



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 11:30 AM EDT

PDB ID : 3HMJ  
Title : Saccharomyces cerevisiae FAS type I  
Authors : Johansson, P.; Mulinacci, B.; Koestler, C.; Vollrath, R.; Oesterhelt, D.;  
Grininger, M.  
Deposited on : 2009-05-29  
Resolution : 4.00 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

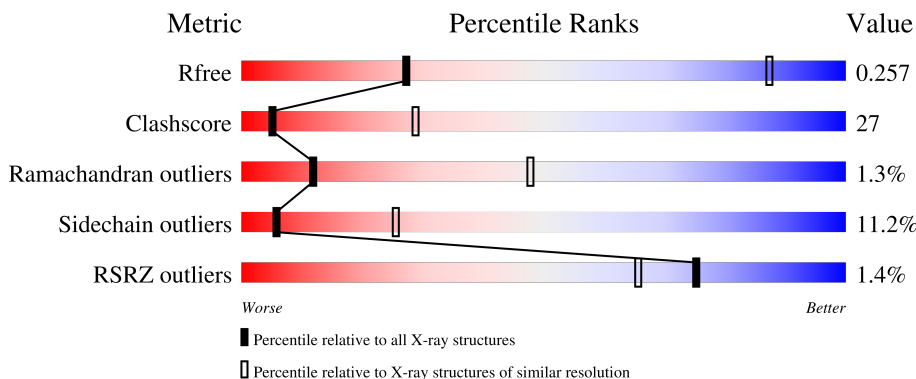
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1087 (4.30-3.70)                                      |
| Clashscore            | 141614                      | 1148 (4.30-3.70)                                      |
| Ramachandran outliers | 138981                      | 1108 (4.30-3.70)                                      |
| Sidechain outliers    | 138945                      | 1099 (4.30-3.70)                                      |
| RSRZ outliers         | 127900                      | 1028 (4.34-3.66)                                      |

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     | 1887   | <br>2% 55% 32% 5% 7% |
| 1   | B     | 1887   | <br>2% 55% 32% 5% 7% |
| 1   | C     | 1887   | <br>3% 54% 33% 5% 7% |
| 2   | G     | 2051   | <br>51% 40% 8% .     |
| 2   | H     | 2051   | <br>51% 40% 8% .     |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | I     | 2051   | <br>51% 40% 8% |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 88830 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.

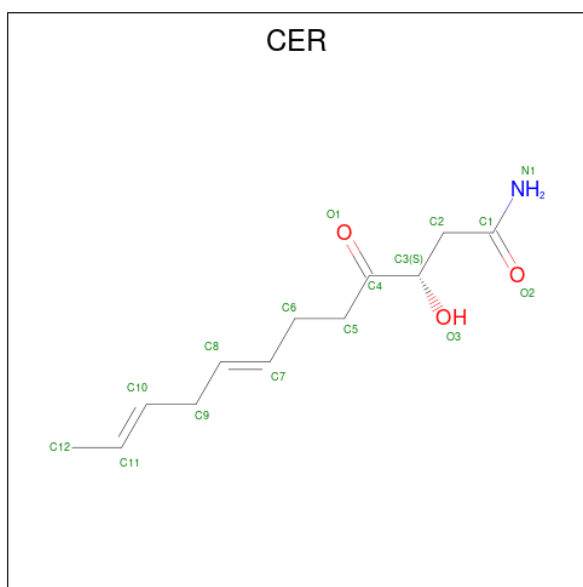
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
|     |       |          | Total | C    | N    | O    | S  |         |         |       |
| 1   | A     | 1750     | 13572 | 8594 | 2292 | 2637 | 49 | 0       | 0       | 0     |
| 1   | B     | 1750     | 13572 | 8594 | 2292 | 2637 | 49 | 0       | 0       | 0     |
| 1   | C     | 1750     | 13572 | 8594 | 2292 | 2637 | 49 | 0       | 0       | 0     |

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

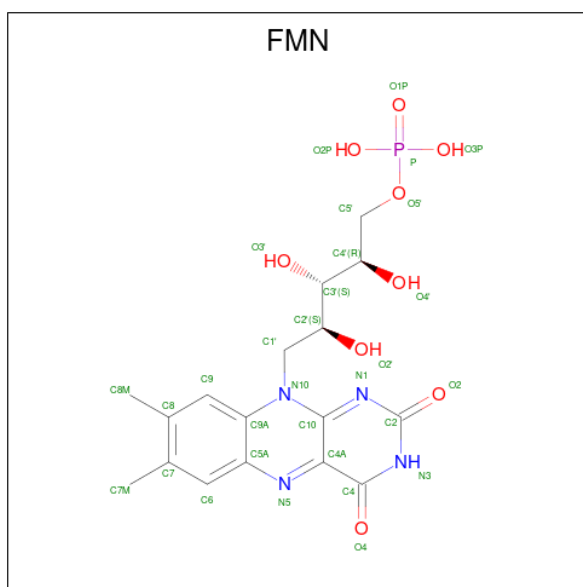
| Mol | Chain | Residues | Atoms |       |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|---------|-------|
|     |       |          | Total | C     | N    | O    | S  |         |         |       |
| 2   | G     | 2033     | 15995 | 10253 | 2660 | 3026 | 56 | 0       | 0       | 0     |
| 2   | H     | 2033     | 15995 | 10253 | 2660 | 3026 | 56 | 0       | 0       | 0     |
| 2   | I     | 2033     | 15995 | 10253 | 2660 | 3026 | 56 | 0       | 0       | 0     |

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: C<sub>12</sub>H<sub>19</sub>NO<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 8 | 1 | 3 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 8 | 1 | 3 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 8 | 1 | 3 |         |         |

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 4   | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |         |

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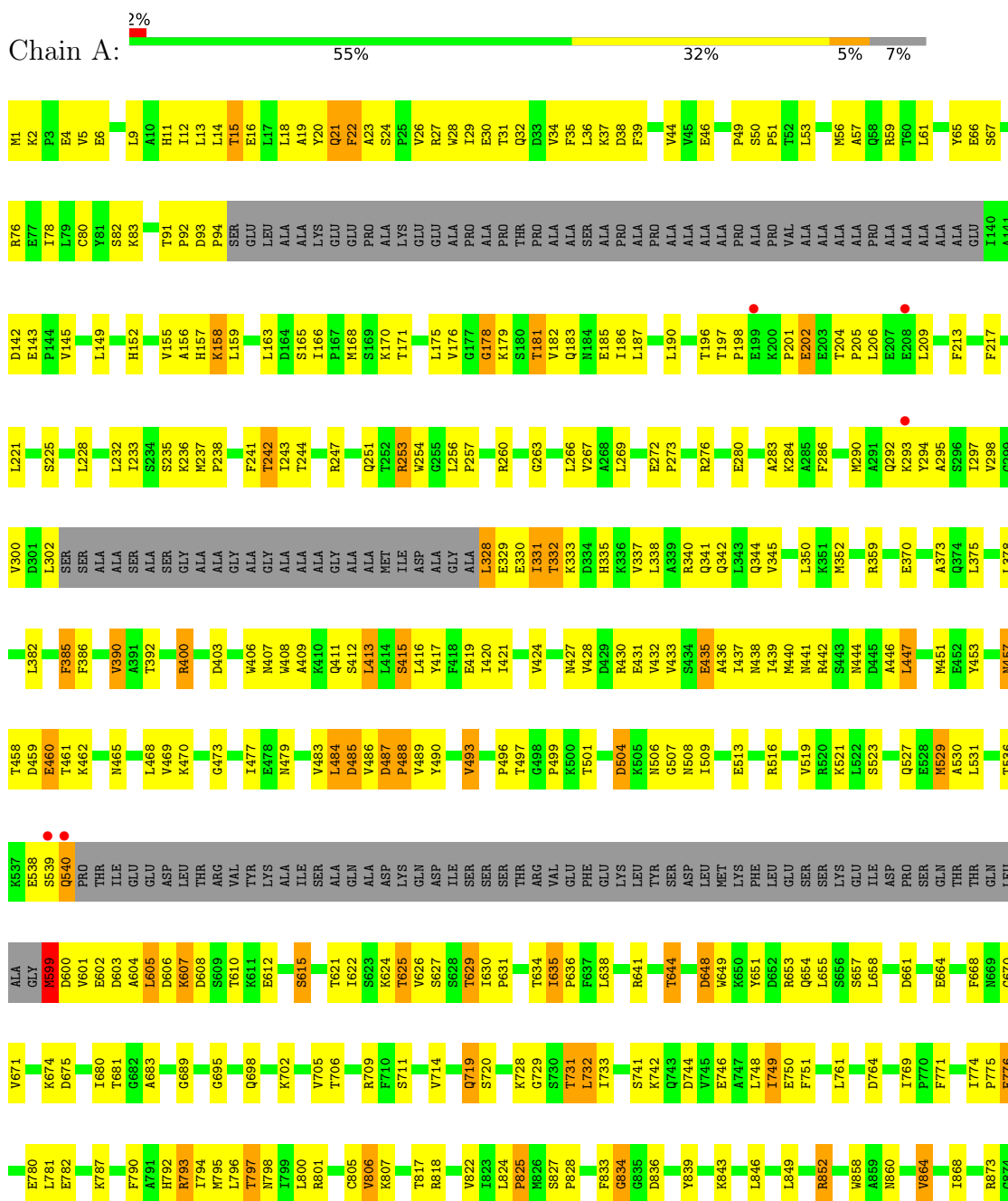
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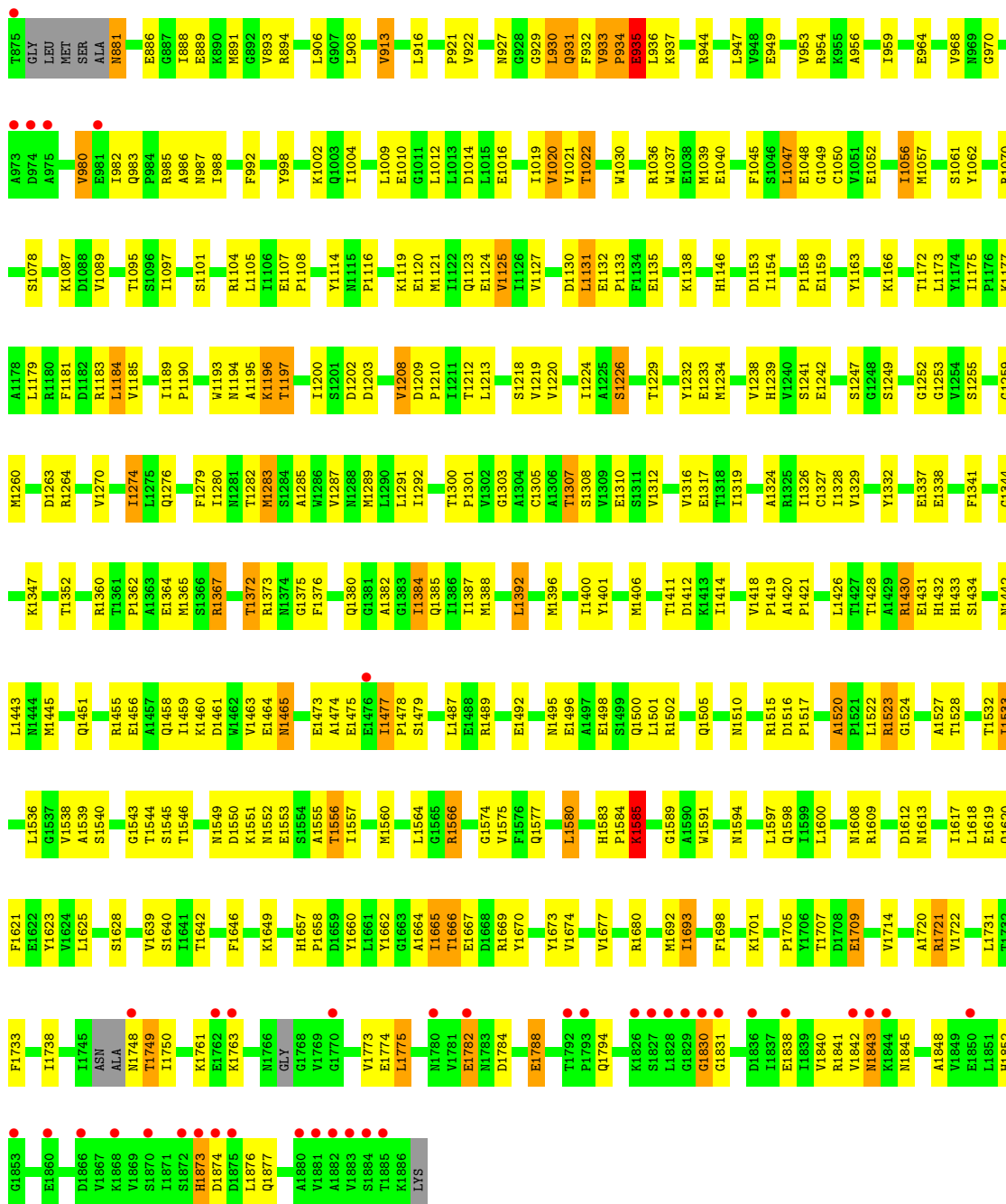
| <b>Mol</b> | <b>Chain</b> | <b>Residues</b> | <b>Atoms</b> |    |   |   |   | <b>ZeroOcc</b> | <b>AltConf</b> |
|------------|--------------|-----------------|--------------|----|---|---|---|----------------|----------------|
| 4          | H            | 1               | Total        | C  | N | O | P | 0              | 0              |
|            |              |                 | 31           | 17 | 4 | 9 | 1 |                |                |
| 4          | I            | 1               | Total        | C  | N | O | P | 0              | 0              |
|            |              |                 | 31           | 17 | 4 | 9 | 1 |                |                |

### 3 Residue-property plots

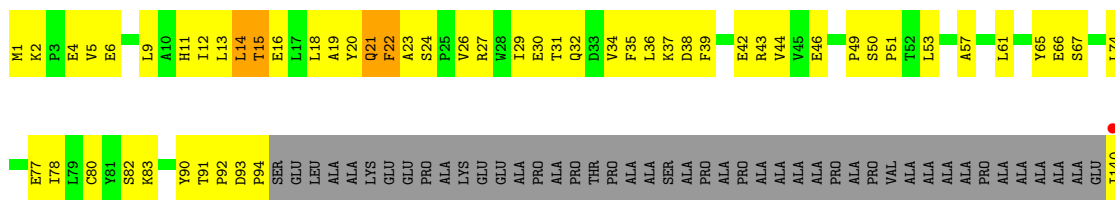
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fatty acid synthase subunit alpha



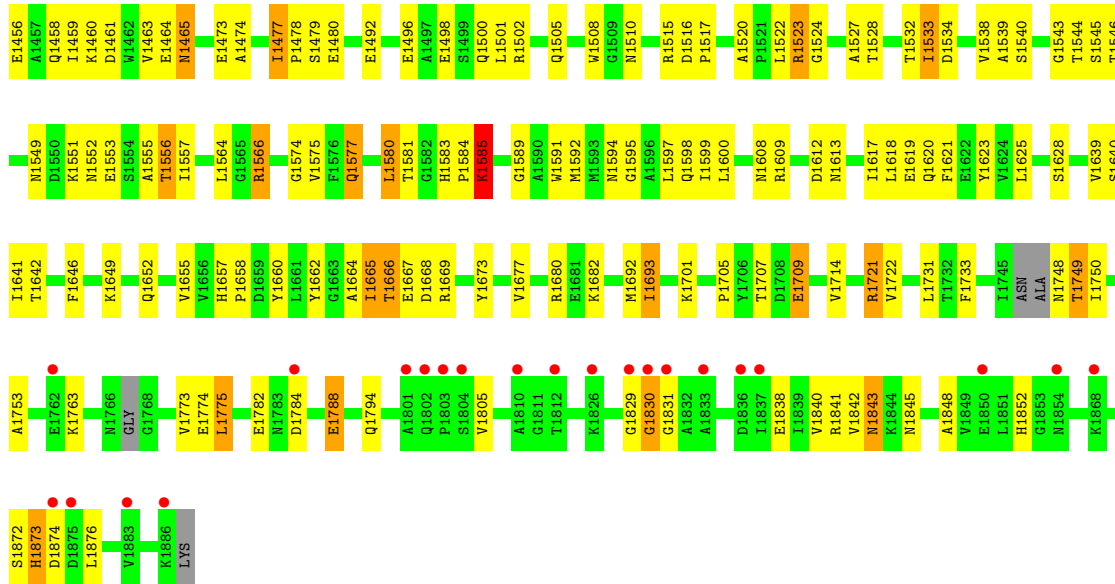


● Molecule 1: Fatty acid synthase subunit alpha

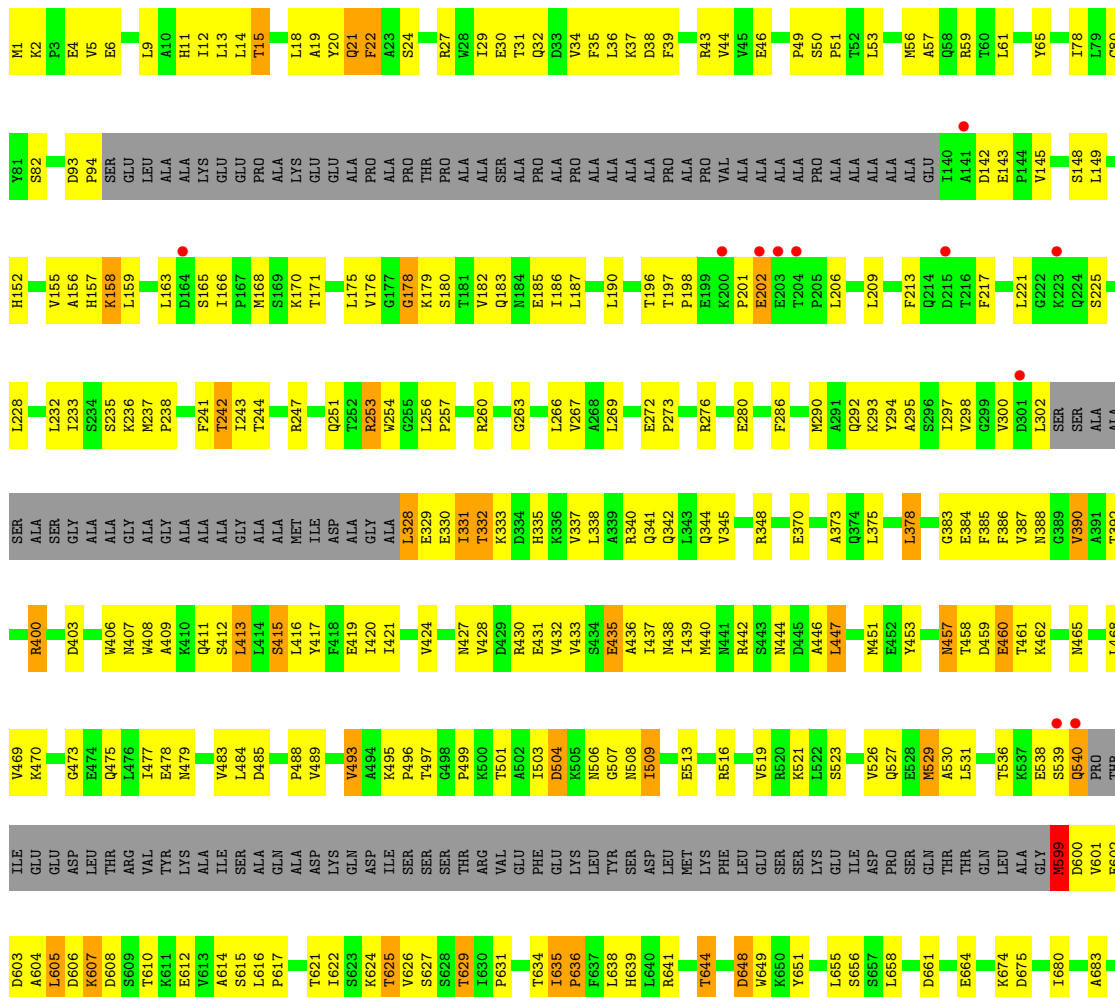


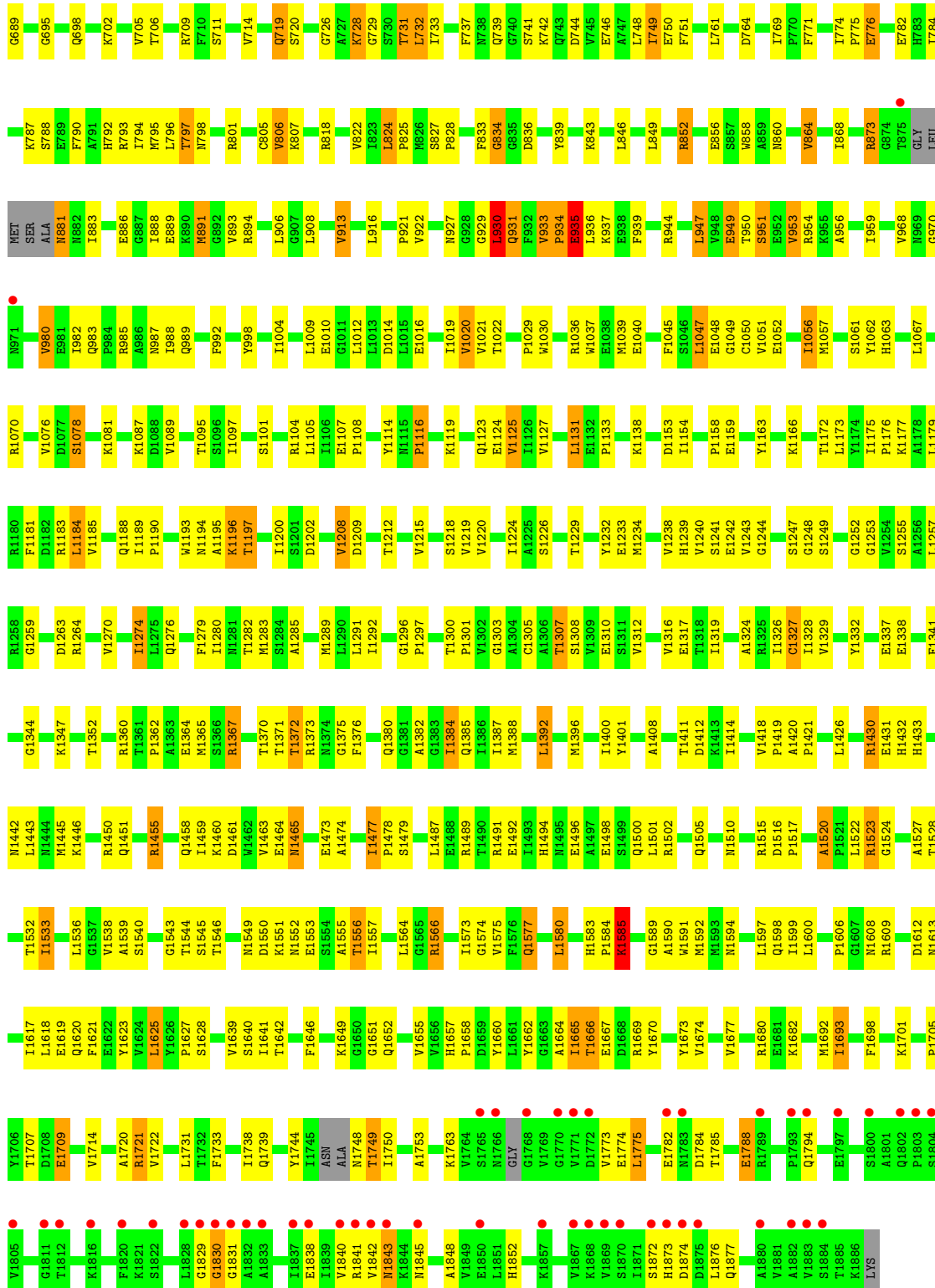


|       |       |       |       |       |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|
| S1366 | I1280 | W1193 | K1087 | Y982  | SER  | G689 | GLY  | E538 | D469 | F386 | L302 | S225 | A141 |
| R1367 | M1281 | M1194 | D1088 | R985  | ALA  | G695 | M899 | S539 | E460 | V390 | SER  | S235 | D142 |
| T1370 | M1282 | A1195 | V1089 | R885  | M882 | T788 | D600 | Q540 | T461 | A391 | ALA  | L228 | E143 |
| T1371 | S1284 | K1196 | T1095 | I883  | F790 | Q698 | V601 | THR  | K462 | T392 | SER  | L232 | V145 |
| T1372 | A1285 | T1197 | S1096 | Q989  | A604 | K702 | A604 | ILE  | M465 | R400 | ALA  | L233 | L149 |
| R1373 | W1200 | T1197 | I1097 | F992  | G887 | R705 | L605 | GLU  | L466 | T401 | SER  | S294 | H152 |
| M1374 | M1287 | S1201 | S1101 | Y998  | I888 | T706 | D606 | ASP  | V469 | F402 | GLY  | K236 | V155 |
| F1376 | M1289 | D1202 | R1104 | Y998  | E889 | M795 | K607 | LEU  | K470 | D403 | ALA  | M237 | A156 |
| Q1380 | I1292 | V1208 | L1105 | I1004 | M891 | R709 | S609 | ARG  | G473 | W406 | GLY  | P238 | H157 |
| P1297 | T1212 | D1209 | Y1114 | L1009 | G892 | F710 | T610 | VAL  | I477 | W407 | ALA  | F241 | K188 |
| T1300 | M1115 | T1212 | M1115 | L1010 | R801 | S711 | K611 | TYR  | E478 | W408 | GLY  | T242 | L163 |
| P1301 | P1116 | L1216 | P1116 | G1011 | V714 | V714 | E812 | LYS  | E479 | A409 | ALA  | T244 | D164 |
| V1302 | K1119 | L1013 | L1013 | L908  | C805 | Q719 | S615 | ILE  | M479 | K410 | ALA  | R247 | S165 |
| G1303 | L1014 | S1218 | D1014 | L908  | V806 | S720 | T621 | ALA  | V483 | S412 | GLY  | Q251 | K170 |
| A1304 | V1219 | V1219 | L1015 | V913  | K807 | S720 | I622 | GLN  | L484 | L413 | ALA  | R247 | T171 |
| C1305 | E1124 | E1124 | L1016 | V913  | R818 | G726 | S623 | ALA  | P488 | S415 | ALA  | Q251 | L175 |
| S1306 | V1125 | V1125 | E1016 | L916  | A727 | A727 | K624 | ASP  | V488 | L416 | MET  | T252 | G177 |
| T1307 | I1126 | I1126 | I1019 | P921  | K728 | K728 | T625 | ASP  | V489 | L416 | ILE  | R253 | S169 |
| S1308 | V1127 | V1127 | V1020 | P921  | G729 | G729 | V626 | LYS  | Y417 | Y417 | ASP  | W254 | K170 |
| V1309 | E1128 | E1128 | V1021 | V922  | S730 | S730 | S627 | ASP  | V493 | F418 | ALA  | G255 | T171 |
| E1310 | E1129 | E1129 | T1022 | P825  | T731 | T731 | S828 | ILE  | K495 | E419 | GLY  | L256 | L176 |
| S1311 | D1130 | D1130 | P1029 | M826  | I732 | I732 | T629 | SER  | P496 | L420 | ALA  | P257 | L175 |
| M1312 | E1131 | E1131 | W1030 | R827  | I733 | I733 | I630 | SER  | G498 | W424 | ALA  | R260 | G178 |
| V1316 | P1133 | P1133 | R1036 | P828  | F737 | F737 | P631 | SER  | P499 | V424 | ALA  | R260 | K179 |
| E1317 | K1138 | K1138 | G834  | F833  | T634 | T634 | T634 | ARG  | N427 | N427 | ALA  | G263 | S180 |
| V1240 | E1037 | E1037 | G834  | G834  | I685 | I685 | I685 | VAL  | T501 | T501 | ALA  | L266 | L181 |
| S1241 | E1038 | E1038 | G835  | G835  | K742 | K742 | P636 | GLU  | A502 | A502 | ALA  | V267 | V182 |
| V1243 | M1039 | M1039 | D836  | D836  | Q743 | Q743 | F637 | PHE  | D429 | D429 | ALA  | E185 | N184 |
| G1244 | E1040 | E1040 | G837  | G837  | L638 | L638 | L638 | GLU  | D504 | D504 | ALA  | L269 | E185 |
| S1247 | F1045 | F1045 | M838  | M838  | V745 | V745 | T644 | LEU  | V432 | V432 | ALA  | E272 | I186 |
| G1248 | S1046 | S1046 | Y839  | Y839  | E746 | E746 | A747 | TYR  | G507 | G507 | ALA  | P273 | L187 |
| S1249 | L1047 | L1047 | K843  | K843  | L748 | L748 | D648 | ASP  | N508 | N508 | ALA  | R276 | L190 |
| G1252 | E1048 | E1048 | L846  | L846  | I749 | I749 | E436 | ASP  | A436 | A436 | ALA  | E280 | G195 |
| V1253 | G1049 | G1049 | L846  | L846  | E750 | E750 | Y651 | LEU  | L437 | L437 | ALA  | P196 | T196 |
| V1254 | C1050 | C1050 | S951  | S951  | F751 | F751 | L655 | MET  | N438 | N438 | ALA  | T197 | T197 |
| S1255 | V1051 | V1051 | L849  | L849  | L761 | L761 | L655 | PHE  | M440 | M440 | ALA  | A283 | P196 |
| A1256 | E1052 | E1052 | R852  | R852  | D764 | D764 | D661 | LEU  | M441 | M441 | ALA  | K284 | P201 |
| L1257 | M1057 | M1057 | W858  | W858  | I769 | I769 | E664 | SER  | S443 | S443 | ALA  | A285 | E202 |
| G1258 | L1173 | L1173 | A859  | A859  | F770 | F770 | N669 | SER  | N444 | N444 | ALA  | F286 | E202 |
| R1259 | I1175 | I1175 | M860  | M860  | F771 | F771 | G670 | GLU  | D445 | D445 | ALA  | M290 | L206 |
| G1259 | P1176 | P1176 | V864  | V864  | I774 | I774 | G670 | ASP  | L447 | L447 | ALA  | A291 | L206 |
| R1263 | K1177 | K1177 | V864  | V864  | P775 | P775 | K674 | PRG  | M451 | M451 | ALA  | Q292 | L209 |
| R1264 | A1178 | A1178 | I868  | I868  | E776 | E776 | D675 | SER  | E452 | E452 | ALA  | K293 | L209 |
| R1283 | L1179 | L1179 | R873  | R873  | E780 | E780 | I680 | GLN  | M529 | M529 | ALA  | Y294 | F213 |
| R1284 | R1183 | R1183 | G970  | G970  | L781 | L781 | T681 | THR  | H454 | H454 | ALA  | I297 | F217 |
| V1270 | L1184 | L1184 | T875  | T875  | GLY  | GLY  | A683 | LEU  | A530 | A530 | ALA  | V288 | S218 |
| V1270 | V1185 | V1185 | A876  | A876  | H782 | H782 | G682 | GLN  | L531 | L531 | ALA  | G299 | G219 |
| L1274 | S1078 | S1078 | V980  | V980  | I784 | I784 | A683 | ALA  | T536 | T536 | ALA  | V300 | A220 |
| L1275 | K1079 | K1079 | E981  | E981  |      |      |      |      | R537 | R537 | ALA  | D301 | L221 |



• Molecule 1: Fatty acid synthase subunit alpha





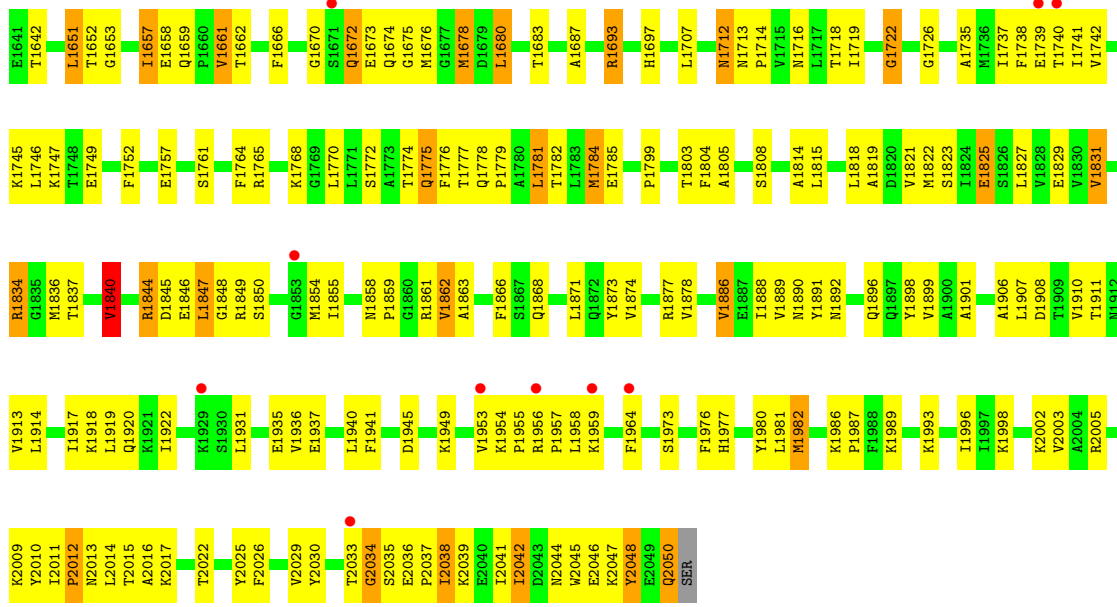
● Molecule 2: Fatty acid synthase subunit beta



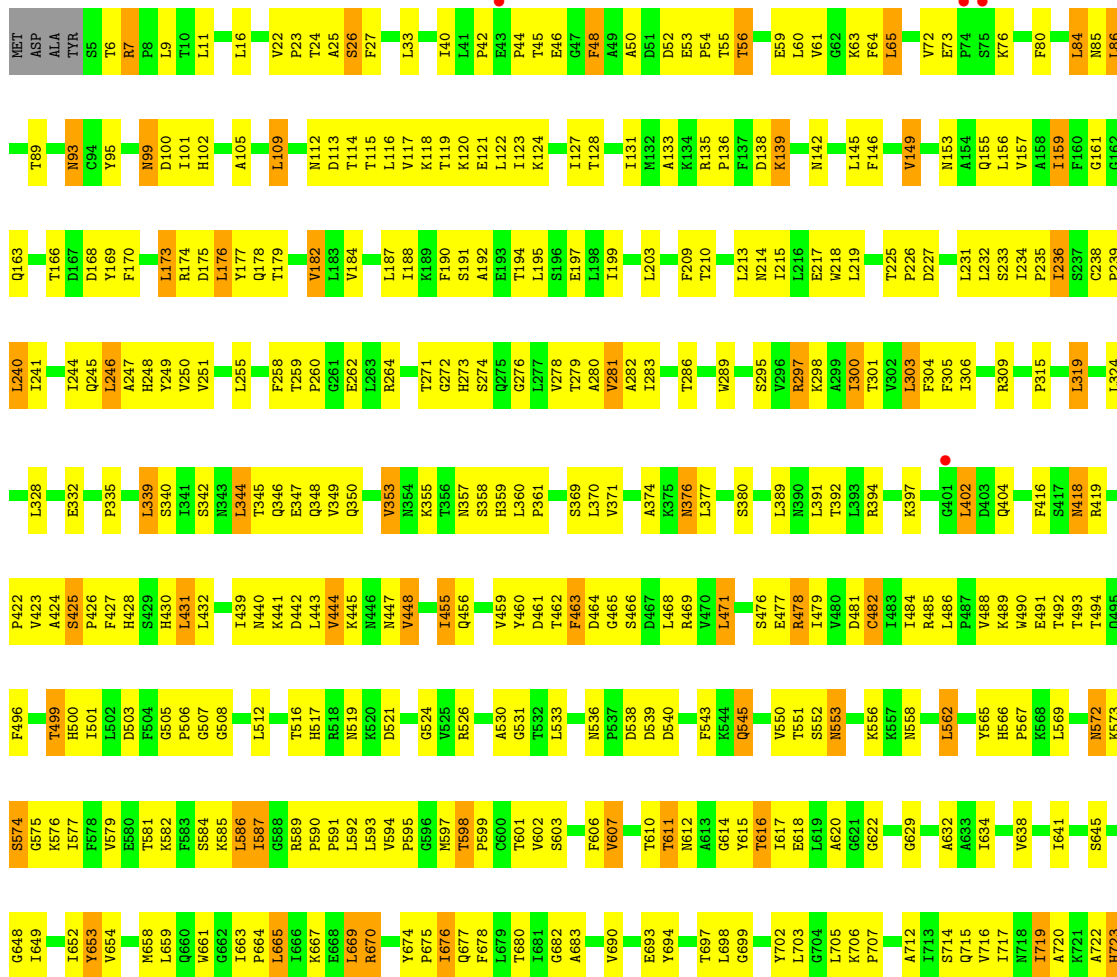




|       |       |       |       |       |      |      |       |      |      |      |
|-------|-------|-------|-------|-------|------|------|-------|------|------|------|
| V1556 | D1468 | F1279 | L1040 | T945  | A858 | E784 | I1717 | P567 | I483 | L402 |
| S1557 | K1462 | D1280 | E1041 | F946  | T859 | W785 | H718  | K568 | I484 | L403 |
| L1560 | T1463 | P1281 | E1042 | F947  | R860 | S786 | A719  | L569 | R485 | Q404 |
| P1561 | V1377 | V1284 | V1043 | G948  | W865 | T787 | A720  | I641 | L486 | Q404 |
| I1563 | I1378 | V1292 | D1044 | D949  | V866 | K788 | K721  | N572 | P487 | P408 |
| I1564 | V1381 | I1293 | D1045 | F950  | K866 | F789 | A722  | K573 | V468 | F409 |
| I1469 | V1382 | I1294 | Q1046 | L951  | F867 | D790 | H723  | S574 | K489 | F409 |
| T1470 | SER   | V1047 | V1047 | R952  | F868 | Y791 | F726  | K575 | W490 | F416 |
| E1471 | SER   | R953  | D1048 | R953  | D869 | P792 | F727  | K576 | E491 | F416 |
| V1472 | VAL   | Q1049 | Q1049 | V954  | E870 | F799 | F727  | S417 | N418 | S417 |
| S1566 | VAL   | E955  | R1050 | E955  | T871 | M794 | F728  | I577 | T492 | N418 |
| R1567 | SER   | E956  | T1051 | E956  | R872 | F795 | A729  | F578 | T493 | N418 |
| H1568 | GIU   | C1052 | C1052 | E956  | R873 | F796 | L730  | V579 | T494 | R419 |
| K4475 | D1123 | I1053 | I1053 | K960  | F879 | D797 | Q731  | F580 | Q495 | R420 |
| N1574 | K1128 | L1054 | L1054 | K960  | R879 | G798 | W732  | T581 | Q496 | L421 |
| L1575 | A1129 | L964  | L964  | L964  | L880 | F799 | W732  | K582 | P422 | P422 |
| I1579 | M1221 | I1130 | V1058 | I967  | V881 | F799 | W733  | F583 | V423 | V423 |
| T1580 | M1223 | M1223 | V1059 | I967  | L800 | L800 | W733  | H500 | A424 | A424 |
| M1583 | M1227 | R1228 | A1060 | Y970  | R804 | R804 | R736  | S425 | S425 | S425 |
| F1584 | E1492 | E1492 | Q1061 | S971  | R805 | R805 | G739  | F504 | F427 | F427 |
| L1493 | S1408 | R1314 | F1062 | S971  | R806 | R806 | H741  | G505 | H428 | H428 |
| P1494 | S1408 | R1314 | T1063 | L972  | I807 | I807 | S742  | P506 | L431 | L431 |
| K1496 | W1138 | W1138 | I1066 | Y987  | E810 | E810 | D745  | L512 | V433 | V433 |
| E1497 | S1145 | E1146 | D1067 | Q993  | R834 | R834 | A746  | T516 | P434 | P434 |
| L1498 | E1147 | E1147 | E1068 | Q993  | T813 | T813 | H747  | H517 | I439 | I439 |
| V1499 | N1148 | N1148 | V1069 | R994  | R887 | R887 | T748  | K520 | N440 | N440 |
| E1500 | W1149 | W1149 | K1071 | L995  | R888 | R888 | F749  | K521 | K441 | K441 |
| I1501 | R1150 | R1150 | M1074 | Q998  | F899 | F899 | D816  | D521 | D442 | D442 |
| G1502 | H1151 | H1151 | M1075 | Q998  | Q900 | Q900 | L751  | G522 | L443 | L443 |
| F1503 | A1152 | A1152 | D1075 | D999  | K901 | K901 | Q752  | G600 | V527 | V527 |
| L1504 | I1159 | I1159 | G1076 | I1000 | P902 | P902 | Y754  | T601 | K445 | K445 |
| V1505 | Q1161 | Q1161 | H1078 | F1002 | A822 | A822 | F678  | S603 | N446 | N446 |
| Y1506 | D1162 | D1162 | D1079 | F1003 | C824 | C824 | I757  | F606 | N447 | N447 |
| A1510 | K1163 | K1163 | G1080 | L1004 | T906 | T906 | I758  | V607 | V448 | V448 |
| H1511 | V1166 | V1166 | H1081 | S1005 | V907 | V907 | R759  | T610 | I485 | I485 |
| P1515 | S1167 | S1167 | I1082 | M1006 | Q910 | Q910 | H760  | T610 | Q456 | Q456 |
| T1526 | E1266 | E1266 | K1083 | P1010 | A911 | A911 | N762  | T611 | D540 | D540 |
| L1527 | D1257 | D1257 | K1084 | P1011 | R912 | R912 | I763  | N612 | V459 | V459 |
| E1528 | P1258 | P1258 | L1085 | Q1012 | D913 | D913 | M764  | F543 | Y460 | Y460 |
| Q1529 | W1259 | W1259 | L1086 | Q1012 | D913 | D913 | L765  | K544 | D461 | D461 |
| K1530 | Q1260 | Q1260 | Y1090 | V1015 | T916 | T916 | T687  | Q645 | T462 | T462 |
| L1533 | R1261 | R1261 | G1091 | P1016 | T845 | T845 | F767  | T616 | P463 | P463 |
| L1527 | R1261 | R1261 | D1092 | F1017 | T846 | T846 | G768  | I617 | D464 | D464 |
| S1625 | R1262 | R1262 | D1093 | F1018 | P839 | P839 | S769  | E618 | G465 | G465 |
| Q1627 | K1263 | K1263 | D1093 | I1018 | T840 | T840 | Y702  | L619 | T551 | T551 |
| Q1627 | E1264 | E1264 | K1096 | P1019 | L926 | L926 | G772  | A620 | S552 | S552 |
| G1630 | M1265 | M1265 | I1097 | V1020 | L929 | L929 | G772  | G621 | N653 | N653 |
| H1631 | Y1266 | Y1266 | I1097 | L1021 | L929 | L929 | S773  | G622 | R469 | R469 |
| N1632 | L1269 | L1269 | V1100 | R1024 | I932 | I932 | A774  | G622 | V470 | V470 |
| N1633 | M1180 | M1180 | E1101 | F1025 | I932 | I932 | D775  | Y624 | L471 | L471 |
| G1634 | M1270 | M1270 | Y1102 | I1026 | V938 | V938 | D775  | K706 | N560 | N560 |
| R1635 | M1355 | M1355 | F1103 | I1027 | F939 | F939 | T777  | P707 | W661 | W661 |
| K1636 | D1272 | D1272 | F1103 | I1027 | P939 | P939 | Y778  | G629 | S476 | S476 |
| L1637 | E1273 | E1273 | P1109 | K1031 | T942 | T942 | P779  | T631 | R478 | R478 |
| I1638 | F1274 | F1274 | V1109 | W109  | R855 | R855 | Y780  | A632 | E564 | E564 |
| P1552 | F1275 | F1275 | ASP   | D1032 | R944 | R944 | L781  | A632 | Y565 | Y565 |
| F1640 | T1196 | T1196 | ASP   | D1032 | R944 | R944 | L781  | I634 | H566 | H566 |



● Molecule 2: Fatty acid synthase subunit beta







|       |       |
|-------|-------|
| V2029 | Y2030 |
| T2033 | G2034 |
| S2035 | E2036 |
| P2037 | I2038 |
| K2039 | E2040 |
| I2041 | L2042 |
| D2043 | M2044 |
| W2045 | E2046 |
| K2047 | Y2048 |
| E2049 | Q2050 |
| SER   |       |

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 43 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 231.88Å 231.88Å 756.78Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 20.00 – 4.00<br>20.00 – 4.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.3 (20.00-4.00)<br>97.3 (20.00-4.00)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.71 (at 3.94Å)   | Xtrriage         |
| Refinement program  | PHENIX  | Depositor        |
| R, $R_{free}$   | 0.266 , 0.267<br>0.257 , 0.257                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8521 reflections (5.07%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 130.2   | Xtrriage         |
| Anisotropy  | 0.319   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.23 , 74.8   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 88830   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 168.0   | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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 i

### 5.1 Standard geometry i

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

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     | 0.43         | 5/13822 (0.0%)  | 0.59        | 6/18682 (0.0%)   |
| 1   | B     | 0.43         | 3/13822 (0.0%)  | 0.61        | 9/18682 (0.0%)   |
| 1   | C     | 0.43         | 4/13822 (0.0%)  | 0.59        | 4/18682 (0.0%)   |
| 2   | G     | 0.41         | 7/16360 (0.0%)  | 0.58        | 6/22198 (0.0%)   |
| 2   | H     | 0.40         | 7/16360 (0.0%)  | 0.57        | 3/22198 (0.0%)   |
| 2   | I     | 0.40         | 5/16360 (0.0%)  | 0.58        | 10/22198 (0.0%)  |
| All | All   | 0.42         | 31/90546 (0.0%) | 0.59        | 38/122640 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | G     | 0                   | 1                   |
| 2   | H     | 0                   | 2                   |
| 2   | I     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (31) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 992  | PHE  | C-N   | 13.35 | 1.59        | 1.34     |
| 1   | C     | 992  | PHE  | C-N   | 13.18 | 1.59        | 1.34     |
| 2   | I     | 842  | GLY  | C-N   | 11.12 | 1.59        | 1.34     |
| 2   | G     | 315  | PRO  | C-N   | 10.45 | 1.58        | 1.34     |
| 1   | C     | 485  | ASP  | C-N   | 9.61  | 1.56        | 1.34     |
| 2   | H     | 1256 | GLU  | C-N   | 9.35  | 1.55        | 1.34     |
| 2   | H     | 138  | ASP  | C-N   | 9.07  | 1.54        | 1.34     |
| 2   | H     | 1840 | VAL  | C-N   | 8.47  | 1.53        | 1.34     |
| 2   | G     | 1657 | ILE  | C-N   | 8.15  | 1.52        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | I     | 315  | PRO  | C-N   | 7.84  | 1.52        | 1.34     |
| 1   | A     | 668  | PHE  | C-N   | 7.73  | 1.51        | 1.34     |
| 2   | I     | 1980 | TYR  | C-N   | 7.70  | 1.51        | 1.34     |
| 1   | A     | 181  | THR  | C-N   | 7.05  | 1.50        | 1.34     |
| 2   | G     | 422  | PRO  | C-N   | 6.97  | 1.50        | 1.34     |
| 2   | I     | 1018 | VAL  | C-N   | -6.57 | 1.21        | 1.34     |
| 2   | G     | 1256 | GLU  | C-N   | 6.43  | 1.48        | 1.34     |
| 1   | C     | 1520 | ALA  | C-N   | -6.36 | 1.22        | 1.34     |
| 2   | I     | 903  | TRP  | C-N   | 6.33  | 1.48        | 1.34     |
| 2   | H     | 1053 | ILE  | C-N   | 6.30  | 1.48        | 1.34     |
| 2   | H     | 422  | PRO  | C-N   | 6.29  | 1.48        | 1.34     |
| 2   | G     | 842  | GLY  | C-N   | 6.06  | 1.48        | 1.34     |
| 2   | H     | 137  | PHE  | C-N   | 5.95  | 1.47        | 1.34     |
| 1   | A     | 1520 | ALA  | C-N   | 5.79  | 1.45        | 1.34     |
| 2   | H     | 1982 | MET  | C-N   | 5.67  | 1.47        | 1.34     |
| 1   | B     | 181  | THR  | C-N   | -5.65 | 1.21        | 1.34     |
| 2   | G     | 1529 | GLN  | C-N   | -5.50 | 1.21        | 1.34     |
| 2   | G     | 1980 | TYR  | C-N   | 5.38  | 1.46        | 1.34     |
| 1   | C     | 636  | PRO  | C-N   | -5.29 | 1.21        | 1.34     |
| 1   | B     | 668  | PHE  | C-N   | 5.29  | 1.46        | 1.34     |
| 1   | B     | 1430 | ARG  | C-N   | -5.19 | 1.22        | 1.34     |
| 1   | A     | 1181 | PHE  | C-N   | 5.13  | 1.45        | 1.34     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 1   | B     | 1116 | PRO  | O-C-N  | -11.67 | 104.02      | 122.70   |
| 2   | I     | 1982 | MET  | O-C-N  | -9.44  | 107.59      | 122.70   |
| 2   | G     | 842  | GLY  | O-C-N  | -8.86  | 108.52      | 122.70   |
| 2   | G     | 1053 | ILE  | O-C-N  | -8.58  | 108.97      | 122.70   |
| 1   | B     | 992  | PHE  | O-C-N  | 8.47   | 137.19      | 121.10   |
| 2   | I     | 422  | PRO  | O-C-N  | -8.30  | 109.42      | 122.70   |
| 1   | B     | 992  | PHE  | C-N-CD | 8.15   | 145.52      | 128.40   |
| 2   | I     | 1982 | MET  | C-N-CA | 8.08   | 141.89      | 121.70   |
| 1   | B     | 1116 | PRO  | CA-C-N | 8.00   | 134.79      | 117.20   |
| 2   | I     | 1657 | ILE  | O-C-N  | -7.47  | 110.75      | 122.70   |
| 1   | C     | 1520 | ALA  | O-C-N  | 7.43   | 135.22      | 121.10   |
| 1   | A     | 1430 | ARG  | O-C-N  | -7.40  | 110.85      | 122.70   |
| 1   | B     | 1116 | PRO  | C-N-CA | 7.29   | 139.94      | 121.70   |
| 1   | B     | 599  | MET  | N-CA-C | -6.93  | 92.27       | 111.00   |
| 1   | C     | 599  | MET  | N-CA-C | -6.92  | 92.32       | 111.00   |
| 1   | A     | 599  | MET  | N-CA-C | -6.90  | 92.37       | 111.00   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 992  | PHE  | C-N-CD | 6.65  | 142.37      | 128.40   |
| 2   | I     | 422  | PRO  | CA-C-N | 6.52  | 131.55      | 117.20   |
| 2   | H     | 1840 | VAL  | O-C-N  | -6.51 | 112.29      | 122.70   |
| 2   | I     | 1982 | MET  | CA-C-N | 6.50  | 131.50      | 117.20   |
| 1   | C     | 1116 | PRO  | O-C-N  | -6.36 | 112.52      | 122.70   |
| 1   | B     | 992  | PHE  | CA-C-N | -6.11 | 100.00      | 117.10   |
| 2   | G     | 1053 | ILE  | CA-C-N | 6.05  | 130.50      | 117.20   |
| 1   | A     | 992  | PHE  | O-C-N  | 5.97  | 132.45      | 121.10   |
| 2   | I     | 315  | PRO  | O-C-N  | -5.75 | 113.50      | 122.70   |
| 1   | B     | 540  | GLN  | N-CA-C | -5.65 | 95.74       | 111.00   |
| 1   | A     | 540  | GLN  | N-CA-C | -5.64 | 95.77       | 111.00   |
| 1   | C     | 540  | GLN  | N-CA-C | -5.63 | 95.80       | 111.00   |
| 1   | B     | 178  | GLY  | O-C-N  | 5.57  | 131.61      | 122.70   |
| 2   | I     | 422  | PRO  | C-N-CA | 5.52  | 135.50      | 121.70   |
| 2   | G     | 138  | ASP  | O-C-N  | -5.44 | 113.99      | 122.70   |
| 1   | A     | 1520 | ALA  | O-C-N  | 5.44  | 131.44      | 121.10   |
| 2   | H     | 1256 | GLU  | CA-C-N | -5.39 | 105.35      | 117.20   |
| 2   | I     | 1657 | ILE  | CA-C-N | 5.34  | 128.95      | 117.20   |
| 2   | G     | 842  | GLY  | CA-C-N | 5.30  | 128.86      | 117.20   |
| 2   | H     | 138  | ASP  | O-C-N  | -5.08 | 114.56      | 122.70   |
| 2   | G     | 138  | ASP  | C-N-CA | 5.05  | 134.32      | 121.70   |
| 2   | I     | 1657 | ILE  | C-N-CA | 5.03  | 134.27      | 121.70   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 2   | G     | 1108 | PRO  | Peptide   |
| 2   | H     | 1108 | PRO  | Peptide   |
| 2   | H     | 1256 | GLU  | Mainchain |
| 2   | I     | 1108 | PRO  | Peptide   |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 13572 | 0        | 13489    | 663     | 15           |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 13572 | 0        | 13490    | 618     | 6            |
| 1   | C     | 13572 | 0        | 13490    | 638     | 22           |
| 2   | G     | 15995 | 0        | 15978    | 1026    | 32           |
| 2   | H     | 15995 | 0        | 15978    | 1023    | 7            |
| 2   | I     | 15995 | 0        | 15977    | 983     | 26           |
| 3   | A     | 12    | 0        | 10       | 3       | 0            |
| 3   | B     | 12    | 0        | 10       | 4       | 0            |
| 3   | C     | 12    | 0        | 10       | 4       | 0            |
| 4   | G     | 31    | 0        | 19       | 7       | 0            |
| 4   | H     | 31    | 0        | 19       | 6       | 0            |
| 4   | I     | 31    | 0        | 19       | 8       | 0            |
| All | All   | 88830 | 0        | 88489    | 4773    | 54           |

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 27.

All (4773) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1749:THR:CB  | 1:A:1874:ASP:HB3  | 1.53                     | 1.37              |
| 1:B:1749:THR:CB  | 1:B:1874:ASP:HB3  | 1.56                     | 1.34              |
| 1:B:1749:THR:CB  | 1:B:1873:HIS:O    | 1.75                     | 1.32              |
| 1:A:1464:GLU:HG3 | 1:A:1773:VAL:CG1  | 1.58                     | 1.32              |
| 1:C:1749:THR:CB  | 1:C:1874:ASP:HB3  | 1.62                     | 1.29              |
| 1:A:1464:GLU:CG  | 1:A:1773:VAL:HG12 | 1.65                     | 1.26              |
| 1:A:1749:THR:CB  | 1:A:1873:HIS:O    | 1.88                     | 1.21              |
| 1:C:1749:THR:CB  | 1:C:1874:ASP:CA   | 2.20                     | 1.19              |
| 2:H:1956:ARG:HB2 | 2:H:1957:PRO:HD3  | 1.24                     | 1.18              |
| 1:C:1749:THR:CB  | 1:C:1874:ASP:CB   | 2.22                     | 1.16              |
| 1:C:1464:GLU:CG  | 1:C:1773:VAL:HG12 | 1.75                     | 1.16              |
| 2:G:28:PHE:CE2   | 2:H:7:ARG:HD2     | 1.80                     | 1.16              |
| 2:G:1859:PRO:HG3 | 2:G:1871:LEU:HD12 | 1.29                     | 1.15              |
| 1:C:1501:LEU:CD1 | 1:C:1775:LEU:HD21 | 1.75                     | 1.15              |
| 2:H:1834:ARG:HG2 | 2:H:1834:ARG:HH11 | 1.06                     | 1.15              |
| 1:C:1460:LYS:NZ  | 1:C:1774:GLU:OE2  | 1.80                     | 1.15              |
| 1:C:1464:GLU:HG3 | 1:C:1773:VAL:CG1  | 1.77                     | 1.14              |
| 1:C:1498:GLU:HG3 | 1:C:1876:LEU:HD13 | 1.19                     | 1.14              |
| 2:H:490:TRP:HE1  | 2:H:516:THR:HG22  | 1.12                     | 1.14              |
| 2:H:499:THR:HB   | 2:H:500:HIS:HD2   | 1.10                     | 1.12              |
| 2:I:490:TRP:HE1  | 2:I:516:THR:HG22  | 1.10                     | 1.12              |
| 2:G:1956:ARG:HB2 | 2:G:1957:PRO:HD3  | 1.23                     | 1.12              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:131:ILE:HD12  | 2:G:182:VAL:HB    | 1.18                     | 1.12              |
| 2:H:131:ILE:HD12  | 2:H:182:VAL:CB    | 1.79                     | 1.11              |
| 2:I:601:THR:HG21  | 2:I:618:GLU:O     | 1.50                     | 1.11              |
| 2:I:1956:ARG:HB2  | 2:I:1957:PRO:HD3  | 1.23                     | 1.11              |
| 1:A:253:ARG:HG3   | 1:A:254:TRP:HD1   | 1.15                     | 1.10              |
| 1:A:1721:ARG:HG2  | 1:A:1721:ARG:HH11 | 1.16                     | 1.10              |
| 2:H:601:THR:HG21  | 2:H:618:GLU:O     | 1.50                     | 1.10              |
| 2:G:601:THR:HG21  | 2:G:618:GLU:O     | 1.52                     | 1.10              |
| 1:B:1464:GLU:HG3  | 1:B:1773:VAL:HG12 | 1.31                     | 1.09              |
| 2:G:499:THR:HB    | 2:G:500:HIS:HD2   | 1.08                     | 1.09              |
| 2:H:131:ILE:CB    | 2:H:182:VAL:HG11  | 1.82                     | 1.09              |
| 2:I:297:ARG:HD3   | 2:I:447:ASN:HD21  | 1.15                     | 1.09              |
| 2:G:131:ILE:HB    | 2:G:182:VAL:HG11  | 1.31                     | 1.09              |
| 2:G:490:TRP:HE1   | 2:G:516:THR:HG22  | 1.12                     | 1.08              |
| 2:I:499:THR:HB    | 2:I:500:HIS:HD2   | 1.07                     | 1.08              |
| 1:B:1460:LYS:NZ   | 1:B:1774:GLU:OE2  | 1.85                     | 1.08              |
| 1:B:1749:THR:CB   | 1:B:1874:ASP:CB   | 2.32                     | 1.08              |
| 1:A:1749:THR:CB   | 1:A:1874:ASP:CB   | 2.31                     | 1.08              |
| 1:C:852:ARG:HG2   | 1:C:852:ARG:HH11  | 1.14                     | 1.08              |
| 1:C:1498:GLU:CG   | 1:C:1876:LEU:HD13 | 1.84                     | 1.07              |
| 2:H:131:ILE:HG21  | 2:H:182:VAL:HG12  | 1.35                     | 1.07              |
| 2:H:128:THR:HA    | 2:H:182:VAL:HG21  | 1.31                     | 1.07              |
| 2:I:1227:ARG:HH11 | 2:I:1227:ARG:HG3  | 1.18                     | 1.07              |
| 2:G:297:ARG:HD3   | 2:G:447:ASN:HD21  | 1.17                     | 1.06              |
| 2:G:28:PHE:CZ     | 2:H:7:ARG:HD2     | 1.91                     | 1.06              |
| 1:C:1367:ARG:NH1  | 1:C:1372:THR:HB   | 1.71                     | 1.06              |
| 2:I:1834:ARG:HG2  | 2:I:1834:ARG:HH11 | 1.16                     | 1.06              |
| 2:G:903:TRP:O     | 2:G:906:THR:HG22  | 1.57                     | 1.05              |
| 1:C:1721:ARG:HG2  | 1:C:1721:ARG:HH11 | 1.19                     | 1.05              |
| 2:G:1834:ARG:HG2  | 2:G:1834:ARG:HH11 | 1.16                     | 1.05              |
| 2:I:7:ARG:HH21    | 2:I:27:PHE:HB3    | 1.20                     | 1.05              |
| 1:B:253:ARG:HG3   | 1:B:254:TRP:HD1   | 1.17                     | 1.04              |
| 1:A:1367:ARG:NH1  | 1:A:1372:THR:HB   | 1.72                     | 1.04              |
| 1:C:253:ARG:HG3   | 1:C:254:TRP:HD1   | 1.15                     | 1.04              |
| 2:G:932:ILE:HD11  | 2:G:1042:ALA:HB2  | 1.36                     | 1.04              |
| 2:I:1739:GLU:HB2  | 2:I:1987:PRO:HB3  | 1.40                     | 1.04              |
| 1:B:1367:ARG:NH1  | 1:B:1372:THR:HB   | 1.73                     | 1.04              |
| 2:H:1227:ARG:HH11 | 2:H:1227:ARG:HG3  | 1.19                     | 1.03              |
| 2:G:1227:ARG:HG3  | 2:G:1227:ARG:HH11 | 1.18                     | 1.03              |
| 2:H:297:ARG:HD3   | 2:H:447:ASN:HD21  | 1.16                     | 1.03              |
| 1:B:1721:ARG:HH11 | 1:B:1721:ARG:HG2  | 1.21                     | 1.03              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1722:VAL:HG11 | 1:B:1731:LEU:HB3  | 1.37                     | 1.03              |
| 1:C:1722:VAL:HG11 | 1:C:1731:LEU:HB3  | 1.37                     | 1.02              |
| 2:G:7:ARG:HH21    | 2:G:27:PHE:HB3    | 1.22                     | 1.02              |
| 1:B:599:MET:HB2   | 1:B:624:LYS:HD2   | 1.42                     | 1.02              |
| 2:H:7:ARG:HH21    | 2:H:27:PHE:HB3    | 1.22                     | 1.02              |
| 1:A:852:ARG:HG2   | 1:A:852:ARG:HH11  | 1.23                     | 1.02              |
| 1:B:852:ARG:HH11  | 1:B:852:ARG:HG2   | 1.20                     | 1.02              |
| 1:C:1498:GLU:HG3  | 1:C:1876:LEU:CD1  | 1.84                     | 1.02              |
| 1:C:1501:LEU:HD12 | 1:C:1775:LEU:HD21 | 1.38                     | 1.02              |
| 2:H:1739:GLU:HB2  | 2:H:1987:PRO:HB3  | 1.42                     | 1.02              |
| 2:H:1859:PRO:HG3  | 2:H:1871:LEU:HD12 | 1.37                     | 1.01              |
| 2:I:1859:PRO:HG3  | 2:I:1871:LEU:HD12 | 1.41                     | 1.01              |
| 2:H:131:ILE:HB    | 2:H:182:VAL:CG1   | 1.89                     | 1.01              |
| 1:C:1219:VAL:HA   | 1:C:1384:ILE:HD11 | 1.40                     | 1.01              |
| 2:H:131:ILE:CD1   | 2:H:182:VAL:HB    | 1.91                     | 1.00              |
| 1:C:1014:ASP:H    | 1:C:1510:ASN:HD21 | 1.03                     | 1.00              |
| 2:H:903:TRP:O     | 2:H:906:THR:HG22  | 1.59                     | 1.00              |
| 1:A:1722:VAL:HG11 | 1:A:1731:LEU:HB3  | 1.40                     | 1.00              |
| 2:I:741:HIS:NE2   | 2:I:855:HIS:CE1   | 2.30                     | 1.00              |
| 1:A:599:MET:HB2   | 1:A:624:LYS:HD2   | 1.43                     | 0.99              |
| 2:H:1567:ARG:HG3  | 2:H:1567:ARG:HH11 | 1.27                     | 0.99              |
| 1:C:1749:THR:CB   | 1:C:1874:ASP:HA   | 1.90                     | 0.99              |
| 1:C:599:MET:HB2   | 1:C:624:LYS:HD2   | 1.43                     | 0.99              |
| 1:C:253:ARG:HG3   | 1:C:254:TRP:CD1   | 1.98                     | 0.99              |
| 2:G:499:THR:HB    | 2:G:500:HIS:CD2   | 1.97                     | 0.98              |
| 2:I:892:ILE:HD11  | 2:I:903:TRP:CE2   | 1.98                     | 0.98              |
| 1:A:253:ARG:HG3   | 1:A:254:TRP:CD1   | 1.98                     | 0.98              |
| 1:B:1219:VAL:HA   | 1:B:1384:ILE:HD11 | 1.45                     | 0.98              |
| 1:C:1460:LYS:HE3  | 1:C:1774:GLU:CD   | 1.83                     | 0.98              |
| 2:H:1803:THR:HG22 | 2:H:2009:LYS:HA   | 1.45                     | 0.98              |
| 2:H:762:ASN:HD22  | 2:H:762:ASN:H     | 1.03                     | 0.98              |
| 2:H:131:ILE:HB    | 2:H:182:VAL:HG11  | 1.00                     | 0.98              |
| 2:I:499:THR:HB    | 2:I:500:HIS:CD2   | 1.97                     | 0.98              |
| 2:I:903:TRP:O     | 2:I:906:THR:HG22  | 1.63                     | 0.98              |
| 2:G:1844:ARG:HG2  | 2:G:1844:ARG:HH11 | 1.26                     | 0.97              |
| 1:A:400:ARG:HG2   | 1:A:400:ARG:HH11  | 1.28                     | 0.97              |
| 2:G:892:ILE:HD11  | 2:G:903:TRP:CE2   | 1.98                     | 0.97              |
| 1:A:400:ARG:HH11  | 1:A:400:ARG:CG    | 1.76                     | 0.97              |
| 2:H:499:THR:HB    | 2:H:500:HIS:CD2   | 1.99                     | 0.97              |
| 2:H:1172:LYS:HE3  | 2:H:1574:ASN:OD1  | 1.64                     | 0.97              |
| 1:B:198:PRO:HG3   | 1:B:209:LEU:HD21  | 1.47                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:253:ARG:HG3   | 1:B:254:TRP:CD1   | 1.99                     | 0.96              |
| 2:H:594:VAL:HB    | 2:H:617:ILE:HG13  | 1.44                     | 0.96              |
| 2:I:490:TRP:NE1   | 2:I:516:THR:HG22  | 1.79                     | 0.96              |
| 2:I:762:ASN:H     | 2:I:762:ASN:HD22  | 1.08                     | 0.96              |
| 1:A:1014:ASP:H    | 1:A:1510:ASN:HD21 | 1.10                     | 0.96              |
| 2:H:490:TRP:NE1   | 2:H:516:THR:HG22  | 1.81                     | 0.96              |
| 2:H:131:ILE:HD12  | 2:H:182:VAL:HB    | 0.96                     | 0.96              |
| 1:A:12:ILE:HD11   | 2:G:2041:ILE:HD12 | 1.47                     | 0.95              |
| 1:C:198:PRO:HG3   | 1:C:209:LEU:HD21  | 1.48                     | 0.95              |
| 2:G:490:TRP:NE1   | 2:G:516:THR:HG22  | 1.81                     | 0.95              |
| 2:H:892:ILE:HD11  | 2:H:903:TRP:CE2   | 2.01                     | 0.95              |
| 2:H:1567:ARG:HH11 | 2:H:1567:ARG:CG   | 1.79                     | 0.95              |
| 2:G:1803:THR:HG22 | 2:G:2009:LYS:HA   | 1.48                     | 0.95              |
| 1:B:1460:LYS:CE   | 1:B:1773:VAL:O    | 2.15                     | 0.95              |
| 2:I:594:VAL:HB    | 2:I:617:ILE:HG13  | 1.46                     | 0.95              |
| 2:I:1567:ARG:HH11 | 2:I:1567:ARG:HG3  | 1.29                     | 0.95              |
| 2:I:1567:ARG:HH11 | 2:I:1567:ARG:CG   | 1.79                     | 0.95              |
| 2:H:1199:GLU:OE2  | 2:H:1567:ARG:NH1  | 2.00                     | 0.95              |
| 2:G:1741:ILE:HD12 | 2:G:1986:LYS:HD2  | 1.47                     | 0.95              |
| 2:G:1878:VAL:HG11 | 2:G:1910:VAL:HG22 | 1.48                     | 0.95              |
| 1:A:198:PRO:HG3   | 1:A:209:LEU:HD21  | 1.47                     | 0.95              |
| 2:I:741:HIS:CE1   | 2:I:855:HIS:CE1   | 2.55                     | 0.95              |
| 2:G:1567:ARG:HH11 | 2:G:1567:ARG:CG   | 1.80                     | 0.95              |
| 1:A:444:ASN:HB2   | 1:A:447:LEU:H     | 1.31                     | 0.95              |
| 1:B:1464:GLU:HG3  | 1:B:1773:VAL:CG1  | 1.95                     | 0.95              |
| 2:H:741:HIS:HE1   | 2:H:845:THR:CG2   | 1.80                     | 0.95              |
| 2:H:835:THR:HG21  | 2:H:855:HIS:CD2   | 1.99                     | 0.94              |
| 2:G:1739:GLU:HB2  | 2:G:1987:PRO:HB3  | 1.43                     | 0.94              |
| 2:G:1589:VAL:HA   | 2:G:1592:LEU:HD12 | 1.49                     | 0.94              |
| 1:B:1460:LYS:HE3  | 1:B:1773:VAL:O    | 1.68                     | 0.94              |
| 2:H:55:THR:HG22   | 2:H:56:THR:HG22   | 1.48                     | 0.94              |
| 1:B:444:ASN:HB2   | 1:B:447:LEU:H     | 1.31                     | 0.94              |
| 1:C:400:ARG:HG2   | 1:C:400:ARG:HH11  | 1.33                     | 0.94              |
| 1:C:1498:GLU:OE2  | 1:C:1876:LEU:HA   | 1.65                     | 0.94              |
| 2:I:1741:ILE:HD12 | 2:I:1986:LYS:HD2  | 1.49                     | 0.94              |
| 1:C:2:LYS:HD2     | 2:I:2050:GLN:HB3  | 1.50                     | 0.94              |
| 2:I:1878:VAL:HG11 | 2:I:1910:VAL:HG22 | 1.50                     | 0.94              |
| 2:H:1314:ARG:HH11 | 2:H:1314:ARG:HG3  | 1.31                     | 0.94              |
| 2:G:762:ASN:H     | 2:G:762:ASN:HD22  | 1.03                     | 0.93              |
| 2:G:942:THR:HB    | 2:G:1012:GLN:HG2  | 1.50                     | 0.93              |
| 1:A:1219:VAL:HA   | 1:A:1384:ILE:HD11 | 1.45                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:529:MET:HA    | 1:B:529:MET:HE3   | 1.47                     | 0.93              |
| 1:A:1501:LEU:CD1  | 1:A:1775:LEU:HD21 | 1.98                     | 0.93              |
| 2:I:741:HIS:HE1   | 2:I:845:THR:CG2   | 1.81                     | 0.93              |
| 2:H:652:ILE:H     | 2:H:658:MET:HE3   | 1.30                     | 0.93              |
| 2:H:1845:ASP:HB2  | 2:H:1849:ARG:H    | 1.34                     | 0.93              |
| 1:B:400:ARG:HH11  | 1:B:400:ARG:CG    | 1.81                     | 0.93              |
| 2:H:1589:VAL:HA   | 2:H:1592:LEU:HD12 | 1.49                     | 0.93              |
| 2:G:565:TYR:CZ    | 2:G:758:ARG:HD2   | 2.04                     | 0.93              |
| 2:I:1314:ARG:HG3  | 2:I:1314:ARG:HH11 | 1.32                     | 0.93              |
| 1:A:12:ILE:HD11   | 2:G:2041:ILE:CD1  | 1.99                     | 0.93              |
| 2:I:56:THR:HG23   | 2:I:59:GLU:HG3    | 1.49                     | 0.93              |
| 1:C:1501:LEU:HD11 | 1:C:1775:LEU:CD2  | 1.99                     | 0.93              |
| 2:G:1567:ARG:HH11 | 2:G:1567:ARG:HG3  | 1.30                     | 0.93              |
| 2:G:128:THR:HA    | 2:G:182:VAL:HG21  | 1.51                     | 0.92              |
| 1:A:1523:ARG:HH11 | 1:A:1523:ARG:HG3  | 1.33                     | 0.92              |
| 1:C:1523:ARG:HG3  | 1:C:1523:ARG:HH11 | 1.32                     | 0.92              |
| 1:C:1501:LEU:CD1  | 1:C:1775:LEU:CD2  | 2.47                     | 0.92              |
| 2:I:741:HIS:CE1   | 2:I:845:THR:CG2   | 2.52                     | 0.92              |
| 2:G:55:THR:HG21   | 2:G:113:ASP:HB2   | 1.52                     | 0.92              |
| 1:A:152:His:CD2   | 1:A:163:LEU:HB2   | 2.05                     | 0.92              |
| 1:A:1460:LYS:CE   | 1:A:1773:VAL:O    | 2.17                     | 0.92              |
| 2:G:741:HIS:NE2   | 2:G:855:HIS:CE1   | 2.38                     | 0.92              |
| 1:B:1749:THR:CB   | 1:B:1873:HIS:C    | 2.37                     | 0.92              |
| 2:G:1844:ARG:HH11 | 2:G:1844:ARG:CG   | 1.82                     | 0.92              |
| 2:I:55:THR:HG22   | 2:I:56:THR:HG22   | 1.51                     | 0.91              |
| 2:I:667:LYS:HD2   | 2:I:697:THR:HG22  | 1.51                     | 0.91              |
| 2:I:741:HIS:CE1   | 2:I:845:THR:HG22  | 2.04                     | 0.91              |
| 1:A:1721:ARG:HH11 | 1:A:1721:ARG:CG   | 1.84                     | 0.91              |
| 1:C:400:ARG:HH11  | 1:C:400:ARG:CG    | 1.81                     | 0.91              |
| 2:G:1314:ARG:HH11 | 2:G:1314:ARG:HG3  | 1.32                     | 0.91              |
| 1:C:152:His:CD2   | 1:C:163:LEU:HB2   | 2.05                     | 0.91              |
| 2:G:56:THR:HG23   | 2:G:59:GLU:HG3    | 1.50                     | 0.91              |
| 2:G:741:HIS:CE1   | 2:G:855:HIS:CE1   | 2.57                     | 0.91              |
| 2:I:1803:THR:HG22 | 2:I:2009:LYS:HA   | 1.51                     | 0.91              |
| 2:I:707:PRO:HG3   | 2:I:716:VAL:HG21  | 1.52                     | 0.91              |
| 1:A:1693:ILE:HD11 | 2:G:998:GLN:HB2   | 1.51                     | 0.91              |
| 1:B:1523:ARG:HH11 | 1:B:1523:ARG:HG3  | 1.36                     | 0.91              |
| 1:C:1464:GLU:HG3  | 1:C:1773:VAL:HG12 | 0.91                     | 0.91              |
| 1:C:793:ARG:HA    | 1:C:797:THR:HG23  | 1.52                     | 0.90              |
| 2:H:1741:ILE:HD12 | 2:H:1986:LYS:HD2  | 1.54                     | 0.90              |
| 2:I:942:THR:HB    | 2:I:1012:GLN:HG2  | 1.52                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:707:PRO:HG3   | 2:H:716:VAL:HG21  | 1.54                     | 0.90              |
| 1:C:1498:GLU:HG3  | 1:C:1876:LEU:HB3  | 1.53                     | 0.90              |
| 2:I:652:ILE:H     | 2:I:658:MET:HE3   | 1.36                     | 0.90              |
| 2:I:1441:ILE:HD11 | 2:I:1445:ARG:CZ   | 2.02                     | 0.90              |
| 1:C:1498:GLU:CG   | 1:C:1876:LEU:HB3  | 2.02                     | 0.90              |
| 2:G:55:THR:HG22   | 2:G:56:THR:HG22   | 1.52                     | 0.90              |
| 2:H:565:TYR:CZ    | 2:H:758:ARG:HD2   | 2.06                     | 0.90              |
| 1:B:1456:GLU:OE1  | 1:B:1775:LEU:HD23 | 1.71                     | 0.89              |
| 2:G:131:ILE:HD12  | 2:G:182:VAL:CB    | 2.01                     | 0.89              |
| 1:C:1431:GLU:HG3  | 1:C:1433:HIS:CE1  | 2.07                     | 0.89              |
| 2:G:1847:LEU:H    | 2:G:1847:LEU:HD12 | 1.37                     | 0.89              |
| 1:C:444:ASN:HB2   | 1:C:447:LEU:H     | 1.33                     | 0.89              |
| 2:G:594:VAL:HB    | 2:G:617:ILE:HG13  | 1.52                     | 0.89              |
| 1:B:793:ARG:HA    | 1:B:797:THR:HG23  | 1.54                     | 0.89              |
| 1:B:1721:ARG:HH11 | 1:B:1721:ARG:CG   | 1.85                     | 0.89              |
| 2:I:1589:VAL:HA   | 2:I:1592:LEU:HD12 | 1.51                     | 0.89              |
| 1:A:253:ARG:HE    | 1:A:254:TRP:HE1   | 1.21                     | 0.89              |
| 2:G:1441:ILE:HD11 | 2:G:1445:ARG:CZ   | 2.02                     | 0.89              |
| 2:H:55:THR:HG21   | 2:H:113:ASP:HB2   | 1.53                     | 0.89              |
| 2:H:1847:LEU:HD12 | 2:H:1847:LEU:H    | 1.37                     | 0.89              |
| 1:A:529:MET:HA    | 1:A:529:MET:HE3   | 1.53                     | 0.89              |
| 2:H:56:THR:HG23   | 2:H:59:GLU:HG3    | 1.54                     | 0.89              |
| 1:A:1474:ALA:HA   | 1:A:1478:PRO:HG2  | 1.54                     | 0.88              |
| 1:B:1749:THR:CB   | 1:B:1874:ASP:CA   | 2.51                     | 0.88              |
| 2:G:667:LYS:HD2   | 2:G:697:THR:HG22  | 1.55                     | 0.88              |
| 1:A:1501:LEU:HD11 | 1:A:1775:LEU:CD2  | 2.01                     | 0.88              |
| 2:H:667:LYS:HD2   | 2:H:697:THR:HG22  | 1.55                     | 0.88              |
| 1:A:403:ASP:HB2   | 1:A:1613:ASN:HD21 | 1.38                     | 0.88              |
| 1:A:1367:ARG:HH12 | 1:A:1372:THR:HB   | 1.35                     | 0.88              |
| 1:B:31:THR:HG23   | 2:H:2011:ILE:HG21 | 1.56                     | 0.88              |
| 2:H:942:THR:HB    | 2:H:1012:GLN:HG2  | 1.54                     | 0.88              |
| 2:I:55:THR:HG21   | 2:I:113:ASP:HB2   | 1.53                     | 0.88              |
| 1:B:152:HIS:CD2   | 1:B:163:LEU:HB2   | 2.09                     | 0.88              |
| 1:B:1367:ARG:HH12 | 1:B:1372:THR:HB   | 1.38                     | 0.88              |
| 1:B:1464:GLU:CG   | 1:B:1773:VAL:HG12 | 2.01                     | 0.88              |
| 2:I:1227:ARG:HH11 | 2:I:1227:ARG:CG   | 1.87                     | 0.88              |
| 1:C:1721:ARG:HH11 | 1:C:1721:ARG:CG   | 1.87                     | 0.87              |
| 2:G:707:PRO:HG3   | 2:G:716:VAL:HG21  | 1.56                     | 0.87              |
| 2:H:1441:ILE:HD11 | 2:H:1445:ARG:CZ   | 2.04                     | 0.87              |
| 2:I:131:ILE:HD12  | 2:I:182:VAL:HB    | 1.55                     | 0.87              |
| 1:B:1501:LEU:HD11 | 1:B:1775:LEU:HD21 | 1.56                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1422:THR:CG2  | 2:G:1474:PHE:HB2  | 2.05                     | 0.87              |
| 1:A:793:ARG:HA    | 1:A:797:THR:HG23  | 1.53                     | 0.87              |
| 1:C:59:ARG:HH11   | 2:I:1896:GLN:NE2  | 1.71                     | 0.87              |
| 2:I:298:LYS:HG2   | 2:I:448:VAL:HG22  | 1.56                     | 0.87              |
| 2:I:369:SER:OG    | 2:I:380:SER:HB3   | 1.74                     | 0.87              |
| 1:C:529:MET:HA    | 1:C:529:MET:HE3   | 1.57                     | 0.87              |
| 1:C:1498:GLU:OE2  | 1:C:1876:LEU:CA   | 2.12                     | 0.87              |
| 2:H:131:ILE:CG2   | 2:H:182:VAL:HG12  | 2.04                     | 0.87              |
| 2:I:1845:ASP:HB2  | 2:I:1849:ARG:H    | 1.38                     | 0.87              |
| 1:B:260:ARG:HH12  | 1:B:300:VAL:HG21  | 1.38                     | 0.87              |
| 2:I:932:ILE:HD11  | 2:I:1042:ALA:HB2  | 1.57                     | 0.87              |
| 1:C:253:ARG:HE    | 1:C:254:TRP:HE1   | 1.21                     | 0.87              |
| 1:A:1119:LYS:HD3  | 1:A:1121:MET:HE2  | 1.55                     | 0.87              |
| 1:A:340:ARG:NH1   | 1:A:344:GLN:HG2   | 1.88                     | 0.87              |
| 1:B:893:VAL:HG11  | 1:B:930:LEU:HD23  | 1.55                     | 0.87              |
| 2:H:741:HIS:HE1   | 2:H:845:THR:HG22  | 1.38                     | 0.86              |
| 2:H:1422:THR:CG2  | 2:H:1474:PHE:HB2  | 2.04                     | 0.86              |
| 1:C:1474:ALA:HA   | 1:C:1478:PRO:HG2  | 1.57                     | 0.86              |
| 2:H:1878:VAL:HG11 | 2:H:1910:VAL:HG22 | 1.55                     | 0.86              |
| 2:I:1739:GLU:HB3  | 2:I:1746:LEU:HD11 | 1.58                     | 0.86              |
| 1:B:1474:ALA:HA   | 1:B:1478:PRO:HG2  | 1.58                     | 0.86              |
| 2:G:741:HIS:HE1   | 2:G:845:THR:CG2   | 1.88                     | 0.86              |
| 2:H:1533:LEU:HD13 | 2:H:1630:GLY:HA2  | 1.55                     | 0.86              |
| 1:B:400:ARG:HH11  | 1:B:400:ARG:HG2   | 1.41                     | 0.85              |
| 2:H:1739:GLU:HB3  | 2:H:1746:LEU:HD11 | 1.56                     | 0.85              |
| 2:G:741:HIS:CE1   | 2:G:845:THR:CG2   | 2.59                     | 0.85              |
| 2:I:1533:LEU:HD13 | 2:I:1630:GLY:HA2  | 1.59                     | 0.85              |
| 2:I:1422:THR:O    | 2:I:1422:THR:HG23 | 1.77                     | 0.85              |
| 1:A:1749:THR:CB   | 1:A:1874:ASP:CA   | 2.55                     | 0.85              |
| 2:H:774:ALA:HB1   | 2:H:1081:HIS:HD2  | 1.41                     | 0.85              |
| 2:I:1847:LEU:H    | 2:I:1847:LEU:HD12 | 1.40                     | 0.85              |
| 1:B:340:ARG:NH1   | 1:B:344:GLN:HG2   | 1.91                     | 0.85              |
| 2:G:28:PHE:HE2    | 2:H:7:ARG:HD2     | 1.36                     | 0.85              |
| 2:H:1844:ARG:CG   | 2:H:1844:ARG:HH11 | 1.89                     | 0.85              |
| 1:A:1119:LYS:HD3  | 1:A:1121:MET:CE   | 2.07                     | 0.85              |
| 2:G:28:PHE:CZ     | 2:H:7:ARG:CD      | 2.59                     | 0.85              |
| 2:H:1844:ARG:HH11 | 2:H:1844:ARG:HG2  | 1.41                     | 0.85              |
| 2:H:297:ARG:HD3   | 2:H:447:ASN:ND2   | 1.91                     | 0.84              |
| 2:H:932:ILE:HD11  | 2:H:1042:ALA:HB2  | 1.58                     | 0.84              |
| 2:G:369:SER:OG    | 2:G:380:SER:HB3   | 1.75                     | 0.84              |
| 2:H:777:THR:CG2   | 2:H:1081:HIS:NE2  | 2.41                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:131:ILE:HG21  | 2:G:182:VAL:HG12  | 1.57                     | 0.84              |
| 1:C:340:ARG:NH1   | 1:C:344:GLN:HG2   | 1.91                     | 0.84              |
| 2:I:297:ARG:HD3   | 2:I:447:ASN:ND2   | 1.92                     | 0.84              |
| 2:G:1054:LEU:HB2  | 4:G:3051:FMN:HM72 | 1.60                     | 0.84              |
| 2:G:652:ILE:H     | 2:G:658:MET:HE3   | 1.42                     | 0.84              |
| 2:H:369:SER:OG    | 2:H:380:SER:HB3   | 1.78                     | 0.84              |
| 2:H:2038:ILE:HG22 | 2:H:2042:ILE:HD11 | 1.60                     | 0.84              |
| 1:C:852:ARG:HG2   | 1:C:852:ARG:NH1   | 1.93                     | 0.84              |
| 2:I:774:ALA:HB2   | 2:I:1077:ILE:HA   | 1.58                     | 0.84              |
| 1:B:11:HIS:ND1    | 2:H:1998:LYS:HA   | 1.93                     | 0.84              |
| 1:C:1303:GLY:HA2  | 1:C:1649:LYS:HE2  | 1.58                     | 0.84              |
| 2:I:995:LEU:HD23  | 2:I:1000:ILE:HD13 | 1.60                     | 0.84              |
| 1:C:31:THR:HG23   | 2:I:2011:ILE:HG21 | 1.59                     | 0.84              |
| 2:H:741:HIS:CE1   | 2:H:845:THR:HG22  | 2.12                     | 0.84              |
| 2:G:1425:LYS:HG2  | 2:G:1471:GLU:HG3  | 1.58                     | 0.83              |
| 2:G:1533:LEU:HD13 | 2:G:1630:GLY:HA2  | 1.60                     | 0.83              |
| 1:A:980:VAL:HG23  | 2:G:968:GLN:OE1   | 1.78                     | 0.83              |
| 2:G:774:ALA:HB2   | 2:G:1077:ILE:HA   | 1.61                     | 0.83              |
| 1:B:253:ARG:HE    | 1:B:254:TRP:HE1   | 1.21                     | 0.83              |
| 2:G:1227:ARG:HH11 | 2:G:1227:ARG:CG   | 1.89                     | 0.83              |
| 2:I:774:ALA:HB1   | 2:I:1081:HIS:HD2  | 1.43                     | 0.83              |
| 2:H:741:HIS:CE1   | 2:H:845:THR:CG2   | 2.60                     | 0.83              |
| 2:H:1227:ARG:HH11 | 2:H:1227:ARG:CG   | 1.90                     | 0.83              |
| 2:H:1672:GLN:HG2  | 2:H:1777:THR:HG23 | 1.59                     | 0.83              |
| 2:I:1844:ARG:HG2  | 2:I:1844:ARG:HH11 | 1.43                     | 0.83              |
| 2:G:1293:THR:HG23 | 2:G:1296:GLU:H    | 1.44                     | 0.83              |
| 2:I:598:THR:HG22  | 2:I:622:GLY:HA3   | 1.61                     | 0.83              |
| 1:B:403:ASP:HB2   | 1:B:1613:ASN:HD21 | 1.44                     | 0.82              |
| 1:A:20:TYR:CG     | 2:G:2033:THR:OG1  | 2.32                     | 0.82              |
| 2:G:297:ARG:HD3   | 2:G:447:ASN:ND2   | 1.94                     | 0.82              |
| 2:G:777:THR:CG2   | 2:G:1081:HIS:NE2  | 2.41                     | 0.82              |
| 2:H:85:ASN:HD22   | 2:H:135:ARG:HH11  | 1.26                     | 0.82              |
| 1:C:1367:ARG:HH12 | 1:C:1372:THR:HB   | 1.37                     | 0.82              |
| 2:G:131:ILE:CB    | 2:G:182:VAL:HG11  | 2.07                     | 0.82              |
| 2:G:298:LYS:HG2   | 2:G:448:VAL:HG22  | 1.61                     | 0.82              |
| 2:G:1739:GLU:HB3  | 2:G:1746:LEU:HD11 | 1.60                     | 0.82              |
| 2:I:1672:GLN:HG2  | 2:I:1777:THR:HG23 | 1.61                     | 0.82              |
| 1:A:36:LEU:HD22   | 1:A:61:LEU:HD21   | 1.60                     | 0.82              |
| 1:A:1249:SER:HB3  | 1:A:1280:ILE:HG23 | 1.62                     | 0.82              |
| 1:B:1014:ASP:H    | 1:B:1510:ASN:HD21 | 1.28                     | 0.82              |
| 2:H:995:LEU:HD23  | 2:H:1000:ILE:HD13 | 1.58                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1931:LEU:HB3  | 2:I:1935:GLU:HG2  | 1.62                     | 0.82              |
| 2:I:2038:ILE:HG22 | 2:I:2042:ILE:HD11 | 1.61                     | 0.82              |
| 1:A:335:HIS:HE1   | 1:B:335:HIS:CE1   | 1.98                     | 0.82              |
| 1:B:12:ILE:HD11   | 2:H:2041:ILE:CD1  | 2.10                     | 0.82              |
| 1:C:333:LYS:O     | 1:C:337:VAL:HG23  | 1.80                     | 0.81              |
| 2:G:995:LEU:HD23  | 2:G:1000:ILE:HD13 | 1.60                     | 0.81              |
| 2:G:1847:LEU:HD13 | 2:G:1849:ARG:HD2  | 1.62                     | 0.81              |
| 2:I:128:THR:HA    | 2:I:182:VAL:HG21  | 1.62                     | 0.81              |
| 1:A:1464:GLU:HG3  | 1:A:1773:VAL:HG12 | 0.85                     | 0.81              |
| 1:A:1501:LEU:HD11 | 1:A:1775:LEU:HD21 | 1.61                     | 0.81              |
| 2:H:543:PHE:HB2   | 2:H:545:GLN:HE22  | 1.45                     | 0.81              |
| 2:H:1159:ILE:HG12 | 2:H:1168:ASN:HA   | 1.61                     | 0.81              |
| 2:I:1054:LEU:HB2  | 4:I:3051:FMN:C7M  | 2.11                     | 0.81              |
| 2:I:1844:ARG:HH11 | 2:I:1844:ARG:CG   | 1.93                     | 0.81              |
| 1:B:1249:SER:HB3  | 1:B:1280:ILE:HG23 | 1.62                     | 0.81              |
| 2:G:543:PHE:HB2   | 2:G:545:GLN:HE22  | 1.46                     | 0.81              |
| 2:I:345:THR:HG22  | 2:I:347:GLU:H     | 1.46                     | 0.81              |
| 2:I:777:THR:CG2   | 2:I:1081:HIS:NE2  | 2.43                     | 0.81              |
| 2:G:1931:LEU:HB3  | 2:G:1935:GLU:HG2  | 1.61                     | 0.81              |
| 1:A:1460:LYS:HE2  | 1:A:1773:VAL:O    | 1.80                     | 0.81              |
| 1:C:59:ARG:HH11   | 2:I:1896:GLN:HE22 | 1.25                     | 0.81              |
| 2:H:1149:TRP:HA   | 2:H:1242:PHE:CE1  | 2.15                     | 0.81              |
| 1:B:93:ASP:HB3    | 1:B:94:PRO:HD2    | 1.62                     | 0.81              |
| 1:B:881:ASN:HA    | 1:B:944:ARG:NH2   | 1.96                     | 0.81              |
| 1:A:1203:ASP:HB3  | 1:B:179:LYS:NZ    | 1.95                     | 0.81              |
| 2:G:2038:ILE:HG22 | 2:G:2042:ILE:HD11 | 1.60                     | 0.81              |
| 1:A:335:HIS:CE1   | 1:C:335:HIS:HE1   | 1.98                     | 0.81              |
| 2:I:345:THR:HB    | 2:I:348:GLN:H     | 1.46                     | 0.81              |
| 1:A:93:ASP:HB3    | 1:A:94:PRO:HD2    | 1.63                     | 0.81              |
| 2:I:1159:ILE:HG12 | 2:I:1168:ASN:HA   | 1.63                     | 0.81              |
| 1:A:400:ARG:HG2   | 1:A:400:ARG:NH1   | 1.91                     | 0.80              |
| 2:I:1693:ARG:HD2  | 2:I:1825:GLU:OE2  | 1.80                     | 0.80              |
| 1:A:333:LYS:O     | 1:A:337:VAL:HG23  | 1.82                     | 0.80              |
| 1:A:1552:ASN:O    | 1:A:1556:THR:HG22 | 1.80                     | 0.80              |
| 2:G:1693:ARG:HD2  | 2:G:1825:GLU:OE2  | 1.81                     | 0.80              |
| 2:I:584:SER:HB3   | 2:I:591:PRO:HG3   | 1.63                     | 0.80              |
| 1:B:1030:TRP:CD1  | 1:B:1580:LEU:HD22 | 2.17                     | 0.80              |
| 2:H:298:LYS:HG2   | 2:H:448:VAL:HG22  | 1.63                     | 0.80              |
| 2:H:1931:LEU:HB3  | 2:H:1935:GLU:HG2  | 1.62                     | 0.80              |
| 1:A:20:TYR:CE1    | 2:G:2035:SER:HB2  | 2.17                     | 0.80              |
| 1:A:340:ARG:HH12  | 1:A:344:GLN:HG2   | 1.45                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:259:THR:HG22  | 2:I:262:GLU:HG3   | 1.63                     | 0.80              |
| 2:G:1672:GLN:HG2  | 2:G:1777:THR:HG23 | 1.61                     | 0.80              |
| 1:B:36:LEU:HD22   | 1:B:61:LEU:HD21   | 1.64                     | 0.80              |
| 2:H:1159:ILE:HG12 | 2:H:1169:PRO:HD3  | 1.63                     | 0.80              |
| 1:B:24:SER:CB     | 2:H:2014:LEU:HD12 | 2.11                     | 0.80              |
| 2:G:741:HIS:CE1   | 2:G:845:THR:HG22  | 2.17                     | 0.80              |
| 2:H:1847:LEU:HD13 | 2:H:1849:ARG:HD2  | 1.63                     | 0.80              |
| 2:I:192:ALA:HA    | 2:I:215:ILE:HD12  | 1.64                     | 0.80              |
| 1:C:1249:SER:HB3  | 1:C:1280:ILE:HG23 | 1.63                     | 0.80              |
| 1:C:1460:LYS:CE   | 1:C:1774:GLU:OE2  | 2.29                     | 0.80              |
| 2:I:1242:PHE:HE2  | 2:I:1244:PRO:HG3  | 1.46                     | 0.80              |
| 1:A:484:LEU:O     | 1:A:485:ASP:HB2   | 1.82                     | 0.79              |
| 1:A:1501:LEU:HD12 | 1:A:1775:LEU:HD21 | 1.63                     | 0.79              |
| 2:H:598:THR:HG22  | 2:H:622:GLY:HA3   | 1.64                     | 0.79              |
| 2:H:907:VAL:HG21  | 2:H:921:GLU:HG2   | 1.64                     | 0.79              |
| 2:I:455:ILE:HD11  | 2:I:469:ARG:HD3   | 1.63                     | 0.79              |
| 1:C:1460:LYS:CE   | 1:C:1774:GLU:CD   | 2.50                     | 0.79              |
| 2:I:1293:THR:HG23 | 2:I:1296:GLU:H    | 1.47                     | 0.79              |
| 2:H:1199:GLU:OE2  | 2:H:1567:ARG:CZ   | 2.31                     | 0.79              |
| 2:I:55:THR:CG2    | 2:I:113:ASP:HB2   | 2.12                     | 0.79              |
| 1:A:31:THR:HG23   | 2:G:2011:ILE:HG21 | 1.64                     | 0.79              |
| 1:C:1501:LEU:HD11 | 1:C:1775:LEU:HD21 | 1.55                     | 0.79              |
| 2:I:1310:ASP:OD2  | 2:I:1602:SER:HB3  | 1.82                     | 0.79              |
| 2:H:455:ILE:HD11  | 2:H:469:ARG:HD3   | 1.63                     | 0.79              |
| 2:H:774:ALA:HB2   | 2:H:1077:ILE:HA   | 1.64                     | 0.79              |
| 2:H:1636:LYS:N    | 2:H:1657:ILE:O    | 2.14                     | 0.79              |
| 2:I:238:CYS:HB2   | 2:I:239:PRO:HD3   | 1.64                     | 0.79              |
| 2:I:543:PHE:HB2   | 2:I:545:GLN:HE22  | 1.46                     | 0.79              |
| 2:G:634:ILE:HD11  | 2:G:649:ILE:HD11  | 1.63                     | 0.79              |
| 2:I:907:VAL:HG21  | 2:I:921:GLU:HG2   | 1.65                     | 0.79              |
| 2:G:1314:ARG:HH11 | 2:G:1314:ARG:CG   | 1.95                     | 0.79              |
| 1:B:260:ARG:NH1   | 1:B:300:VAL:HG21  | 1.97                     | 0.79              |
| 1:C:403:ASP:HB2   | 1:C:1613:ASN:HD21 | 1.46                     | 0.79              |
| 2:G:774:ALA:HB1   | 2:G:1081:HIS:HD2  | 1.47                     | 0.79              |
| 1:B:1303:GLY:HA2  | 1:B:1649:LYS:HE2  | 1.63                     | 0.79              |
| 2:G:55:THR:CG2    | 2:G:113:ASP:HB2   | 2.13                     | 0.79              |
| 2:H:105:ALA:HB1   | 2:H:119:THR:HG23  | 1.65                     | 0.79              |
| 2:H:757:ILE:HG21  | 2:H:765:LEU:HD13  | 1.64                     | 0.79              |
| 2:I:1847:LEU:HD13 | 2:I:1849:ARG:HD2  | 1.64                     | 0.79              |
| 1:B:1722:VAL:CG1  | 1:B:1731:LEU:HB3  | 2.13                     | 0.78              |
| 1:C:1523:ARG:HH11 | 1:C:1523:ARG:CG   | 1.96                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:85:ASN:HD22   | 2:G:135:ARG:HH11  | 1.28                     | 0.78              |
| 2:I:1149:TRP:HA   | 2:I:1242:PHE:CE1  | 2.19                     | 0.78              |
| 1:C:328:LEU:O     | 1:C:331:ILE:HG22  | 1.84                     | 0.78              |
| 2:H:345:THR:HB    | 2:H:348:GLN:H     | 1.48                     | 0.78              |
| 2:H:960:LYS:HE2   | 2:H:960:LYS:HA    | 1.65                     | 0.78              |
| 2:H:1567:ARG:HG3  | 2:H:1567:ARG:NH1  | 1.98                     | 0.78              |
| 2:I:85:ASN:HD22   | 2:I:135:ARG:HH11  | 1.28                     | 0.78              |
| 1:B:12:ILE:HD11   | 2:H:2041:ILE:HD12 | 1.63                     | 0.78              |
| 2:G:7:ARG:NH2     | 2:G:27:PHE:HB3    | 1.99                     | 0.78              |
| 2:H:131:ILE:CB    | 2:H:182:VAL:CG1   | 2.53                     | 0.78              |
| 1:A:328:LEU:O     | 1:A:331:ILE:HG22  | 1.84                     | 0.78              |
| 1:B:333:LYS:O     | 1:B:337:VAL:HG23  | 1.81                     | 0.78              |
| 2:I:741:HIS:HE1   | 2:I:845:THR:HG22  | 1.41                     | 0.78              |
| 1:C:1014:ASP:N    | 1:C:1510:ASN:HD21 | 1.82                     | 0.78              |
| 2:I:138:ASP:O     | 2:I:139:LYS:HG3   | 1.83                     | 0.78              |
| 2:I:1770:LEU:HD23 | 2:I:1776:PHE:CE2  | 2.19                     | 0.78              |
| 1:A:2:LYS:HD2     | 2:G:2050:GLN:HB3  | 1.66                     | 0.78              |
| 1:B:24:SER:O      | 2:H:1977:HIS:HD2  | 1.67                     | 0.78              |
| 1:B:198:PRO:HG3   | 1:B:209:LEU:CD2   | 2.13                     | 0.78              |
| 2:H:55:THR:CG2    | 2:H:113:ASP:HB2   | 2.13                     | 0.78              |
| 1:C:1498:GLU:CG   | 1:C:1876:LEU:CD1  | 2.51                     | 0.78              |
| 2:I:7:ARG:NH2     | 2:I:27:PHE:HB3    | 1.97                     | 0.78              |
| 2:I:634:ILE:HD11  | 2:I:649:ILE:HD11  | 1.66                     | 0.78              |
| 2:G:1227:ARG:HD2  | 2:G:1565:VAL:HG11 | 1.66                     | 0.77              |
| 2:G:1770:LEU:HD23 | 2:G:1776:PHE:CE2  | 2.20                     | 0.77              |
| 2:H:1693:ARG:HD2  | 2:H:1825:GLU:OE2  | 1.83                     | 0.77              |
| 1:A:335:HIS:CE1   | 1:C:335:HIS:CE1   | 2.72                     | 0.77              |
| 1:C:1463:VAL:HG11 | 1:C:1877:GLN:HE22 | 1.48                     | 0.77              |
| 2:H:1293:THR:HG23 | 2:H:1296:GLU:H    | 1.49                     | 0.77              |
| 1:C:1665:ILE:HG13 | 1:C:1669:ARG:HD3  | 1.66                     | 0.77              |
| 2:G:455:ILE:HD11  | 2:G:469:ARG:HD3   | 1.66                     | 0.77              |
| 2:G:28:PHE:HZ     | 2:H:7:ARG:CD      | 1.97                     | 0.77              |
| 2:G:355:LYS:O     | 2:G:358:SER:HB3   | 1.84                     | 0.77              |
| 2:H:131:ILE:CG2   | 2:H:182:VAL:CG1   | 2.63                     | 0.77              |
| 2:I:741:HIS:CE1   | 2:I:855:HIS:NE2   | 2.52                     | 0.77              |
| 1:A:1523:ARG:HH11 | 1:A:1523:ARG:CG   | 1.97                     | 0.77              |
| 2:H:1310:ASP:OD2  | 2:H:1602:SER:HB3  | 1.82                     | 0.77              |
| 1:A:24:SER:HB3    | 2:G:2014:LEU:HD12 | 1.64                     | 0.77              |
| 1:B:1239:HIS:HD2  | 1:B:1241:SER:OG   | 1.67                     | 0.77              |
| 2:I:1314:ARG:HH11 | 2:I:1314:ARG:CG   | 1.98                     | 0.77              |
| 2:I:1423:PHE:HD1  | 2:I:1423:PHE:H    | 1.30                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1030:TRP:CD1  | 1:C:1580:LEU:HD22 | 2.20                     | 0.77              |
| 1:C:1693:ILE:HD11 | 2:I:998:GLN:HB2   | 1.67                     | 0.77              |
| 2:G:345:THR:HG22  | 2:G:347:GLU:H     | 1.47                     | 0.77              |
| 2:G:598:THR:HG22  | 2:G:622:GLY:HA3   | 1.67                     | 0.77              |
| 2:G:1284:VAL:HG13 | 2:G:1377:VAL:HG22 | 1.65                     | 0.77              |
| 1:B:29:ILE:HG13   | 2:H:1891:TYR:O    | 1.85                     | 0.77              |
| 1:C:93:ASP:HB3    | 1:C:94:PRO:HD2    | 1.65                     | 0.77              |
| 1:C:12:ILE:HD11   | 2:I:2041:ILE:HD12 | 1.67                     | 0.77              |
| 1:C:340:ARG:HH12  | 1:C:344:GLN:HG2   | 1.49                     | 0.77              |
| 1:C:1030:TRP:NE1  | 1:C:1580:LEU:HD22 | 2.00                     | 0.77              |
| 2:G:907:VAL:HG21  | 2:G:921:GLU:HG2   | 1.65                     | 0.77              |
| 1:A:1665:ILE:HG13 | 1:A:1669:ARG:HD3  | 1.66                     | 0.76              |
| 2:H:1834:ARG:HG2  | 2:H:1834:ARG:NH1  | 1.86                     | 0.76              |
| 2:I:1567:ARG:HG3  | 2:I:1567:ARG:NH1  | 2.00                     | 0.76              |
| 2:I:1834:ARG:HG2  | 2:I:1834:ARG:NH1  | 1.93                     | 0.76              |
| 2:I:1956:ARG:CB   | 2:I:1957:PRO:HD3  | 2.09                     | 0.76              |
| 1:A:1030:TRP:NE1  | 1:A:1580:LEU:HD22 | 1.99                     | 0.76              |
| 1:B:1030:TRP:NE1  | 1:B:1580:LEU:HD22 | 2.00                     | 0.76              |
| 1:A:198:PRO:HG3   | 1:A:209:LEU:CD2   | 2.14                     | 0.76              |
| 1:C:198:PRO:HG3   | 1:C:209:LEU:CD2   | 2.15                     | 0.76              |
| 2:G:1678:MET:HE3  | 2:G:1707:LEU:HD22 | 1.66                     | 0.76              |
| 1:C:400:ARG:HG2   | 1:C:400:ARG:NH1   | 1.94                     | 0.76              |
| 2:H:762:ASN:HD22  | 2:H:762:ASN:N     | 1.82                     | 0.76              |
| 2:G:146:PHE:HA    | 2:G:149:VAL:CG1   | 2.15                     | 0.76              |
| 2:G:345:THR:HB    | 2:G:348:GLN:H     | 1.50                     | 0.76              |
| 2:I:355:LYS:O     | 2:I:358:SER:HB3   | 1.85                     | 0.76              |
| 1:A:1030:TRP:CD1  | 1:A:1580:LEU:HD22 | 2.21                     | 0.76              |
| 2:G:964:LEU:HD23  | 2:G:964:LEU:H     | 1.50                     | 0.76              |
| 2:G:1149:TRP:HA   | 2:G:1242:PHE:CE1  | 2.20                     | 0.76              |
| 2:H:598:THR:OG1   | 2:H:599:PRO:HD3   | 1.86                     | 0.76              |
| 2:I:2015:THR:HG22 | 2:I:2017:LYS:H    | 1.51                     | 0.76              |
| 1:C:24:SER:O      | 2:I:1977:HIS:HD2  | 1.68                     | 0.76              |
| 1:C:1722:VAL:CG1  | 1:C:1731:LEU:HB3  | 2.14                     | 0.76              |
| 2:H:1638:ILE:HD12 | 2:H:1657:ILE:HG13 | 1.67                     | 0.76              |
| 2:H:1956:ARG:HB2  | 2:H:1957:PRO:CD   | 2.12                     | 0.76              |
| 1:C:1239:HIS:HD2  | 1:C:1241:SER:OG   | 1.68                     | 0.76              |
| 2:H:584:SER:HB3   | 2:H:591:PRO:HG3   | 1.67                     | 0.76              |
| 1:A:988:ILE:HD13  | 1:A:1048:GLU:CB   | 2.15                     | 0.75              |
| 1:B:1501:LEU:CD1  | 1:B:1775:LEU:HD21 | 2.16                     | 0.75              |
| 2:G:2015:THR:HG22 | 2:G:2017:LYS:H    | 1.51                     | 0.75              |
| 2:H:317:THR:HG21  | 2:I:1309:GLU:HG3  | 1.67                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1314:ARG:HH11 | 2:H:1314:ARG:CG   | 1.97                     | 0.75              |
| 2:I:707:PRO:CG    | 2:I:716:VAL:HG21  | 2.15                     | 0.75              |
| 1:B:340:ARG:HH12  | 1:B:344:GLN:HG2   | 1.48                     | 0.75              |
| 1:B:1523:ARG:HH11 | 1:B:1523:ARG:CG   | 1.98                     | 0.75              |
| 2:H:192:ALA:HA    | 2:H:215:ILE:HD12  | 1.68                     | 0.75              |
| 2:I:1054:LEU:HB2  | 4:I:3051:FMN:HM72 | 1.66                     | 0.75              |
| 1:B:1665:ILE:HG13 | 1:B:1669:ARG:HD3  | 1.66                     | 0.75              |
| 2:G:1159:ILE:HG12 | 2:G:1168:ASN:HA   | 1.67                     | 0.75              |
| 2:G:1956:ARG:HB2  | 2:G:1957:PRO:CD   | 2.11                     | 0.75              |
| 2:H:7:ARG:NH2     | 2:H:27:PHE:HB3    | 1.99                     | 0.75              |
| 2:I:856:LYS:HG2   | 2:I:1054:LEU:HD12 | 1.68                     | 0.75              |
| 1:A:1460:LYS:HE3  | 1:A:1773:VAL:O    | 1.86                     | 0.75              |
| 2:G:960:LYS:HE2   | 2:G:960:LYS:HA    | 1.67                     | 0.75              |
| 2:H:84:LEU:HD13   | 2:H:133:ALA:HB2   | 1.69                     | 0.75              |
| 2:H:355:LYS:O     | 2:H:358:SER:HB3   | 1.85                     | 0.75              |
| 1:B:328:LEU:O     | 1:B:331:ILE:HG22  | 1.86                     | 0.75              |
| 2:H:259:THR:HG22  | 2:H:262:GLU:HG3   | 1.68                     | 0.75              |
| 2:H:1770:LEU:HD23 | 2:H:1776:PHE:CE2  | 2.22                     | 0.75              |
| 1:A:1498:GLU:HB2  | 1:A:1876:LEU:HD13 | 1.67                     | 0.75              |
| 1:B:1460:LYS:HE2  | 1:B:1773:VAL:O    | 1.86                     | 0.75              |
| 1:B:1208:VAL:HG13 | 1:B:1212:THR:HB   | 1.68                     | 0.75              |
| 2:H:579:VAL:HG23  | 2:H:1078:HIS:CD2  | 2.21                     | 0.75              |
| 2:H:2015:THR:HG22 | 2:H:2017:LYS:H    | 1.51                     | 0.75              |
| 1:A:1303:GLY:HA2  | 1:A:1649:LYS:HE2  | 1.68                     | 0.75              |
| 1:A:1310:GLU:OE1  | 1:A:1649:LYS:HE3  | 1.86                     | 0.75              |
| 2:G:192:ALA:HA    | 2:G:215:ILE:HD12  | 1.67                     | 0.75              |
| 2:G:572:ASN:HB3   | 2:G:576:LYS:H     | 1.52                     | 0.75              |
| 2:H:455:ILE:HD11  | 2:H:469:ARG:CD    | 2.17                     | 0.75              |
| 2:H:741:HIS:CB    | 2:H:853:PRO:HB2   | 2.16                     | 0.75              |
| 2:I:960:LYS:HE2   | 2:I:960:LYS:HA    | 1.67                     | 0.75              |
| 2:I:572:ASN:HB3   | 2:I:576:LYS:H     | 1.52                     | 0.75              |
| 2:I:757:ILE:HG21  | 2:I:765:LEU:HD13  | 1.69                     | 0.75              |
| 2:I:1129:ALA:HB2  | 2:I:1138:TRP:CZ3  | 2.22                     | 0.75              |
| 2:I:1956:ARG:HB2  | 2:I:1957:PRO:CD   | 2.11                     | 0.75              |
| 2:H:943:TRP:CH2   | 2:H:1016:PRO:HG3  | 2.22                     | 0.74              |
| 2:H:1834:ARG:HH11 | 2:H:1834:ARG:CG   | 1.92                     | 0.74              |
| 2:I:1159:ILE:HG12 | 2:I:1169:PRO:HD3  | 1.67                     | 0.74              |
| 2:I:1284:VAL:HG13 | 2:I:1377:VAL:HG22 | 1.69                     | 0.74              |
| 1:A:427:ASN:HD21  | 1:A:610:THR:H     | 1.33                     | 0.74              |
| 1:B:1552:ASN:O    | 1:B:1556:THR:HG22 | 1.88                     | 0.74              |
| 2:H:1678:MET:HE3  | 2:H:1707:LEU:HD22 | 1.67                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:20:TYR:CD2    | 2:G:2033:THR:OG1  | 2.40                     | 0.74              |
| 2:H:1242:PHE:HE2  | 2:H:1244:PRO:HG3  | 1.51                     | 0.74              |
| 2:H:1672:GLN:HA   | 2:H:1676:MET:HE1  | 1.68                     | 0.74              |
| 2:I:943:TRP:CH2   | 2:I:1016:PRO:HG3  | 2.21                     | 0.74              |
| 2:H:1784:MET:HG3  | 2:H:1785:GLU:N    | 2.03                     | 0.74              |
| 1:A:335:HIS:CE1   | 1:B:335:HIS:CE1   | 2.74                     | 0.74              |
| 1:A:1239:HIS:HD2  | 1:A:1241:SER:OG   | 1.69                     | 0.74              |
| 1:B:335:HIS:HE1   | 1:C:335:HIS:CE1   | 2.06                     | 0.74              |
| 1:C:749:ILE:HD13  | 1:C:806:VAL:HG12  | 1.70                     | 0.74              |
| 2:H:1129:ALA:HB2  | 2:H:1138:TRP:CZ3  | 2.21                     | 0.74              |
| 2:H:1672:GLN:HA   | 2:H:1676:MET:CE   | 2.18                     | 0.74              |
| 2:H:1956:ARG:CB   | 2:H:1957:PRO:HD3  | 2.11                     | 0.74              |
| 2:I:105:ALA:HB1   | 2:I:119:THR:HG23  | 1.67                     | 0.74              |
| 2:I:131:ILE:HB    | 2:I:182:VAL:HG11  | 1.69                     | 0.74              |
| 1:A:1749:THR:CB   | 1:A:1873:HIS:C    | 2.56                     | 0.74              |
| 1:C:1552:ASN:O    | 1:C:1556:THR:HG22 | 1.88                     | 0.74              |
| 2:G:1310:ASP:OD2  | 2:G:1602:SER:HB3  | 1.88                     | 0.74              |
| 2:I:835:THR:HG21  | 2:I:855:HIS:CD2   | 2.23                     | 0.74              |
| 2:I:2035:SER:HB3  | 2:I:2038:ILE:HG13 | 1.69                     | 0.74              |
| 1:B:1551:LYS:HD2  | 1:B:1617:ILE:HG21 | 1.70                     | 0.74              |
| 2:G:705:LEU:HD12  | 2:G:716:VAL:HG13  | 1.70                     | 0.74              |
| 2:I:741:HIS:CE1   | 2:I:845:THR:HG21  | 2.22                     | 0.74              |
| 1:A:1456:GLU:OE1  | 1:A:1775:LEU:HD23 | 1.87                     | 0.74              |
| 2:G:757:ILE:HG21  | 2:G:765:LEU:HD13  | 1.67                     | 0.74              |
| 1:B:18:LEU:HD21   | 2:H:1815:LEU:HD12 | 1.70                     | 0.74              |
| 2:I:1889:VAL:HG13 | 2:I:1977:HIS:HB2  | 1.69                     | 0.74              |
| 1:A:44:VAL:CG1    | 1:A:78:ILE:HG12   | 2.18                     | 0.73              |
| 1:B:833:PHE:HA    | 1:B:937:LYS:HD2   | 1.69                     | 0.73              |
| 2:H:7:ARG:NH1     | 2:H:24:THR:HG23   | 2.03                     | 0.73              |
| 2:H:1194:VAL:HG22 | 2:H:1212:LYS:HB3  | 1.70                     | 0.73              |
| 2:H:1004:LEU:HD21 | 2:H:1020:VAL:HG23 | 1.70                     | 0.73              |
| 1:A:982:ILE:HD11  | 2:G:965:SER:HB2   | 1.69                     | 0.73              |
| 1:C:36:LEU:HD22   | 1:C:61:LEU:HD21   | 1.68                     | 0.73              |
| 2:G:1159:ILE:HG12 | 2:G:1169:PRO:HD3  | 1.71                     | 0.73              |
| 2:H:705:LEU:HD12  | 2:H:716:VAL:HG13  | 1.70                     | 0.73              |
| 1:C:888:ILE:HD11  | 1:C:930:LEU:HD21  | 1.71                     | 0.73              |
| 2:H:1680:LEU:HD13 | 2:H:1687:ALA:HB2  | 1.71                     | 0.73              |
| 2:I:1784:MET:HG3  | 2:I:1785:GLU:N    | 2.02                     | 0.73              |
| 2:G:7:ARG:NH1     | 2:G:24:THR:HG23   | 2.03                     | 0.73              |
| 2:G:105:ALA:HB1   | 2:G:119:THR:HG23  | 1.70                     | 0.73              |
| 2:I:455:ILE:HD11  | 2:I:469:ARG:CD    | 2.19                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:749:ILE:HD13  | 1:B:806:VAL:HG12  | 1.70                     | 0.73              |
| 1:C:1431:GLU:CG   | 1:C:1433:HIS:CE1  | 2.72                     | 0.73              |
| 2:G:259:THR:HG22  | 2:G:262:GLU:HG3   | 1.68                     | 0.73              |
| 2:G:777:THR:HG22  | 2:G:1081:HIS:NE2  | 2.03                     | 0.73              |
| 2:I:7:ARG:NH1     | 2:I:24:THR:HG23   | 2.03                     | 0.73              |
| 1:A:1551:LYS:HD2  | 1:A:1617:ILE:HG21 | 1.70                     | 0.73              |
| 2:G:194:THR:HG23  | 2:G:300:ILE:HD11  | 1.70                     | 0.73              |
| 2:H:345:THR:HG22  | 2:H:347:GLU:H     | 1.51                     | 0.73              |
| 2:H:1300:PHE:CA   | 2:H:1556:VAL:HG11 | 2.19                     | 0.73              |
| 2:H:1422:THR:HG21 | 2:H:1474:PHE:HB2  | 1.70                     | 0.73              |
| 1:C:260:ARG:HH12  | 1:C:300:VAL:HG21  | 1.52                     | 0.73              |
| 2:G:562:LEU:HG    | 2:G:793:PRO:HG2   | 1.71                     | 0.73              |
| 2:G:652:ILE:H     | 2:G:658:MET:CE    | 2.01                     | 0.73              |
| 2:H:194:THR:HG23  | 2:H:300:ILE:HD11  | 1.71                     | 0.73              |
| 2:H:1331:TRP:CZ2  | 2:H:1335:ILE:HG13 | 2.23                     | 0.73              |
| 2:H:1355:ASN:HA   | 2:H:1407:THR:O    | 1.88                     | 0.73              |
| 2:H:7:ARG:HH21    | 2:H:27:PHE:CB     | 2.01                     | 0.73              |
| 2:H:146:PHE:HA    | 2:H:149:VAL:CG1   | 2.18                     | 0.73              |
| 2:H:1300:PHE:HA   | 2:H:1556:VAL:HG11 | 1.70                     | 0.73              |
| 1:B:44:VAL:CG1    | 1:B:78:ILE:HG12   | 2.18                     | 0.72              |
| 2:H:579:VAL:HG23  | 2:H:1078:HIS:NE2  | 2.03                     | 0.72              |
| 2:H:1284:VAL:HG13 | 2:H:1377:VAL:HG22 | 1.71                     | 0.72              |
| 2:I:707:PRO:HG3   | 2:I:716:VAL:CG2   | 2.18                     | 0.72              |
| 2:G:762:ASN:HD22  | 2:G:762:ASN:N     | 1.82                     | 0.72              |
| 2:I:579:VAL:HG23  | 2:I:1078:HIS:CD2  | 2.24                     | 0.72              |
| 1:A:655:LEU:HD22  | 1:A:916:LEU:HD11  | 1.71                     | 0.72              |
| 1:A:1045:PHE:HB3  | 1:A:1049:GLY:HA3  | 1.71                     | 0.72              |
| 1:C:1208:VAL:HG13 | 1:C:1212:THR:HB   | 1.71                     | 0.72              |
| 1:C:1551:LYS:HD2  | 1:C:1617:ILE:HG21 | 1.70                     | 0.72              |
| 2:G:1889:VAL:HG13 | 2:G:1977:HIS:HB2  | 1.72                     | 0.72              |
| 2:H:128:THR:HA    | 2:H:182:VAL:CG2   | 2.16                     | 0.72              |
| 2:H:634:ILE:HD11  | 2:H:649:ILE:HD11  | 1.71                     | 0.72              |
| 2:I:1672:GLN:HA   | 2:I:1676:MET:HE1  | 1.70                     | 0.72              |
| 1:A:1722:VAL:CG1  | 1:A:1731:LEU:HB3  | 2.19                     | 0.72              |
| 1:C:473:GLY:O     | 1:C:477:ILE:HG13  | 1.88                     | 0.72              |
| 2:I:191:SER:HA    | 2:I:194:THR:HG22  | 1.71                     | 0.72              |
| 2:I:194:THR:HG23  | 2:I:300:ILE:HD11  | 1.70                     | 0.72              |
| 1:A:24:SER:CB     | 2:G:2014:LEU:HD12 | 2.19                     | 0.72              |
| 1:C:427:ASN:HD21  | 1:C:610:THR:H     | 1.38                     | 0.72              |
| 2:H:109:LEU:HD11  | 2:H:116:LEU:HD23  | 1.72                     | 0.72              |
| 1:A:1208:VAL:HG13 | 1:A:1212:THR:HB   | 1.70                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:254:TRP:CZ3   | 1:B:302:LEU:HD13  | 2.24                     | 0.72              |
| 1:B:1668:ASP:OD2  | 1:B:1805:VAL:HB   | 1.90                     | 0.72              |
| 2:I:7:ARG:HH21    | 2:I:27:PHE:CB     | 1.99                     | 0.72              |
| 2:I:777:THR:HG22  | 2:I:1081:HIS:NE2  | 2.04                     | 0.72              |
| 2:I:1672:GLN:HA   | 2:I:1676:MET:CE   | 2.20                     | 0.72              |
| 1:B:24:SER:HB3    | 2:H:2014:LEU:HD12 | 1.69                     | 0.72              |
| 2:G:584:SER:HB3   | 2:G:591:PRO:HG3   | 1.70                     | 0.72              |
| 2:H:455:ILE:CD1   | 2:H:469:ARG:HD3   | 2.20                     | 0.72              |
| 2:H:455:ILE:CG1   | 2:H:469:ARG:HD3   | 2.20                     | 0.72              |
| 2:I:259:THR:HG22  | 2:I:262:GLU:CG    | 2.20                     | 0.72              |
| 1:B:473:GLY:O     | 1:B:477:ILE:HG13  | 1.89                     | 0.72              |
| 2:G:598:THR:OG1   | 2:G:599:PRO:HD3   | 1.89                     | 0.72              |
| 2:G:1680:LEU:HD13 | 2:G:1687:ALA:HB2  | 1.71                     | 0.72              |
| 2:H:572:ASN:HB3   | 2:H:576:LYS:H     | 1.54                     | 0.72              |
| 2:G:131:ILE:CD1   | 2:G:182:VAL:HB    | 2.09                     | 0.72              |
| 2:H:777:THR:HG22  | 2:H:1081:HIS:NE2  | 2.04                     | 0.72              |
| 2:G:741:HIS:CE1   | 2:G:845:THR:HG21  | 2.24                     | 0.72              |
| 2:G:741:HIS:CE1   | 2:G:855:HIS:NE2   | 2.58                     | 0.72              |
| 2:G:751:LEU:HD23  | 2:G:791:TYR:CE2   | 2.25                     | 0.72              |
| 2:I:84:LEU:HD13   | 2:I:133:ALA:HB2   | 1.71                     | 0.72              |
| 2:I:1086:LEU:HG   | 2:I:1092:ASP:HA   | 1.72                     | 0.72              |
| 1:B:1232:TYR:CZ   | 1:B:1701:LYS:HD2  | 2.26                     | 0.71              |
| 2:G:161:GLY:H     | 2:G:505:GLY:HA3   | 1.54                     | 0.71              |
| 2:G:1567:ARG:HG3  | 2:G:1567:ARG:NH1  | 2.02                     | 0.71              |
| 2:I:2036:GLU:HB2  | 2:I:2037:PRO:HD3  | 1.72                     | 0.71              |
| 1:A:1501:LEU:CD1  | 1:A:1775:LEU:CD2  | 2.62                     | 0.71              |
| 1:B:888:ILE:HD12  | 1:B:939:PHE:HE2   | 1.55                     | 0.71              |
| 1:C:59:ARG:NH1    | 2:I:1896:GLN:NE2  | 2.38                     | 0.71              |
| 2:H:652:ILE:H     | 2:H:658:MET:CE    | 2.03                     | 0.71              |
| 2:H:741:HIS:NE2   | 2:H:855:HIS:CE1   | 2.58                     | 0.71              |
| 2:I:1673:GLU:H    | 2:I:1676:MET:HE3  | 1.55                     | 0.71              |
| 1:B:1030:TRP:NE1  | 1:B:1580:LEU:CD2  | 2.54                     | 0.71              |
| 2:G:762:ASN:H     | 2:G:762:ASN:ND2   | 1.85                     | 0.71              |
| 2:G:1638:ILE:HD12 | 2:G:1657:ILE:HD12 | 1.71                     | 0.71              |
| 2:H:1227:ARG:HD2  | 2:H:1565:VAL:HG11 | 1.71                     | 0.71              |
| 2:I:1670:GLY:H    | 2:I:1672:GLN:HE21 | 1.38                     | 0.71              |
| 1:A:733:ILE:HD13  | 1:A:761:LEU:HD11  | 1.71                     | 0.71              |
| 1:A:982:ILE:HD11  | 2:G:965:SER:CB    | 2.21                     | 0.71              |
| 1:A:983:GLN:NE2   | 2:G:962:LYS:HD2   | 2.05                     | 0.71              |
| 1:B:2:LYS:HD2     | 2:H:2050:GLN:HB3  | 1.72                     | 0.71              |
| 2:G:50:ALA:HB3    | 2:G:53:GLU:HG3    | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:2036:GLU:HB2  | 2:G:2037:PRO:HD3  | 1.73                     | 0.71              |
| 2:H:1819:ALA:HA   | 2:H:2005:ARG:HH11 | 1.55                     | 0.71              |
| 2:I:455:ILE:CG1   | 2:I:469:ARG:HD3   | 2.21                     | 0.71              |
| 2:I:1331:TRP:CZ2  | 2:I:1335:ILE:HG13 | 2.25                     | 0.71              |
| 1:C:733:ILE:HD13  | 1:C:761:LEU:HD11  | 1.72                     | 0.71              |
| 2:H:1054:LEU:HB2  | 4:H:3051:FMN:C7M  | 2.21                     | 0.71              |
| 2:I:732:TRP:CG    | 2:I:750:MET:CE    | 2.73                     | 0.71              |
| 1:A:1208:VAL:CG1  | 1:A:1212:THR:HB   | 2.21                     | 0.71              |
| 1:C:1219:VAL:HG22 | 1:C:1384:ILE:HD12 | 1.73                     | 0.71              |
| 2:G:238:CYS:HB2   | 2:G:239:PRO:HD3   | 1.71                     | 0.71              |
| 2:G:949:ASP:HB3   | 2:G:1006:MET:HE2  | 1.71                     | 0.71              |
| 2:G:1199:GLU:OE2  | 2:G:1567:ARG:NH1  | 2.23                     | 0.71              |
| 2:G:1672:GLN:HA   | 2:G:1676:MET:HE1  | 1.72                     | 0.71              |
| 2:G:1917:ILE:HG23 | 2:G:1922:ILE:HB   | 1.72                     | 0.71              |
| 2:H:238:CYS:HB2   | 2:H:239:PRO:HD3   | 1.71                     | 0.71              |
| 2:I:1058:VAL:O    | 2:I:1061:GLN:HG2  | 1.90                     | 0.71              |
| 2:G:109:LEU:HD11  | 2:G:116:LEU:HD23  | 1.71                     | 0.71              |
| 1:B:18:LEU:HD21   | 2:H:1815:LEU:CD1  | 2.20                     | 0.71              |
| 1:B:655:LEU:HD22  | 1:B:916:LEU:HD11  | 1.72                     | 0.71              |
| 1:C:1498:GLU:CB   | 1:C:1876:LEU:HD13 | 2.21                     | 0.71              |
| 2:G:707:PRO:CG    | 2:G:716:VAL:HG21  | 2.20                     | 0.71              |
| 2:H:964:LEU:HD23  | 2:H:964:LEU:H     | 1.56                     | 0.71              |
| 1:C:59:ARG:NH1    | 2:I:1896:GLN:HE22 | 1.88                     | 0.70              |
| 1:C:459:ASP:HB3   | 1:C:462:LYS:HG3   | 1.73                     | 0.70              |
| 1:C:1498:GLU:HG3  | 1:C:1876:LEU:CB   | 2.09                     | 0.70              |
| 2:I:751:LEU:HD23  | 2:I:791:TYR:CE2   | 2.25                     | 0.70              |
| 2:I:1242:PHE:CE2  | 2:I:1244:PRO:HG3  | 2.26                     | 0.70              |
| 1:A:1119:LYS:HE2  | 1:A:1341:PHE:CD1  | 2.27                     | 0.70              |
| 1:B:1721:ARG:HG2  | 1:B:1721:ARG:NH1  | 2.00                     | 0.70              |
| 2:H:562:LEU:O     | 2:H:566:HIS:HB2   | 1.90                     | 0.70              |
| 2:H:707:PRO:CG    | 2:H:716:VAL:HG21  | 2.21                     | 0.70              |
| 1:A:1:MET:CE      | 1:A:6:GLU:HA      | 2.21                     | 0.70              |
| 1:B:1460:LYS:HZ1  | 1:B:1774:GLU:CD   | 1.92                     | 0.70              |
| 1:C:12:ILE:HD11   | 2:I:2041:ILE:CD1  | 2.21                     | 0.70              |
| 1:C:631:PRO:HB2   | 1:C:634:THR:OG1   | 1.91                     | 0.70              |
| 2:G:1672:GLN:HA   | 2:G:1676:MET:CE   | 2.21                     | 0.70              |
| 2:I:964:LEU:HD23  | 2:I:964:LEU:H     | 1.56                     | 0.70              |
| 1:C:881:ASN:HA    | 1:C:944:ARG:NH2   | 2.06                     | 0.70              |
| 2:G:650:ASN:HD21  | 4:G:3051:FMN:HN3  | 1.40                     | 0.70              |
| 2:I:732:TRP:CG    | 2:I:750:MET:HE1   | 2.26                     | 0.70              |
| 2:I:1680:LEU:HD13 | 2:I:1687:ALA:HB2  | 1.72                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:90:TYR:HE2    | 2:H:1659:GLN:OE1  | 1.73                     | 0.70              |
| 1:B:1208:VAL:CG1  | 1:B:1212:THR:HB   | 2.20                     | 0.70              |
| 1:B:1501:LEU:HD11 | 1:B:1775:LEU:CD2  | 2.22                     | 0.70              |
| 2:G:123:ILE:HD11  | 2:G:533:LEU:CD2   | 2.21                     | 0.70              |
| 2:G:579:VAL:HG23  | 2:G:1078:HIS:CD2  | 2.27                     | 0.70              |
| 2:I:455:ILE:CD1   | 2:I:469:ARG:HD3   | 2.20                     | 0.70              |
| 2:I:748:THR:HB    | 2:I:749:PRO:HD3   | 1.74                     | 0.70              |
| 1:B:459:ASP:HB3   | 1:B:462:LYS:HG3   | 1.73                     | 0.70              |
| 2:G:707:PRO:HG3   | 2:G:716:VAL:CG2   | 2.22                     | 0.70              |
| 2:G:732:TRP:CG    | 2:G:750:MET:HE1   | 2.27                     | 0.70              |
| 2:G:1956:ARG:CB   | 2:G:1957:PRO:HD3  | 2.10                     | 0.70              |
| 2:I:146:PHE:HA    | 2:I:149:VAL:CG1   | 2.20                     | 0.70              |
| 1:A:1312:VAL:HG22 | 1:A:1329:VAL:HG11 | 1.73                     | 0.70              |
| 1:B:1:MET:CE      | 1:B:6:GLU:HA      | 2.21                     | 0.70              |
| 1:B:968:VAL:HG23  | 2:H:1515:PRO:HG3  | 1.74                     | 0.70              |
| 2:G:1242:PHE:HE2  | 2:G:1244:PRO:HG3  | 1.55                     | 0.70              |
| 1:C:260:ARG:NH1   | 1:C:300:VAL:HG21  | 2.06                     | 0.70              |
| 2:G:1355:ASN:HA   | 2:G:1407:THR:O    | 1.92                     | 0.70              |
| 2:H:234:ILE:HG13  | 2:H:235:PRO:HD3   | 1.73                     | 0.70              |
| 2:I:1264:GLU:HA   | 2:I:1275:PHE:CE1  | 2.27                     | 0.70              |
| 1:C:655:LEU:HD22  | 1:C:916:LEU:HD11  | 1.74                     | 0.70              |
| 2:G:455:ILE:HD11  | 2:G:469:ARG:CD    | 2.22                     | 0.70              |
| 2:H:741:HIS:CE1   | 2:H:845:THR:HG21  | 2.26                     | 0.70              |
| 1:A:12:ILE:HA     | 1:A:15:THR:CG2    | 2.21                     | 0.70              |
| 2:G:1331:TRP:CZ2  | 2:G:1335:ILE:HG13 | 2.26                     | 0.70              |
| 2:G:1673:GLU:H    | 2:G:1676:MET:HE3  | 1.57                     | 0.70              |
| 2:H:2036:GLU:HB2  | 2:H:2037:PRO:HD3  | 1.72                     | 0.70              |
| 1:A:1232:TYR:CZ   | 1:A:1701:LYS:HD2  | 2.27                     | 0.69              |
| 2:G:7:ARG:HH21    | 2:G:27:PHE:CB     | 2.01                     | 0.69              |
| 2:H:499:THR:CB    | 2:H:500:HIS:HD2   | 1.99                     | 0.69              |
| 2:H:835:THR:HB    | 2:H:845:THR:HG23  | 1.73                     | 0.69              |
| 2:H:1673:GLU:H    | 2:H:1676:MET:HE3  | 1.57                     | 0.69              |
| 2:I:926:LEU:HD13  | 2:I:947:THR:HG22  | 1.73                     | 0.69              |
| 1:B:427:ASN:HD21  | 1:B:610:THR:H     | 1.40                     | 0.69              |
| 2:G:1194:VAL:HG22 | 2:G:1212:LYS:HB3  | 1.74                     | 0.69              |
| 2:G:1422:THR:HG21 | 2:G:1474:PHE:HB2  | 1.72                     | 0.69              |
| 2:H:1670:GLY:H    | 2:H:1672:GLN:HE21 | 1.40                     | 0.69              |
| 2:I:1862:VAL:HG11 | 2:I:1866:PHE:CD1  | 2.26                     | 0.69              |
| 1:A:749:ILE:HD13  | 1:A:806:VAL:HG12  | 1.72                     | 0.69              |
| 1:C:12:ILE:HA     | 1:C:15:THR:CG2    | 2.22                     | 0.69              |
| 1:C:852:ARG:HH11  | 1:C:852:ARG:CG    | 2.00                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1054:LEU:HB2  | 4:G:3051:FMN:C7M  | 2.22                     | 0.69              |
| 2:H:567:PRO:HG3   | 2:H:781:LEU:CD1   | 2.22                     | 0.69              |
| 2:H:1195:VAL:CG1  | 2:H:1211:LEU:HB3  | 2.23                     | 0.69              |
| 2:H:1381:VAL:HG13 | 2:H:1390:VAL:HG22 | 1.74                     | 0.69              |
| 2:I:652:ILE:H     | 2:I:658:MET:CE    | 2.04                     | 0.69              |
| 1:A:254:TRP:CZ3   | 1:A:292:GLN:HG3   | 2.26                     | 0.69              |
| 1:B:254:TRP:CZ3   | 1:B:292:GLN:HG3   | 2.27                     | 0.69              |
| 2:I:1770:LEU:HD23 | 2:I:1776:PHE:HE2  | 1.55                     | 0.69              |
| 2:G:84:LEU:HD13   | 2:G:133:ALA:HB2   | 1.75                     | 0.69              |
| 2:G:964:LEU:H     | 2:G:964:LEU:CD2   | 2.05                     | 0.69              |
| 2:I:1678:MET:HE3  | 2:I:1707:LEU:HD22 | 1.75                     | 0.69              |
| 1:C:1208:VAL:CG1  | 1:C:1212:THR:HB   | 2.23                     | 0.69              |
| 2:G:856:LYS:HG2   | 2:G:1054:LEU:HD12 | 1.73                     | 0.69              |
| 2:H:1889:VAL:HG13 | 2:H:1977:HIS:CB   | 2.22                     | 0.69              |
| 2:H:1917:ILE:HG23 | 2:H:1922:ILE:HB   | 1.74                     | 0.69              |
| 1:A:749:ILE:HD11  | 1:A:805:CYS:HB3   | 1.75                     | 0.69              |
| 1:A:1721:ARG:HG2  | 1:A:1721:ARG:NH1  | 1.97                     | 0.69              |
| 1:B:1376:PHE:HB3  | 1:B:1544:THR:HG22 | 1.74                     | 0.69              |
| 2:G:191:SER:HA    | 2:G:194:THR:HG22  | 1.74                     | 0.69              |
| 2:I:109:LEU:HD11  | 2:I:116:LEU:HD23  | 1.73                     | 0.69              |
| 2:I:1194:VAL:HG22 | 2:I:1212:LYS:HB3  | 1.75                     | 0.69              |
| 1:A:479:ASN:O     | 1:A:483:VAL:HG23  | 1.91                     | 0.69              |
| 1:A:1693:ILE:CD1  | 2:G:998:GLN:HB2   | 2.23                     | 0.69              |
| 2:G:1172:LYS:HE3  | 2:G:1574:ASN:OD1  | 1.92                     | 0.69              |
| 2:G:1670:GLY:H    | 2:G:1672:GLN:HE21 | 1.39                     | 0.69              |
| 2:H:663:ILE:HB    | 2:H:664:PRO:HD3   | 1.75                     | 0.69              |
| 2:H:751:LEU:HD23  | 2:H:791:TYR:CE2   | 2.27                     | 0.69              |
| 2:H:1889:VAL:HG13 | 2:H:1977:HIS:HB2  | 1.72                     | 0.69              |
| 2:H:2022:THR:HG23 | 2:H:2025:TYR:H    | 1.58                     | 0.69              |
| 2:I:652:ILE:N     | 2:I:658:MET:HE3   | 2.08                     | 0.69              |
| 1:A:631:PRO:HB2   | 1:A:634:THR:OG1   | 1.92                     | 0.69              |
| 1:C:1838:GLU:OE1  | 1:C:1852:HIS:HE1  | 1.76                     | 0.69              |
| 2:G:1264:GLU:HA   | 2:G:1275:PHE:CE1  | 2.28                     | 0.69              |
| 2:G:1496:LYS:HE2  | 2:G:1693:ARG:HH21 | 1.57                     | 0.69              |
| 2:H:305:PHE:CE1   | 2:H:442:ASP:HB3   | 2.28                     | 0.69              |
| 2:H:1172:LYS:CE   | 2:H:1574:ASN:OD1  | 2.40                     | 0.69              |
| 2:H:1739:GLU:CB   | 2:H:1987:PRO:HB3  | 2.21                     | 0.69              |
| 2:I:663:ILE:HB    | 2:I:664:PRO:HD3   | 1.75                     | 0.69              |
| 2:I:768:GLY:HA3   | 2:I:800:LEU:HD21  | 1.74                     | 0.69              |
| 2:I:1739:GLU:CB   | 2:I:1987:PRO:HB3  | 2.20                     | 0.69              |
| 1:A:257:PRO:HD2   | 1:A:260:ARG:HB2   | 1.75                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1376:PHE:HB3  | 1:A:1544:THR:HG22 | 1.74                     | 0.69              |
| 1:C:1021:VAL:HG11 | 1:C:1597:LEU:HD11 | 1.74                     | 0.69              |
| 1:C:1219:VAL:HA   | 1:C:1384:ILE:CD1  | 2.20                     | 0.69              |
| 1:C:1431:GLU:OE2  | 1:C:1433:HIS:HE1  | 1.76                     | 0.69              |
| 2:G:663:ILE:HB    | 2:G:664:PRO:HD3   | 1.74                     | 0.69              |
| 2:H:54:PRO:HG3    | 2:H:63:LYS:HG3    | 1.72                     | 0.69              |
| 2:H:652:ILE:N     | 2:H:658:MET:HE3   | 2.05                     | 0.69              |
| 2:I:499:THR:CB    | 2:I:500:HIS:HD2   | 1.95                     | 0.69              |
| 2:I:1917:ILE:HG23 | 2:I:1922:ILE:HB   | 1.74                     | 0.69              |
| 1:A:1838:GLU:OE1  | 1:A:1852:HIS:HE1  | 1.75                     | 0.68              |
| 2:H:259:THR:HG22  | 2:H:262:GLU:CG    | 2.22                     | 0.68              |
| 2:I:234:ILE:HG13  | 2:I:235:PRO:HD3   | 1.73                     | 0.68              |
| 1:A:1203:ASP:HB3  | 1:B:179:LYS:HZ3   | 1.58                     | 0.68              |
| 2:G:1058:VAL:O    | 2:G:1061:GLN:HG2  | 1.93                     | 0.68              |
| 1:A:1431:GLU:HG3  | 1:A:1433:HIS:CE1  | 2.28                     | 0.68              |
| 1:C:1045:PHE:HB3  | 1:C:1049:GLY:HA3  | 1.74                     | 0.68              |
| 2:G:2035:SER:HB3  | 2:G:2038:ILE:HG13 | 1.74                     | 0.68              |
| 2:H:161:GLY:H     | 2:H:505:GLY:HA3   | 1.59                     | 0.68              |
| 2:H:1101:GLU:HB3  | 2:H:1147:ILE:HG22 | 1.76                     | 0.68              |
| 1:C:1376:PHE:HB3  | 1:C:1544:THR:HG22 | 1.74                     | 0.68              |
| 2:G:1834:ARG:HG2  | 2:G:1834:ARG:NH1  | 1.93                     | 0.68              |
| 2:I:598:THR:CG2   | 2:I:622:GLY:HA3   | 2.23                     | 0.68              |
| 2:I:1227:ARG:HG3  | 2:I:1227:ARG:NH1  | 2.00                     | 0.68              |
| 1:A:888:ILE:HD11  | 1:A:930:LEU:HD21  | 1.75                     | 0.68              |
| 1:B:400:ARG:HG2   | 1:B:400:ARG:NH1   | 2.00                     | 0.68              |
| 1:B:1312:VAL:HG22 | 1:B:1329:VAL:HG11 | 1.73                     | 0.68              |
| 1:C:985:ARG:NH1   | 2:I:953:ARG:CZ    | 2.57                     | 0.68              |
| 2:I:161:GLY:H     | 2:I:505:GLY:HA3   | 1.56                     | 0.68              |
| 2:I:187:LEU:HA    | 2:I:190:PHE:HB3   | 1.76                     | 0.68              |
| 1:B:90:TYR:CE2    | 2:H:1659:GLN:OE1  | 2.47                     | 0.68              |
| 1:C:1014:ASP:H    | 1:C:1510:ASN:ND2  | 1.84                     | 0.68              |
| 2:G:54:PRO:HG3    | 2:G:63:LYS:HG3    | 1.76                     | 0.68              |
| 2:G:259:THR:HG22  | 2:G:262:GLU:CG    | 2.22                     | 0.68              |
| 2:G:732:TRP:CG    | 2:G:750:MET:CE    | 2.76                     | 0.68              |
| 2:G:1784:MET:HG3  | 2:G:1785:GLU:N    | 2.07                     | 0.68              |
| 2:I:594:VAL:HG21  | 2:I:610:THR:HG21  | 1.75                     | 0.68              |
| 2:I:1638:ILE:HD12 | 2:I:1657:ILE:HD12 | 1.75                     | 0.68              |
| 1:A:1474:ALA:HA   | 1:A:1478:PRO:CG   | 2.24                     | 0.68              |
| 1:C:987:ASN:HD22  | 2:I:957:ARG:HD2   | 1.58                     | 0.68              |
| 2:H:648:GLY:HA3   | 2:H:678:PHE:CE2   | 2.29                     | 0.68              |
| 1:A:332:THR:HG22  | 1:B:331:ILE:HD11  | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:504:ASP:HB3   | 1:A:508:ASN:H     | 1.56                     | 0.68              |
| 1:C:1460:LYS:HE3  | 1:C:1774:GLU:OE1  | 1.92                     | 0.68              |
| 2:G:455:ILE:CG1   | 2:G:469:ARG:HD3   | 2.23                     | 0.68              |
| 2:H:187:LEU:HA    | 2:H:190:PHE:HB3   | 1.75                     | 0.68              |
| 2:I:305:PHE:CE1   | 2:I:442:ASP:HB3   | 2.28                     | 0.68              |
| 1:B:1219:VAL:HG22 | 1:B:1384:ILE:HD12 | 1.75                     | 0.68              |
| 1:C:1310:GLU:OE1  | 1:C:1649:LYS:HE3  | 1.93                     | 0.68              |
| 2:G:455:ILE:CD1   | 2:G:469:ARG:HD3   | 2.24                     | 0.68              |
| 2:H:641:ILE:HG12  | 2:H:645:SER:HB2   | 1.76                     | 0.68              |
| 1:A:1056:ILE:HD13 | 1:A:1193:TRP:HD1  | 1.59                     | 0.68              |
| 1:B:1838:GLU:OE1  | 1:B:1852:HIS:HE1  | 1.76                     | 0.68              |
| 2:G:1176:PRO:O    | 2:G:1177:SER:HB3  | 1.93                     | 0.68              |
| 2:H:1058:VAL:O    | 2:H:1061:GLN:HG2  | 1.94                     | 0.68              |
| 1:A:1303:GLY:H    | 1:A:1307:THR:HG22 | 1.59                     | 0.67              |
| 1:A:1594:ASN:O    | 1:A:1598:GLN:HG3  | 1.94                     | 0.67              |
| 1:B:183:GLN:HE21  | 1:B:202:GLU:HG2   | 1.59                     | 0.67              |
| 1:C:44:VAL:CG1    | 1:C:78:ILE:HG12   | 2.24                     | 0.67              |
| 1:C:254:TRP:CZ3   | 1:C:292:GLN:HG3   | 2.29                     | 0.67              |
| 1:C:1303:GLY:H    | 1:C:1307:THR:HG22 | 1.60                     | 0.67              |
| 2:G:187:LEU:HA    | 2:G:190:PHE:HB3   | 1.74                     | 0.67              |
| 2:G:1475:LYS:CG   | 2:G:1481:SER:HB2  | 2.24                     | 0.67              |
| 2:H:707:PRO:HG3   | 2:H:716:VAL:CG2   | 2.24                     | 0.67              |
| 2:H:1054:LEU:HB2  | 4:H:3051:FMN:HM72 | 1.76                     | 0.67              |
| 2:H:191:SER:HA    | 2:H:194:THR:HG22  | 1.77                     | 0.67              |
| 1:C:1232:TYR:CZ   | 1:C:1701:LYS:HD2  | 2.29                     | 0.67              |
| 1:C:1455:ARG:HH11 | 1:C:1458:GLN:HE21 | 1.42                     | 0.67              |
| 2:G:163:GLN:HG2   | 2:G:423:VAL:HG12  | 1.77                     | 0.67              |
| 2:G:1889:VAL:HG13 | 2:G:1977:HIS:CB   | 2.24                     | 0.67              |
| 2:H:50:ALA:HB3    | 2:H:53:GLU:HG3    | 1.76                     | 0.67              |
| 2:I:579:VAL:HG23  | 2:I:1078:HIS:NE2  | 2.10                     | 0.67              |
| 1:C:504:ASP:HB3   | 1:C:508:ASN:H     | 1.60                     | 0.67              |
| 2:G:1129:ALA:HB2  | 2:G:1138:TRP:CZ3  | 2.30                     | 0.67              |
| 2:I:598:THR:OG1   | 2:I:599:PRO:HD3   | 1.94                     | 0.67              |
| 1:A:459:ASP:HB3   | 1:A:462:LYS:HG3   | 1.76                     | 0.67              |
| 1:B:1303:GLY:H    | 1:B:1307:THR:HG22 | 1.59                     | 0.67              |
| 1:C:409:ALA:HB2   | 1:C:442:ARG:HD2   | 1.76                     | 0.67              |
| 1:C:1056:ILE:HD13 | 1:C:1193:TRP:HD1  | 1.60                     | 0.67              |
| 1:C:1523:ARG:CG   | 1:C:1523:ARG:NH1  | 2.57                     | 0.67              |
| 2:G:768:GLY:HA3   | 2:G:800:LEU:HD21  | 1.76                     | 0.67              |
| 2:G:910:GLN:HE21  | 2:G:912:ARG:HH21  | 1.42                     | 0.67              |
| 2:H:902:PRO:HG2   | 2:H:929:LEU:HD21  | 1.74                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:904:PHE:HB2   | 2:I:1017:PHE:CD1  | 2.28                     | 0.67              |
| 2:I:910:GLN:HE21  | 2:I:912:ARG:HH21  | 1.40                     | 0.67              |
| 1:A:1360:ARG:HH11 | 1:A:1364:GLU:HG2  | 1.60                     | 0.67              |
| 1:B:1039:MET:O    | 1:B:1609:ARG:NH2  | 2.27                     | 0.67              |
| 2:G:1741:ILE:HG12 | 2:G:1746:LEU:HD13 | 1.77                     | 0.67              |
| 1:B:1310:GLU:OE1  | 1:B:1649:LYS:HE3  | 1.94                     | 0.67              |
| 2:I:1675:GLY:O    | 2:I:1678:MET:HB2  | 1.94                     | 0.67              |
| 1:A:328:LEU:O     | 1:A:328:LEU:HD22  | 1.94                     | 0.67              |
| 1:C:746:GLU:O     | 1:C:750:GLU:HG3   | 1.95                     | 0.67              |
| 2:H:545:GLN:HE21  | 2:H:545:GLN:H     | 1.41                     | 0.67              |
| 2:H:594:VAL:HG21  | 2:H:610:THR:HG21  | 1.77                     | 0.67              |
| 2:H:768:GLY:HA3   | 2:H:800:LEU:HD21  | 1.77                     | 0.67              |
| 2:I:54:PRO:HG3    | 2:I:63:LYS:HG3    | 1.75                     | 0.67              |
| 2:G:1004:LEU:HD21 | 2:G:1020:VAL:HG23 | 1.77                     | 0.67              |
| 2:G:1676:MET:HE1  | 2:G:1781:LEU:HD21 | 1.76                     | 0.67              |
| 2:G:1770:LEU:HD23 | 2:G:1776:PHE:HE2  | 1.58                     | 0.67              |
| 2:H:315:PRO:O     | 2:I:1314:ARG:NH2  | 2.28                     | 0.67              |
| 2:H:1086:LEU:HG   | 2:H:1092:ASP:HA   | 1.77                     | 0.67              |
| 2:H:1242:PHE:CE2  | 2:H:1244:PRO:HG3  | 2.30                     | 0.67              |
| 2:H:1264:GLU:HA   | 2:H:1275:PHE:CE1  | 2.29                     | 0.67              |
| 2:I:703:LEU:HD21  | 2:I:705:LEU:HD21  | 1.76                     | 0.67              |
| 2:G:353:VAL:HG23  | 2:G:357:ASN:ND2   | 2.10                     | 0.67              |
| 2:H:1256:GLU:O    | 2:H:1257:ASP:HB2  | 1.93                     | 0.67              |
| 2:I:949:ASP:HB3   | 2:I:1006:MET:HE2  | 1.77                     | 0.67              |
| 2:I:1889:VAL:HG13 | 2:I:1977:HIS:CB   | 2.24                     | 0.67              |
| 1:A:1030:TRP:NE1  | 1:A:1580:LEU:CD2  | 2.57                     | 0.66              |
| 1:C:257:PRO:HD2   | 1:C:260:ARG:HB2   | 1.76                     | 0.66              |
| 1:C:888:ILE:HD12  | 1:C:939:PHE:HE2   | 1.60                     | 0.66              |
| 2:G:670:ARG:HD3   | 2:G:699:GLY:O     | 1.95                     | 0.66              |
| 2:H:1159:ILE:CG1  | 2:H:1169:PRO:HD3  | 2.24                     | 0.66              |
| 2:H:1862:VAL:HG11 | 2:H:1866:PHE:CD1  | 2.30                     | 0.66              |
| 2:I:50:ALA:HB3    | 2:I:53:GLU:HG3    | 1.76                     | 0.66              |
| 2:I:163:GLN:HG2   | 2:I:423:VAL:HG12  | 1.76                     | 0.66              |
| 2:I:1227:ARG:HD2  | 2:I:1565:VAL:HG11 | 1.77                     | 0.66              |
| 1:A:473:GLY:O     | 1:A:477:ILE:HG13  | 1.95                     | 0.66              |
| 1:A:1662:TYR:O    | 1:A:1665:ILE:HG22 | 1.95                     | 0.66              |
| 1:B:328:LEU:O     | 1:B:328:LEU:HD22  | 1.95                     | 0.66              |
| 1:B:335:HIS:CE1   | 1:C:335:HIS:CE1   | 2.82                     | 0.66              |
| 1:C:294:TYR:CE1   | 1:C:298:VAL:HG21  | 2.29                     | 0.66              |
| 1:C:328:LEU:O     | 1:C:328:LEU:HD22  | 1.95                     | 0.66              |
| 1:C:1430:ARG:HG2  | 1:C:1430:ARG:O    | 1.94                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:670:ARG:HD3   | 2:H:699:GLY:O     | 1.95                     | 0.66              |
| 2:I:1739:GLU:O    | 2:I:1987:PRO:HG3  | 1.95                     | 0.66              |
| 2:I:1920:GLN:HG2  | 2:I:1922:ILE:HD11 | 1.75                     | 0.66              |
| 1:A:183:GLN:HE21  | 1:A:202:GLU:HG2   | 1.59                     | 0.66              |
| 1:B:27:ARG:HB2    | 2:H:2016:ALA:HB2  | 1.76                     | 0.66              |
| 1:B:1045:PHE:HB3  | 1:B:1049:GLY:HA3  | 1.76                     | 0.66              |
| 1:C:460:GLU:HG2   | 1:C:470:LYS:HD3   | 1.77                     | 0.66              |
| 1:C:507:GLY:N     | 1:C:954:ARG:HG2   | 2.11                     | 0.66              |
| 1:C:1030:TRP:NE1  | 1:C:1580:LEU:CD2  | 2.58                     | 0.66              |
| 2:H:910:GLN:HE21  | 2:H:912:ARG:HH21  | 1.43                     | 0.66              |
| 2:I:750:MET:HG3   | 2:I:796:PHE:HZ    | 1.60                     | 0.66              |
| 2:I:762:ASN:H     | 2:I:762:ASN:ND2   | 1.88                     | 0.66              |
| 1:A:864:VAL:HG22  | 1:A:921:PRO:HB3   | 1.78                     | 0.66              |
| 1:B:12:ILE:HA     | 1:B:15:THR:CG2    | 2.25                     | 0.66              |
| 2:I:705:LEU:HD12  | 2:I:716:VAL:HG13  | 1.75                     | 0.66              |
| 1:B:504:ASP:HB3   | 1:B:508:ASN:H     | 1.60                     | 0.66              |
| 1:C:934:PRO:O     | 1:C:935:GLU:C     | 2.34                     | 0.66              |
| 2:G:61:VAL:O      | 2:G:65:LEU:HB2    | 1.96                     | 0.66              |
| 2:G:560:ASN:O     | 2:G:561:TRP:C     | 2.34                     | 0.66              |
| 2:G:1300:PHE:HA   | 2:G:1556:VAL:HG11 | 1.77                     | 0.66              |
| 2:G:1862:VAL:HG11 | 2:G:1866:PHE:CD1  | 2.30                     | 0.66              |
| 2:H:741:HIS:CE1   | 2:H:855:HIS:CE1   | 2.84                     | 0.66              |
| 2:H:826:GLY:HA3   | 2:H:1061:GLN:HB3  | 1.75                     | 0.66              |
| 2:H:835:THR:HG21  | 2:H:855:HIS:HD2   | 1.59                     | 0.66              |
| 1:A:988:ILE:HD13  | 1:A:1048:GLU:HB3  | 1.76                     | 0.66              |
| 1:B:1749:THR:CB   | 1:B:1874:ASP:N    | 2.58                     | 0.66              |
| 2:G:579:VAL:HG23  | 2:G:1078:HIS:NE2  | 2.10                     | 0.66              |
| 2:H:1173:VAL:HG21 | 2:H:1221:MET:HE1  | 1.77                     | 0.66              |
| 2:H:1986:LYS:N    | 2:H:1987:PRO:HD2  | 2.11                     | 0.66              |
| 1:A:836:ASP:HB3   | 1:A:839:TYR:HB3   | 1.76                     | 0.66              |
| 1:B:497:THR:OG1   | 1:B:513:GLU:HG2   | 1.95                     | 0.66              |
| 1:B:1540:SER:HA   | 1:B:1575:VAL:HG22 | 1.78                     | 0.66              |
| 1:C:1431:GLU:OE2  | 1:C:1433:HIS:CE1  | 2.48                     | 0.66              |
| 2:G:1920:GLN:HG2  | 2:G:1922:ILE:HD11 | 1.78                     | 0.66              |
| 2:H:61:VAL:O      | 2:H:65:LEU:HB2    | 1.96                     | 0.66              |
| 2:H:904:PHE:HB2   | 2:H:1017:PHE:CD1  | 2.30                     | 0.66              |
| 2:H:1741:ILE:HG12 | 2:H:1746:LEU:HD13 | 1.76                     | 0.66              |
| 1:B:733:ILE:HD13  | 1:B:761:LEU:HD11  | 1.78                     | 0.66              |
| 2:G:1457:PHE:CZ   | 2:G:1501:ILE:HD11 | 2.30                     | 0.66              |
| 2:G:1808:SER:H    | 2:G:2013:ASN:ND2  | 1.93                     | 0.66              |
| 2:H:131:ILE:HG21  | 2:H:182:VAL:CG1   | 2.18                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1173:VAL:HG21 | 2:I:1221:MET:HE1  | 1.77                     | 0.66              |
| 2:I:1195:VAL:CG1  | 2:I:1211:LEU:HB3  | 2.25                     | 0.66              |
| 1:A:254:TRP:CH2   | 1:A:292:GLN:HG3   | 2.31                     | 0.66              |
| 1:B:1219:VAL:HA   | 1:B:1384:ILE:CD1  | 2.24                     | 0.66              |
| 1:C:295:ALA:HB2   | 1:C:302:LEU:HD11  | 1.77                     | 0.66              |
| 2:H:560:ASN:O     | 2:H:561:TRP:C     | 2.33                     | 0.66              |
| 2:H:1770:LEU:HD23 | 2:H:1776:PHE:HE2  | 1.59                     | 0.66              |
| 2:I:1381:VAL:HG13 | 2:I:1390:VAL:HG22 | 1.78                     | 0.66              |
| 2:I:1808:SER:H    | 2:I:2013:ASN:ND2  | 1.94                     | 0.66              |
| 1:B:501:THR:N     | 1:B:886:GLU:OE1   | 2.21                     | 0.66              |
| 1:C:1360:ARG:HH11 | 1:C:1364:GLU:HG2  | 1.60                     | 0.66              |
| 2:G:33:LEU:HD11   | 2:G:80:PHE:HD2    | 1.61                     | 0.66              |
| 2:G:843:ILE:HD11  | 2:G:1055:HIS:HB3  | 1.78                     | 0.66              |
| 2:G:904:PHE:HB2   | 2:G:1017:PHE:CD1  | 2.30                     | 0.66              |
| 2:G:1352:HIS:CD2  | 2:G:1410:PHE:CE2  | 2.84                     | 0.66              |
| 2:I:1819:ALA:HA   | 2:I:2005:ARG:HH11 | 1.61                     | 0.66              |
| 1:A:497:THR:OG1   | 1:A:513:GLU:HG2   | 1.96                     | 0.65              |
| 1:B:529:MET:CG    | 1:B:638:LEU:HG    | 2.26                     | 0.65              |
| 1:C:1:MET:CE      | 1:C:6:GLU:HA      | 2.25                     | 0.65              |
| 1:C:1317:GLU:OE1  | 1:C:1317:GLU:HA   | 1.96                     | 0.65              |
| 2:G:652:ILE:N     | 2:G:658:MET:HE3   | 2.11                     | 0.65              |
| 2:G:1976:PHE:HA   | 2:G:1981:LEU:HD22 | 1.78                     | 0.65              |
| 2:H:2035:SER:HB3  | 2:H:2038:ILE:HG13 | 1.78                     | 0.65              |
| 1:B:836:ASP:HB3   | 1:B:839:TYR:HB3   | 1.79                     | 0.65              |
| 1:C:330:GLU:HA    | 1:C:333:LYS:HD2   | 1.79                     | 0.65              |
| 1:C:836:ASP:HB3   | 1:C:839:TYR:HB3   | 1.77                     | 0.65              |
| 1:C:1312:VAL:HG22 | 1:C:1329:VAL:HG11 | 1.78                     | 0.65              |
| 2:G:1352:HIS:HE1  | 2:G:1583:MET:HE1  | 1.60                     | 0.65              |
| 2:G:1986:LYS:N    | 2:G:1987:PRO:HD2  | 2.12                     | 0.65              |
| 2:H:732:TRP:CG    | 2:H:750:MET:CE    | 2.79                     | 0.65              |
| 2:H:1325:PHE:CZ   | 2:H:1328:VAL:HG11 | 2.32                     | 0.65              |
| 2:I:1782:THR:HG22 | 2:I:1827:LEU:HD21 | 1.78                     | 0.65              |
| 1:A:27:ARG:HB2    | 2:G:2016:ALA:HB2  | 1.77                     | 0.65              |
| 1:A:934:PRO:O     | 1:A:935:GLU:C     | 2.35                     | 0.65              |
| 2:G:597:MET:HA    | 4:G:3051:FMN:N5   | 2.10                     | 0.65              |
| 1:A:27:ARG:HD2    | 1:A:30:GLU:OE2    | 1.97                     | 0.65              |
| 1:A:331:ILE:HD11  | 1:C:332:THR:HG22  | 1.79                     | 0.65              |
| 1:B:460:GLU:HG2   | 1:B:470:LYS:HD3   | 1.78                     | 0.65              |
| 1:B:1317:GLU:OE1  | 1:B:1317:GLU:HA   | 1.96                     | 0.65              |
| 1:C:32:GLN:HA     | 1:C:35:PHE:CE2    | 2.31                     | 0.65              |
| 2:G:234:ILE:HG13  | 2:G:235:PRO:HD3   | 1.77                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:259:THR:HG23  | 2:G:262:GLU:H     | 1.62                     | 0.65              |
| 2:G:902:PRO:HG2   | 2:G:929:LEU:HD21  | 1.79                     | 0.65              |
| 2:G:1086:LEU:HG   | 2:G:1092:ASP:HA   | 1.77                     | 0.65              |
| 2:H:1719:ILE:O    | 2:H:1761:SER:HB2  | 1.97                     | 0.65              |
| 2:I:251:VAL:O     | 2:I:255:LEU:HB2   | 1.96                     | 0.65              |
| 1:B:257:PRO:HD2   | 1:B:260:ARG:HB2   | 1.78                     | 0.65              |
| 1:B:749:ILE:HD11  | 1:B:805:CYS:HB3   | 1.77                     | 0.65              |
| 2:G:736:ARG:NH1   | 2:G:769:SER:O     | 2.29                     | 0.65              |
| 1:A:331:ILE:CD1   | 1:C:332:THR:HG22  | 2.26                     | 0.65              |
| 1:A:1219:VAL:HG22 | 1:A:1384:ILE:HD12 | 1.77                     | 0.65              |
| 2:G:131:ILE:HG21  | 2:G:182:VAL:CG1   | 2.26                     | 0.65              |
| 2:I:545:GLN:HE21  | 2:I:545:GLN:H     | 1.42                     | 0.65              |
| 1:A:968:VAL:O     | 2:G:1512:HIS:HB2  | 1.97                     | 0.65              |
| 1:C:435:GLU:O     | 1:C:439:ILE:HG13  | 1.96                     | 0.65              |
| 2:G:1381:VAL:HG13 | 2:G:1390:VAL:HG22 | 1.77                     | 0.65              |
| 2:G:1740:THR:HG22 | 2:G:1742:VAL:HG23 | 1.78                     | 0.65              |
| 1:B:294:TYR:CE1   | 1:B:298:VAL:HG21  | 2.32                     | 0.65              |
| 1:C:497:THR:OG1   | 1:C:513:GLU:HG2   | 1.97                     | 0.65              |
| 2:G:826:GLY:HA3   | 2:G:1061:GLN:HB3  | 1.77                     | 0.65              |
| 2:H:667:LYS:HB2   | 2:H:698:LEU:HD23  | 1.79                     | 0.65              |
| 2:H:748:THR:HB    | 2:H:749:PRO:HD3   | 1.78                     | 0.65              |
| 2:H:949:ASP:HB3   | 2:H:1006:MET:HE2  | 1.79                     | 0.65              |
| 1:A:340:ARG:HH12  | 1:A:344:GLN:CG    | 2.09                     | 0.65              |
| 1:A:529:MET:CG    | 1:A:638:LEU:HG    | 2.27                     | 0.65              |
| 1:A:1219:VAL:HA   | 1:A:1384:ILE:CD1  | 2.23                     | 0.65              |
| 2:G:259:THR:CG2   | 2:G:262:GLU:H     | 2.10                     | 0.65              |
| 2:G:1242:PHE:CE2  | 2:G:1244:PRO:HG3  | 2.31                     | 0.65              |
| 2:G:1418:ASP:O    | 2:G:1420:GLU:N    | 2.30                     | 0.65              |
| 2:H:567:PRO:HG3   | 2:H:781:LEU:HD12  | 1.77                     | 0.65              |
| 1:A:294:TYR:CE1   | 1:A:298:VAL:HG21  | 2.32                     | 0.65              |
| 1:C:11:HIS:ND1    | 2:I:1998:LYS:HA   | 2.12                     | 0.65              |
| 1:C:1292:ILE:CD1  | 1:C:1328:ILE:HD11 | 2.27                     | 0.65              |
| 2:I:1176:PRO:O    | 2:I:1177:SER:HB3  | 1.95                     | 0.65              |
| 1:B:254:TRP:CH2   | 1:B:292:GLN:HG3   | 2.32                     | 0.64              |
| 2:G:1841:ALA:O    | 2:G:1842:VAL:HG23 | 1.97                     | 0.64              |
| 2:H:741:HIS:HB3   | 2:H:853:PRO:HB2   | 1.77                     | 0.64              |
| 2:H:1195:VAL:HG13 | 2:H:1211:LEU:HB3  | 1.80                     | 0.64              |
| 2:I:490:TRP:HE1   | 2:I:516:THR:CG2   | 2.00                     | 0.64              |
| 2:I:1475:LYS:CG   | 2:I:1481:SER:HB2  | 2.27                     | 0.64              |
| 1:B:599:MET:HB2   | 1:B:624:LYS:CD    | 2.24                     | 0.64              |
| 1:C:1721:ARG:CG   | 1:C:1721:ARG:NH1  | 2.56                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:353:VAL:HG23  | 2:G:357:ASN:HD22  | 1.61                     | 0.64              |
| 2:G:1906:ALA:O    | 2:G:1910:VAL:HG23 | 1.97                     | 0.64              |
| 2:H:1859:PRO:O    | 2:H:1862:VAL:HG13 | 1.98                     | 0.64              |
| 2:I:719:ILE:O     | 2:I:722:ALA:HB3   | 1.97                     | 0.64              |
| 2:I:1355:ASN:HA   | 2:I:1407:THR:O    | 1.97                     | 0.64              |
| 1:A:421:ILE:CG1   | 1:A:469:VAL:HG21  | 2.28                     | 0.64              |
| 1:A:893:VAL:HG11  | 1:A:930:LEU:HD23  | 1.80                     | 0.64              |
| 1:B:864:VAL:HG22  | 1:B:921:PRO:HB3   | 1.77                     | 0.64              |
| 1:C:749:ILE:HD11  | 1:C:805:CYS:HB3   | 1.78                     | 0.64              |
| 2:H:115:THR:HB    | 2:H:118:LYS:HB2   | 1.80                     | 0.64              |
| 2:H:1635:ARG:HG2  | 2:H:1658:GLU:CD   | 2.18                     | 0.64              |
| 1:C:604:ALA:HB3   | 1:C:612:GLU:HG2   | 1.80                     | 0.64              |
| 2:G:138:ASP:O     | 2:G:139:LYS:HG3   | 1.97                     | 0.64              |
| 2:H:259:THR:HG23  | 2:H:262:GLU:H     | 1.63                     | 0.64              |
| 2:H:1352:HIS:CD2  | 2:H:1410:PHE:CE2  | 2.85                     | 0.64              |
| 2:H:1906:ALA:O    | 2:H:1910:VAL:HG23 | 1.98                     | 0.64              |
| 2:I:1265:MET:HE1  | 2:I:1562:PRO:HG2  | 1.78                     | 0.64              |
| 1:A:1039:MET:O    | 1:A:1609:ARG:NH2  | 2.30                     | 0.64              |
| 1:B:746:GLU:O     | 1:B:750:GLU:HG3   | 1.97                     | 0.64              |
| 2:G:490:TRP:HE1   | 2:G:516:THR:CG2   | 1.99                     | 0.64              |
| 2:G:1359:MET:HE3  | 2:G:1404:MET:HB3  | 1.79                     | 0.64              |
| 2:H:259:THR:CG2   | 2:H:262:GLU:H     | 2.10                     | 0.64              |
| 2:H:658:MET:HA    | 2:H:661:TRP:NE1   | 2.13                     | 0.64              |
| 2:H:1823:SER:OG   | 2:H:1825:GLU:HG2  | 1.96                     | 0.64              |
| 1:B:504:ASP:HB2   | 1:B:508:ASN:HB2   | 1.79                     | 0.64              |
| 1:C:1540:SER:HA   | 1:C:1575:VAL:HG22 | 1.79                     | 0.64              |
| 1:C:1594:ASN:O    | 1:C:1598:GLN:HG3  | 1.97                     | 0.64              |
| 2:G:1103:PHE:O    | 2:G:1247:GLY:HA3  | 1.97                     | 0.64              |
| 2:G:1195:VAL:CG1  | 2:G:1211:LEU:HB3  | 2.27                     | 0.64              |
| 2:G:1840:VAL:O    | 2:G:1840:VAL:CG1  | 2.44                     | 0.64              |
| 2:I:61:VAL:O      | 2:I:65:LEU:HB2    | 1.96                     | 0.64              |
| 2:I:826:GLY:HA3   | 2:I:1061:GLN:HB3  | 1.78                     | 0.64              |
| 1:A:504:ASP:HB2   | 1:A:508:ASN:HB2   | 1.78                     | 0.64              |
| 1:A:746:GLU:O     | 1:A:750:GLU:HG3   | 1.97                     | 0.64              |
| 1:A:1022:THR:HG22 | 1:A:1226:SER:HB2  | 1.80                     | 0.64              |
| 1:C:833:PHE:HA    | 1:C:937:LYS:HD2   | 1.78                     | 0.64              |
| 1:C:1460:LYS:NZ   | 1:C:1774:GLU:CD   | 2.51                     | 0.64              |
| 2:G:499:THR:CB    | 2:G:500:HIS:HD2   | 1.97                     | 0.64              |
| 2:H:1808:SER:H    | 2:H:2013:ASN:HD21 | 1.46                     | 0.64              |
| 2:I:7:ARG:HE      | 2:I:27:PHE:HB2    | 1.62                     | 0.64              |
| 2:I:1457:PHE:CZ   | 2:I:1501:ILE:HD11 | 2.33                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:330:GLU:HA    | 1:B:333:LYS:HD2   | 1.80                     | 0.64              |
| 1:B:852:ARG:HG2   | 1:B:852:ARG:NH1   | 1.98                     | 0.64              |
| 1:C:1194:ASN:HB3  | 1:C:1197:THR:CG2  | 2.27                     | 0.64              |
| 2:G:1739:GLU:CB   | 2:G:1987:PRO:HB3  | 2.23                     | 0.64              |
| 2:G:1838:MET:O    | 2:G:1974:VAL:HG21 | 1.98                     | 0.64              |
| 2:H:232:LEU:O     | 2:H:232:LEU:HD23  | 1.98                     | 0.64              |
| 2:H:1457:PHE:CZ   | 2:H:1501:ILE:HD11 | 2.32                     | 0.64              |
| 2:I:648:GLY:HA3   | 2:I:678:PHE:CE2   | 2.32                     | 0.64              |
| 2:I:1676:MET:HE1  | 2:I:1781:LEU:HD21 | 1.79                     | 0.64              |
| 2:I:2022:THR:HG23 | 2:I:2025:TYR:H    | 1.63                     | 0.64              |
| 1:A:1317:GLU:HA   | 1:A:1317:GLU:OE1  | 1.96                     | 0.64              |
| 1:B:421:ILE:CG1   | 1:B:469:VAL:HG21  | 2.27                     | 0.64              |
| 2:G:545:GLN:HE21  | 2:G:545:GLN:H     | 1.46                     | 0.64              |
| 2:H:1205:LEU:O    | 2:H:1206:LYS:HG3  | 1.97                     | 0.64              |
| 2:H:1676:MET:HE1  | 2:H:1781:LEU:HD21 | 1.80                     | 0.64              |
| 2:I:892:ILE:HD11  | 2:I:903:TRP:NE1   | 2.12                     | 0.64              |
| 2:I:964:LEU:H     | 2:I:964:LEU:CD2   | 2.11                     | 0.64              |
| 1:B:1474:ALA:HA   | 1:B:1478:PRO:CG   | 2.27                     | 0.64              |
| 2:G:305:PHE:CE1   | 2:G:442:ASP:HB3   | 2.32                     | 0.64              |
| 2:H:163:GLN:HG2   | 2:H:423:VAL:HG12  | 1.79                     | 0.64              |
| 2:H:703:LEU:HD21  | 2:H:705:LEU:HD21  | 1.79                     | 0.64              |
| 2:I:670:ARG:HD3   | 2:I:699:GLY:O     | 1.98                     | 0.64              |
| 1:A:152:HIS:HD2   | 1:A:163:LEU:HB2   | 1.61                     | 0.63              |
| 1:A:1021:VAL:HG11 | 1:A:1597:LEU:HD11 | 1.79                     | 0.63              |
| 1:C:24:SER:CB     | 2:I:2014:LEU:HD12 | 2.27                     | 0.63              |
| 1:C:934:PRO:O     | 1:C:936:LEU:N     | 2.30                     | 0.63              |
| 1:C:1474:ALA:HA   | 1:C:1478:PRO:CG   | 2.27                     | 0.63              |
| 2:G:648:GLY:HA3   | 2:G:678:PHE:CE2   | 2.33                     | 0.63              |
| 2:H:964:LEU:H     | 2:H:964:LEU:CD2   | 2.09                     | 0.63              |
| 2:H:1176:PRO:O    | 2:H:1177:SER:HB3  | 1.97                     | 0.63              |
| 2:H:1266:TYR:CB   | 2:H:1347:LEU:HD23 | 2.28                     | 0.63              |
| 2:I:641:ILE:HG12  | 2:I:645:SER:HB2   | 1.79                     | 0.63              |
| 1:A:504:ASP:CB    | 1:A:508:ASN:H     | 2.10                     | 0.63              |
| 1:B:438:ASN:HD21  | 1:B:698:GLN:HE21  | 1.46                     | 0.63              |
| 1:C:436:ALA:O     | 1:C:440:MET:HG3   | 1.98                     | 0.63              |
| 1:C:504:ASP:HB2   | 1:C:508:ASN:HB2   | 1.80                     | 0.63              |
| 1:C:989:GLN:NE2   | 2:I:993:GLN:OE1   | 2.32                     | 0.63              |
| 2:G:1205:LEU:O    | 2:G:1206:LYS:HG3  | 1.98                     | 0.63              |
| 2:G:2022:THR:HG23 | 2:G:2025:TYR:H    | 1.63                     | 0.63              |
| 2:H:1227:ARG:CG   | 2:H:1227:ARG:NH1  | 2.57                     | 0.63              |
| 2:H:1808:SER:H    | 2:H:2013:ASN:ND2  | 1.95                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:902:PRO:HG2   | 2:I:929:LEU:HD21  | 1.79                     | 0.63              |
| 2:I:1266:TYR:CB   | 2:I:1347:LEU:HD23 | 2.28                     | 0.63              |
| 2:I:1279:PHE:HB2  | 2:I:1340:PRO:HG3  | 1.79                     | 0.63              |
| 2:I:1378:ILE:HD11 | 2:I:1381:VAL:CG2  | 2.28                     | 0.63              |
| 1:A:956:ALA:O     | 1:A:959:ILE:HG22  | 1.98                     | 0.63              |
| 1:A:1292:ILE:CD1  | 1:A:1328:ILE:HD11 | 2.28                     | 0.63              |
| 1:A:1461:ASP:O    | 1:A:1465:ASN:HB2  | 1.99                     | 0.63              |
| 1:B:992:PHE:CE2   | 1:B:1399:PRO:HG3  | 2.34                     | 0.63              |
| 1:C:1721:ARG:HG2  | 1:C:1721:ARG:NH1  | 2.00                     | 0.63              |
| 2:G:7:ARG:HE      | 2:G:27:PHE:HB2    | 1.63                     | 0.63              |
| 2:G:259:THR:OG1   | 2:G:260:PRO:HD2   | 1.97                     | 0.63              |
| 2:G:745:ASP:HA    | 2:G:832:TRP:HH2   | 1.64                     | 0.63              |
| 2:H:353:VAL:HG23  | 2:H:357:ASN:ND2   | 2.13                     | 0.63              |
| 2:I:1890:ASN:HB2  | 2:I:1899:VAL:HB   | 1.81                     | 0.63              |
| 2:I:1976:PHE:HA   | 2:I:1981:LEU:HD22 | 1.81                     | 0.63              |
| 1:A:824:LEU:HD12  | 1:A:846:LEU:HB3   | 1.80                     | 0.63              |
| 1:A:852:ARG:HG2   | 1:A:852:ARG:NH1   | 2.00                     | 0.63              |
| 1:B:881:ASN:HA    | 1:B:944:ARG:HH21  | 1.63                     | 0.63              |
| 1:C:599:MET:HB2   | 1:C:624:LYS:CD    | 2.25                     | 0.63              |
| 1:C:680:ILE:HG13  | 1:C:769:ILE:HB    | 1.80                     | 0.63              |
| 2:G:835:THR:HG21  | 2:G:855:HIS:CD2   | 2.33                     | 0.63              |
| 2:G:1266:TYR:CB   | 2:G:1347:LEU:HD23 | 2.29                     | 0.63              |
| 2:H:1740:THR:HG22 | 2:H:1742:VAL:HG23 | 1.79                     | 0.63              |
| 2:I:1159:ILE:CG1  | 2:I:1169:PRO:HD3  | 2.28                     | 0.63              |
| 1:B:421:ILE:HG13  | 1:B:469:VAL:HG21  | 1.81                     | 0.63              |
| 2:G:1738:PHE:CE1  | 2:G:1837:THR:HG23 | 2.34                     | 0.63              |
| 2:G:1859:PRO:O    | 2:G:1862:VAL:HG13 | 1.99                     | 0.63              |
| 2:H:598:THR:CG2   | 2:H:622:GLY:HA3   | 2.28                     | 0.63              |
| 2:I:159:ILE:HD11  | 2:I:512:LEU:HG    | 1.80                     | 0.63              |
| 2:I:1195:VAL:HG13 | 2:I:1211:LEU:HB3  | 1.79                     | 0.63              |
| 1:A:330:GLU:HA    | 1:A:333:LYS:HD2   | 1.80                     | 0.63              |
| 1:A:484:LEU:O     | 1:A:485:ASP:CB    | 2.47                     | 0.63              |
| 1:B:1:MET:HE3     | 1:B:5:VAL:HG12    | 1.81                     | 0.63              |
| 1:B:444:ASN:HB3   | 1:B:446:ALA:H     | 1.63                     | 0.63              |
| 1:B:1721:ARG:CG   | 1:B:1721:ARG:NH1  | 2.55                     | 0.63              |
| 2:G:115:THR:HB    | 2:G:118:LYS:HB2   | 1.80                     | 0.63              |
| 2:G:251:VAL:O     | 2:G:255:LEU:HB2   | 1.99                     | 0.63              |
| 2:H:601:THR:CG2   | 2:H:618:GLU:O     | 2.38                     | 0.63              |
| 2:H:835:THR:HG22  | 2:H:845:THR:N     | 2.14                     | 0.63              |
| 2:H:1475:LYS:CG   | 2:H:1481:SER:HB2  | 2.29                     | 0.63              |
| 2:I:1741:ILE:HG12 | 2:I:1746:LEU:HD13 | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1859:PRO:O    | 2:I:1862:VAL:HG13 | 1.98                     | 0.63              |
| 1:A:233:ILE:HD13  | 1:A:237:MET:HE2   | 1.81                     | 0.63              |
| 1:A:436:ALA:O     | 1:A:440:MET:HG3   | 1.99                     | 0.63              |
| 1:A:1194:ASN:HB3  | 1:A:1197:THR:CG2  | 2.28                     | 0.63              |
| 2:I:241:ILE:HG23  | 2:I:506:PRO:HG3   | 1.81                     | 0.63              |
| 1:B:27:ARG:HH21   | 2:H:2015:THR:HA   | 1.64                     | 0.63              |
| 1:C:864:VAL:HG22  | 1:C:921:PRO:HB3   | 1.79                     | 0.63              |
| 2:G:748:THR:HB    | 2:G:749:PRO:HD3   | 1.78                     | 0.63              |
| 2:G:1360:ILE:HG23 | 2:G:1403:VAL:O    | 1.99                     | 0.63              |
| 2:H:892:ILE:HD11  | 2:H:903:TRP:NE1   | 2.14                     | 0.63              |
| 2:I:1194:VAL:O    | 2:I:1194:VAL:HG12 | 1.99                     | 0.63              |
| 1:A:460:GLU:HG2   | 1:A:470:LYS:HD3   | 1.79                     | 0.63              |
| 1:C:742:LYS:HD3   | 1:C:746:GLU:OE2   | 1.98                     | 0.63              |
| 2:G:490:TRP:O     | 2:G:494:THR:HG22  | 1.99                     | 0.63              |
| 2:I:115:THR:HB    | 2:I:118:LYS:HB2   | 1.80                     | 0.63              |
| 2:I:259:THR:HG23  | 2:I:262:GLU:H     | 1.64                     | 0.63              |
| 2:I:259:THR:OG1   | 2:I:260:PRO:HD2   | 1.98                     | 0.63              |
| 1:A:411:GLN:HE22  | 1:A:1628:SER:H    | 1.47                     | 0.62              |
| 1:B:1056:ILE:HD13 | 1:B:1193:TRP:HD1  | 1.64                     | 0.62              |
| 1:C:956:ALA:O     | 1:C:959:ILE:HG22  | 1.98                     | 0.62              |
| 1:C:1753:ALA:HB2  | 1:C:1872:SER:OG   | 1.98                     | 0.62              |
| 2:G:1227:ARG:HG3  | 2:G:1227:ARG:NH1  | 2.00                     | 0.62              |
| 2:H:33:LEU:HD11   | 2:H:80:PHE:HD2    | 1.63                     | 0.62              |
| 2:H:1874:VAL:O    | 2:H:1878:VAL:HG12 | 1.98                     | 0.62              |
| 1:A:13:LEU:HB2    | 2:G:2026:PHE:CE1  | 2.34                     | 0.62              |
| 1:A:158:LYS:HD3   | 1:A:185:GLU:HB3   | 1.81                     | 0.62              |
| 1:B:529:MET:HG3   | 1:B:638:LEU:HG    | 1.80                     | 0.62              |
| 2:G:85:ASN:ND2    | 2:G:135:ARG:HH11  | 1.97                     | 0.62              |
| 2:G:943:TRP:CH2   | 2:G:1016:PRO:HG3  | 2.34                     | 0.62              |
| 2:G:1173:VAL:HG21 | 2:G:1221:MET:HE1  | 1.80                     | 0.62              |
| 2:G:1378:ILE:HD11 | 2:G:1381:VAL:CG2  | 2.29                     | 0.62              |
| 2:H:251:VAL:O     | 2:H:255:LEU:HB2   | 1.99                     | 0.62              |
| 2:H:1374:THR:HG23 | 2:H:1396:LEU:HD12 | 1.81                     | 0.62              |
| 2:H:1931:LEU:HD22 | 2:H:1935:GLU:HG2  | 1.81                     | 0.62              |
| 1:A:1259:GLY:HA2  | 1:A:1263:ASP:HB2  | 1.81                     | 0.62              |
| 1:C:254:TRP:CH2   | 1:C:292:GLN:HG3   | 2.34                     | 0.62              |
| 1:C:529:MET:CG    | 1:C:638:LEU:HG    | 2.30                     | 0.62              |
| 2:G:726:PHE:O     | 2:G:762:ASN:HB2   | 1.98                     | 0.62              |
| 2:H:750:MET:HG3   | 2:H:796:PHE:HZ    | 1.64                     | 0.62              |
| 2:H:856:LYS:HG2   | 2:H:1054:LEU:HD12 | 1.81                     | 0.62              |
| 2:I:324:LEU:HD12  | 2:I:328:LEU:HG    | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1472:VAL:HG22 | 2:I:1483:VAL:HG22 | 1.81                     | 0.62              |
| 2:I:1624:THR:HB   | 2:I:1642:THR:HG23 | 1.81                     | 0.62              |
| 2:H:871:THR:HB    | 2:H:872:ILE:HD12  | 1.80                     | 0.62              |
| 2:H:1472:VAL:HG22 | 2:H:1483:VAL:HG22 | 1.79                     | 0.62              |
| 2:I:1868:GLN:HG3  | 2:I:1898:TYR:OH   | 1.99                     | 0.62              |
| 2:I:1906:ALA:O    | 2:I:1910:VAL:HG23 | 2.00                     | 0.62              |
| 1:A:1292:ILE:HD11 | 1:A:1328:ILE:HD11 | 1.81                     | 0.62              |
| 1:A:1455:ARG:HH11 | 1:A:1458:GLN:HE21 | 1.46                     | 0.62              |
| 1:B:507:GLY:N     | 1:B:954:ARG:HG2   | 2.15                     | 0.62              |
| 1:B:1584:PRO:HG3  | 1:B:1591:TRP:CZ3  | 2.35                     | 0.62              |
| 1:C:1039:MET:O    | 1:C:1609:ARG:NH2  | 2.31                     | 0.62              |
| 2:G:1102:TYR:HB3  | 2:G:1244:PRO:HA   | 1.80                     | 0.62              |
| 2:G:1782:THR:HG22 | 2:G:1827:LEU:HD21 | 1.81                     | 0.62              |
| 2:G:1819:ALA:HA   | 2:G:2005:ARG:HH11 | 1.65                     | 0.62              |
| 2:H:601:THR:HG22  | 2:H:601:THR:O     | 2.00                     | 0.62              |
| 1:B:1455:ARG:HH11 | 1:B:1458:GLN:HE21 | 1.47                     | 0.62              |
| 1:C:822:VAL:HG12  | 1:C:824:LEU:HD22  | 1.82                     | 0.62              |
| 2:H:1168:ASN:ND2  | 2:H:1171:ARG:HB2  | 2.14                     | 0.62              |
| 2:I:464:ASP:HB3   | 2:I:466:SER:HB3   | 1.80                     | 0.62              |
| 2:I:846:VAL:HG13  | 2:I:865:TRP:NE1   | 2.15                     | 0.62              |
| 2:I:1740:THR:HG22 | 2:I:1742:VAL:HG23 | 1.79                     | 0.62              |
| 1:A:749:ILE:CD1   | 1:A:805:CYS:HB3   | 2.29                     | 0.62              |
| 1:A:1540:SER:HA   | 1:A:1575:VAL:HG22 | 1.81                     | 0.62              |
| 1:C:233:ILE:HD13  | 1:C:237:MET:CE    | 2.30                     | 0.62              |
| 2:G:241:ILE:HG23  | 2:G:506:PRO:HG3   | 1.80                     | 0.62              |
| 2:G:871:THR:HB    | 2:G:872:ILE:HD12  | 1.82                     | 0.62              |
| 2:G:1908:ASP:HB2  | 2:G:1958:LEU:HD21 | 1.81                     | 0.62              |
| 2:H:131:ILE:HD12  | 2:H:182:VAL:CG1   | 2.29                     | 0.62              |
| 2:I:184:VAL:HG13  | 2:I:187:LEU:HD21  | 1.80                     | 0.62              |
| 2:I:259:THR:CG2   | 2:I:262:GLU:H     | 2.11                     | 0.62              |
| 1:C:444:ASN:HB3   | 1:C:446:ALA:H     | 1.65                     | 0.62              |
| 2:G:159:ILE:HD11  | 2:G:512:LEU:HG    | 1.80                     | 0.62              |
| 2:G:641:ILE:HG12  | 2:G:645:SER:HB2   | 1.80                     | 0.62              |
| 2:G:1300:PHE:CA   | 2:G:1556:VAL:HG11 | 2.29                     | 0.62              |
| 2:H:85:ASN:ND2    | 2:H:135:ARG:HH11  | 1.96                     | 0.62              |
| 2:I:1805:ALA:HB2  | 2:I:2011:ILE:HB   | 1.82                     | 0.62              |
| 1:A:20:TYR:HE1    | 2:G:2035:SER:HB2  | 1.60                     | 0.62              |
| 1:A:1523:ARG:CG   | 1:A:1523:ARG:NH1  | 2.57                     | 0.62              |
| 1:B:27:ARG:HD2    | 1:B:30:GLU:OE2    | 2.00                     | 0.62              |
| 1:C:501:THR:N     | 1:C:886:GLU:OE1   | 2.21                     | 0.62              |
| 2:G:750:MET:HG3   | 2:G:796:PHE:HZ    | 1.65                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:490:TRP:O     | 2:H:494:THR:HG22  | 2.00                     | 0.62              |
| 1:A:1326:ILE:HG12 | 1:A:1388:MET:HG3  | 1.82                     | 0.62              |
| 2:G:1719:ILE:O    | 2:G:1761:SER:HB2  | 2.00                     | 0.62              |
| 2:G:1931:LEU:HD22 | 2:G:1935:GLU:HG2  | 1.82                     | 0.62              |
| 2:H:1149:TRP:CD1  | 2:H:1213:LEU:HD12 | 2.34                     | 0.62              |
| 2:I:745:ASP:HA    | 2:I:832:TRP:HH2   | 1.65                     | 0.62              |
| 2:I:1086:LEU:HD12 | 2:I:1090:TYR:HB2  | 1.82                     | 0.62              |
| 2:I:1823:SER:OG   | 2:I:1825:GLU:HG2  | 2.00                     | 0.62              |
| 1:C:233:ILE:HD13  | 1:C:237:MET:HE2   | 1.80                     | 0.61              |
| 1:C:509:ILE:HG12  | 1:C:951:SER:HB2   | 1.82                     | 0.61              |
| 1:C:1057:MET:SD   | 1:C:1097:ILE:HG23 | 2.40                     | 0.61              |
| 2:G:719:ILE:O     | 2:G:722:ALA:HB3   | 2.00                     | 0.61              |
| 2:G:1199:GLU:OE2  | 2:G:1567:ARG:CZ   | 2.46                     | 0.61              |
| 2:H:100:ASP:OD2   | 2:H:102:HIS:HD2   | 1.82                     | 0.61              |
| 2:H:159:ILE:HD11  | 2:H:512:LEU:HG    | 1.82                     | 0.61              |
| 2:H:1675:GLY:O    | 2:H:1678:MET:HB2  | 1.99                     | 0.61              |
| 1:A:934:PRO:O     | 1:A:936:LEU:N     | 2.33                     | 0.61              |
| 1:B:631:PRO:HB2   | 1:B:634:THR:OG1   | 2.00                     | 0.61              |
| 1:B:1292:ILE:CD1  | 1:B:1328:ILE:HD11 | 2.30                     | 0.61              |
| 2:H:7:ARG:HE      | 2:H:27:PHE:HB2    | 1.64                     | 0.61              |
| 2:H:353:VAL:HG23  | 2:H:357:ASN:HD22  | 1.65                     | 0.61              |
| 1:B:158:LYS:HD3   | 1:B:185:GLU:HB3   | 1.82                     | 0.61              |
| 1:B:340:ARG:HH12  | 1:B:344:GLN:CG    | 2.13                     | 0.61              |
| 1:B:824:LEU:HD12  | 1:B:846:LEU:HB3   | 1.82                     | 0.61              |
| 1:C:1498:GLU:HB2  | 1:C:1876:LEU:HD13 | 1.82                     | 0.61              |
| 2:H:589:ARG:HB3   | 2:H:590:PRO:HD2   | 1.82                     | 0.61              |
| 2:H:856:LYS:NZ    | 2:H:1052:CYS:SG   | 2.70                     | 0.61              |
| 2:H:1528:GLU:O    | 2:H:1530:LYS:N    | 2.30                     | 0.61              |
| 2:I:860:ARG:HB3   | 2:I:898:ASP:HB3   | 1.81                     | 0.61              |
| 2:I:1054:LEU:HB2  | 4:I:3051:FMN:HM71 | 1.82                     | 0.61              |
| 1:A:1721:ARG:CG   | 1:A:1721:ARG:NH1  | 2.52                     | 0.61              |
| 1:B:1555:ALA:HA   | 1:B:1621:PHE:CE1  | 2.36                     | 0.61              |
| 1:C:20:TYR:CE1    | 2:I:2035:SER:HB2  | 2.35                     | 0.61              |
| 2:G:1739:GLU:O    | 2:G:1987:PRO:HG3  | 2.00                     | 0.61              |
| 2:H:835:THR:HG21  | 2:H:855:HIS:NE2   | 2.14                     | 0.61              |
| 2:H:1378:ILE:HD11 | 2:H:1381:VAL:CG2  | 2.31                     | 0.61              |
| 2:I:100:ASP:OD2   | 2:I:102:HIS:HD2   | 1.83                     | 0.61              |
| 2:I:1808:SER:H    | 2:I:2013:ASN:HD21 | 1.47                     | 0.61              |
| 1:A:24:SER:O      | 2:G:1977:HIS:HD2  | 1.84                     | 0.61              |
| 1:B:20:TYR:CE1    | 2:H:2035:SER:HB2  | 2.35                     | 0.61              |
| 1:B:644:THR:HG23  | 1:B:648:ASP:H     | 1.65                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:20:TYR:CG     | 2:I:2033:THR:OG1  | 2.53                     | 0.61              |
| 1:C:1292:ILE:HD11 | 1:C:1328:ILE:HD11 | 1.81                     | 0.61              |
| 2:G:324:LEU:HD12  | 2:G:328:LEU:HG    | 1.81                     | 0.61              |
| 2:H:33:LEU:HD11   | 2:H:80:PHE:CD2    | 2.35                     | 0.61              |
| 2:H:174:ARG:NH2   | 2:H:225:THR:OG1   | 2.33                     | 0.61              |
| 2:H:1086:LEU:HD12 | 2:H:1090:TYR:HB2  | 1.83                     | 0.61              |
| 2:H:1279:PHE:HB2  | 2:H:1340:PRO:HG3  | 1.81                     | 0.61              |
| 2:H:1419:PHE:O    | 2:H:1421:ASN:N    | 2.33                     | 0.61              |
| 2:I:56:THR:HG23   | 2:I:59:GLU:CG     | 2.28                     | 0.61              |
| 1:A:705:VAL:HG23  | 1:A:732:LEU:HD21  | 1.82                     | 0.61              |
| 1:B:24:SER:O      | 2:H:1977:HIS:CD2  | 2.53                     | 0.61              |
| 1:B:1431:GLU:HG3  | 1:B:1433:HIS:CE1  | 2.36                     | 0.61              |
| 1:B:1693:ILE:HD11 | 2:H:998:GLN:HB2   | 1.83                     | 0.61              |
| 2:H:603:SER:O     | 2:H:607:VAL:HG12  | 2.00                     | 0.61              |
| 1:A:644:THR:HG23  | 1:A:648:ASP:H     | 1.65                     | 0.61              |
| 1:A:822:VAL:HG12  | 1:A:824:LEU:HD22  | 1.82                     | 0.61              |
| 1:B:1194:ASN:HB3  | 1:B:1197:THR:CG2  | 2.30                     | 0.61              |
| 1:C:24:SER:HB3    | 2:I:2014:LEU:HD12 | 1.82                     | 0.61              |
| 1:C:824:LEU:HD12  | 1:C:846:LEU:HB3   | 1.82                     | 0.61              |
| 2:I:663:ILE:HG13  | 2:I:694:TYR:HE1   | 1.66                     | 0.61              |
| 2:I:1325:PHE:CZ   | 2:I:1328:VAL:HG11 | 2.36                     | 0.61              |
| 2:I:1352:HIS:HE1  | 2:I:1583:MET:HE1  | 1.65                     | 0.61              |
| 1:B:1052:GLU:O    | 1:B:1056:ILE:HG23 | 2.01                     | 0.61              |
| 1:B:1594:ASN:O    | 1:B:1598:GLN:HG3  | 2.00                     | 0.61              |
| 1:A:11:HIS:ND1    | 2:G:1998:LYS:HA   | 2.15                     | 0.61              |
| 1:A:599:MET:HB2   | 1:A:624:LYS:CD    | 2.25                     | 0.61              |
| 1:B:1292:ILE:HD11 | 1:B:1328:ILE:HD11 | 1.82                     | 0.61              |
| 1:B:1360:ARG:HH11 | 1:B:1364:GLU:HG2  | 1.66                     | 0.61              |
| 2:G:601:THR:O     | 2:G:601:THR:HG22  | 2.01                     | 0.61              |
| 2:G:1123:ASP:N    | 2:G:1123:ASP:OD1  | 2.34                     | 0.61              |
| 2:G:1976:PHE:HB3  | 2:G:1981:LEU:HD21 | 1.82                     | 0.61              |
| 2:H:260:PRO:HD3   | 2:H:289:TRP:CE2   | 2.36                     | 0.61              |
| 1:A:1:MET:HE3     | 1:A:5:VAL:HG12    | 1.82                     | 0.61              |
| 1:C:1501:LEU:HD11 | 1:C:1775:LEU:HD23 | 1.79                     | 0.61              |
| 2:G:856:LYS:NZ    | 2:G:1052:CYS:SG   | 2.69                     | 0.61              |
| 2:G:1472:VAL:HG22 | 2:G:1483:VAL:HG22 | 1.83                     | 0.61              |
| 2:H:184:VAL:HG13  | 2:H:187:LEU:HD21  | 1.83                     | 0.61              |
| 2:H:1805:ALA:HB2  | 2:H:2011:ILE:HB   | 1.83                     | 0.61              |
| 2:I:1219:ILE:HD11 | 2:I:1242:PHE:HB2  | 1.83                     | 0.61              |
| 1:C:504:ASP:CB    | 1:C:508:ASN:H     | 2.14                     | 0.60              |
| 2:G:1417:THR:C    | 2:G:1419:PHE:H    | 2.04                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:846:VAL:HG13  | 2:H:865:TRP:NE1   | 2.16                     | 0.60              |
| 2:I:565:TYR:CZ    | 2:I:758:ARG:HD2   | 2.35                     | 0.60              |
| 1:A:32:GLN:HA     | 1:A:35:PHE:CE2    | 2.35                     | 0.60              |
| 1:B:233:ILE:HD13  | 1:B:237:MET:HE2   | 1.82                     | 0.60              |
| 1:C:2:LYS:CD      | 2:I:2050:GLN:HB3  | 2.30                     | 0.60              |
| 2:G:33:LEU:HD11   | 2:G:80:PHE:CD2    | 2.35                     | 0.60              |
| 2:G:174:ARG:NH2   | 2:G:225:THR:OG1   | 2.34                     | 0.60              |
| 2:I:33:LEU:HD11   | 2:I:80:PHE:CD2    | 2.36                     | 0.60              |
| 2:I:856:LYS:NZ    | 2:I:1052:CYS:SG   | 2.70                     | 0.60              |
| 2:I:1300:PHE:HA   | 2:I:1556:VAL:HG11 | 1.84                     | 0.60              |
| 1:A:232:LEU:HD22  | 1:A:269:LEU:HA    | 1.83                     | 0.60              |
| 2:G:607:VAL:HA    | 2:G:617:ILE:HD13  | 1.82                     | 0.60              |
| 2:G:747:HIS:HE1   | 2:G:780:TYR:OH    | 1.84                     | 0.60              |
| 2:G:1808:SER:H    | 2:G:2013:ASN:HD21 | 1.47                     | 0.60              |
| 2:G:1844:ARG:CG   | 2:G:1844:ARG:NH1  | 2.49                     | 0.60              |
| 2:I:1198:SER:HB3  | 2:I:1205:LEU:HD21 | 1.82                     | 0.60              |
| 2:I:1908:ASP:HB2  | 2:I:1958:LEU:HD21 | 1.83                     | 0.60              |
| 1:A:20:TYR:OH     | 2:G:2035:SER:HB2  | 2.01                     | 0.60              |
| 1:A:1842:VAL:O    | 1:A:1845:ASN:HB2  | 2.02                     | 0.60              |
| 1:B:400:ARG:HH11  | 1:B:400:ARG:HG3   | 1.64                     | 0.60              |
| 2:G:846:VAL:HG13  | 2:G:865:TRP:NE1   | 2.16                     | 0.60              |
| 2:H:324:LEU:HD12  | 2:H:328:LEU:HG    | 1.84                     | 0.60              |
| 2:H:1198:SER:HB3  | 2:H:1205:LEU:HD21 | 1.83                     | 0.60              |
| 2:H:1219:ILE:HD11 | 2:H:1242:PHE:HB2  | 1.83                     | 0.60              |
| 2:I:674:TYR:HB3   | 2:I:676:ILE:HG22  | 1.84                     | 0.60              |
| 2:I:1352:HIS:CD2  | 2:I:1410:PHE:CE2  | 2.90                     | 0.60              |
| 2:I:1360:ILE:HG23 | 2:I:1403:VAL:O    | 2.01                     | 0.60              |
| 1:B:509:ILE:HG12  | 1:B:951:SER:HB2   | 1.82                     | 0.60              |
| 1:B:1523:ARG:CG   | 1:B:1523:ARG:NH1  | 2.59                     | 0.60              |
| 1:C:221:LEU:O     | 1:C:225:SER:HB3   | 2.02                     | 0.60              |
| 2:G:61:VAL:HG21   | 2:G:95:TYR:HE1    | 1.67                     | 0.60              |
| 2:G:499:THR:CB    | 2:G:500:HIS:CD2   | 2.80                     | 0.60              |
| 2:G:926:LEU:HD13  | 2:G:947:THR:HG22  | 1.84                     | 0.60              |
| 2:G:1325:PHE:CZ   | 2:G:1328:VAL:HG11 | 2.37                     | 0.60              |
| 2:H:745:ASP:HA    | 2:H:832:TRP:HH2   | 1.66                     | 0.60              |
| 2:I:667:LYS:HB2   | 2:I:698:LEU:HD23  | 1.82                     | 0.60              |
| 2:I:817:ALA:O     | 2:I:821:ILE:HG13  | 2.01                     | 0.60              |
| 2:I:1123:ASP:N    | 2:I:1123:ASP:OD1  | 2.35                     | 0.60              |
| 2:I:1205:LEU:O    | 2:I:1206:LYS:HG3  | 2.00                     | 0.60              |
| 1:C:644:THR:HG23  | 1:C:648:ASP:H     | 1.65                     | 0.60              |
| 2:G:561:TRP:O     | 2:G:562:LEU:C     | 2.39                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:816:ASP:HB3   | 2:G:1048:VAL:HG21 | 1.83                     | 0.60              |
| 2:G:1822:MET:HE2  | 2:G:1996:ILE:HG12 | 1.84                     | 0.60              |
| 2:H:1624:THR:HB   | 2:H:1642:THR:HG23 | 1.82                     | 0.60              |
| 2:I:589:ARG:HB3   | 2:I:590:PRO:HD2   | 1.83                     | 0.60              |
| 2:I:1976:PHE:HB3  | 2:I:1981:LEU:HD21 | 1.83                     | 0.60              |
| 1:A:529:MET:HG3   | 1:A:638:LEU:HG    | 1.84                     | 0.60              |
| 1:A:1194:ASN:O    | 1:A:1197:THR:HG23 | 2.02                     | 0.60              |
| 1:B:513:GLU:OE2   | 1:B:873:ARG:NH1   | 2.33                     | 0.60              |
| 2:G:184:VAL:HG13  | 2:G:187:LEU:HD21  | 1.84                     | 0.60              |
| 2:G:271:THR:OG1   | 2:G:460:TYR:HB2   | 2.01                     | 0.60              |
| 2:I:33:LEU:HD11   | 2:I:80:PHE:HD2    | 1.65                     | 0.60              |
| 1:A:233:ILE:HD13  | 1:A:237:MET:CE    | 2.32                     | 0.60              |
| 1:C:1062:TYR:CD2  | 1:C:1693:ILE:HG23 | 2.36                     | 0.60              |
| 2:H:1149:TRP:CD1  | 2:H:1213:LEU:CD1  | 2.85                     | 0.60              |
| 2:H:1739:GLU:O    | 2:H:1987:PRO:HG3  | 2.02                     | 0.60              |
| 2:I:1986:LYS:N    | 2:I:1987:PRO:HD2  | 2.16                     | 0.60              |
| 1:B:604:ALA:HB3   | 1:B:612:GLU:HG2   | 1.82                     | 0.60              |
| 1:B:1657:HIS:ND1  | 1:B:1658:PRO:HD2  | 2.17                     | 0.60              |
| 1:C:529:MET:HG3   | 1:C:638:LEU:HG    | 1.82                     | 0.60              |
| 2:G:732:TRP:CD2   | 2:G:750:MET:CE    | 2.85                     | 0.60              |
| 2:G:892:ILE:HD11  | 2:G:903:TRP:NE1   | 2.17                     | 0.60              |
| 2:H:719:ILE:O     | 2:H:722:ALA:HB3   | 2.02                     | 0.60              |
| 1:B:1021:VAL:HG11 | 1:B:1597:LEU:HD11 | 1.83                     | 0.60              |
| 1:B:1057:MET:SD   | 1:B:1097:ILE:HG23 | 2.42                     | 0.60              |
| 1:C:1662:TYR:O    | 1:C:1665:ILE:HG22 | 2.01                     | 0.60              |
| 1:C:1842:VAL:O    | 1:C:1845:ASN:HB2  | 2.02                     | 0.60              |
| 2:H:1093:ASP:HB3  | 2:H:1096:LYS:HG3  | 1.84                     | 0.60              |
| 2:I:601:THR:O     | 2:I:601:THR:HG22  | 2.02                     | 0.60              |
| 2:I:741:HIS:CB    | 2:I:853:PRO:HB2   | 2.32                     | 0.60              |
| 2:I:1874:VAL:O    | 2:I:1878:VAL:HG12 | 2.02                     | 0.60              |
| 2:I:1989:LYS:O    | 2:I:1993:LYS:HG3  | 2.02                     | 0.60              |
| 1:A:1119:LYS:HE2  | 1:A:1341:PHE:CG   | 2.37                     | 0.59              |
| 1:B:1189:ILE:HD12 | 1:B:1380:GLN:HG3  | 1.82                     | 0.59              |
| 1:C:1461:ASP:O    | 1:C:1465:ASN:HB2  | 2.02                     | 0.59              |
| 1:C:1585:LYS:HB3  | 3:C:2748:CER:H52  | 1.84                     | 0.59              |
| 2:G:100:ASP:OD2   | 2:G:102:HIS:HD2   | 1.85                     | 0.59              |
| 2:G:598:THR:CG2   | 2:G:622:GLY:HA3   | 2.30                     | 0.59              |
| 2:G:1417:THR:HG22 | 2:G:1419:PHE:CE2  | 2.37                     | 0.59              |
| 2:G:1425:LYS:HG2  | 2:G:1471:GLU:CG   | 2.30                     | 0.59              |
| 2:H:1494:PRO:HB2  | 2:H:1823:SER:HB2  | 1.84                     | 0.59              |
| 2:I:732:TRP:CD2   | 2:I:750:MET:CE    | 2.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:37:LYS:HB2    | 1:A:65:TYR:HE1    | 1.67                     | 0.59              |
| 1:A:67:SER:OG     | 2:I:359:HIS:HE1   | 1.85                     | 0.59              |
| 1:A:1475:GLU:CG   | 1:A:1761:LYS:O    | 2.50                     | 0.59              |
| 1:B:80:CYS:SG     | 1:B:82:SER:HB3    | 2.42                     | 0.59              |
| 1:B:1062:TYR:CD2  | 1:B:1693:ILE:HG23 | 2.36                     | 0.59              |
| 1:B:1184:LEU:HB2  | 1:B:1352:THR:HG21 | 1.83                     | 0.59              |
| 2:H:813:THR:HB    | 2:H:818:LYS:HE3   | 1.84                     | 0.59              |
| 2:I:163:GLN:CG    | 2:I:423:VAL:HG12  | 2.32                     | 0.59              |
| 2:I:1378:ILE:HD11 | 2:I:1381:VAL:HG21 | 1.84                     | 0.59              |
| 1:A:435:GLU:O     | 1:A:439:ILE:HG13  | 2.03                     | 0.59              |
| 1:B:32:GLN:HA     | 1:B:35:PHE:CE2    | 2.38                     | 0.59              |
| 1:B:680:ILE:HG13  | 1:B:769:ILE:HB    | 1.83                     | 0.59              |
| 1:B:1460:LYS:NZ   | 1:B:1774:GLU:CD   | 2.51                     | 0.59              |
| 1:C:705:VAL:HG23  | 1:C:732:LEU:HD21  | 1.83                     | 0.59              |
| 2:G:594:VAL:HG21  | 2:G:610:THR:HG21  | 1.84                     | 0.59              |
| 2:H:1314:ARG:CG   | 2:H:1314:ARG:NH1  | 2.62                     | 0.59              |
| 2:I:1575:LEU:HD13 | 2:I:1579:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:1584:PRO:HG3  | 1:A:1591:TRP:CZ3  | 2.37                     | 0.59              |
| 1:B:221:LEU:O     | 1:B:225:SER:HB3   | 2.02                     | 0.59              |
| 1:B:1259:GLY:HA2  | 1:B:1263:ASP:HB2  | 1.84                     | 0.59              |
| 1:C:56:MET:HG3    | 2:I:1893:VAL:CG2  | 2.32                     | 0.59              |
| 1:C:421:ILE:CG1   | 1:C:469:VAL:HG21  | 2.32                     | 0.59              |
| 2:G:754:TYR:CD2   | 2:G:794:MET:HG3   | 2.38                     | 0.59              |
| 2:G:2038:ILE:O    | 2:G:2042:ILE:HG12 | 2.02                     | 0.59              |
| 2:H:241:ILE:HG23  | 2:H:506:PRO:HG3   | 1.83                     | 0.59              |
| 2:H:409:PHE:HB3   | 2:H:833:GLU:OE1   | 2.02                     | 0.59              |
| 2:H:860:ARG:HB3   | 2:H:898:ASP:HB3   | 1.83                     | 0.59              |
| 2:H:1223:MET:HE3  | 2:H:1238:LEU:HD12 | 1.84                     | 0.59              |
| 2:I:658:MET:HA    | 2:I:661:TRP:NE1   | 2.17                     | 0.59              |
| 1:A:1432:HIS:CE1  | 1:A:1434:SER:OG   | 2.55                     | 0.59              |
| 1:A:1749:THR:CB   | 1:A:1874:ASP:HA   | 2.31                     | 0.59              |
| 1:B:233:ILE:HD13  | 1:B:237:MET:CE    | 2.32                     | 0.59              |
| 1:B:956:ALA:O     | 1:B:959:ILE:HG22  | 2.02                     | 0.59              |
| 1:B:1842:VAL:O    | 1:B:1845:ASN:HB2  | 2.02                     | 0.59              |
| 1:C:1194:ASN:O    | 1:C:1197:THR:HG23 | 2.02                     | 0.59              |
| 1:C:1492:GLU:O    | 1:C:1496:GLU:HG3  | 2.01                     | 0.59              |
| 2:G:443:LEU:HD22  | 2:G:448:VAL:HG11  | 1.84                     | 0.59              |
| 2:G:1805:ALA:HB2  | 2:G:2011:ILE:HB   | 1.84                     | 0.59              |
| 2:I:85:ASN:ND2    | 2:I:135:ARG:HH11  | 1.99                     | 0.59              |
| 2:I:402:LEU:O     | 2:I:402:LEU:HD13  | 2.02                     | 0.59              |
| 2:I:1149:TRP:CD1  | 2:I:1213:LEU:HD12 | 2.37                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:504:ASP:CB    | 1:B:508:ASN:H     | 2.15                     | 0.59              |
| 1:C:1584:PRO:HG3  | 1:C:1591:TRP:CZ3  | 2.38                     | 0.59              |
| 2:G:603:SER:O     | 2:G:607:VAL:HG12  | 2.03                     | 0.59              |
| 2:G:932:ILE:HD11  | 2:G:1042:ALA:CB   | 2.24                     | 0.59              |
| 2:G:1195:VAL:HG13 | 2:G:1211:LEU:HB3  | 1.84                     | 0.59              |
| 2:H:817:ALA:O     | 2:H:821:ILE:HG13  | 2.02                     | 0.59              |
| 2:I:1422:THR:O    | 2:I:1422:THR:CG2  | 2.49                     | 0.59              |
| 1:A:417:TYR:OH    | 1:A:458:THR:HG22  | 2.02                     | 0.59              |
| 1:A:516:ARG:NH2   | 1:A:889:GLU:OE1   | 2.35                     | 0.59              |
| 1:B:1585:LYS:HB3  | 3:B:2748:CER:H52  | 1.85                     | 0.59              |
| 1:C:733:ILE:HD12  | 1:C:761:LEU:HD21  | 1.85                     | 0.59              |
| 2:G:1417:THR:O    | 2:G:1419:PHE:N    | 2.30                     | 0.59              |
| 2:H:663:ILE:HG13  | 2:H:694:TYR:HE1   | 1.66                     | 0.59              |
| 2:H:726:PHE:O     | 2:H:762:ASN:HB2   | 2.03                     | 0.59              |
| 2:I:99:ASN:HA     | 2:I:550:VAL:CG2   | 2.32                     | 0.59              |
| 2:I:1086:LEU:HD12 | 2:I:1090:TYR:CB   | 2.33                     | 0.59              |
| 2:I:1496:LYS:HE2  | 2:I:1693:ARG:HH21 | 1.67                     | 0.59              |
| 1:A:409:ALA:HB2   | 1:A:442:ARG:HD2   | 1.84                     | 0.59              |
| 2:G:131:ILE:CG2   | 2:G:182:VAL:CG1   | 2.80                     | 0.59              |
| 2:G:1417:THR:HG22 | 2:G:1419:PHE:CD2  | 2.37                     | 0.59              |
| 2:H:197:GLU:OE1   | 2:H:197:GLU:HA    | 2.02                     | 0.59              |
| 2:H:455:ILE:HG13  | 2:H:469:ARG:HD3   | 1.83                     | 0.59              |
| 1:A:50:SER:HB2    | 1:A:51:PRO:HD3    | 1.85                     | 0.59              |
| 1:A:1002:LYS:NZ   | 1:A:1782:GLU:HG2  | 2.17                     | 0.59              |
| 1:C:1555:ALA:HA   | 1:C:1621:PHE:CE1  | 2.38                     | 0.59              |
| 2:G:402:LEU:O     | 2:G:402:LEU:HD13  | 2.03                     | 0.59              |
| 2:G:1086:LEU:HD12 | 2:G:1090:TYR:HB2  | 1.84                     | 0.59              |
| 2:H:2038:ILE:O    | 2:H:2042:ILE:HG12 | 2.03                     | 0.59              |
| 1:A:440:MET:HB3   | 1:A:483:VAL:HG21  | 1.85                     | 0.59              |
| 1:B:417:TYR:OH    | 1:B:458:THR:HG22  | 2.03                     | 0.59              |
| 1:B:1474:ALA:O    | 1:B:1478:PRO:HD2  | 2.03                     | 0.59              |
| 2:G:1210:ILE:HB   | 2:G:1222:GLU:HB3  | 1.85                     | 0.59              |
| 2:G:1293:THR:CG2  | 2:G:1296:GLU:H    | 2.14                     | 0.59              |
| 2:G:1374:THR:HG23 | 2:G:1396:LEU:HD12 | 1.85                     | 0.59              |
| 2:H:259:THR:OG1   | 2:H:260:PRO:HD2   | 2.03                     | 0.59              |
| 2:H:1130:THR:H    | 2:H:1133:THR:HG23 | 1.68                     | 0.59              |
| 2:I:174:ARG:NH2   | 2:I:225:THR:OG1   | 2.36                     | 0.59              |
| 2:I:353:VAL:HG23  | 2:I:357:ASN:ND2   | 2.18                     | 0.59              |
| 2:I:490:TRP:O     | 2:I:494:THR:HG22  | 2.03                     | 0.59              |
| 1:A:1524:GLY:O    | 1:A:1528:THR:HG23 | 2.03                     | 0.58              |
| 1:A:1585:LYS:HB3  | 3:A:2748:CER:H52  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1234:MET:HG2  | 1:B:1326:ILE:HD12 | 1.85                     | 0.58              |
| 1:C:488:PRO:HG3   | 1:C:728:LYS:HG3   | 1.83                     | 0.58              |
| 2:G:1198:SER:HB3  | 2:G:1205:LEU:HD21 | 1.85                     | 0.58              |
| 2:G:1279:PHE:HB2  | 2:G:1340:PRO:HG3  | 1.85                     | 0.58              |
| 2:G:1378:ILE:HD11 | 2:G:1381:VAL:HG21 | 1.85                     | 0.58              |
| 2:H:273:HIS:HB3   | 2:H:512:LEU:HD22  | 1.85                     | 0.58              |
| 2:I:455:ILE:HG13  | 2:I:469:ARG:HD3   | 1.85                     | 0.58              |
| 1:A:421:ILE:HG12  | 1:A:469:VAL:HG21  | 1.85                     | 0.58              |
| 1:A:531:LEU:HD21  | 1:A:629:THR:HG22  | 1.85                     | 0.58              |
| 1:B:1392:LEU:HD22 | 1:B:1396:MET:HG3  | 1.84                     | 0.58              |
| 1:C:80:CYS:SG     | 1:C:82:SER:HB3    | 2.42                     | 0.58              |
| 1:C:749:ILE:CD1   | 1:C:805:CYS:HB3   | 2.32                     | 0.58              |
| 1:C:1657:HIS:ND1  | 1:C:1658:PRO:HD2  | 2.17                     | 0.58              |
| 2:G:1149:TRP:CD1  | 2:G:1213:LEU:HD12 | 2.38                     | 0.58              |
| 2:H:665:LEU:O     | 2:H:669:LEU:HB2   | 2.04                     | 0.58              |
| 2:H:1010:PRO:O    | 2:H:1011:MET:HB2  | 2.03                     | 0.58              |
| 2:I:499:THR:CB    | 2:I:500:HIS:CD2   | 2.79                     | 0.58              |
| 2:I:907:VAL:O     | 2:I:910:GLN:HB3   | 2.03                     | 0.58              |
| 2:I:1822:MET:CE   | 2:I:1996:ILE:HG12 | 2.34                     | 0.58              |
| 1:A:1463:VAL:HG11 | 1:A:1877:GLN:HE22 | 1.68                     | 0.58              |
| 1:B:37:LYS:HB2    | 1:B:65:TYR:HE1    | 1.69                     | 0.58              |
| 2:G:28:PHE:CZ     | 2:H:7:ARG:NE      | 2.70                     | 0.58              |
| 2:G:166:THR:HG22  | 2:G:168:ASP:N     | 2.19                     | 0.58              |
| 2:I:601:THR:CG2   | 2:I:618:GLU:O     | 2.39                     | 0.58              |
| 2:I:1227:ARG:CG   | 2:I:1227:ARG:NH1  | 2.55                     | 0.58              |
| 2:I:1374:THR:HG23 | 2:I:1396:LEU:HD12 | 1.83                     | 0.58              |
| 1:A:260:ARG:HH12  | 1:A:300:VAL:HG21  | 1.68                     | 0.58              |
| 1:A:444:ASN:HB3   | 1:A:446:ALA:H     | 1.66                     | 0.58              |
| 1:B:409:ALA:HB2   | 1:B:442:ARG:HD2   | 1.86                     | 0.58              |
| 1:C:24:SER:O      | 2:I:1977:HIS:CD2  | 2.54                     | 0.58              |
| 1:C:1233:GLU:OE2  | 1:C:1680:ARG:NH2  | 2.36                     | 0.58              |
| 2:H:1103:PHE:O    | 2:H:1247:GLY:HA3  | 2.03                     | 0.58              |
| 2:H:1360:ILE:HG23 | 2:H:1403:VAL:O    | 2.04                     | 0.58              |
| 2:I:127:ILE:O     | 2:I:131:ILE:HG13  | 2.03                     | 0.58              |
| 2:I:736:ARG:NH1   | 2:I:769:SER:O     | 2.36                     | 0.58              |
| 1:B:436:ALA:O     | 1:B:440:MET:HG3   | 2.04                     | 0.58              |
| 1:C:232:LEU:HD22  | 1:C:269:LEU:HA    | 1.83                     | 0.58              |
| 1:C:1009:LEU:HA   | 1:C:1445:MET:HE2  | 1.85                     | 0.58              |
| 2:G:807:ILE:CG2   | 2:G:1066:ILE:HA   | 2.34                     | 0.58              |
| 2:G:1597:ALA:HB1  | 2:G:1638:ILE:CD1  | 2.33                     | 0.58              |
| 2:G:1823:SER:OG   | 2:G:1825:GLU:HG2  | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:271:THR:OG1   | 2:H:460:TYR:HB2   | 2.03                     | 0.58              |
| 2:H:499:THR:CB    | 2:H:500:HIS:CD2   | 2.81                     | 0.58              |
| 2:H:762:ASN:H     | 2:H:762:ASN:ND2   | 1.85                     | 0.58              |
| 2:I:1269:LEU:O    | 2:I:1560:LEU:HD23 | 2.03                     | 0.58              |
| 1:A:986:ALA:HB2   | 1:A:1047:LEU:HD13 | 1.85                     | 0.58              |
| 1:B:1461:ASP:O    | 1:B:1465:ASN:HB2  | 2.03                     | 0.58              |
| 1:C:232:LEU:HD13  | 1:C:272:GLU:HB2   | 1.85                     | 0.58              |
| 1:C:340:ARG:HH12  | 1:C:344:GLN:CG    | 2.13                     | 0.58              |
| 1:C:421:ILE:HG13  | 1:C:469:VAL:HG21  | 1.84                     | 0.58              |
| 1:C:1665:ILE:HD11 | 1:C:1669:ARG:HG2  | 1.85                     | 0.58              |
| 2:G:131:ILE:CG2   | 2:G:182:VAL:HG12  | 2.33                     | 0.58              |
| 2:G:907:VAL:O     | 2:G:910:GLN:HB3   | 2.02                     | 0.58              |
| 2:G:1223:MET:HE3  | 2:G:1238:LEU:HD12 | 1.85                     | 0.58              |
| 2:I:707:PRO:HG2   | 2:I:730:LEU:HD13  | 1.85                     | 0.58              |
| 1:A:1600:LEU:HD13 | 1:A:1657:HIS:HA   | 1.85                     | 0.58              |
| 1:B:29:ILE:HG13   | 2:H:1891:TYR:C    | 2.23                     | 0.58              |
| 1:C:419:GLU:HG2   | 1:C:424:VAL:HB    | 1.86                     | 0.58              |
| 1:C:968:VAL:O     | 2:I:1512:HIS:HB2  | 2.04                     | 0.58              |
| 2:G:260:PRO:HD3   | 2:G:289:TRP:CE2   | 2.38                     | 0.58              |
| 2:G:565:TYR:OH    | 2:G:758:ARG:HD2   | 2.02                     | 0.58              |
| 2:G:674:TYR:HB3   | 2:G:676:ILE:HG22  | 1.85                     | 0.58              |
| 2:G:1159:ILE:CG1  | 2:G:1169:PRO:HD3  | 2.33                     | 0.58              |
| 2:H:490:TRP:CH2   | 2:H:512:LEU:HD21  | 2.39                     | 0.58              |
| 2:H:543:PHE:CB    | 2:H:545:GLN:HE22  | 2.17                     | 0.58              |
| 2:I:942:THR:HG21  | 2:I:1012:GLN:HA   | 1.85                     | 0.58              |
| 2:I:1719:ILE:O    | 2:I:1761:SER:HB2  | 2.01                     | 0.58              |
| 1:B:198:PRO:CG    | 1:B:209:LEU:HD21  | 2.26                     | 0.58              |
| 1:B:286:PHE:O     | 1:B:290:MET:HG2   | 2.03                     | 0.58              |
| 1:C:1020:VAL:HG13 | 1:C:1400:ILE:HG23 | 1.84                     | 0.58              |
| 2:G:638:VAL:HA    | 2:G:641:ILE:HG22  | 1.86                     | 0.58              |
| 2:H:163:GLN:CG    | 2:H:423:VAL:HG12  | 2.32                     | 0.58              |
| 2:I:1822:MET:HE2  | 2:I:1996:ILE:HG12 | 1.86                     | 0.58              |
| 1:A:20:TYR:CZ     | 2:G:2035:SER:HB2  | 2.39                     | 0.58              |
| 1:A:198:PRO:CG    | 1:A:209:LEU:HD21  | 2.28                     | 0.58              |
| 1:A:987:ASN:HD22  | 2:G:957:ARG:HD2   | 1.68                     | 0.58              |
| 1:B:232:LEU:HD22  | 1:B:269:LEU:HA    | 1.85                     | 0.58              |
| 1:B:749:ILE:CD1   | 1:B:805:CYS:HB3   | 2.33                     | 0.58              |
| 1:B:1473:GLU:O    | 1:B:1478:PRO:HD3  | 2.04                     | 0.58              |
| 1:B:1662:TYR:O    | 1:B:1665:ILE:HG22 | 2.04                     | 0.58              |
| 1:C:27:ARG:HH21   | 2:I:2015:THR:HA   | 1.68                     | 0.58              |
| 1:C:1247:SER:HB2  | 1:C:1332:TYR:HE2  | 1.68                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:232:LEU:O     | 2:G:232:LEU:HD23  | 2.03                     | 0.58              |
| 2:G:273:HIS:HB3   | 2:G:512:LEU:HD22  | 1.86                     | 0.58              |
| 2:G:611:THR:CG2   | 2:G:641:ILE:HG13  | 2.34                     | 0.58              |
| 2:G:817:ALA:O     | 2:G:821:ILE:HG13  | 2.04                     | 0.58              |
| 2:G:860:ARG:HB3   | 2:G:898:ASP:HB3   | 1.85                     | 0.58              |
| 2:G:1359:MET:HE3  | 2:G:1359:MET:HA   | 1.86                     | 0.58              |
| 2:H:1210:ILE:HB   | 2:H:1222:GLU:HB3  | 1.85                     | 0.58              |
| 1:A:329:GLU:O     | 1:A:333:LYS:HG3   | 2.04                     | 0.57              |
| 1:A:1062:TYR:CD2  | 1:A:1693:ILE:HG23 | 2.39                     | 0.57              |
| 1:A:1189:ILE:HD12 | 1:A:1380:GLN:HG3  | 1.86                     | 0.57              |
| 1:A:1419:PRO:HB3  | 1:A:1646:PHE:CZ   | 2.39                     | 0.57              |
| 1:B:419:GLU:HG2   | 1:B:424:VAL:HB    | 1.86                     | 0.57              |
| 1:B:1247:SER:HB2  | 1:B:1332:TYR:HE2  | 1.69                     | 0.57              |
| 1:C:433:VAL:O     | 1:C:437:ILE:HG13  | 2.04                     | 0.57              |
| 1:C:1219:VAL:CA   | 1:C:1384:ILE:HD11 | 2.27                     | 0.57              |
| 2:G:7:ARG:NH1     | 2:G:24:THR:HA     | 2.19                     | 0.57              |
| 2:G:56:THR:HG23   | 2:G:59:GLU:CG     | 2.29                     | 0.57              |
| 2:G:146:PHE:HA    | 2:G:149:VAL:HG12  | 1.86                     | 0.57              |
| 2:G:376:ASN:HD22  | 2:G:377:LEU:N     | 2.02                     | 0.57              |
| 2:I:239:PRO:HG3   | 2:I:304:PHE:HA    | 1.86                     | 0.57              |
| 2:I:376:ASN:HD22  | 2:I:377:LEU:N     | 2.02                     | 0.57              |
| 1:A:11:HIS:O      | 1:A:15:THR:HG22   | 2.04                     | 0.57              |
| 1:A:1056:ILE:CD1  | 1:A:1193:TRP:HD1  | 2.17                     | 0.57              |
| 1:A:1203:ASP:HB3  | 1:B:179:LYS:HZ1   | 1.68                     | 0.57              |
| 1:A:1247:SER:HB2  | 1:A:1332:TYR:HE2  | 1.66                     | 0.57              |
| 1:A:1464:GLU:CD   | 1:A:1773:VAL:HG12 | 2.23                     | 0.57              |
| 1:B:232:LEU:HD13  | 1:B:272:GLU:HB2   | 1.87                     | 0.57              |
| 1:B:1496:GLU:O    | 1:B:1500:GLN:HG3  | 2.03                     | 0.57              |
| 1:C:1052:GLU:O    | 1:C:1056:ILE:HG23 | 2.04                     | 0.57              |
| 1:C:1431:GLU:CD   | 1:C:1433:HIS:HE1  | 2.08                     | 0.57              |
| 2:G:658:MET:HA    | 2:G:661:TRP:NE1   | 2.19                     | 0.57              |
| 2:G:1149:TRP:CD1  | 2:G:1213:LEU:CD1  | 2.87                     | 0.57              |
| 2:H:722:ALA:HB1   | 2:H:723:HIS:CE1   | 2.38                     | 0.57              |
| 2:H:1331:TRP:CE2  | 2:H:1335:ILE:HG13 | 2.38                     | 0.57              |
| 2:I:726:PHE:O     | 2:I:762:ASN:HB2   | 2.04                     | 0.57              |
| 1:A:1538:VAL:HB   | 1:A:1639:VAL:HG22 | 1.86                     | 0.57              |
| 1:B:50:SER:HB2    | 1:B:51:PRO:HD3    | 1.86                     | 0.57              |
| 1:B:1022:THR:HG22 | 1:B:1226:SER:HB2  | 1.87                     | 0.57              |
| 1:B:1125:VAL:HG21 | 1:B:1175:ILE:HD12 | 1.86                     | 0.57              |
| 1:C:1056:ILE:CD1  | 1:C:1193:TRP:HD1  | 2.16                     | 0.57              |
| 2:G:826:GLY:O     | 2:G:827:VAL:HG23  | 2.03                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:942:THR:HG21  | 2:G:1012:GLN:HA   | 1.86                     | 0.57              |
| 2:H:124:LYS:HG2   | 2:H:179:THR:HA    | 1.86                     | 0.57              |
| 1:B:413:LEU:HD13  | 1:B:451:MET:HG2   | 1.85                     | 0.57              |
| 1:B:705:VAL:HG23  | 1:B:732:LEU:HD21  | 1.85                     | 0.57              |
| 1:C:183:GLN:HE21  | 1:C:202:GLU:HG2   | 1.69                     | 0.57              |
| 2:G:163:GLN:CG    | 2:G:423:VAL:HG12  | 2.33                     | 0.57              |
| 2:H:601:THR:HG22  | 2:H:620:ALA:H     | 1.69                     | 0.57              |
| 2:H:732:TRP:CG    | 2:H:750:MET:HE3   | 2.39                     | 0.57              |
| 2:H:907:VAL:O     | 2:H:910:GLN:HB3   | 2.03                     | 0.57              |
| 2:H:1086:LEU:HD12 | 2:H:1090:TYR:CB   | 2.34                     | 0.57              |
| 2:H:1231:GLY:O    | 2:H:1233:PRO:HD3  | 2.04                     | 0.57              |
| 2:H:1567:ARG:HH12 | 2:H:1568:HIS:HB3  | 1.70                     | 0.57              |
| 2:H:1908:ASP:HB2  | 2:H:1958:LEU:HD21 | 1.86                     | 0.57              |
| 2:I:145:LEU:O     | 2:I:149:VAL:HG12  | 2.03                     | 0.57              |
| 2:I:654:VAL:HG23  | 2:I:683:ALA:HB1   | 1.87                     | 0.57              |
| 1:A:232:LEU:HD13  | 1:A:272:GLU:HB2   | 1.85                     | 0.57              |
| 1:C:198:PRO:CG    | 1:C:209:LEU:HD21  | 2.28                     | 0.57              |
| 1:C:771:PHE:CD1   | 1:C:825:PRO:HG3   | 2.40                     | 0.57              |
| 1:C:1189:ILE:HD12 | 1:C:1380:GLN:HG3  | 1.86                     | 0.57              |
| 1:C:1600:LEU:HD13 | 1:C:1657:HIS:HA   | 1.87                     | 0.57              |
| 2:G:562:LEU:O     | 2:G:566:HIS:HB2   | 2.05                     | 0.57              |
| 2:G:932:ILE:CD1   | 2:G:1042:ALA:HB2  | 2.24                     | 0.57              |
| 2:G:1010:PRO:O    | 2:G:1011:MET:HB2  | 2.05                     | 0.57              |
| 2:H:89:THR:O      | 2:H:93:ASN:HB2    | 2.04                     | 0.57              |
| 2:H:736:ARG:NH1   | 2:H:769:SER:O     | 2.36                     | 0.57              |
| 2:I:1130:THR:H    | 2:I:1133:THR:HG23 | 1.69                     | 0.57              |
| 1:A:604:ALA:HB3   | 1:A:612:GLU:HG2   | 1.86                     | 0.57              |
| 1:A:828:PRO:HG3   | 1:A:868:ILE:HG22  | 1.86                     | 0.57              |
| 1:B:980:VAL:HG21  | 2:H:952:ARG:HH21  | 1.70                     | 0.57              |
| 1:C:251:GLN:HA    | 1:C:256:LEU:H     | 1.69                     | 0.57              |
| 1:C:1184:LEU:HB2  | 1:C:1352:THR:HG21 | 1.85                     | 0.57              |
| 1:C:1473:GLU:O    | 1:C:1478:PRO:HD3  | 2.05                     | 0.57              |
| 2:G:517:HIS:C     | 2:G:517:HIS:CD2   | 2.78                     | 0.57              |
| 2:G:1314:ARG:CG   | 2:G:1314:ARG:NH1  | 2.61                     | 0.57              |
| 2:G:1954:LYS:HD3  | 2:G:1958:LEU:HD13 | 1.86                     | 0.57              |
| 2:H:732:TRP:CG    | 2:H:750:MET:HE1   | 2.40                     | 0.57              |
| 2:H:1782:THR:HG22 | 2:H:1827:LEU:HD21 | 1.86                     | 0.57              |
| 2:I:813:THR:HB    | 2:I:818:LYS:HE3   | 1.85                     | 0.57              |
| 2:I:2038:ILE:O    | 2:I:2042:ILE:HG12 | 2.04                     | 0.57              |
| 1:A:655:LEU:CD2   | 1:A:916:LEU:HD11  | 2.35                     | 0.57              |
| 1:A:988:ILE:HA    | 1:A:1048:GLU:HG2  | 1.84                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:741:HIS:HE1   | 2:G:845:THR:HG22  | 1.58                     | 0.57              |
| 2:G:1775:GLN:HG2  | 2:G:1836:MET:SD   | 2.44                     | 0.57              |
| 2:G:1778:GLN:HB3  | 2:G:1831:VAL:HG13 | 1.85                     | 0.57              |
| 2:G:1890:ASN:HB2  | 2:G:1899:VAL:HB   | 1.86                     | 0.57              |
| 2:H:61:VAL:HG21   | 2:H:95:TYR:HE1    | 1.69                     | 0.57              |
| 2:H:166:THR:HG22  | 2:H:168:ASP:N     | 2.19                     | 0.57              |
| 2:H:561:TRP:CD1   | 2:H:754:TYR:HE2   | 2.22                     | 0.57              |
| 2:I:665:LEU:O     | 2:I:669:LEU:HB2   | 2.05                     | 0.57              |
| 1:A:680:ILE:HG13  | 1:A:769:ILE:HB    | 1.87                     | 0.57              |
| 1:A:1285:ALA:O    | 1:A:1289:MET:HG3  | 2.04                     | 0.57              |
| 1:A:1474:ALA:O    | 1:A:1478:PRO:HD2  | 2.04                     | 0.57              |
| 1:B:140:ILE:HD13  | 1:B:255:GLY:O     | 2.05                     | 0.57              |
| 1:B:440:MET:HE3   | 1:B:483:VAL:HG21  | 1.87                     | 0.57              |
| 2:G:703:LEU:HD21  | 2:G:705:LEU:HD21  | 1.86                     | 0.57              |
| 2:G:1266:TYR:CG   | 2:G:1347:LEU:HD23 | 2.40                     | 0.57              |
| 2:H:732:TRP:CD2   | 2:H:750:MET:CE    | 2.87                     | 0.57              |
| 2:H:1100:VAL:HG21 | 2:H:1147:ILE:CD1  | 2.34                     | 0.57              |
| 2:H:1123:ASP:OD1  | 2:H:1123:ASP:N    | 2.36                     | 0.57              |
| 2:H:1575:LEU:HD13 | 2:H:1579:ILE:HD12 | 1.85                     | 0.57              |
| 2:H:2029:VAL:O    | 2:H:2033:THR:HG22 | 2.05                     | 0.57              |
| 2:I:273:HIS:HB3   | 2:I:512:LEU:HD22  | 1.87                     | 0.57              |
| 2:I:353:VAL:HG23  | 2:I:357:ASN:HD22  | 1.69                     | 0.57              |
| 2:I:1292:ILE:O    | 2:I:1368:VAL:O    | 2.23                     | 0.57              |
| 1:A:80:CYS:SG     | 1:A:82:SER:HB3    | 2.45                     | 0.57              |
| 1:A:415:SER:O     | 1:A:419:GLU:HB2   | 2.05                     | 0.57              |
| 1:C:1474:ALA:O    | 1:C:1478:PRO:HD2  | 2.04                     | 0.57              |
| 2:G:89:THR:O      | 2:G:93:ASN:HB2    | 2.05                     | 0.57              |
| 2:G:455:ILE:HG13  | 2:G:469:ARG:HD3   | 1.86                     | 0.57              |
| 2:G:463:PHE:HD1   | 2:G:486:LEU:HD13  | 1.70                     | 0.57              |
| 2:G:584:SER:HA    | 2:G:587:ILE:HG23  | 1.87                     | 0.57              |
| 2:G:667:LYS:HB2   | 2:G:698:LEU:HD23  | 1.85                     | 0.57              |
| 2:G:1168:ASN:ND2  | 2:G:1171:ARG:HB2  | 2.20                     | 0.57              |
| 2:G:1547:PRO:HD3  | 2:G:1584:PHE:CE2  | 2.40                     | 0.57              |
| 2:H:127:ILE:O     | 2:H:131:ILE:HG13  | 2.04                     | 0.57              |
| 2:H:777:THR:CG2   | 2:H:1081:HIS:CE1  | 2.88                     | 0.57              |
| 2:H:1589:VAL:HG11 | 2:H:1640:PHE:CE1  | 2.39                     | 0.57              |
| 2:I:463:PHE:HD1   | 2:I:486:LEU:HD13  | 1.70                     | 0.57              |
| 2:I:777:THR:CG2   | 2:I:1081:HIS:CE1  | 2.88                     | 0.57              |
| 2:I:807:ILE:CG2   | 2:I:1066:ILE:HA   | 2.35                     | 0.57              |
| 2:I:1199:GLU:OE2  | 2:I:1567:ARG:NH1  | 2.37                     | 0.57              |
| 1:B:529:MET:HE3   | 1:B:529:MET:CA    | 2.31                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:742:LYS:HD3   | 1:B:746:GLU:OE2   | 2.05                     | 0.57              |
| 1:B:1431:GLU:HB3  | 1:B:1520:ALA:HB2  | 1.86                     | 0.57              |
| 1:C:341:GLN:O     | 1:C:345:VAL:HG12  | 2.05                     | 0.57              |
| 2:G:1675:GLY:O    | 2:G:1678:MET:HB2  | 2.05                     | 0.57              |
| 2:H:565:TYR:OH    | 2:H:758:ARG:HD2   | 2.04                     | 0.57              |
| 2:H:1266:TYR:CG   | 2:H:1347:LEU:HD23 | 2.40                     | 0.57              |
| 2:H:1871:LEU:HD22 | 2:H:1888:ILE:HD11 | 1.85                     | 0.57              |
| 2:H:1976:PHE:HA   | 2:H:1981:LEU:HD22 | 1.86                     | 0.57              |
| 2:I:607:VAL:HA    | 2:I:617:ILE:HD13  | 1.86                     | 0.57              |
| 2:I:1210:ILE:HB   | 2:I:1222:GLU:HB3  | 1.85                     | 0.57              |
| 2:I:1231:GLY:O    | 2:I:1233:PRO:HD3  | 2.05                     | 0.57              |
| 2:I:2029:VAL:O    | 2:I:2033:THR:HG22 | 2.05                     | 0.57              |
| 1:A:263:GLY:O     | 1:A:267:VAL:HG23  | 2.05                     | 0.56              |
| 1:A:742:LYS:HD3   | 1:A:746:GLU:OE2   | 2.05                     | 0.56              |
| 1:B:152:HIS:HD2   | 1:B:163:LEU:HB2   | 1.66                     | 0.56              |
| 1:B:251:GLN:HA    | 1:B:256:LEU:H     | 1.70                     | 0.56              |
| 1:B:964:GLU:HG2   | 2:H:1515:PRO:HB3  | 1.86                     | 0.56              |
| 1:B:1524:GLY:O    | 1:B:1528:THR:HG23 | 2.05                     | 0.56              |
| 1:C:893:VAL:HG11  | 1:C:930:LEU:HD23  | 1.87                     | 0.56              |
| 2:G:653:TYR:CD1   | 2:G:659:LEU:HD21  | 2.39                     | 0.56              |
| 2:G:1868:GLN:HG3  | 2:G:1898:TYR:OH   | 2.04                     | 0.56              |
| 2:H:56:THR:HG23   | 2:H:59:GLU:CG     | 2.32                     | 0.56              |
| 2:H:517:HIS:C     | 2:H:517:HIS:CD2   | 2.78                     | 0.56              |
| 2:H:653:TYR:CD1   | 2:H:659:LEU:HD21  | 2.40                     | 0.56              |
| 2:H:740:HIS:CE1   | 2:H:852:GLU:OE1   | 2.58                     | 0.56              |
| 2:I:120:LYS:O     | 2:I:124:LYS:HG3   | 2.05                     | 0.56              |
| 2:I:2030:TYR:CE1  | 2:I:2034:GLY:HA2  | 2.39                     | 0.56              |
| 1:A:419:GLU:HG2   | 1:A:424:VAL:HB    | 1.86                     | 0.56              |
| 1:C:20:TYR:HE1    | 2:I:2035:SER:HB2  | 1.69                     | 0.56              |
| 1:C:626:VAL:HG23  | 1:C:664:GLU:OE2   | 2.05                     | 0.56              |
| 1:C:1326:ILE:HG12 | 1:C:1388:MET:HG3  | 1.86                     | 0.56              |
| 1:C:1524:GLY:O    | 1:C:1528:THR:HG23 | 2.05                     | 0.56              |
| 1:C:1538:VAL:HB   | 1:C:1639:VAL:HG22 | 1.86                     | 0.56              |
| 2:G:28:PHE:HZ     | 2:H:7:ARG:NE      | 2.02                     | 0.56              |
| 2:G:654:VAL:HG23  | 2:G:683:ALA:HB1   | 1.87                     | 0.56              |
| 2:G:1567:ARG:HG3  | 2:G:1568:HIS:N    | 2.20                     | 0.56              |
| 2:G:1804:PHE:CZ   | 2:G:2010:TYR:HB2  | 2.40                     | 0.56              |
| 2:H:638:VAL:HA    | 2:H:641:ILE:HG22  | 1.86                     | 0.56              |
| 2:H:839:PRO:HA    | 2:H:844:VAL:HG13  | 1.86                     | 0.56              |
| 2:H:926:LEU:HD13  | 2:H:947:THR:HG22  | 1.86                     | 0.56              |
| 2:H:1352:HIS:HE1  | 2:H:1583:MET:HE1  | 1.69                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:89:THR:O      | 2:I:93:ASN:HB2    | 2.05                     | 0.56              |
| 2:I:197:GLU:OE1   | 2:I:197:GLU:HA    | 2.05                     | 0.56              |
| 2:I:281:VAL:HG23  | 2:I:459:VAL:HG11  | 1.87                     | 0.56              |
| 2:I:741:HIS:HB3   | 2:I:853:PRO:HB2   | 1.86                     | 0.56              |
| 2:I:1223:MET:HE3  | 2:I:1238:LEU:HD12 | 1.87                     | 0.56              |
| 1:A:1014:ASP:N    | 1:A:1510:ASN:HD21 | 1.92                     | 0.56              |
| 1:B:152:HIS:CE1   | 1:B:168:MET:HG3   | 2.40                     | 0.56              |
| 2:G:663:ILE:HG13  | 2:G:694:TYR:HE1   | 1.70                     | 0.56              |
| 2:G:1086:LEU:HD12 | 2:G:1090:TYR:CB   | 2.35                     | 0.56              |
| 2:G:1194:VAL:O    | 2:G:1194:VAL:HG12 | 2.05                     | 0.56              |
| 2:G:1989:LYS:O    | 2:G:1993:LYS:HG3  | 2.05                     | 0.56              |
| 2:H:522:GLY:HA3   | 2:H:561:TRP:CZ3   | 2.40                     | 0.56              |
| 2:H:561:TRP:O     | 2:H:562:LEU:C     | 2.42                     | 0.56              |
| 2:H:702:TYR:CB    | 2:H:727:PRO:HB2   | 2.36                     | 0.56              |
| 2:I:443:LEU:HD22  | 2:I:448:VAL:HG11  | 1.87                     | 0.56              |
| 2:I:481:ASP:OD2   | 2:I:485:ARG:NH1   | 2.38                     | 0.56              |
| 2:I:490:TRP:CH2   | 2:I:512:LEU:HD21  | 2.40                     | 0.56              |
| 2:I:543:PHE:CB    | 2:I:545:GLN:HE22  | 2.17                     | 0.56              |
| 2:I:1149:TRP:CD1  | 2:I:1213:LEU:CD1  | 2.88                     | 0.56              |
| 1:B:488:PRO:HG3   | 1:B:728:LYS:HG3   | 1.87                     | 0.56              |
| 1:C:635:ILE:HG22  | 1:C:651:TYR:CD1   | 2.41                     | 0.56              |
| 2:G:813:THR:HB    | 2:G:818:LYS:HE3   | 1.87                     | 0.56              |
| 2:H:376:ASN:HD22  | 2:H:377:LEU:N     | 2.03                     | 0.56              |
| 2:H:835:THR:HG22  | 2:H:844:VAL:C     | 2.26                     | 0.56              |
| 2:H:1223:MET:CE   | 2:H:1238:LEU:HD12 | 2.35                     | 0.56              |
| 2:H:1834:ARG:NH1  | 2:H:1834:ARG:CG   | 2.60                     | 0.56              |
| 2:I:1722:GLY:N    | 2:I:1726:GLY:HA3  | 2.21                     | 0.56              |
| 2:I:1804:PHE:CZ   | 2:I:2010:TYR:HB2  | 2.40                     | 0.56              |
| 1:A:21:GLN:O      | 2:G:1977:HIS:CD2  | 2.59                     | 0.56              |
| 1:A:1009:LEU:HA   | 1:A:1445:MET:HE2  | 1.87                     | 0.56              |
| 1:B:411:GLN:HE22  | 1:B:1628:SER:H    | 1.52                     | 0.56              |
| 1:C:152:HIS:HD2   | 1:C:163:LEU:HB2   | 1.63                     | 0.56              |
| 2:G:543:PHE:CB    | 2:G:545:GLN:HE22  | 2.17                     | 0.56              |
| 2:G:758:ARG:NH2   | 2:G:797:ASP:OD1   | 2.33                     | 0.56              |
| 2:G:1834:ARG:HH11 | 2:G:1834:ARG:CG   | 2.03                     | 0.56              |
| 2:H:120:LYS:O     | 2:H:124:LYS:HG3   | 2.06                     | 0.56              |
| 2:H:606:PHE:HZ    | 2:H:805:VAL:HG11  | 1.68                     | 0.56              |
| 1:A:221:LEU:O     | 1:A:225:SER:HB3   | 2.05                     | 0.56              |
| 1:A:1057:MET:SD   | 1:A:1097:ILE:HG23 | 2.45                     | 0.56              |
| 1:B:1419:PRO:HB3  | 1:B:1646:PHE:CZ   | 2.40                     | 0.56              |
| 1:C:741:SER:HB3   | 1:C:744:ASP:HB2   | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1022:THR:HG22 | 1:C:1226:SER:HB2  | 1.87                     | 0.56              |
| 2:H:1920:GLN:HG2  | 2:H:1922:ILE:HD11 | 1.87                     | 0.56              |
| 1:B:1009:LEU:HG   | 1:B:1664:ALA:HB2  | 1.87                     | 0.56              |
| 1:C:695:GLY:HA3   | 1:C:906:LEU:HD11  | 1.88                     | 0.56              |
| 2:G:634:ILE:HD11  | 2:G:649:ILE:CD1   | 2.34                     | 0.56              |
| 2:G:1722:GLY:N    | 2:G:1726:GLY:HA3  | 2.21                     | 0.56              |
| 2:H:443:LEU:HD22  | 2:H:448:VAL:HG11  | 1.86                     | 0.56              |
| 2:H:463:PHE:HD1   | 2:H:486:LEU:HD13  | 1.71                     | 0.56              |
| 2:H:1890:ASN:HB2  | 2:H:1899:VAL:HB   | 1.88                     | 0.56              |
| 2:I:835:THR:HG23  | 2:I:843:ILE:O     | 2.05                     | 0.56              |
| 2:I:1567:ARG:HH12 | 2:I:1568:HIS:HB3  | 1.71                     | 0.56              |
| 1:A:152:HIS:CE1   | 1:A:168:MET:HG3   | 2.41                     | 0.56              |
| 1:A:251:GLN:HA    | 1:A:256:LEU:H     | 1.68                     | 0.56              |
| 1:A:1036:ARG:NH1  | 1:A:1040:GLU:OE1  | 2.39                     | 0.56              |
| 1:B:644:THR:HG22  | 1:B:648:ASP:O     | 2.06                     | 0.56              |
| 1:B:1138:LYS:HG3  | 1:B:1163:TYR:CE1  | 2.41                     | 0.56              |
| 1:B:1492:GLU:O    | 1:B:1496:GLU:HG3  | 2.06                     | 0.56              |
| 2:G:577:ILE:HD13  | 2:G:1097:ILE:CD1  | 2.35                     | 0.56              |
| 2:G:589:ARG:HB3   | 2:G:590:PRO:HD2   | 1.87                     | 0.56              |
| 2:G:599:PRO:HD2   | 4:G:3051:FMN:H6   | 1.88                     | 0.56              |
| 2:H:607:VAL:HA    | 2:H:617:ILE:HD13  | 1.88                     | 0.56              |
| 2:H:1868:GLN:HG3  | 2:H:1898:TYR:OH   | 2.05                     | 0.56              |
| 2:I:601:THR:HG22  | 2:I:620:ALA:H     | 1.71                     | 0.56              |
| 2:I:702:TYR:CB    | 2:I:727:PRO:HB2   | 2.36                     | 0.56              |
| 2:I:732:TRP:CG    | 2:I:750:MET:HE3   | 2.39                     | 0.56              |
| 2:I:774:ALA:HB1   | 2:I:1081:HIS:CD2  | 2.33                     | 0.56              |
| 2:I:871:THR:HB    | 2:I:872:ILE:HD12  | 1.88                     | 0.56              |
| 1:B:529:MET:HG2   | 1:B:638:LEU:CD1   | 2.35                     | 0.56              |
| 1:C:329:GLU:O     | 1:C:333:LYS:HG3   | 2.06                     | 0.56              |
| 1:C:531:LEU:HD21  | 1:C:629:THR:HG22  | 1.88                     | 0.56              |
| 1:C:881:ASN:HA    | 1:C:944:ARG:HH21  | 1.70                     | 0.56              |
| 1:C:1259:GLY:HA2  | 1:C:1263:ASP:HB2  | 1.87                     | 0.56              |
| 2:G:702:TYR:CB    | 2:G:727:PRO:HB2   | 2.35                     | 0.56              |
| 2:G:1130:THR:H    | 2:G:1133:THR:HG23 | 1.70                     | 0.56              |
| 2:G:1567:ARG:HH12 | 2:G:1568:HIS:HB3  | 1.71                     | 0.56              |
| 2:H:553:ASN:O     | 2:H:556:LYS:HE3   | 2.06                     | 0.56              |
| 2:H:1100:VAL:HG21 | 2:H:1147:ILE:HD13 | 1.88                     | 0.56              |
| 2:H:1194:VAL:O    | 2:H:1194:VAL:HG12 | 2.05                     | 0.56              |
| 2:H:1778:GLN:HB3  | 2:H:1831:VAL:HG13 | 1.88                     | 0.56              |
| 2:H:1989:LYS:O    | 2:H:1993:LYS:HG3  | 2.06                     | 0.56              |
| 2:I:1931:LEU:HD22 | 2:I:1935:GLU:HG2  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1052:GLU:O    | 1:A:1056:ILE:HG23 | 2.06                     | 0.56              |
| 1:A:1498:GLU:CB   | 1:A:1876:LEU:HD13 | 1.83                     | 0.56              |
| 1:A:1665:ILE:CG1  | 1:A:1669:ARG:HD3  | 2.36                     | 0.56              |
| 1:C:1419:PRO:HB3  | 1:C:1646:PHE:CZ   | 2.41                     | 0.56              |
| 1:C:1749:THR:CA   | 1:C:1874:ASP:HB3  | 2.32                     | 0.56              |
| 2:G:120:LYS:O     | 2:G:124:LYS:HG3   | 2.05                     | 0.56              |
| 2:G:1308:CYS:HB3  | 2:G:1311:PHE:CD2  | 2.41                     | 0.56              |
| 2:G:1874:VAL:O    | 2:G:1878:VAL:HG12 | 2.05                     | 0.56              |
| 2:H:1308:CYS:HB3  | 2:H:1311:PHE:CD2  | 2.41                     | 0.56              |
| 2:H:1328:VAL:HG23 | 2:H:1557:SER:HA   | 1.88                     | 0.56              |
| 2:I:577:ILE:HD13  | 2:I:1097:ILE:CD1  | 2.36                     | 0.56              |
| 2:I:732:TRP:CD1   | 2:I:750:MET:HE3   | 2.40                     | 0.56              |
| 2:I:826:GLY:HA2   | 2:I:1060:ALA:HB3  | 1.88                     | 0.56              |
| 2:I:1589:VAL:HG11 | 2:I:1640:PHE:CE1  | 2.41                     | 0.56              |
| 1:A:295:ALA:HB2   | 1:A:302:LEU:HD11  | 1.87                     | 0.55              |
| 1:A:1524:GLY:HA2  | 1:A:1527:ALA:HB3  | 1.89                     | 0.55              |
| 1:B:11:HIS:O      | 1:B:15:THR:HG22   | 2.06                     | 0.55              |
| 1:B:1233:GLU:OE2  | 1:B:1680:ARG:NH2  | 2.40                     | 0.55              |
| 1:C:29:ILE:HG13   | 2:I:1891:TYR:O    | 2.06                     | 0.55              |
| 1:C:1496:GLU:O    | 1:C:1500:GLN:HG3  | 2.06                     | 0.55              |
| 2:G:732:TRP:CD2   | 2:G:750:MET:HE1   | 2.41                     | 0.55              |
| 2:G:1475:LYS:HG3  | 2:G:1481:SER:HB2  | 1.88                     | 0.55              |
| 2:G:1561:ASN:OD1  | 2:G:1563:ILE:HB   | 2.05                     | 0.55              |
| 2:H:16:LEU:HG     | 2:H:48:PHE:CZ     | 2.40                     | 0.55              |
| 2:H:239:PRO:HG3   | 2:H:304:PHE:HA    | 1.88                     | 0.55              |
| 2:H:1493:LEU:HD11 | 2:H:1499:VAL:CG2  | 2.36                     | 0.55              |
| 2:I:7:ARG:NH1     | 2:I:24:THR:HA     | 2.20                     | 0.55              |
| 2:I:653:TYR:CD1   | 2:I:659:LEU:HD21  | 2.40                     | 0.55              |
| 2:I:1308:CYS:HB3  | 2:I:1311:PHE:CD2  | 2.40                     | 0.55              |
| 1:A:864:VAL:CG2   | 1:A:921:PRO:HB3   | 2.36                     | 0.55              |
| 1:A:1114:TYR:CD1  | 1:A:1337:GLU:HG3  | 2.41                     | 0.55              |
| 1:A:1555:ALA:HA   | 1:A:1621:PHE:CE1  | 2.41                     | 0.55              |
| 1:B:733:ILE:HD12  | 1:B:761:LEU:HD21  | 1.88                     | 0.55              |
| 1:B:988:ILE:HD13  | 1:B:1048:GLU:HB3  | 1.89                     | 0.55              |
| 1:B:1538:VAL:HB   | 1:B:1639:VAL:HG22 | 1.87                     | 0.55              |
| 1:C:335:HIS:HD2   | 1:C:335:HIS:O     | 1.89                     | 0.55              |
| 2:G:652:ILE:HB    | 2:G:658:MET:CE    | 2.36                     | 0.55              |
| 2:H:7:ARG:NH1     | 2:H:24:THR:HA     | 2.21                     | 0.55              |
| 2:I:232:LEU:HD23  | 2:I:232:LEU:O     | 2.06                     | 0.55              |
| 2:I:1931:LEU:HB3  | 2:I:1935:GLU:CG   | 2.35                     | 0.55              |
| 1:A:1665:ILE:HD11 | 1:A:1669:ARG:HG2  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:433:VAL:O     | 1:B:437:ILE:HG13  | 2.07                     | 0.55              |
| 1:B:1665:ILE:HD11 | 1:B:1669:ARG:HG2  | 1.88                     | 0.55              |
| 1:C:12:ILE:HA     | 1:C:15:THR:HG23   | 1.88                     | 0.55              |
| 1:C:417:TYR:OH    | 1:C:458:THR:HG22  | 2.06                     | 0.55              |
| 2:G:722:ALA:HB1   | 2:G:723:HIS:CE1   | 2.42                     | 0.55              |
| 2:G:1931:LEU:HB3  | 2:G:1935:GLU:CG   | 2.33                     | 0.55              |
| 2:G:2036:GLU:O    | 2:G:2039:LYS:HG2  | 2.06                     | 0.55              |
| 2:H:490:TRP:HA    | 2:H:493:THR:CG2   | 2.36                     | 0.55              |
| 2:H:1822:MET:HE2  | 2:H:1996:ILE:HG12 | 1.89                     | 0.55              |
| 2:I:124:LYS:HG2   | 2:I:179:THR:HA    | 1.87                     | 0.55              |
| 2:I:634:ILE:HD11  | 2:I:649:ILE:CD1   | 2.35                     | 0.55              |
| 1:A:825:PRO:HB2   | 1:A:843:LYS:NZ    | 2.21                     | 0.55              |
| 1:B:1036:ARG:NH1  | 1:B:1040:GLU:OE1  | 2.40                     | 0.55              |
| 1:C:1:MET:HE3     | 1:C:9:LEU:HD12    | 1.89                     | 0.55              |
| 1:C:1347:LYS:O    | 1:C:1347:LYS:HD3  | 2.05                     | 0.55              |
| 2:G:665:LEU:O     | 2:G:669:LEU:HB2   | 2.06                     | 0.55              |
| 2:G:1678:MET:CE   | 2:G:1707:LEU:HD22 | 2.35                     | 0.55              |
| 2:H:1431:TYR:CE1  | 2:H:1526:THR:HG23 | 2.41                     | 0.55              |
| 1:C:27:ARG:HD2    | 1:C:30:GLU:OE2    | 2.06                     | 0.55              |
| 1:C:254:TRP:CZ3   | 1:C:302:LEU:HD13  | 2.41                     | 0.55              |
| 1:C:807:LYS:HG3   | 1:C:858:TRP:HB3   | 1.87                     | 0.55              |
| 1:C:1498:GLU:CG   | 1:C:1876:LEU:CB   | 2.64                     | 0.55              |
| 2:G:1475:LYS:HB2  | 2:G:1481:SER:HB2  | 1.89                     | 0.55              |
| 2:H:1166:VAL:HG12 | 2:H:1167:SER:N    | 2.21                     | 0.55              |
| 2:H:2038:ILE:HG22 | 2:H:2042:ILE:CD1  | 2.36                     | 0.55              |
| 2:I:61:VAL:HG21   | 2:I:95:TYR:HE1    | 1.72                     | 0.55              |
| 2:I:166:THR:HG22  | 2:I:168:ASP:N     | 2.21                     | 0.55              |
| 2:I:638:VAL:HA    | 2:I:641:ILE:HG22  | 1.88                     | 0.55              |
| 2:I:926:LEU:HB3   | 2:I:947:THR:HG22  | 1.88                     | 0.55              |
| 1:A:1238:VAL:HG12 | 1:A:1239:HIS:N    | 2.21                     | 0.55              |
| 1:A:1498:GLU:CB   | 1:A:1876:LEU:CD1  | 2.63                     | 0.55              |
| 1:C:11:HIS:O      | 1:C:15:THR:HG22   | 2.06                     | 0.55              |
| 1:C:152:HIS:CE1   | 1:C:168:MET:HG3   | 2.41                     | 0.55              |
| 1:C:383:GLY:O     | 1:C:387:VAL:HG23  | 2.07                     | 0.55              |
| 1:C:1125:VAL:HG21 | 1:C:1175:ILE:HD12 | 1.88                     | 0.55              |
| 2:G:197:GLU:OE1   | 2:G:197:GLU:HA    | 2.06                     | 0.55              |
| 2:G:1496:LYS:HE2  | 2:G:1693:ARG:NH2  | 2.20                     | 0.55              |
| 2:H:807:ILE:CG2   | 2:H:1066:ILE:HA   | 2.36                     | 0.55              |
| 2:H:1359:MET:HA   | 2:H:1359:MET:HE3  | 1.88                     | 0.55              |
| 2:I:2015:THR:HG22 | 2:I:2017:LYS:N    | 2.21                     | 0.55              |
| 1:A:12:ILE:HD11   | 2:G:2041:ILE:HD11 | 1.83                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:332:THR:HG22  | 1:B:331:ILE:CD1   | 2.36                     | 0.55              |
| 1:A:529:MET:HG2   | 1:A:638:LEU:CD1   | 2.36                     | 0.55              |
| 1:A:771:PHE:CD1   | 1:A:825:PRO:HG3   | 2.42                     | 0.55              |
| 1:A:1056:ILE:HD13 | 1:A:1193:TRP:CD1  | 2.42                     | 0.55              |
| 1:A:1233:GLU:OE2  | 1:A:1680:ARG:NH2  | 2.40                     | 0.55              |
| 1:A:1473:GLU:O    | 1:A:1478:PRO:HD3  | 2.06                     | 0.55              |
| 1:B:328:LEU:HD22  | 1:B:328:LEU:C     | 2.28                     | 0.55              |
| 1:B:1285:ALA:O    | 1:B:1289:MET:HG3  | 2.07                     | 0.55              |
| 1:B:1432:HIS:CE1  | 1:B:1434:SER:OG   | 2.60                     | 0.55              |
| 1:C:883:ILE:HD12  | 1:C:947:LEU:HD12  | 1.88                     | 0.55              |
| 2:G:239:PRO:HG3   | 2:G:304:PHE:HA    | 1.88                     | 0.55              |
| 2:H:584:SER:HA    | 2:H:587:ILE:HG23  | 1.89                     | 0.55              |
| 2:H:707:PRO:HG2   | 2:H:730:LEU:HD13  | 1.89                     | 0.55              |
| 2:I:603:SER:O     | 2:I:607:VAL:HG12  | 2.06                     | 0.55              |
| 2:I:1432:GLN:HB2  | 2:I:1527:LEU:HD12 | 1.88                     | 0.55              |
| 2:I:1873:TYR:HE1  | 2:I:1877:ARG:HH21 | 1.54                     | 0.55              |
| 1:C:635:ILE:HG22  | 1:C:651:TYR:CG    | 2.42                     | 0.55              |
| 2:G:777:THR:CG2   | 2:G:1081:HIS:CE1  | 2.89                     | 0.55              |
| 2:G:1822:MET:CE   | 2:G:1996:ILE:HG12 | 2.37                     | 0.55              |
| 2:H:264:ARG:NH1   | 2:H:456:GLN:HG3   | 2.22                     | 0.55              |
| 2:H:740:HIS:HA    | 2:H:854:ILE:HD13  | 1.89                     | 0.55              |
| 2:H:1173:VAL:CG2  | 2:H:1221:MET:HE1  | 2.35                     | 0.55              |
| 2:H:1822:MET:CE   | 2:H:1996:ILE:HG12 | 2.37                     | 0.55              |
| 2:I:741:HIS:CE1   | 2:I:855:HIS:CD2   | 2.95                     | 0.55              |
| 2:I:1427:VAL:O    | 2:I:1427:VAL:HG12 | 2.07                     | 0.55              |
| 1:A:56:MET:HG3    | 2:G:1893:VAL:CG2  | 2.37                     | 0.55              |
| 1:A:982:ILE:HG13  | 2:G:965:SER:N     | 2.22                     | 0.55              |
| 1:C:50:SER:HB2    | 1:C:51:PRO:HD3    | 1.88                     | 0.55              |
| 1:C:176:VAL:HG12  | 1:C:178:GLY:H     | 1.72                     | 0.55              |
| 2:G:127:ILE:O     | 2:G:131:ILE:HG13  | 2.07                     | 0.55              |
| 2:G:747:HIS:O     | 2:G:751:LEU:HB2   | 2.07                     | 0.55              |
| 2:G:835:THR:HG23  | 2:G:843:ILE:O     | 2.06                     | 0.55              |
| 2:G:1624:THR:HB   | 2:G:1642:THR:HG23 | 1.86                     | 0.55              |
| 2:H:402:LEU:O     | 2:H:402:LEU:HD13  | 2.07                     | 0.55              |
| 2:H:1350:LEU:HD11 | 2:H:1410:PHE:HB3  | 1.89                     | 0.55              |
| 2:H:1567:ARG:CG   | 2:H:1567:ARG:NH1  | 2.50                     | 0.55              |
| 2:H:1697:HIS:CE1  | 2:H:1829:GLU:HG2  | 2.42                     | 0.55              |
| 2:H:1844:ARG:CG   | 2:H:1844:ARG:NH1  | 2.58                     | 0.55              |
| 2:I:1010:PRO:O    | 2:I:1011:MET:HB2  | 2.05                     | 0.55              |
| 2:I:1168:ASN:ND2  | 2:I:1171:ARG:HB2  | 2.22                     | 0.55              |
| 1:A:1392:LEU:HD22 | 1:A:1396:MET:HG3  | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:49:PRO:O      | 1:B:82:SER:HB2    | 2.07                     | 0.55              |
| 1:B:1123:GLN:HG3  | 1:B:1124:GLU:N    | 2.22                     | 0.55              |
| 1:B:1566:ARG:HB3  | 1:B:1623:TYR:CE1  | 2.42                     | 0.55              |
| 1:C:1009:LEU:HD13 | 1:C:1445:MET:HE1  | 1.89                     | 0.55              |
| 1:C:1455:ARG:NH2  | 1:C:1459:ILE:HG12 | 2.22                     | 0.55              |
| 2:G:264:ARG:NH1   | 2:G:456:GLN:HG3   | 2.22                     | 0.55              |
| 2:H:1475:LYS:HB2  | 2:H:1481:SER:HB2  | 1.88                     | 0.55              |
| 2:H:2036:GLU:O    | 2:H:2039:LYS:HG2  | 2.07                     | 0.55              |
| 2:I:260:PRO:HD3   | 2:I:289:TRP:CE2   | 2.42                     | 0.55              |
| 2:I:1293:THR:HG22 | 2:I:1296:GLU:CD   | 2.28                     | 0.55              |
| 2:I:1624:THR:HB   | 2:I:1642:THR:OG1  | 2.06                     | 0.55              |
| 1:A:1194:ASN:HB3  | 1:A:1197:THR:HG22 | 1.88                     | 0.54              |
| 1:B:1373:ARG:HB2  | 1:B:1545:SER:O    | 2.07                     | 0.54              |
| 1:C:1:MET:HE3     | 1:C:5:VAL:HG12    | 1.88                     | 0.54              |
| 1:C:1501:LEU:O    | 1:C:1505:GLN:HG3  | 2.07                     | 0.54              |
| 2:G:598:THR:HG23  | 4:G:3051:FMN:O4   | 2.06                     | 0.54              |
| 2:G:1227:ARG:CG   | 2:G:1227:ARG:NH1  | 2.56                     | 0.54              |
| 2:G:1313:SER:O    | 2:G:1314:ARG:HD3  | 2.07                     | 0.54              |
| 2:H:1159:ILE:HG12 | 2:H:1169:PRO:CD   | 2.36                     | 0.54              |
| 2:I:1493:LEU:HD11 | 2:I:1499:VAL:CG2  | 2.37                     | 0.54              |
| 1:A:236:LYS:HE2   | 1:A:273:PRO:O     | 2.07                     | 0.54              |
| 1:A:733:ILE:CD1   | 1:A:761:LEU:HD11  | 2.37                     | 0.54              |
| 1:A:741:SER:HB3   | 1:A:744:ASP:HB2   | 1.89                     | 0.54              |
| 1:A:1455:ARG:NH2  | 1:A:1459:ILE:HG12 | 2.22                     | 0.54              |
| 1:B:263:GLY:O     | 1:B:267:VAL:HG23  | 2.07                     | 0.54              |
| 1:B:771:PHE:CD1   | 1:B:825:PRO:HG3   | 2.42                     | 0.54              |
| 1:C:286:PHE:O     | 1:C:290:MET:HG2   | 2.07                     | 0.54              |
| 1:C:1373:ARG:HB2  | 1:C:1545:SER:O    | 2.07                     | 0.54              |
| 2:G:464:ASP:HB3   | 2:G:466:SER:HB3   | 1.88                     | 0.54              |
| 2:G:1859:PRO:CG   | 2:G:1871:LEU:HD12 | 2.20                     | 0.54              |
| 2:H:1293:THR:HG22 | 2:H:1296:GLU:CD   | 2.28                     | 0.54              |
| 2:H:1976:PHE:HB3  | 2:H:1981:LEU:HD21 | 1.89                     | 0.54              |
| 2:I:131:ILE:HD12  | 2:I:182:VAL:CB    | 2.33                     | 0.54              |
| 2:I:145:LEU:HD21  | 2:I:156:LEU:HD21  | 1.89                     | 0.54              |
| 2:I:606:PHE:HZ    | 2:I:805:VAL:HG11  | 1.71                     | 0.54              |
| 2:I:1331:TRP:CE2  | 2:I:1335:ILE:HG13 | 2.42                     | 0.54              |
| 1:A:430:ARG:NH2   | 1:A:605:LEU:HD13  | 2.23                     | 0.54              |
| 2:G:332:GLU:OE2   | 2:G:394:ARG:HD3   | 2.07                     | 0.54              |
| 2:G:462:THR:HB    | 2:G:482:CYS:SG    | 2.48                     | 0.54              |
| 2:G:1292:ILE:O    | 2:G:1368:VAL:O    | 2.25                     | 0.54              |
| 2:H:732:TRP:CD2   | 2:H:750:MET:HE3   | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1497:GLU:OE1  | 2:H:2002:LYS:HE3  | 2.07                     | 0.54              |
| 2:H:2015:THR:HG22 | 2:H:2017:LYS:N    | 2.21                     | 0.54              |
| 2:I:517:HIS:CD2   | 2:I:517:HIS:C     | 2.80                     | 0.54              |
| 2:I:1567:ARG:CG   | 2:I:1567:ARG:NH1  | 2.50                     | 0.54              |
| 1:A:20:TYR:CD1    | 2:G:2033:THR:HG21 | 2.42                     | 0.54              |
| 1:A:733:ILE:HD12  | 1:A:761:LEU:HD21  | 1.89                     | 0.54              |
| 1:A:1475:GLU:HG2  | 1:A:1761:LYS:O    | 2.06                     | 0.54              |
| 1:A:1748:ASN:C    | 1:A:1750:ILE:H    | 2.11                     | 0.54              |
| 2:H:490:TRP:HE1   | 2:H:516:THR:CG2   | 2.01                     | 0.54              |
| 2:H:611:THR:CG2   | 2:H:641:ILE:HG13  | 2.38                     | 0.54              |
| 2:H:1102:TYR:HB3  | 2:H:1244:PRO:HA   | 1.90                     | 0.54              |
| 2:I:490:TRP:HA    | 2:I:493:THR:CG2   | 2.38                     | 0.54              |
| 2:I:1093:ASP:HB3  | 2:I:1096:LYS:HG3  | 1.89                     | 0.54              |
| 2:I:1166:VAL:HG12 | 2:I:1167:SER:N    | 2.23                     | 0.54              |
| 1:A:183:GLN:O     | 1:A:187:LEU:HG    | 2.08                     | 0.54              |
| 1:A:1501:LEU:CD1  | 1:A:1775:LEU:CG   | 2.86                     | 0.54              |
| 1:A:1657:HIS:ND1  | 1:A:1658:PRO:HD2  | 2.21                     | 0.54              |
| 1:B:1401:TYR:C    | 1:B:1658:PRO:HG3  | 2.27                     | 0.54              |
| 1:B:1501:LEU:O    | 1:B:1505:GLN:HG3  | 2.08                     | 0.54              |
| 1:B:1749:THR:CB   | 1:B:1874:ASP:HA   | 2.33                     | 0.54              |
| 1:C:479:ASN:O     | 1:C:483:VAL:HG23  | 2.07                     | 0.54              |
| 2:G:344:LEU:HB3   | 2:G:349:VAL:HG23  | 1.90                     | 0.54              |
| 2:G:1575:LEU:HD13 | 2:G:1579:ILE:HD12 | 1.89                     | 0.54              |
| 2:H:85:ASN:HD22   | 2:H:135:ARG:NH1   | 2.02                     | 0.54              |
| 2:I:584:SER:HA    | 2:I:587:ILE:HG23  | 1.89                     | 0.54              |
| 2:I:1475:LYS:HB2  | 2:I:1481:SER:HB2  | 1.89                     | 0.54              |
| 2:I:1547:PRO:HD3  | 2:I:1584:PHE:CE2  | 2.43                     | 0.54              |
| 2:I:2046:GLU:C    | 2:I:2048:TYR:H    | 2.11                     | 0.54              |
| 1:A:328:LEU:HD22  | 1:A:328:LEU:C     | 2.28                     | 0.54              |
| 1:A:1234:MET:CE   | 1:A:1326:ILE:HG21 | 2.38                     | 0.54              |
| 1:B:385:PHE:HD2   | 1:B:787:LYS:HA    | 1.73                     | 0.54              |
| 1:B:824:LEU:HD11  | 1:B:849:LEU:HD12  | 1.89                     | 0.54              |
| 1:C:1123:GLN:HG3  | 1:C:1124:GLU:N    | 2.23                     | 0.54              |
| 2:G:807:ILE:HG21  | 2:G:1066:ILE:HA   | 1.88                     | 0.54              |
| 2:G:1697:HIS:CE1  | 2:G:1829:GLU:HG2  | 2.43                     | 0.54              |
| 2:G:2030:TYR:CE1  | 2:G:2034:GLY:HA2  | 2.43                     | 0.54              |
| 2:H:464:ASP:HB3   | 2:H:466:SER:HB3   | 1.90                     | 0.54              |
| 2:H:1547:PRO:HD3  | 2:H:1584:PHE:CE2  | 2.42                     | 0.54              |
| 2:I:123:ILE:HD11  | 2:I:533:LEU:CD2   | 2.37                     | 0.54              |
| 2:I:611:THR:CG2   | 2:I:641:ILE:HG13  | 2.37                     | 0.54              |
| 2:I:652:ILE:HB    | 2:I:658:MET:CE    | 2.37                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1417:THR:O    | 2:I:1419:PHE:N    | 2.30                     | 0.54              |
| 2:I:1778:GLN:HB3  | 2:I:1831:VAL:HG13 | 1.88                     | 0.54              |
| 1:A:1184:LEU:HB2  | 1:A:1352:THR:HG21 | 1.89                     | 0.54              |
| 1:B:23:ALA:O      | 2:H:1977:HIS:HA   | 2.07                     | 0.54              |
| 2:G:1428:GLU:HB2  | 2:G:1468:THR:HG22 | 1.88                     | 0.54              |
| 2:G:1749:GLU:OE2  | 2:G:1840:VAL:CG1  | 2.56                     | 0.54              |
| 1:B:236:LYS:HE2   | 1:B:273:PRO:O     | 2.07                     | 0.54              |
| 1:B:280:GLU:HG2   | 1:B:280:GLU:O     | 2.08                     | 0.54              |
| 1:B:655:LEU:CD2   | 1:B:916:LEU:HD11  | 2.38                     | 0.54              |
| 1:C:1748:ASN:C    | 1:C:1750:ILE:H    | 2.12                     | 0.54              |
| 2:G:601:THR:CG2   | 2:G:618:GLU:O     | 2.41                     | 0.54              |
| 2:H:964:LEU:CD2   | 2:H:964:LEU:N     | 2.70                     | 0.54              |
| 2:H:1378:ILE:HD11 | 2:H:1381:VAL:HG21 | 1.90                     | 0.54              |
| 2:I:99:ASN:HA     | 2:I:550:VAL:HG21  | 1.90                     | 0.54              |
| 2:I:545:GLN:H     | 2:I:545:GLN:NE2   | 2.06                     | 0.54              |
| 2:I:722:ALA:HB1   | 2:I:723:HIS:CE1   | 2.42                     | 0.54              |
| 2:I:1452:LEU:HA   | 2:I:1502:GLY:HA3  | 1.88                     | 0.54              |
| 1:A:1496:GLU:O    | 1:A:1500:GLN:HG3  | 2.07                     | 0.54              |
| 1:B:695:GLY:HA3   | 1:B:906:LEU:HD11  | 1.90                     | 0.54              |
| 1:C:37:LYS:HB2    | 1:C:65:TYR:HE1    | 1.72                     | 0.54              |
| 1:C:1477:ILE:H    | 1:C:1478:PRO:CD   | 2.20                     | 0.54              |
| 2:I:826:GLY:O     | 2:I:827:VAL:HG23  | 2.07                     | 0.54              |
| 1:A:340:ARG:HH12  | 1:A:344:GLN:NE2   | 2.06                     | 0.54              |
| 1:A:625:THR:HG23  | 1:A:661:ASP:OD1   | 2.08                     | 0.54              |
| 1:A:644:THR:HG22  | 1:A:648:ASP:O     | 2.08                     | 0.54              |
| 1:A:1138:LYS:HG3  | 1:A:1163:TYR:CE1  | 2.43                     | 0.54              |
| 1:B:635:ILE:HG22  | 1:B:651:TYR:CG    | 2.43                     | 0.54              |
| 1:B:1600:LEU:HD13 | 1:B:1657:HIS:HA   | 1.90                     | 0.54              |
| 1:C:516:ARG:NH2   | 1:C:889:GLU:OE1   | 2.41                     | 0.54              |
| 1:C:1682:LYS:HB3  | 2:I:994:PHE:CE2   | 2.43                     | 0.54              |
| 2:G:1231:GLY:O    | 2:G:1233:PRO:HD3  | 2.08                     | 0.54              |
| 2:I:332:GLU:OE2   | 2:I:394:ARG:HD3   | 2.08                     | 0.54              |
| 2:I:868:PHE:HB3   | 2:I:873:PHE:CE2   | 2.43                     | 0.54              |
| 2:I:1054:LEU:CB   | 4:I:3051:FMN:C7M  | 2.85                     | 0.54              |
| 2:I:1172:LYS:HE3  | 2:I:1574:ASN:OD1  | 2.08                     | 0.54              |
| 1:A:1125:VAL:HG21 | 1:A:1175:ILE:HD12 | 1.88                     | 0.53              |
| 1:B:1010:GLU:HA   | 1:B:1664:ALA:HA   | 1.89                     | 0.53              |
| 1:C:529:MET:HG2   | 1:C:638:LEU:CD1   | 2.39                     | 0.53              |
| 1:C:1194:ASN:HB3  | 1:C:1197:THR:HG22 | 1.89                     | 0.53              |
| 2:H:146:PHE:HA    | 2:H:149:VAL:HG12  | 1.89                     | 0.53              |
| 2:H:1313:SER:O    | 2:H:1314:ARG:HD3  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1325:PHE:CE1  | 2:H:1328:VAL:HG11 | 2.43                     | 0.53              |
| 2:I:754:TYR:CD2   | 2:I:794:MET:HG3   | 2.42                     | 0.53              |
| 1:A:1120:GLU:O    | 1:A:1121:MET:CG   | 2.56                     | 0.53              |
| 1:A:1566:ARG:HB3  | 1:A:1623:TYR:CE1  | 2.42                     | 0.53              |
| 1:B:807:LYS:HG3   | 1:B:858:TRP:HB3   | 1.90                     | 0.53              |
| 1:C:825:PRO:HB2   | 1:C:843:LYS:NZ    | 2.24                     | 0.53              |
| 2:G:1331:TRP:CE2  | 2:G:1335:ILE:HG13 | 2.43                     | 0.53              |
| 2:H:606:PHE:CE1   | 2:H:811:VAL:HG13  | 2.43                     | 0.53              |
| 2:H:1177:SER:O    | 2:H:1180:MET:HG2  | 2.08                     | 0.53              |
| 2:I:615:TYR:CZ    | 2:I:1074:MET:HB3  | 2.42                     | 0.53              |
| 2:I:1844:ARG:CG   | 2:I:1844:ARG:NH1  | 2.61                     | 0.53              |
| 2:I:1954:LYS:HD3  | 2:I:1958:LEU:HD13 | 1.89                     | 0.53              |
| 1:A:1123:GLN:HB2  | 1:A:1177:LYS:HE2  | 1.90                     | 0.53              |
| 1:A:1153:ASP:OD2  | 1:B:359:ARG:NH2   | 2.41                     | 0.53              |
| 1:A:1392:LEU:CD2  | 1:A:1396:MET:HG3  | 2.38                     | 0.53              |
| 1:B:1194:ASN:O    | 1:B:1197:THR:HG23 | 2.08                     | 0.53              |
| 1:C:236:LYS:HE2   | 1:C:273:PRO:O     | 2.08                     | 0.53              |
| 2:G:1269:LEU:O    | 2:G:1560:LEU:HD23 | 2.08                     | 0.53              |
| 2:H:281:VAL:HG23  | 2:H:459:VAL:HG11  | 1.90                     | 0.53              |
| 2:H:674:TYR:HB3   | 2:H:676:ILE:HG22  | 1.88                     | 0.53              |
| 2:H:826:GLY:O     | 2:H:827:VAL:HG23  | 2.07                     | 0.53              |
| 2:I:234:ILE:CG1   | 2:I:235:PRO:HD3   | 2.38                     | 0.53              |
| 2:I:491:GLU:HA    | 2:I:494:THR:HG22  | 1.89                     | 0.53              |
| 2:I:582:LYS:HE2   | 2:I:1108:PRO:HB3  | 1.91                     | 0.53              |
| 2:I:873:PHE:CD1   | 2:I:1026:GLU:HB2  | 2.43                     | 0.53              |
| 1:A:807:LYS:HG3   | 1:A:858:TRP:HB3   | 1.91                     | 0.53              |
| 1:A:1373:ARG:HB2  | 1:A:1545:SER:O    | 2.08                     | 0.53              |
| 1:B:1020:VAL:HG13 | 1:B:1400:ILE:HG23 | 1.91                     | 0.53              |
| 1:B:1392:LEU:CD2  | 1:B:1396:MET:HG3  | 2.38                     | 0.53              |
| 1:C:263:GLY:O     | 1:C:267:VAL:HG23  | 2.08                     | 0.53              |
| 1:C:824:LEU:HD11  | 1:C:849:LEU:HD12  | 1.90                     | 0.53              |
| 2:G:741:HIS:CB    | 2:G:853:PRO:HB2   | 2.38                     | 0.53              |
| 2:G:892:ILE:HG12  | 2:G:903:TRP:CG    | 2.43                     | 0.53              |
| 2:G:964:LEU:CD2   | 2:G:964:LEU:N     | 2.68                     | 0.53              |
| 2:H:55:THR:CG2    | 2:H:56:THR:HG22   | 2.30                     | 0.53              |
| 2:I:271:THR:OG1   | 2:I:460:TYR:HB2   | 2.08                     | 0.53              |
| 2:I:1745:LYS:HE2  | 2:I:1747:LYS:HG2  | 1.91                     | 0.53              |
| 1:A:421:ILE:HG13  | 1:A:469:VAL:HG21  | 1.89                     | 0.53              |
| 1:B:607:LYS:HG2   | 1:B:608:ASP:N     | 2.23                     | 0.53              |
| 1:B:751:PHE:CZ    | 1:B:761:LEU:HD13  | 2.42                     | 0.53              |
| 1:B:1665:ILE:CG1  | 1:B:1669:ARG:HD3  | 2.36                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:158:LYS:HD3   | 1:C:185:GLU:HB3   | 1.91                     | 0.53              |
| 1:C:985:ARG:HH12  | 2:I:953:ARG:CZ    | 2.21                     | 0.53              |
| 1:C:1401:TYR:C    | 1:C:1658:PRO:HG3  | 2.29                     | 0.53              |
| 2:G:707:PRO:HG2   | 2:G:730:LEU:HD13  | 1.90                     | 0.53              |
| 2:H:173:LEU:HD13  | 2:H:219:LEU:HD21  | 1.90                     | 0.53              |
| 2:H:816:ASP:HB3   | 2:H:1048:VAL:HG21 | 1.91                     | 0.53              |
| 2:H:1804:PHE:CZ   | 2:H:2010:TYR:HB2  | 2.44                     | 0.53              |
| 2:I:526:ARG:HH11  | 2:I:558:ASN:HD21  | 1.55                     | 0.53              |
| 2:I:1102:TYR:HB3  | 2:I:1244:PRO:HA   | 1.91                     | 0.53              |
| 2:I:1177:SER:O    | 2:I:1180:MET:HG2  | 2.09                     | 0.53              |
| 2:I:1314:ARG:CG   | 2:I:1314:ARG:NH1  | 2.63                     | 0.53              |
| 2:I:1431:TYR:CE1  | 2:I:1526:THR:HG22 | 2.44                     | 0.53              |
| 2:I:1567:ARG:HG3  | 2:I:1568:HIS:N    | 2.22                     | 0.53              |
| 1:A:50:SER:HB2    | 1:A:51:PRO:CD     | 2.39                     | 0.53              |
| 1:A:529:MET:CE    | 1:A:894:ARG:HD2   | 2.38                     | 0.53              |
| 1:A:635:ILE:HG22  | 1:A:651:TYR:CG    | 2.43                     | 0.53              |
| 1:A:1020:VAL:HG13 | 1:A:1400:ILE:HG23 | 1.90                     | 0.53              |
| 1:A:1665:ILE:HG12 | 1:A:1666:THR:N    | 2.23                     | 0.53              |
| 1:C:825:PRO:HB2   | 1:C:843:LYS:HZ2   | 1.73                     | 0.53              |
| 2:G:913:ASP:H     | 2:G:916:THR:CG2   | 2.22                     | 0.53              |
| 2:G:2015:THR:HG22 | 2:G:2017:LYS:N    | 2.22                     | 0.53              |
| 2:H:652:ILE:HB    | 2:H:658:MET:CE    | 2.39                     | 0.53              |
| 2:H:1567:ARG:HG3  | 2:H:1568:HIS:N    | 2.23                     | 0.53              |
| 2:I:1173:VAL:CG2  | 2:I:1221:MET:HE1  | 2.39                     | 0.53              |
| 2:I:1293:THR:HG22 | 2:I:1296:GLU:CG   | 2.39                     | 0.53              |
| 2:I:2036:GLU:HG2  | 2:I:2039:LYS:NZ   | 2.23                     | 0.53              |
| 1:A:1492:GLU:O    | 1:A:1496:GLU:HG3  | 2.09                     | 0.53              |
| 1:B:1123:GLN:HB2  | 1:B:1177:LYS:HE2  | 1.91                     | 0.53              |
| 1:B:1577:GLN:HE22 | 1:B:1591:TRP:C    | 2.12                     | 0.53              |
| 1:C:1012:LEU:HD23 | 1:C:1445:MET:CE   | 2.39                     | 0.53              |
| 1:C:1037:TRP:HB2  | 1:C:1598:GLN:OE1  | 2.09                     | 0.53              |
| 2:G:346:GLN:HA    | 2:G:377:LEU:HD21  | 1.89                     | 0.53              |
| 2:G:606:PHE:HZ    | 2:G:805:VAL:HG11  | 1.74                     | 0.53              |
| 2:G:1166:VAL:HG12 | 2:G:1167:SER:N    | 2.23                     | 0.53              |
| 2:H:402:LEU:HD12  | 2:H:404:GLN:HG2   | 1.90                     | 0.53              |
| 2:H:774:ALA:HB1   | 2:H:1081:HIS:CD2  | 2.32                     | 0.53              |
| 2:H:1913:VAL:O    | 2:H:1917:ILE:HG13 | 2.08                     | 0.53              |
| 2:I:1327:ILE:HG12 | 2:I:1583:MET:HE3  | 1.91                     | 0.53              |
| 1:A:385:PHE:HD2   | 1:A:787:LYS:HA    | 1.74                     | 0.53              |
| 1:A:483:VAL:O     | 1:A:486:VAL:N     | 2.42                     | 0.53              |
| 1:A:1014:ASP:H    | 1:A:1510:ASN:ND2  | 1.93                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:12:ILE:HA     | 1:B:15:THR:HG23   | 1.90                     | 0.53              |
| 1:C:1524:GLY:HA2  | 1:C:1527:ALA:HB3  | 1.91                     | 0.53              |
| 2:G:85:ASN:HD22   | 2:G:135:ARG:NH1   | 2.03                     | 0.53              |
| 2:G:490:TRP:CH2   | 2:G:512:LEU:HD21  | 2.43                     | 0.53              |
| 2:G:750:MET:CG    | 2:G:796:PHE:HZ    | 2.21                     | 0.53              |
| 2:H:346:GLN:HA    | 2:H:377:LEU:HD21  | 1.91                     | 0.53              |
| 2:H:1040:LEU:HD21 | 2:H:1048:VAL:HA   | 1.89                     | 0.53              |
| 2:H:1452:LEU:HA   | 2:H:1502:GLY:HA3  | 1.90                     | 0.53              |
| 2:H:1954:LYS:HD3  | 2:H:1958:LEU:HD13 | 1.90                     | 0.53              |
| 2:I:892:ILE:HG12  | 2:I:903:TRP:CG    | 2.44                     | 0.53              |
| 2:I:1040:LEU:HD21 | 2:I:1048:VAL:HA   | 1.90                     | 0.53              |
| 2:I:1441:ILE:HD11 | 2:I:1445:ARG:NH2  | 2.23                     | 0.53              |
| 2:I:1861:ARG:HD2  | 2:I:1964:PHE:O    | 2.08                     | 0.53              |
| 2:I:2038:ILE:HG22 | 2:I:2042:ILE:CD1  | 2.37                     | 0.53              |
| 1:A:12:ILE:HA     | 1:A:15:THR:HG23   | 1.88                     | 0.53              |
| 1:A:1455:ARG:O    | 1:A:1459:ILE:HG13 | 2.08                     | 0.53              |
| 1:C:1036:ARG:NH1  | 1:C:1040:GLU:OE1  | 2.41                     | 0.53              |
| 2:G:281:VAL:HG23  | 2:G:459:VAL:HG11  | 1.91                     | 0.53              |
| 2:G:1040:LEU:HD21 | 2:G:1048:VAL:HA   | 1.90                     | 0.53              |
| 2:G:2038:ILE:HG22 | 2:G:2042:ILE:CD1  | 2.37                     | 0.53              |
| 2:H:1745:LYS:HE2  | 2:H:1747:LYS:HG2  | 1.91                     | 0.53              |
| 2:I:240:LEU:O     | 2:I:244:ILE:HG13  | 2.08                     | 0.53              |
| 2:I:871:THR:HG21  | 2:I:887:LYS:NZ    | 2.24                     | 0.53              |
| 2:I:1266:TYR:CG   | 2:I:1347:LEU:HD23 | 2.43                     | 0.53              |
| 2:I:2035:SER:HB3  | 2:I:2038:ILE:CG1  | 2.37                     | 0.53              |
| 1:B:1326:ILE:HG12 | 1:B:1388:MET:HG3  | 1.91                     | 0.53              |
| 1:C:625:THR:HG23  | 1:C:661:ASP:OD1   | 2.09                     | 0.53              |
| 1:C:1285:ALA:O    | 1:C:1289:MET:HG3  | 2.09                     | 0.53              |
| 2:G:102:HIS:HE1   | 2:G:180:TYR:OH    | 1.92                     | 0.53              |
| 2:G:1173:VAL:CG2  | 2:G:1221:MET:HE1  | 2.38                     | 0.53              |
| 2:G:1861:ARG:HD2  | 2:G:1964:PHE:O    | 2.09                     | 0.53              |
| 2:H:234:ILE:CG1   | 2:H:235:PRO:HD3   | 2.39                     | 0.53              |
| 2:H:455:ILE:HG12  | 2:H:469:ARG:HG2   | 1.91                     | 0.53              |
| 2:H:1101:GLU:HB2  | 2:H:1147:ILE:O    | 2.09                     | 0.53              |
| 2:H:1697:HIS:HE1  | 2:H:1829:GLU:HG2  | 1.74                     | 0.53              |
| 2:I:264:ARG:NH1   | 2:I:456:GLN:HG3   | 2.24                     | 0.53              |
| 1:A:529:MET:HG2   | 1:A:638:LEU:HG    | 1.89                     | 0.52              |
| 1:B:340:ARG:HH12  | 1:B:344:GLN:NE2   | 2.08                     | 0.52              |
| 1:C:864:VAL:CG2   | 1:C:921:PRO:HB3   | 2.39                     | 0.52              |
| 1:C:929:GLY:C     | 1:C:931:GLN:H     | 2.13                     | 0.52              |
| 2:G:55:THR:CG2    | 2:G:56:THR:HG22   | 2.33                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1418:ASP:C    | 2:G:1420:GLU:N    | 2.63                     | 0.52              |
| 2:H:1418:ASP:O    | 2:H:1419:PHE:C    | 2.46                     | 0.52              |
| 2:I:606:PHE:CE1   | 2:I:811:VAL:HG13  | 2.44                     | 0.52              |
| 2:I:1040:LEU:O    | 2:I:1046:GLN:HG3  | 2.09                     | 0.52              |
| 1:A:156:ALA:HA    | 1:A:166:ILE:CD1   | 2.39                     | 0.52              |
| 1:A:341:GLN:O     | 1:A:345:VAL:HG12  | 2.09                     | 0.52              |
| 1:A:986:ALA:CA    | 1:A:1047:LEU:HD13 | 2.39                     | 0.52              |
| 1:B:12:ILE:HD11   | 2:H:2041:ILE:HD11 | 1.89                     | 0.52              |
| 1:B:1234:MET:CE   | 1:B:1326:ILE:HG21 | 2.40                     | 0.52              |
| 1:C:1749:THR:C    | 1:C:1874:ASP:HB3  | 2.29                     | 0.52              |
| 2:H:145:LEU:O     | 2:H:149:VAL:HG12  | 2.10                     | 0.52              |
| 2:H:1159:ILE:CG1  | 2:H:1169:PRO:CD   | 2.87                     | 0.52              |
| 2:H:1427:VAL:HG12 | 2:H:1427:VAL:O    | 2.08                     | 0.52              |
| 2:H:1697:HIS:HE1  | 2:H:1829:GLU:CG   | 2.22                     | 0.52              |
| 2:H:2026:PHE:CD2  | 2:H:2045:TRP:HZ3  | 2.27                     | 0.52              |
| 2:I:465:GLY:HA2   | 2:I:493:THR:HA    | 1.91                     | 0.52              |
| 2:I:598:THR:O     | 2:I:602:VAL:HB    | 2.09                     | 0.52              |
| 2:I:2036:GLU:O    | 2:I:2039:LYS:HG2  | 2.09                     | 0.52              |
| 1:B:784:ILE:HG23  | 1:B:788:SER:HB2   | 1.92                     | 0.52              |
| 1:B:980:VAL:HG21  | 2:H:952:ARG:NH2   | 2.24                     | 0.52              |
| 1:C:1056:ILE:HD13 | 1:C:1193:TRP:CD1  | 2.41                     | 0.52              |
| 1:C:1305:CYS:SG   | 1:C:1583:HIS:NE2  | 2.82                     | 0.52              |
| 2:G:615:TYR:CZ    | 2:G:1074:MET:HB3  | 2.44                     | 0.52              |
| 2:H:194:THR:CG2   | 2:H:300:ILE:HD11  | 2.39                     | 0.52              |
| 2:H:768:GLY:HA3   | 2:H:800:LEU:CD2   | 2.39                     | 0.52              |
| 2:I:418:ASN:N     | 2:I:418:ASN:HD22  | 2.07                     | 0.52              |
| 1:A:335:HIS:HD2   | 1:A:335:HIS:O     | 1.92                     | 0.52              |
| 1:A:824:LEU:HD11  | 1:A:849:LEU:HD12  | 1.89                     | 0.52              |
| 1:B:329:GLU:O     | 1:B:333:LYS:HG3   | 2.08                     | 0.52              |
| 1:C:260:ARG:HH12  | 1:C:300:VAL:CG2   | 2.22                     | 0.52              |
| 1:C:530:ALA:HA    | 1:C:636:PRO:HB3   | 1.91                     | 0.52              |
| 1:C:1411:THR:HG22 | 1:C:1412:ASP:N    | 2.24                     | 0.52              |
| 2:G:490:TRP:HA    | 2:G:493:THR:CG2   | 2.40                     | 0.52              |
| 2:G:1159:ILE:HG12 | 2:G:1169:PRO:CD   | 2.39                     | 0.52              |
| 2:G:1359:MET:CE   | 2:G:1404:MET:HB3  | 2.39                     | 0.52              |
| 2:G:1438:SER:O    | 2:G:1441:ILE:HG23 | 2.09                     | 0.52              |
| 2:H:955:GLU:HG2   | 2:H:987:TYR:CE2   | 2.45                     | 0.52              |
| 2:I:1486:PHE:HA   | 2:I:1504:VAL:O    | 2.10                     | 0.52              |
| 1:A:988:ILE:HD13  | 1:A:1048:GLU:CA   | 2.39                     | 0.52              |
| 1:C:406:TRP:CE3   | 1:C:1619:GLU:HG3  | 2.44                     | 0.52              |
| 1:C:465:ASN:O     | 1:C:469:VAL:HG23  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:145:LEU:HD21  | 2:G:156:LEU:HD21  | 1.91                     | 0.52              |
| 2:G:871:THR:HG21  | 2:G:887:LYS:NZ    | 2.25                     | 0.52              |
| 2:G:1389:ILE:HG13 | 2:G:1411:PHE:HD1  | 1.75                     | 0.52              |
| 2:H:754:TYR:CD2   | 2:H:794:MET:HG3   | 2.44                     | 0.52              |
| 2:H:1722:GLY:N    | 2:H:1726:GLY:HA3  | 2.24                     | 0.52              |
| 2:I:741:HIS:HE1   | 2:I:855:HIS:NE2   | 2.06                     | 0.52              |
| 2:I:1300:PHE:CA   | 2:I:1556:VAL:HG11 | 2.40                     | 0.52              |
| 2:I:1350:LEU:HD11 | 2:I:1410:PHE:HB3  | 1.91                     | 0.52              |
| 2:I:1438:SER:O    | 2:I:1441:ILE:HG23 | 2.08                     | 0.52              |
| 2:I:1475:LYS:HG3  | 2:I:1481:SER:HB2  | 1.92                     | 0.52              |
| 2:I:1774:THR:HA   | 2:I:1777:THR:HB   | 1.92                     | 0.52              |
| 1:A:501:THR:N     | 1:A:886:GLU:OE1   | 2.30                     | 0.52              |
| 1:A:998:TYR:CE2   | 1:A:1667:GLU:HB2  | 2.44                     | 0.52              |
| 1:A:1477:ILE:H    | 1:A:1478:PRO:CD   | 2.21                     | 0.52              |
| 1:B:341:GLN:O     | 1:B:345:VAL:HG12  | 2.10                     | 0.52              |
| 2:G:1475:LYS:CB   | 2:G:1481:SER:HB2  | 2.39                     | 0.52              |
| 2:G:1567:ARG:HH11 | 2:G:1567:ARG:HG2  | 1.72                     | 0.52              |
| 2:G:1593:ILE:HD13 | 2:G:1626:ILE:HD13 | 1.92                     | 0.52              |
| 2:G:1932:SER:O    | 2:G:1936:VAL:HG22 | 2.10                     | 0.52              |
| 2:H:1359:MET:HE3  | 2:H:1404:MET:HB3  | 1.92                     | 0.52              |
| 2:I:702:TYR:HB2   | 2:I:727:PRO:HB2   | 1.92                     | 0.52              |
| 2:I:964:LEU:CD2   | 2:I:964:LEU:N     | 2.72                     | 0.52              |
| 1:A:2:LYS:CD      | 2:G:2050:GLN:HB3  | 2.38                     | 0.52              |
| 1:A:59:ARG:HH11   | 2:G:1896:GLN:NE2  | 2.07                     | 0.52              |
| 1:A:430:ARG:NH1   | 1:A:493:VAL:O     | 2.40                     | 0.52              |
| 1:A:1305:CYS:SG   | 1:A:1583:HIS:NE2  | 2.83                     | 0.52              |
| 2:G:955:GLU:HG2   | 2:G:987:TYR:CE2   | 2.45                     | 0.52              |
| 2:G:2026:PHE:CD2  | 2:G:2045:TRP:HZ3  | 2.27                     | 0.52              |
| 2:H:615:TYR:CZ    | 2:H:1074:MET:HB3  | 2.43                     | 0.52              |
| 2:H:747:HIS:O     | 2:H:751:LEU:HB2   | 2.10                     | 0.52              |
| 2:H:1292:ILE:O    | 2:H:1368:VAL:O    | 2.27                     | 0.52              |
| 2:H:1776:PHE:O    | 2:H:1779:PRO:HD2  | 2.09                     | 0.52              |
| 2:I:913:ASP:H     | 2:I:916:THR:CG2   | 2.23                     | 0.52              |
| 2:I:1004:LEU:HD21 | 2:I:1020:VAL:HG23 | 1.91                     | 0.52              |
| 2:I:1159:ILE:HG12 | 2:I:1169:PRO:CD   | 2.39                     | 0.52              |
| 1:B:529:MET:HG2   | 1:B:638:LEU:HG    | 1.92                     | 0.52              |
| 1:B:893:VAL:HG11  | 1:B:930:LEU:CD2   | 2.36                     | 0.52              |
| 1:C:27:ARG:HB2    | 2:I:2016:ALA:HB2  | 1.91                     | 0.52              |
| 1:C:607:LYS:HG2   | 1:C:608:ASP:N     | 2.24                     | 0.52              |
| 1:C:1431:GLU:CD   | 1:C:1433:HIS:CE1  | 2.83                     | 0.52              |
| 2:G:926:LEU:HB3   | 2:G:947:THR:HG22  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1177:SER:O    | 2:G:1180:MET:HG2  | 2.09                     | 0.52              |
| 2:H:418:ASN:HD22  | 2:H:418:ASN:N     | 2.08                     | 0.52              |
| 2:H:599:PRO:HD2   | 4:H:3051:FMN:H6   | 1.92                     | 0.52              |
| 2:I:751:LEU:HD23  | 2:I:791:TYR:CZ    | 2.44                     | 0.52              |
| 2:I:1282:ARG:HH21 | 2:I:1423:PHE:HB3  | 1.74                     | 0.52              |
| 2:I:1597:ALA:HB1  | 2:I:1638:ILE:CD1  | 2.39                     | 0.52              |
| 2:I:1918:LYS:HG2  | 2:I:1919:LEU:HD23 | 1.92                     | 0.52              |
| 1:A:521:LYS:HE2   | 1:A:605:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:705:VAL:CG2   | 1:A:732:LEU:HD21  | 2.39                     | 0.52              |
| 1:A:1475:GLU:HG3  | 1:A:1761:LYS:O    | 2.10                     | 0.52              |
| 1:C:340:ARG:HH12  | 1:C:344:GLN:NE2   | 2.08                     | 0.52              |
| 1:C:705:VAL:CG2   | 1:C:732:LEU:HD21  | 2.40                     | 0.52              |
| 1:C:1577:GLN:HE22 | 1:C:1591:TRP:C    | 2.13                     | 0.52              |
| 2:G:121:GLU:HA    | 2:G:124:LYS:HD2   | 1.91                     | 0.52              |
| 2:G:176:LEU:HD22  | 2:G:247:ALA:HB1   | 1.90                     | 0.52              |
| 2:G:768:GLY:HA3   | 2:G:800:LEU:CD2   | 2.38                     | 0.52              |
| 2:G:1093:ASP:HB3  | 2:G:1096:LYS:HG3  | 1.90                     | 0.52              |
| 2:G:1745:LYS:HD3  | 2:G:1747:LYS:HE2  | 1.91                     | 0.52              |
| 2:G:1873:TYR:CE1  | 2:G:1877:ARG:NE   | 2.75                     | 0.52              |
| 2:H:278:VAL:HG11  | 2:H:303:LEU:HD13  | 1.92                     | 0.52              |
| 2:H:553:ASN:O     | 2:H:556:LYS:CE    | 2.58                     | 0.52              |
| 2:I:273:HIS:CB    | 2:I:512:LEU:HD22  | 2.40                     | 0.52              |
| 2:I:747:HIS:O     | 2:I:751:LEU:HB2   | 2.10                     | 0.52              |
| 2:I:1223:MET:CE   | 2:I:1238:LEU:HD12 | 2.40                     | 0.52              |
| 1:A:280:GLU:O     | 1:A:280:GLU:HG2   | 2.10                     | 0.52              |
| 1:A:607:LYS:HG2   | 1:A:608:ASP:N     | 2.25                     | 0.52              |
| 1:A:674:LYS:O     | 1:A:675:ASP:HB2   | 2.09                     | 0.52              |
| 1:A:1183:ARG:NH1  | 1:A:1344:GLY:HA2  | 2.24                     | 0.52              |
| 1:A:1577:GLN:HE22 | 1:A:1591:TRP:C    | 2.13                     | 0.52              |
| 1:C:156:ALA:HA    | 1:C:166:ILE:CD1   | 2.40                     | 0.52              |
| 2:G:278:VAL:HG11  | 2:G:303:LEU:HD13  | 1.92                     | 0.52              |
| 2:H:281:VAL:HG12  | 2:H:282:ALA:N     | 2.24                     | 0.52              |
| 2:H:577:ILE:HD13  | 2:H:1097:ILE:CD1  | 2.40                     | 0.52              |
| 2:H:892:ILE:HG12  | 2:H:903:TRP:CG    | 2.45                     | 0.52              |
| 2:I:1871:LEU:HD22 | 2:I:1888:ILE:HD11 | 1.92                     | 0.52              |
| 2:I:2026:PHE:CD2  | 2:I:2045:TRP:HZ3  | 2.27                     | 0.52              |
| 1:A:881:ASN:HA    | 1:A:944:ARG:NH2   | 2.25                     | 0.51              |
| 1:B:985:ARG:HH12  | 2:H:953:ARG:NH2   | 2.07                     | 0.51              |
| 1:B:1056:ILE:CD1  | 1:B:1193:TRP:HD1  | 2.22                     | 0.51              |
| 1:B:1238:VAL:HG12 | 1:B:1239:HIS:N    | 2.25                     | 0.51              |
| 1:B:1748:ASN:C    | 1:B:1750:ILE:H    | 2.13                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1665:ILE:CG1  | 1:C:1669:ARG:HD3  | 2.36                     | 0.51              |
| 2:G:234:ILE:CG1   | 2:G:235:PRO:HD3   | 2.40                     | 0.51              |
| 2:G:1774:THR:HA   | 2:G:1777:THR:HB   | 1.90                     | 0.51              |
| 2:H:654:VAL:HG23  | 2:H:683:ALA:HB1   | 1.92                     | 0.51              |
| 2:H:1673:GLU:N    | 2:H:1676:MET:HE3  | 2.25                     | 0.51              |
| 2:I:1745:LYS:HD3  | 2:I:1747:LYS:HE2  | 1.93                     | 0.51              |
| 1:A:1123:GLN:HG3  | 1:A:1124:GLU:N    | 2.24                     | 0.51              |
| 1:A:1411:THR:HG22 | 1:A:1412:ASP:N    | 2.25                     | 0.51              |
| 1:B:1104:ARG:O    | 1:B:1185:VAL:HG13 | 2.11                     | 0.51              |
| 1:B:1665:ILE:HG12 | 1:B:1666:THR:N    | 2.25                     | 0.51              |
| 1:C:156:ALA:HA    | 1:C:166:ILE:HD12  | 1.92                     | 0.51              |
| 1:C:1238:VAL:HG12 | 1:C:1239:HIS:N    | 2.25                     | 0.51              |
| 1:C:1303:GLY:N    | 1:C:1307:THR:HG22 | 2.26                     | 0.51              |
| 1:C:1840:VAL:HG23 | 1:C:1848:ALA:HB3  | 1.92                     | 0.51              |
| 2:G:376:ASN:HD22  | 2:G:376:ASN:C     | 2.13                     | 0.51              |
| 2:H:131:ILE:CD1   | 2:H:182:VAL:CG1   | 2.88                     | 0.51              |
| 2:I:715:GLN:O     | 2:I:719:ILE:HG12  | 2.10                     | 0.51              |
| 2:I:1697:HIS:CE1  | 2:I:1829:GLU:HG2  | 2.45                     | 0.51              |
| 2:I:1868:GLN:HG3  | 2:I:1898:TYR:CZ   | 2.45                     | 0.51              |
| 1:A:1303:GLY:N    | 1:A:1307:THR:HG22 | 2.25                     | 0.51              |
| 1:A:1411:THR:HG22 | 1:A:1412:ASP:H    | 1.76                     | 0.51              |
| 1:A:1474:ALA:HA   | 1:A:1478:PRO:CD   | 2.41                     | 0.51              |
| 1:B:985:ARG:NH1   | 2:H:953:ARG:CZ    | 2.73                     | 0.51              |
| 1:C:46:GLU:OE1    | 1:C:53:LEU:HB2    | 2.11                     | 0.51              |
| 1:C:674:LYS:O     | 1:C:675:ASP:HB2   | 2.11                     | 0.51              |
| 2:G:124:LYS:HG2   | 2:G:179:THR:HA    | 1.90                     | 0.51              |
| 2:G:213:LEU:O     | 2:G:213:LEU:HG    | 2.10                     | 0.51              |
| 2:G:489:LYS:O     | 2:G:493:THR:HG22  | 2.10                     | 0.51              |
| 2:G:702:TYR:HB2   | 2:G:727:PRO:HB2   | 1.93                     | 0.51              |
| 2:G:1293:THR:HG22 | 2:G:1296:GLU:CG   | 2.40                     | 0.51              |
| 2:G:1328:VAL:HG23 | 2:G:1557:SER:HA   | 1.92                     | 0.51              |
| 2:G:1493:LEU:HD11 | 2:G:1499:VAL:CG2  | 2.40                     | 0.51              |
| 2:H:545:GLN:H     | 2:H:545:GLN:NE2   | 2.07                     | 0.51              |
| 2:H:758:ARG:NH2   | 2:H:797:ASP:OD1   | 2.35                     | 0.51              |
| 2:H:1293:THR:HG22 | 2:H:1296:GLU:CG   | 2.41                     | 0.51              |
| 2:H:1475:LYS:CB   | 2:H:1481:SER:HB2  | 2.40                     | 0.51              |
| 1:A:12:ILE:CD1    | 2:G:2041:ILE:CD1  | 2.83                     | 0.51              |
| 1:B:335:HIS:O     | 1:B:335:HIS:HD2   | 1.93                     | 0.51              |
| 1:B:1411:THR:HG22 | 1:B:1412:ASP:N    | 2.26                     | 0.51              |
| 1:C:983:GLN:NE2   | 2:I:962:LYS:HD2   | 2.25                     | 0.51              |
| 2:G:654:VAL:O     | 2:G:654:VAL:HG12  | 2.09                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1081:HIS:O    | 2:G:1085:LEU:HB2  | 2.10                     | 0.51              |
| 2:H:582:LYS:HE2   | 2:H:1108:PRO:HB3  | 1.92                     | 0.51              |
| 2:H:1081:HIS:O    | 2:H:1085:LEU:HB2  | 2.10                     | 0.51              |
| 2:H:1475:LYS:HG3  | 2:H:1481:SER:HB2  | 1.93                     | 0.51              |
| 2:H:1491:VAL:HB   | 2:H:1501:ILE:HD12 | 1.92                     | 0.51              |
| 2:I:652:ILE:N     | 2:I:652:ILE:HD12  | 2.25                     | 0.51              |
| 2:I:732:TRP:CD2   | 2:I:750:MET:HE3   | 2.45                     | 0.51              |
| 2:I:732:TRP:CD2   | 2:I:750:MET:HE1   | 2.43                     | 0.51              |
| 2:I:1475:LYS:CB   | 2:I:1481:SER:HB2  | 2.41                     | 0.51              |
| 2:G:816:ASP:HB3   | 2:G:1048:VAL:CG2  | 2.41                     | 0.51              |
| 2:H:1561:ASN:OD1  | 2:H:1563:ILE:HB   | 2.10                     | 0.51              |
| 2:I:460:TYR:HA    | 2:I:466:SER:O     | 2.11                     | 0.51              |
| 1:A:157:HIS:HE1   | 1:A:228:LEU:HD22  | 1.76                     | 0.51              |
| 1:A:1840:VAL:HG23 | 1:A:1848:ALA:HB3  | 1.91                     | 0.51              |
| 1:B:338:LEU:O     | 1:B:342:GLN:HG3   | 2.10                     | 0.51              |
| 1:B:415:SER:O     | 1:B:419:GLU:HB2   | 2.10                     | 0.51              |
| 1:B:1194:ASN:HB3  | 1:B:1197:THR:HG22 | 1.91                     | 0.51              |
| 1:B:1477:ILE:H    | 1:B:1478:PRO:CD   | 2.24                     | 0.51              |
| 1:B:1840:VAL:HG23 | 1:B:1848:ALA:HB3  | 1.92                     | 0.51              |
| 1:C:328:LEU:HD22  | 1:C:328:LEU:C     | 2.30                     | 0.51              |
| 1:C:644:THR:HG22  | 1:C:648:ASP:O     | 2.10                     | 0.51              |
| 2:G:145:LEU:O     | 2:G:149:VAL:HG12  | 2.10                     | 0.51              |
| 2:G:1417:THR:CG2  | 2:G:1419:PHE:CE2  | 2.93                     | 0.51              |
| 2:G:1427:VAL:O    | 2:G:1427:VAL:HG12 | 2.09                     | 0.51              |
| 2:H:55:THR:HB     | 2:H:59:GLU:OE2    | 2.10                     | 0.51              |
| 2:H:432:LEU:HB3   | 2:H:484:ILE:HG23  | 1.92                     | 0.51              |
| 2:H:1493:LEU:HD11 | 2:H:1499:VAL:HG21 | 1.93                     | 0.51              |
| 2:I:1015:VAL:HG11 | 2:I:1017:PHE:CE1  | 2.45                     | 0.51              |
| 1:A:1310:GLU:OE1  | 1:A:1649:LYS:CE   | 2.56                     | 0.51              |
| 2:G:1431:TYR:CE1  | 2:G:1526:THR:HG23 | 2.45                     | 0.51              |
| 2:G:1579:ILE:HD11 | 2:G:1615:MET:SD   | 2.51                     | 0.51              |
| 2:G:1589:VAL:HG11 | 2:G:1640:PHE:CE1  | 2.45                     | 0.51              |
| 2:G:1764:PHE:HB2  | 2:G:1770:LEU:HD21 | 1.93                     | 0.51              |
| 2:H:260:PRO:HD3   | 2:H:289:TRP:CZ2   | 2.46                     | 0.51              |
| 2:H:732:TRP:CD1   | 2:H:750:MET:HE3   | 2.46                     | 0.51              |
| 2:H:1054:LEU:HB3  | 4:H:3051:FMN:HM82 | 1.93                     | 0.51              |
| 2:H:1419:PHE:O    | 2:H:1420:GLU:C    | 2.49                     | 0.51              |
| 2:H:1716:ASN:OD1  | 2:H:1765:ARG:HA   | 2.11                     | 0.51              |
| 2:I:306:ILE:HA    | 2:I:439:ILE:CD1   | 2.40                     | 0.51              |
| 2:I:1428:GLU:HB2  | 2:I:1468:THR:HG22 | 1.93                     | 0.51              |
| 2:I:1566:SER:HB3  | 2:I:1568:HIS:CE1  | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:254:TRP:HZ3   | 1:A:292:GLN:HG3   | 1.75                     | 0.51              |
| 1:A:465:ASN:O     | 1:A:469:VAL:HG23  | 2.11                     | 0.51              |
| 1:A:1498:GLU:HB2  | 1:A:1876:LEU:CD1  | 2.37                     | 0.51              |
| 1:B:864:VAL:CG2   | 1:B:921:PRO:HB3   | 2.40                     | 0.51              |
| 1:C:513:GLU:OE2   | 1:C:873:ARG:NH1   | 2.44                     | 0.51              |
| 1:C:1009:LEU:HG   | 1:C:1664:ALA:HB2  | 1.93                     | 0.51              |
| 1:C:1123:GLN:HB2  | 1:C:1177:LYS:HE2  | 1.93                     | 0.51              |
| 1:C:1411:THR:HG22 | 1:C:1412:ASP:H    | 1.75                     | 0.51              |
| 2:G:1986:LYS:HA   | 2:G:1989:LYS:HB3  | 1.92                     | 0.51              |
| 2:H:533:LEU:HD13  | 2:H:545:GLN:HG3   | 1.92                     | 0.51              |
| 2:H:667:LYS:HD2   | 2:H:697:THR:CG2   | 2.35                     | 0.51              |
| 2:H:1236:LEU:HD11 | 2:H:1262:ILE:HG12 | 1.92                     | 0.51              |
| 2:I:157:VAL:HG11  | 2:I:496:PHE:CZ    | 2.46                     | 0.51              |
| 2:I:346:GLN:HA    | 2:I:377:LEU:HD21  | 1.92                     | 0.51              |
| 2:I:950:PHE:O     | 2:I:954:VAL:HG23  | 2.11                     | 0.51              |
| 1:B:1705:PRO:HB2  | 1:B:1733:PHE:CE1  | 2.46                     | 0.51              |
| 1:C:733:ILE:CD1   | 1:C:761:LEU:HD11  | 2.40                     | 0.51              |
| 2:G:16:LEU:HG     | 2:G:48:PHE:CZ     | 2.45                     | 0.51              |
| 2:G:443:LEU:HD22  | 2:G:448:VAL:CG1   | 2.41                     | 0.51              |
| 2:G:566:HIS:O     | 2:G:568:LYS:HG3   | 2.10                     | 0.51              |
| 2:G:786:SER:CB    | 2:G:794:MET:HE2   | 2.41                     | 0.51              |
| 2:G:1422:THR:CG2  | 2:G:1422:THR:O    | 2.59                     | 0.51              |
| 2:H:332:GLU:OE2   | 2:H:394:ARG:HD3   | 2.10                     | 0.51              |
| 2:H:461:ASP:HB3   | 2:H:464:ASP:HB2   | 1.93                     | 0.51              |
| 2:H:807:ILE:HG21  | 2:H:1066:ILE:HA   | 1.92                     | 0.51              |
| 2:H:2046:GLU:C    | 2:H:2048:TYR:H    | 2.14                     | 0.51              |
| 2:I:807:ILE:HG21  | 2:I:1066:ILE:HA   | 1.93                     | 0.51              |
| 2:I:1313:SER:O    | 2:I:1314:ARG:HD3  | 2.11                     | 0.51              |
| 2:I:1359:MET:HA   | 2:I:1359:MET:HE3  | 1.92                     | 0.51              |
| 1:A:400:ARG:HH11  | 1:A:400:ARG:HG3   | 1.67                     | 0.51              |
| 1:A:889:GLU:HG3   | 1:A:893:VAL:O     | 2.11                     | 0.51              |
| 1:B:822:VAL:HG12  | 1:B:824:LEU:HD22  | 1.93                     | 0.51              |
| 1:B:1455:ARG:NH2  | 1:B:1459:ILE:HG12 | 2.26                     | 0.51              |
| 1:C:157:HIS:HE1   | 1:C:228:LEU:HD22  | 1.75                     | 0.51              |
| 1:C:411:GLN:HE22  | 1:C:1628:SER:H    | 1.58                     | 0.51              |
| 2:G:418:ASN:HD22  | 2:G:418:ASN:N     | 2.09                     | 0.51              |
| 2:G:751:LEU:HD23  | 2:G:791:TYR:CZ    | 2.46                     | 0.51              |
| 2:G:868:PHE:HB3   | 2:G:873:PHE:CE2   | 2.46                     | 0.51              |
| 2:G:1135:GLU:OE2  | 2:G:1175:LYS:HE3  | 2.11                     | 0.51              |
| 2:G:1452:LEU:HA   | 2:G:1502:GLY:HA3  | 1.92                     | 0.51              |
| 2:H:233:SER:HA    | 2:H:424:ALA:CB    | 2.41                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:460:TYR:HA    | 2:H:466:SER:O     | 2.11                     | 0.51              |
| 2:H:741:HIS:HB2   | 2:H:853:PRO:O     | 2.11                     | 0.51              |
| 2:H:1678:MET:CE   | 2:H:1707:LEU:HD22 | 2.40                     | 0.51              |
| 2:H:2026:PHE:HD2  | 2:H:2045:TRP:HZ3  | 1.59                     | 0.51              |
| 1:A:635:ILE:HG22  | 1:A:651:TYR:CD1   | 2.46                     | 0.50              |
| 1:A:985:ARG:NH1   | 2:G:953:ARG:CZ    | 2.74                     | 0.50              |
| 1:A:1105:LEU:HD23 | 1:A:1185:VAL:HG22 | 1.93                     | 0.50              |
| 1:B:50:SER:HB2    | 1:B:51:PRO:CD     | 2.40                     | 0.50              |
| 1:B:386:PHE:O     | 1:B:390:VAL:HB    | 2.11                     | 0.50              |
| 1:B:1524:GLY:HA2  | 1:B:1527:ALA:HB3  | 1.93                     | 0.50              |
| 2:G:194:THR:CG2   | 2:G:300:ILE:HD11  | 2.41                     | 0.50              |
| 2:G:601:THR:HG22  | 2:G:620:ALA:H     | 1.75                     | 0.50              |
| 2:G:1223:MET:CE   | 2:G:1238:LEU:HD12 | 2.40                     | 0.50              |
| 2:G:1697:HIS:HE1  | 2:G:1829:GLU:HG2  | 1.74                     | 0.50              |
| 2:H:408:PRO:HG3   | 2:H:836:TYR:CD2   | 2.46                     | 0.50              |
| 2:H:1265:MET:HE1  | 2:H:1562:PRO:HG2  | 1.92                     | 0.50              |
| 2:I:1493:LEU:HD11 | 2:I:1499:VAL:HG21 | 1.93                     | 0.50              |
| 2:I:1776:PHE:O    | 2:I:1779:PRO:HD2  | 2.10                     | 0.50              |
| 1:A:433:VAL:O     | 1:A:437:ILE:HG13  | 2.12                     | 0.50              |
| 1:A:1533:ILE:HD11 | 1:A:1564:LEU:HD13 | 1.93                     | 0.50              |
| 1:B:635:ILE:HG22  | 1:B:651:TYR:CD1   | 2.46                     | 0.50              |
| 1:B:1158:PRO:HD2  | 1:B:1159:GLU:OE2  | 2.10                     | 0.50              |
| 1:B:1196:LYS:HE3  | 1:B:1202:ASP:CG   | 2.31                     | 0.50              |
| 1:B:1411:THR:HG22 | 1:B:1412:ASP:H    | 1.75                     | 0.50              |
| 1:C:34:VAL:O      | 1:C:38:ASP:HB2    | 2.11                     | 0.50              |
| 1:C:655:LEU:CD2   | 1:C:916:LEU:HD11  | 2.41                     | 0.50              |
| 1:C:828:PRO:HG3   | 1:C:868:ILE:HG22  | 1.94                     | 0.50              |
| 2:G:7:ARG:CZ      | 2:G:24:THR:HA     | 2.41                     | 0.50              |
| 2:G:281:VAL:HG12  | 2:G:282:ALA:N     | 2.26                     | 0.50              |
| 2:G:526:ARG:HH11  | 2:G:558:ASN:HD21  | 1.59                     | 0.50              |
| 2:H:1597:ALA:HB1  | 2:H:1638:ILE:CD1  | 2.41                     | 0.50              |
| 2:H:1861:ARG:HD2  | 2:H:1964:PHE:O    | 2.12                     | 0.50              |
| 2:I:85:ASN:HD22   | 2:I:135:ARG:NH1   | 2.04                     | 0.50              |
| 2:I:281:VAL:HG12  | 2:I:282:ALA:N     | 2.25                     | 0.50              |
| 2:I:611:THR:HA    | 2:I:615:TYR:O     | 2.11                     | 0.50              |
| 2:I:750:MET:CG    | 2:I:796:PHE:HZ    | 2.24                     | 0.50              |
| 1:A:20:TYR:CE1    | 2:G:2033:THR:HG21 | 2.47                     | 0.50              |
| 1:A:24:SER:O      | 2:G:1977:HIS:CD2  | 2.65                     | 0.50              |
| 1:A:34:VAL:O      | 1:A:38:ASP:HB2    | 2.10                     | 0.50              |
| 1:A:59:ARG:HH11   | 2:G:1896:GLN:HE22 | 1.58                     | 0.50              |
| 2:G:652:ILE:CD1   | 2:G:658:MET:HE3   | 2.42                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1272:ASP:O    | 2:G:1273:GLU:HG3  | 2.11                     | 0.50              |
| 2:G:1918:LYS:HG2  | 2:G:1919:LEU:HD23 | 1.93                     | 0.50              |
| 2:H:344:LEU:HB3   | 2:H:349:VAL:HG23  | 1.94                     | 0.50              |
| 2:H:491:GLU:HA    | 2:H:494:THR:HG22  | 1.93                     | 0.50              |
| 2:H:1774:THR:HA   | 2:H:1777:THR:HB   | 1.93                     | 0.50              |
| 2:H:1775:GLN:HG2  | 2:H:1836:MET:SD   | 2.51                     | 0.50              |
| 2:I:173:LEU:HD13  | 2:I:219:LEU:HD21  | 1.94                     | 0.50              |
| 2:I:376:ASN:HD22  | 2:I:376:ASN:C     | 2.14                     | 0.50              |
| 2:I:1027:ILE:O    | 2:I:1031:LYS:HB2  | 2.11                     | 0.50              |
| 2:I:1945:ASP:O    | 2:I:1949:LYS:HG3  | 2.10                     | 0.50              |
| 1:A:286:PHE:O     | 1:A:290:MET:HG2   | 2.10                     | 0.50              |
| 1:B:421:ILE:HG12  | 1:B:469:VAL:HG21  | 1.93                     | 0.50              |
| 1:B:1303:GLY:N    | 1:B:1307:THR:HG22 | 2.25                     | 0.50              |
| 1:C:280:GLU:O     | 1:C:280:GLU:HG2   | 2.11                     | 0.50              |
| 1:C:415:SER:O     | 1:C:419:GLU:HB2   | 2.12                     | 0.50              |
| 1:C:702:LYS:HE2   | 1:C:729:GLY:O     | 2.11                     | 0.50              |
| 1:C:1116:PRO:HB2  | 1:C:1184:LEU:HD12 | 1.93                     | 0.50              |
| 2:G:545:GLN:H     | 2:G:545:GLN:NE2   | 2.09                     | 0.50              |
| 2:H:463:PHE:CE1   | 2:H:486:LEU:HD22  | 2.47                     | 0.50              |
| 2:H:1102:TYR:CE2  | 2:H:1152:ALA:HB2  | 2.47                     | 0.50              |
| 2:H:1148:ASN:ND2  | 2:H:1151:HIS:H    | 2.08                     | 0.50              |
| 2:H:1389:ILE:HG13 | 2:H:1411:PHE:HD1  | 1.76                     | 0.50              |
| 2:H:1435:ILE:O    | 2:H:1435:ILE:HG22 | 2.10                     | 0.50              |
| 2:I:1491:VAL:HB   | 2:I:1501:ILE:HD12 | 1.93                     | 0.50              |
| 1:A:1004:ILE:HG22 | 1:A:1660:TYR:CE2  | 2.46                     | 0.50              |
| 1:B:156:ALA:HA    | 1:B:166:ILE:CD1   | 2.41                     | 0.50              |
| 1:B:156:ALA:HA    | 1:B:166:ILE:HD12  | 1.93                     | 0.50              |
| 1:C:1431:GLU:HB3  | 1:C:1520:ALA:HB2  | 1.92                     | 0.50              |
| 2:G:611:THR:HA    | 2:G:615:TYR:O     | 2.11                     | 0.50              |
| 2:G:663:ILE:HB    | 2:G:664:PRO:CD    | 2.40                     | 0.50              |
| 2:G:676:ILE:O     | 2:G:676:ILE:HG12  | 2.11                     | 0.50              |
| 2:G:732:TRP:CG    | 2:G:750:MET:HE3   | 2.46                     | 0.50              |
| 2:G:784:GLU:O     | 2:G:787:THR:HB    | 2.11                     | 0.50              |
| 2:G:1871:LEU:HD22 | 2:G:1888:ILE:HD11 | 1.93                     | 0.50              |
| 2:H:1428:GLU:HB2  | 2:H:1468:THR:HG22 | 1.94                     | 0.50              |
| 2:I:955:GLU:HG2   | 2:I:987:TYR:CE2   | 2.46                     | 0.50              |
| 2:I:1135:GLU:OE2  | 2:I:1175:LYS:HE3  | 2.12                     | 0.50              |
| 2:I:1716:ASN:OD1  | 2:I:1765:ARG:HA   | 2.11                     | 0.50              |
| 2:I:2035:SER:HB3  | 2:I:2038:ILE:CD1  | 2.40                     | 0.50              |
| 1:A:487:ASP:O     | 1:A:488:PRO:O     | 2.30                     | 0.50              |
| 1:A:1523:ARG:NH2  | 1:A:1564:LEU:O    | 2.45                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1009:LEU:HA   | 1:B:1445:MET:HE2  | 1.93                     | 0.50              |
| 1:C:985:ARG:HH12  | 2:I:953:ARG:NH2   | 2.09                     | 0.50              |
| 1:C:1019:ILE:HG21 | 1:C:1316:VAL:HG22 | 1.94                     | 0.50              |
| 1:C:1474:ALA:HA   | 1:C:1478:PRO:CD   | 2.42                     | 0.50              |
| 2:G:774:ALA:HB1   | 2:G:1081:HIS:CD2  | 2.37                     | 0.50              |
| 2:G:1350:LEU:HD11 | 2:G:1410:PHE:HB3  | 1.94                     | 0.50              |
| 2:G:1840:VAL:O    | 2:G:1840:VAL:HG12 | 2.11                     | 0.50              |
| 2:H:826:GLY:HA2   | 2:H:1060:ALA:HB3  | 1.94                     | 0.50              |
| 2:H:2036:GLU:HG2  | 2:H:2039:LYS:NZ   | 2.27                     | 0.50              |
| 2:I:712:ALA:O     | 2:I:715:GLN:HB3   | 2.12                     | 0.50              |
| 2:I:866:LYS:O     | 2:I:870:GLU:HG3   | 2.12                     | 0.50              |
| 2:I:1953:VAL:O    | 2:I:1953:VAL:HG12 | 2.11                     | 0.50              |
| 1:A:12:ILE:CD1    | 2:G:2041:ILE:HD11 | 2.41                     | 0.50              |
| 1:A:359:ARG:NH2   | 1:C:1153:ASP:OD2  | 2.43                     | 0.50              |
| 1:A:1104:ARG:O    | 1:A:1185:VAL:HG13 | 2.12                     | 0.50              |
| 1:B:20:TYR:OH     | 2:H:2035:SER:HB2  | 2.12                     | 0.50              |
| 1:B:825:PRO:HB2   | 1:B:843:LYS:NZ    | 2.27                     | 0.50              |
| 1:B:1347:LYS:O    | 1:B:1347:LYS:HD3  | 2.11                     | 0.50              |
| 1:C:13:LEU:HB2    | 2:I:2026:PHE:CE1  | 2.45                     | 0.50              |
| 2:G:440:ASN:ND2   | 2:G:477:GLU:HG2   | 2.26                     | 0.50              |
| 2:G:894:ARG:NH1   | 2:G:898:ASP:OD2   | 2.43                     | 0.50              |
| 2:G:949:ASP:CB    | 2:G:1006:MET:HE2  | 2.38                     | 0.50              |
| 2:H:121:GLU:HA    | 2:H:124:LYS:HD2   | 1.93                     | 0.50              |
| 2:H:161:GLY:HA3   | 2:H:506:PRO:HD2   | 1.93                     | 0.50              |
| 2:H:638:VAL:HG22  | 2:H:675:PRO:HG2   | 1.93                     | 0.50              |
| 2:I:1986:LYS:HA   | 2:I:1989:LYS:HB3  | 1.93                     | 0.50              |
| 1:A:930:LEU:HD22  | 1:A:933:VAL:HG11  | 1.93                     | 0.50              |
| 1:B:408:TRP:CZ3   | 1:B:1628:SER:HB3  | 2.47                     | 0.50              |
| 1:C:157:HIS:CE1   | 1:C:228:LEU:HD22  | 2.47                     | 0.50              |
| 1:C:328:LEU:HD13  | 1:C:329:GLU:N     | 2.27                     | 0.50              |
| 1:C:702:LYS:HD3   | 1:C:731:THR:CG2   | 2.41                     | 0.50              |
| 2:G:24:THR:O      | 2:G:26:SER:N      | 2.44                     | 0.50              |
| 2:G:60:LEU:O      | 2:G:63:LYS:HB2    | 2.12                     | 0.50              |
| 2:G:306:ILE:HA    | 2:G:439:ILE:CD1   | 2.42                     | 0.50              |
| 2:G:606:PHE:CE1   | 2:G:811:VAL:HG13  | 2.46                     | 0.50              |
| 2:G:682:GLY:O     | 2:G:683:ALA:HB3   | 2.12                     | 0.50              |
| 2:G:1776:PHE:O    | 2:G:1779:PRO:HD2  | 2.12                     | 0.50              |
| 2:G:2035:SER:HB3  | 2:G:2038:ILE:CD1  | 2.42                     | 0.50              |
| 2:H:747:HIS:HE1   | 2:H:780:TYR:OH    | 1.95                     | 0.50              |
| 2:H:2035:SER:HB3  | 2:H:2038:ILE:CD1  | 2.42                     | 0.50              |
| 2:I:344:LEU:HB3   | 2:I:349:VAL:HG23  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1417:THR:C    | 2:I:1419:PHE:H    | 2.14                     | 0.50              |
| 1:A:156:ALA:HA    | 1:A:166:ILE:HD12  | 1.93                     | 0.50              |
| 1:A:1116:PRO:HB2  | 1:A:1184:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:1125:VAL:HG21 | 1:A:1175:ILE:CD1  | 2.42                     | 0.50              |
| 1:A:1347:LYS:O    | 1:A:1347:LYS:HD3  | 2.11                     | 0.50              |
| 1:A:1459:ILE:O    | 1:A:1463:VAL:HG23 | 2.12                     | 0.50              |
| 1:B:46:GLU:OE1    | 1:B:53:LEU:HB2    | 2.12                     | 0.50              |
| 1:C:385:PHE:HD2   | 1:C:787:LYS:HA    | 1.77                     | 0.50              |
| 1:C:1460:LYS:CE   | 1:C:1774:GLU:OE1  | 2.59                     | 0.50              |
| 1:C:1566:ARG:HB3  | 1:C:1623:TYR:CE1  | 2.46                     | 0.50              |
| 1:C:1705:PRO:HB2  | 1:C:1733:PHE:CE1  | 2.46                     | 0.50              |
| 2:G:428:HIS:CD2   | 2:G:488:VAL:HG23  | 2.47                     | 0.50              |
| 2:G:1552:PRO:O    | 2:G:1556:VAL:HG23 | 2.12                     | 0.50              |
| 2:G:1697:HIS:HE1  | 2:G:1829:GLU:CG   | 2.25                     | 0.50              |
| 2:G:1716:ASN:OD1  | 2:G:1765:ARG:HA   | 2.12                     | 0.50              |
| 2:H:7:ARG:CZ      | 2:H:24:THR:HA     | 2.42                     | 0.50              |
| 2:H:441:LYS:O     | 2:H:444:VAL:HG12  | 2.12                     | 0.50              |
| 2:H:1004:LEU:HD21 | 2:H:1020:VAL:CG2  | 2.41                     | 0.50              |
| 2:H:2030:TYR:CE1  | 2:H:2034:GLY:HA2  | 2.46                     | 0.50              |
| 2:I:455:ILE:HG12  | 2:I:469:ARG:HG2   | 1.93                     | 0.50              |
| 2:I:777:THR:HG23  | 2:I:1081:HIS:CE1  | 2.47                     | 0.50              |
| 2:I:1673:GLU:N    | 2:I:1676:MET:HE3  | 2.25                     | 0.50              |
| 1:A:142:ASP:CG    | 1:A:257:PRO:HB2   | 2.32                     | 0.49              |
| 1:B:413:LEU:HB2   | 1:B:439:ILE:HD13  | 1.94                     | 0.49              |
| 1:B:1451:GLN:OE1  | 1:B:1451:GLN:HA   | 2.12                     | 0.49              |
| 1:B:1533:ILE:HG13 | 1:B:1564:LEU:HB3  | 1.94                     | 0.49              |
| 1:C:267:VAL:O     | 1:C:290:MET:HE1   | 2.12                     | 0.49              |
| 1:C:1665:ILE:HG12 | 1:C:1666:THR:N    | 2.27                     | 0.49              |
| 2:G:131:ILE:CB    | 2:G:182:VAL:CG1   | 2.85                     | 0.49              |
| 2:G:1441:ILE:HD11 | 2:G:1445:ARG:NH2  | 2.25                     | 0.49              |
| 2:G:1868:GLN:HG3  | 2:G:1898:TYR:CZ   | 2.48                     | 0.49              |
| 2:G:2029:VAL:O    | 2:G:2033:THR:HG22 | 2.12                     | 0.49              |
| 2:H:777:THR:HG23  | 2:H:1081:HIS:CE1  | 2.47                     | 0.49              |
| 2:H:1227:ARG:HG3  | 2:H:1227:ARG:NH1  | 2.01                     | 0.49              |
| 2:I:7:ARG:HE      | 2:I:27:PHE:CB     | 2.24                     | 0.49              |
| 2:I:72:VAL:HG12   | 2:I:73:GLU:N      | 2.27                     | 0.49              |
| 2:I:1632:ILE:HG23 | 2:I:1632:ILE:O    | 2.12                     | 0.49              |
| 1:A:335:HIS:O     | 1:A:338:LEU:HB3   | 2.12                     | 0.49              |
| 1:A:1460:LYS:HE3  | 1:A:1774:GLU:HA   | 1.94                     | 0.49              |
| 1:B:674:LYS:O     | 1:B:675:ASP:HB2   | 2.11                     | 0.49              |
| 1:B:1125:VAL:HG21 | 1:B:1175:ILE:CD1  | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1474:ALA:HA   | 1:B:1478:PRO:CD   | 2.41                     | 0.49              |
| 2:G:871:THR:HG21  | 2:G:887:LYS:HZ2   | 1.77                     | 0.49              |
| 2:H:7:ARG:HE      | 2:H:27:PHE:CB     | 2.26                     | 0.49              |
| 2:H:28:PHE:CE1    | 2:I:27:PHE:CE2    | 3.00                     | 0.49              |
| 2:H:871:THR:HG21  | 2:H:887:LYS:NZ    | 2.26                     | 0.49              |
| 2:H:1148:ASN:HD22 | 2:H:1151:HIS:H    | 1.60                     | 0.49              |
| 2:H:1162:ASP:O    | 2:H:1163:LYS:HB2  | 2.11                     | 0.49              |
| 2:H:1745:LYS:HD3  | 2:H:1747:LYS:HE2  | 1.94                     | 0.49              |
| 2:I:24:THR:O      | 2:I:26:SER:N      | 2.45                     | 0.49              |
| 2:I:60:LEU:O      | 2:I:63:LYS:HB2    | 2.11                     | 0.49              |
| 2:I:259:THR:HG22  | 2:I:262:GLU:CB    | 2.41                     | 0.49              |
| 2:I:274:SER:OG    | 2:I:428:HIS:HE1   | 1.95                     | 0.49              |
| 1:A:1276:GLN:O    | 1:A:1282:THR:HG21 | 2.13                     | 0.49              |
| 1:A:1501:LEU:CD1  | 1:A:1775:LEU:HG   | 2.43                     | 0.49              |
| 1:C:889:GLU:HG3   | 1:C:893:VAL:O     | 2.13                     | 0.49              |
| 1:C:1264:ARG:NH1  | 1:C:1270:VAL:HB   | 2.27                     | 0.49              |
| 1:C:1455:ARG:O    | 1:C:1459:ILE:HG13 | 2.12                     | 0.49              |
| 2:G:463:PHE:CE1   | 2:G:486:LEU:HD22  | 2.47                     | 0.49              |
| 2:G:463:PHE:HD2   | 2:G:463:PHE:O     | 1.95                     | 0.49              |
| 2:G:1486:PHE:HA   | 2:G:1504:VAL:O    | 2.12                     | 0.49              |
| 2:G:1493:LEU:HD11 | 2:G:1499:VAL:HG21 | 1.93                     | 0.49              |
| 2:H:894:ARG:NH1   | 2:H:898:ASP:OD2   | 2.41                     | 0.49              |
| 2:I:324:LEU:HD12  | 2:I:324:LEU:O     | 2.12                     | 0.49              |
| 2:I:751:LEU:HA    | 2:I:794:MET:HE3   | 1.94                     | 0.49              |
| 2:I:1352:HIS:HE1  | 2:I:1583:MET:CE   | 2.25                     | 0.49              |
| 1:A:1009:LEU:HD13 | 1:A:1445:MET:HE1  | 1.94                     | 0.49              |
| 1:A:1189:ILE:HG23 | 1:A:1190:PRO:HD2  | 1.95                     | 0.49              |
| 1:A:1460:LYS:CG   | 1:A:1773:VAL:O    | 2.60                     | 0.49              |
| 1:C:790:PHE:CE2   | 1:C:794:ILE:HD11  | 2.48                     | 0.49              |
| 1:C:1392:LEU:HD22 | 1:C:1396:MET:HG3  | 1.93                     | 0.49              |
| 2:G:677:GLN:O     | 2:G:678:PHE:HB3   | 2.13                     | 0.49              |
| 2:G:706:LYS:HE2   | 2:G:731:GLN:OE1   | 2.13                     | 0.49              |
| 2:G:950:PHE:O     | 2:G:954:VAL:HG23  | 2.13                     | 0.49              |
| 2:G:1427:VAL:HG22 | 2:G:1469:GLU:HG2  | 1.94                     | 0.49              |
| 2:H:273:HIS:CB    | 2:H:512:LEU:HD22  | 2.41                     | 0.49              |
| 2:H:682:GLY:O     | 2:H:683:ALA:HB3   | 2.13                     | 0.49              |
| 2:H:942:THR:HG21  | 2:H:1012:GLN:HA   | 1.95                     | 0.49              |
| 2:H:1889:VAL:HG13 | 2:H:1977:HIS:HB3  | 1.93                     | 0.49              |
| 2:I:238:CYS:CB    | 2:I:239:PRO:HD3   | 2.40                     | 0.49              |
| 2:I:1293:THR:CG2  | 2:I:1296:GLU:H    | 2.20                     | 0.49              |
| 2:I:1678:MET:CE   | 2:I:1707:LEU:HD22 | 2.41                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:20:TYR:CD1    | 2:G:2033:THR:OG1  | 2.59                     | 0.49              |
| 1:A:46:GLU:OE1    | 1:A:53:LEU:HB2    | 2.12                     | 0.49              |
| 1:A:1234:MET:HG2  | 1:A:1326:ILE:HD12 | 1.94                     | 0.49              |
| 1:B:435:GLU:O     | 1:B:439:ILE:HG13  | 2.12                     | 0.49              |
| 1:B:1305:CYS:SG   | 1:B:1583:HIS:NE2  | 2.85                     | 0.49              |
| 1:B:1460:LYS:HE3  | 1:B:1774:GLU:CD   | 2.33                     | 0.49              |
| 1:C:50:SER:HB2    | 1:C:51:PRO:CD     | 2.43                     | 0.49              |
| 1:C:1050:CYS:HB3  | 1:C:1089:VAL:HG12 | 1.94                     | 0.49              |
| 2:G:1738:PHE:HE1  | 2:G:1837:THR:HG23 | 1.76                     | 0.49              |
| 2:H:598:THR:O     | 2:H:602:VAL:HB    | 2.11                     | 0.49              |
| 2:H:1303:ALA:HB2  | 2:H:1556:VAL:HG21 | 1.93                     | 0.49              |
| 2:H:1417:THR:O    | 2:H:1419:PHE:N    | 2.45                     | 0.49              |
| 1:A:157:HIS:CE1   | 1:A:228:LEU:HD22  | 2.48                     | 0.49              |
| 1:A:489:VAL:HG22  | 1:A:671:VAL:N     | 2.28                     | 0.49              |
| 1:A:1451:GLN:OE1  | 1:A:1451:GLN:HA   | 2.12                     | 0.49              |
| 1:B:170:LYS:HD3   | 1:B:175:LEU:HD23  | 1.93                     | 0.49              |
| 1:B:764:ASP:OD2   | 1:B:818:ARG:HD3   | 2.11                     | 0.49              |
| 1:B:1362:PRO:HA   | 1:B:1365:MET:HG3  | 1.94                     | 0.49              |
| 1:B:1600:LEU:HD11 | 1:B:1655:VAL:HG12 | 1.94                     | 0.49              |
| 2:G:465:GLY:HA2   | 2:G:493:THR:HA    | 1.95                     | 0.49              |
| 2:H:7:ARG:HH11    | 2:H:24:THR:HG23   | 1.75                     | 0.49              |
| 2:H:22:VAL:HG11   | 2:H:27:PHE:HA     | 1.94                     | 0.49              |
| 2:H:138:ASP:O     | 2:H:139:LYS:HG3   | 2.12                     | 0.49              |
| 2:H:369:SER:O     | 2:H:370:LEU:HD23  | 2.13                     | 0.49              |
| 2:H:715:GLN:O     | 2:H:719:ILE:HG12  | 2.13                     | 0.49              |
| 2:H:949:ASP:CB    | 2:H:1006:MET:HE2  | 2.42                     | 0.49              |
| 2:H:1566:SER:HB3  | 2:H:1568:HIS:CE1  | 2.47                     | 0.49              |
| 2:I:7:ARG:CZ      | 2:I:24:THR:HA     | 2.42                     | 0.49              |
| 2:I:16:LEU:HG     | 2:I:48:PHE:CZ     | 2.48                     | 0.49              |
| 2:I:55:THR:CG2    | 2:I:56:THR:HG22   | 2.33                     | 0.49              |
| 2:I:161:GLY:HA3   | 2:I:506:PRO:HD2   | 1.93                     | 0.49              |
| 2:I:1015:VAL:HG13 | 2:I:1017:PHE:CE2  | 2.47                     | 0.49              |
| 2:I:1265:MET:CE   | 2:I:1562:PRO:HG2  | 2.41                     | 0.49              |
| 2:I:1435:ILE:HG22 | 2:I:1435:ILE:O    | 2.12                     | 0.49              |
| 1:A:18:LEU:HD21   | 2:G:1815:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:256:LEU:HD22  | 1:A:260:ARG:HB3   | 1.94                     | 0.49              |
| 1:A:328:LEU:HD13  | 1:A:329:GLU:N     | 2.27                     | 0.49              |
| 1:A:1264:ARG:NH1  | 1:A:1270:VAL:HB   | 2.28                     | 0.49              |
| 1:A:1705:PRO:HB2  | 1:A:1733:PHE:CE1  | 2.47                     | 0.49              |
| 1:B:1105:LEU:HD23 | 1:B:1185:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:636:PRO:HB2   | 1:C:638:LEU:O     | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:980:VAL:HG23  | 2:I:968:GLN:OE1   | 2.13                     | 0.49              |
| 2:G:618:GLU:HG2   | 2:G:678:PHE:CZ    | 2.48                     | 0.49              |
| 2:G:1266:TYR:HB2  | 2:G:1347:LEU:HD23 | 1.95                     | 0.49              |
| 2:H:161:GLY:N     | 2:H:505:GLY:HA3   | 2.25                     | 0.49              |
| 2:H:455:ILE:HD11  | 2:H:469:ARG:NE    | 2.27                     | 0.49              |
| 2:H:463:PHE:O     | 2:H:463:PHE:HD2   | 1.96                     | 0.49              |
| 2:H:1873:TYR:HE1  | 2:H:1877:ARG:HH21 | 1.59                     | 0.49              |
| 2:I:740:HIS:CE1   | 2:I:852:GLU:OE1   | 2.65                     | 0.49              |
| 2:I:1169:PRO:O    | 2:I:1173:VAL:HG23 | 2.13                     | 0.49              |
| 2:I:1873:TYR:CE2  | 2:I:1940:LEU:HD21 | 2.47                     | 0.49              |
| 1:A:21:GLN:HG3    | 2:G:2013:ASN:HB2  | 1.93                     | 0.49              |
| 1:B:1642:THR:HG22 | 1:B:1652:GLN:HG3  | 1.93                     | 0.49              |
| 1:C:982:ILE:HD11  | 2:I:965:SER:HB2   | 1.95                     | 0.49              |
| 1:C:1114:TYR:CD1  | 1:C:1337:GLU:HG3  | 2.48                     | 0.49              |
| 2:G:157:VAL:HG11  | 2:G:496:PHE:CZ    | 2.47                     | 0.49              |
| 2:G:491:GLU:HA    | 2:G:494:THR:HG22  | 1.95                     | 0.49              |
| 2:G:732:TRP:CD1   | 2:G:750:MET:HE3   | 2.47                     | 0.49              |
| 2:H:173:LEU:O     | 2:H:173:LEU:HD22  | 2.13                     | 0.49              |
| 2:H:569:LEU:HD12  | 2:H:1090:TYR:CD1  | 2.48                     | 0.49              |
| 2:H:702:TYR:HB2   | 2:H:727:PRO:HB2   | 1.94                     | 0.49              |
| 2:H:932:ILE:HD12  | 2:H:939:PHE:HD1   | 1.78                     | 0.49              |
| 2:H:1593:ILE:O    | 2:H:1597:ALA:HB3  | 2.12                     | 0.49              |
| 2:H:1634:GLY:HA3  | 2:H:1799:PRO:HA   | 1.94                     | 0.49              |
| 2:H:1666:PHE:CD1  | 2:H:1814:ALA:HA   | 2.48                     | 0.49              |
| 2:I:11:LEU:HD11   | 2:I:64:PHE:CD2    | 2.48                     | 0.49              |
| 2:I:573:LYS:HE3   | 2:I:1101:GLU:OE1  | 2.12                     | 0.49              |
| 2:I:597:MET:H     | 2:I:601:THR:HB    | 1.78                     | 0.49              |
| 2:I:949:ASP:CB    | 2:I:1006:MET:HE2  | 2.43                     | 0.49              |
| 1:A:1219:VAL:CA   | 1:A:1384:ILE:HD11 | 2.31                     | 0.49              |
| 1:A:1362:PRO:HA   | 1:A:1365:MET:HG3  | 1.95                     | 0.49              |
| 1:B:186:ILE:O     | 1:B:190:LEU:HG    | 2.13                     | 0.49              |
| 1:C:18:LEU:HD21   | 2:I:1815:LEU:HD12 | 1.94                     | 0.49              |
| 1:C:20:TYR:CD2    | 2:I:2033:THR:OG1  | 2.66                     | 0.49              |
| 1:C:267:VAL:HG12  | 1:C:290:MET:CE    | 2.42                     | 0.49              |
| 1:C:1020:VAL:CG1  | 1:C:1400:ILE:HG23 | 2.42                     | 0.49              |
| 2:G:161:GLY:N     | 2:G:505:GLY:HA3   | 2.24                     | 0.49              |
| 2:G:273:HIS:CB    | 2:G:512:LEU:HD22  | 2.42                     | 0.49              |
| 2:G:1130:THR:H    | 2:G:1133:THR:CG2  | 2.26                     | 0.49              |
| 2:H:428:HIS:HD2   | 2:H:486:LEU:O     | 1.96                     | 0.49              |
| 2:H:1749:GLU:OE2  | 2:H:1840:VAL:HG13 | 2.12                     | 0.49              |
| 2:I:173:LEU:O     | 2:I:173:LEU:HD22  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:306:ILE:HA    | 2:I:439:ILE:HD13  | 1.94                     | 0.49              |
| 2:I:1567:ARG:HH11 | 2:I:1567:ARG:HG2  | 1.70                     | 0.49              |
| 1:A:1009:LEU:HG   | 1:A:1664:ALA:HB2  | 1.95                     | 0.49              |
| 1:A:1022:THR:HG22 | 1:A:1226:SER:CB   | 2.43                     | 0.49              |
| 1:A:1749:THR:CB   | 1:A:1874:ASP:N    | 2.75                     | 0.49              |
| 1:B:1312:VAL:CG2  | 1:B:1329:VAL:HG11 | 2.39                     | 0.49              |
| 1:C:32:GLN:NE2    | 1:C:57:ALA:HA     | 2.28                     | 0.49              |
| 1:C:335:HIS:O     | 1:C:335:HIS:CD2   | 2.65                     | 0.49              |
| 2:G:173:LEU:O     | 2:G:173:LEU:HD22  | 2.13                     | 0.49              |
| 2:G:259:THR:HG22  | 2:G:262:GLU:CB    | 2.43                     | 0.49              |
| 2:G:560:ASN:O     | 2:G:560:ASN:OD1   | 2.30                     | 0.49              |
| 2:G:653:TYR:HD1   | 2:G:659:LEU:HD21  | 1.78                     | 0.49              |
| 2:G:715:GLN:O     | 2:G:719:ILE:HG12  | 2.13                     | 0.49              |
| 2:G:807:ILE:HD12  | 2:G:1063:THR:HG23 | 1.95                     | 0.49              |
| 2:G:1666:PHE:CD1  | 2:G:1814:ALA:HA   | 2.48                     | 0.49              |
| 2:G:1913:VAL:O    | 2:G:1917:ILE:HG13 | 2.12                     | 0.49              |
| 2:G:2036:GLU:HG2  | 2:G:2039:LYS:NZ   | 2.28                     | 0.49              |
| 2:H:860:ARG:HB2   | 2:H:1049:GLN:HG3  | 1.94                     | 0.49              |
| 2:H:1002:HIS:NE2  | 2:H:1006:MET:HE3  | 2.27                     | 0.49              |
| 2:I:428:HIS:HD2   | 2:I:486:LEU:O     | 1.95                     | 0.49              |
| 2:I:881:VAL:N     | 2:I:882:PRO:CD    | 2.76                     | 0.49              |
| 2:I:1567:ARG:NH1  | 2:I:1568:HIS:HB3  | 2.28                     | 0.49              |
| 1:A:1021:VAL:HG22 | 1:A:1387:ILE:HG22 | 1.95                     | 0.48              |
| 1:A:1312:VAL:CG2  | 1:A:1329:VAL:HG11 | 2.41                     | 0.48              |
| 1:B:182:VAL:O     | 1:B:186:ILE:HG13  | 2.12                     | 0.48              |
| 1:B:916:LEU:HD22  | 1:B:922:VAL:HG22  | 1.94                     | 0.48              |
| 1:B:1753:ALA:HB2  | 1:B:1872:SER:OG   | 2.13                     | 0.48              |
| 1:C:1105:LEU:HD23 | 1:C:1185:VAL:HG22 | 1.94                     | 0.48              |
| 1:C:1693:ILE:CD1  | 2:I:998:GLN:HB2   | 2.40                     | 0.48              |
| 2:G:402:LEU:HD12  | 2:G:404:GLN:HG2   | 1.95                     | 0.48              |
| 2:G:598:THR:O     | 2:G:602:VAL:HB    | 2.13                     | 0.48              |
| 2:H:465:GLY:HA2   | 2:H:493:THR:HA    | 1.95                     | 0.48              |
| 2:H:739:GLY:HA2   | 2:H:1054:LEU:HG   | 1.95                     | 0.48              |
| 2:H:1931:LEU:HB3  | 2:H:1935:GLU:CG   | 2.36                     | 0.48              |
| 2:I:161:GLY:N     | 2:I:505:GLY:HA3   | 2.24                     | 0.48              |
| 2:I:663:ILE:HB    | 2:I:664:PRO:CD    | 2.42                     | 0.48              |
| 2:I:835:THR:HG22  | 2:I:844:VAL:HA    | 1.95                     | 0.48              |
| 2:I:1697:HIS:HE1  | 2:I:1829:GLU:CG   | 2.26                     | 0.48              |
| 1:B:187:LEU:HD22  | 1:B:201:PRO:HB2   | 1.94                     | 0.48              |
| 1:B:465:ASN:O     | 1:B:469:VAL:HG23  | 2.12                     | 0.48              |
| 2:G:11:LEU:HD11   | 2:G:64:PHE:CD2    | 2.48                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:G:376:ASN:C    | 2:G:376:ASN:ND2   | 2.67                     | 0.48              |
| 2:G:597:MET:H    | 2:G:601:THR:HB    | 1.77                     | 0.48              |
| 2:G:1745:LYS:HE2 | 2:G:1747:LYS:HG2  | 1.95                     | 0.48              |
| 2:G:2046:GLU:C   | 2:G:2048:TYR:H    | 2.15                     | 0.48              |
| 2:H:259:THR:HG22 | 2:H:262:GLU:CB    | 2.42                     | 0.48              |
| 2:H:306:ILE:HA   | 2:H:439:ILE:CD1   | 2.42                     | 0.48              |
| 2:H:786:SER:CB   | 2:H:794:MET:HE2   | 2.43                     | 0.48              |
| 2:H:901:LYS:NZ   | 2:H:1031:LYS:O    | 2.46                     | 0.48              |
| 2:H:1272:ASP:O   | 2:H:1273:GLU:HG3  | 2.13                     | 0.48              |
| 2:H:1868:GLN:HG3 | 2:H:1898:TYR:CZ   | 2.48                     | 0.48              |
| 2:I:629:GLY:O    | 2:I:632:ALA:HB3   | 2.13                     | 0.48              |
| 2:I:682:GLY:O    | 2:I:683:ALA:HB3   | 2.13                     | 0.48              |
| 2:I:970:TYR:O    | 2:I:973:LEU:HB2   | 2.14                     | 0.48              |
| 2:I:1674:GLN:OE1 | 2:I:1712:ASN:HA   | 2.13                     | 0.48              |
| 1:A:1477:ILE:H   | 1:A:1478:PRO:HD3  | 1.78                     | 0.48              |
| 1:B:2:LYS:HE2    | 1:B:4:GLU:CD      | 2.34                     | 0.48              |
| 1:B:157:HIS:HE1  | 1:B:228:LEU:HD22  | 1.77                     | 0.48              |
| 1:B:413:LEU:C    | 1:B:415:SER:H     | 2.17                     | 0.48              |
| 1:C:256:LEU:HD22 | 1:C:260:ARG:HB3   | 1.95                     | 0.48              |
| 1:C:1305:CYS:SG  | 3:C:2748:CER:C5   | 3.01                     | 0.48              |
| 1:C:1523:ARG:NH2 | 1:C:1564:LEU:O    | 2.46                     | 0.48              |
| 2:G:7:ARG:HE     | 2:G:27:PHE:CB     | 2.25                     | 0.48              |
| 2:G:533:LEU:HD13 | 2:G:545:GLN:HG3   | 1.94                     | 0.48              |
| 2:G:754:TYR:CE2  | 2:G:794:MET:HG3   | 2.48                     | 0.48              |
| 2:G:1330:GLY:HA2 | 2:G:1374:THR:HG21 | 1.94                     | 0.48              |
| 2:G:1428:GLU:HG2 | 2:G:1470:THR:HG22 | 1.94                     | 0.48              |
| 2:H:33:LEU:HD21  | 2:H:80:PHE:CE2    | 2.49                     | 0.48              |
| 2:H:40:ILE:O     | 2:H:42:PRO:HD3    | 2.13                     | 0.48              |
| 2:H:463:PHE:CD1  | 2:H:486:LEU:HD22  | 2.48                     | 0.48              |
| 2:H:955:GLU:HG2  | 2:H:987:TYR:HE2   | 1.78                     | 0.48              |
| 2:I:278:VAL:HG11 | 2:I:303:LEU:HD13  | 1.95                     | 0.48              |
| 2:I:786:SER:CB   | 2:I:794:MET:HE2   | 2.42                     | 0.48              |
| 2:I:1130:THR:H   | 2:I:1133:THR:CG2  | 2.25                     | 0.48              |
| 2:I:1873:TYR:CE1 | 2:I:1877:ARG:NE   | 2.77                     | 0.48              |
| 1:A:340:ARG:HH12 | 1:A:344:GLN:HE21  | 1.60                     | 0.48              |
| 1:B:328:LEU:HD13 | 1:B:329:GLU:N     | 2.29                     | 0.48              |
| 1:B:332:THR:HG22 | 1:C:331:ILE:CD1   | 2.44                     | 0.48              |
| 1:B:335:HIS:O    | 1:B:338:LEU:HB3   | 2.14                     | 0.48              |
| 1:B:702:LYS:HD3  | 1:B:731:THR:CG2   | 2.44                     | 0.48              |
| 1:C:331:ILE:HG23 | 1:C:332:THR:N     | 2.28                     | 0.48              |
| 2:G:455:ILE:HG12 | 2:G:469:ARG:HG2   | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:720:ALA:HA    | 2:G:728:ILE:CD1   | 2.43                     | 0.48              |
| 2:G:1980:TYR:HD1  | 2:G:1981:LEU:HD12 | 1.79                     | 0.48              |
| 2:H:428:HIS:CD2   | 2:H:488:VAL:HG23  | 2.49                     | 0.48              |
| 2:H:995:LEU:HB3   | 2:H:1000:ILE:HD11 | 1.94                     | 0.48              |
| 2:H:1422:THR:HG23 | 2:H:1474:PHE:CD1  | 2.48                     | 0.48              |
| 2:H:1624:THR:HB   | 2:H:1642:THR:OG1  | 2.14                     | 0.48              |
| 2:I:146:PHE:HA    | 2:I:149:VAL:HG12  | 1.92                     | 0.48              |
| 2:I:249:TYR:CD2   | 2:I:283:ILE:HD11  | 2.48                     | 0.48              |
| 2:I:402:LEU:HD12  | 2:I:404:GLN:HG2   | 1.94                     | 0.48              |
| 2:I:455:ILE:HG13  | 2:I:455:ILE:O     | 2.13                     | 0.48              |
| 2:I:551:THR:HG22  | 2:I:552:SER:N     | 2.29                     | 0.48              |
| 2:I:593:LEU:HD21  | 2:I:800:LEU:HB3   | 1.95                     | 0.48              |
| 2:I:995:LEU:HB3   | 2:I:1000:ILE:HD11 | 1.95                     | 0.48              |
| 2:I:1850:SER:HB2  | 2:I:1973:SER:HB2  | 1.95                     | 0.48              |
| 1:A:1714:VAL:HG22 | 1:A:1738:ILE:HD11 | 1.96                     | 0.48              |
| 1:B:21:GLN:HG3    | 2:H:2013:ASN:HB2  | 1.95                     | 0.48              |
| 1:B:408:TRP:CH2   | 1:B:1628:SER:HB3  | 2.47                     | 0.48              |
| 1:B:998:TYR:CE2   | 1:B:1667:GLU:HB2  | 2.49                     | 0.48              |
| 1:C:988:ILE:HD13  | 1:C:1048:GLU:CB   | 2.43                     | 0.48              |
| 1:C:1477:ILE:H    | 1:C:1478:PRO:HD3  | 1.78                     | 0.48              |
| 1:C:1642:THR:HG22 | 1:C:1652:GLN:HG3  | 1.96                     | 0.48              |
| 2:G:995:LEU:HB3   | 2:G:1000:ILE:HD11 | 1.96                     | 0.48              |
| 2:G:1567:ARG:CG   | 2:G:1567:ARG:NH1  | 2.51                     | 0.48              |
| 2:H:145:LEU:HD21  | 2:H:156:LEU:HD21  | 1.95                     | 0.48              |
| 2:H:1100:VAL:CG2  | 2:H:1147:ILE:HG21 | 2.43                     | 0.48              |
| 2:H:1918:LYS:HG2  | 2:H:1919:LEU:HD23 | 1.96                     | 0.48              |
| 2:H:1953:VAL:O    | 2:H:1953:VAL:HG12 | 2.14                     | 0.48              |
| 2:H:1986:LYS:HA   | 2:H:1989:LYS:HB3  | 1.95                     | 0.48              |
| 2:I:569:LEU:HD12  | 2:I:1090:TYR:CD1  | 2.48                     | 0.48              |
| 2:I:1081:HIS:O    | 2:I:1085:LEU:HB2  | 2.14                     | 0.48              |
| 2:I:1266:TYR:HB2  | 2:I:1347:LEU:HD23 | 1.95                     | 0.48              |
| 2:I:1382:VAL:HA   | 2:I:1422:THR:OG1  | 2.12                     | 0.48              |
| 1:A:19:ALA:O      | 1:A:22:PHE:HB2    | 2.14                     | 0.48              |
| 1:A:20:TYR:CE1    | 2:G:2033:THR:CG2  | 2.97                     | 0.48              |
| 1:A:444:ASN:HB2   | 1:A:447:LEU:N     | 2.14                     | 0.48              |
| 1:A:1401:TYR:C    | 1:A:1658:PRO:HG3  | 2.33                     | 0.48              |
| 1:B:503:ILE:HD12  | 1:B:950:THR:HG21  | 1.96                     | 0.48              |
| 1:C:430:ARG:NH1   | 1:C:493:VAL:O     | 2.44                     | 0.48              |
| 1:C:764:ASP:OD2   | 1:C:818:ARG:HD3   | 2.12                     | 0.48              |
| 2:G:72:VAL:HG12   | 2:G:73:GLU:N      | 2.28                     | 0.48              |
| 2:G:569:LEU:HD12  | 2:G:1090:TYR:CD1  | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:593:LEU:HD21  | 2:G:800:LEU:HB3   | 1.96                     | 0.48              |
| 2:G:1148:ASN:C    | 2:G:1148:ASN:HD22 | 2.17                     | 0.48              |
| 2:G:1213:LEU:O    | 2:G:1214:LEU:HD23 | 2.12                     | 0.48              |
| 2:H:99:ASN:HA     | 2:H:550:VAL:HG21  | 1.95                     | 0.48              |
| 2:H:397:LYS:HB3   | 2:H:416:PHE:CE2   | 2.48                     | 0.48              |
| 2:H:784:GLU:O     | 2:H:787:THR:HB    | 2.13                     | 0.48              |
| 2:H:1632:ILE:HG23 | 2:H:1632:ILE:O    | 2.13                     | 0.48              |
| 2:I:7:ARG:HH11    | 2:I:24:THR:HG23   | 1.77                     | 0.48              |
| 2:I:121:GLU:HA    | 2:I:124:LYS:HD2   | 1.96                     | 0.48              |
| 2:I:533:LEU:HG    | 2:I:533:LEU:O     | 2.13                     | 0.48              |
| 2:I:586:LEU:HD12  | 2:I:764:MET:SD    | 2.54                     | 0.48              |
| 2:I:1159:ILE:CG1  | 2:I:1169:PRO:CD   | 2.90                     | 0.48              |
| 2:I:1738:PHE:CE1  | 2:I:1837:THR:HG23 | 2.48                     | 0.48              |
| 1:A:182:VAL:O     | 1:A:186:ILE:HG13  | 2.14                     | 0.48              |
| 1:A:420:ILE:HG22  | 1:A:469:VAL:HG22  | 1.96                     | 0.48              |
| 1:A:988:ILE:HA    | 1:A:1048:GLU:CG   | 2.44                     | 0.48              |
| 1:C:852:ARG:NH1   | 1:C:852:ARG:CG    | 2.66                     | 0.48              |
| 1:C:1276:GLN:O    | 1:C:1282:THR:HG21 | 2.13                     | 0.48              |
| 1:C:1300:THR:HA   | 1:C:1301:PRO:HD3  | 1.67                     | 0.48              |
| 1:C:1312:VAL:CG2  | 1:C:1329:VAL:HG11 | 2.44                     | 0.48              |
| 1:C:1396:MET:O    | 1:C:1680:ARG:NH1  | 2.46                     | 0.48              |
| 1:C:1451:GLN:HA   | 1:C:1451:GLN:OE1  | 2.13                     | 0.48              |
| 1:C:1617:ILE:O    | 1:C:1620:GLN:HG2  | 2.13                     | 0.48              |
| 2:G:240:LEU:O     | 2:G:244:ILE:HG13  | 2.13                     | 0.48              |
| 2:G:1590:ARG:HG3  | 2:G:1608:TYR:CD2  | 2.48                     | 0.48              |
| 2:G:2026:PHE:HD2  | 2:G:2045:TRP:HZ3  | 1.59                     | 0.48              |
| 2:H:561:TRP:CZ3   | 2:H:792:PRO:HB2   | 2.49                     | 0.48              |
| 2:H:751:LEU:HD23  | 2:H:791:TYR:CZ    | 2.49                     | 0.48              |
| 2:H:1674:GLN:OE1  | 2:H:1712:ASN:HA   | 2.12                     | 0.48              |
| 2:I:667:LYS:HD2   | 2:I:697:THR:CG2   | 2.35                     | 0.48              |
| 2:I:762:ASN:HD22  | 2:I:762:ASN:N     | 1.88                     | 0.48              |
| 2:I:1697:HIS:HE1  | 2:I:1829:GLU:HG2  | 1.77                     | 0.48              |
| 1:A:539:SER:O     | 1:A:540:GLN:C     | 2.52                     | 0.48              |
| 1:A:1037:TRP:HB2  | 1:A:1598:GLN:OE1  | 2.13                     | 0.48              |
| 1:B:625:THR:HG23  | 1:B:661:ASP:OD1   | 2.13                     | 0.48              |
| 1:B:790:PHE:CE2   | 1:B:794:ILE:HD11  | 2.47                     | 0.48              |
| 1:B:1056:ILE:HD13 | 1:B:1193:TRP:CD1  | 2.45                     | 0.48              |
| 1:B:1183:ARG:NH1  | 1:B:1344:GLY:HA2  | 2.29                     | 0.48              |
| 1:C:888:ILE:HD12  | 1:C:939:PHE:CE2   | 2.47                     | 0.48              |
| 1:C:1738:ILE:O    | 1:C:1739:GLN:HB2  | 2.14                     | 0.48              |
| 2:G:1180:MET:HB2  | 2:G:1197:LEU:HD21 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:169:TYR:CG    | 2:H:170:PHE:N     | 2.81                     | 0.48              |
| 2:H:214:ASN:ND2   | 2:H:217:GLU:HB2   | 2.27                     | 0.48              |
| 2:H:317:THR:HG21  | 2:I:1309:GLU:CG   | 2.42                     | 0.48              |
| 2:H:490:TRP:HA    | 2:H:493:THR:HG22  | 1.96                     | 0.48              |
| 2:H:597:MET:H     | 2:H:601:THR:HB    | 1.78                     | 0.48              |
| 2:H:1040:LEU:O    | 2:H:1046:GLN:HG3  | 2.13                     | 0.48              |
| 2:I:845:THR:HG22  | 2:I:855:HIS:CD2   | 2.49                     | 0.48              |
| 2:I:1325:PHE:CE1  | 2:I:1328:VAL:HG11 | 2.49                     | 0.48              |
| 2:I:1586:SER:O    | 2:I:1590:ARG:HB2  | 2.14                     | 0.48              |
| 1:A:427:ASN:HB2   | 1:A:468:LEU:HD21  | 1.95                     | 0.48              |
| 1:A:695:GLY:HA3   | 1:A:906:LEU:HD11  | 1.94                     | 0.48              |
| 1:B:243:ILE:O     | 1:B:247:ARG:HG3   | 2.13                     | 0.48              |
| 2:G:306:ILE:HA    | 2:G:439:ILE:HD13  | 1.96                     | 0.48              |
| 2:G:432:LEU:HB3   | 2:G:484:ILE:HG23  | 1.96                     | 0.48              |
| 2:G:481:ASP:OD2   | 2:G:485:ARG:NH1   | 2.47                     | 0.48              |
| 2:H:489:LYS:O     | 2:H:493:THR:HG22  | 2.13                     | 0.48              |
| 2:H:868:PHE:HB3   | 2:H:873:PHE:CE2   | 2.48                     | 0.48              |
| 2:I:772:GLY:O     | 2:I:804:ARG:HD3   | 2.14                     | 0.48              |
| 2:I:1159:ILE:HG22 | 2:I:1160:THR:N    | 2.28                     | 0.48              |
| 1:A:328:LEU:N     | 1:A:330:GLU:H     | 2.12                     | 0.48              |
| 1:A:927:ASN:O     | 1:A:929:GLY:N     | 2.41                     | 0.48              |
| 1:A:1639:VAL:HG12 | 1:A:1640:SER:N    | 2.28                     | 0.48              |
| 1:B:328:LEU:N     | 1:B:330:GLU:H     | 2.11                     | 0.48              |
| 1:B:683:ALA:HA    | 1:B:689:GLY:HA3   | 1.95                     | 0.48              |
| 1:B:930:LEU:HD23  | 1:B:930:LEU:HA    | 1.67                     | 0.48              |
| 1:B:1319:ILE:HA   | 1:B:1324:ALA:O    | 2.13                     | 0.48              |
| 1:C:386:PHE:O     | 1:C:390:VAL:HB    | 2.14                     | 0.48              |
| 1:C:751:PHE:CZ    | 1:C:761:LEU:HD13  | 2.49                     | 0.48              |
| 2:G:173:LEU:HD13  | 2:G:219:LEU:HD21  | 1.94                     | 0.48              |
| 2:G:461:ASP:HB3   | 2:G:464:ASP:HB2   | 1.95                     | 0.48              |
| 2:G:1148:ASN:ND2  | 2:G:1151:HIS:H    | 2.12                     | 0.48              |
| 2:G:1325:PHE:CE1  | 2:G:1328:VAL:HG11 | 2.48                     | 0.48              |
| 2:H:157:VAL:HG11  | 2:H:496:PHE:CZ    | 2.49                     | 0.48              |
| 2:H:232:LEU:HD21  | 2:H:423:VAL:HA    | 1.95                     | 0.48              |
| 2:H:706:LYS:HE2   | 2:H:731:GLN:OE1   | 2.14                     | 0.48              |
| 2:I:214:ASN:ND2   | 2:I:217:GLU:HB2   | 2.28                     | 0.48              |
| 2:I:489:LYS:O     | 2:I:493:THR:HG22  | 2.13                     | 0.48              |
| 2:I:753:MET:O     | 2:I:757:ILE:HG13  | 2.14                     | 0.48              |
| 2:I:2026:PHE:HD2  | 2:I:2045:TRP:HZ3  | 1.60                     | 0.48              |
| 1:A:187:LEU:HD22  | 1:A:201:PRO:HB2   | 1.96                     | 0.47              |
| 1:B:1:MET:HE3     | 1:B:9:LEU:HD12    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1646:PHE:CE1  | 3:B:2748:CER:H31  | 2.49                     | 0.47              |
| 1:C:440:MET:HE3   | 1:C:483:VAL:HG21  | 1.95                     | 0.47              |
| 1:C:529:MET:HG2   | 1:C:638:LEU:HG    | 1.95                     | 0.47              |
| 1:C:1392:LEU:CD2  | 1:C:1396:MET:HG3  | 2.44                     | 0.47              |
| 2:G:22:VAL:HG11   | 2:G:27:PHE:HA     | 1.96                     | 0.47              |
| 2:G:567:PRO:HG3   | 2:G:781:LEU:CD1   | 2.44                     | 0.47              |
| 2:G:1027:ILE:O    | 2:G:1031:LYS:HB2  | 2.14                     | 0.47              |
| 2:G:1566:SER:HB3  | 2:G:1568:HIS:CE1  | 2.49                     | 0.47              |
| 2:H:873:PHE:CD1   | 2:H:1026:GLU:HB2  | 2.49                     | 0.47              |
| 2:H:943:TRP:CZ2   | 2:H:1016:PRO:HG3  | 2.49                     | 0.47              |
| 2:H:1590:ARG:NH2  | 2:H:1594:GLU:OE2  | 2.47                     | 0.47              |
| 2:I:176:LEU:HD22  | 2:I:247:ALA:HB1   | 1.96                     | 0.47              |
| 2:I:594:VAL:CG2   | 2:I:610:THR:HG21  | 2.44                     | 0.47              |
| 2:I:900:GLN:NE2   | 2:I:1051:THR:HA   | 2.28                     | 0.47              |
| 2:I:1002:HIS:NE2  | 2:I:1006:MET:HE3  | 2.29                     | 0.47              |
| 2:I:1015:VAL:HA   | 2:I:1016:PRO:HD3  | 1.74                     | 0.47              |
| 2:I:1834:ARG:NH1  | 2:I:1834:ARG:CG   | 2.66                     | 0.47              |
| 1:A:176:VAL:HG12  | 1:A:178:GLY:H     | 1.79                     | 0.47              |
| 1:A:1501:LEU:O    | 1:A:1505:GLN:HG3  | 2.14                     | 0.47              |
| 1:B:256:LEU:HD22  | 1:B:260:ARG:HB3   | 1.95                     | 0.47              |
| 1:B:1367:ARG:HH12 | 1:B:1372:THR:CB   | 2.20                     | 0.47              |
| 1:C:427:ASN:HB2   | 1:C:468:LEU:HD21  | 1.95                     | 0.47              |
| 1:C:1021:VAL:HG11 | 1:C:1597:LEU:CD1  | 2.44                     | 0.47              |
| 1:C:1125:VAL:HG21 | 1:C:1175:ILE:CD1  | 2.43                     | 0.47              |
| 2:G:40:ILE:O      | 2:G:42:PRO:HD3    | 2.14                     | 0.47              |
| 2:G:777:THR:HG23  | 2:G:1081:HIS:CE1  | 2.49                     | 0.47              |
| 2:H:159:ILE:CG2   | 2:H:501:ILE:HG22  | 2.44                     | 0.47              |
| 2:H:213:LEU:HG    | 2:H:213:LEU:O     | 2.14                     | 0.47              |
| 2:H:732:TRP:CD2   | 2:H:750:MET:HE1   | 2.49                     | 0.47              |
| 2:H:950:PHE:O     | 2:H:954:VAL:HG23  | 2.13                     | 0.47              |
| 2:H:1749:GLU:OE2  | 2:H:1840:VAL:CG1  | 2.62                     | 0.47              |
| 1:A:683:ALA:HA    | 1:A:689:GLY:HA3   | 1.95                     | 0.47              |
| 1:A:852:ARG:HB3   | 1:A:858:TRP:HZ2   | 1.80                     | 0.47              |
| 1:A:1238:VAL:CG1  | 1:A:1242:GLU:HB2  | 2.44                     | 0.47              |
| 1:A:1303:GLY:C    | 1:A:1307:THR:HG22 | 2.35                     | 0.47              |
| 1:B:530:ALA:HA    | 1:B:636:PRO:HB3   | 1.97                     | 0.47              |
| 1:B:1116:PRO:HB2  | 1:B:1184:LEU:HD12 | 1.95                     | 0.47              |
| 1:B:1209:ASP:OD2  | 1:B:1253:GLY:HA2  | 2.14                     | 0.47              |
| 1:C:1010:GLU:HA   | 1:C:1664:ALA:HA   | 1.95                     | 0.47              |
| 1:C:1516:ASP:HA   | 1:C:1517:PRO:HD3  | 1.66                     | 0.47              |
| 2:G:428:HIS:HD2   | 2:G:486:LEU:O     | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:804:ARG:NH2   | 2:G:1068:GLU:OE1  | 2.48                     | 0.47              |
| 2:G:1624:THR:HB   | 2:G:1642:THR:OG1  | 2.15                     | 0.47              |
| 2:G:1666:PHE:CD1  | 2:G:1814:ALA:HB2  | 2.49                     | 0.47              |
| 2:H:589:ARG:HB3   | 2:H:590:PRO:CD    | 2.43                     | 0.47              |
| 2:H:1438:SER:O    | 2:H:1441:ILE:HG23 | 2.13                     | 0.47              |
| 2:I:926:LEU:HB3   | 2:I:947:THR:CG2   | 2.43                     | 0.47              |
| 2:I:1579:ILE:HD11 | 2:I:1615:MET:SD   | 2.53                     | 0.47              |
| 2:I:1752:PHE:HZ   | 2:I:1836:MET:HE3  | 1.80                     | 0.47              |
| 1:C:370:GLU:O     | 1:C:373:ALA:HB3   | 2.14                     | 0.47              |
| 1:C:526:VAL:HG12  | 1:C:626:VAL:HG11  | 1.96                     | 0.47              |
| 1:C:987:ASN:HD22  | 2:I:957:ARG:CD    | 2.26                     | 0.47              |
| 1:C:998:TYR:CE2   | 1:C:1667:GLU:HB2  | 2.49                     | 0.47              |
| 1:C:1133:PRO:HG3  | 1:C:1166:LYS:HG3  | 1.96                     | 0.47              |
| 1:C:1138:LYS:HG3  | 1:C:1163:TYR:CE1  | 2.48                     | 0.47              |
| 2:G:33:LEU:HD21   | 2:G:80:PHE:CE2    | 2.50                     | 0.47              |
| 2:G:169:TYR:CG    | 2:G:170:PHE:N     | 2.83                     | 0.47              |
| 2:G:512:LEU:O     | 2:G:516:THR:HG23  | 2.15                     | 0.47              |
| 2:H:597:MET:HA    | 4:H:3051:FMN:N5   | 2.30                     | 0.47              |
| 2:H:634:ILE:HD11  | 2:H:649:ILE:CD1   | 2.40                     | 0.47              |
| 2:H:677:GLN:O     | 2:H:678:PHE:HB3   | 2.15                     | 0.47              |
| 2:H:1425:LYS:HG2  | 2:H:1471:GLU:HG3  | 1.95                     | 0.47              |
| 2:H:1472:VAL:CG2  | 2:H:1483:VAL:HG22 | 2.44                     | 0.47              |
| 2:H:1486:PHE:HA   | 2:H:1504:VAL:O    | 2.14                     | 0.47              |
| 2:I:233:SER:HA    | 2:I:424:ALA:CB    | 2.44                     | 0.47              |
| 2:I:562:LEU:HG    | 2:I:793:PRO:CB    | 2.44                     | 0.47              |
| 2:I:1804:PHE:CD2  | 2:I:1818:LEU:HD22 | 2.49                     | 0.47              |
| 1:A:1012:LEU:HD23 | 1:A:1445:MET:CE   | 2.43                     | 0.47              |
| 1:A:1208:VAL:HG11 | 1:A:1212:THR:HB   | 1.96                     | 0.47              |
| 1:A:1319:ILE:HA   | 1:A:1324:ALA:O    | 2.14                     | 0.47              |
| 1:B:20:TYR:CG     | 2:H:2033:THR:OG1  | 2.67                     | 0.47              |
| 1:B:331:ILE:HG23  | 1:B:332:THR:N     | 2.29                     | 0.47              |
| 1:B:531:LEU:HD21  | 1:B:629:THR:HG22  | 1.97                     | 0.47              |
| 1:B:1477:ILE:H    | 1:B:1478:PRO:HD3  | 1.79                     | 0.47              |
| 1:C:142:ASP:CG    | 1:C:257:PRO:HB2   | 2.34                     | 0.47              |
| 1:C:328:LEU:N     | 1:C:330:GLU:H     | 2.12                     | 0.47              |
| 1:C:1303:GLY:CA   | 1:C:1649:LYS:HE2  | 2.36                     | 0.47              |
| 2:G:123:ILE:CD1   | 2:G:533:LEU:CD2   | 2.93                     | 0.47              |
| 2:G:463:PHE:CD1   | 2:G:486:LEU:HD22  | 2.48                     | 0.47              |
| 2:G:732:TRP:CD2   | 2:G:750:MET:HE3   | 2.48                     | 0.47              |
| 2:G:1651:LEU:O    | 2:G:1652:THR:HG23 | 2.14                     | 0.47              |
| 2:G:1949:LYS:O    | 2:G:1953:VAL:HG23 | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:376:ASN:HD22  | 2:H:376:ASN:C     | 2.18                     | 0.47              |
| 2:H:455:ILE:HG13  | 2:H:455:ILE:O     | 2.13                     | 0.47              |
| 2:H:750:MET:CG    | 2:H:796:PHE:HZ    | 2.25                     | 0.47              |
| 2:H:860:ARG:H     | 2:H:1049:GLN:HG3  | 1.79                     | 0.47              |
| 2:H:2037:PRO:O    | 2:H:2041:ILE:HG13 | 2.15                     | 0.47              |
| 2:I:55:THR:HB     | 2:I:59:GLU:OE2    | 2.13                     | 0.47              |
| 2:I:350:GLN:HA    | 2:I:353:VAL:HG13  | 1.96                     | 0.47              |
| 2:I:873:PHE:CE1   | 2:I:1026:GLU:HB2  | 2.49                     | 0.47              |
| 2:I:1378:ILE:O    | 2:I:1378:ILE:HG12 | 2.14                     | 0.47              |
| 2:I:2037:PRO:O    | 2:I:2041:ILE:HG13 | 2.14                     | 0.47              |
| 1:A:983:GLN:HE22  | 2:G:962:LYS:HD2   | 1.77                     | 0.47              |
| 1:B:157:HIS:CE1   | 1:B:228:LEU:HD22  | 2.49                     | 0.47              |
| 1:B:1305:CYS:SG   | 3:B:2748:CER:C5   | 3.03                     | 0.47              |
| 1:C:335:HIS:O     | 1:C:338:LEU:HB3   | 2.14                     | 0.47              |
| 2:G:1422:THR:O    | 2:G:1422:THR:HG23 | 2.14                     | 0.47              |
| 2:H:355:LYS:HE2   | 2:H:355:LYS:HB3   | 1.65                     | 0.47              |
| 2:H:579:VAL:CG2   | 2:H:1078:HIS:CD2  | 2.95                     | 0.47              |
| 2:H:652:ILE:N     | 2:H:652:ILE:HD12  | 2.30                     | 0.47              |
| 2:H:751:LEU:HD23  | 2:H:791:TYR:CD2   | 2.49                     | 0.47              |
| 2:H:1854:MET:CG   | 2:H:1901:ALA:HB2  | 2.45                     | 0.47              |
| 2:I:455:ILE:HD11  | 2:I:469:ARG:NE    | 2.29                     | 0.47              |
| 2:I:553:ASN:O     | 2:I:556:LYS:HE3   | 2.15                     | 0.47              |
| 2:I:706:LYS:HE2   | 2:I:731:GLN:OE1   | 2.15                     | 0.47              |
| 2:I:748:THR:CB    | 2:I:749:PRO:HD3   | 2.44                     | 0.47              |
| 2:I:1103:PHE:O    | 2:I:1247:GLY:HA3  | 2.14                     | 0.47              |
| 2:I:1389:ILE:HG13 | 2:I:1411:PHE:HD1  | 1.80                     | 0.47              |
| 2:I:1590:ARG:NH2  | 2:I:1594:GLU:OE2  | 2.48                     | 0.47              |
| 1:A:243:ILE:O     | 1:A:247:ARG:HG3   | 2.14                     | 0.47              |
| 1:A:406:TRP:CE3   | 1:A:1619:GLU:HG3  | 2.49                     | 0.47              |
| 1:A:413:LEU:HD13  | 1:A:451:MET:HG2   | 1.97                     | 0.47              |
| 1:A:930:LEU:CD2   | 1:A:933:VAL:HG11  | 2.44                     | 0.47              |
| 1:A:1010:GLU:HA   | 1:A:1664:ALA:HA   | 1.97                     | 0.47              |
| 1:A:1061:SER:HB2  | 1:A:1078:SER:HB3  | 1.96                     | 0.47              |
| 1:A:1158:PRO:HD2  | 1:A:1159:GLU:OE2  | 2.14                     | 0.47              |
| 1:B:34:VAL:O      | 1:B:38:ASP:HB2    | 2.14                     | 0.47              |
| 1:B:705:VAL:CG2   | 1:B:732:LEU:HD21  | 2.43                     | 0.47              |
| 1:B:776:GLU:OE1   | 1:B:795:MET:HE1   | 2.13                     | 0.47              |
| 1:B:827:SER:HA    | 1:B:828:PRO:HD3   | 1.73                     | 0.47              |
| 1:B:889:GLU:HG3   | 1:B:893:VAL:O     | 2.15                     | 0.47              |
| 1:B:968:VAL:O     | 2:H:1512:HIS:HB2  | 2.14                     | 0.47              |
| 1:B:1276:GLN:O    | 1:B:1282:THR:HG21 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:254:TRP:HZ3  | 1:C:292:GLN:HG3   | 1.77                     | 0.47              |
| 1:C:338:LEU:O    | 1:C:342:GLN:HG3   | 2.15                     | 0.47              |
| 1:C:1183:ARG:NH1 | 1:C:1344:GLY:HA2  | 2.30                     | 0.47              |
| 1:C:1305:CYS:SG  | 1:C:1585:LYS:HA   | 2.55                     | 0.47              |
| 2:G:232:LEU:HD21 | 2:G:423:VAL:HA    | 1.97                     | 0.47              |
| 2:G:369:SER:O    | 2:G:370:LEU:HD23  | 2.14                     | 0.47              |
| 2:G:629:GLY:O    | 2:G:632:ALA:HB3   | 2.15                     | 0.47              |
| 2:G:732:TRP:CE2  | 2:G:750:MET:HE3   | 2.50                     | 0.47              |
| 2:G:1102:TYR:HB3 | 2:G:1244:PRO:CA   | 2.44                     | 0.47              |
| 2:G:1567:ARG:NH1 | 2:G:1568:HIS:HB3  | 2.28                     | 0.47              |
| 2:H:11:LEU:HD11  | 2:H:64:PHE:CD2    | 2.50                     | 0.47              |
| 2:H:176:LEU:HD22 | 2:H:247:ALA:HB1   | 1.95                     | 0.47              |
| 2:H:560:ASN:O    | 2:H:560:ASN:OD1   | 2.33                     | 0.47              |
| 2:H:606:PHE:HZ   | 2:H:805:VAL:CG1   | 2.28                     | 0.47              |
| 2:H:741:HIS:HE1  | 2:H:845:THR:HG21  | 1.61                     | 0.47              |
| 2:H:967:ILE:HD12 | 2:H:972:LEU:HD22  | 1.96                     | 0.47              |
| 2:H:1130:THR:H   | 2:H:1133:THR:CG2  | 2.27                     | 0.47              |
| 2:H:1378:ILE:O   | 2:H:1378:ILE:HG12 | 2.13                     | 0.47              |
| 2:H:1819:ALA:CA  | 2:H:2005:ARG:HH11 | 2.26                     | 0.47              |
| 2:H:1980:TYR:HD1 | 2:H:1981:LEU:HD12 | 1.79                     | 0.47              |
| 2:I:22:VAL:HG11  | 2:I:27:PHE:HA     | 1.97                     | 0.47              |
| 2:I:443:LEU:HD22 | 2:I:448:VAL:CG1   | 2.45                     | 0.47              |
| 2:I:461:ASP:HB3  | 2:I:464:ASP:HB2   | 1.95                     | 0.47              |
| 2:I:732:TRP:CE2  | 2:I:750:MET:HE3   | 2.50                     | 0.47              |
| 2:I:747:HIS:HE1  | 2:I:780:TYR:OH    | 1.97                     | 0.47              |
| 2:I:768:GLY:HA3  | 2:I:800:LEU:CD2   | 2.41                     | 0.47              |
| 2:I:955:GLU:HG2  | 2:I:987:TYR:HE2   | 1.79                     | 0.47              |
| 2:I:1004:LEU:CD2 | 2:I:1019:PRO:HB2  | 2.44                     | 0.47              |
| 2:I:1148:ASN:ND2 | 2:I:1151:HIS:H    | 2.13                     | 0.47              |
| 1:A:529:MET:HE3  | 1:A:529:MET:CA    | 2.36                     | 0.47              |
| 1:A:988:ILE:HD13 | 1:A:1048:GLU:HA   | 1.97                     | 0.47              |
| 1:B:142:ASP:CG   | 1:B:257:PRO:HB2   | 2.35                     | 0.47              |
| 1:B:253:ARG:O    | 1:B:254:TRP:CD1   | 2.68                     | 0.47              |
| 1:B:1523:ARG:NH2 | 1:B:1564:LEU:O    | 2.48                     | 0.47              |
| 1:C:1544:THR:O   | 1:C:1545:SER:HB3  | 2.15                     | 0.47              |
| 2:G:55:THR:HB    | 2:G:59:GLU:OE2    | 2.14                     | 0.47              |
| 2:G:1159:ILE:CG1 | 2:G:1169:PRO:CD   | 2.93                     | 0.47              |
| 2:G:1666:PHE:CE1 | 2:G:1814:ALA:HA   | 2.50                     | 0.47              |
| 2:G:1873:TYR:CE2 | 2:G:1940:LEU:HD21 | 2.49                     | 0.47              |
| 2:H:586:LEU:HD12 | 2:H:764:MET:SD    | 2.55                     | 0.47              |
| 2:H:826:GLY:HA3  | 2:H:1061:GLN:CB   | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1004:LEU:CD2  | 2:H:1019:PRO:HB2  | 2.44                     | 0.47              |
| 2:I:42:PRO:HG2    | 2:I:52:ASP:CG     | 2.35                     | 0.47              |
| 2:I:194:THR:CG2   | 2:I:300:ILE:HD11  | 2.40                     | 0.47              |
| 2:I:376:ASN:C     | 2:I:376:ASN:ND2   | 2.68                     | 0.47              |
| 2:I:1418:ASP:C    | 2:I:1420:GLU:H    | 2.18                     | 0.47              |
| 1:B:1305:CYS:SG   | 3:B:2748:CER:H51  | 2.54                     | 0.47              |
| 1:C:18:LEU:HD21   | 2:I:1815:LEU:CD1  | 2.45                     | 0.47              |
| 1:C:237:MET:HG3   | 1:C:241:PHE:HB3   | 1.95                     | 0.47              |
| 1:C:1012:LEU:HD23 | 1:C:1445:MET:HE3  | 1.97                     | 0.47              |
| 2:G:730:LEU:C     | 2:G:730:LEU:HD12  | 2.35                     | 0.47              |
| 2:G:772:GLY:O     | 2:G:804:ARG:HD3   | 2.15                     | 0.47              |
| 2:G:826:GLY:HA2   | 2:G:1060:ALA:HB3  | 1.97                     | 0.47              |
| 2:G:1850:SER:HB2  | 2:G:1973:SER:HB2  | 1.96                     | 0.47              |
| 2:H:127:ILE:HD12  | 2:H:180:TYR:HD2   | 1.80                     | 0.47              |
| 2:H:131:ILE:CD1   | 2:H:182:VAL:CB    | 2.71                     | 0.47              |
| 2:I:606:PHE:HZ    | 2:I:805:VAL:CG1   | 2.28                     | 0.47              |
| 2:I:1553:TYR:OH   | 2:I:1583:MET:HB3  | 2.15                     | 0.47              |
| 1:A:29:ILE:HG13   | 2:G:1891:TYR:O    | 2.15                     | 0.47              |
| 1:A:36:LEU:CD2    | 1:A:61:LEU:HD21   | 2.37                     | 0.47              |
| 1:A:1430:ARG:O    | 1:A:1430:ARG:HG2  | 2.15                     | 0.47              |
| 1:A:1830:GLY:HA2  | 1:A:1831:GLY:HA2  | 1.57                     | 0.47              |
| 1:B:32:GLN:NE2    | 1:B:57:ALA:HA     | 2.29                     | 0.47              |
| 1:B:254:TRP:HZ3   | 1:B:292:GLN:HG3   | 1.76                     | 0.47              |
| 1:B:883:ILE:HD12  | 1:B:947:LEU:HD12  | 1.97                     | 0.47              |
| 1:B:1009:LEU:HD13 | 1:B:1445:MET:HE1  | 1.97                     | 0.47              |
| 1:C:1189:ILE:HG23 | 1:C:1190:PRO:HD2  | 1.97                     | 0.47              |
| 2:G:739:GLY:HA2   | 2:G:1054:LEU:HG   | 1.97                     | 0.47              |
| 2:G:745:ASP:HA    | 2:G:832:TRP:CH2   | 2.48                     | 0.47              |
| 2:G:881:VAL:N     | 2:G:882:PRO:CD    | 2.78                     | 0.47              |
| 2:G:1273:GLU:HB3  | 2:G:1274:PRO:CD   | 2.45                     | 0.47              |
| 2:G:1493:LEU:HB3  | 2:G:1494:PRO:HD2  | 1.96                     | 0.47              |
| 2:G:1844:ARG:HG2  | 2:G:1844:ARG:NH1  | 2.09                     | 0.47              |
| 2:H:238:CYS:CB    | 2:H:239:PRO:HD3   | 2.43                     | 0.47              |
| 2:H:720:ALA:HA    | 2:H:728:ILE:CD1   | 2.45                     | 0.47              |
| 2:H:1015:VAL:HG11 | 2:H:1017:PHE:CE1  | 2.50                     | 0.47              |
| 2:H:1054:LEU:HB2  | 4:H:3051:FMN:HM71 | 1.96                     | 0.47              |
| 2:H:1273:GLU:HB3  | 2:H:1274:PRO:CD   | 2.45                     | 0.47              |
| 2:H:1428:GLU:HG2  | 2:H:1470:THR:HG22 | 1.97                     | 0.47              |
| 2:H:1473:THR:O    | 2:H:1481:SER:HB3  | 2.15                     | 0.47              |
| 2:H:1764:PHE:HB2  | 2:H:1770:LEU:HD21 | 1.97                     | 0.47              |
| 2:I:490:TRP:HA    | 2:I:493:THR:HG22  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1148:ASN:C    | 2:I:1148:ASN:HD22 | 2.19                     | 0.47              |
| 1:A:186:ILE:O     | 1:A:190:LEU:HG    | 2.14                     | 0.46              |
| 1:A:702:LYS:HD3   | 1:A:731:THR:CG2   | 2.44                     | 0.46              |
| 1:B:1544:THR:O    | 1:B:1545:SER:HB3  | 2.15                     | 0.46              |
| 1:C:709:ARG:O     | 1:C:714:VAL:HG21  | 2.16                     | 0.46              |
| 1:C:930:LEU:CD2   | 1:C:933:VAL:HG11  | 2.45                     | 0.46              |
| 2:G:249:TYR:CD2   | 2:G:283:ILE:HD11  | 2.50                     | 0.46              |
| 2:G:1015:VAL:HG11 | 2:G:1017:PHE:CE1  | 2.50                     | 0.46              |
| 2:G:2035:SER:HB3  | 2:G:2038:ILE:CG1  | 2.41                     | 0.46              |
| 2:H:7:ARG:NH2     | 2:H:24:THR:O      | 2.48                     | 0.46              |
| 2:H:440:ASN:ND2   | 2:H:477:GLU:HG2   | 2.30                     | 0.46              |
| 2:I:99:ASN:HA     | 2:I:550:VAL:HG23  | 1.97                     | 0.46              |
| 2:I:533:LEU:HD13  | 2:I:545:GLN:HG3   | 1.97                     | 0.46              |
| 2:I:573:LYS:C     | 2:I:575:GLY:H     | 2.19                     | 0.46              |
| 2:I:1913:VAL:O    | 2:I:1917:ILE:HG13 | 2.15                     | 0.46              |
| 1:A:183:GLN:NE2   | 1:A:202:GLU:HG2   | 2.29                     | 0.46              |
| 1:A:908:LEU:HA    | 1:A:913:VAL:HG21  | 1.96                     | 0.46              |
| 1:A:1056:ILE:HG13 | 1:A:1057:MET:N    | 2.30                     | 0.46              |
| 1:A:1238:VAL:CG1  | 1:A:1239:HIS:N    | 2.78                     | 0.46              |
| 1:B:1133:PRO:HG3  | 1:B:1166:LYS:HG3  | 1.97                     | 0.46              |
| 1:C:293:LYS:O     | 1:C:297:ILE:HG13  | 2.15                     | 0.46              |
| 1:C:499:PRO:HD3   | 1:C:516:ARG:HH21  | 1.80                     | 0.46              |
| 1:C:1303:GLY:C    | 1:C:1307:THR:HG22 | 2.35                     | 0.46              |
| 1:C:1646:PHE:CE1  | 3:C:2748:CER:H31  | 2.50                     | 0.46              |
| 2:G:279:THR:O     | 2:G:283:ILE:HB    | 2.15                     | 0.46              |
| 2:G:598:THR:CB    | 2:G:599:PRO:HD3   | 2.46                     | 0.46              |
| 2:G:652:ILE:N     | 2:G:652:ILE:HD12  | 2.29                     | 0.46              |
| 2:G:751:LEU:HA    | 2:G:794:MET:HE3   | 1.96                     | 0.46              |
| 2:G:1293:THR:HG22 | 2:G:1296:GLU:CD   | 2.35                     | 0.46              |
| 2:H:101:ILE:H     | 2:H:101:ILE:HG13  | 1.30                     | 0.46              |
| 2:H:218:TRP:HB3   | 2:H:225:THR:OG1   | 2.15                     | 0.46              |
| 2:H:736:ARG:H     | 2:H:736:ARG:HG3   | 1.55                     | 0.46              |
| 2:H:926:LEU:HB3   | 2:H:947:THR:HG22  | 1.97                     | 0.46              |
| 2:H:1258:ARG:O    | 2:H:1262:ILE:HG13 | 2.15                     | 0.46              |
| 2:H:1269:LEU:O    | 2:H:1560:LEU:HD23 | 2.15                     | 0.46              |
| 2:H:1804:PHE:CD2  | 2:H:1818:LEU:HD22 | 2.50                     | 0.46              |
| 2:I:213:LEU:O     | 2:I:213:LEU:HG    | 2.16                     | 0.46              |
| 2:I:345:THR:HG22  | 2:I:347:GLU:N     | 2.23                     | 0.46              |
| 2:I:758:ARG:NH2   | 2:I:797:ASP:OD1   | 2.38                     | 0.46              |
| 2:I:1080:GLY:O    | 2:I:1084:LYS:HG3  | 2.15                     | 0.46              |
| 2:I:1148:ASN:HD22 | 2:I:1151:HIS:H    | 1.63                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:232:LEU:HD13  | 1:A:272:GLU:CB    | 2.44                     | 0.46              |
| 1:A:702:LYS:HE2   | 1:A:729:GLY:O     | 2.15                     | 0.46              |
| 1:B:14:LEU:HD11   | 2:H:1821:VAL:HG11 | 1.97                     | 0.46              |
| 1:B:237:MET:HG3   | 1:B:241:PHE:HB3   | 1.97                     | 0.46              |
| 1:B:1114:TYR:CD1  | 1:B:1337:GLU:HG3  | 2.50                     | 0.46              |
| 1:B:1239:HIS:CD2  | 1:B:1241:SER:H    | 2.33                     | 0.46              |
| 1:B:1303:GLY:C    | 1:B:1307:THR:HG22 | 2.35                     | 0.46              |
| 1:B:1639:VAL:CG1  | 1:B:1640:SER:N    | 2.79                     | 0.46              |
| 1:C:186:ILE:O     | 1:C:190:LEU:HG    | 2.15                     | 0.46              |
| 1:C:420:ILE:HG22  | 1:C:469:VAL:HG22  | 1.96                     | 0.46              |
| 1:C:908:LEU:HA    | 1:C:913:VAL:HG21  | 1.96                     | 0.46              |
| 1:C:1004:ILE:HG22 | 1:C:1660:TYR:CE2  | 2.49                     | 0.46              |
| 2:G:7:ARG:NH2     | 2:G:24:THR:O      | 2.48                     | 0.46              |
| 2:G:9:LEU:HB2     | 2:G:27:PHE:HE1    | 1.81                     | 0.46              |
| 2:G:826:GLY:HA3   | 2:G:1061:GLN:CB   | 2.44                     | 0.46              |
| 2:G:1422:THR:HG23 | 2:G:1474:PHE:CD1  | 2.51                     | 0.46              |
| 2:G:1579:ILE:HG22 | 2:G:1580:THR:O    | 2.15                     | 0.46              |
| 2:H:72:VAL:HG12   | 2:H:73:GLU:N      | 2.30                     | 0.46              |
| 2:H:350:GLN:HA    | 2:H:353:VAL:HG13  | 1.97                     | 0.46              |
| 2:H:598:THR:CB    | 2:H:599:PRO:HD3   | 2.44                     | 0.46              |
| 2:H:879:LYS:HA    | 2:H:879:LYS:HD3   | 1.71                     | 0.46              |
| 2:H:1079:ASP:O    | 2:H:1082:ILE:HG22 | 2.16                     | 0.46              |
| 2:H:1359:MET:CE   | 2:H:1404:MET:HB3  | 2.44                     | 0.46              |
| 2:H:1552:PRO:O    | 2:H:1556:VAL:HG23 | 2.15                     | 0.46              |
| 2:H:1945:ASP:O    | 2:H:1949:LYS:HG3  | 2.15                     | 0.46              |
| 2:I:826:GLY:HA3   | 2:I:1061:GLN:CB   | 2.46                     | 0.46              |
| 2:I:1593:ILE:HD13 | 2:I:1626:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:338:LEU:O     | 1:A:342:GLN:HG3   | 2.16                     | 0.46              |
| 1:A:986:ALA:CB    | 1:A:1047:LEU:HD13 | 2.45                     | 0.46              |
| 1:A:1544:THR:O    | 1:A:1545:SER:HB3  | 2.15                     | 0.46              |
| 1:A:1639:VAL:CG1  | 1:A:1640:SER:N    | 2.78                     | 0.46              |
| 1:A:1646:PHE:CE1  | 3:A:2748:CER:H31  | 2.50                     | 0.46              |
| 1:B:741:SER:HB3   | 1:B:744:ASP:HB2   | 1.97                     | 0.46              |
| 1:B:1305:CYS:SG   | 1:B:1585:LYS:HA   | 2.56                     | 0.46              |
| 1:C:451:MET:HB3   | 1:C:451:MET:HE2   | 1.71                     | 0.46              |
| 1:C:784:ILE:HG23  | 1:C:788:SER:HB2   | 1.98                     | 0.46              |
| 1:C:1238:VAL:CG1  | 1:C:1242:GLU:HB2  | 2.45                     | 0.46              |
| 2:G:355:LYS:HB3   | 2:G:355:LYS:HE2   | 1.64                     | 0.46              |
| 2:G:1749:GLU:OE2  | 2:G:1840:VAL:HG13 | 2.16                     | 0.46              |
| 2:H:42:PRO:HG2    | 2:H:52:ASP:CG     | 2.36                     | 0.46              |
| 2:H:573:LYS:HE3   | 2:H:1101:GLU:OE1  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:807:ILE:HD12  | 2:H:1063:THR:HG23 | 1.96                     | 0.46              |
| 2:H:881:VAL:N     | 2:H:882:PRO:CD    | 2.79                     | 0.46              |
| 2:H:1266:TYR:HB2  | 2:H:1347:LEU:HD23 | 1.97                     | 0.46              |
| 2:H:1666:PHE:CD1  | 2:H:1814:ALA:HB2  | 2.49                     | 0.46              |
| 2:H:1908:ASP:HA   | 2:H:1911:THR:HG22 | 1.98                     | 0.46              |
| 2:I:131:ILE:HG21  | 2:I:182:VAL:HG12  | 1.97                     | 0.46              |
| 2:I:1272:ASP:O    | 2:I:1273:GLU:HG3  | 2.15                     | 0.46              |
| 2:I:1624:THR:HB   | 2:I:1642:THR:CG2  | 2.43                     | 0.46              |
| 2:I:1764:PHE:HB2  | 2:I:1770:LEU:HD21 | 1.97                     | 0.46              |
| 1:A:26:VAL:CG2    | 2:G:1890:ASN:ND2  | 2.78                     | 0.46              |
| 1:A:1050:CYS:HB3  | 1:A:1089:VAL:HG12 | 1.98                     | 0.46              |
| 1:B:183:GLN:NE2   | 1:B:202:GLU:HG2   | 2.29                     | 0.46              |
| 1:B:451:MET:HE2   | 1:B:451:MET:HB3   | 1.73                     | 0.46              |
| 1:B:1618:LEU:HD23 | 1:B:1621:PHE:CE2  | 2.51                     | 0.46              |
| 1:C:2:LYS:HE2     | 1:C:4:GLU:CD      | 2.35                     | 0.46              |
| 1:C:256:LEU:HA    | 1:C:257:PRO:HD3   | 1.72                     | 0.46              |
| 2:G:109:LEU:HD11  | 2:G:116:LEU:CD2   | 2.41                     | 0.46              |
| 2:G:455:ILE:HG13  | 2:G:455:ILE:O     | 2.14                     | 0.46              |
| 2:G:702:TYR:HB3   | 2:G:727:PRO:HB2   | 1.97                     | 0.46              |
| 2:G:873:PHE:CD1   | 2:G:1026:GLU:HB2  | 2.50                     | 0.46              |
| 2:G:1834:ARG:NH1  | 2:G:1834:ARG:CG   | 2.68                     | 0.46              |
| 2:H:1169:PRO:O    | 2:H:1173:VAL:HG23 | 2.15                     | 0.46              |
| 2:H:1195:VAL:HG13 | 2:H:1211:LEU:CB   | 2.44                     | 0.46              |
| 2:H:1441:ILE:HD11 | 2:H:1445:ARG:NH2  | 2.27                     | 0.46              |
| 2:H:1567:ARG:NH1  | 2:H:1568:HIS:HB3  | 2.29                     | 0.46              |
| 2:H:1638:ILE:HD12 | 2:H:1657:ILE:CG1  | 2.43                     | 0.46              |
| 2:I:584:SER:CB    | 2:I:591:PRO:HG3   | 2.41                     | 0.46              |
| 2:I:1666:PHE:CD1  | 2:I:1814:ALA:HA   | 2.50                     | 0.46              |
| 1:A:2:LYS:HE2     | 1:A:4:GLU:CD      | 2.36                     | 0.46              |
| 1:A:170:LYS:HD3   | 1:A:175:LEU:HD23  | 1.97                     | 0.46              |
| 1:B:702:LYS:HE2   | 1:B:729:GLY:O     | 2.15                     | 0.46              |
| 1:B:1303:GLY:CA   | 1:B:1649:LYS:HE2  | 2.40                     | 0.46              |
| 1:C:243:ILE:O     | 1:C:247:ARG:HG3   | 2.16                     | 0.46              |
| 1:C:1319:ILE:HA   | 1:C:1324:ALA:O    | 2.14                     | 0.46              |
| 1:C:1362:PRO:HA   | 1:C:1365:MET:HG3  | 1.97                     | 0.46              |
| 1:C:1367:ARG:HH12 | 1:C:1372:THR:CB   | 2.20                     | 0.46              |
| 1:C:1533:ILE:HD11 | 1:C:1564:LEU:HD13 | 1.98                     | 0.46              |
| 2:G:209:PHE:CE2   | 2:G:213:LEU:HD22  | 2.51                     | 0.46              |
| 2:G:214:ASN:ND2   | 2:G:217:GLU:HB2   | 2.30                     | 0.46              |
| 2:G:309:ARG:HD3   | 2:G:309:ARG:HA    | 1.64                     | 0.46              |
| 2:G:441:LYS:O     | 2:G:444:VAL:HG12  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:669:LEU:HA    | 2:G:669:LEU:HD12  | 1.62                     | 0.46              |
| 2:G:719:ILE:HG12  | 2:G:719:ILE:H     | 1.57                     | 0.46              |
| 2:G:844:VAL:HG22  | 2:G:858:ALA:HB2   | 1.98                     | 0.46              |
| 2:G:1886:VAL:HG22 | 2:G:1906:ALA:HB1  | 1.97                     | 0.46              |
| 2:H:321:PRO:HD2   | 2:I:1599:ASP:OD1  | 2.16                     | 0.46              |
| 2:H:582:LYS:HE2   | 2:H:761:PRO:O     | 2.16                     | 0.46              |
| 2:I:843:ILE:HD11  | 2:I:1055:HIS:HB3  | 1.98                     | 0.46              |
| 2:I:1071:LYS:HE3  | 2:I:1075:ASP:OD2  | 2.14                     | 0.46              |
| 2:I:1932:SER:O    | 2:I:1936:VAL:HG22 | 2.16                     | 0.46              |
| 2:I:2026:PHE:HB3  | 2:I:2042:ILE:HD13 | 1.98                     | 0.46              |
| 1:A:709:ARG:O     | 1:A:714:VAL:HG21  | 2.16                     | 0.46              |
| 1:A:1270:VAL:HG11 | 1:A:1274:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:1487:LEU:C    | 1:A:1487:LEU:HD23 | 2.35                     | 0.46              |
| 1:A:1617:ILE:O    | 1:A:1620:GLN:HG2  | 2.16                     | 0.46              |
| 1:B:11:HIS:CD2    | 1:B:11:HIS:C      | 2.89                     | 0.46              |
| 1:B:792:HIS:CE1   | 1:B:796:LEU:HD23  | 2.51                     | 0.46              |
| 1:C:774:ILE:HA    | 1:C:775:PRO:HD3   | 1.74                     | 0.46              |
| 1:C:1233:GLU:CD   | 1:C:1680:ARG:HH21 | 2.19                     | 0.46              |
| 1:C:1263:ASP:HB2  | 1:C:1270:VAL:HG21 | 1.98                     | 0.46              |
| 1:C:1577:GLN:NE2  | 1:C:1591:TRP:HB3  | 2.30                     | 0.46              |
| 2:G:553:ASN:O     | 2:G:556:LYS:HE3   | 2.16                     | 0.46              |
| 2:G:1378:ILE:O    | 2:G:1378:ILE:HG12 | 2.13                     | 0.46              |
| 2:G:1854:MET:CG   | 2:G:1901:ALA:HB2  | 2.46                     | 0.46              |
| 2:H:306:ILE:HA    | 2:H:439:ILE:HD13  | 1.96                     | 0.46              |
| 2:H:481:ASP:OD2   | 2:H:485:ARG:NH1   | 2.48                     | 0.46              |
| 2:H:653:TYR:HD1   | 2:H:659:LEU:HD21  | 1.80                     | 0.46              |
| 2:H:845:THR:HG22  | 2:H:855:HIS:CD2   | 2.51                     | 0.46              |
| 2:H:1180:MET:HB2  | 2:H:1197:LEU:HD21 | 1.98                     | 0.46              |
| 2:H:1624:THR:HB   | 2:H:1642:THR:CG2  | 2.45                     | 0.46              |
| 2:H:1738:PHE:CE1  | 2:H:1837:THR:HG23 | 2.50                     | 0.46              |
| 2:H:1850:SER:HB2  | 2:H:1973:SER:HB2  | 1.97                     | 0.46              |
| 2:H:1858:ASN:HA   | 2:H:1896:GLN:O    | 2.16                     | 0.46              |
| 2:I:109:LEU:HD11  | 2:I:116:LEU:CD2   | 2.43                     | 0.46              |
| 2:I:109:LEU:HD22  | 2:I:114:THR:HG23  | 1.96                     | 0.46              |
| 2:I:589:ARG:HB3   | 2:I:590:PRO:CD    | 2.43                     | 0.46              |
| 2:I:653:TYR:HD1   | 2:I:659:LEU:HD21  | 1.79                     | 0.46              |
| 2:I:860:ARG:HB2   | 2:I:1049:GLN:HG3  | 1.97                     | 0.46              |
| 2:I:1418:ASP:C    | 2:I:1420:GLU:N    | 2.68                     | 0.46              |
| 1:A:37:LYS:HB2    | 1:A:65:TYR:CE1    | 2.48                     | 0.46              |
| 1:A:49:PRO:O      | 1:A:82:SER:HB2    | 2.16                     | 0.46              |
| 1:A:427:ASN:ND2   | 1:A:610:THR:H     | 2.08                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1021:VAL:HG22 | 1:B:1387:ILE:HG22 | 1.98                     | 0.46              |
| 1:B:1595:GLY:O    | 1:B:1599:ILE:HG13 | 2.15                     | 0.46              |
| 1:C:182:VAL:O     | 1:C:186:ILE:HG13  | 2.16                     | 0.46              |
| 2:G:131:ILE:CG2   | 2:G:182:VAL:HG11  | 2.43                     | 0.46              |
| 2:G:785:TRP:CG    | 2:G:786:SER:N     | 2.83                     | 0.46              |
| 2:G:845:THR:HG22  | 2:G:855:HIS:CD2   | 2.50                     | 0.46              |
| 2:G:955:GLU:HG2   | 2:G:987:TYR:HE2   | 1.80                     | 0.46              |
| 2:G:1168:ASN:HA   | 2:G:1169:PRO:HD3  | 1.81                     | 0.46              |
| 2:G:1303:ALA:HB2  | 2:G:1556:VAL:HG21 | 1.98                     | 0.46              |
| 2:G:2037:PRO:O    | 2:G:2041:ILE:HG13 | 2.16                     | 0.46              |
| 2:H:60:LEU:O      | 2:H:63:LYS:HB2    | 2.16                     | 0.46              |
| 2:H:551:THR:HG22  | 2:H:552:SER:N     | 2.30                     | 0.46              |
| 2:H:1344:ASP:O    | 2:H:1416:TYR:HE2  | 1.99                     | 0.46              |
| 2:H:1427:VAL:HG22 | 2:H:1469:GLU:HG2  | 1.96                     | 0.46              |
| 2:H:1491:VAL:HB   | 2:H:1501:ILE:CD1  | 2.45                     | 0.46              |
| 2:H:1651:LEU:O    | 2:H:1652:THR:HG23 | 2.16                     | 0.46              |
| 2:H:1846:GLU:C    | 2:H:1848:GLY:H    | 2.19                     | 0.46              |
| 2:H:1873:TYR:CE1  | 2:H:1877:ARG:NE   | 2.77                     | 0.46              |
| 2:I:490:TRP:CZ2   | 2:I:512:LEU:HD21  | 2.51                     | 0.46              |
| 2:I:1180:MET:HB3  | 2:I:1199:GLU:HG2  | 1.98                     | 0.46              |
| 2:I:1543:ASP:OD1  | 2:I:1623:LYS:HG2  | 2.15                     | 0.46              |
| 1:A:35:PHE:HA     | 1:A:39:PHE:HD2    | 1.81                     | 0.46              |
| 1:A:331:ILE:HG23  | 1:A:332:THR:N     | 2.31                     | 0.46              |
| 1:A:489:VAL:CG2   | 1:A:670:GLY:C     | 2.84                     | 0.46              |
| 1:A:507:GLY:N     | 1:A:954:ARG:HG2   | 2.31                     | 0.46              |
| 1:C:11:HIS:C      | 1:C:11:HIS:CD2    | 2.89                     | 0.46              |
| 1:C:1196:LYS:HE3  | 1:C:1202:ASP:CG   | 2.37                     | 0.46              |
| 1:C:1209:ASP:OD2  | 1:C:1253:GLY:HA2  | 2.16                     | 0.46              |
| 2:G:123:ILE:HD11  | 2:G:533:LEU:HD22  | 1.98                     | 0.46              |
| 2:G:970:TYR:O     | 2:G:973:LEU:HB2   | 2.16                     | 0.46              |
| 2:G:1418:ASP:O    | 2:G:1421:ASN:N    | 2.43                     | 0.46              |
| 2:H:490:TRP:CZ2   | 2:H:512:LEU:HD21  | 2.51                     | 0.46              |
| 2:H:702:TYR:HB3   | 2:H:727:PRO:HB2   | 1.97                     | 0.46              |
| 2:H:1227:ARG:NE   | 2:H:1565:VAL:HG12 | 2.30                     | 0.46              |
| 2:H:1236:LEU:HA   | 2:H:1237:PRO:HD3  | 1.78                     | 0.46              |
| 2:H:1374:THR:HG23 | 2:H:1396:LEU:CD1  | 2.46                     | 0.46              |
| 2:I:740:HIS:HE1   | 2:I:852:GLU:OE1   | 1.99                     | 0.46              |
| 2:I:860:ARG:H     | 2:I:1049:GLN:HG3  | 1.80                     | 0.46              |
| 2:I:1031:LYS:O    | 2:I:1032:ASP:C    | 2.54                     | 0.46              |
| 2:I:1054:LEU:HB3  | 4:I:3051:FMN:HM82 | 1.98                     | 0.46              |
| 2:I:1228:THR:HG21 | 2:I:1234:VAL:HG23 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1418:ASP:O    | 2:I:1420:GLU:N    | 2.49                     | 0.46              |
| 1:A:386:PHE:O     | 1:A:390:VAL:HB    | 2.16                     | 0.46              |
| 1:A:1709:GLU:H    | 1:A:1709:GLU:HG3  | 1.46                     | 0.46              |
| 1:B:143:GLU:H     | 1:B:260:ARG:HG2   | 1.81                     | 0.46              |
| 1:B:601:VAL:O     | 1:B:602:GLU:C     | 2.54                     | 0.46              |
| 1:C:539:SER:O     | 1:C:540:GLN:C     | 2.52                     | 0.46              |
| 1:C:1459:ILE:O    | 1:C:1463:VAL:HG23 | 2.16                     | 0.46              |
| 2:G:233:SER:HA    | 2:G:424:ALA:CB    | 2.46                     | 0.46              |
| 2:G:1002:HIS:NE2  | 2:G:1006:MET:CE   | 2.79                     | 0.46              |
| 2:G:1311:PHE:HD1  | 2:G:1320:LEU:O    | 1.99                     | 0.46              |
| 2:G:1435:ILE:O    | 2:G:1435:ILE:HG22 | 2.15                     | 0.46              |
| 2:H:913:ASP:H     | 2:H:916:THR:CG2   | 2.29                     | 0.46              |
| 2:H:1021:LEU:HD22 | 2:H:1021:LEU:HA   | 1.58                     | 0.46              |
| 2:I:232:LEU:HD21  | 2:I:423:VAL:HA    | 1.98                     | 0.46              |
| 2:I:391:LEU:CD2   | 2:I:394:ARG:NH2   | 2.78                     | 0.46              |
| 2:I:670:ARG:HD2   | 2:I:676:ILE:O     | 2.16                     | 0.46              |
| 2:I:751:LEU:HD11  | 2:I:789:PHE:CD1   | 2.51                     | 0.46              |
| 2:I:785:TRP:CG    | 2:I:786:SER:N     | 2.84                     | 0.46              |
| 2:I:844:VAL:HG22  | 2:I:858:ALA:HB2   | 1.97                     | 0.46              |
| 2:I:1222:GLU:HG3  | 2:I:1235:SER:OG   | 2.16                     | 0.46              |
| 2:I:1282:ARG:NH2  | 2:I:1423:PHE:HB3  | 2.31                     | 0.46              |
| 2:I:1561:ASN:OD1  | 2:I:1563:ILE:HB   | 2.15                     | 0.46              |
| 1:A:411:GLN:NE2   | 1:A:1628:SER:H    | 2.13                     | 0.45              |
| 1:A:792:HIS:CE1   | 1:A:796:LEU:HD23  | 2.51                     | 0.45              |
| 1:A:1533:ILE:HG13 | 1:A:1564:LEU:HB3  | 1.98                     | 0.45              |
| 1:A:1557:ILE:HD11 | 1:A:1642:THR:HG21 | 1.97                     | 0.45              |
| 1:B:516:ARG:NH2   | 1:B:889:GLU:OE1   | 2.49                     | 0.45              |
| 1:B:881:ASN:HA    | 1:B:944:ARG:HH22  | 1.78                     | 0.45              |
| 1:B:1234:MET:HG2  | 1:B:1326:ILE:CD1  | 2.46                     | 0.45              |
| 1:C:400:ARG:HH11  | 1:C:400:ARG:HG3   | 1.72                     | 0.45              |
| 1:C:1040:GLU:HB2  | 1:C:1580:LEU:HD12 | 1.98                     | 0.45              |
| 1:C:1376:PHE:CB   | 1:C:1544:THR:HG22 | 2.45                     | 0.45              |
| 1:C:1573:ILE:HG23 | 1:C:1627:PRO:HG3  | 1.98                     | 0.45              |
| 2:G:159:ILE:CG2   | 2:G:501:ILE:HG22  | 2.46                     | 0.45              |
| 2:G:1586:SER:O    | 2:G:1590:ARG:HB2  | 2.16                     | 0.45              |
| 2:G:1738:PHE:CD1  | 2:G:1837:THR:HG23 | 2.51                     | 0.45              |
| 2:H:391:LEU:CD2   | 2:H:394:ARG:NH2   | 2.80                     | 0.45              |
| 2:H:730:LEU:C     | 2:H:730:LEU:HD12  | 2.36                     | 0.45              |
| 2:H:1031:LYS:O    | 2:H:1032:ASP:C    | 2.54                     | 0.45              |
| 2:H:1135:GLU:OE2  | 2:H:1175:LYS:HE3  | 2.15                     | 0.45              |
| 2:H:1388:LYS:HE3  | 2:H:1418:ASP:OD2  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1417:THR:C    | 2:H:1419:PHE:H    | 2.19                     | 0.45              |
| 2:H:1593:ILE:HD13 | 2:H:1626:ILE:HD13 | 1.97                     | 0.45              |
| 2:H:1666:PHE:CE1  | 2:H:1814:ALA:HA   | 2.50                     | 0.45              |
| 2:H:1873:TYR:CE1  | 2:H:1877:ARG:NH2  | 2.83                     | 0.45              |
| 2:H:2026:PHE:HB3  | 2:H:2042:ILE:HD13 | 1.98                     | 0.45              |
| 2:I:738:GLY:HA3   | 4:I:3051:FMN:HM81 | 1.98                     | 0.45              |
| 2:I:807:ILE:HD12  | 2:I:1063:THR:HG23 | 1.98                     | 0.45              |
| 1:A:408:TRP:CZ3   | 1:A:1628:SER:HB3  | 2.51                     | 0.45              |
| 1:A:764:ASP:OD2   | 1:A:818:ARG:HD3   | 2.17                     | 0.45              |
| 1:A:1114:TYR:CE1  | 1:A:1337:GLU:HG3  | 2.50                     | 0.45              |
| 1:B:2:LYS:HE2     | 1:B:4:GLU:OE1     | 2.15                     | 0.45              |
| 1:B:19:ALA:O      | 1:B:22:PHE:HB2    | 2.15                     | 0.45              |
| 1:B:26:VAL:HG13   | 2:H:2013:ASN:ND2  | 2.31                     | 0.45              |
| 1:B:719:GLN:HG3   | 1:B:720:SER:N     | 2.31                     | 0.45              |
| 1:B:1431:GLU:OE2  | 1:B:1433:HIS:HE1  | 2.00                     | 0.45              |
| 1:C:170:LYS:HD3   | 1:C:175:LEU:HD23  | 1.97                     | 0.45              |
| 1:C:430:ARG:NH2   | 1:C:605:LEU:HD13  | 2.31                     | 0.45              |
| 1:C:529:MET:CE    | 1:C:894:ARG:HD2   | 2.46                     | 0.45              |
| 2:G:161:GLY:HA3   | 2:G:506:PRO:HD2   | 1.98                     | 0.45              |
| 2:G:191:SER:HA    | 2:G:194:THR:CG2   | 2.46                     | 0.45              |
| 2:G:1219:ILE:HD11 | 2:G:1242:PHE:HB2  | 1.98                     | 0.45              |
| 2:G:1222:GLU:HG3  | 2:G:1235:SER:OG   | 2.16                     | 0.45              |
| 2:G:1472:VAL:CG2  | 2:G:1483:VAL:HG22 | 2.46                     | 0.45              |
| 2:G:1673:GLU:N    | 2:G:1676:MET:HE3  | 2.25                     | 0.45              |
| 2:G:1976:PHE:HA   | 2:G:1981:LEU:CD2  | 2.46                     | 0.45              |
| 2:H:246:LEU:HD12  | 2:H:246:LEU:HA    | 1.85                     | 0.45              |
| 2:H:324:LEU:HD12  | 2:H:324:LEU:O     | 2.16                     | 0.45              |
| 2:H:612:ASN:HD21  | 2:H:641:ILE:HA    | 1.81                     | 0.45              |
| 2:H:1579:ILE:HG22 | 2:H:1580:THR:O    | 2.16                     | 0.45              |
| 2:H:1768:LYS:HE2  | 2:H:1772:SER:HB3  | 1.98                     | 0.45              |
| 2:I:369:SER:O     | 2:I:370:LEU:HD23  | 2.16                     | 0.45              |
| 2:I:601:THR:HB    | 2:I:620:ALA:HB2   | 1.98                     | 0.45              |
| 2:I:669:LEU:HD12  | 2:I:669:LEU:HA    | 1.65                     | 0.45              |
| 2:I:1359:MET:HE3  | 2:I:1404:MET:HB3  | 1.98                     | 0.45              |
| 1:A:18:LEU:HD21   | 2:G:1815:LEU:CD1  | 2.46                     | 0.45              |
| 1:A:751:PHE:CZ    | 1:A:761:LEU:HD13  | 2.51                     | 0.45              |
| 1:A:1367:ARG:HH12 | 1:A:1372:THR:CB   | 2.18                     | 0.45              |
| 1:A:1431:GLU:OE2  | 1:A:1523:ARG:NH1  | 2.48                     | 0.45              |
| 1:B:37:LYS:HB2    | 1:B:65:TYR:CE1    | 2.51                     | 0.45              |
| 1:B:235:SER:HA    | 1:B:276:ARG:NH2   | 2.32                     | 0.45              |
| 1:B:444:ASN:HB2   | 1:B:447:LEU:N     | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1639:VAL:HG12 | 1:B:1640:SER:N    | 2.31                     | 0.45              |
| 1:C:827:SER:HA    | 1:C:828:PRO:HD3   | 1.70                     | 0.45              |
| 1:C:982:ILE:HD11  | 2:I:965:SER:CB    | 2.46                     | 0.45              |
| 2:G:247:ALA:O     | 2:G:251:VAL:HG13  | 2.15                     | 0.45              |
| 2:G:460:TYR:HA    | 2:G:466:SER:O     | 2.17                     | 0.45              |
| 2:G:562:LEU:HG    | 2:G:793:PRO:CG    | 2.43                     | 0.45              |
| 2:G:860:ARG:HB2   | 2:G:1049:GLN:HG3  | 1.97                     | 0.45              |
| 2:G:1953:VAL:O    | 2:G:1953:VAL:HG12 | 2.16                     | 0.45              |
| 2:H:249:TYR:CD2   | 2:H:283:ILE:HD11  | 2.52                     | 0.45              |
| 2:H:439:ILE:HD12  | 2:H:484:ILE:CD1   | 2.46                     | 0.45              |
| 2:H:562:LEU:HG    | 2:H:793:PRO:CB    | 2.47                     | 0.45              |
| 2:H:1590:ARG:HG3  | 2:H:1608:TYR:CD2  | 2.51                     | 0.45              |
| 2:H:1776:PHE:C    | 2:H:1779:PRO:HD2  | 2.37                     | 0.45              |
| 2:I:618:GLU:HG2   | 2:I:678:PHE:CZ    | 2.51                     | 0.45              |
| 2:I:739:GLY:HA2   | 2:I:1054:LEU:HG   | 1.97                     | 0.45              |
| 2:I:1180:MET:HB2  | 2:I:1197:LEU:HD21 | 1.97                     | 0.45              |
| 2:I:1775:GLN:HG2  | 2:I:1836:MET:SD   | 2.57                     | 0.45              |
| 2:I:1854:MET:CG   | 2:I:1901:ALA:HB2  | 2.47                     | 0.45              |
| 1:A:168:MET:HA    | 1:A:206:LEU:HB2   | 1.98                     | 0.45              |
| 1:A:413:LEU:C     | 1:A:415:SER:H     | 2.18                     | 0.45              |
| 1:A:625:THR:HG23  | 1:A:627:SER:H     | 1.82                     | 0.45              |
| 1:A:630:ILE:O     | 1:A:653:ARG:NH2   | 2.48                     | 0.45              |
| 1:A:798:ASN:HA    | 1:A:801:ARG:HB2   | 1.98                     | 0.45              |
| 1:B:32:GLN:NE2    | 1:B:57:ALA:CA     | 2.80                     | 0.45              |
| 1:B:988:ILE:HD13  | 1:B:1048:GLU:CB   | 2.47                     | 0.45              |
| 1:B:1310:GLU:OE1  | 1:B:1649:LYS:CE   | 2.62                     | 0.45              |
| 1:C:1533:ILE:HG13 | 1:C:1564:LEU:HB3  | 1.98                     | 0.45              |
| 2:G:582:LYS:HE2   | 2:G:1108:PRO:HB3  | 1.97                     | 0.45              |
| 2:G:807:ILE:HA    | 2:G:818:LYS:HG2   | 1.97                     | 0.45              |
| 2:G:1015:VAL:HG13 | 2:G:1017:PHE:CE2  | 2.52                     | 0.45              |
| 2:G:1148:ASN:HD22 | 2:G:1151:HIS:H    | 1.63                     | 0.45              |
| 2:G:1314:ARG:HD3  | 2:G:1314:ARG:HA   | 1.62                     | 0.45              |
| 2:G:1844:ARG:HA   | 2:G:1849:ARG:O    | 2.16                     | 0.45              |
| 2:H:463:PHE:C     | 2:H:463:PHE:CD2   | 2.90                     | 0.45              |
| 2:H:601:THR:CG2   | 2:H:601:THR:O     | 2.65                     | 0.45              |
| 2:H:835:THR:CB    | 2:H:845:THR:HG23  | 2.43                     | 0.45              |
| 2:H:1735:ALA:O    | 2:H:1737:ILE:HG13 | 2.16                     | 0.45              |
| 2:I:463:PHE:CE1   | 2:I:486:LEU:HD22  | 2.51                     | 0.45              |
| 2:I:1199:GLU:OE2  | 2:I:1567:ARG:CZ   | 2.65                     | 0.45              |
| 2:I:1327:ILE:HD12 | 2:I:1327:ILE:HA   | 1.80                     | 0.45              |
| 2:I:1609:THR:O    | 2:I:1653:GLY:HA3  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:143:GLU:H     | 1:A:260:ARG:HG2   | 1.81                     | 0.45              |
| 1:A:293:LYS:O     | 1:A:297:ILE:HG13  | 2.16                     | 0.45              |
| 1:A:1196:LYS:HE3  | 1:A:1202:ASP:CG   | 2.36                     | 0.45              |
| 1:B:1019:ILE:HG21 | 1:B:1316:VAL:HG22 | 1.98                     | 0.45              |
| 1:B:1020:VAL:CG1  | 1:B:1400:ILE:HG23 | 2.46                     | 0.45              |
| 1:B:1061:SER:HB2  | 1:B:1078:SER:HB3  | 1.99                     | 0.45              |
| 1:B:1376:PHE:CB   | 1:B:1544:THR:HG22 | 2.45                     | 0.45              |
| 1:B:1464:GLU:HG3  | 1:B:1773:VAL:HG11 | 1.91                     | 0.45              |
| 1:C:776:GLU:OE1   | 1:C:795:MET:HE1   | 2.17                     | 0.45              |
| 1:C:1104:ARG:O    | 1:C:1185:VAL:HG13 | 2.17                     | 0.45              |
| 1:C:1682:LYS:HB3  | 2:I:994:PHE:CD2   | 2.51                     | 0.45              |
| 2:G:357:ASN:OD1   | 2:G:365:GLN:HB3   | 2.16                     | 0.45              |
| 2:H:24:THR:O      | 2:H:26:SER:N      | 2.49                     | 0.45              |
| 2:H:319:LEU:HD22  | 2:H:319:LEU:HA    | 1.68                     | 0.45              |
| 2:H:611:THR:HA    | 2:H:615:TYR:O     | 2.16                     | 0.45              |
| 2:H:659:LEU:HD12  | 2:H:659:LEU:HA    | 1.82                     | 0.45              |
| 2:H:754:TYR:CE2   | 2:H:794:MET:HG3   | 2.52                     | 0.45              |
| 2:H:1027:ILE:O    | 2:H:1031:LYS:HB2  | 2.16                     | 0.45              |
| 2:H:1383:ASN:HD21 | 2:H:1418:ASP:CB   | 2.30                     | 0.45              |
| 2:I:894:ARG:NH1   | 2:I:898:ASP:OD2   | 2.42                     | 0.45              |
| 2:I:938:TRP:CD1   | 2:I:944:ARG:HG3   | 2.52                     | 0.45              |
| 2:I:1776:PHE:C    | 2:I:1779:PRO:HD2  | 2.37                     | 0.45              |
| 2:I:1976:PHE:CB   | 2:I:1981:LEU:CD2  | 2.94                     | 0.45              |
| 2:I:2036:GLU:HG2  | 2:I:2039:LYS:HZ3  | 1.82                     | 0.45              |
| 1:A:658:LEU:HD13  | 1:A:916:LEU:HD12  | 1.99                     | 0.45              |
| 1:A:776:GLU:OE1   | 1:A:795:MET:HE1   | 2.16                     | 0.45              |
| 1:A:1120:GLU:O    | 1:A:1121:MET:HG3  | 2.16                     | 0.45              |
| 1:B:332:THR:HG22  | 1:C:331:ILE:HD11  | 1.98                     | 0.45              |
| 1:B:1533:ILE:HD11 | 1:B:1564:LEU:HD13 | 1.98                     | 0.45              |
| 1:C:143:GLU:H     | 1:C:260:ARG:HG2   | 1.81                     | 0.45              |
| 1:C:197:THR:HG22  | 1:C:198:PRO:O     | 2.15                     | 0.45              |
| 1:C:225:SER:OG    | 1:C:266:LEU:HD21  | 2.16                     | 0.45              |
| 1:C:1491:ARG:NH1  | 1:C:1744:TYR:O    | 2.50                     | 0.45              |
| 2:G:142:ASN:HB2   | 2:G:550:VAL:HG13  | 1.99                     | 0.45              |
| 2:G:315:PRO:O     | 2:H:1314:ARG:NH2  | 2.50                     | 0.45              |
| 2:G:712:ALA:O     | 2:G:715:GLN:HB3   | 2.16                     | 0.45              |
| 2:G:1080:GLY:O    | 2:G:1084:LYS:HG3  | 2.16                     | 0.45              |
| 2:G:1241:ASN:N    | 2:G:1252:SER:O    | 2.49                     | 0.45              |
| 2:G:1466:PHE:HE2  | 2:G:1489:ILE:HD13 | 1.81                     | 0.45              |
| 2:G:1976:PHE:CB   | 2:G:1981:LEU:CD2  | 2.95                     | 0.45              |
| 2:H:618:GLU:HG2   | 2:H:678:PHE:CZ    | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:785:TRP:CG    | 2:H:786:SER:N     | 2.84                     | 0.45              |
| 2:H:1085:LEU:HD12 | 2:H:1085:LEU:HA   | 1.85                     | 0.45              |
| 2:H:1159:ILE:HG22 | 2:H:1160:THR:N    | 2.32                     | 0.45              |
| 2:H:1325:PHE:O    | 2:H:1328:VAL:HG12 | 2.16                     | 0.45              |
| 2:I:23:PRO:HG2    | 2:I:86:LEU:HD11   | 1.98                     | 0.45              |
| 2:I:440:ASN:ND2   | 2:I:477:GLU:HG2   | 2.31                     | 0.45              |
| 2:I:1195:VAL:HG13 | 2:I:1211:LEU:CB   | 2.46                     | 0.45              |
| 2:I:1637:LEU:HD23 | 2:I:1637:LEU:HA   | 1.79                     | 0.45              |
| 1:A:1300:THR:HA   | 1:A:1301:PRO:HD3  | 1.70                     | 0.45              |
| 1:B:66:GLU:OE1    | 1:B:66:GLU:HA     | 2.15                     | 0.45              |
| 1:C:21:GLN:HG3    | 2:I:2013:ASN:HB2  | 1.98                     | 0.45              |
| 1:C:521:LYS:HB3   | 1:C:523:SER:HB3   | 1.98                     | 0.45              |
| 1:C:1305:CYS:SG   | 3:C:2748:CER:H51  | 2.57                     | 0.45              |
| 1:C:1670:TYR:O    | 1:C:1674:VAL:HG23 | 2.17                     | 0.45              |
| 2:G:665:LEU:O     | 2:G:665:LEU:HD22  | 2.17                     | 0.45              |
| 2:G:754:TYR:CG    | 2:G:794:MET:HG2   | 2.51                     | 0.45              |
| 2:G:1858:ASN:ND2  | 2:G:1861:ARG:HG3  | 2.32                     | 0.45              |
| 2:G:1873:TYR:HE1  | 2:G:1877:ARG:HH21 | 1.59                     | 0.45              |
| 2:H:594:VAL:CG2   | 2:H:610:THR:HG21  | 2.45                     | 0.45              |
| 2:H:1678:MET:HE3  | 2:H:1707:LEU:CD2  | 2.41                     | 0.45              |
| 2:H:2035:SER:HB3  | 2:H:2038:ILE:CG1  | 2.44                     | 0.45              |
| 2:I:478:ARG:O     | 2:I:482:CYS:HB2   | 2.17                     | 0.45              |
| 2:I:784:GLU:O     | 2:I:787:THR:HB    | 2.17                     | 0.45              |
| 2:I:1162:ASP:O    | 2:I:1163:LYS:HB2  | 2.16                     | 0.45              |
| 2:I:1949:LYS:O    | 2:I:1953:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:1239:HIS:CD2  | 1:A:1241:SER:H    | 2.35                     | 0.45              |
| 1:A:1443:LEU:HD23 | 1:A:1443:LEU:HA   | 1.75                     | 0.45              |
| 1:B:1004:ILE:HG22 | 1:B:1660:TYR:CE2  | 2.52                     | 0.45              |
| 1:B:1239:HIS:HE1  | 1:B:1714:VAL:O    | 2.00                     | 0.45              |
| 1:B:1459:ILE:O    | 1:B:1463:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:1584:PRO:CG   | 1:B:1591:TRP:CZ3  | 3.00                     | 0.45              |
| 2:G:101:ILE:H     | 2:G:101:ILE:HG13  | 1.31                     | 0.45              |
| 2:G:218:TRP:HB3   | 2:G:225:THR:OG1   | 2.16                     | 0.45              |
| 2:G:350:GLN:HA    | 2:G:353:VAL:HG13  | 1.97                     | 0.45              |
| 2:G:455:ILE:HD11  | 2:G:469:ARG:NE    | 2.32                     | 0.45              |
| 2:G:879:LYS:HD3   | 2:G:879:LYS:HA    | 1.68                     | 0.45              |
| 2:G:1265:MET:HE1  | 2:G:1562:PRO:HG2  | 1.98                     | 0.45              |
| 2:H:751:LEU:HA    | 2:H:794:MET:HE3   | 1.98                     | 0.45              |
| 2:H:1100:VAL:HG23 | 2:H:1147:ILE:HB   | 1.99                     | 0.45              |
| 2:H:1845:ASP:HB2  | 2:H:1849:ARG:N    | 2.15                     | 0.45              |
| 2:I:161:GLY:H     | 2:I:505:GLY:CA    | 2.28                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:355:LYS:HB3   | 2:I:355:LYS:HE2   | 1.70                     | 0.45              |
| 2:I:654:VAL:O     | 2:I:654:VAL:HG12  | 2.17                     | 0.45              |
| 2:I:677:GLN:O     | 2:I:678:PHE:HB3   | 2.17                     | 0.45              |
| 2:I:943:TRP:CZ2   | 2:I:1016:PRO:HG3  | 2.52                     | 0.45              |
| 2:I:1002:HIS:NE2  | 2:I:1006:MET:CE   | 2.80                     | 0.45              |
| 2:I:1258:ARG:O    | 2:I:1262:ILE:HG13 | 2.17                     | 0.45              |
| 2:I:1308:CYS:HB3  | 2:I:1311:PHE:CE2  | 2.51                     | 0.45              |
| 1:A:483:VAL:O     | 1:A:484:LEU:C     | 2.56                     | 0.45              |
| 1:A:929:GLY:C     | 1:A:931:GLN:H     | 2.19                     | 0.45              |
| 1:B:340:ARG:HH12  | 1:B:344:GLN:HE21  | 1.64                     | 0.45              |
| 1:B:420:ILE:HG22  | 1:B:469:VAL:HG22  | 1.99                     | 0.45              |
| 1:B:1617:ILE:O    | 1:B:1620:GLN:HG2  | 2.17                     | 0.45              |
| 1:C:378:LEU:HD12  | 1:C:378:LEU:HA    | 1.84                     | 0.45              |
| 1:C:927:ASN:O     | 1:C:929:GLY:N     | 2.41                     | 0.45              |
| 2:G:624:TYR:HB2   | 2:G:630:MET:HE3   | 1.99                     | 0.45              |
| 2:G:1227:ARG:CZ   | 2:G:1565:VAL:HG12 | 2.47                     | 0.45              |
| 2:G:1491:VAL:HB   | 2:G:1501:ILE:HD12 | 1.99                     | 0.45              |
| 2:G:1543:ASP:OD1  | 2:G:1623:LYS:HG2  | 2.16                     | 0.45              |
| 2:H:512:LEU:O     | 2:H:516:THR:HG23  | 2.17                     | 0.45              |
| 2:H:1327:ILE:HG12 | 2:H:1583:MET:HE3  | 1.99                     | 0.45              |
| 2:I:653:TYR:OH    | 2:I:690:VAL:HG11  | 2.17                     | 0.45              |
| 2:I:1491:VAL:HB   | 2:I:1501:ILE:CD1  | 2.47                     | 0.45              |
| 1:A:204:THR:HA    | 1:A:205:PRO:HD3   | 1.85                     | 0.45              |
| 1:A:335:HIS:O     | 1:A:335:HIS:CD2   | 2.69                     | 0.45              |
| 1:A:1516:ASP:HA   | 1:A:1517:PRO:HD3  | 1.61                     | 0.45              |
| 1:B:32:GLN:HE21   | 1:B:57:ALA:HB2    | 1.82                     | 0.45              |
| 1:B:43:ARG:O      | 2:H:1662:THR:HA   | 2.16                     | 0.45              |
| 1:B:44:VAL:HG13   | 1:B:78:ILE:HG12   | 1.98                     | 0.45              |
| 1:B:67:SER:OG     | 2:G:359:HIS:HE1   | 1.99                     | 0.45              |
| 1:B:196:THR:O     | 1:B:213:PHE:HE2   | 2.00                     | 0.45              |
| 1:B:1119:LYS:HE2  | 1:B:1341:PHE:CG   | 2.52                     | 0.45              |
| 1:B:1300:THR:HA   | 1:B:1301:PRO:HD3  | 1.69                     | 0.45              |
| 1:B:1592:MET:HE2  | 1:B:1641:ILE:HG23 | 1.98                     | 0.45              |
| 1:C:478:GLU:OE1   | 1:C:478:GLU:HA    | 2.17                     | 0.45              |
| 1:C:916:LEU:HD22  | 1:C:922:VAL:HG22  | 1.99                     | 0.45              |
| 1:C:1061:SER:HB2  | 1:C:1078:SER:HB3  | 1.99                     | 0.45              |
| 2:G:42:PRO:HG2    | 2:G:52:ASP:CG     | 2.38                     | 0.45              |
| 2:G:109:LEU:HD23  | 2:G:109:LEU:HA    | 1.79                     | 0.45              |
| 2:G:1002:HIS:NE2  | 2:G:1006:MET:HE3  | 2.32                     | 0.45              |
| 2:G:1325:PHE:O    | 2:G:1328:VAL:HG12 | 2.17                     | 0.45              |
| 2:G:1389:ILE:HG13 | 2:G:1411:PHE:CD1  | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1417:THR:C    | 2:G:1419:PHE:N    | 2.69                     | 0.45              |
| 2:G:1418:ASP:C    | 2:G:1420:GLU:H    | 2.19                     | 0.45              |
| 2:H:641:ILE:HG12  | 2:H:645:SER:CB    | 2.46                     | 0.45              |
| 2:I:231:LEU:HA    | 2:I:236:ILE:HD12  | 1.99                     | 0.45              |
| 2:I:298:LYS:HG2   | 2:I:448:VAL:CG2   | 2.38                     | 0.45              |
| 2:I:1256:GLU:O    | 2:I:1257:ASP:HB2  | 2.17                     | 0.45              |
| 1:A:242:THR:HG22  | 1:A:243:ILE:H     | 1.81                     | 0.44              |
| 1:A:636:PRO:HB2   | 1:A:638:LEU:O     | 2.16                     | 0.44              |
| 1:A:1283:MET:O    | 1:A:1287:VAL:HG23 | 2.18                     | 0.44              |
| 1:B:13:LEU:HB2    | 2:H:2026:PHE:CE1  | 2.52                     | 0.44              |
| 1:B:411:GLN:NE2   | 1:B:1628:SER:H    | 2.15                     | 0.44              |
| 1:B:427:ASN:HB2   | 1:B:468:LEU:HD21  | 1.99                     | 0.44              |
| 1:B:612:GLU:O     | 1:B:615:SER:HB3   | 2.17                     | 0.44              |
| 1:B:626:VAL:HG23  | 1:B:664:GLU:OE2   | 2.17                     | 0.44              |
| 1:B:733:ILE:CD1   | 1:B:761:LEU:HD11  | 2.46                     | 0.44              |
| 1:B:1029:PRO:HA   | 1:B:1188:GLN:O    | 2.17                     | 0.44              |
| 1:B:1455:ARG:HD2  | 1:B:1455:ARG:HA   | 1.86                     | 0.44              |
| 1:C:253:ARG:O     | 1:C:254:TRP:CD1   | 2.70                     | 0.44              |
| 1:C:641:ARG:HD3   | 1:C:649:TRP:O     | 2.17                     | 0.44              |
| 1:C:1257:LEU:HD23 | 1:C:1257:LEU:HA   | 1.83                     | 0.44              |
| 1:C:1494:HIS:CE1  | 1:C:1877:GLN:CG   | 2.99                     | 0.44              |
| 2:G:607:VAL:O     | 2:G:611:THR:HB    | 2.17                     | 0.44              |
| 2:G:717:ILE:O     | 2:G:720:ALA:HB3   | 2.18                     | 0.44              |
| 2:G:741:HIS:HE1   | 2:G:855:HIS:NE2   | 2.13                     | 0.44              |
| 2:G:741:HIS:HB3   | 2:G:853:PRO:HB2   | 1.98                     | 0.44              |
| 2:G:926:LEU:HB3   | 2:G:947:THR:CG2   | 2.46                     | 0.44              |
| 2:G:1071:LYS:HE3  | 2:G:1075:ASP:OD2  | 2.16                     | 0.44              |
| 2:G:1294:ALA:HA   | 2:G:1368:VAL:CG2  | 2.47                     | 0.44              |
| 2:G:1855:ILE:HB   | 2:G:1907:LEU:HD12 | 2.00                     | 0.44              |
| 2:H:109:LEU:HD22  | 2:H:114:THR:HG23  | 1.99                     | 0.44              |
| 2:H:443:LEU:HD22  | 2:H:448:VAL:CG1   | 2.46                     | 0.44              |
| 2:H:1308:CYS:HB3  | 2:H:1311:PHE:CE2  | 2.52                     | 0.44              |
| 2:H:1321:ALA:HA   | 2:H:1322:PRO:HD3  | 1.84                     | 0.44              |
| 2:H:1529:GLN:O    | 2:H:1632:ILE:HG13 | 2.16                     | 0.44              |
| 2:I:272:GLY:HA3   | 2:I:276:GLY:C     | 2.37                     | 0.44              |
| 2:I:1159:ILE:CG2  | 2:I:1160:THR:N    | 2.81                     | 0.44              |
| 2:I:1589:VAL:HG21 | 2:I:1651:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:225:SER:OG    | 1:A:266:LEU:HD21  | 2.16                     | 0.44              |
| 1:A:1012:LEU:HD23 | 1:A:1445:MET:HE2  | 1.99                     | 0.44              |
| 1:A:1373:ARG:NE   | 1:A:1550:ASP:HB2  | 2.32                     | 0.44              |
| 1:A:1666:THR:HG23 | 1:A:1669:ARG:CB   | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:168:MET:HA    | 1:B:206:LEU:HB2   | 2.00                     | 0.44              |
| 1:B:256:LEU:HA    | 1:B:257:PRO:HD3   | 1.73                     | 0.44              |
| 1:B:330:GLU:O     | 1:B:330:GLU:HG2   | 2.16                     | 0.44              |
| 1:C:1234:MET:HG2  | 1:C:1326:ILE:HD12 | 1.98                     | 0.44              |
| 1:C:1238:VAL:CG1  | 1:C:1239:HIS:N    | 2.80                     | 0.44              |
| 2:G:7:ARG:HH11    | 2:G:24:THR:HG23   | 1.76                     | 0.44              |
| 2:G:463:PHE:C     | 2:G:463:PHE:CD2   | 2.90                     | 0.44              |
| 2:G:595:PRO:HD3   | 2:G:800:LEU:HB2   | 1.99                     | 0.44              |
| 2:G:1609:THR:O    | 2:G:1653:GLY:HA3  | 2.16                     | 0.44              |
| 2:H:120:LYS:HB3   | 2:H:124:LYS:HE3   | 1.99                     | 0.44              |
| 2:H:560:ASN:H     | 2:H:564:GLU:HG2   | 1.82                     | 0.44              |
| 2:H:786:SER:HB2   | 2:H:794:MET:HE2   | 1.99                     | 0.44              |
| 2:H:854:ILE:HG22  | 2:H:856:LYS:HG3   | 1.99                     | 0.44              |
| 2:H:1330:GLY:HA2  | 2:H:1374:THR:HG21 | 1.98                     | 0.44              |
| 2:H:1543:ASP:OD1  | 2:H:1623:LYS:HG2  | 2.17                     | 0.44              |
| 2:I:191:SER:HA    | 2:I:194:THR:CG2   | 2.43                     | 0.44              |
| 2:I:441:LYS:O     | 2:I:444:VAL:HG12  | 2.17                     | 0.44              |
| 2:I:659:LEU:HD12  | 2:I:659:LEU:HA    | 1.84                     | 0.44              |
| 2:I:1303:ALA:HB2  | 2:I:1556:VAL:HG21 | 1.98                     | 0.44              |
| 2:I:1314:ARG:HD3  | 2:I:1314:ARG:HA   | 1.64                     | 0.44              |
| 1:A:27:ARG:HH21   | 2:G:2015:THR:HA   | 1.82                     | 0.44              |
| 1:A:267:VAL:HG12  | 1:A:290:MET:CE    | 2.48                     | 0.44              |
| 1:A:1431:GLU:HB3  | 1:A:1520:ALA:HB2  | 1.99                     | 0.44              |
| 1:B:183:GLN:O     | 1:B:187:LEU:HG    | 2.17                     | 0.44              |
| 1:B:225:SER:OG    | 1:B:266:LEU:HD21  | 2.18                     | 0.44              |
| 1:B:479:ASN:O     | 1:B:483:VAL:HG23  | 2.17                     | 0.44              |
| 1:B:539:SER:O     | 1:B:540:GLN:C     | 2.54                     | 0.44              |
| 1:B:655:LEU:HD23  | 1:B:655:LEU:HA    | 1.82                     | 0.44              |
| 1:B:833:PHE:O     | 1:B:834:GLY:O     | 2.35                     | 0.44              |
| 1:C:180:SER:O     | 1:C:183:GLN:N     | 2.50                     | 0.44              |
| 1:C:1487:LEU:HD23 | 1:C:1487:LEU:C    | 2.38                     | 0.44              |
| 2:G:120:LYS:HB3   | 2:G:124:LYS:HE3   | 1.99                     | 0.44              |
| 2:G:231:LEU:HA    | 2:G:236:ILE:HD12  | 2.00                     | 0.44              |
| 2:G:566:HIS:O     | 2:G:567:PRO:O     | 2.34                     | 0.44              |
| 2:G:1015:VAL:HA   | 2:G:1016:PRO:HD3  | 1.79                     | 0.44              |
| 2:H:161:GLY:H     | 2:H:505:GLY:CA    | 2.29                     | 0.44              |
| 2:H:427:PHE:HB3   | 2:H:428:HIS:ND1   | 2.32                     | 0.44              |
| 2:H:607:VAL:O     | 2:H:611:THR:HB    | 2.17                     | 0.44              |
| 2:I:703:LEU:HD21  | 2:I:705:LEU:CD2   | 2.45                     | 0.44              |
| 2:I:780:TYR:HB2   | 2:I:799:PHE:CE2   | 2.53                     | 0.44              |
| 2:I:901:LYS:NZ    | 2:I:1031:LYS:O    | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1735:ALA:O    | 2:I:1737:ILE:HG13 | 2.17                     | 0.44              |
| 2:I:1757:GLU:H    | 2:I:1757:GLU:HG3  | 1.50                     | 0.44              |
| 1:A:66:GLU:OE1    | 1:A:66:GLU:HA     | 2.17                     | 0.44              |
| 1:A:1020:VAL:CG1  | 1:A:1400:ILE:HG23 | 2.47                     | 0.44              |
| 1:A:1056:ILE:CD1  | 1:A:1193:TRP:CD1  | 3.00                     | 0.44              |
| 1:B:32:GLN:HE22   | 1:B:57:ALA:N      | 2.16                     | 0.44              |
| 1:B:232:LEU:HD13  | 1:B:272:GLU:CB    | 2.47                     | 0.44              |
| 1:B:1040:GLU:OE2  | 1:B:1577:GLN:HB2  | 2.18                     | 0.44              |
| 1:C:625:THR:HG23  | 1:C:627:SER:H     | 1.83                     | 0.44              |
| 1:C:930:LEU:HD23  | 1:C:930:LEU:HA    | 1.76                     | 0.44              |
| 1:C:1022:THR:HG22 | 1:C:1226:SER:CB   | 2.47                     | 0.44              |
| 1:C:1657:HIS:CG   | 1:C:1658:PRO:HD2  | 2.53                     | 0.44              |
| 2:G:932:ILE:HD12  | 2:G:939:PHE:HD1   | 1.83                     | 0.44              |
| 2:G:1590:ARG:NH2  | 2:G:1594:GLU:OE2  | 2.50                     | 0.44              |
| 2:G:1752:PHE:HZ   | 2:G:1836:MET:HE3  | 1.82                     | 0.44              |
| 2:G:1873:TYR:CE1  | 2:G:1877:ARG:NH2  | 2.84                     | 0.44              |
| 2:G:1908:ASP:HA   | 2:G:1911:THR:HG22 | 2.00                     | 0.44              |
| 2:G:1945:ASP:O    | 2:G:1949:LYS:HG3  | 2.17                     | 0.44              |
| 2:H:209:PHE:CE2   | 2:H:213:LEU:HD22  | 2.52                     | 0.44              |
| 2:H:663:ILE:HB    | 2:H:664:PRO:CD    | 2.44                     | 0.44              |
| 2:H:778:TYR:N     | 2:H:779:PRO:CD    | 2.80                     | 0.44              |
| 2:H:1311:PHE:HD1  | 2:H:1320:LEU:O    | 2.00                     | 0.44              |
| 2:H:1697:HIS:CE1  | 2:H:1829:GLU:CG   | 3.00                     | 0.44              |
| 2:I:665:LEU:O     | 2:I:665:LEU:HD22  | 2.18                     | 0.44              |
| 2:I:1054:LEU:CB   | 4:I:3051:FMN:HM71 | 2.46                     | 0.44              |
| 2:I:1330:GLY:HA2  | 2:I:1374:THR:HG21 | 1.99                     | 0.44              |
| 2:I:1418:ASP:OD1  | 2:I:1420:GLU:HG3  | 2.17                     | 0.44              |
| 2:I:1651:LEU:HD23 | 2:I:1651:LEU:HA   | 1.73                     | 0.44              |
| 1:B:496:PRO:HB2   | 1:B:519:VAL:HG12  | 1.99                     | 0.44              |
| 1:C:44:VAL:HG13   | 1:C:78:ILE:HG12   | 1.99                     | 0.44              |
| 1:C:503:ILE:HD12  | 1:C:950:THR:HG21  | 1.98                     | 0.44              |
| 2:G:109:LEU:HD22  | 2:G:114:THR:HG23  | 2.00                     | 0.44              |
| 2:G:297:ARG:O     | 2:G:301:THR:HG22  | 2.17                     | 0.44              |
| 2:G:490:TRP:HA    | 2:G:493:THR:HG22  | 1.98                     | 0.44              |
| 2:G:589:ARG:HB3   | 2:G:590:PRO:CD    | 2.48                     | 0.44              |
| 2:G:1632:ILE:HG23 | 2:G:1632:ILE:O    | 2.16                     | 0.44              |
| 2:H:109:LEU:HD11  | 2:H:116:LEU:CD2   | 2.43                     | 0.44              |
| 2:H:641:ILE:CG1   | 2:H:645:SER:HB2   | 2.45                     | 0.44              |
| 2:I:9:LEU:HB2     | 2:I:27:PHE:HE1    | 1.82                     | 0.44              |
| 2:I:245:GLN:HG2   | 2:I:505:GLY:HA2   | 2.00                     | 0.44              |
| 2:I:468:LEU:O     | 2:I:471:LEU:HB2   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:835:THR:HG22  | 2:I:844:VAL:CA    | 2.48                     | 0.44              |
| 2:I:1590:ARG:HG3  | 2:I:1608:TYR:CD2  | 2.53                     | 0.44              |
| 2:I:1846:GLU:C    | 2:I:1848:GLY:H    | 2.20                     | 0.44              |
| 1:A:1022:THR:CG2  | 1:A:1226:SER:OG   | 2.66                     | 0.44              |
| 1:A:1135:GLU:CD   | 1:B:242:THR:HG21  | 2.38                     | 0.44              |
| 1:A:1305:CYS:SG   | 1:A:1585:LYS:HA   | 2.57                     | 0.44              |
| 1:B:267:VAL:HG12  | 1:B:290:MET:CE    | 2.48                     | 0.44              |
| 1:B:1238:VAL:CG1  | 1:B:1239:HIS:N    | 2.81                     | 0.44              |
| 1:B:1516:ASP:HA   | 1:B:1517:PRO:HD3  | 1.65                     | 0.44              |
| 1:C:503:ILE:HD11  | 1:C:947:LEU:HD22  | 1.98                     | 0.44              |
| 1:C:1557:ILE:HD11 | 1:C:1642:THR:HG21 | 2.00                     | 0.44              |
| 2:G:551:THR:C     | 2:G:553:ASN:H     | 2.20                     | 0.44              |
| 2:G:551:THR:HG22  | 2:G:552:SER:N     | 2.31                     | 0.44              |
| 2:G:751:LEU:HD23  | 2:G:791:TYR:CD2   | 2.53                     | 0.44              |
| 2:G:751:LEU:HD11  | 2:G:789:PHE:CD1   | 2.53                     | 0.44              |
| 2:G:1784:MET:HE2  | 2:G:1784:MET:O    | 2.17                     | 0.44              |
| 2:H:305:PHE:CD1   | 2:H:442:ASP:HB3   | 2.53                     | 0.44              |
| 2:H:807:ILE:HA    | 2:H:818:LYS:HG2   | 1.99                     | 0.44              |
| 2:H:1389:ILE:HG13 | 2:H:1411:PHE:CD1  | 2.52                     | 0.44              |
| 2:I:40:ILE:O      | 2:I:42:PRO:HD3    | 2.17                     | 0.44              |
| 2:I:159:ILE:CG2   | 2:I:501:ILE:HG22  | 2.47                     | 0.44              |
| 2:I:305:PHE:CD1   | 2:I:442:ASP:HB3   | 2.52                     | 0.44              |
| 2:I:720:ALA:HA    | 2:I:728:ILE:CD1   | 2.47                     | 0.44              |
| 2:I:1257:ASP:O    | 2:I:1261:ARG:HG3  | 2.17                     | 0.44              |
| 2:I:1896:GLN:HE21 | 2:I:1896:GLN:HB3  | 1.58                     | 0.44              |
| 1:A:458:THR:OG1   | 1:A:470:LYS:HD2   | 2.18                     | 0.44              |
| 1:A:1194:ASN:OD1  | 1:A:1196:LYS:HB2  | 2.18                     | 0.44              |
| 1:A:1220:VAL:O    | 1:A:1224:ILE:HG12 | 2.18                     | 0.44              |
| 1:A:1464:GLU:HG3  | 1:A:1773:VAL:HG11 | 1.77                     | 0.44              |
| 1:B:29:ILE:HG12   | 2:H:1892:ASN:C    | 2.37                     | 0.44              |
| 1:B:1012:LEU:HD23 | 1:B:1445:MET:CE   | 2.48                     | 0.44              |
| 1:B:1195:ALA:HB1  | 1:B:1200:ILE:HD12 | 1.99                     | 0.44              |
| 1:C:1673:TYR:CZ   | 1:C:1677:VAL:HG21 | 2.51                     | 0.44              |
| 2:H:272:GLY:HA3   | 2:H:276:GLY:C     | 2.38                     | 0.44              |
| 2:H:376:ASN:C     | 2:H:376:ASN:ND2   | 2.70                     | 0.44              |
| 2:H:455:ILE:C     | 2:H:455:ILE:HD12  | 2.38                     | 0.44              |
| 2:H:1148:ASN:HD22 | 2:H:1148:ASN:C    | 2.21                     | 0.44              |
| 2:H:1579:ILE:HD11 | 2:H:1615:MET:SD   | 2.58                     | 0.44              |
| 2:I:184:VAL:HG12  | 2:I:188:ILE:HG12  | 1.99                     | 0.44              |
| 2:I:297:ARG:O     | 2:I:301:THR:HG22  | 2.18                     | 0.44              |
| 2:I:517:HIS:CE1   | 2:I:540:ASP:O     | 2.71                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1739:GLU:HB2  | 2:I:1987:PRO:CB   | 2.29                     | 0.44              |
| 2:I:1976:PHE:HB3  | 2:I:1981:LEU:CD2  | 2.48                     | 0.44              |
| 1:A:11:HIS:CD2    | 1:A:11:HIS:C      | 2.92                     | 0.44              |
| 1:A:499:PRO:HD3   | 1:A:516:ARG:HH21  | 1.83                     | 0.44              |
| 1:A:530:ALA:HA    | 1:A:636:PRO:HB3   | 1.99                     | 0.44              |
| 1:A:1133:PRO:HG3  | 1:A:1166:LYS:HG3  | 1.99                     | 0.44              |
| 1:B:20:TYR:CD2    | 2:H:2033:THR:OG1  | 2.71                     | 0.44              |
| 1:B:42:GLU:O      | 1:B:77:GLU:N      | 2.47                     | 0.44              |
| 1:B:1037:TRP:HB2  | 1:B:1598:GLN:OE1  | 2.18                     | 0.44              |
| 1:B:1455:ARG:O    | 1:B:1459:ILE:HG13 | 2.18                     | 0.44              |
| 1:B:1842:VAL:O    | 1:B:1843:ASN:C    | 2.57                     | 0.44              |
| 1:C:187:LEU:HD22  | 1:C:201:PRO:HB2   | 1.99                     | 0.44              |
| 1:C:601:VAL:O     | 1:C:602:GLU:C     | 2.56                     | 0.44              |
| 1:C:706:THR:HB    | 1:C:737:PHE:HB3   | 2.00                     | 0.44              |
| 1:C:852:ARG:HB3   | 1:C:858:TRP:HZ2   | 1.83                     | 0.44              |
| 1:C:1234:MET:CE   | 1:C:1326:ILE:HG21 | 2.48                     | 0.44              |
| 1:C:1270:VAL:HG11 | 1:C:1274:ILE:HD13 | 1.99                     | 0.44              |
| 2:G:615:TYR:CE2   | 2:G:1074:MET:HB3  | 2.52                     | 0.44              |
| 2:G:1257:ASP:O    | 2:G:1261:ARG:HG3  | 2.18                     | 0.44              |
| 2:G:1551:GLU:HB2  | 2:G:1552:PRO:HD3  | 2.00                     | 0.44              |
| 2:G:1589:VAL:HG21 | 2:G:1651:LEU:HD12 | 1.99                     | 0.44              |
| 2:G:1662:THR:HB   | 2:G:1799:PRO:HG2  | 1.99                     | 0.44              |
| 2:G:1776:PHE:C    | 2:G:1779:PRO:HD2  | 2.38                     | 0.44              |
| 2:H:184:VAL:HG12  | 2:H:188:ILE:HG12  | 2.00                     | 0.44              |
| 2:H:732:TRP:CE2   | 2:H:750:MET:HE3   | 2.52                     | 0.44              |
| 2:H:780:TYR:HB2   | 2:H:799:PHE:CE2   | 2.53                     | 0.44              |
| 2:H:938:TRP:CE2   | 2:H:944:ARG:HG3   | 2.52                     | 0.44              |
| 2:H:1228:THR:HG21 | 2:H:1234:VAL:HG23 | 2.00                     | 0.44              |
| 2:I:142:ASN:HB2   | 2:I:550:VAL:HG13  | 1.99                     | 0.44              |
| 2:I:1579:ILE:HG22 | 2:I:1580:THR:O    | 2.18                     | 0.44              |
| 2:I:1666:PHE:CE1  | 2:I:1814:ALA:HA   | 2.53                     | 0.44              |
| 2:I:1886:VAL:HG22 | 2:I:1906:ALA:HB1  | 1.98                     | 0.44              |
| 1:A:1501:LEU:HD11 | 1:A:1775:LEU:CG   | 2.47                     | 0.44              |
| 1:A:1842:VAL:O    | 1:A:1843:ASN:C    | 2.57                     | 0.44              |
| 1:B:267:VAL:O     | 1:B:290:MET:HE1   | 2.17                     | 0.44              |
| 1:B:1430:ARG:O    | 1:B:1430:ARG:HG2  | 2.18                     | 0.44              |
| 1:C:295:ALA:HB1   | 1:C:300:VAL:O     | 2.18                     | 0.44              |
| 1:C:833:PHE:O     | 1:C:834:GLY:O     | 2.36                     | 0.44              |
| 1:C:1181:PHE:CZ   | 1:C:1341:PHE:HA   | 2.53                     | 0.44              |
| 1:C:1291:LEU:HD21 | 1:C:1698:PHE:CE1  | 2.53                     | 0.44              |
| 2:G:159:ILE:HD11  | 2:G:512:LEU:CG    | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:459:VAL:HG12  | 2:G:468:LEU:HD12  | 2.00                     | 0.44              |
| 2:G:566:HIS:O     | 2:G:567:PRO:C     | 2.57                     | 0.44              |
| 2:G:901:LYS:NZ    | 2:G:1031:LYS:O    | 2.50                     | 0.44              |
| 2:G:1004:LEU:CD2  | 2:G:1019:PRO:HB2  | 2.48                     | 0.44              |
| 2:G:1352:HIS:HE1  | 2:G:1583:MET:CE   | 2.27                     | 0.44              |
| 2:H:102:HIS:HE1   | 2:H:180:TYR:OH    | 2.00                     | 0.44              |
| 2:H:1496:LYS:HE2  | 2:H:1693:ARG:HH21 | 1.82                     | 0.44              |
| 2:H:1739:GLU:HB2  | 2:H:1987:PRO:CB   | 2.30                     | 0.44              |
| 2:I:218:TRP:HB3   | 2:I:225:THR:OG1   | 2.18                     | 0.44              |
| 2:I:246:LEU:O     | 2:I:250:VAL:HG23  | 2.18                     | 0.44              |
| 2:I:914:LEU:HD21  | 2:I:1003:PHE:CD2  | 2.53                     | 0.44              |
| 2:I:1493:LEU:HB3  | 2:I:1494:PRO:CD   | 2.48                     | 0.44              |
| 2:I:1684:SER:O    | 2:I:1688:GLN:HG3  | 2.18                     | 0.44              |
| 1:A:181:THR:O     | 1:A:185:GLU:HG3   | 2.18                     | 0.43              |
| 1:A:406:TRP:CE3   | 1:A:407:ASN:HB2   | 2.53                     | 0.43              |
| 1:A:933:VAL:O     | 1:A:933:VAL:HG22  | 2.18                     | 0.43              |
| 1:B:35:PHE:HA     | 1:B:39:PHE:HD2    | 1.83                     | 0.43              |
| 1:B:888:ILE:HD12  | 1:B:939:PHE:CE2   | 2.43                     | 0.43              |
| 1:B:1129:GLU:OE1  | 1:C:348:ARG:HD3   | 2.18                     | 0.43              |
| 1:B:1460:LYS:CE   | 1:B:1774:GLU:CD   | 2.86                     | 0.43              |
| 1:C:413:LEU:C     | 1:C:415:SER:H     | 2.21                     | 0.43              |
| 1:C:1332:TYR:HB3  | 1:C:1382:ALA:CB   | 2.48                     | 0.43              |
| 1:C:1373:ARG:NE   | 1:C:1550:ASP:HB2  | 2.33                     | 0.43              |
| 2:G:245:GLN:HG2   | 2:G:505:GLY:HA2   | 1.99                     | 0.43              |
| 2:G:543:PHE:CB    | 2:G:545:GLN:NE2   | 2.81                     | 0.43              |
| 2:G:566:HIS:ND1   | 2:G:567:PRO:HD2   | 2.33                     | 0.43              |
| 2:G:726:PHE:HA    | 2:G:727:PRO:HD3   | 1.89                     | 0.43              |
| 2:G:753:MET:O     | 2:G:757:ILE:HG13  | 2.18                     | 0.43              |
| 2:G:866:LYS:O     | 2:G:870:GLU:HG3   | 2.18                     | 0.43              |
| 2:G:1236:LEU:HD11 | 2:G:1262:ILE:HG12 | 1.99                     | 0.43              |
| 2:H:9:LEU:HB2     | 2:H:27:PHE:HE1    | 1.83                     | 0.43              |
| 2:H:123:ILE:HD11  | 2:H:533:LEU:CD2   | 2.48                     | 0.43              |
| 2:H:567:PRO:CG    | 2:H:781:LEU:CD1   | 2.94                     | 0.43              |
| 2:H:670:ARG:HD2   | 2:H:676:ILE:O     | 2.18                     | 0.43              |
| 2:H:1222:GLU:HG3  | 2:H:1235:SER:OG   | 2.17                     | 0.43              |
| 2:H:1586:SER:O    | 2:H:1590:ARG:HB2  | 2.17                     | 0.43              |
| 2:H:1638:ILE:CD1  | 2:H:1657:ILE:HG13 | 2.41                     | 0.43              |
| 2:I:427:PHE:HB3   | 2:I:428:HIS:ND1   | 2.33                     | 0.43              |
| 2:I:432:LEU:HB3   | 2:I:484:ILE:HG23  | 2.00                     | 0.43              |
| 2:I:932:ILE:HD12  | 2:I:939:PHE:HD1   | 1.83                     | 0.43              |
| 2:I:1427:VAL:HG22 | 2:I:1469:GLU:HG2  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1551:GLU:HB2  | 2:I:1552:PRO:HD3  | 2.00                     | 0.43              |
| 2:I:1782:THR:CG2  | 2:I:1827:LEU:HD21 | 2.45                     | 0.43              |
| 1:A:626:VAL:HG23  | 1:A:664:GLU:OE2   | 2.18                     | 0.43              |
| 1:A:930:LEU:HD23  | 1:A:930:LEU:HA    | 1.75                     | 0.43              |
| 1:A:1584:PRO:CG   | 1:A:1591:TRP:CZ3  | 3.02                     | 0.43              |
| 1:B:1279:PHE:HB2  | 1:B:1282:THR:HG23 | 2.00                     | 0.43              |
| 1:C:168:MET:HA    | 1:C:206:LEU:HB2   | 2.00                     | 0.43              |
| 1:C:196:THR:O     | 1:C:213:PHE:HE2   | 2.01                     | 0.43              |
| 1:C:1279:PHE:HB2  | 1:C:1282:THR:HG23 | 2.00                     | 0.43              |
| 1:C:1720:ALA:O    | 1:C:1721:ARG:HG2  | 2.17                     | 0.43              |
| 2:G:195:LEU:O     | 2:G:199:ILE:HG13  | 2.18                     | 0.43              |
| 2:G:581:THR:O     | 2:G:585:LYS:HB2   | 2.18                     | 0.43              |
| 2:G:754:TYR:CD2   | 2:G:794:MET:CG    | 3.01                     | 0.43              |
| 2:G:900:GLN:NE2   | 2:G:1051:THR:HA   | 2.32                     | 0.43              |
| 2:G:1195:VAL:HG13 | 2:G:1211:LEU:CB   | 2.48                     | 0.43              |
| 2:G:1227:ARG:CD   | 2:G:1565:VAL:HG11 | 2.44                     | 0.43              |
| 2:H:666:ILE:HG22  | 2:H:698:LEU:HD22  | 2.00                     | 0.43              |
| 2:I:428:HIS:CD2   | 2:I:488:VAL:HG23  | 2.53                     | 0.43              |
| 2:I:751:LEU:HD23  | 2:I:791:TYR:CD2   | 2.53                     | 0.43              |
| 2:I:938:TRP:CE2   | 2:I:944:ARG:HG3   | 2.53                     | 0.43              |
| 2:I:1778:GLN:HB2  | 2:I:1779:PRO:HD3  | 2.00                     | 0.43              |
| 2:I:1976:PHE:HA   | 2:I:1981:LEU:CD2  | 2.48                     | 0.43              |
| 1:A:28:TRP:HB3    | 2:G:1892:ASN:HA   | 2.00                     | 0.43              |
| 1:A:235:SER:HA    | 1:A:276:ARG:NH2   | 2.32                     | 0.43              |
| 1:A:237:MET:HG3   | 1:A:241:PHE:HB3   | 2.00                     | 0.43              |
| 1:A:411:GLN:O     | 1:A:415:SER:HB2   | 2.18                     | 0.43              |
| 1:A:1209:ASP:OD2  | 1:A:1253:GLY:HA2  | 2.19                     | 0.43              |
| 1:B:807:LYS:C     | 1:B:807:LYS:HD3   | 2.39                     | 0.43              |
| 1:B:1014:ASP:N    | 1:B:1510:ASN:HD21 | 2.06                     | 0.43              |
| 1:B:1248:GLY:HA3  | 1:B:1301:PRO:HD2  | 1.99                     | 0.43              |
| 1:C:340:ARG:HH12  | 1:C:344:GLN:HE21  | 1.65                     | 0.43              |
| 1:C:421:ILE:HG12  | 1:C:469:VAL:HG21  | 1.98                     | 0.43              |
| 1:C:627:SER:HB3   | 1:C:661:ASP:OD1   | 2.18                     | 0.43              |
| 1:C:639:HIS:HB2   | 1:C:656:SER:OG    | 2.18                     | 0.43              |
| 1:C:988:ILE:HD13  | 1:C:1048:GLU:HB3  | 2.01                     | 0.43              |
| 1:C:1056:ILE:CD1  | 1:C:1193:TRP:CD1  | 2.99                     | 0.43              |
| 2:G:1327:ILE:HD12 | 2:G:1327:ILE:HA   | 1.79                     | 0.43              |
| 2:G:1473:THR:O    | 2:G:1481:SER:HB3  | 2.18                     | 0.43              |
| 2:G:1768:LYS:HE2  | 2:G:1772:SER:HB3  | 2.00                     | 0.43              |
| 2:H:369:SER:C     | 2:H:370:LEU:HD23  | 2.38                     | 0.43              |
| 2:H:439:ILE:HD12  | 2:H:484:ILE:HD11  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:732:TRP:CH2   | 2:H:749:PRO:HG2   | 2.53                     | 0.43              |
| 2:H:772:GLY:O     | 2:H:804:ARG:HD3   | 2.18                     | 0.43              |
| 2:H:856:LYS:CE    | 2:H:1052:CYS:SG   | 3.06                     | 0.43              |
| 2:H:970:TYR:O     | 2:H:973:LEU:HB2   | 2.18                     | 0.43              |
| 2:I:159:ILE:HG12  | 2:I:512:LEU:HD23  | 2.01                     | 0.43              |
| 2:I:551:THR:C     | 2:I:553:ASN:H     | 2.22                     | 0.43              |
| 2:I:572:ASN:CB    | 2:I:576:LYS:H     | 2.27                     | 0.43              |
| 2:I:754:TYR:CG    | 2:I:794:MET:HG2   | 2.53                     | 0.43              |
| 2:I:843:ILE:HD13  | 2:I:1055:HIS:O    | 2.18                     | 0.43              |
| 2:I:1241:ASN:N    | 2:I:1252:SER:O    | 2.50                     | 0.43              |
| 2:I:1624:THR:CB   | 2:I:1642:THR:HG23 | 2.47                     | 0.43              |
| 1:B:176:VAL:HG12  | 1:B:178:GLY:H     | 1.83                     | 0.43              |
| 1:B:1244:GLY:C    | 1:B:1327:CYS:HB2  | 2.38                     | 0.43              |
| 1:C:980:VAL:HG21  | 2:I:952:ARG:HH21  | 1.83                     | 0.43              |
| 2:G:455:ILE:C     | 2:G:455:ILE:HD12  | 2.39                     | 0.43              |
| 2:G:967:ILE:HD12  | 2:G:972:LEU:HD22  | 2.00                     | 0.43              |
| 2:G:1016:PRO:HD2  | 2:G:1017:PHE:CE2  | 2.53                     | 0.43              |
| 2:G:1040:LEU:O    | 2:G:1046:GLN:HG3  | 2.19                     | 0.43              |
| 2:G:1162:ASP:O    | 2:G:1163:LYS:HB2  | 2.19                     | 0.43              |
| 2:G:1223:MET:HE3  | 2:G:1238:LEU:CD1  | 2.49                     | 0.43              |
| 2:G:1308:CYS:HB3  | 2:G:1311:PHE:CE2  | 2.53                     | 0.43              |
| 2:G:1674:GLN:OE1  | 2:G:1712:ASN:HA   | 2.18                     | 0.43              |
| 2:G:1678:MET:HE3  | 2:G:1707:LEU:CD2  | 2.43                     | 0.43              |
| 2:G:1804:PHE:CD2  | 2:G:1818:LEU:HD22 | 2.53                     | 0.43              |
| 2:G:1846:GLU:C    | 2:G:1848:GLY:H    | 2.20                     | 0.43              |
| 2:H:309:ARG:HD3   | 2:H:309:ARG:HA    | 1.63                     | 0.43              |
| 2:I:430:HIS:CE1   | 2:I:431:LEU:HD13  | 2.53                     | 0.43              |
| 2:I:439:ILE:HD12  | 2:I:484:ILE:CD1   | 2.48                     | 0.43              |
| 2:I:835:THR:HG21  | 2:I:855:HIS:NE2   | 2.33                     | 0.43              |
| 2:I:1210:ILE:HG22 | 2:I:1210:ILE:O    | 2.18                     | 0.43              |
| 2:I:1325:PHE:O    | 2:I:1328:VAL:HG12 | 2.18                     | 0.43              |
| 2:I:1428:GLU:HG2  | 2:I:1470:THR:HG22 | 1.99                     | 0.43              |
| 1:A:254:TRP:CZ3   | 1:A:302:LEU:HD13  | 2.53                     | 0.43              |
| 1:A:413:LEU:O     | 1:A:413:LEU:HG    | 2.17                     | 0.43              |
| 1:A:496:PRO:HB2   | 1:A:519:VAL:HG12  | 2.01                     | 0.43              |
| 1:A:893:VAL:HG11  | 1:A:930:LEU:CD2   | 2.46                     | 0.43              |
| 1:A:1291:LEU:HD21 | 1:A:1698:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:1375:GLY:HA2  | 1:A:1546:THR:HG22 | 2.01                     | 0.43              |
| 1:A:1553:GLU:HA   | 1:A:1556:THR:HG23 | 2.01                     | 0.43              |
| 1:A:1556:THR:O    | 1:A:1560:MET:HG2  | 2.18                     | 0.43              |
| 1:A:1673:TYR:CZ   | 1:A:1677:VAL:HG21 | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:242:THR:HB    | 1:B:244:THR:HB    | 2.01                     | 0.43              |
| 1:C:221:LEU:HD23  | 1:C:221:LEU:HA    | 1.89                     | 0.43              |
| 1:C:235:SER:HA    | 1:C:276:ARG:NH2   | 2.33                     | 0.43              |
| 1:C:1021:VAL:HG22 | 1:C:1387:ILE:HG22 | 2.01                     | 0.43              |
| 1:C:1625:LEU:O    | 1:C:1627:PRO:HD3  | 2.18                     | 0.43              |
| 2:G:156:LEU:HD23  | 2:G:500:HIS:HB2   | 1.99                     | 0.43              |
| 2:G:272:GLY:HA3   | 2:G:276:GLY:C     | 2.38                     | 0.43              |
| 2:G:397:LYS:HB3   | 2:G:416:PHE:CE2   | 2.53                     | 0.43              |
| 2:G:653:TYR:OH    | 2:G:690:VAL:HG11  | 2.18                     | 0.43              |
| 2:G:1458:ASP:O    | 2:G:1462:LYS:HE3  | 2.19                     | 0.43              |
| 2:G:1493:LEU:HB3  | 2:G:1494:PRO:CD   | 2.48                     | 0.43              |
| 2:H:726:PHE:HA    | 2:H:727:PRO:HD3   | 1.88                     | 0.43              |
| 2:H:745:ASP:HA    | 2:H:832:TRP:CH2   | 2.51                     | 0.43              |
| 2:H:1015:VAL:HG13 | 2:H:1017:PHE:CE2  | 2.53                     | 0.43              |
| 2:H:1422:THR:CG2  | 2:H:1422:THR:O    | 2.66                     | 0.43              |
| 2:I:397:LYS:HB3   | 2:I:416:PHE:CE2   | 2.53                     | 0.43              |
| 2:I:439:ILE:HD12  | 2:I:484:ILE:HD11  | 1.99                     | 0.43              |
| 2:I:562:LEU:HD23  | 2:I:562:LEU:HA    | 1.79                     | 0.43              |
| 2:I:852:GLU:H     | 2:I:852:GLU:HG3   | 1.39                     | 0.43              |
| 2:I:972:LEU:HD23  | 2:I:979:ALA:HB2   | 2.00                     | 0.43              |
| 2:I:1496:LYS:CE   | 2:I:1693:ARG:HH21 | 2.31                     | 0.43              |
| 2:I:1651:LEU:O    | 2:I:1652:THR:HG23 | 2.17                     | 0.43              |
| 1:A:242:THR:HB    | 1:A:244:THR:HB    | 2.00                     | 0.43              |
| 1:A:627:SER:HB2   | 1:A:657:SER:CB    | 2.48                     | 0.43              |
| 1:A:641:ARG:HD3   | 1:A:649:TRP:O     | 2.18                     | 0.43              |
| 1:A:790:PHE:CE2   | 1:A:794:ILE:HD11  | 2.53                     | 0.43              |
| 1:B:1208:VAL:HG11 | 1:B:1212:THR:HB   | 1.97                     | 0.43              |
| 1:B:1270:VAL:HG11 | 1:B:1274:ILE:HD13 | 2.00                     | 0.43              |
| 1:C:232:LEU:HD13  | 1:C:272:GLU:CB    | 2.48                     | 0.43              |
| 1:C:1234:MET:HE3  | 1:C:1326:ILE:HG21 | 2.01                     | 0.43              |
| 1:C:1446:LYS:O    | 1:C:1450:ARG:HG3  | 2.18                     | 0.43              |
| 2:G:99:ASN:HA     | 2:G:550:VAL:CG2   | 2.49                     | 0.43              |
| 2:G:419:ARG:HG3   | 2:G:420:PHE:N     | 2.33                     | 0.43              |
| 2:G:1889:VAL:HG13 | 2:G:1977:HIS:HB3  | 1.97                     | 0.43              |
| 2:H:73:GLU:OE2    | 2:H:76:LYS:HD2    | 2.18                     | 0.43              |
| 2:H:160:PHE:CE2   | 2:H:504:PHE:HB2   | 2.54                     | 0.43              |
| 2:H:360:LEU:HA    | 2:H:361:PRO:HD3   | 1.90                     | 0.43              |
| 2:H:1241:ASN:N    | 2:H:1252:SER:O    | 2.51                     | 0.43              |
| 2:H:1419:PHE:C    | 2:H:1421:ASN:N    | 2.71                     | 0.43              |
| 2:I:279:THR:O     | 2:I:283:ILE:HB    | 2.19                     | 0.43              |
| 2:I:871:THR:HG21  | 2:I:887:LYS:HZ1   | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1079:ASP:O    | 2:I:1082:ILE:HG22 | 2.19                     | 0.43              |
| 2:I:1236:LEU:HD22 | 2:I:1238:LEU:HG   | 1.99                     | 0.43              |
| 2:I:1959:LYS:O    | 2:I:1959:LYS:HG2  | 2.19                     | 0.43              |
| 1:A:267:VAL:O     | 1:A:290:MET:HE1   | 2.19                     | 0.43              |
| 1:A:988:ILE:CD1   | 1:A:1048:GLU:HA   | 2.48                     | 0.43              |
| 1:A:1431:GLU:OE2  | 1:A:1433:HIS:HE1  | 2.02                     | 0.43              |
| 1:B:370:GLU:O     | 1:B:373:ALA:HB3   | 2.19                     | 0.43              |
| 1:B:1219:VAL:CA   | 1:B:1384:ILE:HD11 | 2.32                     | 0.43              |
| 1:B:1233:GLU:CD   | 1:B:1680:ARG:HH21 | 2.22                     | 0.43              |
| 1:C:49:PRO:O      | 1:C:82:SER:HB2    | 2.19                     | 0.43              |
| 1:C:1248:GLY:HA3  | 1:C:1301:PRO:HD2  | 2.01                     | 0.43              |
| 1:C:1375:GLY:HA2  | 1:C:1546:THR:HG22 | 1.99                     | 0.43              |
| 1:C:1539:ALA:O    | 1:C:1574:GLY:HA2  | 2.18                     | 0.43              |
| 1:C:1553:GLU:HA   | 1:C:1556:THR:HG23 | 2.01                     | 0.43              |
| 1:C:1599:ILE:HD11 | 1:C:1606:PRO:HD2  | 2.01                     | 0.43              |
| 2:G:184:VAL:HG12  | 2:G:188:ILE:HG12  | 2.00                     | 0.43              |
| 2:G:184:VAL:HG12  | 2:G:184:VAL:O     | 2.19                     | 0.43              |
| 2:G:324:LEU:HD12  | 2:G:324:LEU:O     | 2.18                     | 0.43              |
| 2:G:566:HIS:ND1   | 2:G:566:HIS:C     | 2.72                     | 0.43              |
| 2:G:573:LYS:C     | 2:G:575:GLY:H     | 2.21                     | 0.43              |
| 2:G:652:ILE:HD13  | 2:G:658:MET:HE3   | 1.99                     | 0.43              |
| 2:G:854:ILE:HG22  | 2:G:856:LYS:HG3   | 2.01                     | 0.43              |
| 2:H:573:LYS:C     | 2:H:575:GLY:H     | 2.21                     | 0.43              |
| 2:H:629:GLY:O     | 2:H:632:ALA:HB3   | 2.18                     | 0.43              |
| 2:H:643:LYS:HA    | 2:H:1163:LYS:HG2  | 1.99                     | 0.43              |
| 2:H:653:TYR:OH    | 2:H:690:VAL:HG11  | 2.18                     | 0.43              |
| 2:H:1223:MET:HE3  | 2:H:1238:LEU:CD1  | 2.46                     | 0.43              |
| 2:I:7:ARG:NH2     | 2:I:24:THR:O      | 2.52                     | 0.43              |
| 2:I:607:VAL:O     | 2:I:611:THR:HB    | 2.18                     | 0.43              |
| 1:A:335:HIS:ND1   | 1:C:335:HIS:HE1   | 2.17                     | 0.43              |
| 1:A:644:THR:HG23  | 1:A:648:ASP:N     | 2.34                     | 0.43              |
| 1:A:827:SER:HA    | 1:A:828:PRO:HD3   | 1.70                     | 0.43              |
| 1:A:1009:LEU:CD1  | 1:A:1445:MET:HE1  | 2.48                     | 0.43              |
| 1:B:681:THR:HA    | 1:B:706:THR:OG1   | 2.19                     | 0.43              |
| 1:B:1375:GLY:HA2  | 1:B:1546:THR:HG22 | 2.01                     | 0.43              |
| 1:B:1446:LYS:O    | 1:B:1450:ARG:HG3  | 2.19                     | 0.43              |
| 1:B:1498:GLU:HG2  | 1:B:1876:LEU:HB3  | 1.89                     | 0.43              |
| 1:C:384:GLU:O     | 1:C:388:ASN:HB2   | 2.19                     | 0.43              |
| 1:C:1158:PRO:HD2  | 1:C:1159:GLU:OE2  | 2.18                     | 0.43              |
| 2:G:324:LEU:O     | 2:G:328:LEU:HG    | 2.18                     | 0.43              |
| 2:G:601:THR:O     | 2:G:601:THR:CG2   | 2.67                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:786:SER:HB3   | 2:G:794:MET:HE2   | 2.01                     | 0.43              |
| 2:G:860:ARG:H     | 2:G:1049:GLN:HG3  | 1.83                     | 0.43              |
| 2:G:1004:LEU:HD21 | 2:G:1020:VAL:CG2  | 2.48                     | 0.43              |
| 2:G:1175:LYS:HG3  | 2:G:1176:PRO:HD2  | 2.00                     | 0.43              |
| 2:H:654:VAL:O     | 2:H:654:VAL:HG12  | 2.18                     | 0.43              |
| 2:H:1567:ARG:HH11 | 2:H:1567:ARG:HG2  | 1.72                     | 0.43              |
| 2:H:1940:LEU:HD12 | 2:H:1941:PHE:N    | 2.34                     | 0.43              |
| 2:I:169:TYR:CG    | 2:I:170:PHE:N     | 2.87                     | 0.43              |
| 2:I:425:SER:HA    | 2:I:426:PRO:HD3   | 1.78                     | 0.43              |
| 2:I:846:VAL:CG1   | 2:I:865:TRP:NE1   | 2.82                     | 0.43              |
| 2:I:1168:ASN:HA   | 2:I:1169:PRO:HD3  | 1.84                     | 0.43              |
| 2:I:1552:PRO:O    | 2:I:1556:VAL:HG23 | 2.19                     | 0.43              |
| 2:I:2030:TYR:CD1  | 2:I:2034:GLY:HA2  | 2.54                     | 0.43              |
| 1:A:833:PHE:HA    | 1:A:937:LYS:HD2   | 2.00                     | 0.43              |
| 1:A:1431:GLU:CG   | 1:A:1433:HIS:CE1  | 3.00                     | 0.43              |
| 1:A:1670:TYR:O    | 1:A:1674:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:460:GLU:CG    | 1:B:470:LYS:HD3   | 2.48                     | 0.43              |
| 1:B:1431:GLU:CG   | 1:B:1433:HIS:CE1  | 3.02                     | 0.43              |
| 1:B:1657:HIS:HA   | 1:B:1658:PRO:HD3  | 1.89                     | 0.43              |
| 1:C:1600:LEU:HD11 | 1:C:1655:VAL:HG12 | 2.00                     | 0.43              |
| 2:G:15:SER:H      | 2:G:48:PHE:HE2    | 1.67                     | 0.43              |
| 2:G:28:PHE:CE2    | 2:H:7:ARG:CD      | 2.73                     | 0.43              |
| 2:G:486:LEU:HA    | 2:G:487:PRO:HD3   | 1.90                     | 0.43              |
| 2:G:835:THR:HG22  | 2:G:844:VAL:HA    | 2.00                     | 0.43              |
| 2:G:884:LEU:HD22  | 2:G:1021:LEU:CD1  | 2.49                     | 0.43              |
| 2:G:1219:ILE:HB   | 2:G:1240:TYR:HB2  | 2.01                     | 0.43              |
| 2:G:1875:VAL:HG22 | 2:G:1910:VAL:HG11 | 2.01                     | 0.43              |
| 2:G:2042:ILE:HG12 | 2:G:2042:ILE:H    | 1.39                     | 0.43              |
| 2:H:543:PHE:CB    | 2:H:545:GLN:NE2   | 2.81                     | 0.43              |
| 2:H:717:ILE:HG23  | 2:H:760:HIS:CE1   | 2.54                     | 0.43              |
| 2:H:1862:VAL:HG22 | 2:H:1863:ALA:N    | 2.33                     | 0.43              |
| 2:I:209:PHE:CE2   | 2:I:213:LEU:HD22  | 2.53                     | 0.43              |
| 2:I:573:LYS:C     | 2:I:575:GLY:N     | 2.72                     | 0.43              |
| 2:I:615:TYR:CE2   | 2:I:1074:MET:HB3  | 2.53                     | 0.43              |
| 2:I:702:TYR:HB3   | 2:I:727:PRO:HB2   | 2.00                     | 0.43              |
| 2:I:967:ILE:HD12  | 2:I:972:LEU:HD22  | 2.00                     | 0.43              |
| 2:I:1561:ASN:HA   | 2:I:1562:PRO:HD3  | 1.80                     | 0.43              |
| 2:I:1662:THR:HB   | 2:I:1799:PRO:HG2  | 2.00                     | 0.43              |
| 2:I:1873:TYR:CE1  | 2:I:1877:ARG:NH2  | 2.81                     | 0.43              |
| 1:A:32:GLN:HE22   | 1:A:57:ALA:N      | 2.16                     | 0.43              |
| 1:A:44:VAL:HG11   | 1:A:78:ILE:HG12   | 1.96                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:196:THR:O     | 1:A:213:PHE:HE2   | 2.01                     | 0.43              |
| 1:A:460:GLU:CG    | 1:A:470:LYS:HD3   | 2.49                     | 0.43              |
| 1:A:1107:GLU:HA   | 1:A:1108:PRO:HD3  | 1.90                     | 0.43              |
| 1:A:1498:GLU:HG2  | 1:A:1876:LEU:HB3  | 1.68                     | 0.43              |
| 1:B:260:ARG:HH12  | 1:B:300:VAL:CG2   | 2.20                     | 0.43              |
| 1:B:335:HIS:C     | 1:B:335:HIS:CD2   | 2.92                     | 0.43              |
| 1:B:411:GLN:O     | 1:B:415:SER:HB2   | 2.18                     | 0.43              |
| 1:B:1283:MET:O    | 1:B:1287:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:1553:GLU:HA   | 1:B:1556:THR:HG23 | 2.00                     | 0.43              |
| 1:C:852:ARG:NH1   | 1:C:856:GLU:OE1   | 2.52                     | 0.43              |
| 1:C:1047:LEU:O    | 1:C:1051:VAL:HG23 | 2.19                     | 0.43              |
| 1:C:1107:GLU:HA   | 1:C:1108:PRO:HD3  | 1.89                     | 0.43              |
| 1:C:1208:VAL:HG11 | 1:C:1212:THR:HB   | 1.98                     | 0.43              |
| 2:G:339:LEU:HD23  | 2:G:419:ARG:O     | 2.19                     | 0.43              |
| 2:G:441:LYS:O     | 2:G:445:LYS:HG3   | 2.18                     | 0.43              |
| 2:G:634:ILE:CD1   | 2:G:649:ILE:HD11  | 2.43                     | 0.43              |
| 2:G:1327:ILE:HG12 | 2:G:1583:MET:HE3  | 2.01                     | 0.43              |
| 2:G:1339:PHE:N    | 2:G:1340:PRO:CD   | 2.82                     | 0.43              |
| 2:G:1348:LEU:HD12 | 2:G:1348:LEU:HA   | 1.81                     | 0.43              |
| 2:G:1858:ASN:HA   | 2:G:1896:GLN:O    | 2.18                     | 0.43              |
| 2:H:595:PRO:HD3   | 2:H:800:LEU:HB2   | 2.01                     | 0.43              |
| 2:H:1293:THR:CG2  | 2:H:1296:GLU:H    | 2.24                     | 0.43              |
| 2:I:652:ILE:CD1   | 2:I:658:MET:HE3   | 2.48                     | 0.43              |
| 2:I:950:PHE:O     | 2:I:953:ARG:HB3   | 2.19                     | 0.43              |
| 1:A:2:LYS:HE2     | 1:A:4:GLU:OE1     | 2.19                     | 0.42              |
| 1:A:155:VAL:O     | 1:A:159:LEU:HG    | 2.19                     | 0.42              |
| 1:A:705:VAL:HG23  | 1:A:732:LEU:CD2   | 2.48                     | 0.42              |
| 1:A:1396:MET:O    | 1:A:1680:ARG:NH1  | 2.52                     | 0.42              |
| 1:A:1539:ALA:O    | 1:A:1574:GLY:HA2  | 2.18                     | 0.42              |
| 1:B:335:HIS:O     | 1:B:335:HIS:CD2   | 2.70                     | 0.42              |
| 1:B:350:LEU:HB2   | 1:B:352:MET:HG2   | 2.01                     | 0.42              |
| 1:B:430:ARG:NH2   | 1:B:605:LEU:HD13  | 2.33                     | 0.42              |
| 1:B:1050:CYS:HB3  | 1:B:1089:VAL:HG12 | 2.00                     | 0.42              |
| 1:B:1263:ASP:HB2  | 1:B:1270:VAL:HG21 | 2.00                     | 0.42              |
| 1:B:1406:MET:HE1  | 1:B:1428:THR:HB   | 2.01                     | 0.42              |
| 1:C:1175:ILE:HA   | 1:C:1176:PRO:HD3  | 1.89                     | 0.42              |
| 1:C:1243:VAL:O    | 1:C:1296:GLY:HA3  | 2.18                     | 0.42              |
| 2:G:23:PRO:HG2    | 2:G:86:LEU:HD11   | 2.00                     | 0.42              |
| 2:G:561:TRP:O     | 2:G:563:GLU:N     | 2.51                     | 0.42              |
| 2:H:551:THR:C     | 2:H:553:ASN:H     | 2.21                     | 0.42              |
| 2:H:1257:ASP:O    | 2:H:1261:ARG:HG3  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1458:ASP:O    | 2:H:1462:LYS:HE3  | 2.19                     | 0.42              |
| 2:H:1847:LEU:H    | 2:H:1847:LEU:CD1  | 2.12                     | 0.42              |
| 2:I:7:ARG:CG      | 2:I:22:VAL:O      | 2.67                     | 0.42              |
| 2:I:516:THR:O     | 2:I:519:ASN:HB2   | 2.19                     | 0.42              |
| 2:I:736:ARG:H     | 2:I:736:ARG:HG3   | 1.57                     | 0.42              |
| 2:I:835:THR:HB    | 2:I:845:THR:HG23  | 2.01                     | 0.42              |
| 2:I:1311:PHE:HD1  | 2:I:1320:LEU:O    | 2.02                     | 0.42              |
| 2:I:1868:GLN:HG3  | 2:I:1898:TYR:HH   | 1.83                     | 0.42              |
| 2:I:1878:VAL:CG1  | 2:I:1910:VAL:HG22 | 2.36                     | 0.42              |
| 1:A:32:GLN:NE2    | 1:A:57:ALA:HA     | 2.34                     | 0.42              |
| 1:A:1195:ALA:HB1  | 1:A:1200:ILE:HD12 | 2.02                     | 0.42              |
| 1:A:1495:ASN:HD22 | 1:A:1495:ASN:HA   | 1.67                     | 0.42              |
| 1:B:12:ILE:CD1    | 2:H:2041:ILE:HD11 | 2.49                     | 0.42              |
| 1:B:417:TYR:HH    | 1:B:458:THR:HG22  | 1.84                     | 0.42              |
| 1:B:1119:LYS:HE2  | 1:B:1341:PHE:CD1  | 2.54                     | 0.42              |
| 1:C:949:GLU:O     | 1:C:953:VAL:CG1   | 2.67                     | 0.42              |
| 1:C:1239:HIS:HE1  | 1:C:1714:VAL:O    | 2.02                     | 0.42              |
| 1:C:1308:SER:HB3  | 1:C:1589:GLY:HA3  | 2.01                     | 0.42              |
| 1:C:1618:LEU:HD23 | 1:C:1621:PHE:CE2  | 2.55                     | 0.42              |
| 1:C:1657:HIS:CE1  | 1:C:1658:PRO:HD2  | 2.54                     | 0.42              |
| 2:G:238:CYS:CB    | 2:G:239:PRO:HD3   | 2.45                     | 0.42              |
| 2:G:612:ASN:HD21  | 2:G:641:ILE:HA    | 1.85                     | 0.42              |
| 2:G:1320:LEU:HD12 | 2:G:1320:LEU:HA   | 1.88                     | 0.42              |
| 2:H:127:ILE:HD12  | 2:H:180:TYR:CD2   | 2.54                     | 0.42              |
| 2:H:245:GLN:HG2   | 2:H:505:GLY:HA2   | 2.00                     | 0.42              |
| 2:H:274:SER:OG    | 2:H:428:HIS:HE1   | 2.02                     | 0.42              |
| 2:H:279:THR:O     | 2:H:283:ILE:HB    | 2.20                     | 0.42              |
| 2:H:665:LEU:O     | 2:H:665:LEU:HD22  | 2.19                     | 0.42              |
| 2:H:866:LYS:O     | 2:H:870:GLU:HG3   | 2.19                     | 0.42              |
| 2:H:938:TRP:CD1   | 2:H:944:ARG:HG3   | 2.53                     | 0.42              |
| 2:H:1070:ILE:CD1  | 2:H:1074:MET:HG2  | 2.49                     | 0.42              |
| 2:H:1149:TRP:HA   | 2:H:1242:PHE:CD1  | 2.54                     | 0.42              |
| 2:H:1335:ILE:O    | 2:H:1338:ILE:HG12 | 2.19                     | 0.42              |
| 2:I:503:ASP:O     | 2:I:530:ALA:HB3   | 2.19                     | 0.42              |
| 2:I:538:ASP:HB2   | 2:I:540:ASP:HB2   | 2.01                     | 0.42              |
| 2:I:810:GLU:OE2   | 2:I:1070:ILE:N    | 2.43                     | 0.42              |
| 2:I:856:LYS:CE    | 2:I:1052:CYS:SG   | 3.07                     | 0.42              |
| 2:I:896:ASN:O     | 2:I:1050:ARG:NH2  | 2.52                     | 0.42              |
| 2:I:1321:ALA:HA   | 2:I:1322:PRO:HD3  | 1.83                     | 0.42              |
| 2:I:1666:PHE:CD1  | 2:I:1814:ALA:HB2  | 2.54                     | 0.42              |
| 1:A:290:MET:HB3   | 1:A:290:MET:HE2   | 1.93                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1131:LEU:HD12 | 1:A:1131:LEU:HA   | 1.76                     | 0.42              |
| 1:A:1132:GLU:HA   | 1:A:1133:PRO:HD3  | 1.94                     | 0.42              |
| 1:B:155:VAL:HG22  | 1:B:186:ILE:CG2   | 2.50                     | 0.42              |
| 1:B:280:GLU:O     | 1:B:284:LYS:HG3   | 2.20                     | 0.42              |
| 1:B:828:PRO:HG3   | 1:B:868:ILE:HG22  | 2.00                     | 0.42              |
| 1:B:908:LEU:HA    | 1:B:913:VAL:HG21  | 2.00                     | 0.42              |
| 1:B:1145:LYS:HD3  | 1:B:1154:ILE:HG12 | 2.01                     | 0.42              |
| 1:B:1420:ALA:HA   | 1:B:1421:PRO:HD3  | 1.74                     | 0.42              |
| 1:C:330:GLU:HG2   | 1:C:330:GLU:O     | 2.18                     | 0.42              |
| 1:C:408:TRP:CH2   | 1:C:1628:SER:HB3  | 2.55                     | 0.42              |
| 1:C:1114:TYR:CE1  | 1:C:1337:GLU:HG3  | 2.55                     | 0.42              |
| 2:G:421:LEU:HA    | 2:G:422:PRO:HD3   | 1.81                     | 0.42              |
| 2:G:543:PHE:HB2   | 2:G:545:GLN:NE2   | 2.25                     | 0.42              |
| 2:G:586:LEU:HD12  | 2:G:764:MET:SD    | 2.59                     | 0.42              |
| 2:G:1031:LYS:O    | 2:G:1032:ASP:C    | 2.57                     | 0.42              |
| 2:G:1986:LYS:N    | 2:G:1987:PRO:CD   | 2.82                     | 0.42              |
| 2:G:2026:PHE:HB3  | 2:G:2042:ILE:HD13 | 2.00                     | 0.42              |
| 2:H:38:ASN:HA     | 2:H:41:LEU:HD12   | 2.01                     | 0.42              |
| 2:H:240:LEU:HD12  | 2:H:240:LEU:HA    | 1.78                     | 0.42              |
| 2:H:258:PHE:N     | 2:H:258:PHE:CD1   | 2.87                     | 0.42              |
| 2:H:967:ILE:CD1   | 2:H:972:LEU:HD22  | 2.50                     | 0.42              |
| 2:H:1080:GLY:O    | 2:H:1084:LYS:HG3  | 2.19                     | 0.42              |
| 2:H:1159:ILE:CG2  | 2:H:1160:THR:N    | 2.82                     | 0.42              |
| 2:H:1383:ASN:HD21 | 2:H:1418:ASP:HB3  | 1.84                     | 0.42              |
| 2:H:1497:GLU:OE1  | 2:H:2002:LYS:CE   | 2.66                     | 0.42              |
| 2:H:1551:GLU:HB2  | 2:H:1552:PRO:HD3  | 2.00                     | 0.42              |
| 2:I:190:PHE:O     | 2:I:194:THR:HG22  | 2.19                     | 0.42              |
| 2:I:234:ILE:HG13  | 2:I:235:PRO:CD    | 2.46                     | 0.42              |
| 2:I:309:ARG:HA    | 2:I:309:ARG:HD3   | 1.61                     | 0.42              |
| 2:I:726:PHE:HA    | 2:I:727:PRO:HD3   | 1.86                     | 0.42              |
| 2:I:778:TYR:N     | 2:I:779:PRO:CD    | 2.82                     | 0.42              |
| 2:I:1085:LEU:HD12 | 2:I:1085:LEU:HA   | 1.82                     | 0.42              |
| 1:A:460:GLU:H     | 1:A:460:GLU:HG3   | 1.34                     | 0.42              |
| 1:A:1002:LYS:HZ1  | 1:A:1782:GLU:HG2  | 1.83                     | 0.42              |
| 1:B:874:GLY:O     | 1:B:875:THR:C     | 2.58                     | 0.42              |
| 1:C:21:GLN:HE21   | 1:C:21:GLN:HB3    | 1.69                     | 0.42              |
| 1:C:406:TRP:CE3   | 1:C:407:ASN:HB2   | 2.53                     | 0.42              |
| 1:C:798:ASN:HA    | 1:C:801:ARG:HB2   | 2.02                     | 0.42              |
| 1:C:1219:VAL:CA   | 1:C:1384:ILE:CD1  | 2.94                     | 0.42              |
| 2:G:503:ASP:OD2   | 2:G:513:GLY:N     | 2.50                     | 0.42              |
| 2:G:1878:VAL:CG1  | 2:G:1910:VAL:HG22 | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:176:LEU:CD2   | 2:H:184:VAL:HG21  | 2.50                     | 0.42              |
| 2:H:520:LYS:O     | 2:H:521:ASP:C     | 2.58                     | 0.42              |
| 2:H:536:ASN:HD21  | 2:H:540:ASP:HB3   | 1.84                     | 0.42              |
| 2:H:741:HIS:CE1   | 2:H:855:HIS:NE2   | 2.88                     | 0.42              |
| 2:H:1159:ILE:HG13 | 2:H:1169:PRO:CD   | 2.50                     | 0.42              |
| 2:H:1427:VAL:HG22 | 2:H:1469:GLU:CG   | 2.50                     | 0.42              |
| 2:H:1986:LYS:N    | 2:H:1987:PRO:CD   | 2.81                     | 0.42              |
| 2:I:120:LYS:HB3   | 2:I:124:LYS:HE3   | 2.01                     | 0.42              |
| 2:I:441:LYS:O     | 2:I:445:LYS:HG3   | 2.19                     | 0.42              |
| 2:I:674:TYR:HA    | 2:I:675:PRO:HD3   | 1.69                     | 0.42              |
| 2:I:1102:TYR:HB3  | 2:I:1244:PRO:CA   | 2.49                     | 0.42              |
| 2:I:1175:LYS:HG3  | 2:I:1176:PRO:HD2  | 2.00                     | 0.42              |
| 2:I:1590:ARG:HG3  | 2:I:1608:TYR:CG   | 2.54                     | 0.42              |
| 2:I:2042:ILE:HG12 | 2:I:2042:ILE:H    | 1.36                     | 0.42              |
| 1:A:382:LEU:HA    | 1:A:382:LEU:HD23  | 1.79                     | 0.42              |
| 1:A:1195:ALA:CB   | 1:A:1213:LEU:HD13 | 2.49                     | 0.42              |
| 1:B:20:TYR:HE1    | 2:H:2035:SER:HB2  | 1.82                     | 0.42              |
| 1:B:157:HIS:CE1   | 1:B:269:LEU:HD11  | 2.55                     | 0.42              |
| 1:B:272:GLU:HA    | 1:B:273:PRO:HD3   | 1.92                     | 0.42              |
| 1:B:1022:THR:HG22 | 1:B:1226:SER:CB   | 2.49                     | 0.42              |
| 1:B:1234:MET:HE3  | 1:B:1326:ILE:HG21 | 2.01                     | 0.42              |
| 1:B:1385:GLN:HE21 | 1:B:1385:GLN:HB3  | 1.66                     | 0.42              |
| 1:B:1534:ASP:OD1  | 1:B:1566:ARG:HD3  | 2.19                     | 0.42              |
| 1:C:32:GLN:NE2    | 1:C:57:ALA:CA     | 2.82                     | 0.42              |
| 1:C:408:TRP:CZ3   | 1:C:1628:SER:HB3  | 2.54                     | 0.42              |
| 1:C:413:LEU:O     | 1:C:413:LEU:HG    | 2.19                     | 0.42              |
| 1:C:1455:ARG:HD2  | 1:C:1455:ARG:HA   | 1.82                     | 0.42              |
| 1:C:1592:MET:HE2  | 1:C:1641:ILE:HG23 | 2.00                     | 0.42              |
| 2:G:517:HIS:CE1   | 2:G:540:ASP:O     | 2.73                     | 0.42              |
| 2:G:638:VAL:HG22  | 2:G:675:PRO:HG2   | 2.01                     | 0.42              |
| 2:G:1135:GLU:HG2  | 2:G:1176:PRO:HG2  | 2.02                     | 0.42              |
| 2:H:676:ILE:O     | 2:H:676:ILE:HG12  | 2.17                     | 0.42              |
| 2:H:751:LEU:HD11  | 2:H:789:PHE:CD1   | 2.55                     | 0.42              |
| 2:H:1149:TRP:NE1  | 2:H:1213:LEU:HD12 | 2.34                     | 0.42              |
| 2:H:1294:ALA:HA   | 2:H:1368:VAL:CG2  | 2.49                     | 0.42              |
| 2:I:463:PHE:CD1   | 2:I:486:LEU:HD22  | 2.54                     | 0.42              |
| 2:I:730:LEU:C     | 2:I:730:LEU:HD12  | 2.40                     | 0.42              |
| 2:I:754:TYR:CE2   | 2:I:794:MET:HG3   | 2.53                     | 0.42              |
| 2:I:786:SER:HB3   | 2:I:794:MET:HE2   | 2.01                     | 0.42              |
| 2:I:835:THR:HG22  | 2:I:844:VAL:C     | 2.40                     | 0.42              |
| 1:A:529:MET:HG2   | 1:A:638:LEU:CG    | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1420:ALA:HA   | 1:A:1421:PRO:HD3  | 1.75                     | 0.42              |
| 1:B:706:THR:HB    | 1:B:737:PHE:HB3   | 2.01                     | 0.42              |
| 1:B:982:ILE:HG23  | 2:H:956:GLU:HG2   | 2.01                     | 0.42              |
| 1:B:1239:HIS:CD2  | 1:B:1241:SER:OG   | 2.59                     | 0.42              |
| 1:B:1784:ASP:O    | 1:B:1788:GLU:HB2  | 2.20                     | 0.42              |
| 1:C:406:TRP:CD2   | 1:C:1619:GLU:HG3  | 2.55                     | 0.42              |
| 1:C:475:GLN:CD    | 1:C:614:ALA:HB2   | 2.40                     | 0.42              |
| 1:C:1220:VAL:O    | 1:C:1224:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:1639:VAL:CG1  | 1:C:1640:SER:N    | 2.82                     | 0.42              |
| 2:G:786:SER:HB2   | 2:G:794:MET:HE2   | 2.00                     | 0.42              |
| 2:G:1180:MET:HB3  | 2:G:1199:GLU:HG2  | 2.00                     | 0.42              |
| 2:G:1418:ASP:O    | 2:G:1419:PHE:C    | 2.58                     | 0.42              |
| 2:H:60:LEU:O      | 2:H:60:LEU:HD23   | 2.20                     | 0.42              |
| 2:H:345:THR:HG22  | 2:H:347:GLU:N     | 2.25                     | 0.42              |
| 2:H:562:LEU:HG    | 2:H:793:PRO:HG2   | 2.02                     | 0.42              |
| 2:H:900:GLN:NE2   | 2:H:1051:THR:HA   | 2.34                     | 0.42              |
| 2:I:33:LEU:HD21   | 2:I:80:PHE:CE2    | 2.54                     | 0.42              |
| 2:I:298:LYS:HA    | 2:I:448:VAL:CG2   | 2.49                     | 0.42              |
| 2:I:1217:ASN:HD22 | 2:I:1217:ASN:HA   | 1.60                     | 0.42              |
| 2:I:1344:ASP:O    | 2:I:1416:TYR:HE2  | 2.02                     | 0.42              |
| 2:I:1359:MET:CE   | 2:I:1404:MET:HB3  | 2.50                     | 0.42              |
| 1:A:1:MET:HE3     | 1:A:9:LEU:HD12    | 2.01                     | 0.42              |
| 1:A:181:THR:HG22  | 1:A:185:GLU:OE2   | 2.19                     | 0.42              |
| 1:A:489:VAL:CG2   | 1:A:671:VAL:N     | 2.83                     | 0.42              |
| 1:A:1019:ILE:HG13 | 1:A:1316:VAL:HG13 | 2.01                     | 0.42              |
| 1:A:1263:ASP:HB2  | 1:A:1270:VAL:HG21 | 2.01                     | 0.42              |
| 1:B:242:THR:HG22  | 1:B:243:ILE:H     | 1.83                     | 0.42              |
| 1:B:625:THR:HG23  | 1:B:627:SER:H     | 1.84                     | 0.42              |
| 1:B:1238:VAL:CG1  | 1:B:1242:GLU:HB2  | 2.49                     | 0.42              |
| 1:B:1244:GLY:O    | 1:B:1327:CYS:HB2  | 2.20                     | 0.42              |
| 1:B:1264:ARG:NH1  | 1:B:1270:VAL:HB   | 2.35                     | 0.42              |
| 1:B:1682:LYS:HB3  | 2:H:994:PHE:CE2   | 2.54                     | 0.42              |
| 1:C:438:ASN:HD21  | 1:C:698:GLN:HE21  | 1.66                     | 0.42              |
| 1:C:1067:LEU:HD23 | 1:C:1067:LEU:HA   | 1.76                     | 0.42              |
| 2:G:507:GLY:O     | 2:G:508:GLY:C     | 2.58                     | 0.42              |
| 2:G:810:GLU:OE2   | 2:G:1070:ILE:N    | 2.44                     | 0.42              |
| 2:G:856:LYS:CE    | 2:G:1052:CYS:SG   | 3.08                     | 0.42              |
| 2:G:938:TRP:CE2   | 2:G:944:ARG:HG3   | 2.54                     | 0.42              |
| 2:G:1044:VAL:HG21 | 2:G:1050:ARG:NE   | 2.34                     | 0.42              |
| 2:G:1149:TRP:NE1  | 2:G:1213:LEU:HD12 | 2.35                     | 0.42              |
| 2:H:567:PRO:HG3   | 2:H:781:LEU:HD11  | 1.99                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:581:THR:O     | 2:H:585:LYS:HB2   | 2.20                     | 0.42              |
| 2:H:712:ALA:O     | 2:H:716:VAL:HG23  | 2.20                     | 0.42              |
| 2:H:754:TYR:CG    | 2:H:794:MET:HG2   | 2.55                     | 0.42              |
| 2:H:804:ARG:NH1   | 2:H:1062:PHE:O    | 2.52                     | 0.42              |
| 2:H:949:ASP:HB3   | 2:H:1006:MET:CE   | 2.47                     | 0.42              |
| 2:H:1002:HIS:NE2  | 2:H:1006:MET:CE   | 2.82                     | 0.42              |
| 2:H:1175:LYS:HG3  | 2:H:1176:PRO:HD2  | 2.02                     | 0.42              |
| 2:H:1339:PHE:N    | 2:H:1340:PRO:CD   | 2.83                     | 0.42              |
| 2:I:44:PRO:HA     | 2:I:53:GLU:OE2    | 2.19                     | 0.42              |
| 2:I:73:GLU:OE2    | 2:I:76:LYS:HD2    | 2.18                     | 0.42              |
| 2:I:703:LEU:CD2   | 2:I:705:LEU:HG    | 2.50                     | 0.42              |
| 2:I:740:HIS:HA    | 2:I:854:ILE:HD13  | 2.01                     | 0.42              |
| 2:I:745:ASP:HA    | 2:I:832:TRP:CH2   | 2.49                     | 0.42              |
| 2:I:1129:ALA:HB2  | 2:I:1138:TRP:CH2  | 2.55                     | 0.42              |
| 2:I:1273:GLU:HB3  | 2:I:1274:PRO:CD   | 2.50                     | 0.42              |
| 2:I:1343:VAL:HG22 | 2:I:1343:VAL:O    | 2.20                     | 0.42              |
| 2:I:1989:LYS:NZ   | 2:I:2037:PRO:HG2  | 2.35                     | 0.42              |
| 2:I:2046:GLU:C    | 2:I:2048:TYR:N    | 2.73                     | 0.42              |
| 1:A:408:TRP:CH2   | 1:A:1628:SER:HB3  | 2.55                     | 0.42              |
| 1:A:655:LEU:HD23  | 1:A:655:LEU:HA    | 1.81                     | 0.42              |
| 1:A:800:LEU:HD23  | 1:A:800:LEU:HA    | 1.84                     | 0.42              |
| 1:A:987:ASN:HD22  | 2:G:957:ARG:CD    | 2.30                     | 0.42              |
| 1:A:1260:MET:HB2  | 1:A:1274:ILE:HD12 | 2.02                     | 0.42              |
| 1:B:458:THR:OG1   | 1:B:470:LYS:HD2   | 2.20                     | 0.42              |
| 1:B:798:ASN:HA    | 1:B:801:ARG:HB2   | 2.02                     | 0.42              |
| 1:B:1012:LEU:HD23 | 1:B:1445:MET:HE3  | 2.00                     | 0.42              |
| 1:B:1830:GLY:HA2  | 1:B:1831:GLY:HA2  | 1.57                     | 0.42              |
| 1:C:2:LYS:HE2     | 1:C:4:GLU:OE1     | 2.19                     | 0.42              |
| 1:C:37:LYS:HB2    | 1:C:65:TYR:CE1    | 2.52                     | 0.42              |
| 1:C:155:VAL:O     | 1:C:159:LEU:HG    | 2.19                     | 0.42              |
| 1:C:1310:GLU:OE1  | 1:C:1649:LYS:CE   | 2.65                     | 0.42              |
| 1:C:1842:VAL:O    | 1:C:1843:ASN:C    | 2.57                     | 0.42              |
| 2:G:7:ARG:NH1     | 2:G:24:THR:CG2    | 2.79                     | 0.42              |
| 2:G:237:SER:O     | 2:G:241:ILE:HG13  | 2.20                     | 0.42              |
| 2:G:258:PHE:N     | 2:G:258:PHE:HD1   | 2.18                     | 0.42              |
| 2:G:732:TRP:CH2   | 2:G:749:PRO:HG2   | 2.55                     | 0.42              |
| 2:G:827:VAL:HG21  | 2:G:840:THR:CG2   | 2.49                     | 0.42              |
| 2:G:1014:PRO:HG2  | 2:G:1032:ASP:HB2  | 2.01                     | 0.42              |
| 2:G:1079:ASP:O    | 2:G:1082:ILE:HG22 | 2.19                     | 0.42              |
| 2:G:1217:ASN:HD22 | 2:G:1217:ASN:HA   | 1.62                     | 0.42              |
| 2:G:1383:ASN:OD1  | 2:G:1388:LYS:HG3  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:33:LEU:HD13   | 2:H:68:VAL:HG22   | 2.02                     | 0.42              |
| 2:H:624:TYR:HB2   | 2:H:630:MET:HE3   | 2.02                     | 0.42              |
| 2:H:844:VAL:HG22  | 2:H:858:ALA:HB2   | 2.01                     | 0.42              |
| 2:H:1642:THR:HB   | 2:H:1651:LEU:HB2  | 2.01                     | 0.42              |
| 2:I:732:TRP:CH2   | 2:I:749:PRO:HG2   | 2.55                     | 0.42              |
| 1:A:155:VAL:HG22  | 1:A:186:ILE:CG2   | 2.50                     | 0.42              |
| 1:A:335:HIS:CD2   | 1:A:335:HIS:C     | 2.92                     | 0.42              |
| 1:A:444:ASN:CB    | 1:A:446:ALA:H     | 2.32                     | 0.42              |
| 1:A:453:TYR:O     | 1:A:457:ASN:HB2   | 2.20                     | 0.42              |
| 1:A:1332:TYR:HB3  | 1:A:1382:ALA:CB   | 2.50                     | 0.42              |
| 1:A:1618:LEU:HD23 | 1:A:1621:PHE:CE2  | 2.54                     | 0.42              |
| 1:B:1:MET:HE3     | 1:B:6:GLU:HA      | 2.01                     | 0.42              |
| 1:B:20:TYR:CZ     | 2:H:2035:SER:HB2  | 2.53                     | 0.42              |
| 1:B:31:THR:CG2    | 2:H:2011:ILE:HG21 | 2.40                     | 0.42              |
| 1:B:44:VAL:HG11   | 1:B:78:ILE:HG12   | 2.00                     | 0.42              |
| 1:B:780:GLU:O     | 1:B:781:LEU:C     | 2.58                     | 0.42              |
| 1:B:1189:ILE:HG23 | 1:B:1190:PRO:HD2  | 2.01                     | 0.42              |
| 1:B:1539:ALA:O    | 1:B:1574:GLY:HA2  | 2.20                     | 0.42              |
| 1:B:1705:PRO:HB2  | 1:B:1733:PHE:CD1  | 2.55                     | 0.42              |
| 1:C:1012:LEU:HD23 | 1:C:1445:MET:HE2  | 2.02                     | 0.42              |
| 1:C:1154:ILE:O    | 1:C:1154:ILE:HG13 | 2.20                     | 0.42              |
| 1:C:1244:GLY:HA3  | 1:C:1297:PRO:HD2  | 2.02                     | 0.42              |
| 2:G:892:ILE:HD11  | 2:G:903:TRP:CD2   | 2.51                     | 0.42              |
| 2:G:1666:PHE:CD1  | 2:G:1814:ALA:CB   | 3.02                     | 0.42              |
| 2:G:1840:VAL:O    | 2:G:1840:VAL:HG13 | 2.18                     | 0.42              |
| 2:G:2036:GLU:HB2  | 2:G:2037:PRO:CD   | 2.48                     | 0.42              |
| 2:H:433:VAL:N     | 2:H:434:PRO:CD    | 2.83                     | 0.42              |
| 2:H:641:ILE:CD1   | 2:H:645:SER:HB2   | 2.50                     | 0.42              |
| 2:H:995:LEU:HB3   | 2:H:1000:ILE:CD1  | 2.50                     | 0.42              |
| 2:H:1889:VAL:HG22 | 2:H:1977:HIS:O    | 2.19                     | 0.42              |
| 2:I:360:LEU:HA    | 2:I:361:PRO:HD3   | 1.89                     | 0.42              |
| 2:I:879:LYS:HD3   | 2:I:879:LYS:HA    | 1.73                     | 0.42              |
| 2:I:1135:GLU:HG2  | 2:I:1176:PRO:HG2  | 2.02                     | 0.42              |
| 2:I:1223:MET:HE3  | 2:I:1238:LEU:CD1  | 2.49                     | 0.42              |
| 2:I:1593:ILE:O    | 2:I:1597:ALA:HB3  | 2.20                     | 0.42              |
| 1:A:32:GLN:HE21   | 1:A:57:ALA:HB2    | 1.85                     | 0.42              |
| 1:A:350:LEU:HD23  | 1:A:350:LEU:HA    | 1.89                     | 0.42              |
| 1:A:521:LYS:HB3   | 1:A:523:SER:HB3   | 2.01                     | 0.42              |
| 1:A:780:GLU:O     | 1:A:781:LEU:C     | 2.59                     | 0.42              |
| 1:A:998:TYR:CD2   | 1:A:1667:GLU:HG3  | 2.55                     | 0.42              |
| 1:A:1234:MET:HE3  | 1:A:1326:ILE:HG21 | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:140:ILE:CG2   | 1:B:141:ALA:N     | 2.83                     | 0.42              |
| 1:B:438:ASN:ND2   | 1:B:698:GLN:HE21  | 2.14                     | 0.42              |
| 1:B:1175:ILE:HA   | 1:B:1176:PRO:HD3  | 1.89                     | 0.42              |
| 1:C:19:ALA:O      | 1:C:22:PHE:HB2    | 2.19                     | 0.42              |
| 1:C:1029:PRO:HA   | 1:C:1188:GLN:O    | 2.20                     | 0.42              |
| 1:C:1370:THR:HG22 | 1:C:1371:THR:N    | 2.35                     | 0.42              |
| 2:G:298:LYS:HA    | 2:G:448:VAL:CG2   | 2.50                     | 0.42              |
| 2:G:427:PHE:HB3   | 2:G:428:HIS:ND1   | 2.34                     | 0.42              |
| 2:G:468:LEU:O     | 2:G:471:LEU:HB2   | 2.20                     | 0.42              |
| 2:G:670:ARG:HD2   | 2:G:676:ILE:O     | 2.20                     | 0.42              |
| 2:G:736:ARG:H     | 2:G:736:ARG:HG3   | 1.59                     | 0.42              |
| 2:G:1236:LEU:HA   | 2:G:1237:PRO:HD3  | 1.76                     | 0.42              |
| 2:G:1360:ILE:HA   | 2:G:1361:PRO:HD3  | 1.91                     | 0.42              |
| 2:G:1782:THR:CG2  | 2:G:1827:LEU:HD21 | 2.48                     | 0.42              |
| 2:H:23:PRO:HG2    | 2:H:86:LEU:HD11   | 2.01                     | 0.42              |
| 2:H:234:ILE:HG13  | 2:H:235:PRO:CD    | 2.47                     | 0.42              |
| 2:H:421:LEU:HA    | 2:H:422:PRO:HD3   | 1.78                     | 0.42              |
| 2:H:1180:MET:HB3  | 2:H:1199:GLU:HG2  | 2.02                     | 0.42              |
| 2:H:1343:VAL:O    | 2:H:1343:VAL:HG22 | 2.20                     | 0.42              |
| 2:H:1666:PHE:CD1  | 2:H:1814:ALA:CB   | 3.03                     | 0.42              |
| 2:H:1855:ILE:HB   | 2:H:1907:LEU:HD12 | 2.01                     | 0.42              |
| 2:H:2036:GLU:HB2  | 2:H:2037:PRO:CD   | 2.47                     | 0.42              |
| 2:I:258:PHE:N     | 2:I:258:PHE:CD1   | 2.87                     | 0.42              |
| 2:I:804:ARG:NH2   | 2:I:1068:GLU:OE1  | 2.53                     | 0.42              |
| 2:I:1214:LEU:HD11 | 2:I:1220:GLN:NE2  | 2.35                     | 0.42              |
| 2:I:1335:ILE:O    | 2:I:1338:ILE:HG12 | 2.20                     | 0.42              |
| 2:I:1738:PHE:HE1  | 2:I:1837:THR:HG23 | 1.85                     | 0.42              |
| 1:A:32:GLN:NE2    | 1:A:57:ALA:CA     | 2.83                     | 0.41              |
| 1:A:1019:ILE:HG21 | 1:A:1316:VAL:HG22 | 2.01                     | 0.41              |
| 1:A:1279:PHE:HB2  | 1:A:1282:THR:HG23 | 2.01                     | 0.41              |
| 1:A:1308:SER:HB3  | 1:A:1589:GLY:HA3  | 2.01                     | 0.41              |
| 1:A:1657:HIS:CG   | 1:A:1658:PRO:HD2  | 2.55                     | 0.41              |
| 1:B:1019:ILE:HG13 | 1:B:1316:VAL:HG13 | 2.02                     | 0.41              |
| 1:B:1673:TYR:CZ   | 1:B:1677:VAL:HG21 | 2.55                     | 0.41              |
| 1:C:12:ILE:HD11   | 2:I:2041:ILE:HD11 | 2.01                     | 0.41              |
| 1:C:616:LEU:HB2   | 1:C:617:PRO:HD3   | 2.01                     | 0.41              |
| 1:C:635:ILE:CG2   | 1:C:651:TYR:CG    | 3.03                     | 0.41              |
| 1:C:1215:VAL:O    | 1:C:1219:VAL:HG23 | 2.20                     | 0.41              |
| 2:G:439:ILE:HD12  | 2:G:484:ILE:HD11  | 2.01                     | 0.41              |
| 2:G:638:VAL:HA    | 2:G:641:ILE:CG2   | 2.50                     | 0.41              |
| 2:G:1128:LYS:HG2  | 2:G:1181:VAL:HG22 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1496:LYS:CE   | 2:G:1693:ARG:HH21 | 2.28                     | 0.41              |
| 2:G:1579:ILE:CD1  | 2:G:1615:MET:SD   | 3.08                     | 0.41              |
| 2:H:240:LEU:O     | 2:H:244:ILE:HG13  | 2.19                     | 0.41              |
| 2:H:258:PHE:N     | 2:H:258:PHE:HD1   | 2.18                     | 0.41              |
| 2:H:896:ASN:O     | 2:H:1050:ARG:NH2  | 2.53                     | 0.41              |
| 2:H:2010:TYR:O    | 2:H:2012:PRO:HD3  | 2.20                     | 0.41              |
| 2:I:441:LYS:HG2   | 2:I:445:LYS:HE3   | 2.02                     | 0.41              |
| 2:I:512:LEU:O     | 2:I:516:THR:HG23  | 2.20                     | 0.41              |
| 2:I:659:LEU:O     | 2:I:663:ILE:HG12  | 2.20                     | 0.41              |
| 2:I:1697:HIS:CE1  | 2:I:1829:GLU:CG   | 3.03                     | 0.41              |
| 2:I:1815:LEU:O    | 2:I:1821:VAL:HG23 | 2.20                     | 0.41              |
| 2:I:1980:TYR:HD1  | 2:I:1981:LEU:HD12 | 1.85                     | 0.41              |
| 1:A:28:TRP:CE2    | 1:A:53:LEU:HD22   | 2.55                     | 0.41              |
| 1:A:29:ILE:HD13   | 2:G:1894:GLU:HA   | 2.01                     | 0.41              |
| 1:A:50:SER:CB     | 1:A:51:PRO:CD     | 2.98                     | 0.41              |
| 1:A:280:GLU:O     | 1:A:284:LYS:HG3   | 2.21                     | 0.41              |
| 1:A:340:ARG:NH1   | 1:A:344:GLN:CG    | 2.70                     | 0.41              |
| 1:A:983:GLN:HE21  | 2:G:962:LYS:HD2   | 1.80                     | 0.41              |
| 1:A:1233:GLU:CD   | 1:A:1680:ARG:HH21 | 2.24                     | 0.41              |
| 1:B:290:MET:HB3   | 1:B:290:MET:HE2   | 1.96                     | 0.41              |
| 1:C:12:ILE:O      | 1:C:15:THR:HG23   | 2.20                     | 0.41              |
| 1:C:889:GLU:C     | 1:C:891:MET:H     | 2.24                     | 0.41              |
| 1:C:1584:PRO:CG   | 1:C:1591:TRP:CZ3  | 3.03                     | 0.41              |
| 2:G:717:ILE:HG23  | 2:G:760:HIS:CE1   | 2.55                     | 0.41              |
| 2:G:992:GLU:OE1   | 2:G:992:GLU:HA    | 2.20                     | 0.41              |
| 2:G:1553:TYR:OH   | 2:G:1583:MET:HB3  | 2.20                     | 0.41              |
| 2:G:1755:ILE:HD11 | 2:G:1762:TYR:HB2  | 2.03                     | 0.41              |
| 2:G:2035:SER:OG   | 2:G:2037:PRO:HD2  | 2.21                     | 0.41              |
| 2:H:15:SER:H      | 2:H:48:PHE:HE2    | 1.66                     | 0.41              |
| 2:H:142:ASN:HB2   | 2:H:550:VAL:HG13  | 2.01                     | 0.41              |
| 2:H:584:SER:CB    | 2:H:591:PRO:HG3   | 2.46                     | 0.41              |
| 2:H:1713:ASN:HA   | 2:H:1714:PRO:HD3  | 1.89                     | 0.41              |
| 2:I:84:LEU:HD23   | 2:I:84:LEU:HA     | 1.89                     | 0.41              |
| 2:I:524:GLY:HA2   | 2:I:558:ASN:O     | 2.20                     | 0.41              |
| 2:I:592:LEU:O     | 2:I:616:THR:HG23  | 2.19                     | 0.41              |
| 2:I:1149:TRP:HA   | 2:I:1242:PHE:CD1  | 2.54                     | 0.41              |
| 2:I:1495:THR:O    | 2:I:1496:LYS:HB2  | 2.20                     | 0.41              |
| 1:A:1666:THR:HG23 | 1:A:1669:ARG:HB2  | 2.01                     | 0.41              |
| 1:A:1784:ASP:O    | 1:A:1788:GLU:HB2  | 2.20                     | 0.41              |
| 1:B:455:ILE:HD13  | 1:B:455:ILE:HA    | 1.84                     | 0.41              |
| 1:B:852:ARG:HB3   | 1:B:858:TRP:HZ2   | 1.83                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1047:LEU:O    | 1:B:1051:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:335:HIS:CD2   | 1:C:335:HIS:C     | 2.91                     | 0.41              |
| 1:C:792:HIS:CE1   | 1:C:796:LEU:HD23  | 2.55                     | 0.41              |
| 1:C:1047:LEU:HD23 | 1:C:1047:LEU:HA   | 1.89                     | 0.41              |
| 1:C:1208:VAL:HG13 | 1:C:1209:ASP:O    | 2.20                     | 0.41              |
| 2:G:520:LYS:O     | 2:G:521:ASP:C     | 2.58                     | 0.41              |
| 2:G:667:LYS:HD2   | 2:G:697:THR:CG2   | 2.38                     | 0.41              |
| 2:G:888:ARG:O     | 2:G:892:ILE:HB    | 2.21                     | 0.41              |
| 2:G:1258:ARG:O    | 2:G:1262:ILE:HG13 | 2.20                     | 0.41              |
| 2:G:1359:MET:HB3  | 2:G:1606:ARG:NH2  | 2.35                     | 0.41              |
| 2:G:1380:SER:HB3  | 2:G:1424:GLN:HB2  | 2.02                     | 0.41              |
| 2:G:1624:THR:HB   | 2:G:1642:THR:CG2  | 2.50                     | 0.41              |
| 2:H:1314:ARG:HD3  | 2:H:1314:ARG:HA   | 1.63                     | 0.41              |
| 2:I:195:LEU:O     | 2:I:199:ILE:HG13  | 2.20                     | 0.41              |
| 2:I:339:LEU:HD23  | 2:I:419:ARG:O     | 2.20                     | 0.41              |
| 2:I:507:GLY:O     | 2:I:508:GLY:C     | 2.59                     | 0.41              |
| 2:I:581:THR:O     | 2:I:585:LYS:HB2   | 2.20                     | 0.41              |
| 2:I:807:ILE:HA    | 2:I:818:LYS:HG2   | 2.02                     | 0.41              |
| 2:I:1493:LEU:HB3  | 2:I:1494:PRO:HD2  | 2.02                     | 0.41              |
| 1:A:12:ILE:O      | 1:A:15:THR:HG23   | 2.20                     | 0.41              |
| 1:A:28:TRP:CZ2    | 1:A:53:LEU:HD22   | 2.56                     | 0.41              |
| 1:A:330:GLU:O     | 1:A:330:GLU:HG2   | 2.20                     | 0.41              |
| 1:A:807:LYS:HD3   | 1:A:807:LYS:C     | 2.40                     | 0.41              |
| 1:A:1154:ILE:O    | 1:A:1154:ILE:HG13 | 2.19                     | 0.41              |
| 1:A:1305:CYS:SG   | 3:A:2748:CER:C5   | 3.08                     | 0.41              |
| 1:A:1720:ALA:O    | 1:A:1721:ARG:HG2  | 2.21                     | 0.41              |
| 1:B:378:LEU:HD12  | 1:B:378:LEU:HA    | 1.75                     | 0.41              |
| 1:B:992:PHE:CD2   | 1:B:1399:PRO:HG3  | 2.55                     | 0.41              |
| 1:B:1216:LEU:HD23 | 1:B:1216:LEU:HA   | 1.93                     | 0.41              |
| 1:B:1448:ARG:HD2  | 1:B:1508:TRP:O    | 2.21                     | 0.41              |
| 1:C:495:LYS:HA    | 1:C:496:PRO:HD3   | 1.86                     | 0.41              |
| 1:C:496:PRO:HB2   | 1:C:519:VAL:HG12  | 2.02                     | 0.41              |
| 1:C:521:LYS:HE2   | 1:C:605:LEU:HD11  | 2.02                     | 0.41              |
| 1:C:719:GLN:HG3   | 1:C:720:SER:N     | 2.35                     | 0.41              |
| 2:G:439:ILE:HD12  | 2:G:484:ILE:CD1   | 2.50                     | 0.41              |
| 2:G:760:HIS:HA    | 2:G:761:PRO:HD3   | 1.85                     | 0.41              |
| 2:G:846:VAL:HG13  | 2:G:865:TRP:CD1   | 2.55                     | 0.41              |
| 2:G:950:PHE:O     | 2:G:953:ARG:HB3   | 2.20                     | 0.41              |
| 2:H:455:ILE:HG12  | 2:H:469:ARG:CG    | 2.49                     | 0.41              |
| 2:H:561:TRP:CG    | 2:H:754:TYR:HE2   | 2.39                     | 0.41              |
| 2:H:601:THR:HB    | 2:H:620:ALA:HB2   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1071:LYS:HE3  | 2:H:1075:ASP:OD2  | 2.20                     | 0.41              |
| 2:H:1752:PHE:HZ   | 2:H:1836:MET:HE3  | 1.84                     | 0.41              |
| 2:H:1886:VAL:HG22 | 2:H:1906:ALA:HB1  | 2.02                     | 0.41              |
| 2:I:156:LEU:HD23  | 2:I:500:HIS:HB2   | 2.02                     | 0.41              |
| 2:I:258:PHE:N     | 2:I:258:PHE:HD1   | 2.18                     | 0.41              |
| 2:I:654:VAL:CG2   | 2:I:683:ALA:HB1   | 2.50                     | 0.41              |
| 2:I:949:ASP:HB3   | 2:I:1006:MET:CE   | 2.48                     | 0.41              |
| 2:I:1021:LEU:HD22 | 2:I:1021:LEU:HA   | 1.61                     | 0.41              |
| 2:I:1457:PHE:CD2  | 2:I:1459:LEU:HD23 | 2.55                     | 0.41              |
| 2:I:1458:ASP:O    | 2:I:1462:LYS:HE3  | 2.21                     | 0.41              |
| 1:A:9:LEU:HD21    | 2:G:2047:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:12:ILE:O      | 1:A:16:GLU:HG2    | 2.20                     | 0.41              |
| 1:A:82:SER:OG     | 1:A:83:LYS:HG3    | 2.20                     | 0.41              |
| 1:A:601:VAL:O     | 1:A:602:GLU:C     | 2.59                     | 0.41              |
| 1:A:1477:ILE:N    | 1:A:1478:PRO:CD   | 2.83                     | 0.41              |
| 1:B:2:LYS:CD      | 2:H:2050:GLN:HB3  | 2.44                     | 0.41              |
| 1:B:453:TYR:O     | 1:B:457:ASN:HB2   | 2.21                     | 0.41              |
| 1:B:504:ASP:CB    | 1:B:508:ASN:HB2   | 2.49                     | 0.41              |
| 1:B:949:GLU:O     | 1:B:953:VAL:HG12  | 2.21                     | 0.41              |
| 1:B:1232:TYR:CE2  | 1:B:1701:LYS:HD2  | 2.55                     | 0.41              |
| 1:B:1244:GLY:HA3  | 1:B:1297:PRO:HD2  | 2.03                     | 0.41              |
| 1:B:1257:LEU:HA   | 1:B:1257:LEU:HD23 | 1.76                     | 0.41              |
| 1:B:1303:GLY:H    | 1:B:1307:THR:CG2  | 2.31                     | 0.41              |
| 1:B:1308:SER:HB3  | 1:B:1589:GLY:HA3  | 2.03                     | 0.41              |
| 1:C:242:THR:HB    | 1:C:244:THR:HB    | 2.02                     | 0.41              |
| 1:C:1408:ALA:O    | 1:C:1651:GLY:HA2  | 2.21                     | 0.41              |
| 1:C:1443:LEU:HD23 | 1:C:1443:LEU:HA   | 1.77                     | 0.41              |
| 1:C:1830:GLY:HA2  | 1:C:1831:GLY:HA2  | 1.57                     | 0.41              |
| 2:G:1676:MET:HE1  | 2:G:1781:LEU:CD2  | 2.47                     | 0.41              |
| 2:G:1706:ILE:HD12 | 2:G:1706:ILE:HA   | 1.89                     | 0.41              |
| 2:G:1862:VAL:HG22 | 2:G:1863:ALA:N    | 2.36                     | 0.41              |
| 2:H:231:LEU:HA    | 2:H:236:ILE:HD12  | 2.03                     | 0.41              |
| 2:H:339:LEU:HD23  | 2:H:419:ARG:O     | 2.20                     | 0.41              |
| 2:H:478:ARG:O     | 2:H:482:CYS:HB2   | 2.20                     | 0.41              |
| 2:I:177:TYR:CD1   | 2:I:188:ILE:HG21  | 2.55                     | 0.41              |
| 2:I:566:HIS:ND1   | 2:I:567:PRO:HD2   | 2.35                     | 0.41              |
| 2:I:572:ASN:HD22  | 2:I:572:ASN:HA    | 1.70                     | 0.41              |
| 2:I:712:ALA:O     | 2:I:716:VAL:HG23  | 2.21                     | 0.41              |
| 2:I:780:TYR:HB2   | 2:I:799:PHE:HE2   | 1.85                     | 0.41              |
| 2:I:786:SER:HB2   | 2:I:794:MET:HE2   | 2.02                     | 0.41              |
| 2:I:800:LEU:HD23  | 2:I:800:LEU:H     | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1940:LEU:HD12 | 2:I:1941:PHE:N    | 2.35                     | 0.41              |
| 1:A:370:GLU:O     | 1:A:373:ALA:HB3   | 2.20                     | 0.41              |
| 1:A:529:MET:HE1   | 1:A:894:ARG:HD2   | 2.00                     | 0.41              |
| 1:A:825:PRO:HB2   | 1:A:843:LYS:HZ2   | 1.86                     | 0.41              |
| 1:A:932:PHE:O     | 1:A:934:PRO:HD3   | 2.20                     | 0.41              |
| 1:A:1842:VAL:O    | 1:A:1843:ASN:O    | 2.39                     | 0.41              |
| 1:B:238:PRO:CG    | 1:B:283:ALA:HB2   | 2.50                     | 0.41              |
| 1:B:406:TRP:CD2   | 1:B:1619:GLU:HG3  | 2.55                     | 0.41              |
| 1:B:495:LYS:HA    | 1:B:496:PRO:HD3   | 1.89                     | 0.41              |
| 1:B:1066:ASN:HD22 | 1:B:1071:PRO:HA   | 1.86                     | 0.41              |
| 1:C:1709:GLU:H    | 1:C:1709:GLU:HG3  | 1.42                     | 0.41              |
| 1:C:1784:ASP:O    | 1:C:1788:GLU:HB2  | 2.20                     | 0.41              |
| 2:G:490:TRP:CZ2   | 2:G:512:LEU:HD21  | 2.55                     | 0.41              |
| 2:G:597:MET:HA    | 4:G:3051:FMN:C5A  | 2.51                     | 0.41              |
| 2:G:754:TYR:CG    | 2:G:794:MET:CG    | 3.04                     | 0.41              |
| 2:G:1169:PRO:O    | 2:G:1173:VAL:HG23 | 2.20                     | 0.41              |
| 2:G:1352:HIS:HD2  | 2:G:1410:PHE:CD2  | 2.38                     | 0.41              |
| 2:G:1495:THR:O    | 2:G:1496:LYS:HB2  | 2.20                     | 0.41              |
| 2:G:1642:THR:HB   | 2:G:1651:LEU:HB2  | 2.01                     | 0.41              |
| 2:G:1815:LEU:O    | 2:G:1821:VAL:HG23 | 2.20                     | 0.41              |
| 2:G:1979:THR:O    | 2:G:1982:MET:HB2  | 2.21                     | 0.41              |
| 2:H:624:TYR:CD1   | 2:H:630:MET:HE2   | 2.56                     | 0.41              |
| 2:H:712:ALA:O     | 2:H:715:GLN:HB3   | 2.20                     | 0.41              |
| 2:H:717:ILE:CG2   | 2:H:760:HIS:CE1   | 3.04                     | 0.41              |
| 2:H:722:ALA:CB    | 2:H:723:HIS:CE1   | 3.04                     | 0.41              |
| 2:H:950:PHE:O     | 2:H:953:ARG:HB3   | 2.20                     | 0.41              |
| 2:H:1236:LEU:HD22 | 2:H:1238:LEU:HG   | 2.03                     | 0.41              |
| 2:H:1680:LEU:HD13 | 2:H:1687:ALA:CB   | 2.45                     | 0.41              |
| 2:I:638:VAL:HG22  | 2:I:675:PRO:HG2   | 2.03                     | 0.41              |
| 2:I:663:ILE:HG13  | 2:I:694:TYR:CE1   | 2.51                     | 0.41              |
| 2:I:1054:LEU:HD22 | 4:I:3051:FMN:HM72 | 2.03                     | 0.41              |
| 2:I:1417:THR:C    | 2:I:1419:PHE:N    | 2.74                     | 0.41              |
| 2:I:1423:PHE:CD1  | 2:I:1423:PHE:N    | 2.71                     | 0.41              |
| 1:A:32:GLN:O      | 1:A:36:LEU:HB2    | 2.21                     | 0.41              |
| 1:A:774:ILE:HA    | 1:A:775:PRO:HD3   | 1.76                     | 0.41              |
| 1:A:988:ILE:HD13  | 1:A:1048:GLU:CG   | 2.50                     | 0.41              |
| 1:B:1105:LEU:HD23 | 1:B:1105:LEU:HA   | 1.89                     | 0.41              |
| 1:B:1126:ILE:CD1  | 1:B:1172:THR:HG22 | 2.51                     | 0.41              |
| 1:B:1666:THR:HG23 | 1:B:1669:ARG:CB   | 2.50                     | 0.41              |
| 1:C:35:PHE:HA     | 1:C:39:PHE:HD2    | 1.86                     | 0.41              |
| 1:C:1119:LYS:HE2  | 1:C:1341:PHE:CG   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1131:LEU:HA   | 1:C:1131:LEU:HD12 | 1.69                     | 0.41              |
| 1:C:1418:VAL:N    | 1:C:1419:PRO:CD   | 2.83                     | 0.41              |
| 2:G:246:LEU:HD12  | 2:G:246:LEU:HA    | 1.82                     | 0.41              |
| 2:G:425:SER:HA    | 2:G:426:PRO:HD3   | 1.79                     | 0.41              |
| 2:G:571:LYS:HB2   | 2:G:1099:ALA:HB2  | 2.02                     | 0.41              |
| 2:G:587:ILE:HD11  | 2:G:589:ARG:HB2   | 2.03                     | 0.41              |
| 2:G:835:THR:HG21  | 2:G:855:HIS:NE2   | 2.35                     | 0.41              |
| 2:G:843:ILE:CD1   | 2:G:1055:HIS:HB3  | 2.50                     | 0.41              |
| 2:G:1344:ASP:O    | 2:G:1416:TYR:HE2  | 2.03                     | 0.41              |
| 2:G:1427:VAL:HG22 | 2:G:1469:GLU:CG   | 2.51                     | 0.41              |
| 2:H:11:LEU:HD23   | 2:H:11:LEU:HA     | 1.93                     | 0.41              |
| 2:H:236:ILE:C     | 2:H:236:ILE:HD13  | 2.40                     | 0.41              |
| 2:H:821:ILE:HA    | 2:H:857:ILE:HD11  | 2.02                     | 0.41              |
| 2:H:827:VAL:HG12  | 2:H:828:PRO:O     | 2.19                     | 0.41              |
| 2:H:1128:LYS:HG2  | 2:H:1181:VAL:HG22 | 2.01                     | 0.41              |
| 2:H:1503:ILE:HG22 | 2:H:1504:VAL:C    | 2.41                     | 0.41              |
| 2:I:159:ILE:HD11  | 2:I:512:LEU:CG    | 2.49                     | 0.41              |
| 2:I:463:PHE:O     | 2:I:463:PHE:HD2   | 2.04                     | 0.41              |
| 2:I:595:PRO:HD3   | 2:I:800:LEU:HB2   | 2.01                     | 0.41              |
| 2:I:634:ILE:CD1   | 2:I:649:ILE:HD11  | 2.44                     | 0.41              |
| 2:I:1357:TYR:HD1  | 2:I:1406:VAL:HG22 | 1.85                     | 0.41              |
| 2:I:1642:THR:HB   | 2:I:1651:LEU:HB2  | 2.03                     | 0.41              |
| 2:I:1981:LEU:HD12 | 2:I:1981:LEU:N    | 2.36                     | 0.41              |
| 1:A:16:GLU:OE2    | 1:A:16:GLU:HA     | 2.21                     | 0.41              |
| 1:A:91:THR:HA     | 1:A:92:PRO:HD3    | 1.81                     | 0.41              |
| 1:A:441:ASN:OD1   | 1:A:488:PRO:HA    | 2.21                     | 0.41              |
| 1:A:1239:HIS:HE1  | 1:A:1714:VAL:O    | 2.03                     | 0.41              |
| 1:B:521:LYS:HB3   | 1:B:523:SER:HB3   | 2.03                     | 0.41              |
| 1:B:949:GLU:O     | 1:B:953:VAL:CG1   | 2.68                     | 0.41              |
| 1:C:658:LEU:HD13  | 1:C:916:LEU:HD12  | 2.02                     | 0.41              |
| 1:C:1420:ALA:HA   | 1:C:1421:PRO:HD3  | 1.78                     | 0.41              |
| 2:G:123:ILE:CD1   | 2:G:533:LEU:HD23  | 2.50                     | 0.41              |
| 2:G:131:ILE:HD12  | 2:G:182:VAL:CG1   | 2.49                     | 0.41              |
| 2:G:236:ILE:HG12  | 2:G:240:LEU:HD22  | 2.02                     | 0.41              |
| 2:G:270:ALA:O     | 2:G:459:VAL:HA    | 2.20                     | 0.41              |
| 2:G:1070:ILE:HD13 | 2:G:1070:ILE:O    | 2.21                     | 0.41              |
| 2:G:1428:GLU:CG   | 2:G:1468:THR:HG22 | 2.51                     | 0.41              |
| 2:H:159:ILE:HG12  | 2:H:512:LEU:HD23  | 2.02                     | 0.41              |
| 2:H:320:PRO:HA    | 2:H:321:PRO:HD3   | 1.92                     | 0.41              |
| 2:H:674:TYR:HA    | 2:H:675:PRO:HD3   | 1.73                     | 0.41              |
| 2:H:719:ILE:HG12  | 2:H:719:ILE:H     | 1.63                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:805:VAL:O     | 2:H:805:VAL:HG12  | 2.21                     | 0.41              |
| 2:H:1662:THR:HB   | 2:H:1799:PRO:HG2  | 2.02                     | 0.41              |
| 2:H:1959:LYS:O    | 2:H:1959:LYS:HG2  | 2.20                     | 0.41              |
| 2:I:705:LEU:HD23  | 2:I:705:LEU:HA    | 1.80                     | 0.41              |
| 2:I:1374:THR:HG23 | 2:I:1396:LEU:CD1  | 2.49                     | 0.41              |
| 2:I:2035:SER:OG   | 2:I:2037:PRO:HD2  | 2.21                     | 0.41              |
| 1:A:152:HIS:HD2   | 1:A:163:LEU:CB    | 2.32                     | 0.41              |
| 1:A:253:ARG:O     | 1:A:254:TRP:CD1   | 2.74                     | 0.41              |
| 1:A:438:ASN:HD21  | 1:A:698:GLN:HE21  | 1.68                     | 0.41              |
| 1:A:612:GLU:O     | 1:A:615:SER:HB3   | 2.21                     | 0.41              |
| 1:A:719:GLN:HG3   | 1:A:720:SER:N     | 2.36                     | 0.41              |
| 1:A:930:LEU:HD22  | 1:A:933:VAL:CG1   | 2.51                     | 0.41              |
| 1:A:1460:LYS:CE   | 1:A:1774:GLU:OE1  | 2.62                     | 0.41              |
| 1:B:444:ASN:CB    | 1:B:446:ALA:H     | 2.31                     | 0.41              |
| 1:B:1418:VAL:N    | 1:B:1419:PRO:CD   | 2.83                     | 0.41              |
| 1:B:1618:LEU:HD23 | 1:B:1621:PHE:HE2  | 1.85                     | 0.41              |
| 1:B:1657:HIS:CG   | 1:B:1658:PRO:HD2  | 2.55                     | 0.41              |
| 1:B:1709:GLU:H    | 1:B:1709:GLU:HG3  | 1.45                     | 0.41              |
| 1:C:32:GLN:HE22   | 1:C:57:ALA:N      | 2.19                     | 0.41              |
| 1:C:453:TYR:O     | 1:C:457:ASN:HB2   | 2.19                     | 0.41              |
| 1:C:683:ALA:HA    | 1:C:689:GLY:HA3   | 2.02                     | 0.41              |
| 1:C:739:GLN:HB3   | 1:C:794:ILE:HG23  | 2.03                     | 0.41              |
| 1:C:949:GLU:O     | 1:C:953:VAL:HG12  | 2.21                     | 0.41              |
| 1:C:1076:VAL:CG1  | 1:C:1081:LYS:HA   | 2.50                     | 0.41              |
| 1:C:1239:HIS:CD2  | 1:C:1241:SER:H    | 2.38                     | 0.41              |
| 1:C:1244:GLY:C    | 1:C:1327:CYS:HB2  | 2.41                     | 0.41              |
| 1:C:1431:GLU:HG3  | 1:C:1431:GLU:O    | 2.19                     | 0.41              |
| 1:C:1705:PRO:HB2  | 1:C:1733:PHE:CD1  | 2.56                     | 0.41              |
| 1:C:1829:GLY:O    | 1:C:1830:GLY:O    | 2.39                     | 0.41              |
| 1:C:1842:VAL:O    | 1:C:1843:ASN:O    | 2.39                     | 0.41              |
| 2:G:258:PHE:N     | 2:G:258:PHE:CD1   | 2.87                     | 0.41              |
| 2:G:260:PRO:HD3   | 2:G:289:TRP:CZ2   | 2.54                     | 0.41              |
| 2:G:735:GLY:O     | 2:G:741:HIS:CD2   | 2.73                     | 0.41              |
| 2:G:748:THR:CB    | 2:G:749:PRO:HD3   | 2.47                     | 0.41              |
| 2:G:780:TYR:HB2   | 2:G:799:PHE:CE2   | 2.56                     | 0.41              |
| 2:G:995:LEU:HB3   | 2:G:1000:ILE:CD1  | 2.50                     | 0.41              |
| 2:G:1210:ILE:O    | 2:G:1210:ILE:HG22 | 2.19                     | 0.41              |
| 2:G:1352:HIS:CD2  | 2:G:1410:PHE:CD2  | 3.09                     | 0.41              |
| 2:G:1778:GLN:HB2  | 2:G:1779:PRO:HD3  | 2.02                     | 0.41              |
| 2:G:1884:TRP:HB3  | 2:G:1885:LEU:H    | 1.74                     | 0.41              |
| 2:G:1889:VAL:HG22 | 2:G:1977:HIS:O    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1981:LEU:HD12 | 2:G:1981:LEU:N    | 2.36                     | 0.41              |
| 2:G:1989:LYS:NZ   | 2:G:2037:PRO:HG2  | 2.35                     | 0.41              |
| 2:H:195:LEU:O     | 2:H:199:ILE:HG13  | 2.20                     | 0.41              |
| 2:H:425:SER:HA    | 2:H:426:PRO:HD3   | 1.78                     | 0.41              |
| 2:H:615:TYR:CE2   | 2:H:1074:MET:HB3  | 2.56                     | 0.41              |
| 2:H:753:MET:O     | 2:H:757:ILE:HG13  | 2.21                     | 0.41              |
| 2:H:804:ARG:NH2   | 2:H:1068:GLU:OE1  | 2.54                     | 0.41              |
| 2:H:827:VAL:HG21  | 2:H:840:THR:CG2   | 2.51                     | 0.41              |
| 2:H:892:ILE:HD11  | 2:H:903:TRP:CD2   | 2.53                     | 0.41              |
| 2:H:1213:LEU:O    | 2:H:1214:LEU:HD23 | 2.19                     | 0.41              |
| 2:H:1270:TRP:HZ3  | 2:H:1347:LEU:HD21 | 1.85                     | 0.41              |
| 2:H:1300:PHE:CB   | 2:H:1556:VAL:HG11 | 2.50                     | 0.41              |
| 2:H:1589:VAL:HG21 | 2:H:1651:LEU:HD12 | 2.02                     | 0.41              |
| 2:H:1815:LEU:O    | 2:H:1821:VAL:HG23 | 2.21                     | 0.41              |
| 2:H:1868:GLN:HG3  | 2:H:1898:TYR:HH   | 1.83                     | 0.41              |
| 2:I:248:HIS:CE1   | 2:I:531:GLY:HA2   | 2.55                     | 0.41              |
| 2:I:455:ILE:C     | 2:I:455:ILE:HD12  | 2.42                     | 0.41              |
| 2:I:582:LYS:HE2   | 2:I:761:PRO:O     | 2.21                     | 0.41              |
| 2:I:827:VAL:HG12  | 2:I:828:PRO:O     | 2.20                     | 0.41              |
| 2:I:1219:ILE:HB   | 2:I:1240:TYR:HB2  | 2.03                     | 0.41              |
| 2:I:1503:ILE:HG22 | 2:I:1504:VAL:C    | 2.41                     | 0.41              |
| 2:I:1514:ASN:HA   | 2:I:1515:PRO:HD3  | 1.86                     | 0.41              |
| 2:I:1579:ILE:CD1  | 2:I:1615:MET:SD   | 3.09                     | 0.41              |
| 1:A:36:LEU:O      | 1:A:76:ARG:NH1    | 2.53                     | 0.41              |
| 1:A:908:LEU:O     | 1:A:913:VAL:HG22  | 2.21                     | 0.41              |
| 1:A:1705:PRO:HB2  | 1:A:1733:PHE:CD1  | 2.56                     | 0.41              |
| 1:B:32:GLN:HE22   | 1:B:57:ALA:CA     | 2.34                     | 0.41              |
| 1:B:82:SER:OG     | 1:B:83:LYS:HG3    | 2.20                     | 0.41              |
| 1:B:187:LEU:CD2   | 1:B:201:PRO:HB2   | 2.51                     | 0.41              |
| 1:B:197:THR:HG22  | 1:B:198:PRO:O     | 2.21                     | 0.41              |
| 1:B:427:ASN:ND2   | 1:B:610:THR:H     | 2.14                     | 0.41              |
| 1:B:489:VAL:HG22  | 1:B:670:GLY:HA3   | 2.02                     | 0.41              |
| 1:B:504:ASP:O     | 1:B:954:ARG:HD3   | 2.21                     | 0.41              |
| 1:B:1029:PRO:HG2  | 1:B:1581:THR:O    | 2.21                     | 0.41              |
| 1:C:237:MET:HA    | 1:C:238:PRO:HD3   | 1.93                     | 0.41              |
| 1:C:294:TYR:CZ    | 1:C:298:VAL:HG21  | 2.55                     | 0.41              |
| 1:C:427:ASN:HB2   | 1:C:468:LEU:CD2   | 2.51                     | 0.41              |
| 1:C:644:THR:HG23  | 1:C:648:ASP:N     | 2.34                     | 0.41              |
| 1:C:1019:ILE:HG13 | 1:C:1316:VAL:HG13 | 2.03                     | 0.41              |
| 1:C:1666:THR:HG23 | 1:C:1669:ARG:CB   | 2.51                     | 0.41              |
| 2:G:44:PRO:HA     | 2:G:53:GLU:OE2    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:339:LEU:HB2   | 2:G:386:LEU:HD22  | 2.03                     | 0.41              |
| 2:G:455:ILE:HD13  | 2:G:457:ILE:O     | 2.21                     | 0.41              |
| 2:G:2049:GLU:O    | 2:G:2050:GLN:C    | 2.59                     | 0.41              |
| 2:H:1063:THR:O    | 2:H:1063:THR:HG22 | 2.21                     | 0.41              |
| 2:H:1387:GLY:HA2  | 2:H:1414:GLY:O    | 2.21                     | 0.41              |
| 2:H:1949:LYS:O    | 2:H:1953:VAL:HG23 | 2.21                     | 0.41              |
| 2:I:118:LYS:O     | 2:I:121:GLU:HB2   | 2.20                     | 0.41              |
| 2:I:319:LEU:HD22  | 2:I:319:LEU:HA    | 1.67                     | 0.41              |
| 2:I:717:ILE:O     | 2:I:720:ALA:HB3   | 2.21                     | 0.41              |
| 2:I:754:TYR:CG    | 2:I:794:MET:CG    | 3.04                     | 0.41              |
| 2:I:827:VAL:HG21  | 2:I:840:THR:CG2   | 2.51                     | 0.41              |
| 2:I:1327:ILE:O    | 2:I:1331:TRP:HB2  | 2.21                     | 0.41              |
| 2:I:2020:GLN:HA   | 2:I:2020:GLN:NE2  | 2.36                     | 0.41              |
| 1:A:29:ILE:HG21   | 2:G:1894:GLU:HB2  | 2.04                     | 0.40              |
| 1:A:197:THR:HG22  | 1:A:198:PRO:O     | 2.21                     | 0.40              |
| 1:A:232:LEU:O     | 1:A:236:LYS:HB2   | 2.21                     | 0.40              |
| 1:A:681:THR:HA    | 1:A:706:THR:OG1   | 2.21                     | 0.40              |
| 1:A:1418:VAL:N    | 1:A:1419:PRO:CD   | 2.84                     | 0.40              |
| 1:B:91:THR:HA     | 1:B:92:PRO:HD3    | 1.81                     | 0.40              |
| 1:B:483:VAL:O     | 1:B:483:VAL:HG12  | 2.21                     | 0.40              |
| 1:B:933:VAL:HA    | 1:B:934:PRO:HD3   | 1.63                     | 0.40              |
| 1:B:989:GLN:NE2   | 2:H:993:GLN:OE1   | 2.53                     | 0.40              |
| 1:B:998:TYR:CD2   | 1:B:1667:GLU:HG3  | 2.56                     | 0.40              |
| 1:B:1056:ILE:HG13 | 1:B:1057:MET:N    | 2.36                     | 0.40              |
| 1:B:1557:ILE:HD11 | 1:B:1642:THR:HG21 | 2.03                     | 0.40              |
| 1:C:187:LEU:CD2   | 1:C:201:PRO:HB2   | 2.51                     | 0.40              |
| 1:C:1308:SER:OG   | 1:C:1590:ALA:N    | 2.54                     | 0.40              |
| 2:G:73:GLU:OE2    | 2:G:76:LYS:HD2    | 2.21                     | 0.40              |
| 2:G:159:ILE:HG12  | 2:G:512:LEU:HD23  | 2.03                     | 0.40              |
| 2:G:430:HIS:CE1   | 2:G:431:LEU:HD13  | 2.56                     | 0.40              |
| 2:G:938:TRP:CD1   | 2:G:944:ARG:HG3   | 2.56                     | 0.40              |
| 2:G:1343:VAL:O    | 2:G:1343:VAL:HG22 | 2.20                     | 0.40              |
| 2:G:1844:ARG:HD2  | 2:G:1848:GLY:O    | 2.21                     | 0.40              |
| 2:H:338:MET:HG3   | 2:H:423:VAL:HG21  | 2.02                     | 0.40              |
| 2:H:566:HIS:O     | 2:H:567:PRO:C     | 2.59                     | 0.40              |
| 2:H:888:ARG:O     | 2:H:892:ILE:HB    | 2.21                     | 0.40              |
| 2:H:1227:ARG:CZ   | 2:H:1565:VAL:HG12 | 2.51                     | 0.40              |
| 2:I:247:ALA:O     | 2:I:251:VAL:HG13  | 2.21                     | 0.40              |
| 2:I:280:ALA:O     | 2:I:283:ILE:HG22  | 2.21                     | 0.40              |
| 2:I:846:VAL:CG2   | 2:I:866:LYS:HB2   | 2.51                     | 0.40              |
| 2:I:1676:MET:HE1  | 2:I:1781:LEU:CD2  | 2.50                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1880:LYS:HE3  | 2:I:1880:LYS:HB2  | 1.90                     | 0.40              |
| 2:I:1889:VAL:HG21 | 2:I:1901:ALA:HB3  | 2.03                     | 0.40              |
| 2:I:2036:GLU:HB2  | 2:I:2037:PRO:CD   | 2.47                     | 0.40              |
| 2:I:2039:LYS:HA   | 2:I:2042:ILE:HG13 | 2.03                     | 0.40              |
| 1:A:23:ALA:O      | 2:G:1977:HIS:HA   | 2.20                     | 0.40              |
| 1:A:44:VAL:HG13   | 1:A:78:ILE:HG12   | 1.99                     | 0.40              |
| 1:A:833:PHE:O     | 1:A:834:GLY:O     | 2.39                     | 0.40              |
| 1:A:1021:VAL:HG11 | 1:A:1597:LEU:CD1  | 2.50                     | 0.40              |
| 1:A:1146:HIS:O    | 1:A:1146:HIS:HD2  | 2.04                     | 0.40              |
| 1:A:1665:ILE:HD11 | 1:A:1669:ARG:CG   | 2.51                     | 0.40              |
| 1:B:1583:HIS:HA   | 1:B:1584:PRO:HD3  | 1.84                     | 0.40              |
| 1:B:1829:GLY:O    | 1:B:1830:GLY:O    | 2.39                     | 0.40              |
| 1:C:148:SER:O     | 1:C:152:HIS:HB2   | 2.21                     | 0.40              |
| 1:C:411:GLN:O     | 1:C:415:SER:HB2   | 2.21                     | 0.40              |
| 1:C:1105:LEU:HD23 | 1:C:1105:LEU:HA   | 1.84                     | 0.40              |
| 2:G:562:LEU:HD23  | 2:G:562:LEU:HA    | 1.85                     | 0.40              |
| 2:G:601:THR:HB    | 2:G:620:ALA:HB2   | 2.01                     | 0.40              |
| 2:G:638:VAL:O     | 2:G:641:ILE:HG22  | 2.20                     | 0.40              |
| 2:G:805:VAL:O     | 2:G:805:VAL:HG12  | 2.21                     | 0.40              |
| 2:G:827:VAL:HG12  | 2:G:828:PRO:O     | 2.21                     | 0.40              |
| 2:G:1227:ARG:NE   | 2:G:1565:VAL:HG12 | 2.36                     | 0.40              |
| 2:G:1678:MET:HG2  | 2:G:1711:ILE:HG12 | 2.03                     | 0.40              |
| 2:G:1940:LEU:HD12 | 2:G:1941:PHE:N    | 2.37                     | 0.40              |
| 2:H:203:LEU:HD12  | 2:H:203:LEU:HA    | 1.91                     | 0.40              |
| 2:H:462:THR:HB    | 2:H:482:CYS:SG    | 2.61                     | 0.40              |
| 2:H:573:LYS:C     | 2:H:575:GLY:N     | 2.75                     | 0.40              |
| 2:H:590:PRO:HA    | 2:H:591:PRO:HD3   | 1.81                     | 0.40              |
| 2:H:638:VAL:HA    | 2:H:641:ILE:CG2   | 2.52                     | 0.40              |
| 2:H:723:HIS:ND1   | 2:H:723:HIS:N     | 2.70                     | 0.40              |
| 2:H:960:LYS:HA    | 2:H:960:LYS:CE    | 2.44                     | 0.40              |
| 2:H:1214:LEU:HD11 | 2:H:1220:GLN:NE2  | 2.36                     | 0.40              |
| 2:H:1506:TYR:CZ   | 2:H:1515:PRO:HG2  | 2.56                     | 0.40              |
| 2:H:1609:THR:O    | 2:H:1653:GLY:HA3  | 2.21                     | 0.40              |
| 2:I:246:LEU:HA    | 2:I:246:LEU:HD12  | 1.79                     | 0.40              |
| 2:I:536:ASN:HD21  | 2:I:540:ASP:HB3   | 1.85                     | 0.40              |
| 2:I:543:PHE:CB    | 2:I:545:GLN:NE2   | 2.82                     | 0.40              |
| 2:I:703:LEU:HD23  | 2:I:705:LEU:HG    | 2.04                     | 0.40              |
| 2:I:816:ASP:HB3   | 2:I:1048:VAL:HG21 | 2.03                     | 0.40              |
| 2:I:1091:GLY:O    | 2:I:1093:ASP:N    | 2.55                     | 0.40              |
| 2:I:1339:PHE:N    | 2:I:1340:PRO:CD   | 2.85                     | 0.40              |
| 2:I:1359:MET:HB3  | 2:I:1606:ARG:NH2  | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1889:VAL:HG13 | 2:I:1977:HIS:HB3  | 2.00                     | 0.40              |
| 1:A:238:PRO:CG    | 1:A:283:ALA:HB2   | 2.51                     | 0.40              |
| 1:A:852:ARG:NH1   | 1:A:852:ARG:CG    | 2.73                     | 0.40              |
| 1:B:221:LEU:HD23  | 1:B:221:LEU:HA    | 1.94                     | 0.40              |
| 1:B:293:LYS:O     | 1:B:297:ILE:HG13  | 2.20                     | 0.40              |
| 1:B:774:ILE:HA    | 1:B:775:PRO:HD3   | 1.74                     | 0.40              |
| 1:B:1303:GLY:CA   | 1:B:1307:THR:HG22 | 2.52                     | 0.40              |
| 1:C:43:ARG:O      | 2:I:1662:THR:HA   | 2.22                     | 0.40              |
| 1:C:1303:GLY:CA   | 1:C:1307:THR:HG22 | 2.52                     | 0.40              |
| 2:G:248:HIS:CE1   | 2:G:531:GLY:HA2   | 2.56                     | 0.40              |
| 2:G:319:LEU:HA    | 2:G:319:LEU:HD22  | 1.62                     | 0.40              |
| 2:G:391:LEU:CD2   | 2:G:394:ARG:NH2   | 2.85                     | 0.40              |
| 2:G:441:LYS:HG2   | 2:G:445:LYS:HE3   | 2.02                     | 0.40              |
| 2:G:573:LYS:C     | 2:G:575:GLY:N     | 2.75                     | 0.40              |
| 2:G:582:LYS:HE2   | 2:G:761:PRO:O     | 2.22                     | 0.40              |
| 2:G:852:GLU:H     | 2:G:852:GLU:HG3   | 1.40                     | 0.40              |
| 2:G:1637:LEU:HD23 | 2:G:1637:LEU:HA   | 1.77                     | 0.40              |
| 2:G:1875:VAL:HA   | 2:G:1878:VAL:CG1  | 2.52                     | 0.40              |
| 2:H:517:HIS:HB2   | 2:H:527:VAL:HG21  | 2.04                     | 0.40              |
| 2:H:517:HIS:CE1   | 2:H:540:ASP:O     | 2.75                     | 0.40              |
| 2:H:560:ASN:O     | 2:H:562:LEU:N     | 2.54                     | 0.40              |
| 2:H:810:GLU:OE2   | 2:H:1070:ILE:N    | 2.45                     | 0.40              |
| 2:H:912:ARG:HB2   | 2:H:916:THR:HG23  | 2.03                     | 0.40              |
| 2:H:1166:VAL:CG1  | 2:H:1167:SER:N    | 2.85                     | 0.40              |
| 2:H:1528:GLU:C    | 2:H:1530:LYS:H    | 2.17                     | 0.40              |
| 2:H:1597:ALA:HB1  | 2:H:1657:ILE:HD12 | 2.02                     | 0.40              |
| 2:I:612:ASN:HD21  | 2:I:641:ILE:HA    | 1.84                     | 0.40              |
| 2:I:864:LEU:HD13  | 2:I:894:ARG:HB3   | 2.04                     | 0.40              |
| 2:I:1213:LEU:O    | 2:I:1214:LEU:HD23 | 2.20                     | 0.40              |
| 2:I:1271:ILE:HG22 | 2:I:1273:GLU:HB2  | 2.04                     | 0.40              |
| 2:I:1855:ILE:HB   | 2:I:1907:LEU:HD12 | 2.02                     | 0.40              |
| 1:A:157:HIS:CE1   | 1:A:269:LEU:HD11  | 2.57                     | 0.40              |
| 1:A:916:LEU:HD22  | 1:A:922:VAL:HG22  | 2.02                     | 0.40              |
| 1:A:1209:ASP:OD1  | 1:A:1210:PRO:HD2  | 2.21                     | 0.40              |
| 1:A:1406:MET:CE   | 1:A:1428:THR:HB   | 2.52                     | 0.40              |
| 1:B:12:ILE:O      | 1:B:16:GLU:HG2    | 2.20                     | 0.40              |
| 1:B:74:LEU:HD12   | 1:B:74:LEU:O      | 2.22                     | 0.40              |
| 1:B:509:ILE:H     | 1:B:509:ILE:HG13  | 1.50                     | 0.40              |
| 1:B:1370:THR:HG22 | 1:B:1371:THR:N    | 2.36                     | 0.40              |
| 1:C:406:TRP:CZ3   | 1:C:407:ASN:HB2   | 2.57                     | 0.40              |
| 1:C:655:LEU:HA    | 1:C:655:LEU:HD23  | 1.79                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1063:HIS:CE1  | 1:C:1067:LEU:CD2  | 3.04                     | 0.40              |
| 1:C:1195:ALA:HB1  | 1:C:1200:ILE:HD12 | 2.03                     | 0.40              |
| 1:C:1639:VAL:HG12 | 1:C:1640:SER:N    | 2.35                     | 0.40              |
| 1:C:1749:THR:O    | 1:C:1874:ASP:HB3  | 2.21                     | 0.40              |
| 2:G:260:PRO:HD3   | 2:G:289:TRP:CD2   | 2.56                     | 0.40              |
| 2:G:612:ASN:C     | 2:G:614:GLY:H     | 2.24                     | 0.40              |
| 2:H:538:ASP:HB2   | 2:H:540:ASP:HB2   | 2.03                     | 0.40              |
| 2:H:607:VAL:HG23  | 2:H:617:ILE:CG2   | 2.51                     | 0.40              |
| 2:H:1281:PRO:O    | 2:H:1378:ILE:HG23 | 2.22                     | 0.40              |
| 2:H:1593:ILE:HD13 | 2:H:1626:ILE:CD1  | 2.51                     | 0.40              |
| 2:H:1716:ASN:HA   | 2:H:1770:LEU:HD11 | 2.04                     | 0.40              |
| 2:I:240:LEU:HD12  | 2:I:240:LEU:HA    | 1.81                     | 0.40              |
| 2:I:717:ILE:CG2   | 2:I:760:HIS:CE1   | 3.05                     | 0.40              |
| 2:I:812:LYS:HD3   | 2:I:812:LYS:HA    | 1.82                     | 0.40              |
| 1:A:350:LEU:HB2   | 1:A:352:MET:HG2   | 2.03                     | 0.40              |
| 1:A:427:ASN:HB2   | 1:A:468:LEU:CD2   | 2.51                     | 0.40              |
| 1:B:709:ARG:O     | 1:B:714:VAL:HG21  | 2.21                     | 0.40              |
| 1:B:1577:GLN:NE2  | 1:B:1591:TRP:HB3  | 2.36                     | 0.40              |
| 1:C:187:LEU:HD11  | 1:C:202:GLU:HG3   | 2.03                     | 0.40              |
| 1:C:413:LEU:HD13  | 1:C:451:MET:HG2   | 2.03                     | 0.40              |
| 2:G:119:THR:HG22  | 2:G:120:LYS:N     | 2.36                     | 0.40              |
| 2:G:533:LEU:O     | 2:G:533:LEU:HG    | 2.21                     | 0.40              |
| 2:G:606:PHE:HZ    | 2:G:805:VAL:CG1   | 2.33                     | 0.40              |
| 2:G:1830:VAL:HA   | 2:G:1991:PHE:HE2  | 1.86                     | 0.40              |
| 2:G:2039:LYS:HA   | 2:G:2042:ILE:HG13 | 2.03                     | 0.40              |
| 2:H:156:LEU:HD23  | 2:H:500:HIS:HB2   | 2.04                     | 0.40              |
| 2:H:233:SER:HA    | 2:H:424:ALA:HB3   | 2.03                     | 0.40              |
| 2:H:283:ILE:HD12  | 2:H:283:ILE:HA    | 1.89                     | 0.40              |
| 2:H:298:LYS:HA    | 2:H:448:VAL:CG2   | 2.52                     | 0.40              |
| 2:H:441:LYS:O     | 2:H:445:LYS:HG3   | 2.22                     | 0.40              |
| 2:H:816:ASP:HB3   | 2:H:1048:VAL:CG2  | 2.52                     | 0.40              |
| 2:H:1172:LYS:HZ1  | 2:H:1574:ASN:HA   | 1.85                     | 0.40              |
| 2:H:1327:ILE:HA   | 2:H:1327:ILE:HD12 | 1.77                     | 0.40              |
| 2:I:225:THR:HA    | 2:I:226:PRO:HD3   | 1.98                     | 0.40              |
| 2:I:601:THR:O     | 2:I:601:THR:CG2   | 2.68                     | 0.40              |
| 2:I:612:ASN:C     | 2:I:614:GLY:H     | 2.25                     | 0.40              |

All (54) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 1:C:1784:ASP:CA  | 2:G:1087:HIS:CE1[7_655] | 0.16                     | 2.04              |
| 1:A:1784:ASP:CG  | 2:I:1087:HIS:CE1[7_545] | 0.52                     | 1.68              |
| 1:C:1784:ASP:C   | 2:G:1087:HIS:NE2[7_655] | 0.54                     | 1.66              |
| 1:C:1784:ASP:CB  | 2:G:1087:HIS:ND1[7_655] | 0.56                     | 1.64              |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:ND1[7_545] | 0.58                     | 1.62              |
| 1:B:1480:GLU:OE2 | 2:H:290:GLU:CB[6_555]   | 0.74                     | 1.46              |
| 1:C:1784:ASP:CB  | 2:G:1087:HIS:CG[7_655]  | 0.83                     | 1.37              |
| 1:A:1784:ASP:CG  | 2:I:1087:HIS:NE2[7_545] | 0.91                     | 1.29              |
| 1:A:1784:ASP:CB  | 2:I:1087:HIS:NE2[7_545] | 0.97                     | 1.23              |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:CE1[7_545] | 1.05                     | 1.15              |
| 1:C:1784:ASP:CA  | 2:G:1087:HIS:ND1[7_655] | 1.19                     | 1.01              |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:CG[7_545]  | 1.20                     | 1.00              |
| 1:C:1784:ASP:O   | 2:G:1087:HIS:NE2[7_655] | 1.22                     | 0.98              |
| 1:B:1480:GLU:CD  | 2:H:290:GLU:CB[6_555]   | 1.29                     | 0.91              |
| 2:G:77:VAL:CB    | 2:I:1929:LYS:CD[6_455]  | 1.31                     | 0.89              |
| 1:A:1784:ASP:OD1 | 2:I:1087:HIS:CE1[7_545] | 1.38                     | 0.82              |
| 1:C:1784:ASP:C   | 2:G:1087:HIS:CE1[7_655] | 1.38                     | 0.82              |
| 1:C:1784:ASP:CA  | 2:G:1087:HIS:NE2[7_655] | 1.42                     | 0.78              |
| 1:B:1480:GLU:OE2 | 2:H:290:GLU:CG[6_555]   | 1.43                     | 0.77              |
| 1:C:1784:ASP:N   | 2:G:1087:HIS:CE1[7_655] | 1.46                     | 0.74              |
| 2:G:77:VAL:CG2   | 2:I:1929:LYS:NZ[6_455]  | 1.46                     | 0.74              |
| 1:C:1784:ASP:CG  | 2:G:1087:HIS:ND1[7_655] | 1.47                     | 0.73              |
| 2:G:77:VAL:CG2   | 2:I:1929:LYS:CE[6_455]  | 1.51                     | 0.69              |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:NE2[7_545] | 1.60                     | 0.60              |
| 1:A:1784:ASP:CG  | 2:I:1087:HIS:ND1[7_545] | 1.64                     | 0.56              |
| 1:C:1784:ASP:CB  | 2:G:1087:HIS:CE1[7_655] | 1.64                     | 0.56              |
| 2:G:79:GLN:OE1   | 2:I:1930:SER:O[6_455]   | 1.64                     | 0.56              |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:CD2[7_545] | 1.68                     | 0.52              |
| 1:C:1785:THR:N   | 2:G:1087:HIS:NE2[7_655] | 1.70                     | 0.50              |
| 2:G:77:VAL:CB    | 2:I:1929:LYS:CE[6_455]  | 1.71                     | 0.49              |
| 1:C:1784:ASP:CB  | 2:G:1087:HIS:CD2[7_655] | 1.81                     | 0.39              |
| 1:B:1480:GLU:OE1 | 2:H:290:GLU:CB[6_555]   | 1.83                     | 0.37              |
| 1:A:1784:ASP:CB  | 2:I:1087:HIS:CE1[7_545] | 1.84                     | 0.36              |
| 1:C:1784:ASP:C   | 2:G:1087:HIS:CD2[7_655] | 1.86                     | 0.34              |
| 2:G:77:VAL:O     | 2:I:1929:LYS:CB[6_455]  | 1.92                     | 0.28              |
| 2:G:77:VAL:O     | 2:I:1929:LYS:CA[6_455]  | 1.93                     | 0.27              |
| 1:A:1784:ASP:CG  | 2:I:1087:HIS:CD2[7_545] | 1.94                     | 0.26              |
| 2:G:77:VAL:CG1   | 2:I:1929:LYS:CD[6_455]  | 1.95                     | 0.25              |
| 1:C:1784:ASP:CG  | 2:G:1087:HIS:CG[7_655]  | 1.97                     | 0.23              |
| 2:G:77:VAL:O     | 2:I:1929:LYS:CG[6_455]  | 1.97                     | 0.23              |
| 1:A:1784:ASP:OD1 | 2:I:1087:HIS:NE2[7_545] | 1.98                     | 0.22              |
| 1:C:1784:ASP:N   | 2:G:1087:HIS:ND1[7_655] | 1.98                     | 0.22              |

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| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 1:C:1784:ASP:CB  | 2:G:1087:HIS:CB[7_655]  | 2.03                     | 0.17              |
| 1:C:1784:ASP:OD2 | 2:G:1087:HIS:CB[7_655]  | 2.03                     | 0.17              |
| 2:H:6:THR:CG2    | 2:I:1935:GLU:OE2[6_455] | 2.05                     | 0.15              |
| 2:H:6:THR:CG2    | 2:I:1935:GLU:CD[6_455]  | 2.06                     | 0.14              |
| 1:C:1784:ASP:OD1 | 2:G:1087:HIS:ND1[7_655] | 2.11                     | 0.09              |
| 1:C:1784:ASP:CB  | 2:G:1087:HIS:NE2[7_655] | 2.11                     | 0.09              |
| 1:C:1784:ASP:O   | 2:G:1087:HIS:CD2[7_655] | 2.12                     | 0.08              |
| 1:C:1784:ASP:CA  | 2:G:1087:HIS:CG[7_655]  | 2.13                     | 0.07              |
| 1:A:1784:ASP:CB  | 2:I:1087:HIS:CD2[7_545] | 2.15                     | 0.05              |
| 2:G:77:VAL:CB    | 2:I:1929:LYS:CG[6_455]  | 2.15                     | 0.05              |
| 1:A:852:ARG:NH2  | 1:B:837:GLY:O[7_645]    | 2.19                     | 0.01              |
| 1:B:1480:GLU:OE1 | 2:H:290:GLU:CA[6_555]   | 2.19                     | 0.01              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 1736/1887 (92%)   | 1614 (93%)  | 100 (6%) | 22 (1%)  | 12          | 48 |
| 1   | B     | 1736/1887 (92%)   | 1619 (93%)  | 100 (6%) | 17 (1%)  | 15          | 53 |
| 1   | C     | 1736/1887 (92%)   | 1618 (93%)  | 96 (6%)  | 22 (1%)  | 12          | 48 |
| 2   | G     | 2029/2051 (99%)   | 1825 (90%)  | 173 (8%) | 31 (2%)  | 10          | 45 |
| 2   | H     | 2029/2051 (99%)   | 1826 (90%)  | 173 (8%) | 30 (2%)  | 10          | 45 |
| 2   | I     | 2029/2051 (99%)   | 1829 (90%)  | 174 (9%) | 26 (1%)  | 12          | 48 |
| All | All   | 11295/11814 (96%) | 10331 (92%) | 816 (7%) | 148 (1%) | 12          | 48 |

All (148) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 488 | PRO  |
| 1   | A     | 504 | ASP  |
| 1   | A     | 538 | GLU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 605        | LEU         |
| 1          | A            | 834        | GLY         |
| 1          | A            | 935        | GLU         |
| 1          | A            | 1763       | LYS         |
| 1          | A            | 1830       | GLY         |
| 1          | A            | 1843       | ASN         |
| 1          | B            | 504        | ASP         |
| 1          | B            | 538        | GLU         |
| 1          | B            | 605        | LEU         |
| 1          | B            | 834        | GLY         |
| 1          | B            | 1763       | LYS         |
| 1          | B            | 1830       | GLY         |
| 1          | B            | 1843       | ASN         |
| 1          | C            | 504        | ASP         |
| 1          | C            | 538        | GLU         |
| 1          | C            | 605        | LEU         |
| 1          | C            | 834        | GLY         |
| 1          | C            | 935        | GLU         |
| 1          | C            | 1763       | LYS         |
| 1          | C            | 1830       | GLY         |
| 1          | C            | 1843       | ASN         |
| 2          | G            | 521        | ASP         |
| 2          | G            | 561        | TRP         |
| 2          | G            | 1177       | SER         |
| 2          | G            | 1955       | PRO         |
| 2          | H            | 521        | ASP         |
| 2          | H            | 561        | TRP         |
| 2          | H            | 1418       | ASP         |
| 2          | H            | 1955       | PRO         |
| 2          | I            | 521        | ASP         |
| 2          | I            | 1955       | PRO         |
| 1          | A            | 1252       | GLY         |
| 1          | A            | 1585       | LYS         |
| 1          | A            | 1608       | ASN         |
| 1          | B            | 179        | LYS         |
| 1          | B            | 1252       | GLY         |
| 1          | B            | 1585       | LYS         |
| 1          | B            | 1608       | ASN         |
| 1          | C            | 1252       | GLY         |
| 1          | C            | 1585       | LYS         |
| 1          | C            | 1608       | ASN         |
| 2          | G            | 203        | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | G            | 562        | LEU         |
| 2          | G            | 1044       | VAL         |
| 2          | G            | 1418       | ASP         |
| 2          | G            | 1419       | PHE         |
| 2          | G            | 1722       | GLY         |
| 2          | H            | 203        | LEU         |
| 2          | H            | 1044       | VAL         |
| 2          | H            | 1177       | SER         |
| 2          | H            | 1420       | GLU         |
| 2          | H            | 1529       | GLN         |
| 2          | H            | 1722       | GLY         |
| 2          | I            | 203        | LEU         |
| 2          | I            | 1044       | VAL         |
| 2          | I            | 1177       | SER         |
| 2          | I            | 1418       | ASP         |
| 2          | I            | 1722       | GLY         |
| 1          | A            | 179        | LYS         |
| 1          | A            | 1749       | THR         |
| 1          | B            | 1749       | THR         |
| 1          | C            | 1749       | THR         |
| 2          | G            | 112        | ASN         |
| 2          | G            | 139        | LYS         |
| 2          | G            | 567        | PRO         |
| 2          | G            | 1101       | GLU         |
| 2          | G            | 2034       | GLY         |
| 2          | H            | 112        | ASN         |
| 2          | H            | 562        | LEU         |
| 2          | H            | 1101       | GLU         |
| 2          | I            | 374        | ALA         |
| 2          | I            | 1092       | ASP         |
| 2          | I            | 1101       | GLU         |
| 2          | I            | 2034       | GLY         |
| 2          | G            | 25         | ALA         |
| 2          | G            | 26         | SER         |
| 2          | G            | 374        | ALA         |
| 2          | G            | 742        | SER         |
| 2          | G            | 769        | SER         |
| 2          | G            | 1092       | ASP         |
| 2          | G            | 1510       | ALA         |
| 2          | H            | 26         | SER         |
| 2          | H            | 374        | ALA         |
| 2          | H            | 567        | PRO         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 742        | SER         |
| 2          | H            | 823        | ALA         |
| 2          | H            | 1510       | ALA         |
| 2          | H            | 2034       | GLY         |
| 2          | I            | 26         | SER         |
| 2          | I            | 112        | ASN         |
| 2          | I            | 742        | SER         |
| 2          | I            | 1419       | PHE         |
| 1          | A            | 485        | ASP         |
| 1          | A            | 1130       | ASP         |
| 1          | A            | 1477       | ILE         |
| 1          | A            | 1536       | LEU         |
| 1          | B            | 970        | GLY         |
| 1          | B            | 1477       | ILE         |
| 1          | C            | 179        | LYS         |
| 1          | C            | 934        | PRO         |
| 1          | C            | 1477       | ILE         |
| 2          | H            | 769        | SER         |
| 2          | H            | 1092       | ASP         |
| 2          | H            | 1257       | ASP         |
| 2          | I            | 25         | ALA         |
| 2          | I            | 136        | PRO         |
| 2          | I            | 769        | SER         |
| 2          | I            | 823        | ALA         |
| 2          | I            | 1510       | ALA         |
| 1          | A            | 178        | GLY         |
| 1          | A            | 970        | GLY         |
| 1          | C            | 930        | LEU         |
| 1          | C            | 970        | GLY         |
| 1          | C            | 1536       | LEU         |
| 2          | G            | 574        | SER         |
| 2          | H            | 1419       | PHE         |
| 2          | I            | 139        | LYS         |
| 2          | I            | 574        | SER         |
| 1          | A            | 1543       | GLY         |
| 1          | B            | 1543       | GLY         |
| 1          | C            | 1543       | GLY         |
| 2          | G            | 136        | PRO         |
| 2          | G            | 335        | PRO         |
| 2          | H            | 136        | PRO         |
| 2          | H            | 335        | PRO         |
| 2          | H            | 1661       | VAL         |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 178  | GLY  |
| 2   | G     | 1340 | PRO  |
| 2   | G     | 1956 | ARG  |
| 2   | H     | 772  | GLY  |
| 1   | A     | 934  | PRO  |
| 1   | C     | 178  | GLY  |
| 1   | C     | 1240 | VAL  |
| 2   | G     | 772  | GLY  |
| 2   | G     | 1176 | PRO  |
| 2   | G     | 1840 | VAL  |
| 2   | I     | 772  | GLY  |
| 1   | B     | 726  | GLY  |
| 1   | C     | 726  | GLY  |
| 2   | G     | 470  | VAL  |
| 2   | H     | 470  | VAL  |
| 2   | H     | 2012 | PRO  |
| 2   | I     | 335  | PRO  |
| 2   | I     | 1956 | ARG  |
| 2   | I     | 1340 | PRO  |

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 1460/1566 (93%)  | 1308 (90%) | 152 (10%)  | 7           | 28 |
| 1   | B     | 1460/1566 (93%)  | 1312 (90%) | 148 (10%)  | 7           | 29 |
| 1   | C     | 1460/1566 (93%)  | 1310 (90%) | 150 (10%)  | 7           | 28 |
| 2   | G     | 1772/1789 (99%)  | 1563 (88%) | 209 (12%)  | 5           | 24 |
| 2   | H     | 1772/1789 (99%)  | 1560 (88%) | 212 (12%)  | 5           | 23 |
| 2   | I     | 1772/1789 (99%)  | 1561 (88%) | 211 (12%)  | 5           | 24 |
| All | All   | 9696/10065 (96%) | 8614 (89%) | 1082 (11%) | 6           | 25 |

All (1082) residues with a non-rotameric sidechain are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | LEU  |
| 1   | A     | 15  | THR  |
| 1   | A     | 21  | GLN  |
| 1   | A     | 22  | PHE  |
| 1   | A     | 145 | VAL  |
| 1   | A     | 149 | LEU  |
| 1   | A     | 158 | LYS  |
| 1   | A     | 165 | SER  |
| 1   | A     | 171 | THR  |
| 1   | A     | 202 | GLU  |
| 1   | A     | 217 | PHE  |
| 1   | A     | 242 | THR  |
| 1   | A     | 253 | ARG  |
| 1   | A     | 328 | LEU  |
| 1   | A     | 331 | ILE  |
| 1   | A     | 332 | THR  |
| 1   | A     | 375 | LEU  |
| 1   | A     | 378 | LEU  |
| 1   | A     | 385 | PHE  |
| 1   | A     | 390 | VAL  |
| 1   | A     | 392 | THR  |
| 1   | A     | 400 | ARG  |
| 1   | A     | 412 | SER  |
| 1   | A     | 413 | LEU  |
| 1   | A     | 415 | SER  |
| 1   | A     | 416 | LEU  |
| 1   | A     | 428 | VAL  |
| 1   | A     | 431 | GLU  |
| 1   | A     | 432 | VAL  |
| 1   | A     | 435 | GLU  |
| 1   | A     | 447 | LEU  |
| 1   | A     | 457 | ASN  |
| 1   | A     | 460 | GLU  |
| 1   | A     | 461 | THR  |
| 1   | A     | 484 | LEU  |
| 1   | A     | 487 | ASP  |
| 1   | A     | 490 | TYR  |
| 1   | A     | 493 | VAL  |
| 1   | A     | 506 | ASN  |
| 1   | A     | 509 | ILE  |
| 1   | A     | 527 | GLN  |
| 1   | A     | 529 | MET  |
| 1   | A     | 536 | THR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 599        | MET         |
| 1          | A            | 600        | ASP         |
| 1          | A            | 603        | ASP         |
| 1          | A            | 606        | ASP         |
| 1          | A            | 607        | LYS         |
| 1          | A            | 615        | SER         |
| 1          | A            | 621        | THR         |
| 1          | A            | 622        | ILE         |
| 1          | A            | 625        | THR         |
| 1          | A            | 629        | THR         |
| 1          | A            | 635        | ILE         |
| 1          | A            | 644        | THR         |
| 1          | A            | 648        | ASP         |
| 1          | A            | 654        | GLN         |
| 1          | A            | 711        | SER         |
| 1          | A            | 719        | GLN         |
| 1          | A            | 728        | LYS         |
| 1          | A            | 731        | THR         |
| 1          | A            | 732        | LEU         |
| 1          | A            | 748        | LEU         |
| 1          | A            | 749        | ILE         |
| 1          | A            | 776        | GLU         |
| 1          | A            | 782        | GLU         |
| 1          | A            | 793        | ARG         |
| 1          | A            | 797        | THR         |
| 1          | A            | 806        | VAL         |
| 1          | A            | 817        | THR         |
| 1          | A            | 825        | PRO         |
| 1          | A            | 852        | ARG         |
| 1          | A            | 860        | ASN         |
| 1          | A            | 864        | VAL         |
| 1          | A            | 873        | ARG         |
| 1          | A            | 881        | ASN         |
| 1          | A            | 891        | MET         |
| 1          | A            | 913        | VAL         |
| 1          | A            | 930        | LEU         |
| 1          | A            | 931        | GLN         |
| 1          | A            | 933        | VAL         |
| 1          | A            | 935        | GLU         |
| 1          | A            | 947        | LEU         |
| 1          | A            | 949        | GLU         |
| 1          | A            | 953        | VAL         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 964        | GLU         |
| 1          | A            | 980        | VAL         |
| 1          | A            | 1016       | GLU         |
| 1          | A            | 1020       | VAL         |
| 1          | A            | 1022       | THR         |
| 1          | A            | 1047       | LEU         |
| 1          | A            | 1056       | ILE         |
| 1          | A            | 1070       | ARG         |
| 1          | A            | 1087       | LYS         |
| 1          | A            | 1095       | THR         |
| 1          | A            | 1101       | SER         |
| 1          | A            | 1125       | VAL         |
| 1          | A            | 1127       | VAL         |
| 1          | A            | 1131       | LEU         |
| 1          | A            | 1172       | THR         |
| 1          | A            | 1173       | LEU         |
| 1          | A            | 1179       | LEU         |
| 1          | A            | 1184       | LEU         |
| 1          | A            | 1196       | LYS         |
| 1          | A            | 1197       | THR         |
| 1          | A            | 1208       | VAL         |
| 1          | A            | 1218       | SER         |
| 1          | A            | 1226       | SER         |
| 1          | A            | 1229       | THR         |
| 1          | A            | 1255       | SER         |
| 1          | A            | 1274       | ILE         |
| 1          | A            | 1283       | MET         |
| 1          | A            | 1307       | THR         |
| 1          | A            | 1327       | CYS         |
| 1          | A            | 1338       | GLU         |
| 1          | A            | 1367       | ARG         |
| 1          | A            | 1372       | THR         |
| 1          | A            | 1384       | ILE         |
| 1          | A            | 1385       | GLN         |
| 1          | A            | 1392       | LEU         |
| 1          | A            | 1414       | ILE         |
| 1          | A            | 1426       | LEU         |
| 1          | A            | 1442       | ASN         |
| 1          | A            | 1465       | ASN         |
| 1          | A            | 1479       | SER         |
| 1          | A            | 1489       | ARG         |
| 1          | A            | 1502       | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1515       | ARG         |
| 1          | A            | 1522       | LEU         |
| 1          | A            | 1523       | ARG         |
| 1          | A            | 1532       | THR         |
| 1          | A            | 1533       | ILE         |
| 1          | A            | 1549       | ASN         |
| 1          | A            | 1556       | THR         |
| 1          | A            | 1566       | ARG         |
| 1          | A            | 1580       | LEU         |
| 1          | A            | 1585       | LYS         |
| 1          | A            | 1612       | ASP         |
| 1          | A            | 1625       | LEU         |
| 1          | A            | 1665       | ILE         |
| 1          | A            | 1666       | THR         |
| 1          | A            | 1692       | MET         |
| 1          | A            | 1693       | ILE         |
| 1          | A            | 1707       | THR         |
| 1          | A            | 1709       | GLU         |
| 1          | A            | 1721       | ARG         |
| 1          | A            | 1775       | LEU         |
| 1          | A            | 1782       | GLU         |
| 1          | A            | 1788       | GLU         |
| 1          | A            | 1794       | GLN         |
| 1          | A            | 1841       | ARG         |
| 1          | A            | 1873       | HIS         |
| 1          | B            | 14         | LEU         |
| 1          | B            | 15         | THR         |
| 1          | B            | 21         | GLN         |
| 1          | B            | 22         | PHE         |
| 1          | B            | 145        | VAL         |
| 1          | B            | 149        | LEU         |
| 1          | B            | 158        | LYS         |
| 1          | B            | 165        | SER         |
| 1          | B            | 171        | THR         |
| 1          | B            | 202        | GLU         |
| 1          | B            | 217        | PHE         |
| 1          | B            | 242        | THR         |
| 1          | B            | 253        | ARG         |
| 1          | B            | 300        | VAL         |
| 1          | B            | 328        | LEU         |
| 1          | B            | 331        | ILE         |
| 1          | B            | 332        | THR         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 375        | LEU         |
| 1          | B            | 385        | PHE         |
| 1          | B            | 390        | VAL         |
| 1          | B            | 392        | THR         |
| 1          | B            | 400        | ARG         |
| 1          | B            | 401        | THR         |
| 1          | B            | 412        | SER         |
| 1          | B            | 413        | LEU         |
| 1          | B            | 415        | SER         |
| 1          | B            | 416        | LEU         |
| 1          | B            | 428        | VAL         |
| 1          | B            | 432        | VAL         |
| 1          | B            | 435        | GLU         |
| 1          | B            | 447        | LEU         |
| 1          | B            | 457        | ASN         |
| 1          | B            | 460        | GLU         |
| 1          | B            | 461        | THR         |
| 1          | B            | 484        | LEU         |
| 1          | B            | 489        | VAL         |
| 1          | B            | 493        | VAL         |
| 1          | B            | 499        | PRO         |
| 1          | B            | 506        | ASN         |
| 1          | B            | 509        | ILE         |
| 1          | B            | 510        | THR         |
| 1          | B            | 527        | GLN         |
| 1          | B            | 529        | MET         |
| 1          | B            | 536        | THR         |
| 1          | B            | 599        | MET         |
| 1          | B            | 600        | ASP         |
| 1          | B            | 603        | ASP         |
| 1          | B            | 606        | ASP         |
| 1          | B            | 607        | LYS         |
| 1          | B            | 615        | SER         |
| 1          | B            | 621        | THR         |
| 1          | B            | 622        | ILE         |
| 1          | B            | 625        | THR         |
| 1          | B            | 629        | THR         |
| 1          | B            | 635        | ILE         |
| 1          | B            | 644        | THR         |
| 1          | B            | 648        | ASP         |
| 1          | B            | 711        | SER         |
| 1          | B            | 719        | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 728        | LYS         |
| 1          | B            | 731        | THR         |
| 1          | B            | 732        | LEU         |
| 1          | B            | 748        | LEU         |
| 1          | B            | 749        | ILE         |
| 1          | B            | 776        | GLU         |
| 1          | B            | 782        | GLU         |
| 1          | B            | 793        | ARG         |
| 1          | B            | 797        | THR         |
| 1          | B            | 806        | VAL         |
| 1          | B            | 852        | ARG         |
| 1          | B            | 860        | ASN         |
| 1          | B            | 864        | VAL         |
| 1          | B            | 873        | ARG         |
| 1          | B            | 881        | ASN         |
| 1          | B            | 891        | MET         |
| 1          | B            | 913        | VAL         |
| 1          | B            | 930        | LEU         |
| 1          | B            | 933        | VAL         |
| 1          | B            | 947        | LEU         |
| 1          | B            | 949        | GLU         |
| 1          | B            | 953        | VAL         |
| 1          | B            | 964        | GLU         |
| 1          | B            | 980        | VAL         |
| 1          | B            | 1016       | GLU         |
| 1          | B            | 1020       | VAL         |
| 1          | B            | 1047       | LEU         |
| 1          | B            | 1056       | ILE         |
| 1          | B            | 1070       | ARG         |
| 1          | B            | 1078       | SER         |
| 1          | B            | 1080       | THR         |
| 1          | B            | 1087       | LYS         |
| 1          | B            | 1095       | THR         |
| 1          | B            | 1101       | SER         |
| 1          | B            | 1125       | VAL         |
| 1          | B            | 1127       | VAL         |
| 1          | B            | 1131       | LEU         |
| 1          | B            | 1172       | THR         |
| 1          | B            | 1173       | LEU         |
| 1          | B            | 1179       | LEU         |
| 1          | B            | 1184       | LEU         |
| 1          | B            | 1196       | LYS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 1197       | THR         |
| 1          | B            | 1208       | VAL         |
| 1          | B            | 1218       | SER         |
| 1          | B            | 1229       | THR         |
| 1          | B            | 1255       | SER         |
| 1          | B            | 1274       | ILE         |
| 1          | B            | 1283       | MET         |
| 1          | B            | 1307       | THR         |
| 1          | B            | 1327       | CYS         |
| 1          | B            | 1338       | GLU         |
| 1          | B            | 1367       | ARG         |
| 1          | B            | 1372       | THR         |
| 1          | B            | 1384       | ILE         |
| 1          | B            | 1385       | GLN         |
| 1          | B            | 1392       | LEU         |
| 1          | B            | 1414       | ILE         |
| 1          | B            | 1426       | LEU         |
| 1          | B            | 1442       | ASN         |
| 1          | B            | 1465       | ASN         |
| 1          | B            | 1479       | SER         |
| 1          | B            | 1502       | ARG         |
| 1          | B            | 1515       | ARG         |
| 1          | B            | 1522       | LEU         |
| 1          | B            | 1523       | ARG         |
| 1          | B            | 1532       | THR         |
| 1          | B            | 1533       | ILE         |
| 1          | B            | 1549       | ASN         |
| 1          | B            | 1556       | THR         |
| 1          | B            | 1566       | ARG         |
| 1          | B            | 1577       | GLN         |
| 1          | B            | 1580       | LEU         |
| 1          | B            | 1585       | LYS         |
| 1          | B            | 1612       | ASP         |
| 1          | B            | 1625       | LEU         |
| 1          | B            | 1665       | ILE         |
| 1          | B            | 1666       | THR         |
| 1          | B            | 1692       | MET         |
| 1          | B            | 1693       | ILE         |
| 1          | B            | 1707       | THR         |
| 1          | B            | 1709       | GLU         |
| 1          | B            | 1721       | ARG         |
| 1          | B            | 1775       | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 1782       | GLU         |
| 1          | B            | 1788       | GLU         |
| 1          | B            | 1794       | GLN         |
| 1          | B            | 1841       | ARG         |
| 1          | B            | 1873       | HIS         |
| 1          | C            | 14         | LEU         |
| 1          | C            | 15         | THR         |
| 1          | C            | 21         | GLN         |
| 1          | C            | 22         | PHE         |
| 1          | C            | 145        | VAL         |
| 1          | C            | 149        | LEU         |
| 1          | C            | 158        | LYS         |
| 1          | C            | 165        | SER         |
| 1          | C            | 171        | THR         |
| 1          | C            | 202        | GLU         |
| 1          | C            | 217        | PHE         |
| 1          | C            | 242        | THR         |
| 1          | C            | 253        | ARG         |
| 1          | C            | 328        | LEU         |
| 1          | C            | 331        | ILE         |
| 1          | C            | 332        | THR         |
| 1          | C            | 375        | LEU         |
| 1          | C            | 378        | LEU         |
| 1          | C            | 390        | VAL         |
| 1          | C            | 392        | THR         |
| 1          | C            | 400        | ARG         |
| 1          | C            | 412        | SER         |
| 1          | C            | 413        | LEU         |
| 1          | C            | 415        | SER         |
| 1          | C            | 416        | LEU         |
| 1          | C            | 428        | VAL         |
| 1          | C            | 431        | GLU         |
| 1          | C            | 432        | VAL         |
| 1          | C            | 435        | GLU         |
| 1          | C            | 447        | LEU         |
| 1          | C            | 457        | ASN         |
| 1          | C            | 460        | GLU         |
| 1          | C            | 461        | THR         |
| 1          | C            | 484        | LEU         |
| 1          | C            | 489        | VAL         |
| 1          | C            | 493        | VAL         |
| 1          | C            | 506        | ASN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 509        | ILE         |
| 1          | C            | 527        | GLN         |
| 1          | C            | 529        | MET         |
| 1          | C            | 536        | THR         |
| 1          | C            | 599        | MET         |
| 1          | C            | 600        | ASP         |
| 1          | C            | 603        | ASP         |
| 1          | C            | 606        | ASP         |
| 1          | C            | 607        | LYS         |
| 1          | C            | 615        | SER         |
| 1          | C            | 621        | THR         |
| 1          | C            | 622        | ILE         |
| 1          | C            | 625        | THR         |
| 1          | C            | 629        | THR         |
| 1          | C            | 635        | ILE         |
| 1          | C            | 644        | THR         |
| 1          | C            | 648        | ASP         |
| 1          | C            | 711        | SER         |
| 1          | C            | 719        | GLN         |
| 1          | C            | 728        | LYS         |
| 1          | C            | 731        | THR         |
| 1          | C            | 732        | LEU         |
| 1          | C            | 748        | LEU         |
| 1          | C            | 749        | ILE         |
| 1          | C            | 776        | GLU         |
| 1          | C            | 782        | GLU         |
| 1          | C            | 797        | THR         |
| 1          | C            | 806        | VAL         |
| 1          | C            | 824        | LEU         |
| 1          | C            | 852        | ARG         |
| 1          | C            | 860        | ASN         |
| 1          | C            | 864        | VAL         |
| 1          | C            | 873        | ARG         |
| 1          | C            | 881        | ASN         |
| 1          | C            | 891        | MET         |
| 1          | C            | 913        | VAL         |
| 1          | C            | 930        | LEU         |
| 1          | C            | 931        | GLN         |
| 1          | C            | 933        | VAL         |
| 1          | C            | 935        | GLU         |
| 1          | C            | 947        | LEU         |
| 1          | C            | 949        | GLU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 951        | SER         |
| 1          | C            | 953        | VAL         |
| 1          | C            | 980        | VAL         |
| 1          | C            | 1016       | GLU         |
| 1          | C            | 1020       | VAL         |
| 1          | C            | 1047       | LEU         |
| 1          | C            | 1056       | ILE         |
| 1          | C            | 1070       | ARG         |
| 1          | C            | 1078       | SER         |
| 1          | C            | 1087       | LYS         |
| 1          | C            | 1095       | THR         |
| 1          | C            | 1101       | SER         |
| 1          | C            | 1125       | VAL         |
| 1          | C            | 1127       | VAL         |
| 1          | C            | 1131       | LEU         |
| 1          | C            | 1172       | THR         |
| 1          | C            | 1173       | LEU         |
| 1          | C            | 1179       | LEU         |
| 1          | C            | 1184       | LEU         |
| 1          | C            | 1196       | LYS         |
| 1          | C            | 1197       | THR         |
| 1          | C            | 1208       | VAL         |
| 1          | C            | 1218       | SER         |
| 1          | C            | 1229       | THR         |
| 1          | C            | 1255       | SER         |
| 1          | C            | 1274       | ILE         |
| 1          | C            | 1283       | MET         |
| 1          | C            | 1307       | THR         |
| 1          | C            | 1327       | CYS         |
| 1          | C            | 1338       | GLU         |
| 1          | C            | 1367       | ARG         |
| 1          | C            | 1372       | THR         |
| 1          | C            | 1384       | ILE         |
| 1          | C            | 1385       | GLN         |
| 1          | C            | 1392       | LEU         |
| 1          | C            | 1414       | ILE         |
| 1          | C            | 1426       | LEU         |
| 1          | C            | 1430       | ARG         |
| 1          | C            | 1432       | HIS         |
| 1          | C            | 1442       | ASN         |
| 1          | C            | 1455       | ARG         |
| 1          | C            | 1465       | ASN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 1479       | SER         |
| 1          | C            | 1489       | ARG         |
| 1          | C            | 1502       | ARG         |
| 1          | C            | 1515       | ARG         |
| 1          | C            | 1522       | LEU         |
| 1          | C            | 1523       | ARG         |
| 1          | C            | 1532       | THR         |
| 1          | C            | 1533       | ILE         |
| 1          | C            | 1549       | ASN         |
| 1          | C            | 1556       | THR         |
| 1          | C            | 1566       | ARG         |
| 1          | C            | 1577       | GLN         |
| 1          | C            | 1580       | LEU         |
| 1          | C            | 1585       | LYS         |
| 1          | C            | 1612       | ASP         |
| 1          | C            | 1625       | LEU         |
| 1          | C            | 1665       | ILE         |
| 1          | C            | 1666       | THR         |
| 1          | C            | 1692       | MET         |
| 1          | C            | 1693       | ILE         |
| 1          | C            | 1707       | THR         |
| 1          | C            | 1709       | GLU         |
| 1          | C            | 1721       | ARG         |
| 1          | C            | 1775       | LEU         |
| 1          | C            | 1782       | GLU         |
| 1          | C            | 1788       | GLU         |
| 1          | C            | 1794       | GLN         |
| 1          | C            | 1841       | ARG         |
| 1          | C            | 1873       | HIS         |
| 2          | G            | 6          | THR         |
| 2          | G            | 7          | ARG         |
| 2          | G            | 45         | THR         |
| 2          | G            | 46         | GLU         |
| 2          | G            | 48         | PHE         |
| 2          | G            | 56         | THR         |
| 2          | G            | 65         | LEU         |
| 2          | G            | 84         | LEU         |
| 2          | G            | 86         | LEU         |
| 2          | G            | 93         | ASN         |
| 2          | G            | 99         | ASN         |
| 2          | G            | 101        | ILE         |
| 2          | G            | 109        | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | G            | 117        | VAL         |
| 2          | G            | 122        | LEU         |
| 2          | G            | 149        | VAL         |
| 2          | G            | 153        | ASN         |
| 2          | G            | 155        | GLN         |
| 2          | G            | 159        | ILE         |
| 2          | G            | 173        | LEU         |
| 2          | G            | 175        | ASP         |
| 2          | G            | 176        | LEU         |
| 2          | G            | 178        | GLN         |
| 2          | G            | 182        | VAL         |
| 2          | G            | 210        | THR         |
| 2          | G            | 227        | ASP         |
| 2          | G            | 236        | ILE         |
| 2          | G            | 240        | LEU         |
| 2          | G            | 246        | LEU         |
| 2          | G            | 281        | VAL         |
| 2          | G            | 286        | THR         |
| 2          | G            | 295        | SER         |
| 2          | G            | 297        | ARG         |
| 2          | G            | 300        | ILE         |
| 2          | G            | 303        | LEU         |
| 2          | G            | 319        | LEU         |
| 2          | G            | 339        | LEU         |
| 2          | G            | 340        | SER         |
| 2          | G            | 342        | SER         |
| 2          | G            | 344        | LEU         |
| 2          | G            | 353        | VAL         |
| 2          | G            | 371        | VAL         |
| 2          | G            | 376        | ASN         |
| 2          | G            | 389        | LEU         |
| 2          | G            | 392        | THR         |
| 2          | G            | 402        | LEU         |
| 2          | G            | 418        | ASN         |
| 2          | G            | 425        | SER         |
| 2          | G            | 431        | LEU         |
| 2          | G            | 448        | VAL         |
| 2          | G            | 455        | ILE         |
| 2          | G            | 462        | THR         |
| 2          | G            | 463        | PHE         |
| 2          | G            | 471        | LEU         |
| 2          | G            | 476        | SER         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | G            | 478        | ARG         |
| 2          | G            | 482        | CYS         |
| 2          | G            | 492        | THR         |
| 2          | G            | 499        | THR         |
| 2          | G            | 539        | ASP         |
| 2          | G            | 545        | GLN         |
| 2          | G            | 553        | ASN         |
| 2          | G            | 562        | LEU         |
| 2          | G            | 566        | HIS         |
| 2          | G            | 574        | SER         |
| 2          | G            | 586        | LEU         |
| 2          | G            | 587        | ILE         |
| 2          | G            | 598        | THR         |
| 2          | G            | 607        | VAL         |
| 2          | G            | 611        | THR         |
| 2          | G            | 616        | THR         |
| 2          | G            | 653        | TYR         |
| 2          | G            | 665        | LEU         |
| 2          | G            | 669        | LEU         |
| 2          | G            | 670        | ARG         |
| 2          | G            | 676        | ILE         |
| 2          | G            | 693        | GLU         |
| 2          | G            | 714        | SER         |
| 2          | G            | 719        | ILE         |
| 2          | G            | 723        | HIS         |
| 2          | G            | 730        | LEU         |
| 2          | G            | 736        | ARG         |
| 2          | G            | 741        | HIS         |
| 2          | G            | 750        | MET         |
| 2          | G            | 751        | LEU         |
| 2          | G            | 762        | ASN         |
| 2          | G            | 767        | PHE         |
| 2          | G            | 775        | ASP         |
| 2          | G            | 777        | THR         |
| 2          | G            | 787        | THR         |
| 2          | G            | 794        | MET         |
| 2          | G            | 800        | LEU         |
| 2          | G            | 810        | GLU         |
| 2          | G            | 825        | THR         |
| 2          | G            | 832        | TRP         |
| 2          | G            | 835        | THR         |
| 2          | G            | 844        | VAL         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | G            | 852        | GLU         |
| 2          | G            | 855        | HIS         |
| 2          | G            | 857        | ILE         |
| 2          | G            | 869        | ASP         |
| 2          | G            | 880        | LEU         |
| 2          | G            | 881        | VAL         |
| 2          | G            | 892        | ILE         |
| 2          | G            | 907        | VAL         |
| 2          | G            | 929        | LEU         |
| 2          | G            | 945        | THR         |
| 2          | G            | 952        | ARG         |
| 2          | G            | 953        | ARG         |
| 2          | G            | 964        | LEU         |
| 2          | G            | 971        | SER         |
| 2          | G            | 993        | GLN         |
| 2          | G            | 1015       | VAL         |
| 2          | G            | 1021       | LEU         |
| 2          | G            | 1024       | ARG         |
| 2          | G            | 1048       | VAL         |
| 2          | G            | 1066       | ILE         |
| 2          | G            | 1070       | ILE         |
| 2          | G            | 1082       | ILE         |
| 2          | G            | 1109       | VAL         |
| 2          | G            | 1123       | ASP         |
| 2          | G            | 1124       | SER         |
| 2          | G            | 1145       | SER         |
| 2          | G            | 1148       | ASN         |
| 2          | G            | 1160       | THR         |
| 2          | G            | 1171       | ARG         |
| 2          | G            | 1189       | THR         |
| 2          | G            | 1197       | LEU         |
| 2          | G            | 1211       | LEU         |
| 2          | G            | 1219       | ILE         |
| 2          | G            | 1227       | ARG         |
| 2          | G            | 1260       | GLN         |
| 2          | G            | 1265       | MET         |
| 2          | G            | 1284       | VAL         |
| 2          | G            | 1314       | ARG         |
| 2          | G            | 1318       | THR         |
| 2          | G            | 1328       | VAL         |
| 2          | G            | 1335       | ILE         |
| 2          | G            | 1348       | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | G            | 1359       | MET         |
| 2          | G            | 1360       | ILE         |
| 2          | G            | 1378       | ILE         |
| 2          | G            | 1397       | SER         |
| 2          | G            | 1407       | THR         |
| 2          | G            | 1408       | SER         |
| 2          | G            | 1417       | THR         |
| 2          | G            | 1418       | ASP         |
| 2          | G            | 1420       | GLU         |
| 2          | G            | 1424       | GLN         |
| 2          | G            | 1426       | THR         |
| 2          | G            | 1434       | HIS         |
| 2          | G            | 1437       | THR         |
| 2          | G            | 1441       | ILE         |
| 2          | G            | 1443       | VAL         |
| 2          | G            | 1446       | SER         |
| 2          | G            | 1452       | LEU         |
| 2          | G            | 1463       | THR         |
| 2          | G            | 1468       | THR         |
| 2          | G            | 1470       | THR         |
| 2          | G            | 1472       | VAL         |
| 2          | G            | 1473       | THR         |
| 2          | G            | 1501       | ILE         |
| 2          | G            | 1511       | SER         |
| 2          | G            | 1526       | THR         |
| 2          | G            | 1527       | LEU         |
| 2          | G            | 1528       | GLU         |
| 2          | G            | 1533       | LEU         |
| 2          | G            | 1549       | THR         |
| 2          | G            | 1563       | ILE         |
| 2          | G            | 1567       | ARG         |
| 2          | G            | 1590       | ARG         |
| 2          | G            | 1602       | SER         |
| 2          | G            | 1605       | VAL         |
| 2          | G            | 1609       | THR         |
| 2          | G            | 1616       | VAL         |
| 2          | G            | 1624       | THR         |
| 2          | G            | 1627       | GLN         |
| 2          | G            | 1632       | ILE         |
| 2          | G            | 1637       | LEU         |
| 2          | G            | 1651       | LEU         |
| 2          | G            | 1672       | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | G            | 1678       | MET         |
| 2          | G            | 1680       | LEU         |
| 2          | G            | 1683       | THR         |
| 2          | G            | 1712       | ASN         |
| 2          | G            | 1718       | THR         |
| 2          | G            | 1757       | GLU         |
| 2          | G            | 1775       | GLN         |
| 2          | G            | 1781       | LEU         |
| 2          | G            | 1784       | MET         |
| 2          | G            | 1825       | GLU         |
| 2          | G            | 1831       | VAL         |
| 2          | G            | 1834       | ARG         |
| 2          | G            | 1844       | ARG         |
| 2          | G            | 1847       | LEU         |
| 2          | G            | 1857       | ILE         |
| 2          | G            | 1862       | VAL         |
| 2          | G            | 1886       | VAL         |
| 2          | G            | 1914       | LEU         |
| 2          | G            | 1936       | VAL         |
| 2          | G            | 1937       | GLU         |
| 2          | G            | 1941       | PHE         |
| 2          | G            | 1982       | MET         |
| 2          | G            | 2003       | VAL         |
| 2          | G            | 2042       | ILE         |
| 2          | G            | 2044       | ASN         |
| 2          | G            | 2047       | LYS         |
| 2          | G            | 2048       | TYR         |
| 2          | G            | 2050       | GLN         |
| 2          | H            | 6          | THR         |
| 2          | H            | 7          | ARG         |
| 2          | H            | 45         | THR         |
| 2          | H            | 46         | GLU         |
| 2          | H            | 48         | PHE         |
| 2          | H            | 56         | THR         |
| 2          | H            | 65         | LEU         |
| 2          | H            | 84         | LEU         |
| 2          | H            | 86         | LEU         |
| 2          | H            | 93         | ASN         |
| 2          | H            | 99         | ASN         |
| 2          | H            | 101        | ILE         |
| 2          | H            | 109        | LEU         |
| 2          | H            | 117        | VAL         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 122        | LEU         |
| 2          | H            | 149        | VAL         |
| 2          | H            | 153        | ASN         |
| 2          | H            | 155        | GLN         |
| 2          | H            | 159        | ILE         |
| 2          | H            | 173        | LEU         |
| 2          | H            | 176        | LEU         |
| 2          | H            | 178        | GLN         |
| 2          | H            | 182        | VAL         |
| 2          | H            | 186        | ASP         |
| 2          | H            | 198        | LEU         |
| 2          | H            | 210        | THR         |
| 2          | H            | 227        | ASP         |
| 2          | H            | 236        | ILE         |
| 2          | H            | 240        | LEU         |
| 2          | H            | 246        | LEU         |
| 2          | H            | 281        | VAL         |
| 2          | H            | 286        | THR         |
| 2          | H            | 295        | SER         |
| 2          | H            | 297        | ARG         |
| 2          | H            | 300        | ILE         |
| 2          | H            | 317        | THR         |
| 2          | H            | 319        | LEU         |
| 2          | H            | 339        | LEU         |
| 2          | H            | 340        | SER         |
| 2          | H            | 342        | SER         |
| 2          | H            | 344        | LEU         |
| 2          | H            | 353        | VAL         |
| 2          | H            | 371        | VAL         |
| 2          | H            | 376        | ASN         |
| 2          | H            | 389        | LEU         |
| 2          | H            | 392        | THR         |
| 2          | H            | 402        | LEU         |
| 2          | H            | 418        | ASN         |
| 2          | H            | 425        | SER         |
| 2          | H            | 431        | LEU         |
| 2          | H            | 448        | VAL         |
| 2          | H            | 455        | ILE         |
| 2          | H            | 462        | THR         |
| 2          | H            | 463        | PHE         |
| 2          | H            | 471        | LEU         |
| 2          | H            | 476        | SER         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 478        | ARG         |
| 2          | H            | 482        | CYS         |
| 2          | H            | 492        | THR         |
| 2          | H            | 499        | THR         |
| 2          | H            | 545        | GLN         |
| 2          | H            | 553        | ASN         |
| 2          | H            | 562        | LEU         |
| 2          | H            | 566        | HIS         |
| 2          | H            | 572        | ASN         |
| 2          | H            | 574        | SER         |
| 2          | H            | 586        | LEU         |
| 2          | H            | 587        | ILE         |
| 2          | H            | 598        | THR         |
| 2          | H            | 607        | VAL         |
| 2          | H            | 611        | THR         |
| 2          | H            | 616        | THR         |
| 2          | H            | 653        | TYR         |
| 2          | H            | 665        | LEU         |
| 2          | H            | 669        | LEU         |
| 2          | H            | 670        | ARG         |
| 2          | H            | 676        | ILE         |
| 2          | H            | 693        | GLU         |
| 2          | H            | 714        | SER         |
| 2          | H            | 719        | ILE         |
| 2          | H            | 723        | HIS         |
| 2          | H            | 730        | LEU         |
| 2          | H            | 733        | THR         |
| 2          | H            | 736        | ARG         |
| 2          | H            | 741        | HIS         |
| 2          | H            | 751        | LEU         |
| 2          | H            | 762        | ASN         |
| 2          | H            | 767        | PHE         |
| 2          | H            | 775        | ASP         |
| 2          | H            | 777        | THR         |
| 2          | H            | 787        | THR         |
| 2          | H            | 794        | MET         |
| 2          | H            | 797        | ASP         |
| 2          | H            | 800        | LEU         |
| 2          | H            | 810        | GLU         |
| 2          | H            | 825        | THR         |
| 2          | H            | 832        | TRP         |
| 2          | H            | 835        | THR         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 844        | VAL         |
| 2          | H            | 852        | GLU         |
| 2          | H            | 855        | HIS         |
| 2          | H            | 857        | ILE         |
| 2          | H            | 869        | ASP         |
| 2          | H            | 880        | LEU         |
| 2          | H            | 881        | VAL         |
| 2          | H            | 892        | ILE         |
| 2          | H            | 907        | VAL         |
| 2          | H            | 929        | LEU         |
| 2          | H            | 945        | THR         |
| 2          | H            | 952        | ARG         |
| 2          | H            | 953        | ARG         |
| 2          | H            | 964        | LEU         |
| 2          | H            | 971        | SER         |
| 2          | H            | 993        | GLN         |
| 2          | H            | 1015       | VAL         |
| 2          | H            | 1021       | LEU         |
| 2          | H            | 1024       | ARG         |
| 2          | H            | 1048       | VAL         |
| 2          | H            | 1066       | ILE         |
| 2          | H            | 1070       | ILE         |
| 2          | H            | 1082       | ILE         |
| 2          | H            | 1109       | VAL         |
| 2          | H            | 1123       | ASP         |
| 2          | H            | 1145       | SER         |
| 2          | H            | 1148       | ASN         |
| 2          | H            | 1160       | THR         |
| 2          | H            | 1171       | ARG         |
| 2          | H            | 1189       | THR         |
| 2          | H            | 1197       | LEU         |
| 2          | H            | 1211       | LEU         |
| 2          | H            | 1219       | ILE         |
| 2          | H            | 1227       | ARG         |
| 2          | H            | 1260       | GLN         |
| 2          | H            | 1265       | MET         |
| 2          | H            | 1284       | VAL         |
| 2          | H            | 1314       | ARG         |
| 2          | H            | 1318       | THR         |
| 2          | H            | 1328       | VAL         |
| 2          | H            | 1335       | ILE         |
| 2          | H            | 1348       | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 1359       | MET         |
| 2          | H            | 1360       | ILE         |
| 2          | H            | 1378       | ILE         |
| 2          | H            | 1397       | SER         |
| 2          | H            | 1407       | THR         |
| 2          | H            | 1408       | SER         |
| 2          | H            | 1420       | GLU         |
| 2          | H            | 1422       | THR         |
| 2          | H            | 1426       | THR         |
| 2          | H            | 1434       | HIS         |
| 2          | H            | 1437       | THR         |
| 2          | H            | 1441       | ILE         |
| 2          | H            | 1443       | VAL         |
| 2          | H            | 1446       | SER         |
| 2          | H            | 1452       | LEU         |
| 2          | H            | 1463       | THR         |
| 2          | H            | 1468       | THR         |
| 2          | H            | 1470       | THR         |
| 2          | H            | 1472       | VAL         |
| 2          | H            | 1473       | THR         |
| 2          | H            | 1501       | ILE         |
| 2          | H            | 1511       | SER         |
| 2          | H            | 1526       | THR         |
| 2          | H            | 1527       | LEU         |
| 2          | H            | 1528       | GLU         |
| 2          | H            | 1530       | LYS         |
| 2          | H            | 1533       | LEU         |
| 2          | H            | 1549       | THR         |
| 2          | H            | 1563       | ILE         |
| 2          | H            | 1567       | ARG         |
| 2          | H            | 1590       | ARG         |
| 2          | H            | 1602       | SER         |
| 2          | H            | 1605       | VAL         |
| 2          | H            | 1609       | THR         |
| 2          | H            | 1616       | VAL         |
| 2          | H            | 1624       | THR         |
| 2          | H            | 1627       | GLN         |
| 2          | H            | 1632       | ILE         |
| 2          | H            | 1637       | LEU         |
| 2          | H            | 1651       | LEU         |
| 2          | H            | 1657       | ILE         |
| 2          | H            | 1661       | VAL         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 1672       | GLN         |
| 2          | H            | 1678       | MET         |
| 2          | H            | 1680       | LEU         |
| 2          | H            | 1683       | THR         |
| 2          | H            | 1693       | ARG         |
| 2          | H            | 1712       | ASN         |
| 2          | H            | 1718       | THR         |
| 2          | H            | 1757       | GLU         |
| 2          | H            | 1775       | GLN         |
| 2          | H            | 1781       | LEU         |
| 2          | H            | 1784       | MET         |
| 2          | H            | 1825       | GLU         |
| 2          | H            | 1831       | VAL         |
| 2          | H            | 1834       | ARG         |
| 2          | H            | 1840       | VAL         |
| 2          | H            | 1844       | ARG         |
| 2          | H            | 1847       | LEU         |
| 2          | H            | 1862       | VAL         |
| 2          | H            | 1886       | VAL         |
| 2          | H            | 1914       | LEU         |
| 2          | H            | 1936       | VAL         |
| 2          | H            | 1937       | GLU         |
| 2          | H            | 1982       | MET         |
| 2          | H            | 2003       | VAL         |
| 2          | H            | 2038       | ILE         |
| 2          | H            | 2042       | ILE         |
| 2          | H            | 2044       | ASN         |
| 2          | H            | 2047       | LYS         |
| 2          | H            | 2048       | TYR         |
| 2          | H            | 2050       | GLN         |
| 2          | I            | 6          | THR         |
| 2          | I            | 7          | ARG         |
| 2          | I            | 45         | THR         |
| 2          | I            | 46         | GLU         |
| 2          | I            | 48         | PHE         |
| 2          | I            | 56         | THR         |
| 2          | I            | 65         | LEU         |
| 2          | I            | 84         | LEU         |
| 2          | I            | 86         | LEU         |
| 2          | I            | 93         | ASN         |
| 2          | I            | 99         | ASN         |
| 2          | I            | 101        | ILE         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | I            | 109        | LEU         |
| 2          | I            | 117        | VAL         |
| 2          | I            | 122        | LEU         |
| 2          | I            | 149        | VAL         |
| 2          | I            | 153        | ASN         |
| 2          | I            | 155        | GLN         |
| 2          | I            | 159        | ILE         |
| 2          | I            | 173        | LEU         |
| 2          | I            | 175        | ASP         |
| 2          | I            | 176        | LEU         |
| 2          | I            | 178        | GLN         |
| 2          | I            | 182        | VAL         |
| 2          | I            | 210        | THR         |
| 2          | I            | 227        | ASP         |
| 2          | I            | 236        | ILE         |
| 2          | I            | 240        | LEU         |
| 2          | I            | 246        | LEU         |
| 2          | I            | 281        | VAL         |
| 2          | I            | 286        | THR         |
| 2          | I            | 295        | SER         |
| 2          | I            | 297        | ARG         |
| 2          | I            | 300        | ILE         |
| 2          | I            | 303        | LEU         |
| 2          | I            | 319        | LEU         |
| 2          | I            | 339        | LEU         |
| 2          | I            | 340        | SER         |
| 2          | I            | 342        | SER         |
| 2          | I            | 344        | LEU         |
| 2          | I            | 353        | VAL         |
| 2          | I            | 371        | VAL         |
| 2          | I            | 376        | ASN         |
| 2          | I            | 389        | LEU         |
| 2          | I            | 392        | THR         |
| 2          | I            | 402        | LEU         |
| 2          | I            | 418        | ASN         |
| 2          | I            | 425        | SER         |
| 2          | I            | 431        | LEU         |
| 2          | I            | 444        | VAL         |
| 2          | I            | 448        | VAL         |
| 2          | I            | 455        | ILE         |
| 2          | I            | 462        | THR         |
| 2          | I            | 463        | PHE         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | I            | 471        | LEU         |
| 2          | I            | 476        | SER         |
| 2          | I            | 478        | ARG         |
| 2          | I            | 479        | ILE         |
| 2          | I            | 482        | CYS         |
| 2          | I            | 492        | THR         |
| 2          | I            | 499        | THR         |
| 2          | I            | 539        | ASP         |
| 2          | I            | 545        | GLN         |
| 2          | I            | 553        | ASN         |
| 2          | I            | 562        | LEU         |
| 2          | I            | 572        | ASN         |
| 2          | I            | 574        | SER         |
| 2          | I            | 586        | LEU         |
| 2          | I            | 587        | ILE         |
| 2          | I            | 598        | THR         |
| 2          | I            | 607        | VAL         |
| 2          | I            | 611        | THR         |
| 2          | I            | 616        | THR         |
| 2          | I            | 653        | TYR         |
| 2          | I            | 665        | LEU         |
| 2          | I            | 669        | LEU         |
| 2          | I            | 670        | ARG         |
| 2          | I            | 676        | ILE         |
| 2          | I            | 680        | THR         |
| 2          | I            | 693        | GLU         |
| 2          | I            | 714        | SER         |
| 2          | I            | 719        | ILE         |
| 2          | I            | 723        | HIS         |
| 2          | I            | 730        | LEU         |
| 2          | I            | 733        | THR         |
| 2          | I            | 736        | ARG         |
| 2          | I            | 741        | HIS         |
| 2          | I            | 750        | MET         |
| 2          | I            | 751        | LEU         |
| 2          | I            | 762        | ASN         |
| 2          | I            | 767        | PHE         |
| 2          | I            | 775        | ASP         |
| 2          | I            | 777        | THR         |
| 2          | I            | 787        | THR         |
| 2          | I            | 794        | MET         |
| 2          | I            | 800        | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | I            | 810        | GLU         |
| 2          | I            | 825        | THR         |
| 2          | I            | 832        | TRP         |
| 2          | I            | 835        | THR         |
| 2          | I            | 844        | VAL         |
| 2          | I            | 846        | VAL         |
| 2          | I            | 852        | GLU         |
| 2          | I            | 855        | HIS         |
| 2          | I            | 857        | ILE         |
| 2          | I            | 865        | TRP         |
| 2          | I            | 869        | ASP         |
| 2          | I            | 880        | LEU         |
| 2          | I            | 881        | VAL         |
| 2          | I            | 892        | ILE         |
| 2          | I            | 907        | VAL         |
| 2          | I            | 929        | LEU         |
| 2          | I            | 945        | THR         |
| 2          | I            | 952        | ARG         |
| 2          | I            | 953        | ARG         |
| 2          | I            | 964        | LEU         |
| 2          | I            | 971        | SER         |
| 2          | I            | 993        | GLN         |
| 2          | I            | 1015       | VAL         |
| 2          | I            | 1021       | LEU         |
| 2          | I            | 1024       | ARG         |
| 2          | I            | 1048       | VAL         |
| 2          | I            | 1066       | ILE         |
| 2          | I            | 1070       | ILE         |
| 2          | I            | 1082       | ILE         |
| 2          | I            | 1109       | VAL         |
| 2          | I            | 1123       | ASP         |
| 2          | I            | 1124       | SER         |
| 2          | I            | 1145       | SER         |
| 2          | I            | 1148       | ASN         |
| 2          | I            | 1160       | THR         |
| 2          | I            | 1171       | ARG         |
| 2          | I            | 1189       | THR         |
| 2          | I            | 1197       | LEU         |
| 2          | I            | 1211       | LEU         |
| 2          | I            | 1219       | ILE         |
| 2          | I            | 1227       | ARG         |
| 2          | I            | 1260       | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | I            | 1265       | MET         |
| 2          | I            | 1284       | VAL         |
| 2          | I            | 1314       | ARG         |
| 2          | I            | 1318       | THR         |
| 2          | I            | 1328       | VAL         |
| 2          | I            | 1335       | ILE         |
| 2          | I            | 1348       | LEU         |
| 2          | I            | 1359       | MET         |
| 2          | I            | 1360       | ILE         |
| 2          | I            | 1378       | ILE         |
| 2          | I            | 1397       | SER         |
| 2          | I            | 1407       | THR         |
| 2          | I            | 1408       | SER         |
| 2          | I            | 1420       | GLU         |
| 2          | I            | 1421       | ASN         |
| 2          | I            | 1423       | PHE         |
| 2          | I            | 1434       | HIS         |
| 2          | I            | 1437       | THR         |
| 2          | I            | 1441       | ILE         |
| 2          | I            | 1443       | VAL         |
| 2          | I            | 1446       | SER         |
| 2          | I            | 1452       | LEU         |
| 2          | I            | 1463       | THR         |
| 2          | I            | 1468       | THR         |
| 2          | I            | 1470       | THR         |
| 2          | I            | 1472       | VAL         |
| 2          | I            | 1473       | THR         |
| 2          | I            | 1501       | ILE         |
| 2          | I            | 1511       | SER         |
| 2          | I            | 1527       | LEU         |
| 2          | I            | 1528       | GLU         |
| 2          | I            | 1533       | LEU         |
| 2          | I            | 1549       | THR         |
| 2          | I            | 1563       | ILE         |
| 2          | I            | 1567       | ARG         |
| 2          | I            | 1590       | ARG         |
| 2          | I            | 1602       | SER         |
| 2          | I            | 1605       | VAL         |
| 2          | I            | 1609       | THR         |
| 2          | I            | 1616       | VAL         |
| 2          | I            | 1624       | THR         |
| 2          | I            | 1627       | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | I            | 1632       | ILE         |
| 2          | I            | 1637       | LEU         |
| 2          | I            | 1651       | LEU         |
| 2          | I            | 1672       | GLN         |
| 2          | I            | 1678       | MET         |
| 2          | I            | 1680       | LEU         |
| 2          | I            | 1683       | THR         |
| 2          | I            | 1712       | ASN         |
| 2          | I            | 1718       | THR         |
| 2          | I            | 1757       | GLU         |
| 2          | I            | 1775       | GLN         |
| 2          | I            | 1781       | LEU         |
| 2          | I            | 1784       | MET         |
| 2          | I            | 1825       | GLU         |
| 2          | I            | 1831       | VAL         |
| 2          | I            | 1834       | ARG         |
| 2          | I            | 1844       | ARG         |
| 2          | I            | 1847       | LEU         |
| 2          | I            | 1862       | VAL         |
| 2          | I            | 1871       | LEU         |
| 2          | I            | 1886       | VAL         |
| 2          | I            | 1914       | LEU         |
| 2          | I            | 1936       | VAL         |
| 2          | I            | 1937       | GLU         |
| 2          | I            | 1982       | MET         |
| 2          | I            | 2003       | VAL         |
| 2          | I            | 2042       | ILE         |
| 2          | I            | 2044       | ASN         |
| 2          | I            | 2047       | LYS         |
| 2          | I            | 2048       | TYR         |
| 2          | I            | 2050       | GLN         |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (294) such sidechains are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 11         | HIS         |
| 1          | A            | 21         | GLN         |
| 1          | A            | 32         | GLN         |
| 1          | A            | 58         | GLN         |
| 1          | A            | 63         | ASN         |
| 1          | A            | 157        | HIS         |
| 1          | A            | 183        | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 214        | GLN         |
| 1          | A            | 271        | ASN         |
| 1          | A            | 335        | HIS         |
| 1          | A            | 341        | GLN         |
| 1          | A            | 344        | GLN         |
| 1          | A            | 374        | GLN         |
| 1          | A            | 411        | GLN         |
| 1          | A            | 427        | ASN         |
| 1          | A            | 438        | ASN         |
| 1          | A            | 506        | ASN         |
| 1          | A            | 527        | GLN         |
| 1          | A            | 618        | ASN         |
| 1          | A            | 694        | GLN         |
| 1          | A            | 738        | ASN         |
| 1          | A            | 758        | ASN         |
| 1          | A            | 792        | HIS         |
| 1          | A            | 860        | ASN         |
| 1          | A            | 898        | GLN         |
| 1          | A            | 983        | GLN         |
| 1          | A            | 987        | ASN         |
| 1          | A            | 989        | GLN         |
| 1          | A            | 1000       | GLN         |
| 1          | A            | 1003       | GLN         |
| 1          | A            | 1063       | HIS         |
| 1          | A            | 1064       | ASN         |
| 1          | A            | 1066       | ASN         |
| 1          | A            | 1146       | HIS         |
| 1          | A            | 1239       | HIS         |
| 1          | A            | 1385       | GLN         |
| 1          | A            | 1432       | HIS         |
| 1          | A            | 1433       | HIS         |
| 1          | A            | 1442       | ASN         |
| 1          | A            | 1458       | GLN         |
| 1          | A            | 1482       | GLN         |
| 1          | A            | 1494       | HIS         |
| 1          | A            | 1495       | ASN         |
| 1          | A            | 1505       | GLN         |
| 1          | A            | 1510       | ASN         |
| 1          | A            | 1542       | HIS         |
| 1          | A            | 1549       | ASN         |
| 1          | A            | 1563       | HIS         |
| 1          | A            | 1577       | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1610       | ASN         |
| 1          | A            | 1652       | GLN         |
| 1          | A            | 1690       | ASN         |
| 1          | A            | 1852       | HIS         |
| 1          | B            | 11         | HIS         |
| 1          | B            | 21         | GLN         |
| 1          | B            | 32         | GLN         |
| 1          | B            | 58         | GLN         |
| 1          | B            | 63         | ASN         |
| 1          | B            | 157        | HIS         |
| 1          | B            | 183        | GLN         |
| 1          | B            | 214        | GLN         |
| 1          | B            | 271        | ASN         |
| 1          | B            | 335        | HIS         |
| 1          | B            | 341        | GLN         |
| 1          | B            | 344        | GLN         |
| 1          | B            | 374        | GLN         |
| 1          | B            | 407        | ASN         |
| 1          | B            | 411        | GLN         |
| 1          | B            | 427        | ASN         |
| 1          | B            | 438        | ASN         |
| 1          | B            | 506        | ASN         |
| 1          | B            | 527        | GLN         |
| 1          | B            | 618        | ASN         |
| 1          | B            | 694        | GLN         |
| 1          | B            | 738        | ASN         |
| 1          | B            | 758        | ASN         |
| 1          | B            | 792        | HIS         |
| 1          | B            | 898        | GLN         |
| 1          | B            | 987        | ASN         |
| 1          | B            | 989        | GLN         |
| 1          | B            | 1000       | GLN         |
| 1          | B            | 1003       | GLN         |
| 1          | B            | 1063       | HIS         |
| 1          | B            | 1064       | ASN         |
| 1          | B            | 1066       | ASN         |
| 1          | B            | 1146       | HIS         |
| 1          | B            | 1239       | HIS         |
| 1          | B            | 1385       | GLN         |
| 1          | B            | 1432       | HIS         |
| 1          | B            | 1433       | HIS         |
| 1          | B            | 1442       | ASN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 1458       | GLN         |
| 1          | B            | 1482       | GLN         |
| 1          | B            | 1494       | HIS         |
| 1          | B            | 1495       | ASN         |
| 1          | B            | 1505       | GLN         |
| 1          | B            | 1510       | ASN         |
| 1          | B            | 1542       | HIS         |
| 1          | B            | 1549       | ASN         |
| 1          | B            | 1563       | HIS         |
| 1          | B            | 1577       | GLN         |
| 1          | B            | 1610       | ASN         |
| 1          | B            | 1652       | GLN         |
| 1          | B            | 1690       | ASN         |
| 1          | B            | 1794       | GLN         |
| 1          | B            | 1852       | HIS         |
| 1          | C            | 11         | HIS         |
| 1          | C            | 21         | GLN         |
| 1          | C            | 32         | GLN         |
| 1          | C            | 58         | GLN         |
| 1          | C            | 63         | ASN         |
| 1          | C            | 157        | HIS         |
| 1          | C            | 183        | GLN         |
| 1          | C            | 214        | GLN         |
| 1          | C            | 271        | ASN         |
| 1          | C            | 335        | HIS         |
| 1          | C            | 341        | GLN         |
| 1          | C            | 344        | GLN         |
| 1          | C            | 374        | GLN         |
| 1          | C            | 411        | GLN         |
| 1          | C            | 427        | ASN         |
| 1          | C            | 438        | ASN         |
| 1          | C            | 506        | ASN         |
| 1          | C            | 527        | GLN         |
| 1          | C            | 618        | ASN         |
| 1          | C            | 694        | GLN         |
| 1          | C            | 738        | ASN         |
| 1          | C            | 758        | ASN         |
| 1          | C            | 792        | HIS         |
| 1          | C            | 860        | ASN         |
| 1          | C            | 898        | GLN         |
| 1          | C            | 987        | ASN         |
| 1          | C            | 989        | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 1000       | GLN         |
| 1          | C            | 1003       | GLN         |
| 1          | C            | 1063       | HIS         |
| 1          | C            | 1064       | ASN         |
| 1          | C            | 1066       | ASN         |
| 1          | C            | 1146       | HIS         |
| 1          | C            | 1239       | HIS         |
| 1          | C            | 1385       | GLN         |
| 1          | C            | 1432       | HIS         |
| 1          | C            | 1433       | HIS         |
| 1          | C            | 1442       | ASN         |
| 1          | C            | 1458       | GLN         |
| 1          | C            | 1482       | GLN         |
| 1          | C            | 1495       | ASN         |
| 1          | C            | 1505       | GLN         |
| 1          | C            | 1510       | ASN         |
| 1          | C            | 1542       | HIS         |
| 1          | C            | 1549       | ASN         |
| 1          | C            | 1563       | HIS         |
| 1          | C            | 1577       | GLN         |
| 1          | C            | 1610       | ASN         |
| 1          | C            | 1652       | GLN         |
| 1          | C            | 1690       | ASN         |
| 1          | C            | 1852       | HIS         |
| 2          | G            | 34         | GLN         |
| 2          | G            | 36         | GLN         |
| 2          | G            | 85         | ASN         |
| 2          | G            | 102        | HIS         |
| 2          | G            | 178        | GLN         |
| 2          | G            | 359        | HIS         |
| 2          | G            | 376        | ASN         |
| 2          | G            | 418        | ASN         |
| 2          | G            | 428        | HIS         |
| 2          | G            | 440        | ASN         |
| 2          | G            | 447        | ASN         |
| 2          | G            | 500        | HIS         |
| 2          | G            | 517        | HIS         |
| 2          | G            | 545        | GLN         |
| 2          | G            | 558        | ASN         |
| 2          | G            | 572        | ASN         |
| 2          | G            | 612        | ASN         |
| 2          | G            | 650        | ASN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | G            | 718        | ASN         |
| 2          | G            | 740        | HIS         |
| 2          | G            | 741        | HIS         |
| 2          | G            | 747        | HIS         |
| 2          | G            | 752        | GLN         |
| 2          | G            | 762        | ASN         |
| 2          | G            | 855        | HIS         |
| 2          | G            | 900        | GLN         |
| 2          | G            | 910        | GLN         |
| 2          | G            | 1046       | GLN         |
| 2          | G            | 1148       | ASN         |
| 2          | G            | 1217       | ASN         |
| 2          | G            | 1220       | GLN         |
| 2          | G            | 1260       | GLN         |
| 2          | G            | 1341       | ASN         |
| 2          | G            | 1352       | HIS         |
| 2          | G            | 1355       | ASN         |
| 2          | G            | 1367       | GLN         |
| 2          | G            | 1384       | GLN         |
| 2          | G            | 1595       | ASN         |
| 2          | G            | 1659       | GLN         |
| 2          | G            | 1669       | GLN         |
| 2          | G            | 1672       | GLN         |
| 2          | G            | 1697       | HIS         |
| 2          | G            | 1890       | ASN         |
| 2          | G            | 1896       | GLN         |
| 2          | G            | 1977       | HIS         |
| 2          | G            | 2013       | ASN         |
| 2          | G            | 2020       | GLN         |
| 2          | H            | 34         | GLN         |
| 2          | H            | 85         | ASN         |
| 2          | H            | 102        | HIS         |
| 2          | H            | 178        | GLN         |
| 2          | H            | 359        | HIS         |
| 2          | H            | 376        | ASN         |
| 2          | H            | 418        | ASN         |
| 2          | H            | 428        | HIS         |
| 2          | H            | 440        | ASN         |
| 2          | H            | 447        | ASN         |
| 2          | H            | 500        | HIS         |
| 2          | H            | 517        | HIS         |
| 2          | H            | 545        | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 558        | ASN         |
| 2          | H            | 572        | ASN         |
| 2          | H            | 612        | ASN         |
| 2          | H            | 650        | ASN         |
| 2          | H            | 718        | ASN         |
| 2          | H            | 740        | HIS         |
| 2          | H            | 741        | HIS         |
| 2          | H            | 747        | HIS         |
| 2          | H            | 752        | GLN         |
| 2          | H            | 762        | ASN         |
| 2          | H            | 900        | GLN         |
| 2          | H            | 910        | GLN         |
| 2          | H            | 1039       | HIS         |
| 2          | H            | 1046       | GLN         |
| 2          | H            | 1148       | ASN         |
| 2          | H            | 1217       | ASN         |
| 2          | H            | 1220       | GLN         |
| 2          | H            | 1260       | GLN         |
| 2          | H            | 1341       | ASN         |
| 2          | H            | 1352       | HIS         |
| 2          | H            | 1355       | ASN         |
| 2          | H            | 1367       | GLN         |
| 2          | H            | 1669       | GLN         |
| 2          | H            | 1672       | GLN         |
| 2          | H            | 1697       | HIS         |
| 2          | H            | 1890       | ASN         |
| 2          | H            | 1896       | GLN         |
| 2          | H            | 1977       | HIS         |
| 2          | H            | 2013       | ASN         |
| 2          | H            | 2020       | GLN         |
| 2          | I            | 34         | GLN         |
| 2          | I            | 36         | GLN         |
| 2          | I            | 85         | ASN         |
| 2          | I            | 102        | HIS         |
| 2          | I            | 178        | GLN         |
| 2          | I            | 359        | HIS         |
| 2          | I            | 376        | ASN         |
| 2          | I            | 418        | ASN         |
| 2          | I            | 428        | HIS         |
| 2          | I            | 440        | ASN         |
| 2          | I            | 447        | ASN         |
| 2          | I            | 500        | HIS         |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 517  | HIS  |
| 2   | I     | 545  | GLN  |
| 2   | I     | 558  | ASN  |
| 2   | I     | 572  | ASN  |
| 2   | I     | 612  | ASN  |
| 2   | I     | 718  | ASN  |
| 2   | I     | 740  | HIS  |
| 2   | I     | 741  | HIS  |
| 2   | I     | 747  | HIS  |
| 2   | I     | 752  | GLN  |
| 2   | I     | 762  | ASN  |
| 2   | I     | 855  | HIS  |
| 2   | I     | 900  | GLN  |
| 2   | I     | 910  | GLN  |
| 2   | I     | 1046 | GLN  |
| 2   | I     | 1055 | HIS  |
| 2   | I     | 1148 | ASN  |
| 2   | I     | 1217 | ASN  |
| 2   | I     | 1220 | GLN  |
| 2   | I     | 1260 | GLN  |
| 2   | I     | 1341 | ASN  |
| 2   | I     | 1352 | HIS  |
| 2   | I     | 1355 | ASN  |
| 2   | I     | 1367 | GLN  |
| 2   | I     | 1421 | ASN  |
| 2   | I     | 1595 | ASN  |
| 2   | I     | 1669 | GLN  |
| 2   | I     | 1672 | GLN  |
| 2   | I     | 1697 | HIS  |
| 2   | I     | 1868 | GLN  |
| 2   | I     | 1890 | ASN  |
| 2   | I     | 1896 | GLN  |
| 2   | I     | 1977 | HIS  |
| 2   | I     | 2013 | ASN  |
| 2   | I     | 2020 | GLN  |

### 5.3.3 RNA ⓘ

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 monosaccharides 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   | CER  | A     | 2748 | -    | 10,11,15     | 4.19 | 3 (30%)  | 9,13,17     | 3.18 | 3 (33%)  |
| 3   | CER  | B     | 2748 | -    | 10,11,15     | 4.19 | 3 (30%)  | 9,13,17     | 3.05 | 3 (33%)  |
| 4   | FMN  | I     | 3051 | -    | 33,33,33     | 6.32 | 24 (72%) | 48,50,50    | 1.30 | 7 (14%)  |
| 4   | FMN  | H     | 3051 | -    | 33,33,33     | 6.23 | 21 (63%) | 48,50,50    | 1.31 | 8 (16%)  |
| 3   | CER  | C     | 2748 | -    | 10,11,15     | 4.21 | 3 (30%)  | 9,13,17     | 3.18 | 3 (33%)  |
| 4   | FMN  | G     | 3051 | -    | 33,33,33     | 6.32 | 21 (63%) | 48,50,50    | 1.30 | 5 (10%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | CER  | A     | 2748 | -    | -       | 5/12/12/16 | -       |
| 3   | CER  | B     | 2748 | -    | -       | 5/12/12/16 | -       |
| 4   | FMN  | I     | 3051 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 4   | FMN  | H     | 3051 | -    | -       | 5/18/18/18 | 0/3/3/3 |
| 3   | CER  | C     | 2748 | -    | -       | 5/12/12/16 | -       |
| 4   | FMN  | G     | 3051 | -    | -       | 5/18/18/18 | 0/3/3/3 |

All (75) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | G     | 3051 | FMN  | C6-C7   | 12.51 | 1.57        | 1.39     |
| 4   | G     | 3051 | FMN  | C9-C9A  | 12.29 | 1.59        | 1.39     |
| 4   | I     | 3051 | FMN  | C6-C7   | 12.18 | 1.57        | 1.39     |
| 4   | I     | 3051 | FMN  | C6-C5A  | 12.15 | 1.59        | 1.40     |
| 4   | H     | 3051 | FMN  | C9-C9A  | 12.15 | 1.59        | 1.39     |
| 4   | I     | 3051 | FMN  | C9-C9A  | 12.09 | 1.59        | 1.39     |
| 4   | H     | 3051 | FMN  | C6-C7   | 11.89 | 1.57        | 1.39     |
| 4   | G     | 3051 | FMN  | C6-C5A  | 11.87 | 1.58        | 1.40     |
| 3   | C     | 2748 | CER  | O1-C4   | 11.69 | 1.41        | 1.21     |
| 4   | H     | 3051 | FMN  | C6-C5A  | 11.67 | 1.58        | 1.40     |
| 3   | A     | 2748 | CER  | O1-C4   | 11.67 | 1.41        | 1.21     |
| 3   | B     | 2748 | CER  | O1-C4   | 11.63 | 1.41        | 1.21     |
| 4   | I     | 3051 | FMN  | C9-C8   | 11.52 | 1.56        | 1.39     |
| 4   | G     | 3051 | FMN  | C9-C8   | 11.11 | 1.55        | 1.39     |
| 4   | H     | 3051 | FMN  | C9-C8   | 10.93 | 1.55        | 1.39     |
| 4   | G     | 3051 | FMN  | C4A-N5  | 10.64 | 1.51        | 1.30     |
| 4   | I     | 3051 | FMN  | C4A-N5  | 10.32 | 1.50        | 1.30     |
| 4   | H     | 3051 | FMN  | C4A-N5  | 10.28 | 1.50        | 1.30     |
| 4   | G     | 3051 | FMN  | O4-C4   | 9.99  | 1.42        | 1.23     |
| 4   | H     | 3051 | FMN  | O4-C4   | 9.87  | 1.42        | 1.23     |
| 4   | I     | 3051 | FMN  | O4-C4   | 9.68  | 1.42        | 1.23     |
| 4   | H     | 3051 | FMN  | O2-C2   | 9.21  | 1.41        | 1.24     |
| 4   | I     | 3051 | FMN  | O2-C2   | 9.13  | 1.41        | 1.24     |
| 4   | G     | 3051 | FMN  | O2-C2   | 8.88  | 1.40        | 1.24     |
| 4   | I     | 3051 | FMN  | C9A-C5A | 8.71  | 1.55        | 1.41     |
| 4   | G     | 3051 | FMN  | C9A-C5A | 8.37  | 1.55        | 1.41     |
| 4   | H     | 3051 | FMN  | C9A-C5A | 8.05  | 1.54        | 1.41     |
| 4   | I     | 3051 | FMN  | C8-C7   | 7.29  | 1.59        | 1.40     |
| 4   | G     | 3051 | FMN  | C10-N1  | 7.19  | 1.48        | 1.33     |
| 4   | H     | 3051 | FMN  | C10-N1  | 7.11  | 1.47        | 1.33     |
| 4   | G     | 3051 | FMN  | C2-N1   | 7.00  | 1.53        | 1.36     |
| 4   | G     | 3051 | FMN  | C8-C7   | 6.89  | 1.58        | 1.40     |
| 4   | H     | 3051 | FMN  | C2-N1   | 6.85  | 1.53        | 1.36     |
| 4   | I     | 3051 | FMN  | C10-N1  | 6.81  | 1.47        | 1.33     |
| 4   | I     | 3051 | FMN  | C2-N1   | 6.80  | 1.52        | 1.36     |
| 4   | H     | 3051 | FMN  | C8-C7   | 6.72  | 1.57        | 1.40     |
| 4   | I     | 3051 | FMN  | C10-N10 | 6.57  | 1.51        | 1.37     |
| 4   | H     | 3051 | FMN  | C10-N10 | 6.56  | 1.51        | 1.37     |
| 4   | G     | 3051 | FMN  | C10-N10 | 6.50  | 1.51        | 1.37     |
| 4   | H     | 3051 | FMN  | C4-N3   | 6.46  | 1.50        | 1.38     |
| 4   | I     | 3051 | FMN  | C5A-N5  | 6.32  | 1.51        | 1.39     |
| 4   | G     | 3051 | FMN  | C5A-N5  | 6.19  | 1.51        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | H     | 3051 | FMN  | C2-N3   | 6.18 | 1.53        | 1.39     |
| 4   | G     | 3051 | FMN  | C4-N3   | 6.12 | 1.50        | 1.38     |
| 4   | I     | 3051 | FMN  | C4-N3   | 6.10 | 1.50        | 1.38     |
| 4   | H     | 3051 | FMN  | C5A-N5  | 6.06 | 1.51        | 1.39     |
| 4   | G     | 3051 | FMN  | C2-N3   | 5.82 | 1.52        | 1.39     |
| 4   | I     | 3051 | FMN  | C2-N3   | 5.68 | 1.52        | 1.39     |
| 4   | G     | 3051 | FMN  | C9A-N10 | 5.17 | 1.50        | 1.41     |
| 4   | H     | 3051 | FMN  | C9A-N10 | 4.90 | 1.49        | 1.41     |
| 4   | I     | 3051 | FMN  | C9A-N10 | 4.86 | 1.49        | 1.41     |
| 3   | C     | 2748 | CER  | C1-N1   | 4.46 | 1.47        | 1.32     |
| 3   | B     | 2748 | CER  | C1-N1   | 4.44 | 1.47        | 1.32     |
| 3   | A     | 2748 | CER  | C1-N1   | 4.39 | 1.47        | 1.32     |
| 4   | G     | 3051 | FMN  | C4A-C10 | 3.62 | 1.54        | 1.44     |
| 3   | B     | 2748 | CER  | C5-C4   | 3.49 | 1.56        | 1.51     |
| 3   | C     | 2748 | CER  | C5-C4   | 3.47 | 1.55        | 1.51     |
| 3   | A     | 2748 | CER  | C5-C4   | 3.38 | 1.55        | 1.51     |
| 4   | H     | 3051 | FMN  | C4A-C10 | 3.31 | 1.53        | 1.44     |
| 4   | H     | 3051 | FMN  | C1'-C2' | 3.21 | 1.57        | 1.52     |
| 4   | I     | 3051 | FMN  | C4A-C10 | 3.21 | 1.53        | 1.44     |
| 4   | I     | 3051 | FMN  | C1'-C2' | 3.07 | 1.57        | 1.52     |
| 4   | I     | 3051 | FMN  | P-O2P   | 3.04 | 1.66        | 1.54     |
| 4   | G     | 3051 | FMN  | C1'-C2' | 2.98 | 1.56        | 1.52     |
| 4   | H     | 3051 | FMN  | P-O2P   | 2.92 | 1.66        | 1.54     |
| 4   | G     | 3051 | FMN  | P-O2P   | 2.89 | 1.66        | 1.54     |
| 4   | I     | 3051 | FMN  | P-O3P   | 2.84 | 1.65        | 1.54     |
| 4   | H     | 3051 | FMN  | P-O3P   | 2.81 | 1.65        | 1.54     |
| 4   | G     | 3051 | FMN  | P-O3P   | 2.60 | 1.64        | 1.54     |
| 4   | G     | 3051 | FMN  | C4A-C4  | 2.47 | 1.53        | 1.44     |
| 4   | H     | 3051 | FMN  | C4A-C4  | 2.35 | 1.53        | 1.44     |
| 4   | I     | 3051 | FMN  | C8M-C8  | 2.26 | 1.55        | 1.51     |
| 4   | I     | 3051 | FMN  | C4A-C4  | 2.24 | 1.52        | 1.44     |
| 4   | I     | 3051 | FMN  | C7M-C7  | 2.10 | 1.55        | 1.51     |
| 4   | I     | 3051 | FMN  | C5'-C4' | 2.04 | 1.54        | 1.51     |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | C     | 2748 | CER  | O1-C4-C5 | -7.72 | 107.97      | 121.70   |
| 3   | A     | 2748 | CER  | O1-C4-C5 | -7.67 | 108.06      | 121.70   |
| 3   | B     | 2748 | CER  | O1-C4-C5 | -7.34 | 108.64      | 121.70   |
| 3   | A     | 2748 | CER  | C5-C4-C3 | -3.86 | 110.87      | 117.94   |
| 3   | B     | 2748 | CER  | C5-C4-C3 | -3.77 | 111.03      | 117.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | C     | 2748 | CER  | C5-C4-C3    | -3.76 | 111.05      | 117.94   |
| 3   | A     | 2748 | CER  | C6-C5-C4    | -3.35 | 108.47      | 113.88   |
| 3   | C     | 2748 | CER  | C6-C5-C4    | -3.30 | 108.56      | 113.88   |
| 4   | I     | 3051 | FMN  | C4A-C10-N10 | 3.08  | 120.99      | 116.48   |
| 4   | G     | 3051 | FMN  | C4A-C10-N10 | 3.08  | 120.98      | 116.48   |
| 4   | H     | 3051 | FMN  | C4A-C10-N10 | 3.05  | 120.94      | 116.48   |
| 3   | B     | 2748 | CER  | C6-C5-C4    | -3.05 | 108.95      | 113.88   |
| 4   | I     | 3051 | FMN  | C4'-C3'-C2' | -2.76 | 107.62      | 113.36   |
| 4   | G     | 3051 | FMN  | C10-C4A-N5  | -2.72 | 119.08      | 124.86   |
| 4   | H     | 3051 | FMN  | C4'-C3'-C2' | -2.72 | 107.71      | 113.36   |
| 4   | G     | 3051 | FMN  | C4'-C3'-C2' | -2.70 | 107.74      | 113.36   |
| 4   | H     | 3051 | FMN  | C10-C4A-N5  | -2.67 | 119.20      | 124.86   |
| 4   | I     | 3051 | FMN  | C4-N3-C2    | -2.48 | 121.05      | 125.64   |
| 4   | I     | 3051 | FMN  | C10-C4A-N5  | -2.48 | 119.59      | 124.86   |
| 4   | G     | 3051 | FMN  | C4-N3-C2    | -2.33 | 121.33      | 125.64   |
| 4   | H     | 3051 | FMN  | O2-C2-N1    | -2.29 | 118.04      | 121.83   |
| 4   | H     | 3051 | FMN  | C4-N3-C2    | -2.27 | 121.44      | 125.64   |
| 4   | I     | 3051 | FMN  | O4-C4-C4A   | -2.22 | 120.72      | 126.60   |
| 4   | I     | 3051 | FMN  | O2-C2-N1    | -2.11 | 118.33      | 121.83   |
| 4   | I     | 3051 | FMN  | C4A-C4-N3   | 2.06  | 118.41      | 113.19   |
| 4   | H     | 3051 | FMN  | C4-C4A-C10  | 2.05  | 120.24      | 116.79   |
| 4   | H     | 3051 | FMN  | O5'-C5'-C4' | -2.03 | 103.94      | 109.36   |
| 4   | G     | 3051 | FMN  | O2-C2-N1    | -2.03 | 118.46      | 121.83   |
| 4   | H     | 3051 | FMN  | O4-C4-C4A   | -2.02 | 121.24      | 126.60   |

There are no chirality outliers.

All (30) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 2748 | CER  | C2-C3-C4-O1     |
| 3   | B     | 2748 | CER  | C2-C3-C4-O1     |
| 3   | C     | 2748 | CER  | C2-C3-C4-O1     |
| 4   | G     | 3051 | FMN  | C2'-C3'-C4'-C5' |
| 4   | G     | 3051 | FMN  | O3'-C3'-C4'-C5' |
| 4   | H     | 3051 | FMN  | C2'-C3'-C4'-C5' |
| 4   | H     | 3051 | FMN  | O3'-C3'-C4'-C5' |
| 4   | I     | 3051 | FMN  | C2'-C3'-C4'-C5' |
| 4   | I     | 3051 | FMN  | O3'-C3'-C4'-C5' |
| 4   | H     | 3051 | FMN  | O3'-C3'-C4'-O4' |
| 4   | I     | 3051 | FMN  | O3'-C3'-C4'-O4' |
| 4   | I     | 3051 | FMN  | C2'-C3'-C4'-O4' |
| 4   | H     | 3051 | FMN  | C2'-C3'-C4'-O4' |

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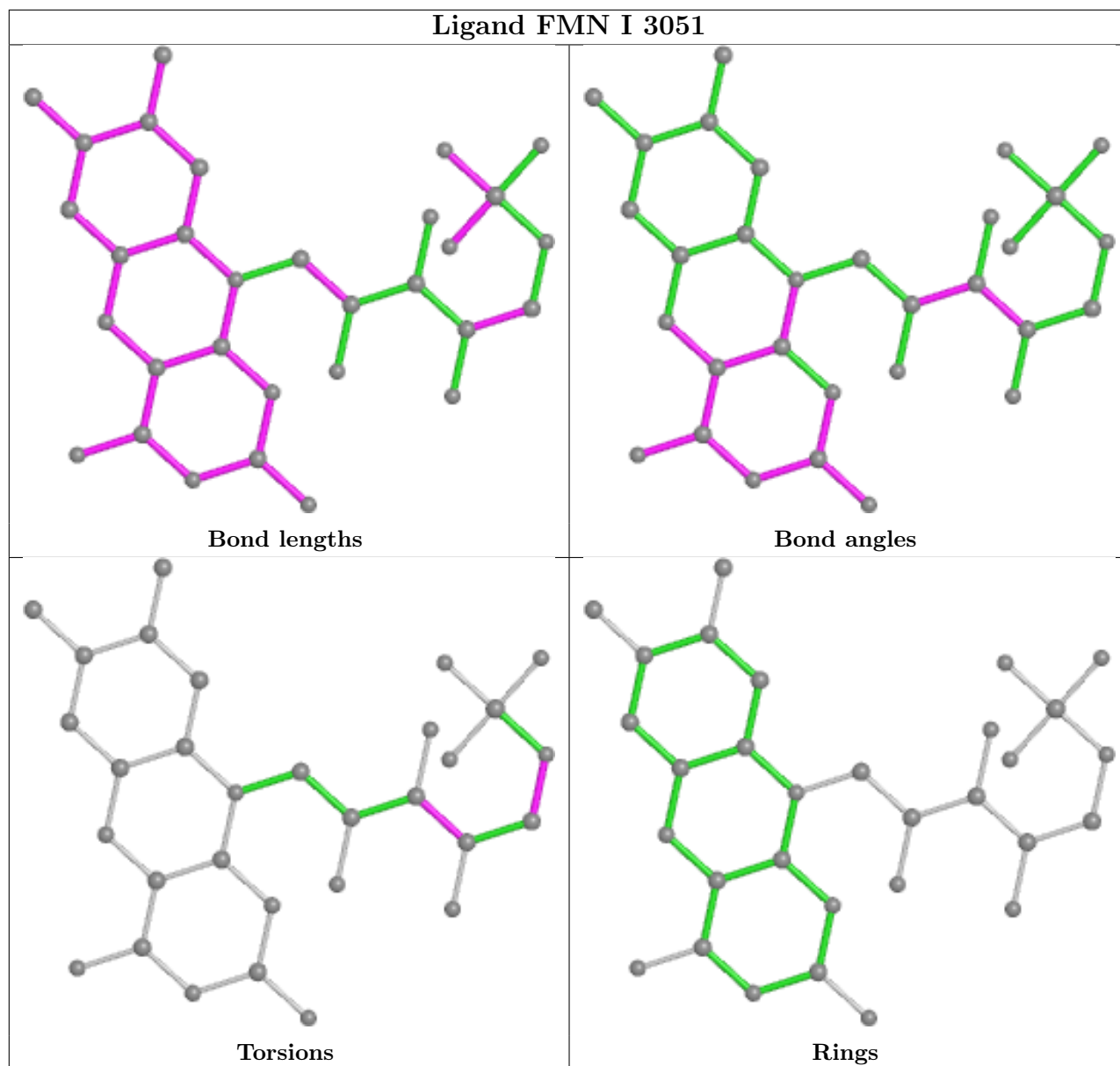
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 2748 | CER  | O2-C1-C2-C3     |
| 3   | B     | 2748 | CER  | O2-C1-C2-C3     |
| 3   | C     | 2748 | CER  | O2-C1-C2-C3     |
| 4   | G     | 3051 | FMN  | C2'-C3'-C4'-O4' |
| 4   | G     | 3051 | FMN  | O3'-C3'-C4'-O4' |
| 3   | A     | 2748 | CER  | N1-C1-C2-C3     |
| 3   | B     | 2748 | CER  | N1-C1-C2-C3     |
| 3   | C     | 2748 | CER  | N1-C1-C2-C3     |
| 3   | C     | 2748 | CER  | C5-C6-C7-C8     |
| 3   | A     | 2748 | CER  | O3-C3-C4-O1     |
| 3   | B     | 2748 | CER  | O3-C3-C4-O1     |
| 3   | C     | 2748 | CER  | O3-C3-C4-O1     |
| 3   | A     | 2748 | CER  | C5-C6-C7-C8     |
| 3   | B     | 2748 | CER  | C5-C6-C7-C8     |
| 4   | G     | 3051 | FMN  | C4'-C5'-O5'-P   |
| 4   | H     | 3051 | FMN  | C4'-C5'-O5'-P   |
| 4   | I     | 3051 | FMN  | C4'-C5'-O5'-P   |

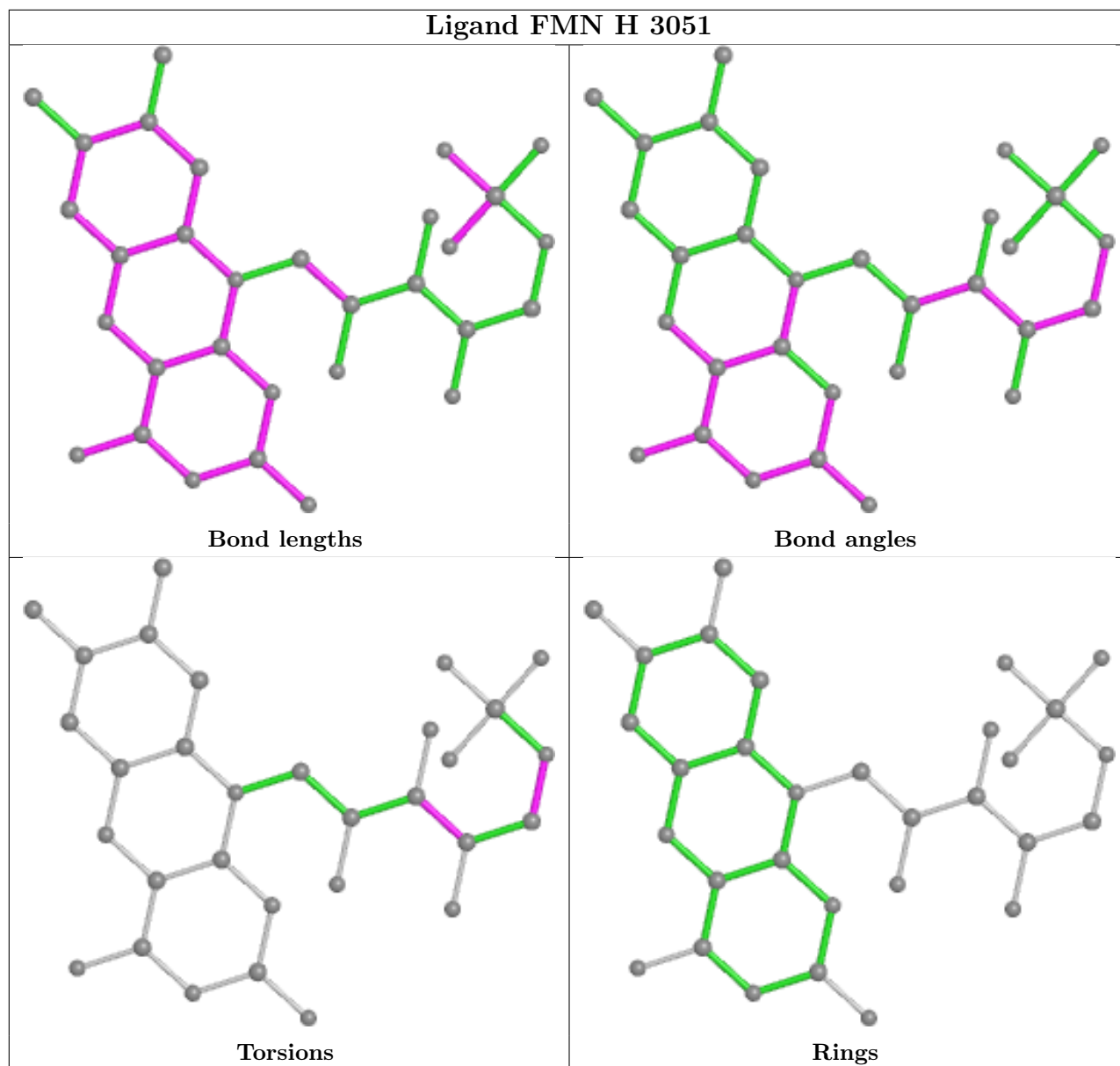
There are no ring outliers.

6 monomers are involved in 32 short contacts:

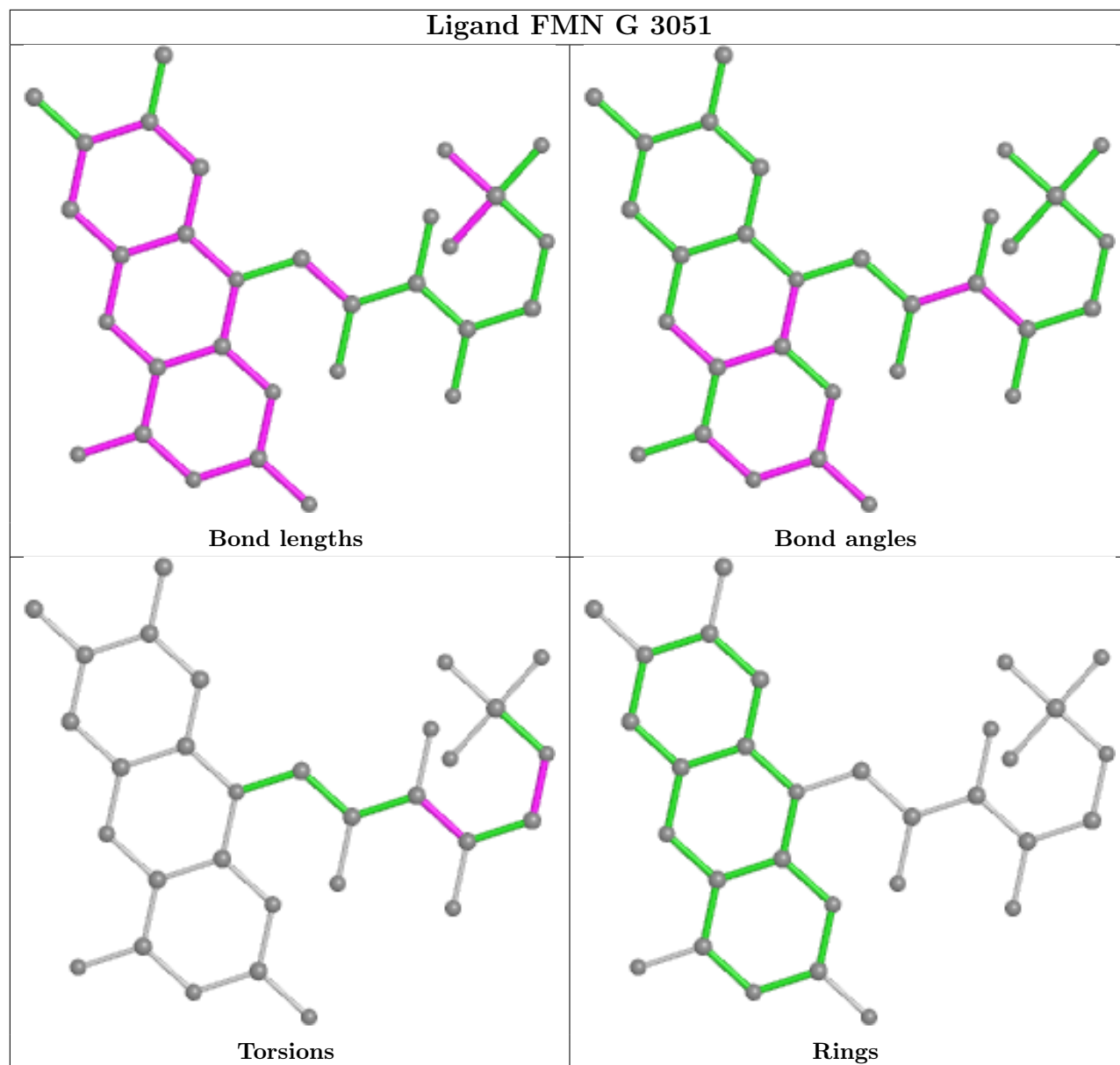
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 2748 | CER  | 3       | 0            |
| 3   | B     | 2748 | CER  | 4       | 0            |
| 4   | I     | 3051 | FMN  | 8       | 0            |
| 4   | H     | 3051 | FMN  | 6       | 0            |
| 3   | C     | 2748 | CER  | 4       | 0            |
| 4   | G     | 3051 | FMN  | 7       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 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     | 1750/1887 (92%)   | -0.30  | 46 (2%) 56 46  | 95, 134, 347, 457     | 0     |
| 1   | B     | 1750/1887 (92%)   | -0.34  | 32 (1%) 68 59  | 96, 132, 302, 419     | 0     |
| 1   | C     | 1750/1887 (92%)   | -0.26  | 62 (3%) 44 35  | 98, 135, 423, 568     | 0     |
| 2   | G     | 2033/2051 (99%)   | -0.45  | 1 (0%) 100 100 | 131, 169, 218, 267    | 0     |
| 2   | H     | 2033/2051 (99%)   | -0.36  | 10 (0%) 91 85  | 130, 170, 215, 265    | 0     |
| 2   | I     | 2033/2051 (99%)   | -0.43  | 6 (0%) 94 90   | 131, 171, 215, 261    | 0     |
| All | All   | 11349/11814 (96%) | -0.36  | 157 (1%) 75 65 | 95, 162, 239, 568     | 0     |

All (157) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 1882 | ALA  | 10.4 |
| 1   | C     | 1831 | GLY  | 9.1  |
| 1   | A     | 1829 | GLY  | 8.0  |
| 1   | C     | 1830 | GLY  | 7.7  |
| 1   | C     | 1870 | SER  | 7.6  |
| 1   | C     | 1850 | GLU  | 7.3  |
| 1   | C     | 1884 | SER  | 7.3  |
| 1   | C     | 1838 | GLU  | 7.2  |
| 1   | C     | 1832 | ALA  | 6.8  |
| 1   | C     | 1883 | VAL  | 6.1  |
| 1   | A     | 1827 | SER  | 5.7  |
| 1   | A     | 1763 | LYS  | 5.3  |
| 1   | A     | 1882 | ALA  | 5.2  |
| 1   | C     | 1872 | SER  | 5.2  |
| 1   | C     | 875  | THR  | 5.1  |
| 1   | C     | 1869 | VAL  | 5.0  |
| 1   | C     | 1794 | GLN  | 4.8  |
| 1   | A     | 1881 | VAL  | 4.8  |
| 1   | B     | 875  | THR  | 4.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1830 | GLY  | 4.5  |
| 1   | C     | 1797 | GLU  | 4.5  |
| 1   | B     | 539  | SER  | 4.5  |
| 1   | C     | 1766 | ASN  | 4.4  |
| 1   | C     | 1833 | ALA  | 4.4  |
| 1   | C     | 1857 | LYS  | 4.3  |
| 1   | A     | 974  | ASP  | 4.2  |
| 1   | C     | 1803 | PRO  | 4.2  |
| 1   | A     | 539  | SER  | 4.2  |
| 1   | C     | 1874 | ASP  | 4.1  |
| 1   | B     | 141  | ALA  | 4.1  |
| 1   | A     | 875  | THR  | 4.0  |
| 1   | C     | 1804 | SER  | 4.0  |
| 1   | C     | 1873 | HIS  | 4.0  |
| 1   | A     | 1762 | GLU  | 3.9  |
| 1   | C     | 1868 | LYS  | 3.9  |
| 1   | A     | 975  | ALA  | 3.9  |
| 1   | A     | 1843 | ASN  | 3.8  |
| 1   | A     | 1875 | ASP  | 3.8  |
| 1   | C     | 1880 | ALA  | 3.8  |
| 1   | B     | 1833 | ALA  | 3.7  |
| 2   | G     | 1956 | ARG  | 3.7  |
| 1   | B     | 599  | MET  | 3.6  |
| 2   | H     | 1929 | LYS  | 3.6  |
| 1   | A     | 1853 | GLY  | 3.6  |
| 1   | B     | 1762 | GLU  | 3.6  |
| 1   | C     | 540  | GLN  | 3.5  |
| 1   | A     | 208  | GLU  | 3.5  |
| 1   | B     | 1830 | GLY  | 3.5  |
| 1   | A     | 1880 | ALA  | 3.5  |
| 1   | C     | 1837 | ILE  | 3.5  |
| 1   | C     | 1783 | ASN  | 3.5  |
| 1   | B     | 140  | ILE  | 3.5  |
| 1   | A     | 1866 | ASP  | 3.4  |
| 1   | C     | 200  | LYS  | 3.4  |
| 1   | C     | 1842 | VAL  | 3.4  |
| 1   | B     | 1854 | ASN  | 3.4  |
| 1   | A     | 1826 | LYS  | 3.4  |
| 1   | A     | 1850 | GLU  | 3.4  |
| 1   | B     | 1874 | ASP  | 3.4  |
| 2   | H     | 1953 | VAL  | 3.3  |
| 1   | C     | 1765 | SER  | 3.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 1793       | PRO         | 3.3         |
| 2          | I            | 1928       | GLN         | 3.3         |
| 2          | H            | 1671       | SER         | 3.3         |
| 1          | A            | 1770       | GLY         | 3.3         |
| 1          | B            | 540        | GLN         | 3.2         |
| 1          | A            | 1870       | SER         | 3.2         |
| 1          | B            | 976        | ALA         | 3.1         |
| 1          | A            | 1831       | GLY         | 3.1         |
| 2          | H            | 1959       | LYS         | 3.0         |
| 1          | B            | 1875       | ASP         | 3.0         |
| 1          | B            | 1837       | ILE         | 3.0         |
| 1          | C            | 1816       | LYS         | 3.0         |
| 1          | A            | 1884       | SER         | 3.0         |
| 1          | B            | 1868       | LYS         | 2.9         |
| 1          | A            | 1873       | HIS         | 2.9         |
| 1          | C            | 1875       | ASP         | 2.9         |
| 2          | H            | 1964       | PHE         | 2.9         |
| 1          | C            | 1793       | PRO         | 2.9         |
| 1          | B            | 1829       | GLY         | 2.9         |
| 1          | C            | 141        | ALA         | 2.9         |
| 1          | C            | 1843       | ASN         | 2.9         |
| 1          | A            | 540        | GLN         | 2.8         |
| 1          | A            | 1883       | VAL         | 2.8         |
| 1          | C            | 1771       | VAL         | 2.8         |
| 1          | B            | 1836       | ASP         | 2.8         |
| 1          | B            | 1883       | VAL         | 2.8         |
| 1          | B            | 219        | GLY         | 2.8         |
| 1          | C            | 204        | THR         | 2.7         |
| 1          | B            | 1802       | GLN         | 2.7         |
| 1          | B            | 1850       | GLU         | 2.7         |
| 1          | B            | 1826       | LYS         | 2.7         |
| 2          | H            | 1956       | ARG         | 2.7         |
| 1          | B            | 1784       | ASP         | 2.6         |
| 1          | C            | 202        | GLU         | 2.6         |
| 1          | C            | 1820       | PHE         | 2.6         |
| 1          | C            | 1841       | ARG         | 2.6         |
| 2          | I            | 401        | GLY         | 2.6         |
| 1          | B            | 1804       | SER         | 2.6         |
| 1          | A            | 1476       | GLU         | 2.6         |
| 1          | B            | 600        | ASP         | 2.6         |
| 1          | C            | 1770       | GLY         | 2.6         |
| 1          | A            | 1780       | ASN         | 2.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | C            | 215        | ASP         | 2.6         |
| 1          | A            | 1860       | GLU         | 2.5         |
| 1          | C            | 1840       | VAL         | 2.5         |
| 1          | C            | 539        | SER         | 2.5         |
| 1          | C            | 164        | ASP         | 2.4         |
| 1          | C            | 1768       | GLY         | 2.4         |
| 1          | C            | 1800       | SER         | 2.4         |
| 2          | I            | 43         | GLU         | 2.4         |
| 1          | A            | 1748       | ASN         | 2.4         |
| 1          | A            | 1868       | LYS         | 2.4         |
| 1          | C            | 1829       | GLY         | 2.4         |
| 1          | C            | 1812       | THR         | 2.4         |
| 1          | B            | 195        | GLY         | 2.4         |
| 1          | C            | 1789       | ARG         | 2.3         |
| 1          | C            | 203        | GLU         | 2.3         |
| 1          | C            | 301        | ASP         | 2.3         |
| 1          | A            | 1792       | THR         | 2.3         |
| 1          | C            | 223        | LYS         | 2.3         |
| 2          | H            | 2033       | THR         | 2.3         |
| 1          | C            | 1828       | LEU         | 2.3         |
| 2          | H            | 1853       | GLY         | 2.3         |
| 2          | I            | 1880       | LYS         | 2.3         |
| 1          | C            | 1822       | SER         | 2.3         |
| 1          | A            | 1842       | VAL         | 2.2         |
| 1          | A            | 1844       | LYS         | 2.2         |
| 1          | A            | 1885       | THR         | 2.2         |
| 1          | C            | 1845       | ASN         | 2.2         |
| 1          | A            | 1874       | ASP         | 2.2         |
| 1          | B            | 1801       | ALA         | 2.2         |
| 1          | A            | 1838       | GLU         | 2.2         |
| 1          | A            | 1872       | SER         | 2.2         |
| 1          | B            | 1831       | GLY         | 2.2         |
| 1          | A            | 293        | LYS         | 2.2         |
| 1          | C            | 1867       | VAL         | 2.2         |
| 1          | A            | 1782       | GLU         | 2.2         |
| 1          | A            | 1828       | LEU         | 2.2         |
| 1          | B            | 1803       | PRO         | 2.2         |
| 1          | A            | 1836       | ASP         | 2.2         |
| 1          | C            | 1805       | VAL         | 2.2         |
| 2          | I            | 75         | SER         | 2.2         |
| 1          | C            | 1782       | GLU         | 2.2         |
| 1          | C            | 971        | ASN         | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 973  | ALA  | 2.1  |
| 1   | A     | 981  | GLU  | 2.1  |
| 1   | C     | 1811 | GLY  | 2.1  |
| 2   | I     | 74   | PRO  | 2.1  |
| 1   | B     | 1886 | LYS  | 2.1  |
| 2   | H     | 1739 | GLU  | 2.1  |
| 1   | B     | 1812 | THR  | 2.0  |
| 1   | C     | 1772 | ASP  | 2.0  |
| 1   | B     | 1810 | ALA  | 2.0  |
| 1   | A     | 199  | GLU  | 2.0  |
| 2   | H     | 1740 | THR  | 2.0  |
| 1   | C     | 1802 | GLN  | 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

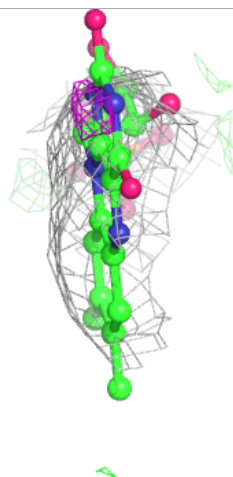
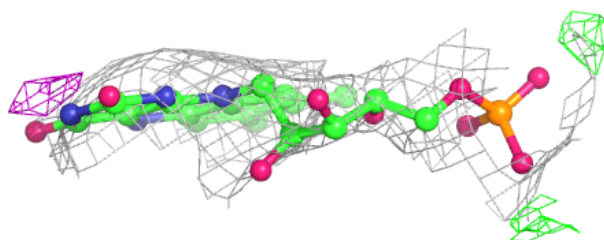
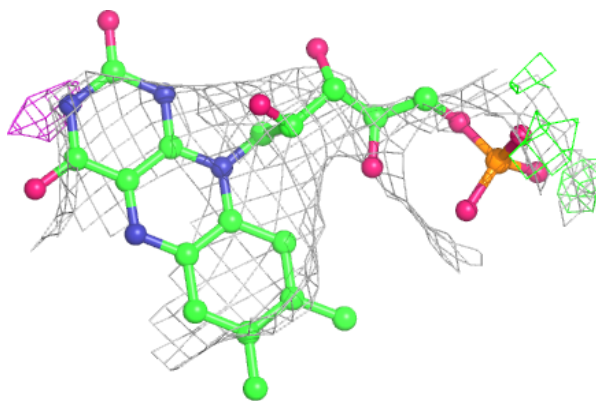
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 4   | FMN  | H     | 3051 | 31/31 | 0.80 | 0.32 | 131,157,181,186            | 0     |
| 4   | FMN  | G     | 3051 | 31/31 | 0.82 | 0.27 | 135,158,184,203            | 0     |
| 4   | FMN  | I     | 3051 | 31/31 | 0.82 | 0.26 | 129,161,178,201            | 0     |
| 3   | CER  | A     | 2748 | 12/16 | 0.84 | 0.30 | 67,131,240,249             | 0     |
| 3   | CER  | C     | 2748 | 12/16 | 0.90 | 0.34 | 67,131,249,250             | 0     |
| 3   | CER  | B     | 2748 | 12/16 | 0.91 | 0.20 | 67,131,249,250             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

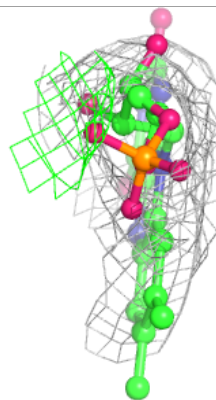
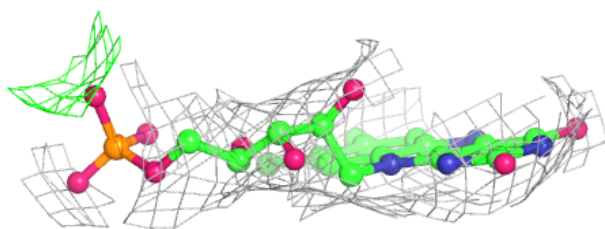
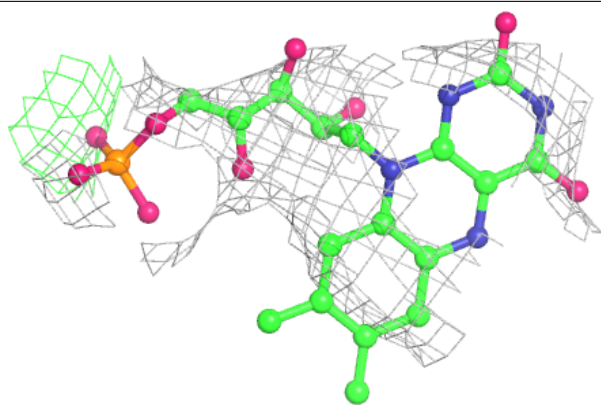
**Electron density around FMN H 3051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

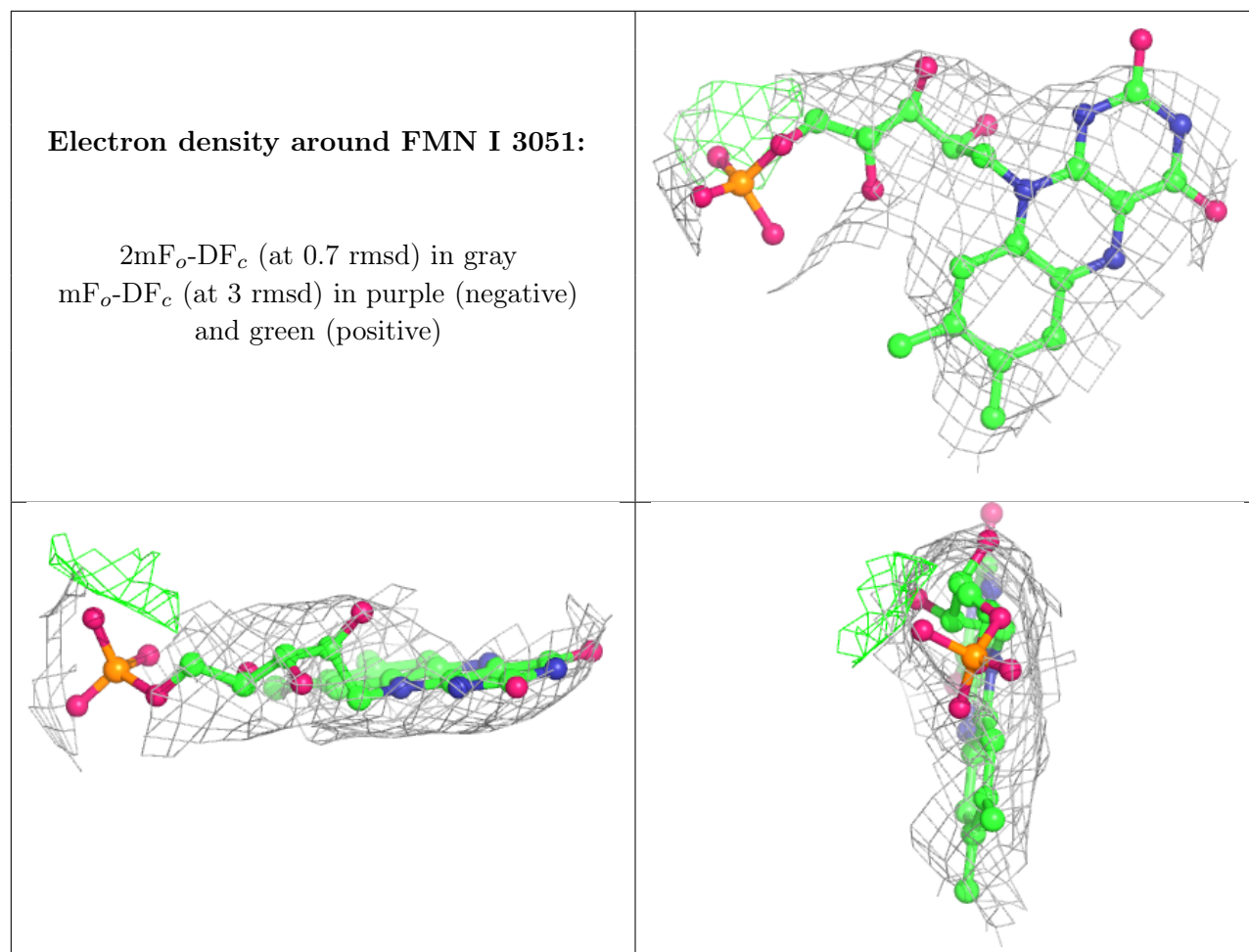


**Electron density around FMN G 3051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.