.42              |
| 2:B:1349:VAL:CG2  | 2:B:1363:LEU:HD12 | 2.50                     | 0.42              |
| 2:B:1397:LEU:HD12 | 2:B:1397:LEU:HA   | 1.75                     | 0.42              |
| 1:C:20:GLU:O      | 1:C:20:GLU:CG     | 2.61                     | 0.42              |
| 1:C:565:GLU:HG2   | 1:C:565:GLU:O     | 2.20                     | 0.42              |
| 1:C:578:ASP:O     | 1:C:579:ALA:C     | 2.63                     | 0.42              |
| 1:C:621:GLU:H     | 1:C:621:GLU:HG3   | 1.74                     | 0.42              |
| 1:C:1060:ARG:CG   | 1:C:1061:ASN:N    | 2.83                     | 0.42              |
| 1:C:1091:LYS:H    | 1:C:1091:LYS:HG3  | 1.43                     | 0.42              |
| 1:C:1194:ALA:O    | 1:C:1195:LEU:C    | 2.63                     | 0.42              |
| 1:C:1212:LEU:O    | 1:C:1215:GLU:HB2  | 2.20                     | 0.42              |
| 1:C:1279:ARG:CZ   | 1:C:1280:TYR:CD2  | 3.03                     | 0.42              |
| 1:C:1327:LYS:C    | 1:C:1328:MET:HE2  | 2.45                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1545:ALA:CB   | 1:C:1660:PHE:CE1  | 3.03                     | 0.42              |
| 1:C:1636:ILE:O    | 1:C:1636:ILE:CG2  | 2.68                     | 0.42              |
| 2:D:296:ARG:NH1   | 2:D:296:ARG:CG    | 2.83                     | 0.42              |
| 2:D:435:TYR:OH    | 2:D:617:ASN:HB3   | 2.20                     | 0.42              |
| 2:D:485:ASN:O     | 2:D:486:LYS:HB2   | 2.18                     | 0.42              |
| 2:D:739:PHE:CE1   | 2:D:901:GLN:HB2   | 2.55                     | 0.42              |
| 2:D:830:VAL:HG23  | 2:D:831:GLU:N     | 2.34                     | 0.42              |
| 2:D:857:CYS:HB3   | 2:D:885:VAL:HG22  | 2.01                     | 0.42              |
| 2:D:860:SER:OG    | 2:D:866:TYR:HB3   | 2.20                     | 0.42              |
| 2:D:1294:TYR:O    | 2:D:1294:TYR:HD2  | 2.02                     | 0.42              |
| 2:D:1386:MET:HA   | 2:D:1386:MET:CE   | 2.39                     | 0.42              |
| 2:D:1424:ILE:N    | 2:D:1424:ILE:CD1  | 2.76                     | 0.42              |
| 2:D:1602:THR:H    | 2:D:1605:THR:HB   | 1.85                     | 0.42              |
| 1:A:21:GLN:HB3    | 1:A:44:TYR:O      | 2.20                     | 0.42              |
| 1:A:144:ARG:HD2   | 1:A:146:TYR:CZ    | 2.55                     | 0.42              |
| 1:A:289:ASN:OD1   | 1:A:289:ASN:N     | 2.52                     | 0.42              |
| 1:A:296:ILE:CG2   | 1:A:297:ALA:N     | 2.82                     | 0.42              |
| 1:A:371:ILE:CG2   | 1:A:371:ILE:O     | 2.67                     | 0.42              |
| 1:A:472:ASN:O     | 1:A:473:HIS:CB    | 2.67                     | 0.42              |
| 1:A:575:LEU:O     | 1:A:576:SER:C     | 2.63                     | 0.42              |
| 1:A:578:ASP:C     | 1:A:579:ALA:O     | 2.63                     | 0.42              |
| 1:A:663:GLN:O     | 1:A:664:GLU:HB2   | 2.20                     | 0.42              |
| 1:A:691:LYS:C     | 1:A:693:SER:N     | 2.75                     | 0.42              |
| 1:A:780:VAL:HA    | 1:A:781:PRO:HD3   | 1.85                     | 0.42              |
| 1:A:827:MET:HB3   | 1:A:829:ILE:HD13  | 2.01                     | 0.42              |
| 1:A:1075:SER:O    | 1:A:1076:THR:C    | 2.63                     | 0.42              |
| 1:A:1212:LEU:HD13 | 1:A:1228:TRP:NE1  | 2.35                     | 0.42              |
| 1:A:1229:LYS:HZ1  | 1:A:1240:PRO:HD2  | 1.85                     | 0.42              |
| 2:B:1385:SER:OG   | 2:B:1455:SER:N    | 2.46                     | 0.42              |
| 1:C:96:GLN:HG3    | 1:C:97:ASN:N      | 2.35                     | 0.42              |
| 1:C:654:LEU:HA    | 1:C:654:LEU:HD23  | 1.58                     | 0.42              |
| 1:C:1016:VAL:HG11 | 1:C:1291:ILE:CD1  | 2.50                     | 0.42              |
| 1:C:1057:MET:O    | 1:C:1058:SER:C    | 2.63                     | 0.42              |
| 1:C:1153:ARG:NH2  | 1:C:1168:LEU:HD13 | 2.35                     | 0.42              |
| 2:D:76:ASN:CB     | 2:D:77:PRO:HD2    | 2.44                     | 0.42              |
| 2:D:171:ILE:H     | 2:D:171:ILE:HG13  | 1.59                     | 0.42              |
| 2:D:485:ASN:C     | 2:D:487:GLY:N     | 2.78                     | 0.42              |
| 2:D:603:GLU:C     | 2:D:605:SER:N     | 2.74                     | 0.42              |
| 2:D:1275:LEU:HD13 | 2:D:1321:ALA:HB2  | 2.02                     | 0.42              |
| 1:A:126:LEU:C     | 1:A:127:PHE:HD1   | 2.29                     | 0.41              |
| 1:A:354:LEU:N     | 1:A:354:LEU:CD2   | 2.83                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:606:ASP:HB2   | 1:A:797:TRP:HZ3   | 1.85                     | 0.41              |
| 1:A:773:TRP:CZ3   | 1:A:774:LEU:HB2   | 2.55                     | 0.41              |
| 1:A:871:PRO:O     | 1:A:872:VAL:C     | 2.63                     | 0.41              |
| 1:A:901:LEU:HA    | 1:A:902:PRO:HD3   | 1.78                     | 0.41              |
| 1:A:1061:ASN:HB2  | 1:A:1065:SER:O    | 2.20                     | 0.41              |
| 1:A:1311:MET:HE3  | 1:A:1311:MET:HB2  | 1.66                     | 0.41              |
| 1:A:1641:SER:O    | 1:A:1643:THR:HG23 | 2.20                     | 0.41              |
| 2:B:36:ASP:OD1    | 2:B:90:PRO:HA     | 2.19                     | 0.41              |
| 2:B:138:THR:HG22  | 2:B:139:PRO:O     | 2.20                     | 0.41              |
| 2:B:343:TYR:HE1   | 2:B:420:LEU:HD11  | 1.84                     | 0.41              |
| 2:B:415:THR:OG1   | 2:B:415:THR:O     | 2.35                     | 0.41              |
| 2:B:748:ARG:NH1   | 2:B:784:ILE:HG23  | 2.35                     | 0.41              |
| 2:B:811:MET:HG3   | 2:B:812:LYS:N     | 2.34                     | 0.41              |
| 1:C:135:TYR:CE1   | 1:C:141:VAL:HG13  | 2.51                     | 0.41              |
| 1:C:163:PHE:HE1   | 1:C:188:PHE:HB2   | 1.85                     | 0.41              |
| 1:C:387:PRO:HG2   | 1:C:438:ASP:O     | 2.20                     | 0.41              |
| 1:C:504:LEU:N     | 1:C:504:LEU:HD13  | 2.35                     | 0.41              |
| 1:C:594:THR:OG1   | 1:C:782:ARG:CA    | 2.68                     | 0.41              |
| 1:C:700:TYR:CZ    | 1:C:757:LEU:HD22  | 2.55                     | 0.41              |
| 1:C:829:ILE:HD12  | 1:C:829:ILE:N     | 2.34                     | 0.41              |
| 1:C:1096:ASN:OD1  | 1:C:1096:ASN:C    | 2.62                     | 0.41              |
| 1:C:1133:LEU:HD12 | 1:C:1133:LEU:N    | 2.32                     | 0.41              |
| 1:C:1313:ILE:HD13 | 1:C:1350:THR:HB   | 2.01                     | 0.41              |
| 2:D:265:PHE:O     | 2:D:276:ILE:HG13  | 2.19                     | 0.41              |
| 2:D:581:ASP:CG    | 2:D:785:THR:HG21  | 2.45                     | 0.41              |
| 2:D:756:LEU:CD2   | 2:D:778:PHE:CE1   | 3.03                     | 0.41              |
| 2:D:1301:ARG:HH11 | 2:D:1301:ARG:CB   | 2.32                     | 0.41              |
| 2:D:1380:THR:HG23 | 2:D:1460:SER:HA   | 2.01                     | 0.41              |
| 2:D:1569:CYS:O    | 2:D:1570:GLN:C    | 2.62                     | 0.41              |
| 1:A:518:PHE:HD2   | 1:A:524:GLN:NE2   | 2.17                     | 0.41              |
| 1:A:621:GLU:H     | 1:A:621:GLU:HG3   | 1.73                     | 0.41              |
| 1:A:683:ILE:O     | 1:A:687:ALA:HB3   | 2.20                     | 0.41              |
| 1:A:804:ILE:HG13  | 1:A:804:ILE:O     | 2.21                     | 0.41              |
| 1:A:824:PHE:CD2   | 1:A:824:PHE:N     | 2.82                     | 0.41              |
| 1:A:1003:LEU:HA   | 1:A:1004:PRO:HD2  | 1.64                     | 0.41              |
| 1:A:1060:ARG:CG   | 1:A:1061:ASN:H    | 2.33                     | 0.41              |
| 1:A:1439:LEU:HD23 | 1:A:1439:LEU:HA   | 1.58                     | 0.41              |
| 1:A:1545:ALA:CB   | 1:A:1660:PHE:CE1  | 3.03                     | 0.41              |
| 1:A:1584:ILE:O    | 1:A:1585:TYR:CB   | 2.68                     | 0.41              |
| 1:A:1641:SER:O    | 1:A:1642:LEU:HB2  | 2.20                     | 0.41              |
| 2:B:27:LEU:HD11   | 2:B:29:THR:HG22   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:264:LEU:HB2   | 2:B:280:LEU:HB2   | 2.01                     | 0.41              |
| 2:B:267:VAL:HG13  | 2:B:313:THR:O     | 2.20                     | 0.41              |
| 2:B:478:TYR:CD1   | 2:B:478:TYR:C     | 2.98                     | 0.41              |
| 2:B:1412:GLU:HB2  | 2:B:1419:GLN:HB2  | 2.01                     | 0.41              |
| 2:B:1445:HIS:CG   | 2:B:1446:PHE:H    | 2.37                     | 0.41              |
| 2:B:1498:SER:O    | 2:B:1573:LEU:CD2  | 2.68                     | 0.41              |
| 1:C:32:ARG:O      | 1:C:33:VAL:C      | 2.63                     | 0.41              |
| 1:C:127:PHE:N     | 1:C:127:PHE:CD1   | 2.87                     | 0.41              |
| 1:C:405:ASP:N     | 1:C:405:ASP:OD1   | 2.52                     | 0.41              |
| 1:C:791:PRO:CD    | 1:C:797:TRP:HE1   | 2.32                     | 0.41              |
| 1:C:1320:LYS:CG   | 1:C:1321:GLY:H    | 2.34                     | 0.41              |
| 1:C:1329:THR:OG1  | 1:C:1331:LYS:HG2  | 2.21                     | 0.41              |
| 1:A:700:TYR:CZ    | 1:A:757:LEU:HD22  | 2.55                     | 0.41              |
| 1:A:701:ASP:N     | 1:A:701:ASP:OD1   | 2.51                     | 0.41              |
| 1:A:1158:ILE:HG22 | 1:A:1158:ILE:O    | 2.19                     | 0.41              |
| 1:A:1336:ARG:HA   | 1:A:1337:PRO:HD3  | 1.95                     | 0.41              |
| 1:A:1632:SER:C    | 1:A:1633:PHE:CG   | 2.97                     | 0.41              |
| 2:B:630:THR:O     | 2:B:631:SER:C     | 2.62                     | 0.41              |
| 2:B:1408:ILE:HD11 | 2:B:1425:ILE:CG1  | 2.44                     | 0.41              |
| 1:C:24:VAL:HG11   | 1:C:543:TYR:HE2   | 1.83                     | 0.41              |
| 1:C:423:ASN:OD1   | 2:D:504:VAL:HG22  | 2.19                     | 0.41              |
| 1:C:545:ILE:H     | 1:C:545:ILE:HG12  | 1.65                     | 0.41              |
| 1:C:977:LEU:CD2   | 1:C:1361:VAL:HG13 | 2.50                     | 0.41              |
| 1:C:984:VAL:O     | 1:C:987:ILE:HB    | 2.19                     | 0.41              |
| 1:C:1047:LYS:O    | 1:C:1048:LYS:C    | 2.62                     | 0.41              |
| 1:C:1056:ILE:O    | 1:C:1057:MET:C    | 2.62                     | 0.41              |
| 1:C:1081:PHE:HD1  | 1:C:1147:PHE:HZ   | 1.68                     | 0.41              |
| 1:C:1226:ARG:HD2  | 1:C:1270:VAL:CG2  | 2.51                     | 0.41              |
| 2:D:41:ILE:O      | 2:D:85:PRO:HD2    | 2.20                     | 0.41              |
| 2:D:219:TYR:CD1   | 2:D:220:VAL:N     | 2.86                     | 0.41              |
| 2:D:454:ILE:HD12  | 2:D:538:VAL:HG11  | 2.02                     | 0.41              |
| 2:D:800:ILE:CG2   | 2:D:801:CYS:N     | 2.72                     | 0.41              |
| 2:D:818:LEU:HD23  | 2:D:911:LYS:CD    | 2.47                     | 0.41              |
| 1:A:40:VAL:HA     | 1:A:82:SER:HB3    | 2.02                     | 0.41              |
| 1:A:292:LEU:CD1   | 1:A:292:LEU:C     | 2.93                     | 0.41              |
| 1:A:309:GLU:N     | 1:A:309:GLU:CD    | 2.78                     | 0.41              |
| 1:A:330:ILE:O     | 1:A:330:ILE:HG13  | 2.20                     | 0.41              |
| 1:A:412:ARG:CD    | 2:B:458:ASP:OD1   | 2.66                     | 0.41              |
| 1:A:931:PRO:HG2   | 1:A:1366:HIS:NE2  | 2.36                     | 0.41              |
| 1:A:1019:PHE:CZ   | 1:A:1088:GLN:HB3  | 2.56                     | 0.41              |
| 1:A:1056:ILE:O    | 1:A:1057:MET:C    | 2.61                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1193:TYR:O    | 1:A:1194:ALA:C    | 2.63                     | 0.41              |
| 2:B:148:PHE:CZ    | 2:B:792:VAL:CG1   | 3.04                     | 0.41              |
| 2:B:1275:LEU:HD13 | 2:B:1321:ALA:HB2  | 2.02                     | 0.41              |
| 2:B:1277:ILE:HG22 | 2:B:1290:TYR:HB2  | 2.02                     | 0.41              |
| 2:B:1606:TRP:C    | 2:B:1606:TRP:HD1  | 2.26                     | 0.41              |
| 1:C:404:LEU:HD22  | 1:C:404:LEU:HA    | 1.85                     | 0.41              |
| 1:C:642:ASN:C     | 1:C:642:ASN:ND2   | 2.73                     | 0.41              |
| 1:C:899:THR:C     | 1:C:900:VAL:HG13  | 2.45                     | 0.41              |
| 1:C:915:GLU:HB3   | 2:D:905:TRP:CZ2   | 2.55                     | 0.41              |
| 1:C:1020:TYR:CZ   | 1:C:1295:GLU:HB2  | 2.55                     | 0.41              |
| 1:C:1364:VAL:O    | 1:C:1364:VAL:HG13 | 2.19                     | 0.41              |
| 1:C:1370:THR:O    | 1:C:1371:SER:C    | 2.63                     | 0.41              |
| 1:C:1381:ILE:HD12 | 1:C:1493:PHE:HD2  | 1.85                     | 0.41              |
| 1:C:1587:THR:HB   | 1:C:1591:VAL:CG2  | 2.50                     | 0.41              |
| 2:D:302:ARG:HG3   | 2:D:303:PHE:CE1   | 2.56                     | 0.41              |
| 2:D:339:VAL:HG23  | 2:D:340:ALA:N     | 2.35                     | 0.41              |
| 2:D:438:GLN:HB2   | 2:D:617:ASN:HD21  | 1.84                     | 0.41              |
| 2:D:1610:TRP:CG   | 2:D:1628:PHE:CD2  | 3.07                     | 0.41              |
| 2:D:1614:ASP:O    | 2:D:1615:GLU:C    | 2.64                     | 0.41              |
| 1:A:36:SER:HA     | 1:A:86:THR:HG22   | 2.02                     | 0.41              |
| 1:A:431:LEU:HD22  | 1:A:432:GLU:N     | 2.35                     | 0.41              |
| 1:A:979:VAL:HG21  | 1:A:1326:TYR:CZ   | 2.49                     | 0.41              |
| 1:A:985:GLY:C     | 1:A:987:ILE:N     | 2.79                     | 0.41              |
| 1:A:1525:CYS:N    | 1:A:1528:VAL:HG13 | 2.36                     | 0.41              |
| 1:A:1660:PHE:HE2  | 1:A:1664:LEU:CD1  | 2.28                     | 0.41              |
| 2:B:41:ILE:O      | 2:B:85:PRO:HD2    | 2.20                     | 0.41              |
| 2:B:133:ASP:OD2   | 2:B:134:LYS:HG2   | 2.19                     | 0.41              |
| 2:B:330:VAL:O     | 2:B:330:VAL:HG23  | 2.20                     | 0.41              |
| 2:B:339:VAL:HG23  | 2:B:340:ALA:N     | 2.35                     | 0.41              |
| 2:B:762:LEU:N     | 2:B:762:LEU:CD1   | 2.82                     | 0.41              |
| 2:B:939:GLY:O     | 2:B:1316:SER:HA   | 2.21                     | 0.41              |
| 1:C:24:VAL:HG11   | 1:C:543:TYR:CZ    | 2.56                     | 0.41              |
| 1:C:74:SER:HA     | 1:C:79:PHE:CE1    | 2.56                     | 0.41              |
| 1:C:371:ILE:O     | 1:C:371:ILE:CG2   | 2.66                     | 0.41              |
| 1:C:960:PRO:HB2   | 1:C:961:TYR:H     | 1.62                     | 0.41              |
| 1:C:961:TYR:CE1   | 1:C:963:ILE:HG12  | 2.55                     | 0.41              |
| 1:C:1025:LEU:HA   | 1:C:1025:LEU:HD23 | 1.75                     | 0.41              |
| 1:C:1208:ILE:O    | 1:C:1208:ILE:HG22 | 2.21                     | 0.41              |
| 2:D:384:PHE:O     | 2:D:385:HIS:C     | 2.64                     | 0.41              |
| 2:D:511:THR:OG1   | 2:D:512:PRO:HD2   | 2.20                     | 0.41              |
| 2:D:885:VAL:HA    | 2:D:886:PRO:HD3   | 1.75                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:902:GLU:O     | 2:D:903:ALA:HB2   | 2.20                     | 0.41              |
| 2:D:1349:VAL:CG2  | 2:D:1363:LEU:HD12 | 2.50                     | 0.41              |
| 2:D:1528:LEU:HD12 | 2:D:1541:VAL:O    | 2.20                     | 0.41              |
| 1:A:59:TYR:N      | 1:A:60:PRO:CD     | 2.84                     | 0.41              |
| 1:A:470:THR:CG2   | 2:B:450:THR:HG22  | 2.40                     | 0.41              |
| 1:A:558:SER:HB3   | 1:A:645:VAL:HG13  | 2.03                     | 0.41              |
| 1:A:775:TRP:CD1   | 1:A:775:TRP:O     | 2.74                     | 0.41              |
| 1:A:829:ILE:HG12  | 1:A:925:LYS:CG    | 2.45                     | 0.41              |
| 1:A:1026:GLU:OE1  | 1:A:1031:TRP:NE1  | 2.53                     | 0.41              |
| 1:A:1455:ILE:N    | 1:A:1455:ILE:CD1  | 2.84                     | 0.41              |
| 1:A:1616:GLN:CD   | 1:A:1648:TRP:CZ3  | 2.99                     | 0.41              |
| 1:C:163:PHE:HE1   | 1:C:188:PHE:CB    | 2.33                     | 0.41              |
| 1:C:342:ILE:HA    | 1:C:343:PRO:HD3   | 1.73                     | 0.41              |
| 1:C:361:LEU:N     | 1:C:361:LEU:CD1   | 2.83                     | 0.41              |
| 1:C:382:LEU:HD13  | 1:C:415:ASP:C     | 2.46                     | 0.41              |
| 1:C:618:LYS:O     | 1:C:619:PRO:C     | 2.63                     | 0.41              |
| 1:C:938:SER:OG    | 1:C:1284:PHE:CZ   | 2.74                     | 0.41              |
| 1:C:987:ILE:O     | 1:C:988:LEU:C     | 2.62                     | 0.41              |
| 1:C:1003:LEU:O    | 1:C:1004:PRO:C    | 2.64                     | 0.41              |
| 1:C:1078:LEU:O    | 1:C:1079:THR:C    | 2.63                     | 0.41              |
| 1:C:1180:LEU:HD21 | 1:C:1208:ILE:HG12 | 2.01                     | 0.41              |
| 1:C:1226:ARG:HD2  | 1:C:1270:VAL:HG23 | 2.02                     | 0.41              |
| 1:C:1560:ALA:HA   | 1:C:1620:MET:HA   | 2.03                     | 0.41              |
| 2:D:104:VAL:CG2   | 2:D:105:VAL:H     | 2.30                     | 0.41              |
| 2:D:391:LEU:C     | 2:D:393:ASP:H     | 2.28                     | 0.41              |
| 2:D:466:VAL:CG1   | 2:D:524:TYR:CE2   | 3.04                     | 0.41              |
| 2:D:1277:ILE:HG12 | 2:D:1278:THR:N    | 2.36                     | 0.41              |
| 2:D:1445:HIS:CG   | 2:D:1446:PHE:H    | 2.38                     | 0.41              |
| 2:D:1512:ILE:CG2  | 2:D:1631:PHE:CD1  | 3.03                     | 0.41              |
| 1:A:354:LEU:HD23  | 1:A:354:LEU:H     | 1.85                     | 0.41              |
| 1:A:484:ILE:HG21  | 1:A:528:ILE:HD11  | 2.03                     | 0.41              |
| 1:A:1133:LEU:HD12 | 1:A:1133:LEU:N    | 2.34                     | 0.41              |
| 1:A:1161:LEU:N    | 1:A:1161:LEU:HD22 | 2.35                     | 0.41              |
| 1:A:1162:VAL:HG11 | 1:C:1064:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:1187:THR:O    | 1:A:1188:LEU:C    | 2.62                     | 0.41              |
| 1:A:1212:LEU:CD1  | 1:A:1228:TRP:NE1  | 2.83                     | 0.41              |
| 2:B:382:GLU:C     | 2:B:384:PHE:H     | 2.28                     | 0.41              |
| 2:B:756:LEU:CD2   | 2:B:778:PHE:CE1   | 3.03                     | 0.41              |
| 2:B:857:CYS:O     | 2:B:885:VAL:HG22  | 2.20                     | 0.41              |
| 2:B:923:SER:O     | 2:B:924:ILE:HD12  | 2.20                     | 0.41              |
| 2:B:1277:ILE:HG12 | 2:B:1278:THR:N    | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1444:LYS:CE   | 2:B:1447:GLU:HA   | 2.45                     | 0.41              |
| 2:B:1522:TYR:HB2  | 2:B:1524:TYR:CE1  | 2.55                     | 0.41              |
| 2:B:1581:TYR:HA   | 2:B:1608:GLU:O    | 2.20                     | 0.41              |
| 1:C:78:LYS:HD2    | 1:C:498:HIS:NE2   | 2.35                     | 0.41              |
| 1:C:97:ASN:HA     | 1:C:98:PRO:HD3    | 1.84                     | 0.41              |
| 1:C:608:ALA:O     | 1:C:609:VAL:C     | 2.64                     | 0.41              |
| 1:C:1013:MET:CE   | 1:C:1287:THR:HB   | 2.47                     | 0.41              |
| 1:C:1566:THR:O    | 1:C:1613:LYS:HE3  | 2.20                     | 0.41              |
| 2:D:25:TYR:CZ     | 2:D:113:VAL:HG22  | 2.55                     | 0.41              |
| 2:D:34:ARG:HG2    | 2:D:34:ARG:HH11   | 1.85                     | 0.41              |
| 2:D:56:ILE:HG12   | 2:D:71:THR:O      | 2.20                     | 0.41              |
| 2:D:285:ILE:O     | 2:D:286:ILE:HD13  | 2.20                     | 0.41              |
| 2:D:512:PRO:HA    | 2:D:515:ILE:HD12  | 2.03                     | 0.41              |
| 2:D:593:ILE:O     | 2:D:593:ILE:HG12  | 2.10                     | 0.41              |
| 2:D:594:SER:O     | 2:D:595:GLN:C     | 2.62                     | 0.41              |
| 2:D:621:PHE:N     | 2:D:621:PHE:CD2   | 2.86                     | 0.41              |
| 2:D:815:PHE:C     | 2:D:815:PHE:CD1   | 2.98                     | 0.41              |
| 1:A:91:GLN:OE1    | 1:A:91:GLN:CA     | 2.58                     | 0.41              |
| 1:A:186:PRO:O     | 1:A:187:ASP:C     | 2.62                     | 0.41              |
| 1:A:571:LEU:HD22  | 1:A:803:GLY:HA3   | 2.03                     | 0.41              |
| 1:A:690:TYR:O     | 1:A:690:TYR:CG    | 2.73                     | 0.41              |
| 1:A:888:VAL:HG13  | 1:A:888:VAL:O     | 2.20                     | 0.41              |
| 1:A:917:TRP:O     | 2:B:813:VAL:CG2   | 2.69                     | 0.41              |
| 1:A:1313:ILE:HD13 | 1:A:1313:ILE:HA   | 1.67                     | 0.41              |
| 1:A:1346:LEU:HA   | 1:A:1346:LEU:HD12 | 1.46                     | 0.41              |
| 1:A:1428:LEU:HD11 | 1:A:1434:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:1527:CYS:O    | 1:A:1528:VAL:C    | 2.62                     | 0.41              |
| 1:A:1537:GLU:O    | 1:A:1539:LEU:N    | 2.54                     | 0.41              |
| 1:A:1574:PHE:HA   | 1:A:1603:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:1667:PHE:CD2  | 1:A:1667:PHE:N    | 2.88                     | 0.41              |
| 2:B:143:VAL:HG23  | 2:B:188:LEU:HD11  | 2.01                     | 0.41              |
| 2:B:306:LEU:HD12  | 2:B:306:LEU:HA    | 1.83                     | 0.41              |
| 2:B:358:MET:HE2   | 2:B:467:LYS:HD2   | 2.02                     | 0.41              |
| 2:B:386:SER:O     | 2:B:398:LEU:HD11  | 2.21                     | 0.41              |
| 2:B:557:GLN:OE1   | 2:B:557:GLN:HA    | 2.19                     | 0.41              |
| 2:B:783:SER:HB2   | 2:B:787:TRP:CZ2   | 2.55                     | 0.41              |
| 2:B:819:GLN:NE2   | 2:B:819:GLN:CA    | 2.84                     | 0.41              |
| 2:B:891:LEU:HB2   | 2:B:912:LYS:CE    | 2.51                     | 0.41              |
| 2:B:952:ASP:O     | 2:B:1331:ALA:CA   | 2.68                     | 0.41              |
| 2:B:952:ASP:O     | 2:B:1331:ALA:HB1  | 2.21                     | 0.41              |
| 2:B:1481:LEU:C    | 2:B:1481:LEU:HD13 | 2.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1623:LYS:HA   | 2:B:1623:LYS:HD2  | 1.66                     | 0.41              |
| 1:C:42:GLN:OE1    | 1:C:500:ASN:ND2   | 2.53                     | 0.41              |
| 1:C:552:ALA:HB3   | 1:C:658:ASN:CG    | 2.45                     | 0.41              |
| 1:C:1013:MET:HA   | 1:C:1016:VAL:HG23 | 2.02                     | 0.41              |
| 1:C:1022:PHE:O    | 1:C:1025:LEU:N    | 2.54                     | 0.41              |
| 1:C:1046:LYS:O    | 1:C:1047:LYS:C    | 2.62                     | 0.41              |
| 1:C:1108:VAL:HG21 | 1:C:1167:ALA:HB2  | 2.02                     | 0.41              |
| 1:C:1133:LEU:H    | 1:C:1133:LEU:CD1  | 2.31                     | 0.41              |
| 1:C:1232:LEU:HD12 | 1:C:1233:GLN:H    | 1.86                     | 0.41              |
| 2:D:229:GLN:HA    | 2:D:229:GLN:OE1   | 2.20                     | 0.41              |
| 2:D:247:ILE:HD11  | 2:D:318:VAL:CG2   | 2.48                     | 0.41              |
| 2:D:285:ILE:C     | 2:D:286:ILE:HD13  | 2.45                     | 0.41              |
| 2:D:839:TYR:HD1   | 2:D:839:TYR:HA    | 1.65                     | 0.41              |
| 2:D:952:ASP:O     | 2:D:1331:ALA:CA   | 2.69                     | 0.41              |
| 2:D:1393:ASP:CB   | 2:D:1443:LEU:HD11 | 2.44                     | 0.41              |
| 2:D:1418:ALA:C    | 2:D:1419:GLN:HE21 | 2.29                     | 0.41              |
| 2:D:1473:HIS:O    | 2:D:1474:PRO:C    | 2.63                     | 0.41              |
| 1:A:31:PHE:O      | 1:A:119:ILE:HA    | 2.21                     | 0.41              |
| 1:A:101:TYR:O     | 1:A:102:VAL:HG23  | 2.21                     | 0.41              |
| 1:A:176:GLU:HB2   | 1:A:185:PHE:CE1   | 2.56                     | 0.41              |
| 1:A:382:LEU:HD23  | 1:A:382:LEU:HA    | 1.87                     | 0.41              |
| 1:A:476:LEU:HD23  | 1:A:476:LEU:HA    | 1.78                     | 0.41              |
| 1:A:539:ARG:HH21  | 1:A:634:CYS:H     | 1.59                     | 0.41              |
| 1:A:541:LEU:HB2   | 1:A:557:ASP:O     | 2.20                     | 0.41              |
| 1:A:599:TRP:HE1   | 1:A:779:LEU:CB    | 2.34                     | 0.41              |
| 1:A:695:VAL:HG13  | 1:A:724:CYS:HA    | 2.02                     | 0.41              |
| 1:A:874:ASP:C     | 1:A:875:HIS:CG    | 2.99                     | 0.41              |
| 1:A:965:LEU:C     | 1:A:965:LEU:HD12  | 2.46                     | 0.41              |
| 1:A:1108:VAL:HG12 | 1:A:1108:VAL:H    | 1.60                     | 0.41              |
| 1:A:1209:VAL:O    | 1:A:1210:SER:C    | 2.63                     | 0.41              |
| 1:A:1213:LYS:HE2  | 1:A:1266:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:1268:ASN:C    | 1:A:1270:VAL:N    | 2.77                     | 0.41              |
| 1:A:1271:ILE:HG21 | 1:A:1300:TYR:CD1  | 2.55                     | 0.41              |
| 1:A:1279:ARG:CZ   | 1:A:1280:TYR:CD2  | 3.04                     | 0.41              |
| 1:A:1280:TYR:O    | 1:A:1280:TYR:CG   | 2.74                     | 0.41              |
| 1:A:1320:LYS:CG   | 1:A:1321:GLY:H    | 2.34                     | 0.41              |
| 1:A:1541:LEU:HD21 | 1:A:1543:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:1582:LEU:C    | 1:A:1594:LYS:NZ   | 2.79                     | 0.41              |
| 2:B:74:ASP:OD1    | 2:B:74:ASP:N      | 2.54                     | 0.41              |
| 2:B:78:ALA:C      | 2:B:80:GLY:N      | 2.78                     | 0.41              |
| 2:B:132:THR:O     | 2:B:133:ASP:C     | 2.63                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:144:LEU:HD23  | 2:B:144:LEU:N     | 2.34                     | 0.41              |
| 2:B:175:SER:C     | 2:B:176:ASN:CG    | 2.89                     | 0.41              |
| 2:B:514:LEU:HG    | 2:B:514:LEU:H     | 1.73                     | 0.41              |
| 2:B:518:PHE:HE2   | 2:B:538:VAL:CG2   | 2.33                     | 0.41              |
| 2:B:739:PHE:CE1   | 2:B:901:GLN:HB2   | 2.56                     | 0.41              |
| 2:B:866:TYR:OH    | 2:B:1388:THR:CG2  | 2.69                     | 0.41              |
| 2:B:1380:THR:HG23 | 2:B:1460:SER:HA   | 2.02                     | 0.41              |
| 2:B:1418:ALA:C    | 2:B:1419:GLN:HE21 | 2.29                     | 0.41              |
| 2:B:1553:ASP:C    | 2:B:1555:ASN:N    | 2.78                     | 0.41              |
| 2:B:1610:TRP:CG   | 2:B:1628:PHE:CD2  | 3.08                     | 0.41              |
| 2:B:1614:ASP:O    | 2:B:1615:GLU:C    | 2.64                     | 0.41              |
| 1:C:20:GLU:CB     | 1:C:551:THR:HG22  | 2.51                     | 0.41              |
| 1:C:443:PRO:O     | 1:C:444:GLU:C     | 2.64                     | 0.41              |
| 1:C:501:TYR:O     | 1:C:501:TYR:CD1   | 2.73                     | 0.41              |
| 1:C:515:ARG:HG3   | 1:C:526:ILE:HG23  | 2.03                     | 0.41              |
| 1:C:599:TRP:HE1   | 1:C:779:LEU:HB2   | 1.86                     | 0.41              |
| 1:C:625:GLN:O     | 1:C:626:PHE:C     | 2.64                     | 0.41              |
| 1:C:663:GLN:O     | 1:C:664:GLU:HB2   | 2.21                     | 0.41              |
| 1:C:811:VAL:O     | 1:C:811:VAL:CG1   | 2.64                     | 0.41              |
| 1:C:1265:ASN:C    | 1:C:1267:VAL:N    | 2.76                     | 0.41              |
| 2:D:36:ASP:O      | 2:D:154:THR:HG22  | 2.20                     | 0.41              |
| 2:D:148:PHE:HB2   | 2:D:800:ILE:HD11  | 2.02                     | 0.41              |
| 2:D:226:VAL:HG21  | 2:D:320:VAL:CG1   | 2.51                     | 0.41              |
| 2:D:238:ASP:OD1   | 2:D:238:ASP:O     | 2.39                     | 0.41              |
| 2:D:350:THR:O     | 2:D:350:THR:CG2   | 2.69                     | 0.41              |
| 2:D:355:LYS:HA    | 2:D:356:PRO:HD3   | 1.91                     | 0.41              |
| 2:D:407:GLN:HA    | 2:D:407:GLN:HE21  | 1.84                     | 0.41              |
| 2:D:557:GLN:NE2   | 2:D:563:MET:HE3   | 2.36                     | 0.41              |
| 2:D:750:ASP:OD1   | 2:D:750:ASP:C     | 2.64                     | 0.41              |
| 2:D:829:GLN:HE21  | 2:D:829:GLN:C     | 2.28                     | 0.41              |
| 2:D:954:VAL:HG12  | 2:D:955:PRO:HD2   | 2.03                     | 0.41              |
| 2:D:1391:LEU:CG   | 2:D:1417:MET:HE2  | 2.50                     | 0.41              |
| 2:D:1632:SER:O    | 2:D:1636:THR:CB   | 2.68                     | 0.41              |
| 1:A:311:SER:C     | 1:A:313:TYR:H     | 2.29                     | 0.41              |
| 1:A:392:ALA:HB1   | 1:A:432:GLU:O     | 2.21                     | 0.41              |
| 1:A:510:ILE:HD12  | 1:A:533:ASN:HB2   | 2.02                     | 0.41              |
| 1:A:543:TYR:HD1   | 1:A:543:TYR:H     | 1.68                     | 0.41              |
| 1:A:567:CYS:HB3   | 1:A:570:GLN:HB3   | 2.03                     | 0.41              |
| 1:A:1013:MET:HA   | 1:A:1016:VAL:CG2  | 2.51                     | 0.41              |
| 1:A:1159:CYS:O    | 1:A:1164:ILE:HD11 | 2.21                     | 0.41              |
| 1:A:1379:LEU:HD12 | 1:A:1505:CYS:SG   | 2.61                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1426:ILE:O    | 1:A:1426:ILE:HG22 | 2.20                     | 0.41              |
| 1:A:1535:MET:HE2  | 1:A:1645:ILE:HG21 | 2.02                     | 0.41              |
| 1:A:1658:GLN:N    | 1:A:1658:GLN:HE21 | 2.17                     | 0.41              |
| 2:B:76:ASN:CB     | 2:B:77:PRO:HD2    | 2.44                     | 0.41              |
| 2:B:217:ARG:HG2   | 2:B:218:LYS:N     | 2.33                     | 0.41              |
| 2:B:243:PHE:CE1   | 2:B:336:ILE:HG21  | 2.56                     | 0.41              |
| 2:B:529:ASN:OD1   | 2:B:529:ASN:C     | 2.64                     | 0.41              |
| 2:B:943:GLU:HB2   | 2:B:1313:VAL:HG23 | 2.03                     | 0.41              |
| 2:B:1501:ASN:H    | 2:B:1501:ASN:ND2  | 2.16                     | 0.41              |
| 2:B:1575:LEU:N    | 2:B:1575:LEU:CD2  | 2.84                     | 0.41              |
| 2:B:1584:TRP:CD1  | 2:B:1584:TRP:C    | 2.99                     | 0.41              |
| 2:B:1614:ASP:C    | 2:B:1616:CYS:N    | 2.79                     | 0.41              |
| 1:C:38:ASN:ND2    | 1:C:509:ILE:O     | 2.51                     | 0.41              |
| 1:C:367:ILE:HD13  | 1:C:466:TYR:HD2   | 1.83                     | 0.41              |
| 1:C:544:TYR:C     | 1:C:544:TYR:CD2   | 2.99                     | 0.41              |
| 1:C:970:LYS:O     | 1:C:971:THR:HG22  | 2.21                     | 0.41              |
| 1:C:1570:VAL:HG22 | 1:C:1575:VAL:HA   | 2.02                     | 0.41              |
| 2:D:147:VAL:O     | 2:D:147:VAL:CG1   | 2.68                     | 0.41              |
| 2:D:295:LYS:HD2   | 2:D:295:LYS:HA    | 1.87                     | 0.41              |
| 2:D:599:TRP:O     | 2:D:600:ASP:C     | 2.63                     | 0.41              |
| 2:D:764:GLU:O     | 2:D:765:GLU:C     | 2.64                     | 0.41              |
| 2:D:860:SER:OG    | 2:D:866:TYR:CB    | 2.69                     | 0.41              |
| 2:D:885:VAL:HG23  | 2:D:887:LEU:CD2   | 2.49                     | 0.41              |
| 2:D:1519:ASN:O    | 2:D:1520:VAL:CG2  | 2.69                     | 0.41              |
| 1:A:40:VAL:CG2    | 1:A:41:ILE:N      | 2.84                     | 0.40              |
| 1:A:60:PRO:HD2    | 1:A:61:ASP:N      | 2.17                     | 0.40              |
| 1:A:99:VAL:HG13   | 1:A:119:ILE:HD11  | 2.03                     | 0.40              |
| 1:A:463:SER:CB    | 1:A:491:PRO:HA    | 2.51                     | 0.40              |
| 1:A:862:VAL:CG1   | 1:A:907:LEU:HD21  | 2.50                     | 0.40              |
| 1:A:949:ILE:O     | 1:A:949:ILE:CG2   | 2.69                     | 0.40              |
| 1:A:987:ILE:HG22  | 1:A:988:LEU:N     | 2.34                     | 0.40              |
| 1:A:1020:TYR:CZ   | 1:A:1295:GLU:HB2  | 2.55                     | 0.40              |
| 1:A:1226:ARG:HD2  | 1:A:1270:VAL:HG23 | 2.03                     | 0.40              |
| 1:A:1568:ILE:CG2  | 1:A:1577:TYR:HE1  | 2.30                     | 0.40              |
| 1:A:1625:LEU:O    | 1:A:1627:ILE:HG23 | 2.20                     | 0.40              |
| 2:B:146:ARG:HA    | 2:B:183:PHE:CE2   | 2.56                     | 0.40              |
| 2:B:384:PHE:O     | 2:B:385:HIS:C     | 2.64                     | 0.40              |
| 2:B:402:ILE:HD13  | 2:B:402:ILE:N     | 2.36                     | 0.40              |
| 2:B:1371:TYR:HB2  | 2:B:1377:SER:HB3  | 2.03                     | 0.40              |
| 1:C:36:SER:HA     | 1:C:86:THR:HG22   | 2.03                     | 0.40              |
| 1:C:163:PHE:CE2   | 1:C:201:ILE:HG12  | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:331:GLU:CD    | 1:C:333:THR:HG23  | 2.46                     | 0.40              |
| 1:C:459:SER:C     | 1:C:461:SER:N     | 2.79                     | 0.40              |
| 1:C:518:PHE:HD2   | 1:C:524:GLN:NE2   | 2.19                     | 0.40              |
| 1:C:651:LEU:HA    | 1:C:651:LEU:HD23  | 1.76                     | 0.40              |
| 1:C:758:LEU:CB    | 1:C:759:PRO:HD2   | 2.50                     | 0.40              |
| 1:C:832:SER:HA    | 1:C:928:ARG:HB3   | 2.03                     | 0.40              |
| 1:C:1202:HIS:CG   | 1:C:1203:PRO:HD2  | 2.56                     | 0.40              |
| 1:C:1245:ALA:HB2  | 1:C:1285:TYR:HB3  | 2.02                     | 0.40              |
| 1:C:1406:ALA:O    | 1:C:1472:PHE:HA   | 2.21                     | 0.40              |
| 1:C:1541:LEU:HD21 | 1:C:1543:ILE:HD12 | 2.03                     | 0.40              |
| 2:D:148:PHE:CZ    | 2:D:792:VAL:HG11  | 2.55                     | 0.40              |
| 2:D:386:SER:O     | 2:D:398:LEU:HD11  | 2.21                     | 0.40              |
| 2:D:466:VAL:HG12  | 2:D:524:TYR:HE2   | 1.86                     | 0.40              |
| 2:D:602:ILE:O     | 2:D:603:GLU:C     | 2.64                     | 0.40              |
| 2:D:857:CYS:O     | 2:D:885:VAL:HG22  | 2.21                     | 0.40              |
| 2:D:1369:THR:OG1  | 2:D:1370:ARG:N    | 2.54                     | 0.40              |
| 2:D:1459:TYR:HB3  | 2:D:1466:GLU:HB3  | 2.03                     | 0.40              |
| 1:A:256:TYR:HE2   | 1:A:826:GLU:CD    | 2.29                     | 0.40              |
| 1:A:327:VAL:HG12  | 1:A:328:THR:N     | 2.36                     | 0.40              |
| 1:A:330:ILE:HG22  | 1:A:337:SER:CB    | 2.38                     | 0.40              |
| 1:A:354:LEU:CD2   | 1:A:450:GLU:HG3   | 2.51                     | 0.40              |
| 1:A:404:LEU:HD22  | 1:A:404:LEU:HA    | 1.85                     | 0.40              |
| 1:A:577:PRO:CD    | 1:A:588:VAL:HG23  | 2.51                     | 0.40              |
| 1:A:700:TYR:HD1   | 1:A:758:LEU:HD12  | 1.86                     | 0.40              |
| 1:A:800:GLN:HE21  | 1:A:800:GLN:HB2   | 1.69                     | 0.40              |
| 1:A:885:ARG:HD3   | 1:A:885:ARG:HA    | 1.88                     | 0.40              |
| 1:A:931:PRO:C     | 1:A:932:GLU:OE1   | 2.65                     | 0.40              |
| 1:A:934:VAL:HG13  | 1:A:935:LYS:N     | 2.36                     | 0.40              |
| 1:A:1127:ILE:HD12 | 1:A:1127:ILE:N    | 2.15                     | 0.40              |
| 1:A:1161:LEU:HA   | 1:A:1161:LEU:HD13 | 1.85                     | 0.40              |
| 1:A:1168:LEU:HD22 | 1:A:1168:LEU:HA   | 1.77                     | 0.40              |
| 1:A:1217:LEU:HD12 | 1:A:1227:PHE:HE1  | 1.86                     | 0.40              |
| 1:A:1580:THR:HG23 | 1:A:1597:GLU:OE2  | 2.21                     | 0.40              |
| 2:B:354:PHE:CE2   | 2:B:409:LEU:HB2   | 2.57                     | 0.40              |
| 2:B:391:LEU:C     | 2:B:393:ASP:H     | 2.29                     | 0.40              |
| 2:B:424:ARG:O     | 2:B:425:GLN:C     | 2.64                     | 0.40              |
| 2:B:750:ASP:OD1   | 2:B:750:ASP:C     | 2.64                     | 0.40              |
| 1:C:196:TYR:CE1   | 1:C:221:GLU:CB    | 3.03                     | 0.40              |
| 1:C:459:SER:OG    | 1:C:461:SER:HB3   | 2.22                     | 0.40              |
| 1:C:577:PRO:HD2   | 1:C:588:VAL:HG23  | 2.02                     | 0.40              |
| 1:C:773:TRP:CZ3   | 1:C:774:LEU:HB2   | 2.54                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:871:PRO:O     | 1:C:872:VAL:C     | 2.64                     | 0.40              |
| 1:C:953:ILE:HD12  | 1:C:955:ARG:HH21  | 1.87                     | 0.40              |
| 1:C:1075:SER:O    | 1:C:1076:THR:C    | 2.64                     | 0.40              |
| 1:C:1226:ARG:NE   | 1:C:1266:TYR:CE1  | 2.89                     | 0.40              |
| 1:C:1226:ARG:HD3  | 1:C:1266:TYR:CE1  | 2.56                     | 0.40              |
| 1:C:1285:TYR:O    | 1:C:1286:SER:O    | 2.39                     | 0.40              |
| 1:C:1328:MET:HE2  | 1:C:1328:MET:CA   | 2.51                     | 0.40              |
| 1:C:1499:HIS:C    | 1:C:1500:ARG:CG   | 2.93                     | 0.40              |
| 1:C:1562:LYS:HB2  | 1:C:1583:ASP:O    | 2.21                     | 0.40              |
| 2:D:41:ILE:HG23   | 2:D:87:ILE:HD11   | 2.04                     | 0.40              |
| 2:D:167:THR:HG23  | 2:D:171:ILE:N     | 2.37                     | 0.40              |
| 2:D:484:LEU:HD11  | 2:D:626:LEU:CD1   | 2.51                     | 0.40              |
| 2:D:511:THR:O     | 2:D:513:ASP:N     | 2.54                     | 0.40              |
| 2:D:1446:PHE:C    | 2:D:1448:VAL:H    | 2.29                     | 0.40              |
| 2:D:1635:LEU:HA   | 2:D:1635:LEU:HD23 | 1.83                     | 0.40              |
| 1:A:49:ALA:HB2    | 1:A:74:SER:HB2    | 2.03                     | 0.40              |
| 1:A:113:LYS:CG    | 1:A:114:SER:N     | 2.69                     | 0.40              |
| 1:A:115:LYS:HE3   | 1:A:654:LEU:HD11  | 2.02                     | 0.40              |
| 1:A:419:SER:C     | 1:A:420:PHE:CD2   | 3.00                     | 0.40              |
| 1:A:575:LEU:HD23  | 1:A:590:LEU:HD13  | 2.04                     | 0.40              |
| 1:A:942:VAL:HG11  | 1:A:957:LYS:HG2   | 2.03                     | 0.40              |
| 1:A:942:VAL:CG2   | 1:A:1359:VAL:HB   | 2.52                     | 0.40              |
| 1:A:961:TYR:CE1   | 1:A:963:ILE:HG12  | 2.56                     | 0.40              |
| 1:A:987:ILE:O     | 1:A:988:LEU:C     | 2.64                     | 0.40              |
| 1:A:1078:LEU:O    | 1:A:1079:THR:C    | 2.62                     | 0.40              |
| 1:A:1083:LEU:CD2  | 1:A:1104:LEU:CD2  | 2.99                     | 0.40              |
| 1:A:1091:LYS:NZ   | 1:A:1091:LYS:HB2  | 2.37                     | 0.40              |
| 1:A:1127:ILE:HG13 | 1:A:1143:TYR:CE2  | 2.45                     | 0.40              |
| 1:A:1467:ILE:HA   | 1:A:1468:PRO:HD3  | 1.78                     | 0.40              |
| 1:A:1622:LYS:NZ   | 1:A:1642:LEU:HB3  | 2.23                     | 0.40              |
| 2:B:89:ILE:CD1    | 2:B:121:LEU:HD11  | 2.52                     | 0.40              |
| 2:B:285:ILE:C     | 2:B:286:ILE:HD13  | 2.45                     | 0.40              |
| 2:B:495:GLN:OE1   | 2:B:506:MET:HB2   | 2.22                     | 0.40              |
| 2:B:580:VAL:CG1   | 2:B:581:ASP:N     | 2.84                     | 0.40              |
| 2:B:736:GLU:CD    | 2:B:737:ASP:H     | 2.29                     | 0.40              |
| 2:B:825:VAL:HA    | 2:B:916:VAL:O     | 2.22                     | 0.40              |
| 2:B:1619:GLU:HA   | 2:B:1622:GLN:NE2  | 2.36                     | 0.40              |
| 1:C:29:LYS:HB3    | 1:C:29:LYS:HE3    | 1.88                     | 0.40              |
| 1:C:141:VAL:HG23  | 1:C:188:PHE:O     | 2.21                     | 0.40              |
| 1:C:354:LEU:HD23  | 1:C:354:LEU:H     | 1.86                     | 0.40              |
| 1:C:1054:LEU:O    | 1:C:1057:MET:HB2  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1432:ILE:HD13 | 1:C:1432:ILE:N    | 2.35                     | 0.40              |
| 1:C:1560:ALA:O    | 1:C:1561:TYR:CB   | 2.69                     | 0.40              |
| 1:C:1568:ILE:HD11 | 1:C:1613:LYS:HB2  | 2.03                     | 0.40              |
| 1:C:1573:VAL:HG12 | 1:C:1603:LYS:CB   | 2.50                     | 0.40              |
| 1:C:1578:LYS:HA   | 1:C:1578:LYS:HD3  | 1.87                     | 0.40              |
| 1:C:1622:LYS:HB2  | 1:C:1643:THR:HG22 | 2.02                     | 0.40              |
| 2:D:27:LEU:HD11   | 2:D:29:THR:HG22   | 2.03                     | 0.40              |
| 2:D:341:SER:HA    | 2:D:342:PRO:HD3   | 1.82                     | 0.40              |
| 2:D:364:VAL:O     | 2:D:395:THR:HA    | 2.21                     | 0.40              |
| 2:D:536:VAL:HG22  | 2:D:537:TRP:N     | 2.37                     | 0.40              |
| 2:D:736:GLU:CD    | 2:D:737:ASP:H     | 2.29                     | 0.40              |
| 2:D:742:ASP:OD1   | 2:D:743:SER:N     | 2.55                     | 0.40              |
| 2:D:1273:LEU:HD13 | 2:D:1275:LEU:HG   | 2.04                     | 0.40              |
| 1:A:215:ALA:C     | 1:A:216:TYR:HD2   | 2.30                     | 0.40              |
| 1:A:238:ILE:HG12  | 1:A:246:PHE:HE1   | 1.84                     | 0.40              |
| 1:A:336:PHE:HB3   | 1:A:337:SER:H     | 1.76                     | 0.40              |
| 1:A:500:ASN:CB    | 1:A:543:TYR:CD1   | 2.94                     | 0.40              |
| 1:A:625:GLN:O     | 1:A:626:PHE:C     | 2.63                     | 0.40              |
| 1:A:1263:ASP:O    | 1:A:1264:ILE:C    | 2.64                     | 0.40              |
| 1:A:1305:LYS:CB   | 1:C:116:ARG:HH21  | 2.35                     | 0.40              |
| 1:A:1570:VAL:C    | 1:A:1571:GLU:HG3  | 2.45                     | 0.40              |
| 2:B:41:ILE:HG23   | 2:B:87:ILE:HD11   | 2.04                     | 0.40              |
| 2:B:75:MET:HG2    | 2:B:81:MET:HE1    | 2.02                     | 0.40              |
| 2:B:151:ASP:HB2   | 2:B:794:PHE:CZ    | 2.56                     | 0.40              |
| 2:B:202:LYS:CG    | 2:B:203:TYR:N     | 2.84                     | 0.40              |
| 2:B:296:ARG:NH1   | 2:B:296:ARG:CG    | 2.85                     | 0.40              |
| 2:B:302:ARG:HG3   | 2:B:303:PHE:CE1   | 2.56                     | 0.40              |
| 2:B:511:THR:H     | 2:B:514:LEU:HD11  | 1.87                     | 0.40              |
| 2:B:574:ARG:HH21  | 2:B:759:THR:HG21  | 1.87                     | 0.40              |
| 2:B:884:ILE:HG21  | 2:B:884:ILE:HD13  | 1.84                     | 0.40              |
| 2:B:1327:THR:CG2  | 2:B:1328:PHE:N    | 2.84                     | 0.40              |
| 1:C:308:LYS:HA    | 1:C:313:TYR:O     | 2.21                     | 0.40              |
| 1:C:350:SER:OG    | 1:C:352:TYR:O     | 2.40                     | 0.40              |
| 1:C:398:ASN:O     | 1:C:399:GLN:CB    | 2.69                     | 0.40              |
| 1:C:689:LYS:O     | 1:C:691:LYS:N     | 2.52                     | 0.40              |
| 1:C:775:TRP:CD1   | 1:C:775:TRP:O     | 2.75                     | 0.40              |
| 1:C:1016:VAL:N    | 1:C:1017:PRO:HD2  | 2.33                     | 0.40              |
| 1:C:1244:THR:O    | 1:C:1248:VAL:HG23 | 2.22                     | 0.40              |
| 1:C:1267:VAL:O    | 1:C:1270:VAL:HB   | 2.20                     | 0.40              |
| 1:C:1296:GLY:O    | 1:C:1297:LEU:C    | 2.64                     | 0.40              |
| 1:C:1304:VAL:HG12 | 1:C:1305:LYS:H    | 1.83                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1347:ILE:O    | 1:C:1347:ILE:HG22 | 2.20                     | 0.40              |
| 1:C:1616:GLN:HB2  | 1:C:1648:TRP:O    | 2.21                     | 0.40              |
| 2:D:42:LEU:HD22   | 2:D:492:VAL:HG21  | 2.04                     | 0.40              |
| 2:D:151:ASP:HB2   | 2:D:794:PHE:CZ    | 2.57                     | 0.40              |
| 2:D:343:TYR:HE1   | 2:D:420:LEU:HD11  | 1.85                     | 0.40              |
| 2:D:763:THR:C     | 2:D:764:GLU:HG2   | 2.47                     | 0.40              |
| 2:D:824:VAL:CG1   | 2:D:913:LEU:HD21  | 2.51                     | 0.40              |
| 2:D:895:GLU:HA    | 2:D:909:VAL:O     | 2.21                     | 0.40              |
| 2:D:965:ILE:HD12  | 2:D:1277:ILE:HD13 | 2.03                     | 0.40              |
| 2:D:1391:LEU:HD12 | 2:D:1417:MET:CE   | 2.52                     | 0.40              |
| 2:D:1506:ILE:CD1  | 2:D:1628:PHE:CE1  | 3.05                     | 0.40              |
| 1:A:40:VAL:HB     | 1:A:82:SER:HB3    | 2.02                     | 0.40              |
| 1:A:449:ARG:O     | 1:A:450:GLU:HG2   | 2.21                     | 0.40              |
| 1:A:545:ILE:H     | 1:A:545:ILE:HG12  | 1.63                     | 0.40              |
| 1:A:578:ASP:O     | 1:A:579:ALA:C     | 2.61                     | 0.40              |
| 1:A:1003:LEU:HD12 | 1:A:1498:TYR:CE2  | 2.56                     | 0.40              |
| 1:A:1151:GLY:O    | 1:A:1154:LYS:N    | 2.52                     | 0.40              |
| 1:A:1274:LEU:HA   | 1:A:1274:LEU:HD23 | 1.84                     | 0.40              |
| 1:A:1324:HIS:CG   | 1:A:1336:ARG:NH2  | 2.89                     | 0.40              |
| 1:A:1381:ILE:HB   | 1:A:1493:PHE:CD2  | 2.57                     | 0.40              |
| 1:A:1560:ALA:HA   | 1:A:1620:MET:HA   | 2.04                     | 0.40              |
| 2:B:60:ASP:N      | 2:B:68:LEU:HD21   | 2.37                     | 0.40              |
| 2:B:295:LYS:HD2   | 2:B:295:LYS:HA    | 1.89                     | 0.40              |
| 2:B:358:MET:HB2   | 2:B:358:MET:HE3   | 1.73                     | 0.40              |
| 2:B:376:HIS:HA    | 2:B:389:THR:HG22  | 2.04                     | 0.40              |
| 2:B:524:TYR:C     | 2:B:524:TYR:CD1   | 3.00                     | 0.40              |
| 2:B:902:GLU:O     | 2:B:902:GLU:HG3   | 2.22                     | 0.40              |
| 2:B:1459:TYR:HB3  | 2:B:1466:GLU:HB3  | 2.03                     | 0.40              |
| 2:B:1498:SER:O    | 2:B:1573:LEU:HD21 | 2.22                     | 0.40              |
| 1:C:23:TYR:CE1    | 1:C:655:THR:CB    | 3.05                     | 0.40              |
| 1:C:61:ASP:O      | 1:C:62:LYS:HB2    | 2.22                     | 0.40              |
| 1:C:436:LYS:HA    | 1:C:448:ALA:O     | 2.22                     | 0.40              |
| 1:C:495:LYS:HA    | 1:C:495:LYS:HD3   | 1.57                     | 0.40              |
| 1:C:1226:ARG:NH1  | 1:C:1266:TYR:CE1  | 2.86                     | 0.40              |
| 1:C:1386:ILE:HG22 | 1:C:1399:TYR:HB2  | 2.03                     | 0.40              |
| 1:C:1612:VAL:HB   | 1:C:1615:ARG:CB   | 2.51                     | 0.40              |
| 1:C:1646:GLU:OE2  | 1:C:1660:PHE:HZ   | 2.04                     | 0.40              |
| 2:D:405:ASN:OD1   | 2:D:405:ASN:N     | 2.54                     | 0.40              |
| 2:D:1598:SER:C    | 2:D:1599:TYR:HD1  | 2.30                     | 0.40              |
| 2:D:1623:LYS:N    | 2:D:1623:LYS:HD2  | 2.36                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 1617/1676 (96%) | 1173 (72%) | 292 (18%) | 152 (9%) | 0           | 8  |
| 1   | C     | 1617/1676 (96%) | 1179 (73%) | 288 (18%) | 150 (9%) | 0           | 8  |
| 2   | B     | 1215/1642 (74%) | 998 (82%)  | 161 (13%) | 56 (5%)  | 2           | 17 |
| 2   | D     | 1215/1642 (74%) | 995 (82%)  | 162 (13%) | 58 (5%)  | 2           | 16 |
| All | All   | 5664/6636 (85%) | 4345 (77%) | 903 (16%) | 416 (7%) | 1           | 11 |

All (416) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 48  | GLU  |
| 1   | A     | 60  | PRO  |
| 1   | A     | 89  | PRO  |
| 1   | A     | 96  | GLN  |
| 1   | A     | 97  | ASN  |
| 1   | A     | 154 | PRO  |
| 1   | A     | 155 | ALA  |
| 1   | A     | 181 | GLY  |
| 1   | A     | 208 | ASP  |
| 1   | A     | 255 | PHE  |
| 1   | A     | 285 | THR  |
| 1   | A     | 287 | MET  |
| 1   | A     | 308 | LYS  |
| 1   | A     | 309 | GLU  |
| 1   | A     | 312 | TYR  |
| 1   | A     | 489 | LYS  |
| 1   | A     | 490 | SER  |
| 1   | A     | 519 | SER  |
| 1   | A     | 522 | SER  |
| 1   | A     | 579 | ALA  |
| 1   | A     | 619 | PRO  |
| 1   | A     | 621 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 656  | ASN  |
| 1   | A     | 692  | HIS  |
| 1   | A     | 754  | MET  |
| 1   | A     | 759  | PRO  |
| 1   | A     | 793  | SER  |
| 1   | A     | 873  | ILE  |
| 1   | A     | 884  | VAL  |
| 1   | A     | 885  | ARG  |
| 1   | A     | 931  | PRO  |
| 1   | A     | 946  | PRO  |
| 1   | A     | 948  | GLY  |
| 1   | A     | 960  | PRO  |
| 1   | A     | 1091 | LYS  |
| 1   | A     | 1143 | TYR  |
| 1   | A     | 1284 | PHE  |
| 1   | A     | 1286 | SER  |
| 1   | A     | 1352 | PHE  |
| 1   | A     | 1386 | ILE  |
| 1   | A     | 1452 | ASP  |
| 1   | A     | 1534 | GLN  |
| 1   | A     | 1584 | ILE  |
| 1   | A     | 1585 | TYR  |
| 1   | A     | 1589 | GLU  |
| 1   | A     | 1628 | LYS  |
| 1   | A     | 1638 | PRO  |
| 1   | A     | 1639 | LEU  |
| 1   | A     | 1651 | ASP  |
| 1   | A     | 1654 | CYS  |
| 1   | A     | 1674 | ASN  |
| 2   | B     | 48   | ASP  |
| 2   | B     | 207  | PRO  |
| 2   | B     | 220  | VAL  |
| 2   | B     | 349  | LYS  |
| 2   | B     | 418  | GLY  |
| 2   | B     | 490  | PHE  |
| 2   | B     | 545  | MET  |
| 2   | B     | 583  | ALA  |
| 2   | B     | 641  | ALA  |
| 2   | B     | 643  | LYS  |
| 2   | B     | 647  | PRO  |
| 2   | B     | 736  | GLU  |
| 2   | B     | 937  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1297 | ALA  |
| 2   | B     | 1449 | GLY  |
| 2   | B     | 1529 | LEU  |
| 2   | B     | 1597 | ILE  |
| 1   | C     | 48   | GLU  |
| 1   | C     | 60   | PRO  |
| 1   | C     | 89   | PRO  |
| 1   | C     | 96   | GLN  |
| 1   | C     | 97   | ASN  |
| 1   | C     | 154  | PRO  |
| 1   | C     | 155  | ALA  |
| 1   | C     | 181  | GLY  |
| 1   | C     | 208  | ASP  |
| 1   | C     | 255  | PHE  |
| 1   | C     | 285  | THR  |
| 1   | C     | 287  | MET  |
| 1   | C     | 308  | LYS  |
| 1   | C     | 309  | GLU  |
| 1   | C     | 312  | TYR  |
| 1   | C     | 489  | LYS  |
| 1   | C     | 490  | SER  |
| 1   | C     | 522  | SER  |
| 1   | C     | 616  | ALA  |
| 1   | C     | 621  | GLU  |
| 1   | C     | 656  | ASN  |
| 1   | C     | 692  | HIS  |
| 1   | C     | 754  | MET  |
| 1   | C     | 759  | PRO  |
| 1   | C     | 793  | SER  |
| 1   | C     | 820  | PHE  |
| 1   | C     | 873  | ILE  |
| 1   | C     | 884  | VAL  |
| 1   | C     | 885  | ARG  |
| 1   | C     | 931  | PRO  |
| 1   | C     | 946  | PRO  |
| 1   | C     | 948  | GLY  |
| 1   | C     | 960  | PRO  |
| 1   | C     | 1091 | LYS  |
| 1   | C     | 1143 | TYR  |
| 1   | C     | 1284 | PHE  |
| 1   | C     | 1286 | SER  |
| 1   | C     | 1352 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1386 | ILE  |
| 1   | C     | 1452 | ASP  |
| 1   | C     | 1534 | GLN  |
| 1   | C     | 1584 | ILE  |
| 1   | C     | 1585 | TYR  |
| 1   | C     | 1589 | GLU  |
| 1   | C     | 1628 | LYS  |
| 1   | C     | 1638 | PRO  |
| 1   | C     | 1639 | LEU  |
| 1   | C     | 1651 | ASP  |
| 1   | C     | 1654 | CYS  |
| 1   | C     | 1674 | ASN  |
| 2   | D     | 48   | ASP  |
| 2   | D     | 220  | VAL  |
| 2   | D     | 348  | THR  |
| 2   | D     | 349  | LYS  |
| 2   | D     | 418  | GLY  |
| 2   | D     | 490  | PHE  |
| 2   | D     | 545  | MET  |
| 2   | D     | 583  | ALA  |
| 2   | D     | 641  | ALA  |
| 2   | D     | 643  | LYS  |
| 2   | D     | 647  | PRO  |
| 2   | D     | 736  | GLU  |
| 2   | D     | 937  | VAL  |
| 2   | D     | 1297 | ALA  |
| 2   | D     | 1449 | GLY  |
| 2   | D     | 1529 | LEU  |
| 2   | D     | 1597 | ILE  |
| 1   | A     | 459  | SER  |
| 1   | A     | 474  | LYS  |
| 1   | A     | 475  | ALA  |
| 1   | A     | 552  | ALA  |
| 1   | A     | 569  | ASN  |
| 1   | A     | 616  | ALA  |
| 1   | A     | 623  | VAL  |
| 1   | A     | 627  | LEU  |
| 1   | A     | 638  | GLY  |
| 1   | A     | 664  | GLU  |
| 1   | A     | 806  | ASN  |
| 1   | A     | 820  | PHE  |
| 1   | A     | 889  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 890  | GLY  |
| 1   | A     | 939  | TYR  |
| 1   | A     | 981  | GLY  |
| 1   | A     | 998  | ASN  |
| 1   | A     | 1001 | THR  |
| 1   | A     | 1004 | PRO  |
| 1   | A     | 1009 | GLU  |
| 1   | A     | 1096 | ASN  |
| 1   | A     | 1122 | SER  |
| 1   | A     | 1140 | ASN  |
| 1   | A     | 1238 | SER  |
| 1   | A     | 1321 | GLY  |
| 1   | A     | 1324 | HIS  |
| 1   | A     | 1334 | LEU  |
| 1   | A     | 1382 | ASP  |
| 1   | A     | 1421 | HIS  |
| 1   | A     | 1471 | ASP  |
| 1   | A     | 1538 | GLU  |
| 1   | A     | 1590 | ALA  |
| 2   | B     | 237  | ILE  |
| 2   | B     | 348  | THR  |
| 2   | B     | 604  | LYS  |
| 2   | B     | 842  | GLU  |
| 2   | B     | 862  | LYS  |
| 2   | B     | 873  | LYS  |
| 2   | B     | 1319 | GLY  |
| 2   | B     | 1379 | MET  |
| 2   | B     | 1503 | GLN  |
| 2   | B     | 1558 | ALA  |
| 2   | B     | 1570 | GLN  |
| 1   | C     | 305  | THR  |
| 1   | C     | 459  | SER  |
| 1   | C     | 474  | LYS  |
| 1   | C     | 519  | SER  |
| 1   | C     | 552  | ALA  |
| 1   | C     | 569  | ASN  |
| 1   | C     | 579  | ALA  |
| 1   | C     | 619  | PRO  |
| 1   | C     | 623  | VAL  |
| 1   | C     | 627  | LEU  |
| 1   | C     | 634  | CYS  |
| 1   | C     | 638  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 664  | GLU  |
| 1   | C     | 889  | GLU  |
| 1   | C     | 890  | GLY  |
| 1   | C     | 981  | GLY  |
| 1   | C     | 994  | GLN  |
| 1   | C     | 998  | ASN  |
| 1   | C     | 1001 | THR  |
| 1   | C     | 1004 | PRO  |
| 1   | C     | 1009 | GLU  |
| 1   | C     | 1096 | ASN  |
| 1   | C     | 1140 | ASN  |
| 1   | C     | 1238 | SER  |
| 1   | C     | 1321 | GLY  |
| 1   | C     | 1324 | HIS  |
| 1   | C     | 1334 | LEU  |
| 1   | C     | 1382 | ASP  |
| 1   | C     | 1421 | HIS  |
| 1   | C     | 1471 | ASP  |
| 1   | C     | 1538 | GLU  |
| 1   | C     | 1590 | ALA  |
| 1   | C     | 1609 | ALA  |
| 2   | D     | 142  | PRO  |
| 2   | D     | 207  | PRO  |
| 2   | D     | 237  | ILE  |
| 2   | D     | 470  | ALA  |
| 2   | D     | 604  | LYS  |
| 2   | D     | 842  | GLU  |
| 2   | D     | 873  | LYS  |
| 2   | D     | 1319 | GLY  |
| 2   | D     | 1379 | MET  |
| 2   | D     | 1503 | GLN  |
| 2   | D     | 1558 | ALA  |
| 2   | D     | 1570 | GLN  |
| 1   | A     | 209  | PHE  |
| 1   | A     | 286  | ALA  |
| 1   | A     | 289  | ASN  |
| 1   | A     | 305  | THR  |
| 1   | A     | 440  | PRO  |
| 1   | A     | 441  | ASP  |
| 1   | A     | 472  | ASN  |
| 1   | A     | 624  | PHE  |
| 1   | A     | 634  | CYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 657  | ALA  |
| 1   | A     | 791  | PRO  |
| 1   | A     | 821  | LYS  |
| 1   | A     | 823  | VAL  |
| 1   | A     | 849  | ARG  |
| 1   | A     | 938  | SER  |
| 1   | A     | 994  | GLN  |
| 1   | A     | 1194 | ALA  |
| 1   | A     | 1196 | SER  |
| 1   | A     | 1539 | LEU  |
| 1   | A     | 1588 | GLY  |
| 1   | A     | 1609 | ALA  |
| 1   | A     | 1632 | SER  |
| 1   | A     | 1652 | THR  |
| 2   | B     | 142  | PRO  |
| 2   | B     | 435  | TYR  |
| 2   | B     | 470  | ALA  |
| 2   | B     | 613  | SER  |
| 2   | B     | 780  | LEU  |
| 2   | B     | 1340 | CYS  |
| 2   | B     | 1497 | CYS  |
| 2   | B     | 1557 | ARG  |
| 1   | C     | 167  | GLU  |
| 1   | C     | 440  | PRO  |
| 1   | C     | 441  | ASP  |
| 1   | C     | 472  | ASN  |
| 1   | C     | 475  | ALA  |
| 1   | C     | 488  | PRO  |
| 1   | C     | 520  | ASP  |
| 1   | C     | 624  | PHE  |
| 1   | C     | 657  | ALA  |
| 1   | C     | 760  | VAL  |
| 1   | C     | 791  | PRO  |
| 1   | C     | 806  | ASN  |
| 1   | C     | 821  | LYS  |
| 1   | C     | 823  | VAL  |
| 1   | C     | 849  | ARG  |
| 1   | C     | 938  | SER  |
| 1   | C     | 939  | TYR  |
| 1   | C     | 1122 | SER  |
| 1   | C     | 1194 | ALA  |
| 1   | C     | 1196 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1539 | LEU  |
| 1   | C     | 1632 | SER  |
| 1   | C     | 1652 | THR  |
| 2   | D     | 326  | SER  |
| 2   | D     | 435  | TYR  |
| 2   | D     | 613  | SER  |
| 2   | D     | 780  | LEU  |
| 2   | D     | 862  | LYS  |
| 2   | D     | 1340 | CYS  |
| 2   | D     | 1497 | CYS  |
| 2   | D     | 1557 | ARG  |
| 1   | A     | 234  | GLU  |
| 1   | A     | 256  | TYR  |
| 1   | A     | 520  | ASP  |
| 1   | A     | 667  | GLU  |
| 1   | A     | 690  | TYR  |
| 1   | A     | 760  | VAL  |
| 1   | A     | 882  | LYS  |
| 1   | A     | 909  | ASN  |
| 1   | A     | 988  | LEU  |
| 1   | A     | 1139 | GLU  |
| 1   | A     | 1150 | ILE  |
| 1   | A     | 1513 | ASN  |
| 1   | A     | 1540 | ASP  |
| 1   | A     | 1573 | VAL  |
| 1   | A     | 1655 | SER  |
| 2   | B     | 81   | MET  |
| 2   | B     | 277  | PRO  |
| 2   | B     | 326  | SER  |
| 2   | B     | 959  | ILE  |
| 2   | B     | 1447 | GLU  |
| 2   | B     | 1501 | ASN  |
| 1   | C     | 94   | GLY  |
| 1   | C     | 256  | TYR  |
| 1   | C     | 286  | ALA  |
| 1   | C     | 289  | ASN  |
| 1   | C     | 337  | SER  |
| 1   | C     | 667  | GLU  |
| 1   | C     | 690  | TYR  |
| 1   | C     | 909  | ASN  |
| 1   | C     | 987  | ILE  |
| 1   | C     | 988  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 997  | ILE  |
| 1   | C     | 1098 | ASN  |
| 1   | C     | 1139 | GLU  |
| 1   | C     | 1540 | ASP  |
| 1   | C     | 1573 | VAL  |
| 1   | C     | 1588 | GLY  |
| 1   | C     | 1655 | SER  |
| 2   | D     | 81   | MET  |
| 2   | D     | 277  | PRO  |
| 2   | D     | 471  | ASN  |
| 2   | D     | 821  | PRO  |
| 2   | D     | 959  | ILE  |
| 2   | D     | 1298 | LEU  |
| 2   | D     | 1332 | GLN  |
| 2   | D     | 1447 | GLU  |
| 2   | D     | 1501 | ASN  |
| 2   | D     | 1553 | ASP  |
| 2   | D     | 1560 | THR  |
| 1   | A     | 94   | GLY  |
| 1   | A     | 101  | TYR  |
| 1   | A     | 167  | GLU  |
| 1   | A     | 186  | PRO  |
| 1   | A     | 274  | ASP  |
| 1   | A     | 291  | MET  |
| 1   | A     | 337  | SER  |
| 1   | A     | 488  | PRO  |
| 1   | A     | 576  | SER  |
| 1   | A     | 737  | GLN  |
| 1   | A     | 753  | HIS  |
| 1   | A     | 987  | ILE  |
| 1   | A     | 997  | ILE  |
| 1   | A     | 1098 | ASN  |
| 1   | A     | 1134 | PRO  |
| 1   | A     | 1160 | PRO  |
| 1   | A     | 1272 | LYS  |
| 1   | A     | 1675 | GLY  |
| 2   | B     | 471  | ASN  |
| 2   | B     | 950  | LEU  |
| 2   | B     | 1332 | GLN  |
| 2   | B     | 1556 | PRO  |
| 2   | B     | 1639 | GLY  |
| 1   | C     | 101  | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 186  | PRO  |
| 1   | C     | 234  | GLU  |
| 1   | C     | 291  | MET  |
| 1   | C     | 576  | SER  |
| 1   | C     | 753  | HIS  |
| 1   | C     | 882  | LYS  |
| 1   | C     | 1023 | HIS  |
| 1   | C     | 1134 | PRO  |
| 1   | C     | 1150 | ILE  |
| 1   | C     | 1513 | ASN  |
| 1   | C     | 1675 | GLY  |
| 2   | D     | 1556 | PRO  |
| 2   | D     | 1592 | PRO  |
| 1   | A     | 633  | GLY  |
| 1   | A     | 986  | GLU  |
| 1   | A     | 1002 | HIS  |
| 1   | A     | 1022 | PHE  |
| 1   | A     | 1243 | GLY  |
| 2   | B     | 560  | GLY  |
| 2   | B     | 1514 | LYS  |
| 2   | B     | 1592 | PRO  |
| 1   | C     | 274  | ASP  |
| 1   | C     | 970  | LYS  |
| 1   | C     | 1272 | LYS  |
| 2   | D     | 49   | SER  |
| 2   | D     | 950  | LEU  |
| 2   | B     | 821  | PRO  |
| 1   | C     | 633  | GLY  |
| 1   | C     | 1160 | PRO  |
| 1   | C     | 1243 | GLY  |
| 1   | C     | 1649 | PRO  |
| 2   | D     | 560  | GLY  |
| 1   | A     | 166  | PRO  |
| 1   | A     | 1649 | PRO  |
| 2   | B     | 339  | VAL  |
| 1   | C     | 510  | ILE  |
| 1   | C     | 1671 | ILE  |
| 2   | D     | 339  | VAL  |
| 2   | D     | 403  | PRO  |
| 1   | A     | 93   | PRO  |
| 1   | A     | 171  | VAL  |
| 1   | A     | 999  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1671 | ILE  |
| 2   | B     | 79   | GLY  |
| 2   | B     | 403  | PRO  |
| 2   | B     | 512  | PRO  |
| 2   | B     | 559  | PRO  |
| 1   | C     | 93   | PRO  |
| 1   | C     | 166  | PRO  |
| 1   | C     | 171  | VAL  |
| 2   | D     | 79   | GLY  |
| 2   | D     | 512  | PRO  |
| 2   | D     | 584  | VAL  |
| 1   | A     | 137  | PRO  |
| 1   | A     | 168  | GLY  |
| 1   | C     | 168  | GLY  |
| 1   | C     | 999  | ILE  |
| 1   | C     | 1239 | VAL  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 1446/1484 (97%) | 1068 (74%) | 378 (26%)  | 0           | 3 |
| 1   | C     | 1446/1484 (97%) | 1069 (74%) | 377 (26%)  | 0           | 3 |
| 2   | B     | 1093/1435 (76%) | 834 (76%)  | 259 (24%)  | 1           | 5 |
| 2   | D     | 1093/1435 (76%) | 830 (76%)  | 263 (24%)  | 1           | 4 |
| All | All   | 5078/5838 (87%) | 3801 (75%) | 1277 (25%) | 0           | 4 |

All (1277) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | GLN  |
| 1   | A     | 22  | THR  |
| 1   | A     | 23  | TYR  |
| 1   | A     | 24  | VAL  |
| 1   | A     | 26  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | ILE  |
| 1   | A     | 40  | VAL  |
| 1   | A     | 41  | ILE  |
| 1   | A     | 47  | THR  |
| 1   | A     | 53  | THR  |
| 1   | A     | 55  | SER  |
| 1   | A     | 58  | SER  |
| 1   | A     | 63  | LYS  |
| 1   | A     | 64  | PHE  |
| 1   | A     | 67  | SER  |
| 1   | A     | 71  | VAL  |
| 1   | A     | 73  | LEU  |
| 1   | A     | 84  | ILE  |
| 1   | A     | 85  | LEU  |
| 1   | A     | 87  | ILE  |
| 1   | A     | 89  | PRO  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 99  | VAL  |
| 1   | A     | 102 | VAL  |
| 1   | A     | 104 | LEU  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 110 | HIS  |
| 1   | A     | 125 | PHE  |
| 1   | A     | 126 | LEU  |
| 1   | A     | 128 | ILE  |
| 1   | A     | 131 | ASP  |
| 1   | A     | 136 | THR  |
| 1   | A     | 141 | VAL  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 144 | ARG  |
| 1   | A     | 148 | LEU  |
| 1   | A     | 156 | LYS  |
| 1   | A     | 157 | ARG  |
| 1   | A     | 158 | GLU  |
| 1   | A     | 160 | VAL  |
| 1   | A     | 161 | LEU  |
| 1   | A     | 162 | THR  |
| 1   | A     | 164 | ILE  |
| 1   | A     | 167 | GLU  |
| 1   | A     | 169 | SER  |
| 1   | A     | 171 | VAL  |
| 1   | A     | 176 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 182 | ILE  |
| 1   | A     | 183 | ILE  |
| 1   | A     | 200 | THR  |
| 1   | A     | 208 | ASP  |
| 1   | A     | 211 | THR  |
| 1   | A     | 212 | THR  |
| 1   | A     | 214 | THR  |
| 1   | A     | 218 | GLU  |
| 1   | A     | 223 | VAL  |
| 1   | A     | 224 | LEU  |
| 1   | A     | 228 | SER  |
| 1   | A     | 230 | SER  |
| 1   | A     | 231 | ILE  |
| 1   | A     | 232 | GLU  |
| 1   | A     | 240 | TYR  |
| 1   | A     | 241 | LYS  |
| 1   | A     | 242 | ASN  |
| 1   | A     | 249 | THR  |
| 1   | A     | 261 | THR  |
| 1   | A     | 268 | THR  |
| 1   | A     | 279 | GLN  |
| 1   | A     | 287 | MET  |
| 1   | A     | 289 | ASN  |
| 1   | A     | 291 | MET  |
| 1   | A     | 292 | LEU  |
| 1   | A     | 296 | ILE  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 321 | LYS  |
| 1   | A     | 322 | TYR  |
| 1   | A     | 323 | LEU  |
| 1   | A     | 324 | TYR  |
| 1   | A     | 325 | ILE  |
| 1   | A     | 328 | THR  |
| 1   | A     | 333 | THR  |
| 1   | A     | 337 | SER  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 355 | ASN  |
| 1   | A     | 363 | LEU  |
| 1   | A     | 371 | ILE  |
| 1   | A     | 373 | VAL  |
| 1   | A     | 375 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 383 | VAL  |
| 1   | A     | 389 | THR  |
| 1   | A     | 390 | LEU  |
| 1   | A     | 394 | THR  |
| 1   | A     | 400 | GLU  |
| 1   | A     | 404 | LEU  |
| 1   | A     | 407 | SER  |
| 1   | A     | 412 | ARG  |
| 1   | A     | 414 | ASP  |
| 1   | A     | 419 | SER  |
| 1   | A     | 422 | LEU  |
| 1   | A     | 431 | LEU  |
| 1   | A     | 433 | PHE  |
| 1   | A     | 441 | ASP  |
| 1   | A     | 442 | LEU  |
| 1   | A     | 455 | ILE  |
| 1   | A     | 457 | TYR  |
| 1   | A     | 458 | SER  |
| 1   | A     | 460 | LEU  |
| 1   | A     | 467 | ILE  |
| 1   | A     | 469 | TRP  |
| 1   | A     | 471 | ASP  |
| 1   | A     | 474 | LYS  |
| 1   | A     | 477 | LEU  |
| 1   | A     | 484 | ILE  |
| 1   | A     | 486 | VAL  |
| 1   | A     | 493 | ILE  |
| 1   | A     | 495 | LYS  |
| 1   | A     | 497 | THR  |
| 1   | A     | 501 | TYR  |
| 1   | A     | 504 | LEU  |
| 1   | A     | 506 | LYS  |
| 1   | A     | 509 | ILE  |
| 1   | A     | 516 | GLU  |
| 1   | A     | 522 | SER  |
| 1   | A     | 526 | ILE  |
| 1   | A     | 534 | MET  |
| 1   | A     | 535 | VAL  |
| 1   | A     | 540 | LEU  |
| 1   | A     | 541 | LEU  |
| 1   | A     | 543 | TYR  |
| 1   | A     | 545 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 547 | THR  |
| 1   | A     | 549 | GLU  |
| 1   | A     | 550 | GLN  |
| 1   | A     | 555 | VAL  |
| 1   | A     | 559 | VAL  |
| 1   | A     | 561 | LEU  |
| 1   | A     | 563 | ILE  |
| 1   | A     | 567 | CYS  |
| 1   | A     | 569 | ASN  |
| 1   | A     | 573 | VAL  |
| 1   | A     | 580 | ASP  |
| 1   | A     | 587 | THR  |
| 1   | A     | 596 | MET  |
| 1   | A     | 597 | ASP  |
| 1   | A     | 605 | VAL  |
| 1   | A     | 613 | GLN  |
| 1   | A     | 614 | ARG  |
| 1   | A     | 618 | LYS  |
| 1   | A     | 620 | LEU  |
| 1   | A     | 621 | GLU  |
| 1   | A     | 625 | GLN  |
| 1   | A     | 627 | LEU  |
| 1   | A     | 630 | SER  |
| 1   | A     | 640 | LEU  |
| 1   | A     | 642 | ASN  |
| 1   | A     | 644 | ASN  |
| 1   | A     | 652 | THR  |
| 1   | A     | 653 | PHE  |
| 1   | A     | 654 | LEU  |
| 1   | A     | 663 | GLN  |
| 1   | A     | 664 | GLU  |
| 1   | A     | 667 | GLU  |
| 1   | A     | 672 | ILE  |
| 1   | A     | 692 | HIS  |
| 1   | A     | 695 | VAL  |
| 1   | A     | 697 | LYS  |
| 1   | A     | 699 | CYS  |
| 1   | A     | 704 | CYS  |
| 1   | A     | 707 | ASN  |
| 1   | A     | 710 | THR  |
| 1   | A     | 713 | GLN  |
| 1   | A     | 720 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 732 | CYS  |
| 1   | A     | 753 | HIS  |
| 1   | A     | 756 | THR  |
| 1   | A     | 758 | LEU  |
| 1   | A     | 767 | SER  |
| 1   | A     | 774 | LEU  |
| 1   | A     | 777 | VAL  |
| 1   | A     | 778 | HIS  |
| 1   | A     | 782 | ARG  |
| 1   | A     | 788 | PHE  |
| 1   | A     | 793 | SER  |
| 1   | A     | 795 | THR  |
| 1   | A     | 797 | TRP  |
| 1   | A     | 800 | GLN  |
| 1   | A     | 809 | ILE  |
| 1   | A     | 811 | VAL  |
| 1   | A     | 823 | VAL  |
| 1   | A     | 824 | PHE  |
| 1   | A     | 825 | LEU  |
| 1   | A     | 833 | VAL  |
| 1   | A     | 838 | GLN  |
| 1   | A     | 839 | ILE  |
| 1   | A     | 845 | VAL  |
| 1   | A     | 849 | ARG  |
| 1   | A     | 850 | THR  |
| 1   | A     | 854 | GLN  |
| 1   | A     | 856 | CYS  |
| 1   | A     | 857 | VAL  |
| 1   | A     | 859 | MET  |
| 1   | A     | 865 | ILE  |
| 1   | A     | 867 | THR  |
| 1   | A     | 876 | GLN  |
| 1   | A     | 887 | LYS  |
| 1   | A     | 895 | LEU  |
| 1   | A     | 896 | VAL  |
| 1   | A     | 899 | THR  |
| 1   | A     | 901 | LEU  |
| 1   | A     | 914 | LEU  |
| 1   | A     | 915 | GLU  |
| 1   | A     | 923 | LEU  |
| 1   | A     | 930 | VAL  |
| 1   | A     | 935 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 936  | ARG  |
| 1   | A     | 940  | SER  |
| 1   | A     | 944  | LEU  |
| 1   | A     | 947  | ARG  |
| 1   | A     | 952  | THR  |
| 1   | A     | 953  | ILE  |
| 1   | A     | 965  | LEU  |
| 1   | A     | 967  | LEU  |
| 1   | A     | 972  | GLU  |
| 1   | A     | 975  | ARG  |
| 1   | A     | 977  | LEU  |
| 1   | A     | 980  | LYS  |
| 1   | A     | 983  | LEU  |
| 1   | A     | 984  | VAL  |
| 1   | A     | 986  | GLU  |
| 1   | A     | 988  | LEU  |
| 1   | A     | 1001 | THR  |
| 1   | A     | 1002 | HIS  |
| 1   | A     | 1003 | LEU  |
| 1   | A     | 1007 | SER  |
| 1   | A     | 1011 | GLU  |
| 1   | A     | 1013 | MET  |
| 1   | A     | 1014 | SER  |
| 1   | A     | 1016 | VAL  |
| 1   | A     | 1018 | VAL  |
| 1   | A     | 1033 | ILE  |
| 1   | A     | 1055 | SER  |
| 1   | A     | 1056 | ILE  |
| 1   | A     | 1070 | LYS  |
| 1   | A     | 1076 | THR  |
| 1   | A     | 1078 | LEU  |
| 1   | A     | 1084 | ARG  |
| 1   | A     | 1089 | VAL  |
| 1   | A     | 1091 | LYS  |
| 1   | A     | 1098 | ASN  |
| 1   | A     | 1105 | LEU  |
| 1   | A     | 1107 | LEU  |
| 1   | A     | 1108 | VAL  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1113 | LEU  |
| 1   | A     | 1119 | LYS  |
| 1   | A     | 1127 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1128 | LYS  |
| 1   | A     | 1129 | LEU  |
| 1   | A     | 1140 | ASN  |
| 1   | A     | 1141 | SER  |
| 1   | A     | 1148 | THR  |
| 1   | A     | 1163 | LYS  |
| 1   | A     | 1164 | ILE  |
| 1   | A     | 1166 | THR  |
| 1   | A     | 1168 | LEU  |
| 1   | A     | 1175 | LEU  |
| 1   | A     | 1176 | LEU  |
| 1   | A     | 1179 | THR  |
| 1   | A     | 1180 | LEU  |
| 1   | A     | 1183 | GLN  |
| 1   | A     | 1185 | THR  |
| 1   | A     | 1190 | ILE  |
| 1   | A     | 1196 | SER  |
| 1   | A     | 1200 | LYS  |
| 1   | A     | 1201 | THR  |
| 1   | A     | 1209 | VAL  |
| 1   | A     | 1212 | LEU  |
| 1   | A     | 1218 | VAL  |
| 1   | A     | 1227 | PHE  |
| 1   | A     | 1231 | ASN  |
| 1   | A     | 1236 | ASP  |
| 1   | A     | 1244 | THR  |
| 1   | A     | 1246 | ARG  |
| 1   | A     | 1255 | LEU  |
| 1   | A     | 1257 | THR  |
| 1   | A     | 1259 | LEU  |
| 1   | A     | 1264 | ILE  |
| 1   | A     | 1268 | ASN  |
| 1   | A     | 1280 | TYR  |
| 1   | A     | 1294 | ILE  |
| 1   | A     | 1301 | SER  |
| 1   | A     | 1302 | LEU  |
| 1   | A     | 1303 | LEU  |
| 1   | A     | 1306 | GLN  |
| 1   | A     | 1307 | LEU  |
| 1   | A     | 1309 | LEU  |
| 1   | A     | 1311 | MET  |
| 1   | A     | 1313 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1315 | VAL  |
| 1   | A     | 1323 | LEU  |
| 1   | A     | 1326 | TYR  |
| 1   | A     | 1329 | THR  |
| 1   | A     | 1331 | LYS  |
| 1   | A     | 1333 | PHE  |
| 1   | A     | 1334 | LEU  |
| 1   | A     | 1336 | ARG  |
| 1   | A     | 1338 | VAL  |
| 1   | A     | 1341 | LEU  |
| 1   | A     | 1346 | LEU  |
| 1   | A     | 1347 | ILE  |
| 1   | A     | 1348 | VAL  |
| 1   | A     | 1356 | LEU  |
| 1   | A     | 1358 | THR  |
| 1   | A     | 1361 | VAL  |
| 1   | A     | 1363 | THR  |
| 1   | A     | 1366 | HIS  |
| 1   | A     | 1367 | LYS  |
| 1   | A     | 1372 | GLU  |
| 1   | A     | 1374 | VAL  |
| 1   | A     | 1397 | SER  |
| 1   | A     | 1414 | GLU  |
| 1   | A     | 1421 | HIS  |
| 1   | A     | 1423 | VAL  |
| 1   | A     | 1433 | SER  |
| 1   | A     | 1443 | VAL  |
| 1   | A     | 1454 | GLN  |
| 1   | A     | 1457 | ASP  |
| 1   | A     | 1462 | LEU  |
| 1   | A     | 1464 | LEU  |
| 1   | A     | 1470 | SER  |
| 1   | A     | 1474 | CYS  |
| 1   | A     | 1475 | VAL  |
| 1   | A     | 1479 | ILE  |
| 1   | A     | 1480 | PHE  |
| 1   | A     | 1483 | PHE  |
| 1   | A     | 1487 | PHE  |
| 1   | A     | 1488 | LEU  |
| 1   | A     | 1492 | THR  |
| 1   | A     | 1493 | PHE  |
| 1   | A     | 1494 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1495 | VAL  |
| 1   | A     | 1497 | GLU  |
| 1   | A     | 1500 | ARG  |
| 1   | A     | 1503 | LYS  |
| 1   | A     | 1504 | GLN  |
| 1   | A     | 1506 | THR  |
| 1   | A     | 1507 | MET  |
| 1   | A     | 1512 | SER  |
| 1   | A     | 1535 | MET  |
| 1   | A     | 1542 | THR  |
| 1   | A     | 1544 | SER  |
| 1   | A     | 1548 | ARG  |
| 1   | A     | 1549 | LYS  |
| 1   | A     | 1553 | CYS  |
| 1   | A     | 1557 | ILE  |
| 1   | A     | 1565 | ILE  |
| 1   | A     | 1566 | THR  |
| 1   | A     | 1580 | THR  |
| 1   | A     | 1581 | LEU  |
| 1   | A     | 1582 | LEU  |
| 1   | A     | 1585 | TYR  |
| 1   | A     | 1598 | ILE  |
| 1   | A     | 1602 | LYS  |
| 1   | A     | 1604 | VAL  |
| 1   | A     | 1605 | THR  |
| 1   | A     | 1606 | CYS  |
| 1   | A     | 1616 | GLN  |
| 1   | A     | 1618 | LEU  |
| 1   | A     | 1626 | GLN  |
| 1   | A     | 1627 | ILE  |
| 1   | A     | 1631 | PHE  |
| 1   | A     | 1636 | ILE  |
| 1   | A     | 1639 | LEU  |
| 1   | A     | 1651 | ASP  |
| 1   | A     | 1652 | THR  |
| 1   | A     | 1655 | SER  |
| 1   | A     | 1663 | ASN  |
| 2   | B     | 29   | THR  |
| 2   | B     | 40   | GLN  |
| 2   | B     | 43   | VAL  |
| 2   | B     | 54   | LEU  |
| 2   | B     | 56   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 58  | VAL  |
| 2   | B     | 68  | LEU  |
| 2   | B     | 71  | THR  |
| 2   | B     | 74  | ASP  |
| 2   | B     | 82  | LEU  |
| 2   | B     | 86  | THR  |
| 2   | B     | 87  | ILE  |
| 2   | B     | 100 | GLN  |
| 2   | B     | 103 | TYR  |
| 2   | B     | 105 | VAL  |
| 2   | B     | 106 | VAL  |
| 2   | B     | 108 | VAL  |
| 2   | B     | 113 | VAL  |
| 2   | B     | 114 | ARG  |
| 2   | B     | 119 | VAL  |
| 2   | B     | 120 | LEU  |
| 2   | B     | 121 | LEU  |
| 2   | B     | 124 | GLN  |
| 2   | B     | 144 | LEU  |
| 2   | B     | 147 | VAL  |
| 2   | B     | 161 | VAL  |
| 2   | B     | 162 | ILE  |
| 2   | B     | 167 | THR  |
| 2   | B     | 171 | ILE  |
| 2   | B     | 175 | SER  |
| 2   | B     | 176 | ASN  |
| 2   | B     | 177 | SER  |
| 2   | B     | 178 | VAL  |
| 2   | B     | 179 | ASP  |
| 2   | B     | 183 | PHE  |
| 2   | B     | 190 | ASP  |
| 2   | B     | 191 | LEU  |
| 2   | B     | 196 | THR  |
| 2   | B     | 198 | ARG  |
| 2   | B     | 202 | LYS  |
| 2   | B     | 208 | GLU  |
| 2   | B     | 216 | VAL  |
| 2   | B     | 217 | ARG  |
| 2   | B     | 220 | VAL  |
| 2   | B     | 221 | LEU  |
| 2   | B     | 223 | SER  |
| 2   | B     | 226 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 231 | SER  |
| 2   | B     | 258 | GLU  |
| 2   | B     | 263 | VAL  |
| 2   | B     | 264 | LEU  |
| 2   | B     | 280 | LEU  |
| 2   | B     | 285 | ILE  |
| 2   | B     | 296 | ARG  |
| 2   | B     | 298 | THR  |
| 2   | B     | 301 | SER  |
| 2   | B     | 306 | LEU  |
| 2   | B     | 315 | TYR  |
| 2   | B     | 317 | SER  |
| 2   | B     | 323 | GLU  |
| 2   | B     | 327 | ASP  |
| 2   | B     | 328 | MET  |
| 2   | B     | 329 | VAL  |
| 2   | B     | 344 | GLN  |
| 2   | B     | 345 | ILE  |
| 2   | B     | 348 | THR  |
| 2   | B     | 349 | LYS  |
| 2   | B     | 358 | MET  |
| 2   | B     | 377 | VAL  |
| 2   | B     | 379 | VAL  |
| 2   | B     | 382 | GLU  |
| 2   | B     | 389 | THR  |
| 2   | B     | 390 | THR  |
| 2   | B     | 398 | LEU  |
| 2   | B     | 400 | LEU  |
| 2   | B     | 402 | ILE  |
| 2   | B     | 409 | LEU  |
| 2   | B     | 414 | ARG  |
| 2   | B     | 416 | ASN  |
| 2   | B     | 422 | ARG  |
| 2   | B     | 427 | THR  |
| 2   | B     | 433 | ILE  |
| 2   | B     | 437 | THR  |
| 2   | B     | 449 | ILE  |
| 2   | B     | 460 | LEU  |
| 2   | B     | 465 | ASN  |
| 2   | B     | 466 | VAL  |
| 2   | B     | 469 | ASN  |
| 2   | B     | 473 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 481 | TYR  |
| 2   | B     | 482 | LEU  |
| 2   | B     | 483 | ILE  |
| 2   | B     | 488 | LYS  |
| 2   | B     | 497 | ARG  |
| 2   | B     | 504 | VAL  |
| 2   | B     | 505 | THR  |
| 2   | B     | 511 | THR  |
| 2   | B     | 513 | ASP  |
| 2   | B     | 514 | LEU  |
| 2   | B     | 515 | ILE  |
| 2   | B     | 518 | PHE  |
| 2   | B     | 521 | VAL  |
| 2   | B     | 524 | TYR  |
| 2   | B     | 525 | GLN  |
| 2   | B     | 526 | VAL  |
| 2   | B     | 531 | ILE  |
| 2   | B     | 532 | VAL  |
| 2   | B     | 543 | THR  |
| 2   | B     | 544 | CYS  |
| 2   | B     | 555 | LEU  |
| 2   | B     | 556 | ILE  |
| 2   | B     | 558 | MET  |
| 2   | B     | 563 | MET  |
| 2   | B     | 564 | LYS  |
| 2   | B     | 567 | LEU  |
| 2   | B     | 582 | LYS  |
| 2   | B     | 586 | VAL  |
| 2   | B     | 588 | ASN  |
| 2   | B     | 593 | ILE  |
| 2   | B     | 597 | LYS  |
| 2   | B     | 598 | ILE  |
| 2   | B     | 602 | ILE  |
| 2   | B     | 613 | SER  |
| 2   | B     | 615 | GLN  |
| 2   | B     | 620 | VAL  |
| 2   | B     | 629 | THR  |
| 2   | B     | 638 | GLN  |
| 2   | B     | 735 | ASN  |
| 2   | B     | 736 | GLU  |
| 2   | B     | 742 | ASP  |
| 2   | B     | 745 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 746 | ILE  |
| 2   | B     | 747 | SER  |
| 2   | B     | 764 | GLU  |
| 2   | B     | 769 | GLN  |
| 2   | B     | 773 | SER  |
| 2   | B     | 778 | PHE  |
| 2   | B     | 780 | LEU  |
| 2   | B     | 784 | ILE  |
| 2   | B     | 786 | THR  |
| 2   | B     | 789 | VAL  |
| 2   | B     | 800 | ILE  |
| 2   | B     | 802 | VAL  |
| 2   | B     | 804 | GLU  |
| 2   | B     | 808 | ILE  |
| 2   | B     | 810 | VAL  |
| 2   | B     | 813 | VAL  |
| 2   | B     | 816 | ILE  |
| 2   | B     | 817 | ASP  |
| 2   | B     | 819 | GLN  |
| 2   | B     | 829 | GLN  |
| 2   | B     | 830 | VAL  |
| 2   | B     | 836 | LEU  |
| 2   | B     | 840 | VAL  |
| 2   | B     | 851 | LEU  |
| 2   | B     | 857 | CYS  |
| 2   | B     | 868 | GLN  |
| 2   | B     | 870 | PHE  |
| 2   | B     | 872 | ILE  |
| 2   | B     | 873 | LYS  |
| 2   | B     | 880 | VAL  |
| 2   | B     | 884 | ILE  |
| 2   | B     | 887 | LEU  |
| 2   | B     | 889 | GLN  |
| 2   | B     | 891 | LEU  |
| 2   | B     | 918 | GLU  |
| 2   | B     | 920 | VAL  |
| 2   | B     | 925 | VAL  |
| 2   | B     | 926 | THR  |
| 2   | B     | 944 | VAL  |
| 2   | B     | 946 | LYS  |
| 2   | B     | 948 | ARG  |
| 2   | B     | 949 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 952  | ASP  |
| 2   | B     | 963  | ILE  |
| 2   | B     | 964  | ILE  |
| 2   | B     | 1273 | LEU  |
| 2   | B     | 1274 | ASN  |
| 2   | B     | 1278 | THR  |
| 2   | B     | 1279 | ILE  |
| 2   | B     | 1281 | LEU  |
| 2   | B     | 1291 | ARG  |
| 2   | B     | 1292 | ILE  |
| 2   | B     | 1296 | ASN  |
| 2   | B     | 1301 | ARG  |
| 2   | B     | 1303 | VAL  |
| 2   | B     | 1305 | THR  |
| 2   | B     | 1308 | ASN  |
| 2   | B     | 1313 | VAL  |
| 2   | B     | 1322 | THR  |
| 2   | B     | 1324 | THR  |
| 2   | B     | 1326 | LEU  |
| 2   | B     | 1330 | ASN  |
| 2   | B     | 1332 | GLN  |
| 2   | B     | 1344 | HIS  |
| 2   | B     | 1345 | LEU  |
| 2   | B     | 1346 | ASN  |
| 2   | B     | 1349 | VAL  |
| 2   | B     | 1350 | GLU  |
| 2   | B     | 1351 | ASN  |
| 2   | B     | 1353 | HIS  |
| 2   | B     | 1365 | LEU  |
| 2   | B     | 1367 | ILE  |
| 2   | B     | 1372 | LEU  |
| 2   | B     | 1378 | THR  |
| 2   | B     | 1380 | THR  |
| 2   | B     | 1382 | ILE  |
| 2   | B     | 1388 | THR  |
| 2   | B     | 1398 | THR  |
| 2   | B     | 1401 | SER  |
| 2   | B     | 1404 | VAL  |
| 2   | B     | 1406 | ARG  |
| 2   | B     | 1415 | ASN  |
| 2   | B     | 1423 | VAL  |
| 2   | B     | 1424 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1427 | LEU  |
| 2   | B     | 1429 | LYS  |
| 2   | B     | 1431 | SER  |
| 2   | B     | 1433 | SER  |
| 2   | B     | 1437 | CYS  |
| 2   | B     | 1438 | LEU  |
| 2   | B     | 1442 | ILE  |
| 2   | B     | 1443 | LEU  |
| 2   | B     | 1448 | VAL  |
| 2   | B     | 1451 | ILE  |
| 2   | B     | 1456 | VAL  |
| 2   | B     | 1464 | LEU  |
| 2   | B     | 1475 | ASP  |
| 2   | B     | 1480 | LEU  |
| 2   | B     | 1481 | LEU  |
| 2   | B     | 1490 | CYS  |
| 2   | B     | 1492 | CYS  |
| 2   | B     | 1495 | GLU  |
| 2   | B     | 1496 | THR  |
| 2   | B     | 1497 | CYS  |
| 2   | B     | 1500 | LEU  |
| 2   | B     | 1504 | GLU  |
| 2   | B     | 1516 | CYS  |
| 2   | B     | 1526 | THR  |
| 2   | B     | 1535 | ASP  |
| 2   | B     | 1539 | ILE  |
| 2   | B     | 1566 | GLN  |
| 2   | B     | 1571 | GLU  |
| 2   | B     | 1582 | LEU  |
| 2   | B     | 1583 | ILE  |
| 2   | B     | 1584 | TRP  |
| 2   | B     | 1594 | LYS  |
| 2   | B     | 1598 | SER  |
| 2   | B     | 1599 | TYR  |
| 2   | B     | 1601 | ILE  |
| 2   | B     | 1604 | ASN  |
| 2   | B     | 1605 | THR  |
| 2   | B     | 1606 | TRP  |
| 2   | B     | 1607 | ILE  |
| 2   | B     | 1609 | ARG  |
| 2   | B     | 1613 | GLU  |
| 2   | B     | 1614 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1622 | GLN  |
| 2   | B     | 1623 | LYS  |
| 1   | C     | 21   | GLN  |
| 1   | C     | 22   | THR  |
| 1   | C     | 23   | TYR  |
| 1   | C     | 24   | VAL  |
| 1   | C     | 26   | SER  |
| 1   | C     | 40   | VAL  |
| 1   | C     | 41   | ILE  |
| 1   | C     | 47   | THR  |
| 1   | C     | 53   | THR  |
| 1   | C     | 55   | SER  |
| 1   | C     | 58   | SER  |
| 1   | C     | 63   | LYS  |
| 1   | C     | 64   | PHE  |
| 1   | C     | 67   | SER  |
| 1   | C     | 71   | VAL  |
| 1   | C     | 73   | LEU  |
| 1   | C     | 84   | ILE  |
| 1   | C     | 85   | LEU  |
| 1   | C     | 87   | ILE  |
| 1   | C     | 89   | PRO  |
| 1   | C     | 91   | GLN  |
| 1   | C     | 99   | VAL  |
| 1   | C     | 102  | VAL  |
| 1   | C     | 104  | LEU  |
| 1   | C     | 106  | VAL  |
| 1   | C     | 110  | HIS  |
| 1   | C     | 125  | PHE  |
| 1   | C     | 126  | LEU  |
| 1   | C     | 128  | ILE  |
| 1   | C     | 131  | ASP  |
| 1   | C     | 136  | THR  |
| 1   | C     | 141  | VAL  |
| 1   | C     | 143  | VAL  |
| 1   | C     | 144  | ARG  |
| 1   | C     | 148  | LEU  |
| 1   | C     | 156  | LYS  |
| 1   | C     | 157  | ARG  |
| 1   | C     | 158  | GLU  |
| 1   | C     | 160  | VAL  |
| 1   | C     | 161  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 162 | THR  |
| 1   | C     | 164 | ILE  |
| 1   | C     | 167 | GLU  |
| 1   | C     | 169 | SER  |
| 1   | C     | 171 | VAL  |
| 1   | C     | 176 | GLU  |
| 1   | C     | 182 | ILE  |
| 1   | C     | 183 | ILE  |
| 1   | C     | 200 | THR  |
| 1   | C     | 208 | ASP  |
| 1   | C     | 211 | THR  |
| 1   | C     | 212 | THR  |
| 1   | C     | 214 | THR  |
| 1   | C     | 218 | GLU  |
| 1   | C     | 219 | VAL  |
| 1   | C     | 223 | VAL  |
| 1   | C     | 224 | LEU  |
| 1   | C     | 228 | SER  |
| 1   | C     | 230 | SER  |
| 1   | C     | 231 | ILE  |
| 1   | C     | 232 | GLU  |
| 1   | C     | 240 | TYR  |
| 1   | C     | 241 | LYS  |
| 1   | C     | 242 | ASN  |
| 1   | C     | 249 | THR  |
| 1   | C     | 261 | THR  |
| 1   | C     | 268 | THR  |
| 1   | C     | 279 | GLN  |
| 1   | C     | 287 | MET  |
| 1   | C     | 289 | ASN  |
| 1   | C     | 291 | MET  |
| 1   | C     | 292 | LEU  |
| 1   | C     | 296 | ILE  |
| 1   | C     | 310 | LEU  |
| 1   | C     | 315 | LEU  |
| 1   | C     | 321 | LYS  |
| 1   | C     | 322 | TYR  |
| 1   | C     | 323 | LEU  |
| 1   | C     | 324 | TYR  |
| 1   | C     | 325 | ILE  |
| 1   | C     | 328 | THR  |
| 1   | C     | 333 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 337 | SER  |
| 1   | C     | 354 | LEU  |
| 1   | C     | 355 | ASN  |
| 1   | C     | 363 | LEU  |
| 1   | C     | 371 | ILE  |
| 1   | C     | 373 | VAL  |
| 1   | C     | 375 | VAL  |
| 1   | C     | 383 | VAL  |
| 1   | C     | 389 | THR  |
| 1   | C     | 390 | LEU  |
| 1   | C     | 394 | THR  |
| 1   | C     | 400 | GLU  |
| 1   | C     | 404 | LEU  |
| 1   | C     | 407 | SER  |
| 1   | C     | 412 | ARG  |
| 1   | C     | 414 | ASP  |
| 1   | C     | 419 | SER  |
| 1   | C     | 422 | LEU  |
| 1   | C     | 431 | LEU  |
| 1   | C     | 433 | PHE  |
| 1   | C     | 441 | ASP  |
| 1   | C     | 442 | LEU  |
| 1   | C     | 455 | ILE  |
| 1   | C     | 457 | TYR  |
| 1   | C     | 458 | SER  |
| 1   | C     | 460 | LEU  |
| 1   | C     | 467 | ILE  |
| 1   | C     | 469 | TRP  |
| 1   | C     | 471 | ASP  |
| 1   | C     | 474 | LYS  |
| 1   | C     | 477 | LEU  |
| 1   | C     | 484 | ILE  |
| 1   | C     | 486 | VAL  |
| 1   | C     | 493 | ILE  |
| 1   | C     | 495 | LYS  |
| 1   | C     | 497 | THR  |
| 1   | C     | 501 | TYR  |
| 1   | C     | 504 | LEU  |
| 1   | C     | 506 | LYS  |
| 1   | C     | 509 | ILE  |
| 1   | C     | 516 | GLU  |
| 1   | C     | 522 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 526 | ILE  |
| 1   | C     | 534 | MET  |
| 1   | C     | 535 | VAL  |
| 1   | C     | 540 | LEU  |
| 1   | C     | 541 | LEU  |
| 1   | C     | 543 | TYR  |
| 1   | C     | 545 | ILE  |
| 1   | C     | 547 | THR  |
| 1   | C     | 549 | GLU  |
| 1   | C     | 550 | GLN  |
| 1   | C     | 555 | VAL  |
| 1   | C     | 558 | SER  |
| 1   | C     | 559 | VAL  |
| 1   | C     | 561 | LEU  |
| 1   | C     | 563 | ILE  |
| 1   | C     | 567 | CYS  |
| 1   | C     | 569 | ASN  |
| 1   | C     | 573 | VAL  |
| 1   | C     | 580 | ASP  |
| 1   | C     | 587 | THR  |
| 1   | C     | 596 | MET  |
| 1   | C     | 597 | ASP  |
| 1   | C     | 605 | VAL  |
| 1   | C     | 613 | GLN  |
| 1   | C     | 614 | ARG  |
| 1   | C     | 618 | LYS  |
| 1   | C     | 620 | LEU  |
| 1   | C     | 621 | GLU  |
| 1   | C     | 625 | GLN  |
| 1   | C     | 627 | LEU  |
| 1   | C     | 630 | SER  |
| 1   | C     | 640 | LEU  |
| 1   | C     | 642 | ASN  |
| 1   | C     | 644 | ASN  |
| 1   | C     | 652 | THR  |
| 1   | C     | 653 | PHE  |
| 1   | C     | 654 | LEU  |
| 1   | C     | 663 | GLN  |
| 1   | C     | 664 | GLU  |
| 1   | C     | 667 | GLU  |
| 1   | C     | 672 | ILE  |
| 1   | C     | 692 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 695 | VAL  |
| 1   | C     | 697 | LYS  |
| 1   | C     | 699 | CYS  |
| 1   | C     | 701 | ASP  |
| 1   | C     | 707 | ASN  |
| 1   | C     | 710 | THR  |
| 1   | C     | 713 | GLN  |
| 1   | C     | 720 | LEU  |
| 1   | C     | 732 | CYS  |
| 1   | C     | 753 | HIS  |
| 1   | C     | 756 | THR  |
| 1   | C     | 758 | LEU  |
| 1   | C     | 767 | SER  |
| 1   | C     | 774 | LEU  |
| 1   | C     | 777 | VAL  |
| 1   | C     | 778 | HIS  |
| 1   | C     | 782 | ARG  |
| 1   | C     | 788 | PHE  |
| 1   | C     | 793 | SER  |
| 1   | C     | 795 | THR  |
| 1   | C     | 797 | TRP  |
| 1   | C     | 800 | GLN  |
| 1   | C     | 809 | ILE  |
| 1   | C     | 811 | VAL  |
| 1   | C     | 823 | VAL  |
| 1   | C     | 824 | PHE  |
| 1   | C     | 825 | LEU  |
| 1   | C     | 833 | VAL  |
| 1   | C     | 838 | GLN  |
| 1   | C     | 839 | ILE  |
| 1   | C     | 845 | VAL  |
| 1   | C     | 849 | ARG  |
| 1   | C     | 850 | THR  |
| 1   | C     | 854 | GLN  |
| 1   | C     | 856 | CYS  |
| 1   | C     | 857 | VAL  |
| 1   | C     | 859 | MET  |
| 1   | C     | 865 | ILE  |
| 1   | C     | 867 | THR  |
| 1   | C     | 876 | GLN  |
| 1   | C     | 887 | LYS  |
| 1   | C     | 895 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 896  | VAL  |
| 1   | C     | 899  | THR  |
| 1   | C     | 901  | LEU  |
| 1   | C     | 910  | ILE  |
| 1   | C     | 914  | LEU  |
| 1   | C     | 915  | GLU  |
| 1   | C     | 923  | LEU  |
| 1   | C     | 930  | VAL  |
| 1   | C     | 935  | LYS  |
| 1   | C     | 936  | ARG  |
| 1   | C     | 940  | SER  |
| 1   | C     | 944  | LEU  |
| 1   | C     | 947  | ARG  |
| 1   | C     | 952  | THR  |
| 1   | C     | 953  | ILE  |
| 1   | C     | 967  | LEU  |
| 1   | C     | 972  | GLU  |
| 1   | C     | 975  | ARG  |
| 1   | C     | 977  | LEU  |
| 1   | C     | 980  | LYS  |
| 1   | C     | 983  | LEU  |
| 1   | C     | 984  | VAL  |
| 1   | C     | 986  | GLU  |
| 1   | C     | 988  | LEU  |
| 1   | C     | 1001 | THR  |
| 1   | C     | 1002 | HIS  |
| 1   | C     | 1003 | LEU  |
| 1   | C     | 1007 | SER  |
| 1   | C     | 1011 | GLU  |
| 1   | C     | 1014 | SER  |
| 1   | C     | 1016 | VAL  |
| 1   | C     | 1018 | VAL  |
| 1   | C     | 1033 | ILE  |
| 1   | C     | 1055 | SER  |
| 1   | C     | 1056 | ILE  |
| 1   | C     | 1070 | LYS  |
| 1   | C     | 1076 | THR  |
| 1   | C     | 1078 | LEU  |
| 1   | C     | 1084 | ARG  |
| 1   | C     | 1089 | VAL  |
| 1   | C     | 1091 | LYS  |
| 1   | C     | 1098 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1105 | LEU  |
| 1   | C     | 1107 | LEU  |
| 1   | C     | 1108 | VAL  |
| 1   | C     | 1110 | ASN  |
| 1   | C     | 1113 | LEU  |
| 1   | C     | 1119 | LYS  |
| 1   | C     | 1127 | ILE  |
| 1   | C     | 1128 | LYS  |
| 1   | C     | 1129 | LEU  |
| 1   | C     | 1140 | ASN  |
| 1   | C     | 1148 | THR  |
| 1   | C     | 1163 | LYS  |
| 1   | C     | 1164 | ILE  |
| 1   | C     | 1166 | THR  |
| 1   | C     | 1168 | LEU  |
| 1   | C     | 1175 | LEU  |
| 1   | C     | 1176 | LEU  |
| 1   | C     | 1179 | THR  |
| 1   | C     | 1180 | LEU  |
| 1   | C     | 1183 | GLN  |
| 1   | C     | 1185 | THR  |
| 1   | C     | 1190 | ILE  |
| 1   | C     | 1196 | SER  |
| 1   | C     | 1200 | LYS  |
| 1   | C     | 1201 | THR  |
| 1   | C     | 1209 | VAL  |
| 1   | C     | 1212 | LEU  |
| 1   | C     | 1218 | VAL  |
| 1   | C     | 1227 | PHE  |
| 1   | C     | 1231 | ASN  |
| 1   | C     | 1236 | ASP  |
| 1   | C     | 1244 | THR  |
| 1   | C     | 1246 | ARG  |
| 1   | C     | 1255 | LEU  |
| 1   | C     | 1257 | THR  |
| 1   | C     | 1259 | LEU  |
| 1   | C     | 1264 | ILE  |
| 1   | C     | 1280 | TYR  |
| 1   | C     | 1294 | ILE  |
| 1   | C     | 1301 | SER  |
| 1   | C     | 1302 | LEU  |
| 1   | C     | 1303 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1306 | GLN  |
| 1   | C     | 1307 | LEU  |
| 1   | C     | 1309 | LEU  |
| 1   | C     | 1311 | MET  |
| 1   | C     | 1313 | ILE  |
| 1   | C     | 1323 | LEU  |
| 1   | C     | 1326 | TYR  |
| 1   | C     | 1331 | LYS  |
| 1   | C     | 1333 | PHE  |
| 1   | C     | 1334 | LEU  |
| 1   | C     | 1336 | ARG  |
| 1   | C     | 1338 | VAL  |
| 1   | C     | 1341 | LEU  |
| 1   | C     | 1346 | LEU  |
| 1   | C     | 1347 | ILE  |
| 1   | C     | 1348 | VAL  |
| 1   | C     | 1356 | LEU  |
| 1   | C     | 1358 | THR  |
| 1   | C     | 1361 | VAL  |
| 1   | C     | 1363 | THR  |
| 1   | C     | 1366 | HIS  |
| 1   | C     | 1367 | LYS  |
| 1   | C     | 1372 | GLU  |
| 1   | C     | 1374 | VAL  |
| 1   | C     | 1381 | ILE  |
| 1   | C     | 1397 | SER  |
| 1   | C     | 1414 | GLU  |
| 1   | C     | 1416 | SER  |
| 1   | C     | 1423 | VAL  |
| 1   | C     | 1433 | SER  |
| 1   | C     | 1443 | VAL  |
| 1   | C     | 1454 | GLN  |
| 1   | C     | 1457 | ASP  |
| 1   | C     | 1462 | LEU  |
| 1   | C     | 1464 | LEU  |
| 1   | C     | 1470 | SER  |
| 1   | C     | 1474 | CYS  |
| 1   | C     | 1475 | VAL  |
| 1   | C     | 1479 | ILE  |
| 1   | C     | 1480 | PHE  |
| 1   | C     | 1483 | PHE  |
| 1   | C     | 1487 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1488 | LEU  |
| 1   | C     | 1492 | THR  |
| 1   | C     | 1493 | PHE  |
| 1   | C     | 1494 | THR  |
| 1   | C     | 1495 | VAL  |
| 1   | C     | 1497 | GLU  |
| 1   | C     | 1500 | ARG  |
| 1   | C     | 1503 | LYS  |
| 1   | C     | 1504 | GLN  |
| 1   | C     | 1506 | THR  |
| 1   | C     | 1507 | MET  |
| 1   | C     | 1512 | SER  |
| 1   | C     | 1525 | CYS  |
| 1   | C     | 1535 | MET  |
| 1   | C     | 1542 | THR  |
| 1   | C     | 1544 | SER  |
| 1   | C     | 1548 | ARG  |
| 1   | C     | 1549 | LYS  |
| 1   | C     | 1553 | CYS  |
| 1   | C     | 1557 | ILE  |
| 1   | C     | 1565 | ILE  |
| 1   | C     | 1566 | THR  |
| 1   | C     | 1577 | TYR  |
| 1   | C     | 1580 | THR  |
| 1   | C     | 1581 | LEU  |
| 1   | C     | 1582 | LEU  |
| 1   | C     | 1585 | TYR  |
| 1   | C     | 1598 | ILE  |
| 1   | C     | 1602 | LYS  |
| 1   | C     | 1604 | VAL  |
| 1   | C     | 1605 | THR  |
| 1   | C     | 1606 | CYS  |
| 1   | C     | 1616 | GLN  |
| 1   | C     | 1618 | LEU  |
| 1   | C     | 1626 | GLN  |
| 1   | C     | 1627 | ILE  |
| 1   | C     | 1631 | PHE  |
| 1   | C     | 1636 | ILE  |
| 1   | C     | 1639 | LEU  |
| 1   | C     | 1651 | ASP  |
| 1   | C     | 1652 | THR  |
| 1   | C     | 1655 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1663 | ASN  |
| 2   | D     | 29   | THR  |
| 2   | D     | 40   | GLN  |
| 2   | D     | 43   | VAL  |
| 2   | D     | 54   | LEU  |
| 2   | D     | 56   | ILE  |
| 2   | D     | 58   | VAL  |
| 2   | D     | 68   | LEU  |
| 2   | D     | 71   | THR  |
| 2   | D     | 74   | ASP  |
| 2   | D     | 82   | LEU  |
| 2   | D     | 86   | THR  |
| 2   | D     | 87   | ILE  |
| 2   | D     | 100  | GLN  |
| 2   | D     | 103  | TYR  |
| 2   | D     | 105  | VAL  |
| 2   | D     | 106  | VAL  |
| 2   | D     | 108  | VAL  |
| 2   | D     | 113  | VAL  |
| 2   | D     | 114  | ARG  |
| 2   | D     | 119  | VAL  |
| 2   | D     | 120  | LEU  |
| 2   | D     | 121  | LEU  |
| 2   | D     | 124  | GLN  |
| 2   | D     | 144  | LEU  |
| 2   | D     | 147  | VAL  |
| 2   | D     | 161  | VAL  |
| 2   | D     | 162  | ILE  |
| 2   | D     | 167  | THR  |
| 2   | D     | 171  | ILE  |
| 2   | D     | 175  | SER  |
| 2   | D     | 176  | ASN  |
| 2   | D     | 177  | SER  |
| 2   | D     | 178  | VAL  |
| 2   | D     | 179  | ASP  |
| 2   | D     | 183  | PHE  |
| 2   | D     | 190  | ASP  |
| 2   | D     | 191  | LEU  |
| 2   | D     | 193  | SER  |
| 2   | D     | 196  | THR  |
| 2   | D     | 198  | ARG  |
| 2   | D     | 202  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 208 | GLU  |
| 2   | D     | 214 | PHE  |
| 2   | D     | 216 | VAL  |
| 2   | D     | 217 | ARG  |
| 2   | D     | 220 | VAL  |
| 2   | D     | 221 | LEU  |
| 2   | D     | 223 | SER  |
| 2   | D     | 226 | VAL  |
| 2   | D     | 231 | SER  |
| 2   | D     | 258 | GLU  |
| 2   | D     | 263 | VAL  |
| 2   | D     | 264 | LEU  |
| 2   | D     | 280 | LEU  |
| 2   | D     | 285 | ILE  |
| 2   | D     | 296 | ARG  |
| 2   | D     | 298 | THR  |
| 2   | D     | 301 | SER  |
| 2   | D     | 306 | LEU  |
| 2   | D     | 315 | TYR  |
| 2   | D     | 317 | SER  |
| 2   | D     | 323 | GLU  |
| 2   | D     | 327 | ASP  |
| 2   | D     | 328 | MET  |
| 2   | D     | 329 | VAL  |
| 2   | D     | 338 | ILE  |
| 2   | D     | 344 | GLN  |
| 2   | D     | 345 | ILE  |
| 2   | D     | 348 | THR  |
| 2   | D     | 349 | LYS  |
| 2   | D     | 358 | MET  |
| 2   | D     | 377 | VAL  |
| 2   | D     | 379 | VAL  |
| 2   | D     | 382 | GLU  |
| 2   | D     | 386 | SER  |
| 2   | D     | 389 | THR  |
| 2   | D     | 390 | THR  |
| 2   | D     | 398 | LEU  |
| 2   | D     | 400 | LEU  |
| 2   | D     | 402 | ILE  |
| 2   | D     | 414 | ARG  |
| 2   | D     | 416 | ASN  |
| 2   | D     | 422 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 427 | THR  |
| 2   | D     | 433 | ILE  |
| 2   | D     | 437 | THR  |
| 2   | D     | 449 | ILE  |
| 2   | D     | 460 | LEU  |
| 2   | D     | 466 | VAL  |
| 2   | D     | 469 | ASN  |
| 2   | D     | 473 | LEU  |
| 2   | D     | 481 | TYR  |
| 2   | D     | 482 | LEU  |
| 2   | D     | 483 | ILE  |
| 2   | D     | 488 | LYS  |
| 2   | D     | 497 | ARG  |
| 2   | D     | 504 | VAL  |
| 2   | D     | 505 | THR  |
| 2   | D     | 511 | THR  |
| 2   | D     | 513 | ASP  |
| 2   | D     | 514 | LEU  |
| 2   | D     | 515 | ILE  |
| 2   | D     | 518 | PHE  |
| 2   | D     | 521 | VAL  |
| 2   | D     | 524 | TYR  |
| 2   | D     | 525 | GLN  |
| 2   | D     | 526 | VAL  |
| 2   | D     | 531 | ILE  |
| 2   | D     | 532 | VAL  |
| 2   | D     | 543 | THR  |
| 2   | D     | 544 | CYS  |
| 2   | D     | 545 | MET  |
| 2   | D     | 555 | LEU  |
| 2   | D     | 556 | ILE  |
| 2   | D     | 558 | MET  |
| 2   | D     | 563 | MET  |
| 2   | D     | 564 | LYS  |
| 2   | D     | 567 | LEU  |
| 2   | D     | 582 | LYS  |
| 2   | D     | 586 | VAL  |
| 2   | D     | 588 | ASN  |
| 2   | D     | 593 | ILE  |
| 2   | D     | 597 | LYS  |
| 2   | D     | 598 | ILE  |
| 2   | D     | 602 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 613 | SER  |
| 2   | D     | 615 | GLN  |
| 2   | D     | 620 | VAL  |
| 2   | D     | 629 | THR  |
| 2   | D     | 638 | GLN  |
| 2   | D     | 735 | ASN  |
| 2   | D     | 736 | GLU  |
| 2   | D     | 742 | ASP  |
| 2   | D     | 745 | ILE  |
| 2   | D     | 746 | ILE  |
| 2   | D     | 747 | SER  |
| 2   | D     | 764 | GLU  |
| 2   | D     | 769 | GLN  |
| 2   | D     | 773 | SER  |
| 2   | D     | 778 | PHE  |
| 2   | D     | 780 | LEU  |
| 2   | D     | 784 | ILE  |
| 2   | D     | 786 | THR  |
| 2   | D     | 789 | VAL  |
| 2   | D     | 800 | ILE  |
| 2   | D     | 802 | VAL  |
| 2   | D     | 804 | GLU  |
| 2   | D     | 808 | ILE  |
| 2   | D     | 810 | VAL  |
| 2   | D     | 813 | VAL  |
| 2   | D     | 816 | ILE  |
| 2   | D     | 817 | ASP  |
| 2   | D     | 819 | GLN  |
| 2   | D     | 829 | GLN  |
| 2   | D     | 830 | VAL  |
| 2   | D     | 836 | LEU  |
| 2   | D     | 840 | VAL  |
| 2   | D     | 851 | LEU  |
| 2   | D     | 857 | CYS  |
| 2   | D     | 866 | TYR  |
| 2   | D     | 868 | GLN  |
| 2   | D     | 870 | PHE  |
| 2   | D     | 872 | ILE  |
| 2   | D     | 873 | LYS  |
| 2   | D     | 880 | VAL  |
| 2   | D     | 884 | ILE  |
| 2   | D     | 887 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 889  | GLN  |
| 2   | D     | 891  | LEU  |
| 2   | D     | 918  | GLU  |
| 2   | D     | 920  | VAL  |
| 2   | D     | 925  | VAL  |
| 2   | D     | 926  | THR  |
| 2   | D     | 944  | VAL  |
| 2   | D     | 946  | LYS  |
| 2   | D     | 948  | ARG  |
| 2   | D     | 949  | LYS  |
| 2   | D     | 952  | ASP  |
| 2   | D     | 963  | ILE  |
| 2   | D     | 964  | ILE  |
| 2   | D     | 1273 | LEU  |
| 2   | D     | 1274 | ASN  |
| 2   | D     | 1278 | THR  |
| 2   | D     | 1279 | ILE  |
| 2   | D     | 1281 | LEU  |
| 2   | D     | 1291 | ARG  |
| 2   | D     | 1292 | ILE  |
| 2   | D     | 1296 | ASN  |
| 2   | D     | 1301 | ARG  |
| 2   | D     | 1303 | VAL  |
| 2   | D     | 1305 | THR  |
| 2   | D     | 1308 | ASN  |
| 2   | D     | 1313 | VAL  |
| 2   | D     | 1322 | THR  |
| 2   | D     | 1324 | THR  |
| 2   | D     | 1326 | LEU  |
| 2   | D     | 1330 | ASN  |
| 2   | D     | 1332 | GLN  |
| 2   | D     | 1344 | HIS  |
| 2   | D     | 1345 | LEU  |
| 2   | D     | 1346 | ASN  |
| 2   | D     | 1349 | VAL  |
| 2   | D     | 1350 | GLU  |
| 2   | D     | 1351 | ASN  |
| 2   | D     | 1353 | HIS  |
| 2   | D     | 1365 | LEU  |
| 2   | D     | 1367 | ILE  |
| 2   | D     | 1372 | LEU  |
| 2   | D     | 1378 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 1380 | THR  |
| 2   | D     | 1388 | THR  |
| 2   | D     | 1398 | THR  |
| 2   | D     | 1401 | SER  |
| 2   | D     | 1404 | VAL  |
| 2   | D     | 1406 | ARG  |
| 2   | D     | 1415 | ASN  |
| 2   | D     | 1423 | VAL  |
| 2   | D     | 1424 | ILE  |
| 2   | D     | 1427 | LEU  |
| 2   | D     | 1429 | LYS  |
| 2   | D     | 1431 | SER  |
| 2   | D     | 1433 | SER  |
| 2   | D     | 1437 | CYS  |
| 2   | D     | 1438 | LEU  |
| 2   | D     | 1442 | ILE  |
| 2   | D     | 1443 | LEU  |
| 2   | D     | 1448 | VAL  |
| 2   | D     | 1451 | ILE  |
| 2   | D     | 1456 | VAL  |
| 2   | D     | 1464 | LEU  |
| 2   | D     | 1475 | ASP  |
| 2   | D     | 1480 | LEU  |
| 2   | D     | 1481 | LEU  |
| 2   | D     | 1490 | CYS  |
| 2   | D     | 1492 | CYS  |
| 2   | D     | 1495 | GLU  |
| 2   | D     | 1496 | THR  |
| 2   | D     | 1497 | CYS  |
| 2   | D     | 1500 | LEU  |
| 2   | D     | 1504 | GLU  |
| 2   | D     | 1516 | CYS  |
| 2   | D     | 1526 | THR  |
| 2   | D     | 1535 | ASP  |
| 2   | D     | 1566 | GLN  |
| 2   | D     | 1571 | GLU  |
| 2   | D     | 1582 | LEU  |
| 2   | D     | 1583 | ILE  |
| 2   | D     | 1584 | TRP  |
| 2   | D     | 1590 | LEU  |
| 2   | D     | 1594 | LYS  |
| 2   | D     | 1598 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 1599 | TYR  |
| 2   | D     | 1601 | ILE  |
| 2   | D     | 1604 | ASN  |
| 2   | D     | 1605 | THR  |
| 2   | D     | 1606 | TRP  |
| 2   | D     | 1607 | ILE  |
| 2   | D     | 1609 | ARG  |
| 2   | D     | 1612 | HIS  |
| 2   | D     | 1613 | GLU  |
| 2   | D     | 1614 | ASP  |
| 2   | D     | 1622 | GLN  |
| 2   | D     | 1623 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | GLN  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 97  | ASN  |
| 1   | A     | 139 | GLN  |
| 1   | A     | 242 | ASN  |
| 1   | A     | 257 | ASN  |
| 1   | A     | 288 | GLN  |
| 1   | A     | 298 | GLN  |
| 1   | A     | 355 | ASN  |
| 1   | A     | 391 | ASN  |
| 1   | A     | 472 | ASN  |
| 1   | A     | 473 | HIS  |
| 1   | A     | 483 | ASN  |
| 1   | A     | 569 | ASN  |
| 1   | A     | 570 | GLN  |
| 1   | A     | 574 | HIS  |
| 1   | A     | 613 | GLN  |
| 1   | A     | 647 | HIS  |
| 1   | A     | 692 | HIS  |
| 1   | A     | 706 | ASN  |
| 1   | A     | 785 | GLN  |
| 1   | A     | 787 | GLN  |
| 1   | A     | 800 | GLN  |
| 1   | A     | 847 | ASN  |
| 1   | A     | 854 | GLN  |
| 1   | A     | 875 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 876  | GLN  |
| 1   | A     | 894  | HIS  |
| 1   | A     | 1023 | HIS  |
| 1   | A     | 1061 | ASN  |
| 1   | A     | 1095 | GLN  |
| 1   | A     | 1102 | ASN  |
| 1   | A     | 1112 | GLN  |
| 1   | A     | 1130 | GLN  |
| 1   | A     | 1183 | GLN  |
| 1   | A     | 1234 | HIS  |
| 1   | A     | 1241 | ASN  |
| 1   | A     | 1260 | ASN  |
| 1   | A     | 1268 | ASN  |
| 1   | A     | 1292 | ASN  |
| 1   | A     | 1319 | HIS  |
| 1   | A     | 1366 | HIS  |
| 1   | A     | 1448 | GLN  |
| 1   | A     | 1550 | GLN  |
| 1   | A     | 1608 | ASN  |
| 1   | A     | 1616 | GLN  |
| 1   | A     | 1658 | GLN  |
| 2   | B     | 40   | GLN  |
| 2   | B     | 65   | GLN  |
| 2   | B     | 124  | GLN  |
| 2   | B     | 152  | HIS  |
| 2   | B     | 176  | ASN  |
| 2   | B     | 187  | ASN  |
| 2   | B     | 312  | HIS  |
| 2   | B     | 333  | GLN  |
| 2   | B     | 337  | HIS  |
| 2   | B     | 344  | GLN  |
| 2   | B     | 417  | HIS  |
| 2   | B     | 469  | ASN  |
| 2   | B     | 525  | GLN  |
| 2   | B     | 528  | ASN  |
| 2   | B     | 588  | ASN  |
| 2   | B     | 615  | GLN  |
| 2   | B     | 735  | ASN  |
| 2   | B     | 819  | GLN  |
| 2   | B     | 829  | GLN  |
| 2   | B     | 869  | GLN  |
| 2   | B     | 889  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 901  | GLN  |
| 2   | B     | 921  | GLN  |
| 2   | B     | 1270 | HIS  |
| 2   | B     | 1330 | ASN  |
| 2   | B     | 1341 | ASN  |
| 2   | B     | 1344 | HIS  |
| 2   | B     | 1419 | GLN  |
| 2   | B     | 1473 | HIS  |
| 2   | B     | 1482 | ASN  |
| 2   | B     | 1501 | ASN  |
| 2   | B     | 1503 | GLN  |
| 2   | B     | 1561 | HIS  |
| 2   | B     | 1562 | GLN  |
| 1   | C     | 80   | GLN  |
| 1   | C     | 91   | GLN  |
| 1   | C     | 97   | ASN  |
| 1   | C     | 139  | GLN  |
| 1   | C     | 242  | ASN  |
| 1   | C     | 257  | ASN  |
| 1   | C     | 294  | ASN  |
| 1   | C     | 298  | GLN  |
| 1   | C     | 355  | ASN  |
| 1   | C     | 374  | GLN  |
| 1   | C     | 391  | ASN  |
| 1   | C     | 472  | ASN  |
| 1   | C     | 473  | HIS  |
| 1   | C     | 569  | ASN  |
| 1   | C     | 570  | GLN  |
| 1   | C     | 574  | HIS  |
| 1   | C     | 613  | GLN  |
| 1   | C     | 647  | HIS  |
| 1   | C     | 692  | HIS  |
| 1   | C     | 706  | ASN  |
| 1   | C     | 785  | GLN  |
| 1   | C     | 787  | GLN  |
| 1   | C     | 800  | GLN  |
| 1   | C     | 854  | GLN  |
| 1   | C     | 875  | HIS  |
| 1   | C     | 876  | GLN  |
| 1   | C     | 894  | HIS  |
| 1   | C     | 1023 | HIS  |
| 1   | C     | 1061 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1095 | GLN  |
| 1   | C     | 1102 | ASN  |
| 1   | C     | 1112 | GLN  |
| 1   | C     | 1130 | GLN  |
| 1   | C     | 1183 | GLN  |
| 1   | C     | 1234 | HIS  |
| 1   | C     | 1241 | ASN  |
| 1   | C     | 1260 | ASN  |
| 1   | C     | 1268 | ASN  |
| 1   | C     | 1319 | HIS  |
| 1   | C     | 1324 | HIS  |
| 1   | C     | 1366 | HIS  |
| 1   | C     | 1448 | GLN  |
| 1   | C     | 1534 | GLN  |
| 1   | C     | 1550 | GLN  |
| 1   | C     | 1608 | ASN  |
| 1   | C     | 1616 | GLN  |
| 1   | C     | 1658 | GLN  |
| 2   | D     | 40   | GLN  |
| 2   | D     | 65   | GLN  |
| 2   | D     | 124  | GLN  |
| 2   | D     | 152  | HIS  |
| 2   | D     | 176  | ASN  |
| 2   | D     | 187  | ASN  |
| 2   | D     | 312  | HIS  |
| 2   | D     | 333  | GLN  |
| 2   | D     | 337  | HIS  |
| 2   | D     | 344  | GLN  |
| 2   | D     | 346  | HIS  |
| 2   | D     | 416  | ASN  |
| 2   | D     | 417  | HIS  |
| 2   | D     | 469  | ASN  |
| 2   | D     | 507  | ASN  |
| 2   | D     | 525  | GLN  |
| 2   | D     | 528  | ASN  |
| 2   | D     | 588  | ASN  |
| 2   | D     | 615  | GLN  |
| 2   | D     | 735  | ASN  |
| 2   | D     | 819  | GLN  |
| 2   | D     | 829  | GLN  |
| 2   | D     | 869  | GLN  |
| 2   | D     | 889  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 901  | GLN  |
| 2   | D     | 921  | GLN  |
| 2   | D     | 1270 | HIS  |
| 2   | D     | 1330 | ASN  |
| 2   | D     | 1341 | ASN  |
| 2   | D     | 1344 | HIS  |
| 2   | D     | 1419 | GLN  |
| 2   | D     | 1463 | ASN  |
| 2   | D     | 1473 | HIS  |
| 2   | D     | 1482 | ASN  |
| 2   | D     | 1501 | ASN  |
| 2   | D     | 1503 | GLN  |
| 2   | D     | 1561 | HIS  |
| 2   | D     | 1562 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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 |
| 3   | NAG  | B     | 2001 | 2    | 14,14,15     | 0.85 | 1 (7%)   | 17,19,21    | 2.08 | 3 (17%)  |
| 3   | NAG  | D     | 2002 | 2    | 14,14,15     | 0.94 | 0        | 17,19,21    | 1.18 | 1 (5%)   |
| 3   | NAG  | C     | 2003 | 1    | 14,14,15     | 0.59 | 0        | 17,19,21    | 2.24 | 4 (23%)  |
| 3   | NAG  | B     | 2002 | 2    | 14,14,15     | 0.94 | 0        | 17,19,21    | 1.19 | 1 (5%)   |
| 3   | NAG  | D     | 2001 | 2    | 14,14,15     | 0.78 | 1 (7%)   | 17,19,21    | 2.17 | 3 (17%)  |
| 3   | NAG  | A     | 2003 | 1    | 14,14,15     | 0.61 | 0        | 17,19,21    | 2.22 | 4 (23%)  |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | NAG  | B     | 2001 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | D     | 2002 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 2003 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 2002 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | D     | 2001 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 2003 | 1    | -       | 3/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | B     | 2001 | NAG  | C1-C2 | 2.36 | 1.55        | 1.52     |
| 3   | D     | 2001 | NAG  | C1-C2 | 2.08 | 1.55        | 1.52     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 2001 | NAG  | C1-O5-C5 | 6.65  | 121.10      | 112.19   |
| 3   | B     | 2001 | NAG  | C1-O5-C5 | 6.25  | 120.56      | 112.19   |
| 3   | A     | 2003 | NAG  | C1-O5-C5 | 5.76  | 119.91      | 112.19   |
| 3   | C     | 2003 | NAG  | C1-O5-C5 | 5.74  | 119.87      | 112.19   |
| 3   | C     | 2003 | NAG  | C4-C3-C2 | 4.36  | 117.41      | 111.02   |
| 3   | A     | 2003 | NAG  | C4-C3-C2 | 4.24  | 117.23      | 111.02   |
| 3   | B     | 2001 | NAG  | O5-C1-C2 | 3.99  | 117.46      | 111.29   |
| 3   | B     | 2002 | NAG  | O5-C1-C2 | -3.78 | 105.45      | 111.29   |
| 3   | D     | 2002 | NAG  | O5-C1-C2 | -3.76 | 105.48      | 111.29   |
| 3   | D     | 2001 | NAG  | O5-C1-C2 | 3.70  | 117.02      | 111.29   |
| 3   | C     | 2003 | NAG  | C1-C2-N2 | -3.40 | 105.07      | 110.43   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | A     | 2003 | NAG  | C1-C2-N2 | -3.29 | 105.25      | 110.43   |
| 3   | A     | 2003 | NAG  | C3-C4-C5 | 2.94  | 115.56      | 110.23   |
| 3   | C     | 2003 | NAG  | C3-C4-C5 | 2.90  | 115.50      | 110.23   |
| 3   | D     | 2001 | NAG  | C2-N2-C7 | -2.73 | 119.24      | 122.90   |
| 3   | B     | 2001 | NAG  | C2-N2-C7 | -2.53 | 119.52      | 122.90   |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 3   | A     | 2003 | NAG  | C3-C2-N2-C7 |
| 3   | A     | 2003 | NAG  | C8-C7-N2-C2 |
| 3   | A     | 2003 | NAG  | O7-C7-N2-C2 |
| 3   | B     | 2001 | NAG  | C8-C7-N2-C2 |
| 3   | B     | 2001 | NAG  | O7-C7-N2-C2 |
| 3   | C     | 2003 | NAG  | C3-C2-N2-C7 |
| 3   | C     | 2003 | NAG  | C8-C7-N2-C2 |
| 3   | C     | 2003 | NAG  | O7-C7-N2-C2 |
| 3   | D     | 2001 | NAG  | C8-C7-N2-C2 |
| 3   | D     | 2001 | NAG  | O7-C7-N2-C2 |

There are no ring outliers.

4 monomers are involved in 6 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | B     | 2001 | NAG  | 1       | 0            |
| 3   | C     | 2003 | NAG  | 2       | 0            |
| 3   | D     | 2001 | NAG  | 1       | 0            |
| 3   | A     | 2003 | NAG  | 2       | 0            |

## 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| 1   | A     | 1627/1676 (97%) | 0.23   | 28 (1%)  | 69 | 54 | 90, 187, 312, 465     | 0     |
| 1   | C     | 1627/1676 (97%) | 0.27   | 47 (2%)  | 53 | 41 | 97, 186, 299, 486     | 0     |
| 2   | B     | 1225/1642 (74%) | 0.14   | 14 (1%)  | 78 | 62 | 107, 174, 261, 395    | 0     |
| 2   | D     | 1225/1642 (74%) | 0.17   | 20 (1%)  | 70 | 55 | 114, 181, 263, 371    | 0     |
| All | All   | 5704/6636 (85%) | 0.21   | 109 (1%) | 66 | 51 | 90, 183, 291, 486     | 0     |

All (109) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 490  | SER  | 4.4  |
| 2   | D     | 642  | ALA  | 3.8  |
| 1   | A     | 1449 | LEU  | 3.8  |
| 1   | C     | 997  | ILE  | 3.7  |
| 2   | B     | 111  | PRO  | 3.6  |
| 1   | A     | 760  | VAL  | 3.5  |
| 2   | B     | 1401 | SER  | 3.4  |
| 1   | A     | 255  | PHE  | 3.4  |
| 2   | D     | 23   | ALA  | 3.3  |
| 2   | B     | 123  | TYR  | 3.3  |
| 1   | A     | 44   | TYR  | 3.3  |
| 1   | A     | 310  | LEU  | 3.1  |
| 1   | A     | 628  | GLU  | 3.1  |
| 1   | A     | 318  | LEU  | 3.1  |
| 1   | C     | 999  | ILE  | 3.0  |
| 1   | C     | 492  | TYR  | 3.0  |
| 2   | B     | 1435 | ASP  | 3.0  |
| 1   | A     | 30   | ILE  | 3.0  |
| 1   | A     | 1572 | ASN  | 3.0  |
| 1   | C     | 1676 | CYS  | 2.9  |
| 1   | A     | 33   | VAL  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1628 | LYS  | 2.9  |
| 1   | A     | 1656 | SER  | 2.7  |
| 1   | C     | 870  | SER  | 2.7  |
| 1   | C     | 1656 | SER  | 2.7  |
| 1   | C     | 460  | LEU  | 2.7  |
| 1   | C     | 661  | ASP  | 2.7  |
| 1   | C     | 939  | TYR  | 2.7  |
| 1   | C     | 1662 | ALA  | 2.7  |
| 1   | C     | 861  | ALA  | 2.6  |
| 2   | B     | 190  | ASP  | 2.6  |
| 1   | C     | 489  | LYS  | 2.6  |
| 1   | C     | 1279 | ARG  | 2.6  |
| 1   | C     | 20   | GLU  | 2.6  |
| 2   | D     | 159  | LYS  | 2.6  |
| 1   | C     | 1655 | SER  | 2.6  |
| 1   | A     | 1242 | THR  | 2.6  |
| 1   | C     | 440  | PRO  | 2.6  |
| 1   | C     | 315  | LEU  | 2.5  |
| 1   | C     | 493  | ILE  | 2.5  |
| 2   | B     | 1298 | LEU  | 2.5  |
| 1   | A     | 1335 | GLY  | 2.5  |
| 1   | C     | 44   | TYR  | 2.5  |
| 2   | B     | 1492 | CYS  | 2.4  |
| 1   | A     | 36   | SER  | 2.4  |
| 2   | D     | 1626 | ASP  | 2.4  |
| 1   | C     | 127  | PHE  | 2.4  |
| 1   | C     | 1585 | TYR  | 2.4  |
| 2   | D     | 1625 | CYS  | 2.4  |
| 1   | C     | 627  | LEU  | 2.4  |
| 1   | C     | 240  | TYR  | 2.4  |
| 1   | A     | 921  | GLU  | 2.3  |
| 1   | A     | 1227 | PHE  | 2.3  |
| 1   | C     | 1528 | VAL  | 2.3  |
| 1   | A     | 661  | ASP  | 2.3  |
| 1   | A     | 700  | TYR  | 2.3  |
| 2   | D     | 1624 | LEU  | 2.3  |
| 2   | D     | 1612 | HIS  | 2.3  |
| 1   | A     | 997  | ILE  | 2.3  |
| 2   | B     | 1611 | PRO  | 2.3  |
| 1   | C     | 686  | ILE  | 2.3  |
| 2   | D     | 225  | GLU  | 2.3  |
| 1   | C     | 1238 | SER  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 429  | SER  | 2.3  |
| 2   | D     | 1352 | ILE  | 2.2  |
| 1   | A     | 49   | ALA  | 2.2  |
| 1   | C     | 324  | TYR  | 2.2  |
| 1   | C     | 722  | PRO  | 2.2  |
| 1   | C     | 1644 | TRP  | 2.2  |
| 2   | D     | 1629 | ALA  | 2.2  |
| 1   | A     | 66   | TYR  | 2.2  |
| 2   | D     | 862  | LYS  | 2.2  |
| 1   | C     | 318  | LEU  | 2.2  |
| 2   | D     | 1617 | GLN  | 2.2  |
| 1   | C     | 507  | GLY  | 2.2  |
| 2   | D     | 1515 | ALA  | 2.2  |
| 1   | A     | 470  | THR  | 2.2  |
| 1   | C     | 1640 | ASP  | 2.2  |
| 2   | D     | 647  | PRO  | 2.2  |
| 1   | C     | 1178 | ASN  | 2.2  |
| 1   | A     | 672  | ILE  | 2.2  |
| 2   | B     | 404  | LEU  | 2.2  |
| 2   | D     | 1354 | LEU  | 2.2  |
| 1   | A     | 1219 | LYS  | 2.1  |
| 1   | C     | 682  | LYS  | 2.1  |
| 1   | C     | 47   | THR  | 2.1  |
| 1   | C     | 850  | THR  | 2.1  |
| 1   | C     | 872  | VAL  | 2.1  |
| 1   | A     | 664  | GLU  | 2.1  |
| 2   | B     | 1613 | GLU  | 2.1  |
| 1   | C     | 260  | VAL  | 2.1  |
| 2   | D     | 1333 | LEU  | 2.1  |
| 1   | C     | 519  | SER  | 2.1  |
| 2   | D     | 95   | SER  | 2.1  |
| 1   | A     | 922  | ILE  | 2.0  |
| 1   | A     | 1574 | PHE  | 2.0  |
| 2   | B     | 23   | ALA  | 2.0  |
| 2   | B     | 1445 | HIS  | 2.0  |
| 2   | D     | 1639 | GLY  | 2.0  |
| 1   | C     | 472  | ASN  | 2.0  |
| 1   | C     | 965  | LEU  | 2.0  |
| 1   | C     | 1541 | LEU  | 2.0  |
| 1   | C     | 1673 | LEU  | 2.0  |
| 2   | B     | 1626 | ASP  | 2.0  |
| 1   | C     | 1649 | PRO  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 1513 | ASN  | 2.0  |
| 2   | D     | 568  | GLU  | 2.0  |
| 2   | D     | 1298 | LEU  | 2.0  |
| 1   | C     | 246  | PHE  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | NAG  | B     | 2001 | 14/15 | 0.61 | 0.14 | 275,285,305,313             | 0     |
| 3   | NAG  | A     | 2003 | 14/15 | 0.62 | 0.21 | 284,286,289,289             | 0     |
| 3   | NAG  | B     | 2002 | 14/15 | 0.65 | 0.27 | 321,327,336,339             | 0     |
| 3   | NAG  | D     | 2002 | 14/15 | 0.66 | 0.19 | 289,293,305,308             | 0     |
| 3   | NAG  | D     | 2001 | 14/15 | 0.74 | 0.14 | 285,296,309,310             | 0     |
| 3   | NAG  | C     | 2003 | 14/15 | 0.81 | 0.19 | 260,272,284,287             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.