



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 11, 2018 – 05:17 pm GMT

PDB ID : 4UX2
Title : Cryo-EM structure of antagonist-bound E2P gastric H,K-ATPase (SCH.E2. MgF)
Authors : Abe, K.; Tani, K.; Fujiyoshi, Y.
Deposited on : 2014-08-18
Resolution : 7.00 Å(reported)

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

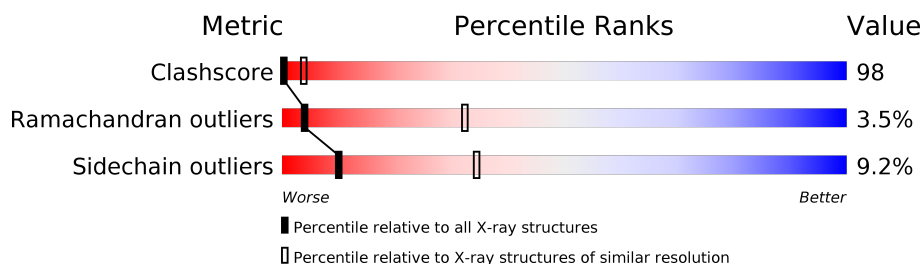
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 7.00 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 122126 | 1146 (10.00-3.80) |
| Ramachandran outliers | 120053 | 1071 (10.00-3.80) |
| Sidechain outliers | 120020 | 1038 (10.00-3.80) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1034 | |
| 2 | B | 290 | |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9161 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 POTASSIUM-TRANSPORTING ATPASE ALPHA CHAIN 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 993 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7718 | 4927 | 1304 | 1434 | 53 | | | |

- Molecule 2 is a protein called POTASSIUM-TRANSPORTING ATPASE SUBUNIT BETA.

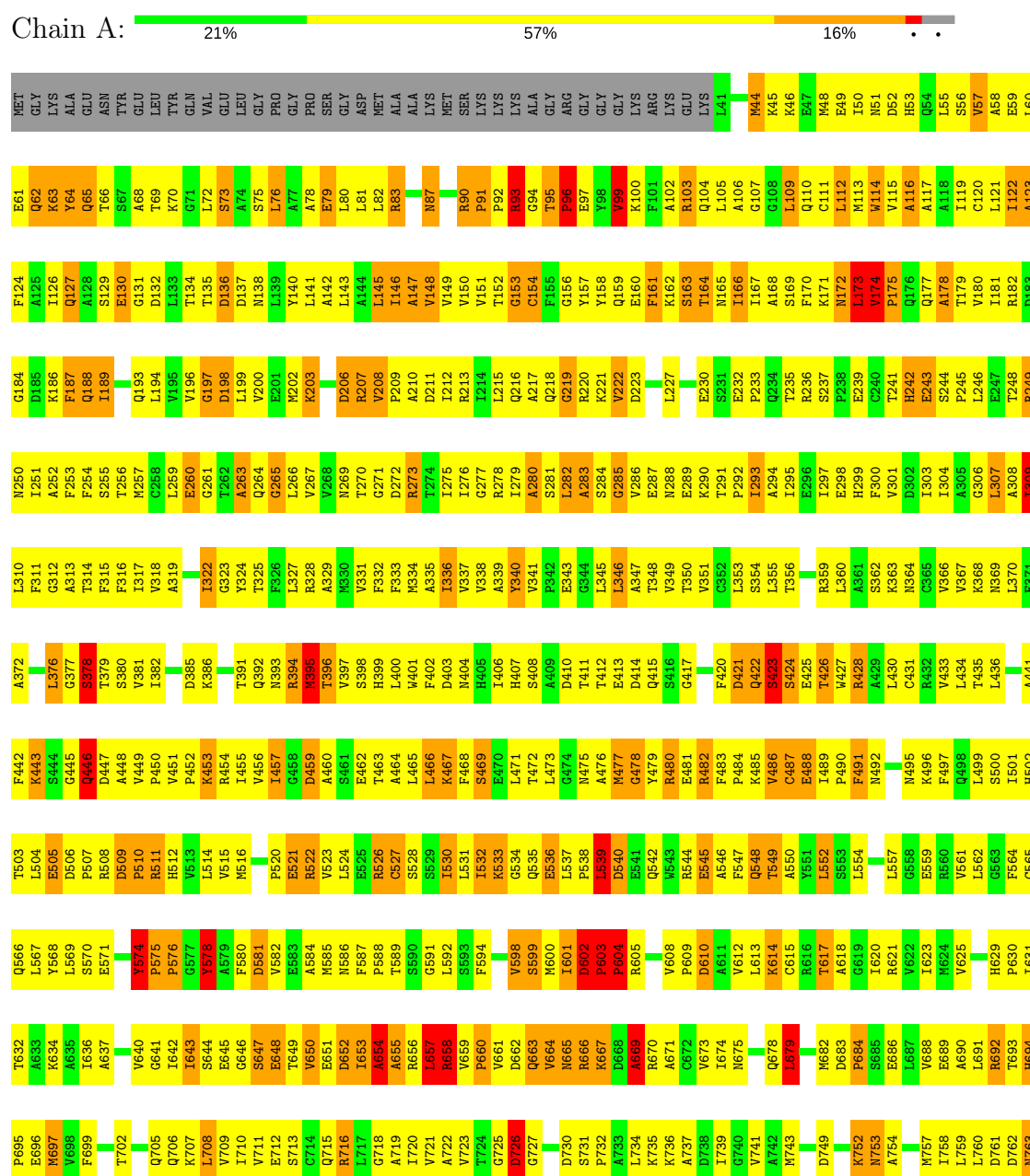
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 175 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1443 | 949 | 237 | 249 | 8 | | | |

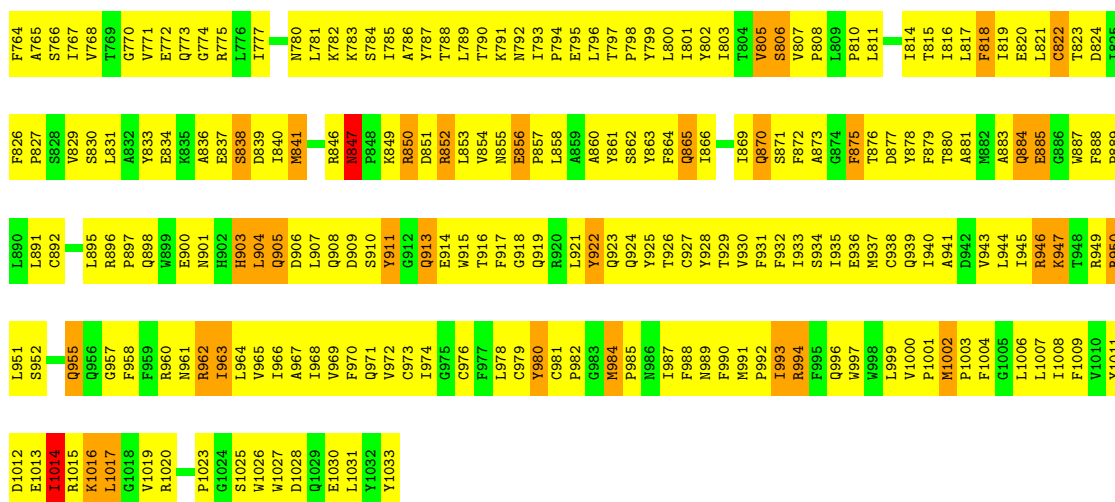
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

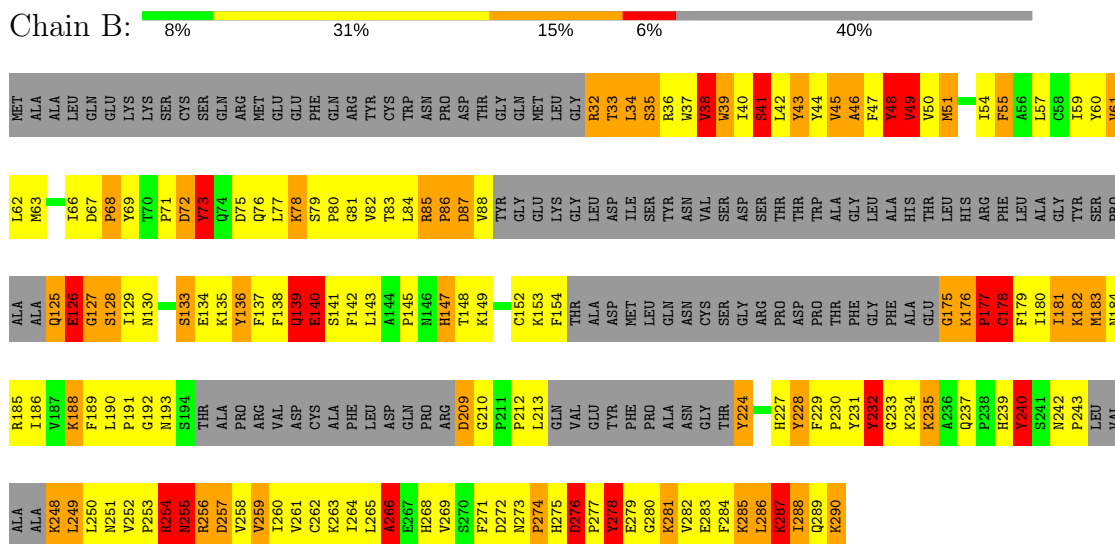
Note EDS was not executed.

• Molecule 1: POTASSIUM-TRANSPORTING ATPASE ALPHA CHAIN 1





- Molecule 2: POTASSIUM-TRANSPORTING ATPASE SUBUNIT BETA



4 Model quality

4.1 Standard geometry

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 | 1.15 | 3/7876 (0.0%) | 1.39 | 37/10694 (0.3%) |
| 2 | B | 1.13 | 1/1486 (0.1%) | 1.42 | 11/2008 (0.5%) |
| All | All | 1.14 | 4/9362 (0.0%) | 1.40 | 48/12702 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 160 |
| 2 | B | 0 | 52 |
| All | All | 0 | 212 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | B | 254 | ARG | CZ-NH2 | 5.23 | 1.39 | 1.33 |
| 1 | A | 950 | ARG | CZ-NH1 | 5.07 | 1.39 | 1.33 |
| 1 | A | 511 | ARG | NE-CZ | 5.06 | 1.39 | 1.33 |
| 1 | A | 273 | ARG | NE-CZ | 5.03 | 1.39 | 1.33 |

All (48) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 140 | TYR | CB-CG-CD1 | 10.11 | 127.07 | 121.00 |
| 2 | B | 68 | PRO | CA-N-CD | -9.05 | 98.84 | 111.50 |
| 1 | A | 960 | ARG | NE-CZ-NH1 | 7.32 | 123.96 | 120.30 |
| 1 | A | 950 | ARG | NE-CZ-NH2 | 7.29 | 123.95 | 120.30 |
| 1 | A | 692 | ARG | NE-CZ-NH1 | -7.25 | 116.67 | 120.30 |
| 1 | A | 64 | TYR | CA-CB-CG | -7.24 | 99.64 | 113.40 |
| 1 | A | 522 | ARG | NE-CZ-NH1 | -7.24 | 116.68 | 120.30 |
| 1 | A | 716 | ARG | NE-CZ-NH1 | -7.14 | 116.73 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 278 | TYR | CB-CG-CD1 | -6.78 | 116.93 | 121.00 |
| 1 | A | 726 | ASP | CB-CA-C | -6.67 | 97.06 | 110.40 |
| 1 | A | 51 | ASN | C-N-CA | 6.48 | 137.90 | 121.70 |
| 1 | A | 574 | TYR | CA-CB-CG | -6.41 | 101.22 | 113.40 |
| 1 | A | 946 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 1 | A | 658 | ARG | NE-CZ-NH1 | 6.15 | 123.37 | 120.30 |
| 1 | A | 340 | TYR | CA-CB-CG | -6.04 | 101.91 | 113.40 |
| 1 | A | 852 | ARG | NE-CZ-NH1 | 5.89 | 123.25 | 120.30 |
| 2 | B | 136 | TYR | CB-CG-CD1 | 5.85 | 124.51 | 121.00 |
| 1 | A | 95 | THR | C-N-CD | -5.83 | 107.78 | 120.60 |
| 1 | A | 875 | PHE | CB-CG-CD2 | -5.78 | 116.75 | 120.80 |
| 1 | A | 207 | ARG | NE-CZ-NH1 | -5.76 | 117.42 | 120.30 |
| 1 | A | 669 | ALA | N-CA-CB | 5.67 | 118.03 | 110.10 |
| 1 | A | 140 | TYR | CB-CG-CD2 | -5.63 | 117.62 | 121.00 |
| 2 | B | 73 | TYR | O-C-N | -5.60 | 113.74 | 122.70 |
| 1 | A | 522 | ARG | CD-NE-CZ | -5.59 | 115.78 | 123.60 |
| 1 | A | 850 | ARG | NE-CZ-NH1 | -5.58 | 117.51 | 120.30 |
| 1 | A | 428 | ARG | NE-CZ-NH1 | -5.56 | 117.52 | 120.30 |
| 2 | B | 140 | GLU | N-CA-CB | 5.55 | 120.59 | 110.60 |
| 1 | A | 818 | PHE | CA-CB-CG | -5.52 | 100.64 | 113.90 |
| 1 | A | 222 | VAL | CB-CA-C | -5.50 | 100.96 | 111.40 |
| 2 | B | 232 | TYR | CA-CB-CG | -5.49 | 102.97 | 113.40 |
| 1 | A | 957 | GLY | N-CA-C | -5.41 | 99.56 | 113.10 |
| 1 | A | 692 | ARG | CD-NE-CZ | -5.35 | 116.10 | 123.60 |
| 1 | A | 207 | ARG | CD-NE-CZ | -5.34 | 116.12 | 123.60 |
| 1 | A | 114 | TRP | CB-CG-CD1 | 5.31 | 133.90 | 127.00 |
| 1 | A | 249 | ARG | CD-NE-CZ | -5.29 | 116.19 | 123.60 |
| 1 | A | 114 | TRP | CG-CD2-CE3 | -5.28 | 129.15 | 133.90 |
| 2 | B | 256 | ARG | NE-CZ-NH1 | -5.25 | 117.67 | 120.30 |
| 1 | A | 850 | ARG | CD-NE-CZ | -5.21 | 116.30 | 123.60 |
| 2 | B | 48 | TYR | CB-CG-CD1 | -5.16 | 117.91 | 121.00 |
| 1 | A | 911 | TYR | CA-CB-CG | -5.12 | 103.67 | 113.40 |
| 1 | A | 206 | ASP | CB-CA-C | -5.12 | 100.16 | 110.40 |
| 2 | B | 133 | SER | N-CA-CB | 5.12 | 118.17 | 110.50 |
| 2 | B | 274 | PRO | N-CA-CB | 5.10 | 109.42 | 103.30 |
| 1 | A | 198 | ASP | CB-CA-C | -5.06 | 100.29 | 110.40 |
| 1 | A | 852 | ARG | NE-CZ-NH2 | -5.05 | 117.77 | 120.30 |
| 1 | A | 905 | GLN | C-N-CA | 5.05 | 134.32 | 121.70 |
| 1 | A | 962 | ARG | NE-CZ-NH2 | -5.03 | 117.78 | 120.30 |
| 2 | B | 249 | LEU | C-N-CA | 5.02 | 134.25 | 121.70 |

There are no chirality outliers.

All (212) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-------------------|
| 1 | A | 1002 | MET | Mainchain |
| 1 | A | 1014 | ILE | Mainchain |
| 1 | A | 1016 | LYS | Mainchain |
| 1 | A | 1017 | LEU | Mainchain |
| 1 | A | 102 | ALA | Mainchain |
| 1 | A | 1023 | PRO | Mainchain |
| 1 | A | 1025 | SER | Mainchain |
| 1 | A | 103 | ARG | Mainchain |
| 1 | A | 111 | CYS | Mainchain |
| 1 | A | 112 | LEU | Mainchain |
| 1 | A | 116 | ALA | Mainchain |
| 1 | A | 123 | ALA | Mainchain |
| 1 | A | 127 | GLN | Mainchain |
| 1 | A | 130 | GLU | Mainchain |
| 1 | A | 131 | GLY | Mainchain |
| 1 | A | 136 | ASP | Mainchain |
| 1 | A | 145 | LEU | Mainchain |
| 1 | A | 147 | ALA | Mainchain |
| 1 | A | 148 | VAL | Mainchain |
| 1 | A | 153 | GLY | Mainchain |
| 1 | A | 154 | CYS | Mainchain |
| 1 | A | 156 | GLY | Mainchain |
| 1 | A | 173 | LEU | Peptide |
| 1 | A | 174 | VAL | Mainchain,Peptide |
| 1 | A | 177 | GLN | Mainchain |
| 1 | A | 178 | ALA | Mainchain |
| 1 | A | 187 | PHE | Mainchain |
| 1 | A | 188 | GLN | Mainchain |
| 1 | A | 189 | ILE | Mainchain |
| 1 | A | 197 | GLY | Mainchain |
| 1 | A | 203 | LYS | Mainchain |
| 1 | A | 206 | ASP | Mainchain |
| 1 | A | 217 | ALA | Mainchain |
| 1 | A | 218 | GLN | Mainchain |
| 1 | A | 219 | GLY | Mainchain |
| 1 | A | 242 | HIS | Mainchain |
| 1 | A | 243 | GLU | Mainchain |
| 1 | A | 260 | GLU | Mainchain |
| 1 | A | 263 | ALA | Mainchain |
| 1 | A | 265 | GLY | Mainchain |
| 1 | A | 278 | ARG | Mainchain |
| 1 | A | 279 | ILE | Mainchain |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 280 | ALA | Mainchain |
| 1 | A | 282 | LEU | Mainchain |
| 1 | A | 287 | GLU | Mainchain |
| 1 | A | 288 | ASN | Mainchain |
| 1 | A | 289 | GLU | Mainchain |
| 1 | A | 290 | LYS | Mainchain |
| 1 | A | 299 | HIS | Mainchain |
| 1 | A | 306 | GLY | Mainchain |
| 1 | A | 309 | ILE | Mainchain |
| 1 | A | 317 | ILE | Mainchain |
| 1 | A | 322 | ILE | Mainchain |
| 1 | A | 323 | GLY | Mainchain |
| 1 | A | 336 | ILE | Mainchain |
| 1 | A | 394 | ARG | Mainchain |
| 1 | A | 395 | MET | Mainchain |
| 1 | A | 396 | THR | Mainchain |
| 1 | A | 417 | GLY | Mainchain |
| 1 | A | 422 | GLN | Mainchain |
| 1 | A | 423 | SER | Mainchain |
| 1 | A | 426 | THR | Mainchain |
| 1 | A | 44 | MET | Mainchain |
| 1 | A | 445 | GLY | Mainchain,Peptide |
| 1 | A | 446 | GLN | Mainchain |
| 1 | A | 457 | ILE | Mainchain |
| 1 | A | 459 | ASP | Mainchain |
| 1 | A | 469 | SER | Mainchain |
| 1 | A | 477 | MET | Mainchain |
| 1 | A | 482 | ARG | Mainchain |
| 1 | A | 486 | VAL | Mainchain |
| 1 | A | 487 | CYS | Mainchain |
| 1 | A | 488 | GLU | Mainchain |
| 1 | A | 491 | PHE | Mainchain |
| 1 | A | 505 | GLU | Mainchain |
| 1 | A | 508 | ARG | Mainchain |
| 1 | A | 509 | ASP | Mainchain,Peptide |
| 1 | A | 521 | GLU | Mainchain |
| 1 | A | 526 | ARG | Mainchain |
| 1 | A | 527 | CYS | Mainchain |
| 1 | A | 530 | ILE | Mainchain |
| 1 | A | 536 | GLU | Mainchain |
| 1 | A | 539 | LEU | Mainchain |
| 1 | A | 540 | ASP | Mainchain |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 545 | GLU | Mainchain |
| 1 | A | 548 | GLN | Mainchain |
| 1 | A | 549 | THR | Mainchain |
| 1 | A | 566 | GLN | Mainchain |
| 1 | A | 571 | GLU | Mainchain |
| 1 | A | 574 | TYR | Mainchain |
| 1 | A | 575 | PRO | Mainchain |
| 1 | A | 576 | PRO | Mainchain |
| 1 | A | 578 | TYR | Mainchain |
| 1 | A | 581 | ASP | Mainchain |
| 1 | A | 585 | MET | Mainchain |
| 1 | A | 586 | ASN | Mainchain |
| 1 | A | 589 | THR | Mainchain |
| 1 | A | 598 | VAL | Mainchain |
| 1 | A | 602 | ASP | Mainchain |
| 1 | A | 603 | PRO | Mainchain |
| 1 | A | 604 | PRO | Mainchain |
| 1 | A | 610 | ASP | Mainchain |
| 1 | A | 614 | LYS | Mainchain |
| 1 | A | 62 | GLN | Mainchain |
| 1 | A | 63 | LYS | Mainchain |
| 1 | A | 641 | GLY | Mainchain |
| 1 | A | 643 | ILE | Mainchain |
| 1 | A | 644 | SER | Mainchain |
| 1 | A | 645 | GLU | Mainchain |
| 1 | A | 646 | GLY | Mainchain |
| 1 | A | 647 | SER | Mainchain |
| 1 | A | 648 | GLU | Mainchain |
| 1 | A | 652 | ASP | Mainchain |
| 1 | A | 653 | ILE | Peptide |
| 1 | A | 654 | ALA | Mainchain,Peptide |
| 1 | A | 655 | ALA | Mainchain |
| 1 | A | 656 | ARG | Mainchain |
| 1 | A | 657 | LEU | Mainchain |
| 1 | A | 658 | ARG | Mainchain |
| 1 | A | 660 | PRO | Mainchain |
| 1 | A | 663 | GLN | Mainchain |
| 1 | A | 664 | VAL | Mainchain |
| 1 | A | 666 | ARG | Mainchain |
| 1 | A | 669 | ALA | Mainchain |
| 1 | A | 679 | LEU | Mainchain |
| 1 | A | 684 | PRO | Mainchain |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 694 | HIS | Mainchain |
| 1 | A | 715 | GLN | Mainchain |
| 1 | A | 718 | GLY | Mainchain |
| 1 | A | 73 | SER | Mainchain |
| 1 | A | 75 | SER | Mainchain |
| 1 | A | 752 | LYS | Mainchain |
| 1 | A | 753 | ASN | Mainchain |
| 1 | A | 76 | LEU | Mainchain |
| 1 | A | 79 | GLU | Mainchain |
| 1 | A | 806 | SER | Mainchain |
| 1 | A | 82 | LEU | Mainchain |
| 1 | A | 822 | CYS | Mainchain |
| 1 | A | 83 | ARG | Mainchain |
| 1 | A | 838 | SER | Mainchain |
| 1 | A | 839 | ASP | Mainchain |
| 1 | A | 847 | ASN | Mainchain |
| 1 | A | 852 | ARG | Mainchain |
| 1 | A | 865 | GLN | Mainchain |
| 1 | A | 870 | GLN | Mainchain |
| 1 | A | 90 | ARG | Sidechain |
| 1 | A | 909 | ASP | Mainchain |
| 1 | A | 944 | LEU | Mainchain |
| 1 | A | 947 | LYS | Mainchain |
| 1 | A | 949 | ARG | Mainchain |
| 1 | A | 952 | SER | Mainchain |
| 1 | A | 955 | GLN | Mainchain |
| 1 | A | 96 | PRO | Mainchain |
| 1 | A | 980 | TYR | Mainchain |
| 1 | A | 99 | VAL | Mainchain |
| 1 | A | 994 | ARG | Mainchain |
| 2 | B | 125 | GLN | Mainchain,Peptide |
| 2 | B | 126 | GLU | Mainchain,Peptide |
| 2 | B | 127 | GLY | Mainchain |
| 2 | B | 128 | SER | Mainchain |
| 2 | B | 133 | SER | Mainchain |
| 2 | B | 138 | PHE | Mainchain |
| 2 | B | 139 | GLN | Mainchain |
| 2 | B | 147 | HIS | Mainchain |
| 2 | B | 175 | GLY | Mainchain |
| 2 | B | 176 | LYS | Mainchain |
| 2 | B | 177 | PRO | Mainchain |
| 2 | B | 178 | CYS | Mainchain |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 2 | B | 181 | ILE | Mainchain |
| 2 | B | 183 | MET | Mainchain |
| 2 | B | 191 | PRO | Mainchain |
| 2 | B | 209 | ASP | Mainchain |
| 2 | B | 210 | GLY | Mainchain,Peptide |
| 2 | B | 212 | PRO | Mainchain |
| 2 | B | 224 | TYR | Mainchain |
| 2 | B | 228 | TYR | Mainchain |
| 2 | B | 232 | TYR | Mainchain |
| 2 | B | 239 | HIS | Mainchain |
| 2 | B | 240 | TYR | Sidechain |
| 2 | B | 248 | LYS | Mainchain |
| 2 | B | 250 | LEU | Mainchain |
| 2 | B | 254 | ARG | Mainchain |
| 2 | B | 255 | ASN | Mainchain |
| 2 | B | 256 | ARG | Mainchain |
| 2 | B | 257 | ASP | Mainchain |
| 2 | B | 258 | VAL | Mainchain |
| 2 | B | 259 | VAL | Mainchain |
| 2 | B | 266 | ALA | Mainchain |
| 2 | B | 278 | TYR | Mainchain |
| 2 | B | 285 | LYS | Mainchain |
| 2 | B | 286 | LEU | Mainchain |
| 2 | B | 287 | LYS | Mainchain |
| 2 | B | 34 | LEU | Mainchain |
| 2 | B | 35 | SER | Mainchain,Peptide |
| 2 | B | 38 | VAL | Mainchain |
| 2 | B | 39 | TRP | Mainchain |
| 2 | B | 41 | SER | Mainchain |
| 2 | B | 46 | ALA | Mainchain |
| 2 | B | 51 | MET | Mainchain |
| 2 | B | 55 | PHE | Mainchain |
| 2 | B | 59 | ILE | Mainchain |
| 2 | B | 62 | LEU | Mainchain |
| 2 | B | 63 | MET | Mainchain |
| 2 | B | 73 | TYR | Mainchain |

4.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 7718 | 0 | 7746 | 1572 | 0 |
| 2 | B | 1443 | 0 | 1430 | 358 | 0 |
| All | All | 9161 | 0 | 9176 | 1793 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 98.

All (1793) 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:901:ASN:HB3 | 1:A:904:LEU:CD1 | 1.26 | 1.65 |
| 1:A:398:SER:CB | 1:A:600:MET:CA | 1.78 | 1.56 |
| 1:A:994:ARG:NH1 | 2:B:73:TYR:CG | 1.70 | 1.55 |
| 1:A:913:GLN:NE2 | 2:B:77:LEU:HD22 | 1.25 | 1.48 |
| 1:A:398:SER:HB2 | 1:A:600:MET:CA | 0.96 | 1.42 |
| 1:A:398:SER:HB2 | 1:A:600:MET:C | 1.41 | 1.38 |
| 1:A:901:ASN:CB | 1:A:904:LEU:HD11 | 1.54 | 1.37 |
| 1:A:398:SER:CB | 1:A:600:MET:N | 1.89 | 1.34 |
| 1:A:398:SER:HB3 | 1:A:600:MET:N | 1.41 | 1.33 |
| 1:A:286:VAL:HB | 1:A:735:LYS:CE | 1.58 | 1.32 |
| 1:A:1011:TYR:CE1 | 2:B:47:PHE:HE1 | 1.48 | 1.32 |
| 1:A:923:GLN:CG | 2:B:76:GLN:HG2 | 1.59 | 1.32 |
| 1:A:65:GLN:NE2 | 1:A:65:GLN:N | 1.78 | 1.30 |
| 1:A:398:SER:CB | 1:A:600:MET:HA | 1.43 | 1.30 |
| 1:A:548:GLN:O | 1:A:552:LEU:HD23 | 1.27 | 1.28 |
| 1:A:913:GLN:HB3 | 2:B:185:ARG:O | 1.17 | 1.28 |
| 1:A:775:ARG:HD2 | 1:A:840:ILE:CG2 | 1.63 | 1.28 |
| 1:A:651:GLU:O | 1:A:654:ALA:HB3 | 1.22 | 1.28 |
| 1:A:775:ARG:NH1 | 1:A:840:ILE:O | 1.66 | 1.26 |
| 1:A:398:SER:HB3 | 1:A:599:SER:C | 1.53 | 1.25 |
| 1:A:906:ASP:OD1 | 2:B:83:THR:HB | 1.07 | 1.23 |
| 1:A:548:GLN:O | 1:A:552:LEU:CD2 | 1.85 | 1.23 |
| 1:A:906:ASP:OD1 | 2:B:83:THR:CB | 1.88 | 1.22 |
| 2:B:240:TYR:CD1 | 2:B:240:TYR:O | 1.92 | 1.21 |
| 1:A:1011:TYR:CE1 | 2:B:47:PHE:CE1 | 2.27 | 1.21 |
| 1:A:207:ARG:HG2 | 1:A:257:MET:HG3 | 1.23 | 1.20 |
| 1:A:363:LYS:HE3 | 1:A:773:GLN:NE2 | 1.56 | 1.20 |
| 1:A:994:ARG:NH1 | 2:B:73:TYR:CD2 | 2.10 | 1.20 |
| 1:A:45:LYS:NZ | 1:A:281:SER:HB2 | 1.56 | 1.20 |
| 1:A:169:SER:HB3 | 1:A:753:ASN:ND2 | 1.57 | 1.19 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:399:HIS:C | 1:A:400:LEU:HD12 | 1.64 | 1.18 |
| 1:A:207:ARG:HG2 | 1:A:257:MET:CG | 1.74 | 1.17 |
| 1:A:394:ARG:NH1 | 1:A:452:PRO:HB2 | 1.57 | 1.17 |
| 1:A:72:LEU:HD13 | 1:A:198:ASP:HA | 1.17 | 1.16 |
| 1:A:913:GLN:NE2 | 2:B:77:LEU:CD2 | 2.09 | 1.16 |
| 1:A:286:VAL:HB | 1:A:735:LYS:HE2 | 1.25 | 1.16 |
| 1:A:169:SER:CB | 1:A:753:ASN:ND2 | 2.09 | 1.16 |
| 1:A:901:ASN:CB | 1:A:904:LEU:CD1 | 2.16 | 1.15 |
| 1:A:170:PHE:O | 1:A:173:LEU:CD1 | 1.95 | 1.15 |
| 1:A:905:GLN:CG | 2:B:278:TYR:HD2 | 1.59 | 1.14 |
| 1:A:119:ILE:HG23 | 1:A:334:MET:CE | 1.77 | 1.14 |
| 1:A:559:GLU:HG2 | 1:A:600:MET:O | 1.45 | 1.14 |
| 1:A:905:GLN:CG | 2:B:83:THR:HG22 | 1.77 | 1.13 |
| 1:A:166:ILE:HD12 | 1:A:753:ASN:HB2 | 1.30 | 1.13 |
| 1:A:163:SER:OG | 1:A:368:LYS:HD3 | 1.48 | 1.13 |
| 1:A:884:GLN:HG2 | 2:B:73:TYR:CD2 | 1.85 | 1.12 |
| 1:A:170:PHE:O | 1:A:173:LEU:HD11 | 1.46 | 1.11 |
| 1:A:775:ARG:HD2 | 1:A:840:ILE:HG22 | 1.16 | 1.11 |
| 1:A:169:SER:OG | 1:A:749:ASP:HB3 | 1.47 | 1.11 |
| 1:A:396:THR:HG22 | 1:A:397:VAL:N | 1.61 | 1.11 |
| 1:A:46:LYS:NZ | 1:A:712:GLU:OE2 | 1.83 | 1.11 |
| 1:A:922:TYR:CE2 | 1:A:991:MET:SD | 2.44 | 1.11 |
| 1:A:552:LEU:HD23 | 1:A:552:LEU:H | 1.08 | 1.10 |
| 1:A:905:GLN:HG2 | 2:B:83:THR:HG22 | 1.18 | 1.10 |
| 2:B:288:ILE:O | 2:B:288:ILE:HG22 | 1.46 | 1.10 |
| 1:A:914:GLU:O | 2:B:184:ASN:HB3 | 1.52 | 1.10 |
| 1:A:679:LEU:HD23 | 1:A:679:LEU:O | 1.51 | 1.10 |
| 1:A:901:ASN:HB3 | 1:A:904:LEU:HD12 | 1.12 | 1.09 |
| 1:A:146:ILE:HD13 | 1:A:146:ILE:O | 1.53 | 1.09 |
| 1:A:786:ALA:HB2 | 1:A:858:LEU:HD21 | 1.33 | 1.09 |
| 1:A:97:GLU:HB3 | 1:A:99:VAL:HG22 | 1.33 | 1.08 |
| 1:A:1007:LEU:HD21 | 2:B:54:ILE:HG21 | 1.22 | 1.08 |
| 1:A:903:HIS:HB2 | 2:B:88:VAL:O | 1.53 | 1.08 |
| 1:A:905:GLN:HG3 | 2:B:278:TYR:CD2 | 1.89 | 1.07 |
| 1:A:775:ARG:CD | 1:A:840:ILE:CG2 | 2.32 | 1.07 |
| 1:A:978:LEU:HD21 | 1:A:990:PHE:CE2 | 1.88 | 1.07 |
| 1:A:994:ARG:NH1 | 2:B:73:TYR:CB | 2.17 | 1.07 |
| 1:A:189:ILE:HD11 | 1:A:194:LEU:HD23 | 1.34 | 1.07 |
| 1:A:443:LYS:HG3 | 1:A:455:ILE:HG23 | 1.26 | 1.07 |
| 2:B:287:LYS:HE2 | 2:B:289:GLN:HE21 | 1.05 | 1.07 |
| 1:A:994:ARG:NH2 | 2:B:75:ASP:HB2 | 1.70 | 1.07 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:394:ARG:HH12 | 1:A:452:PRO:HB2 | 1.03 | 1.06 |
| 1:A:286:VAL:HB | 1:A:735:LYS:HE3 | 1.31 | 1.06 |
| 1:A:396:THR:CG2 | 1:A:397:VAL:H | 1.66 | 1.06 |
| 1:A:601:ILE:HG13 | 1:A:602:ASP:H | 0.94 | 1.06 |
| 1:A:363:LYS:HE3 | 1:A:773:GLN:HE21 | 0.95 | 1.06 |
| 1:A:922:TYR:CD2 | 1:A:991:MET:HE3 | 1.88 | 1.06 |
| 1:A:723:VAL:HG23 | 1:A:737:ALA:HB2 | 1.38 | 1.06 |
| 1:A:283:ALA:O | 1:A:286:VAL:HG23 | 1.55 | 1.06 |
| 1:A:884:GLN:HG2 | 2:B:73:TYR:HD2 | 1.15 | 1.06 |
| 1:A:114:TRP:CZ3 | 1:A:146:ILE:HG12 | 1.91 | 1.06 |
| 1:A:446:GLN:HB2 | 1:A:449:VAL:HG22 | 1.37 | 1.06 |
| 1:A:567:LEU:HD12 | 1:A:592:LEU:CD2 | 1.85 | 1.05 |
| 1:A:601:ILE:HG13 | 1:A:602:ASP:N | 1.63 | 1.05 |
| 1:A:651:GLU:O | 1:A:654:ALA:CB | 2.04 | 1.05 |
| 1:A:386:LYS:HD2 | 1:A:636:ILE:HD12 | 1.37 | 1.05 |
| 1:A:752:LYS:HG3 | 1:A:758:ILE:CD1 | 1.86 | 1.05 |
| 1:A:923:GLN:HG2 | 2:B:76:GLN:HG2 | 1.09 | 1.05 |
| 1:A:905:GLN:O | 2:B:83:THR:HG21 | 1.53 | 1.05 |
| 1:A:994:ARG:HD3 | 2:B:73:TYR:CE1 | 1.92 | 1.05 |
| 1:A:923:GLN:HG2 | 2:B:76:GLN:CG | 1.85 | 1.04 |
| 1:A:601:ILE:CG1 | 1:A:602:ASP:H | 1.67 | 1.04 |
| 1:A:905:GLN:CG | 2:B:278:TYR:CD2 | 2.40 | 1.04 |
| 1:A:360:LEU:HD13 | 1:A:363:LYS:HD2 | 1.35 | 1.04 |
| 1:A:483:PHE:HE2 | 1:A:504:LEU:HD12 | 1.16 | 1.03 |
| 1:A:360:LEU:HD11 | 1:A:773:GLN:HG3 | 1.08 | 1.03 |
| 1:A:913:GLN:CB | 2:B:185:ARG:O | 2.06 | 1.03 |
| 2:B:126:GLU:HG3 | 2:B:127:GLY:H | 1.19 | 1.02 |
| 2:B:254:ARG:HD3 | 2:B:255:ASN:HD22 | 1.22 | 1.02 |
| 1:A:397:VAL:CG1 | 1:A:398:SER:H | 1.72 | 1.02 |
| 1:A:377:GLY:HA3 | 1:A:774:GLY:O | 1.59 | 1.02 |
| 1:A:511:ARG:NH1 | 1:A:511:ARG:HB3 | 1.74 | 1.01 |
| 1:A:922:TYR:CD2 | 1:A:991:MET:CE | 2.44 | 1.01 |
| 1:A:887:TRP:HH2 | 1:A:907:LEU:HG | 1.22 | 1.01 |
| 1:A:119:ILE:HG23 | 1:A:334:MET:HE1 | 1.42 | 1.01 |
| 1:A:360:LEU:HD11 | 1:A:773:GLN:CG | 1.91 | 1.00 |
| 1:A:339:ALA:HB1 | 1:A:796:LEU:HD12 | 1.39 | 1.00 |
| 1:A:903:HIS:HD2 | 1:A:904:LEU:N | 1.58 | 1.00 |
| 1:A:315:PHE:CE2 | 1:A:800:LEU:HD22 | 1.96 | 1.00 |
| 1:A:896:ARG:O | 1:A:900:GLU:HG2 | 1.61 | 1.00 |
| 1:A:915:TRP:CZ2 | 2:B:77:LEU:HB2 | 1.96 | 1.00 |
| 1:A:922:TYR:OH | 2:B:275:HIS:HE1 | 1.43 | 1.00 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:690:ALA:O | 1:A:693:THR:HG22 | 1.60 | 1.00 |
| 1:A:1011:TYR:CZ | 2:B:47:PHE:CE1 | 2.48 | 0.99 |
| 1:A:923:GLN:CG | 2:B:76:GLN:CG | 2.39 | 0.99 |
| 1:A:657:LEU:O | 1:A:658:ARG:HG3 | 1.60 | 0.99 |
| 1:A:901:ASN:HB3 | 1:A:904:LEU:HD11 | 1.00 | 0.99 |
| 1:A:903:HIS:HB2 | 2:B:88:VAL:C | 1.80 | 0.99 |
| 1:A:564:PHE:HE1 | 1:A:598:VAL:HG12 | 1.26 | 0.99 |
| 1:A:602:ASP:OD2 | 1:A:636:ILE:HD11 | 1.63 | 0.99 |
| 1:A:693:THR:HG23 | 1:A:694:HIS:ND1 | 1.75 | 0.99 |
| 1:A:537:LEU:HD12 | 1:A:538:PRO:HD2 | 1.44 | 0.98 |
| 1:A:905:GLN:HG2 | 2:B:83:THR:CG2 | 1.94 | 0.98 |
| 1:A:905:GLN:O | 2:B:83:THR:CG2 | 2.11 | 0.98 |
| 1:A:254:PHE:CE2 | 1:A:276:ILE:HD11 | 1.98 | 0.98 |
| 1:A:567:LEU:HD12 | 1:A:592:LEU:HD23 | 1.45 | 0.98 |
| 1:A:752:LYS:HG3 | 1:A:758:ILE:HD11 | 1.45 | 0.97 |
| 1:A:994:ARG:HD3 | 2:B:73:TYR:CZ | 2.00 | 0.97 |
| 1:A:391:THR:HA | 1:A:604:PRO:HA | 1.43 | 0.97 |
| 1:A:994:ARG:CZ | 2:B:73:TYR:CD1 | 2.47 | 0.97 |
| 1:A:399:HIS:HB3 | 1:A:407:HIS:O | 1.64 | 0.96 |
| 1:A:69:THR:HG23 | 1:A:70:LYS:N | 1.80 | 0.96 |
| 1:A:1007:LEU:CD2 | 2:B:54:ILE:HG21 | 1.96 | 0.96 |
| 1:A:994:ARG:CZ | 2:B:73:TYR:CG | 2.48 | 0.96 |
| 1:A:483:PHE:CE2 | 1:A:504:LEU:HD12 | 2.00 | 0.96 |
| 1:A:93:ARG:HH21 | 1:A:285:GLY:HA3 | 1.27 | 0.96 |
| 1:A:398:SER:CA | 1:A:600:MET:HA | 1.96 | 0.95 |
| 1:A:552:LEU:CD2 | 1:A:552:LEU:H | 1.78 | 0.95 |
| 1:A:905:GLN:C | 2:B:83:THR:HG21 | 1.84 | 0.95 |
| 1:A:487:CYS:SG | 1:A:580:PHE:HB2 | 2.06 | 0.95 |
| 1:A:786:ALA:HB3 | 1:A:946:ARG:HD2 | 1.46 | 0.95 |
| 1:A:363:LYS:CE | 1:A:773:GLN:NE2 | 2.29 | 0.95 |
| 1:A:286:VAL:CB | 1:A:735:LYS:HE3 | 1.97 | 0.95 |
| 1:A:479:TYR:HA | 1:A:482:ARG:HD3 | 1.49 | 0.95 |
| 1:A:479:TYR:HA | 1:A:482:ARG:CD | 1.97 | 0.94 |
| 1:A:57:VAL:CG2 | 1:A:215:LEU:HD23 | 1.95 | 0.94 |
| 1:A:924:GLN:HG2 | 1:A:928:TYR:CE2 | 2.02 | 0.94 |
| 1:A:45:LYS:NZ | 1:A:281:SER:CB | 2.30 | 0.94 |
| 1:A:109:LEU:HG | 1:A:346:LEU:HD22 | 1.50 | 0.94 |
| 2:B:287:LYS:CE | 2:B:289:GLN:HE21 | 1.79 | 0.94 |
| 1:A:1016:LYS:O | 1:A:1019:VAL:HG22 | 1.66 | 0.94 |
| 1:A:905:GLN:C | 2:B:83:THR:CG2 | 2.37 | 0.94 |
| 1:A:397:VAL:HG12 | 1:A:398:SER:N | 1.81 | 0.93 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:903:HIS:CD2 | 1:A:904:LEU:N | 2.36 | 0.93 |
| 2:B:240:TYR:HD1 | 2:B:240:TYR:O | 1.40 | 0.93 |
| 1:A:360:LEU:CD1 | 1:A:773:GLN:HG3 | 1.98 | 0.93 |
| 1:A:814:ILE:HD11 | 1:A:988:PHE:CD1 | 2.03 | 0.93 |
| 1:A:376:LEU:HD22 | 1:A:770:GLY:C | 1.89 | 0.93 |
| 2:B:249:LEU:HD12 | 2:B:286:LEU:HD12 | 1.49 | 0.92 |
| 1:A:667:LYS:HZ3 | 1:A:667:LYS:HA | 1.30 | 0.92 |
| 1:A:57:VAL:HG21 | 1:A:215:LEU:CD2 | 1.98 | 0.92 |
| 1:A:397:VAL:CG1 | 1:A:398:SER:N | 2.28 | 0.92 |
| 1:A:72:LEU:CD1 | 1:A:198:ASP:HA | 1.99 | 0.92 |
| 1:A:775:ARG:CD | 1:A:840:ILE:HG22 | 1.99 | 0.92 |
| 1:A:939:GLN:O | 1:A:943:VAL:HG23 | 1.69 | 0.92 |
| 1:A:914:GLU:O | 2:B:184:ASN:CB | 2.18 | 0.92 |
| 1:A:394:ARG:HH12 | 1:A:452:PRO:CB | 1.83 | 0.92 |
| 1:A:679:LEU:CD2 | 1:A:679:LEU:O | 2.17 | 0.92 |
| 1:A:339:ALA:HB1 | 1:A:796:LEU:CD1 | 1.98 | 0.92 |
| 1:A:925:TYR:HA | 1:A:928:TYR:HD2 | 1.34 | 0.92 |
| 2:B:154:PHE:HD1 | 2:B:228:TYR:HH | 1.08 | 0.91 |
| 1:A:363:LYS:CE | 1:A:773:GLN:HE21 | 1.81 | 0.91 |
| 1:A:433:VAL:HG23 | 1:A:515:VAL:HB | 1.53 | 0.91 |
| 1:A:381:VAL:CG1 | 1:A:721:VAL:HG12 | 2.00 | 0.91 |
| 1:A:166:ILE:HD12 | 1:A:753:ASN:CB | 2.01 | 0.91 |
| 1:A:309:ILE:HG23 | 1:A:310:LEU:N | 1.85 | 0.91 |
| 1:A:913:GLN:HE22 | 2:B:77:LEU:CD2 | 1.77 | 0.91 |
| 1:A:397:VAL:HG13 | 1:A:398:SER:H | 1.36 | 0.90 |
| 1:A:864:PHE:HD1 | 1:A:865:GLN:HG3 | 1.35 | 0.90 |
| 1:A:189:ILE:HD11 | 1:A:194:LEU:CD2 | 2.01 | 0.90 |
| 1:A:994:ARG:HH21 | 2:B:75:ASP:HB2 | 1.36 | 0.90 |
| 1:A:922:TYR:CE2 | 1:A:991:MET:CE | 2.55 | 0.90 |
| 1:A:903:HIS:C | 1:A:903:HIS:CD2 | 2.45 | 0.90 |
| 1:A:254:PHE:CD2 | 1:A:276:ILE:HD11 | 2.07 | 0.89 |
| 1:A:618:ALA:HB3 | 1:A:620:ILE:HD12 | 1.54 | 0.89 |
| 1:A:286:VAL:CB | 1:A:735:LYS:CE | 2.47 | 0.89 |
| 1:A:79:GLU:CD | 1:A:79:GLU:O | 2.09 | 0.89 |
| 1:A:814:ILE:HD11 | 1:A:988:PHE:HD1 | 1.37 | 0.89 |
| 1:A:169:SER:CB | 1:A:753:ASN:HD21 | 1.77 | 0.89 |
| 1:A:171:LYS:O | 1:A:173:LEU:N | 2.03 | 0.89 |
| 1:A:398:SER:HB2 | 1:A:600:MET:HA | 0.94 | 0.89 |
| 1:A:858:LEU:O | 1:A:858:LEU:HD13 | 1.71 | 0.89 |
| 2:B:126:GLU:HG3 | 2:B:127:GLY:N | 1.79 | 0.89 |
| 1:A:913:GLN:HE21 | 2:B:77:LEU:HD22 | 1.36 | 0.89 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:166:ILE:CD1 | 1:A:753:ASN:HB2 | 2.02 | 0.89 |
| 2:B:45:VAL:O | 2:B:49:VAL:HB | 1.71 | 0.89 |
| 1:A:166:ILE:HA | 1:A:753:ASN:ND2 | 1.88 | 0.89 |
| 2:B:287:LYS:HE2 | 2:B:289:GLN:NE2 | 1.88 | 0.89 |
| 1:A:120:CYS:HB2 | 1:A:142:ALA:HB2 | 1.54 | 0.88 |
| 1:A:396:THR:CG2 | 1:A:397:VAL:N | 2.24 | 0.88 |
| 1:A:65:GLN:HE21 | 1:A:65:GLN:N | 1.67 | 0.88 |
| 1:A:994:ARG:NH1 | 2:B:73:TYR:CD1 | 2.40 | 0.88 |
| 1:A:905:GLN:HB2 | 2:B:278:TYR:CD2 | 2.08 | 0.88 |
| 2:B:88:VAL:HG21 | 2:B:284:PHE:CD1 | 2.09 | 0.88 |
| 1:A:905:GLN:CB | 2:B:83:THR:HG22 | 2.03 | 0.88 |
| 1:A:324:TYR:CD1 | 1:A:328:ARG:HG2 | 2.07 | 0.88 |
| 1:A:169:SER:HB2 | 1:A:753:ASN:ND2 | 1.88 | 0.88 |
| 1:A:587:PHE:HB2 | 1:A:588:PRO:HD2 | 1.53 | 0.88 |
| 1:A:65:GLN:NE2 | 1:A:65:GLN:H | 1.60 | 0.88 |
| 1:A:869:ILE:HG12 | 2:B:51:MET:HE2 | 1.56 | 0.88 |
| 1:A:1015:ARG:O | 1:A:1019:VAL:HG13 | 1.73 | 0.88 |
| 1:A:230:GLU:OE1 | 1:A:230:GLU:HA | 1.74 | 0.88 |
| 1:A:166:ILE:HA | 1:A:753:ASN:CB | 2.04 | 0.88 |
| 1:A:169:SER:OG | 1:A:749:ASP:CB | 2.21 | 0.87 |
| 1:A:216:GLN:HG2 | 1:A:264:GLN:HB2 | 1.54 | 0.87 |
| 2:B:288:ILE:CG2 | 2:B:288:ILE:O | 2.21 | 0.87 |
| 1:A:857:PRO:HB3 | 1:A:1030:GLU:O | 1.74 | 0.87 |
| 1:A:286:VAL:CG1 | 1:A:735:LYS:HE3 | 2.05 | 0.87 |
| 1:A:791:LYS:HD2 | 1:A:819:ILE:CG2 | 2.04 | 0.87 |
| 1:A:905:GLN:CB | 2:B:278:TYR:CD2 | 2.57 | 0.87 |
| 1:A:57:VAL:HG22 | 1:A:215:LEU:HD23 | 1.57 | 0.87 |
| 1:A:349:VAL:O | 1:A:353:LEU:HD13 | 1.74 | 0.87 |
| 1:A:442:PHE:CD1 | 1:A:454:ARG:HD2 | 2.10 | 0.87 |
| 1:A:396:THR:HG22 | 1:A:397:VAL:H | 1.20 | 0.86 |
| 1:A:943:VAL:CG1 | 1:A:964:LEU:HD11 | 2.04 | 0.86 |
| 1:A:574:TYR:HD1 | 1:A:578:TYR:CE2 | 1.93 | 0.86 |
| 1:A:146:ILE:O | 1:A:149:VAL:HG22 | 1.76 | 0.86 |
| 1:A:212:ILE:CG2 | 1:A:252:ALA:HB3 | 2.05 | 0.86 |
| 1:A:72:LEU:HD13 | 1:A:198:ASP:CA | 2.04 | 0.86 |
| 1:A:784:SER:HA | 1:A:831:LEU:HD22 | 1.58 | 0.86 |
| 2:B:68:PRO:HD2 | 2:B:69:TYR:H | 1.40 | 0.86 |
| 1:A:705:GLN:O | 1:A:709:VAL:HG23 | 1.74 | 0.86 |
| 1:A:489:ILE:HG12 | 1:A:582:VAL:HG13 | 1.55 | 0.85 |
| 1:A:903:HIS:HD2 | 1:A:904:LEU:CA | 1.88 | 0.85 |
| 1:A:332:PHE:O | 1:A:336:ILE:HG13 | 1.77 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:435:THR:HG23 | 1:A:436:LEU:CD1 | 2.07 | 0.85 |
| 1:A:282:LEU:HG | 1:A:282:LEU:O | 1.75 | 0.85 |
| 1:A:1019:VAL:HB | 1:A:1028:ASP:OD1 | 1.77 | 0.85 |
| 1:A:856:GLU:HG2 | 1:A:857:PRO:HD3 | 1.59 | 0.85 |
| 1:A:421:ASP:OD1 | 1:A:421:ASP:C | 2.15 | 0.85 |
| 1:A:112:LEU:HD21 | 1:A:341:VAL:HG12 | 1.56 | 0.85 |
| 1:A:446:GLN:CB | 1:A:449:VAL:HG22 | 2.06 | 0.85 |
| 1:A:682:MET:SD | 1:A:686:GLU:HG2 | 2.17 | 0.85 |
| 1:A:114:TRP:HZ3 | 1:A:146:ILE:HG12 | 1.38 | 0.84 |
| 1:A:169:SER:HB2 | 1:A:753:ASN:HD21 | 1.40 | 0.84 |
| 1:A:841:MET:CE | 1:A:841:MET:HA | 2.06 | 0.84 |
| 2:B:84:LEU:HB3 | 2:B:86:PRO:HD2 | 1.58 | 0.84 |
| 1:A:765:ALA:O | 1:A:768:VAL:HG12 | 1.77 | 0.84 |
| 1:A:315:PHE:CD2 | 1:A:800:LEU:HD22 | 2.11 | 0.84 |
| 2:B:186:ILE:HG23 | 2:B:189:PHE:HB3 | 1.59 | 0.84 |
| 1:A:574:TYR:HD1 | 1:A:578:TYR:CD2 | 1.96 | 0.84 |
| 1:A:752:LYS:HG3 | 1:A:758:ILE:HD12 | 1.60 | 0.84 |
| 1:A:212:ILE:HG22 | 1:A:252:ALA:HB3 | 1.58 | 0.84 |
| 1:A:1011:TYR:O | 1:A:1014:ILE:HG22 | 1.76 | 0.84 |
| 1:A:552:LEU:HD23 | 1:A:552:LEU:N | 1.91 | 0.84 |
| 1:A:117:ALA:HA | 1:A:145:LEU:HD12 | 1.59 | 0.83 |
| 1:A:291:THR:O | 1:A:295:ILE:HG13 | 1.76 | 0.83 |
| 1:A:463:THR:OG1 | 1:A:467:LYS:HE3 | 1.77 | 0.83 |
| 1:A:212:ILE:HD11 | 1:A:265:GLY:C | 1.98 | 0.83 |
| 1:A:446:GLN:HB2 | 1:A:449:VAL:CG2 | 2.07 | 0.83 |
| 1:A:965:VAL:O | 1:A:968:ILE:HG22 | 1.79 | 0.83 |
| 1:A:670:ARG:HE | 1:A:695:PRO:HG2 | 1.44 | 0.83 |
| 1:A:723:VAL:CG2 | 1:A:737:ALA:HB2 | 2.08 | 0.83 |
| 1:A:207:ARG:CG | 1:A:257:MET:HG3 | 2.07 | 0.83 |
| 1:A:398:SER:CB | 1:A:600:MET:C | 2.27 | 0.83 |
| 1:A:947:LYS:HD2 | 1:A:964:LEU:HD22 | 1.59 | 0.83 |
| 1:A:693:THR:CG2 | 1:A:694:HIS:ND1 | 2.41 | 0.83 |
| 2:B:249:LEU:HD12 | 2:B:286:LEU:CD1 | 2.08 | 0.83 |
| 1:A:124:PHE:HA | 1:A:127:GLN:HG2 | 1.60 | 0.83 |
| 2:B:77:LEU:HG | 2:B:186:ILE:HD12 | 1.58 | 0.83 |
| 1:A:739:ILE:HD11 | 1:A:757:MET:SD | 2.19 | 0.83 |
| 1:A:760:LEU:HD22 | 1:A:760:LEU:H | 1.43 | 0.83 |
| 1:A:1002:MET:HB3 | 1:A:1003:PRO:HD3 | 1.61 | 0.82 |
| 1:A:386:LYS:HD2 | 1:A:636:ILE:CD1 | 2.09 | 0.82 |
| 1:A:169:SER:HB3 | 1:A:753:ASN:HD22 | 1.40 | 0.82 |
| 1:A:915:TRP:CH2 | 2:B:77:LEU:HB2 | 2.13 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:32:ARG:HH11 | 2:B:32:ARG:CG | 1.89 | 0.82 |
| 1:A:1015:ARG:HD2 | 1:A:1031:LEU:CD2 | 2.08 | 0.82 |
| 1:A:648:GLU:HB3 | 1:A:652:ASP:OD1 | 1.79 | 0.82 |
| 1:A:564:PHE:HE1 | 1:A:598:VAL:CG1 | 1.92 | 0.82 |
| 1:A:795:GLU:HB3 | 1:A:816:ILE:HD12 | 1.61 | 0.81 |
| 1:A:90:ARG:NH1 | 1:A:272:ASP:OD2 | 2.12 | 0.81 |
| 1:A:913:GLN:HE22 | 2:B:77:LEU:HD22 | 0.91 | 0.81 |
| 1:A:170:PHE:O | 1:A:173:LEU:HD12 | 1.76 | 0.81 |
| 1:A:166:ILE:CD1 | 1:A:753:ASN:CB | 2.59 | 0.81 |
| 1:A:548:GLN:O | 1:A:552:LEU:HD21 | 1.77 | 0.81 |
| 1:A:922:TYR:OH | 2:B:275:HIS:CE1 | 2.33 | 0.81 |
| 1:A:495:ASN:HB3 | 1:A:497:PHE:CE2 | 2.14 | 0.81 |
| 1:A:97:GLU:HB3 | 1:A:99:VAL:CG2 | 2.10 | 0.81 |
| 1:A:661:VAL:CG2 | 1:A:662:ASP:N | 2.43 | 0.81 |
| 1:A:905:GLN:HG3 | 2:B:278:TYR:HB3 | 1.61 | 0.81 |
| 1:A:79:GLU:HA | 1:A:79:GLU:OE1 | 1.79 | 0.81 |
| 1:A:181:ILE:HG13 | 1:A:199:LEU:HD23 | 1.61 | 0.81 |
| 1:A:315:PHE:HA | 1:A:318:VAL:HG22 | 1.62 | 0.81 |
| 1:A:905:GLN:CB | 2:B:278:TYR:HD2 | 1.93 | 0.81 |
| 2:B:282:VAL:HG13 | 2:B:284:PHE:CE2 | 2.17 | 0.80 |
| 1:A:119:ILE:CG2 | 1:A:334:MET:HB3 | 2.11 | 0.80 |
| 1:A:623:ILE:HG12 | 1:A:697:MET:SD | 2.20 | 0.80 |
| 1:A:166:ILE:HA | 1:A:753:ASN:CG | 2.00 | 0.80 |
| 1:A:53:HIS:HB3 | 1:A:251:ILE:HD11 | 1.63 | 0.80 |
| 1:A:610:ASP:OD1 | 1:A:614:LYS:HE3 | 1.80 | 0.80 |
| 1:A:381:VAL:HG23 | 1:A:621:ARG:O | 1.82 | 0.80 |
| 1:A:759:LEU:CD1 | 1:A:766:SER:HB2 | 2.11 | 0.80 |
| 1:A:791:LYS:HD2 | 1:A:819:ILE:HG21 | 1.62 | 0.80 |
| 2:B:68:PRO:HG2 | 2:B:69:TYR:CZ | 2.16 | 0.80 |
| 1:A:442:PHE:CZ | 1:A:466:LEU:HD13 | 2.16 | 0.80 |
| 1:A:922:TYR:CG | 1:A:991:MET:HE3 | 2.17 | 0.80 |
| 1:A:943:VAL:HG13 | 1:A:964:LEU:HD11 | 1.63 | 0.80 |
| 1:A:731:SER:HB2 | 1:A:732:PRO:HD3 | 1.64 | 0.80 |
| 1:A:92:PRO:HD3 | 1:A:171:LYS:HE3 | 1.62 | 0.80 |
| 1:A:398:SER:N | 1:A:600:MET:HA | 1.96 | 0.80 |
| 2:B:82:VAL:HG13 | 2:B:280:GLY:HA2 | 1.62 | 0.80 |
| 2:B:82:VAL:HG22 | 2:B:281:LYS:N | 1.97 | 0.80 |
| 1:A:574:TYR:CD1 | 1:A:578:TYR:CE2 | 2.70 | 0.79 |
| 1:A:901:ASN:HB2 | 1:A:904:LEU:HD11 | 1.64 | 0.79 |
| 1:A:322:ILE:HG13 | 1:A:322:ILE:O | 1.81 | 0.79 |
| 2:B:85:ARG:HB3 | 2:B:180:ILE:HG13 | 1.63 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:48:MET:HE3 | 1:A:246:LEU:HG | 1.61 | 0.79 |
| 2:B:240:TYR:CD1 | 2:B:240:TYR:C | 2.55 | 0.79 |
| 1:A:905:GLN:HB2 | 2:B:278:TYR:CE2 | 2.18 | 0.79 |
| 1:A:994:ARG:CD | 2:B:73:TYR:CE1 | 2.66 | 0.79 |
| 1:A:491:PHE:HZ | 1:A:496:LYS:HE2 | 1.48 | 0.79 |
| 1:A:826:PHE:HB2 | 1:A:827:PRO:HD3 | 1.64 | 0.79 |
| 1:A:255:SER:HB2 | 1:A:276:ILE:HG12 | 1.65 | 0.79 |
| 1:A:761:ASP:OD1 | 1:A:763:ASN:HB2 | 1.83 | 0.79 |
| 1:A:917:PHE:HB3 | 2:B:278:TYR:CE1 | 2.18 | 0.79 |
| 1:A:807:VAL:HG22 | 1:A:808:PRO:HD2 | 1.64 | 0.79 |
| 1:A:947:LYS:HD2 | 1:A:964:LEU:CD2 | 2.11 | 0.79 |
| 1:A:57:VAL:CG2 | 1:A:215:LEU:CD2 | 2.58 | 0.78 |
| 1:A:64:TYR:C | 1:A:65:GLN:HE21 | 1.85 | 0.78 |
| 1:A:674:ILE:O | 1:A:674:ILE:HG23 | 1.83 | 0.78 |
| 1:A:877:ASP:O | 1:A:880:THR:HG22 | 1.84 | 0.78 |
| 1:A:991:MET:HG3 | 1:A:992:PRO:HD2 | 1.65 | 0.78 |
| 1:A:598:VAL:O | 1:A:598:VAL:HG13 | 1.83 | 0.78 |
| 1:A:173:LEU:N | 1:A:173:LEU:HD12 | 1.98 | 0.78 |
| 2:B:68:PRO:HG2 | 2:B:69:TYR:CE2 | 2.18 | 0.78 |
| 1:A:915:TRP:HZ3 | 2:B:76:GLN:HG3 | 1.49 | 0.78 |
| 1:A:441:ALA:O | 1:A:456:VAL:HG13 | 1.84 | 0.78 |
| 1:A:511:ARG:HB3 | 1:A:511:ARG:HH11 | 1.47 | 0.78 |
| 1:A:479:TYR:O | 1:A:482:ARG:HG2 | 1.83 | 0.78 |
| 1:A:266:LEU:HD23 | 1:A:267:VAL:N | 1.99 | 0.78 |
| 1:A:860:ALA:O | 1:A:864:PHE:HB3 | 1.84 | 0.78 |
| 2:B:83:THR:C | 2:B:84:LEU:HD12 | 2.03 | 0.78 |
| 1:A:481:GLU:O | 1:A:484:PRO:HD3 | 1.84 | 0.78 |
| 1:A:887:TRP:CH2 | 1:A:907:LEU:HG | 2.14 | 0.78 |
| 1:A:690:ALA:C | 1:A:693:THR:HG22 | 2.04 | 0.78 |
| 1:A:994:ARG:HH21 | 2:B:75:ASP:CB | 1.95 | 0.78 |
| 1:A:45:LYS:HZ2 | 1:A:281:SER:HB2 | 1.44 | 0.77 |
| 1:A:667:LYS:HA | 1:A:667:LYS:NZ | 1.98 | 0.77 |
| 1:A:962:ARG:O | 1:A:965:VAL:HG12 | 1.84 | 0.77 |
| 2:B:77:LEU:HD23 | 2:B:186:ILE:HG13 | 1.66 | 0.77 |
| 1:A:657:LEU:O | 1:A:658:ARG:CG | 2.32 | 0.77 |
| 1:A:399:HIS:CD2 | 1:A:408:SER:HA | 2.19 | 0.77 |
| 1:A:511:ARG:HG2 | 1:A:512:HIS:H | 1.49 | 0.77 |
| 1:A:918:GLY:HA3 | 2:B:276:ASP:HB3 | 1.66 | 0.77 |
| 1:A:45:LYS:HZ3 | 1:A:281:SER:HB2 | 1.46 | 0.77 |
| 1:A:891:LEU:O | 1:A:895:LEU:CD2 | 2.32 | 0.77 |
| 1:A:903:HIS:HD2 | 1:A:904:LEU:HA | 1.49 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:891:LEU:HG | 1:A:910:SER:OG | 1.85 | 0.77 |
| 1:A:891:LEU:O | 1:A:895:LEU:HD23 | 1.85 | 0.77 |
| 1:A:303:ILE:O | 1:A:307:LEU:HD23 | 1.84 | 0.76 |
| 1:A:443:LYS:HE2 | 1:A:457:ILE:CG1 | 2.15 | 0.76 |
| 1:A:791:LYS:HG3 | 1:A:935:ILE:HG21 | 1.65 | 0.76 |
| 2:B:32:ARG:HH11 | 2:B:32:ARG:HG3 | 1.49 | 0.76 |
| 1:A:146:ILE:O | 1:A:149:VAL:CG2 | 2.34 | 0.76 |
| 1:A:847:ASN:HD22 | 1:A:849:LYS:H | 1.33 | 0.76 |
| 2:B:136:TYR:CE1 | 2:B:190:LEU:HB3 | 2.20 | 0.76 |
| 1:A:615:CYS:O | 1:A:618:ALA:HB3 | 1.84 | 0.76 |
| 2:B:259:VAL:HG23 | 2:B:259:VAL:O | 1.86 | 0.76 |
| 1:A:934:SER:HA | 1:A:1001:PRO:HG3 | 1.66 | 0.76 |
| 1:A:97:GLU:CB | 1:A:99:VAL:HG22 | 2.14 | 0.76 |
| 1:A:392:GLN:OE1 | 1:A:413:GLU:HB3 | 1.86 | 0.76 |
| 1:A:411:THR:HG21 | 1:A:601:ILE:CG2 | 2.16 | 0.76 |
| 1:A:625:VAL:HG11 | 1:A:707:LYS:HG3 | 1.66 | 0.76 |
| 1:A:786:ALA:HB1 | 1:A:946:ARG:NH1 | 2.01 | 0.76 |
| 1:A:978:LEU:HD21 | 1:A:990:PHE:CD2 | 2.20 | 0.76 |
| 1:A:574:TYR:OH | 1:A:588:PRO:HD3 | 1.85 | 0.76 |
| 1:A:650:VAL:CG1 | 1:A:651:GLU:N | 2.48 | 0.76 |
| 1:A:905:GLN:HG3 | 2:B:278:TYR:CG | 2.20 | 0.76 |
| 2:B:213:LEU:HD23 | 2:B:213:LEU:O | 1.85 | 0.76 |
| 1:A:173:LEU:O | 1:A:173:LEU:HD13 | 1.86 | 0.76 |
| 1:A:564:PHE:CE1 | 1:A:598:VAL:HG12 | 2.17 | 0.76 |
| 1:A:223:ASP:O | 1:A:256:THR:HG23 | 1.86 | 0.76 |
| 1:A:397:VAL:HG21 | 1:A:468:PHE:HB2 | 1.66 | 0.76 |
| 1:A:380:SER:O | 1:A:620:ILE:HG23 | 1.85 | 0.76 |
| 2:B:126:GLU:HA | 2:B:153:LYS:HZ1 | 1.50 | 0.76 |
| 1:A:166:ILE:HA | 1:A:753:ASN:HB3 | 1.67 | 0.76 |
| 2:B:189:PHE:HZ | 2:B:268:HIS:HB3 | 1.48 | 0.76 |
| 1:A:524:LEU:O | 1:A:524:LEU:HD13 | 1.85 | 0.75 |
| 1:A:56:SER:CB | 1:A:59:GLU:OE2 | 2.35 | 0.75 |
| 1:A:916:THR:HG22 | 1:A:919:GLN:HG3 | 1.67 | 0.75 |
| 1:A:242:HIS:HD2 | 1:A:244:SER:H | 1.33 | 0.75 |
| 1:A:377:GLY:O | 1:A:378:SER:OG | 2.03 | 0.75 |
| 1:A:427:TRP:HH2 | 1:A:468:PHE:HE2 | 1.35 | 0.75 |
| 1:A:503:THR:O | 1:A:503:THR:HG23 | 1.86 | 0.75 |
| 2:B:148:THR:O | 2:B:148:THR:HG23 | 1.84 | 0.75 |
| 1:A:430:LEU:O | 1:A:433:VAL:HG12 | 1.86 | 0.75 |
| 1:A:345:LEU:O | 1:A:348:THR:HG22 | 1.85 | 0.75 |
| 1:A:443:LYS:HE2 | 1:A:457:ILE:HD11 | 1.67 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:286:VAL:CB | 1:A:735:LYS:HE2 | 2.13 | 0.75 |
| 1:A:916:THR:HG22 | 1:A:919:GLN:CG | 2.17 | 0.75 |
| 1:A:481:GLU:OE1 | 1:A:481:GLU:HA | 1.86 | 0.75 |
| 1:A:322:ILE:HG23 | 1:A:324:TYR:CD2 | 2.21 | 0.75 |
| 1:A:410:ASP:HB3 | 1:A:415:GLN:OE1 | 1.85 | 0.75 |
| 1:A:1015:ARG:HD2 | 1:A:1031:LEU:HD23 | 1.69 | 0.75 |
| 1:A:917:PHE:CZ | 1:A:921:LEU:HD11 | 2.21 | 0.75 |
| 1:A:1012:ASP:OD2 | 1:A:1016:LYS:HE3 | 1.87 | 0.74 |
| 1:A:254:PHE:HE2 | 1:A:276:ILE:HD11 | 1.52 | 0.74 |
| 2:B:272:ASP:HB3 | 2:B:276:ASP:OD1 | 1.86 | 0.74 |
| 1:A:793:ILE:HB | 1:A:794:PRO:HD3 | 1.69 | 0.74 |
| 1:A:947:LYS:CD | 1:A:964:LEU:HD22 | 2.16 | 0.74 |
| 2:B:143:LEU:HB3 | 2:B:145:PRO:HD2 | 1.69 | 0.74 |
| 1:A:994:ARG:CD | 2:B:73:TYR:CZ | 2.71 | 0.74 |
| 1:A:181:ILE:CD1 | 1:A:186:LYS:HB3 | 2.17 | 0.74 |
| 1:A:70:LYS:HD3 | 1:A:184:GLY:CA | 2.17 | 0.74 |
| 1:A:93:ARG:NH2 | 1:A:285:GLY:HA3 | 2.02 | 0.74 |
| 1:A:495:ASN:HB3 | 1:A:497:PHE:CD2 | 2.22 | 0.74 |
| 1:A:535:GLN:HG2 | 1:A:536:GLU:O | 1.87 | 0.74 |
| 1:A:309:ILE:HG23 | 1:A:310:LEU:H | 1.52 | 0.74 |
| 1:A:381:VAL:HG13 | 1:A:721:VAL:HG12 | 1.70 | 0.74 |
| 1:A:791:LYS:HE3 | 1:A:939:GLN:NE2 | 2.01 | 0.74 |
| 1:A:940:ILE:HD13 | 1:A:968:ILE:HG13 | 1.70 | 0.74 |
| 1:A:69:THR:CG2 | 1:A:70:LYS:N | 2.50 | 0.74 |
| 1:A:820:GLU:HG3 | 1:A:821:LEU:CD1 | 2.18 | 0.74 |
| 1:A:917:PHE:CE2 | 1:A:921:LEU:HD11 | 2.22 | 0.74 |
| 1:A:993:ILE:HD13 | 1:A:993:ILE:H | 1.51 | 0.74 |
| 1:A:311:PHE:O | 1:A:314:THR:HG22 | 1.86 | 0.74 |
| 1:A:552:LEU:CD2 | 1:A:552:LEU:N | 2.44 | 0.74 |
| 1:A:887:TRP:HH2 | 1:A:907:LEU:CG | 1.98 | 0.73 |
| 2:B:68:PRO:HD2 | 2:B:69:TYR:CD2 | 2.24 | 0.73 |
| 1:A:435:THR:HG23 | 1:A:436:LEU:HD12 | 1.69 | 0.73 |
| 1:A:356:THR:HG21 | 1:A:777:ILE:HD12 | 1.69 | 0.73 |
| 1:A:53:HIS:H | 1:A:53:HIS:CD2 | 2.07 | 0.73 |
| 1:A:618:ALA:CB | 1:A:620:ILE:HD12 | 2.18 | 0.73 |
| 1:A:978:LEU:HD21 | 1:A:990:PHE:CZ | 2.23 | 0.73 |
| 1:A:446:GLN:OE1 | 1:A:454:ARG:HB2 | 1.89 | 0.73 |
| 1:A:864:PHE:CD1 | 1:A:865:GLN:HG3 | 2.21 | 0.73 |
| 1:A:537:LEU:CD1 | 1:A:538:PRO:HD2 | 2.19 | 0.73 |
| 1:A:501:ILE:HD13 | 1:A:580:PHE:CD2 | 2.23 | 0.73 |
| 1:A:674:ILE:HG13 | 1:A:678:GLN:CD | 2.09 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:708:LEU:O | 1:A:708:LEU:HD13 | 1.88 | 0.73 |
| 1:A:898:GLN:O | 1:A:904:LEU:HD13 | 1.89 | 0.73 |
| 1:A:915:TRP:CH2 | 1:A:923:GLN:NE2 | 2.56 | 0.73 |
| 1:A:916:THR:HG23 | 1:A:919:GLN:H | 1.53 | 0.73 |
| 2:B:261:VAL:HG22 | 2:B:283:GLU:OE1 | 1.89 | 0.72 |
| 1:A:567:LEU:HB2 | 1:A:592:LEU:HD22 | 1.71 | 0.72 |
| 1:A:994:ARG:NH1 | 2:B:73:TYR:HB3 | 2.04 | 0.72 |
| 2:B:139:GLN:HB2 | 2:B:232:TYR:CZ | 2.24 | 0.72 |
| 1:A:820:GLU:HG3 | 1:A:821:LEU:HD12 | 1.70 | 0.72 |
| 2:B:85:ARG:CB | 2:B:180:ILE:HG13 | 2.19 | 0.72 |
| 1:A:147:ALA:O | 1:A:150:VAL:HG12 | 1.87 | 0.72 |
| 1:A:394:ARG:NH1 | 1:A:452:PRO:CB | 2.44 | 0.72 |
| 1:A:564:PHE:CE1 | 1:A:598:VAL:CG1 | 2.71 | 0.72 |
| 2:B:77:LEU:HD23 | 2:B:186:ILE:CG1 | 2.19 | 0.72 |
| 2:B:68:PRO:HD2 | 2:B:69:TYR:N | 2.03 | 0.72 |
| 1:A:933:ILE:HD11 | 1:A:979:CYS:SG | 2.29 | 0.72 |
| 1:A:827:PRO:HG2 | 1:A:971:GLN:NE2 | 2.04 | 0.72 |
| 1:A:316:PHE:CD1 | 1:A:329:ALA:HB1 | 2.24 | 0.72 |
| 1:A:442:PHE:CE2 | 1:A:466:LEU:HD11 | 2.25 | 0.72 |
| 1:A:818:PHE:O | 1:A:822:CYS:HB2 | 1.89 | 0.72 |
| 1:A:994:ARG:NH2 | 2:B:75:ASP:CB | 2.51 | 0.72 |
| 1:A:119:ILE:HG23 | 1:A:334:MET:HE2 | 1.67 | 0.72 |
| 1:A:434:LEU:HD23 | 1:A:564:PHE:CE2 | 2.24 | 0.72 |
| 1:A:855:ASN:HD22 | 1:A:857:PRO:CD | 2.02 | 0.72 |
| 1:A:905:GLN:O | 1:A:916:THR:HA | 1.89 | 0.72 |
| 1:A:927:CYS:O | 1:A:930:VAL:HG22 | 1.88 | 0.72 |
| 1:A:69:THR:HG23 | 1:A:70:LYS:H | 1.54 | 0.72 |
| 1:A:175:PRO:HA | 1:A:207:ARG:HH21 | 1.54 | 0.72 |
| 1:A:760:LEU:N | 1:A:760:LEU:HD22 | 2.05 | 0.71 |
| 1:A:815:THR:CG2 | 1:A:932:PHE:HB2 | 2.19 | 0.71 |
| 1:A:807:VAL:O | 1:A:896:ARG:HG2 | 1.90 | 0.71 |
| 1:A:359:ARG:O | 1:A:362:SER:HB2 | 1.91 | 0.71 |
| 1:A:486:VAL:HG22 | 1:A:501:ILE:O | 1.90 | 0.71 |
| 1:A:53:HIS:NE2 | 1:A:245:PRO:HG3 | 2.04 | 0.71 |
| 1:A:652:ASP:O | 1:A:655:ALA:N | 2.18 | 0.71 |
| 1:A:743:MET:HE3 | 1:A:762:ASP:HA | 1.73 | 0.71 |
| 1:A:175:PRO:HA | 1:A:207:ARG:NH2 | 2.05 | 0.71 |
| 1:A:65:GLN:NE2 | 1:A:65:GLN:CA | 2.53 | 0.71 |
| 1:A:112:LEU:O | 1:A:115:VAL:HG12 | 1.91 | 0.71 |
| 1:A:520:PRO:O | 1:A:523:VAL:HG12 | 1.90 | 0.71 |
| 1:A:869:ILE:HG12 | 2:B:51:MET:CE | 2.20 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:933:ILE:O | 1:A:936:GLU:HG2 | 1.91 | 0.71 |
| 1:A:250:ASN:C | 1:A:251:ILE:HD12 | 2.11 | 0.70 |
| 1:A:165:ASN:O | 1:A:753:ASN:CG | 2.29 | 0.70 |
| 1:A:693:THR:HG23 | 1:A:694:HIS:CG | 2.25 | 0.70 |
| 1:A:888:PHE:HB3 | 1:A:889:PRO:HD2 | 1.73 | 0.70 |
| 1:A:806:SER:HA | 1:A:896:ARG:HD3 | 1.72 | 0.70 |
| 1:A:768:VAL:O | 1:A:771:VAL:HG22 | 1.90 | 0.70 |
| 1:A:775:ARG:CD | 1:A:840:ILE:HG23 | 2.19 | 0.70 |
| 1:A:916:THR:CG2 | 1:A:919:GLN:HG3 | 2.20 | 0.70 |
| 2:B:57:LEU:O | 2:B:61:VAL:HG13 | 1.91 | 0.70 |
| 1:A:399:HIS:O | 1:A:400:LEU:HD12 | 1.90 | 0.70 |
| 1:A:759:LEU:HD12 | 1:A:763:ASN:O | 1.91 | 0.70 |
| 1:A:915:TRP:CZ3 | 2:B:76:GLN:HG3 | 2.27 | 0.70 |
| 1:A:347:ALA:O | 1:A:350:THR:HG22 | 1.91 | 0.70 |
| 1:A:905:GLN:HG3 | 2:B:278:TYR:CB | 2.20 | 0.70 |
| 1:A:97:GLU:CB | 1:A:99:VAL:CG2 | 2.69 | 0.70 |
| 1:A:463:THR:O | 1:A:467:LYS:HD3 | 1.91 | 0.70 |
| 2:B:41:SER:O | 2:B:45:VAL:HG23 | 1.91 | 0.70 |
| 1:A:396:THR:HG23 | 1:A:397:VAL:H | 1.55 | 0.70 |
| 1:A:315:PHE:HB2 | 1:A:336:ILE:CD1 | 2.21 | 0.70 |
| 1:A:1026:TRP:HE1 | 2:B:40:ILE:HD12 | 1.56 | 0.70 |
| 1:A:426:THR:HA | 1:A:531:LEU:HD23 | 1.72 | 0.69 |
| 1:A:575:PRO:HB3 | 1:A:576:PRO:HD2 | 1.74 | 0.69 |
| 1:A:759:LEU:HD11 | 1:A:766:SER:HB2 | 1.74 | 0.69 |
| 1:A:791:LYS:CD | 1:A:819:ILE:HG21 | 2.21 | 0.69 |
| 1:A:999:LEU:H | 1:A:999:LEU:HD12 | 1.57 | 0.69 |
| 1:A:905:GLN:CD | 2:B:278:TYR:HD2 | 1.95 | 0.69 |
| 1:A:846:ARG:HB2 | 1:A:851:ASP:OD1 | 1.92 | 0.69 |
| 1:A:328:ARG:HG3 | 1:A:332:PHE:CE2 | 2.26 | 0.69 |
| 1:A:76:LEU:O | 1:A:80:LEU:HD13 | 1.92 | 0.69 |
| 2:B:180:ILE:O | 2:B:180:ILE:HD12 | 1.90 | 0.69 |
| 1:A:651:GLU:HA | 1:A:654:ALA:HB2 | 1.74 | 0.69 |
| 1:A:817:LEU:HD23 | 1:A:820:GLU:OE2 | 1.91 | 0.69 |
| 1:A:435:THR:HG23 | 1:A:436:LEU:HD13 | 1.73 | 0.69 |
| 2:B:32:ARG:NH1 | 2:B:32:ARG:CG | 2.51 | 0.69 |
| 1:A:903:HIS:HE1 | 2:B:87:ASP:HB2 | 1.58 | 0.69 |
| 1:A:167:ILE:O | 1:A:171:LYS:HG2 | 1.92 | 0.69 |
| 1:A:614:LYS:O | 1:A:617:THR:HG22 | 1.91 | 0.69 |
| 1:A:806:SER:HA | 1:A:896:ARG:CD | 2.23 | 0.69 |
| 1:A:216:GLN:CG | 1:A:264:GLN:HB2 | 2.21 | 0.69 |
| 1:A:702:THR:HA | 1:A:706:GLN:NE2 | 2.08 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:905:GLN:C | 2:B:83:THR:HG22 | 2.13 | 0.69 |
| 1:A:917:PHE:O | 1:A:921:LEU:HG | 1.93 | 0.69 |
| 1:A:940:ILE:HG12 | 1:A:968:ILE:HD12 | 1.74 | 0.69 |
| 1:A:109:LEU:CG | 1:A:346:LEU:HD22 | 2.22 | 0.69 |
| 1:A:690:ALA:O | 1:A:693:THR:CG2 | 2.38 | 0.69 |
| 1:A:72:LEU:HD22 | 1:A:198:ASP:OD1 | 1.93 | 0.69 |
| 1:A:903:HIS:HD2 | 1:A:903:HIS:C | 1.90 | 0.69 |
| 1:A:937:MET:O | 1:A:940:ILE:HG22 | 1.92 | 0.69 |
| 2:B:229:PHE:HB3 | 2:B:230:PRO:HA | 1.74 | 0.69 |
| 1:A:309:ILE:O | 1:A:309:ILE:HG12 | 1.93 | 0.69 |
| 1:A:442:PHE:CZ | 1:A:466:LEU:CD1 | 2.76 | 0.69 |
| 1:A:811:LEU:HD23 | 1:A:816:ILE:HD11 | 1.73 | 0.69 |
| 1:A:443:LYS:HE2 | 1:A:457:ILE:CD1 | 2.23 | 0.68 |
| 1:A:460:ALA:O | 1:A:463:THR:HG22 | 1.93 | 0.68 |
| 1:A:119:ILE:O | 1:A:122:ILE:HG22 | 1.92 | 0.68 |
| 1:A:605:ARG:HB2 | 1:A:608:VAL:HG23 | 1.75 | 0.68 |
| 1:A:146:ILE:HD13 | 1:A:146:ILE:C | 2.14 | 0.68 |
| 1:A:761:ASP:O | 1:A:762:ASP:HB2 | 1.93 | 0.68 |
| 1:A:791:LYS:CG | 1:A:935:ILE:HG21 | 2.22 | 0.68 |
| 2:B:49:VAL:HG12 | 2:B:50:VAL:N | 2.09 | 0.68 |
| 1:A:847:ASN:ND2 | 1:A:849:LYS:H | 1.91 | 0.68 |
| 2:B:189:PHE:CZ | 2:B:268:HIS:HB3 | 2.28 | 0.68 |
| 1:A:507:PRO:C | 1:A:510:PRO:HD3 | 2.14 | 0.68 |
| 1:A:970:PHE:O | 1:A:974:ILE:HG12 | 1.94 | 0.68 |
| 1:A:366:VAL:HG12 | 1:A:760:LEU:HD21 | 1.74 | 0.68 |
| 1:A:925:TYR:HA | 1:A:928:TYR:CD2 | 2.25 | 0.68 |
| 1:A:253:PHE:CD1 | 1:A:275:ILE:HD13 | 2.28 | 0.68 |
| 1:A:833:TYR:CD1 | 1:A:963:ILE:HG21 | 2.29 | 0.68 |
| 1:A:122:ILE:HD13 | 1:A:126:ILE:HG12 | 1.75 | 0.68 |
| 1:A:315:PHE:HA | 1:A:318:VAL:CG2 | 2.24 | 0.68 |
| 1:A:427:TRP:HH2 | 1:A:468:PHE:CE2 | 2.12 | 0.68 |
| 2:B:249:LEU:CD1 | 2:B:286:LEU:HD12 | 2.24 | 0.68 |
| 1:A:178:ALA:CB | 1:A:194:LEU:HD11 | 2.24 | 0.67 |
| 1:A:723:VAL:HG23 | 1:A:737:ALA:CB | 2.21 | 0.67 |
| 1:A:786:ALA:HB3 | 1:A:946:ARG:CD | 2.23 | 0.67 |
| 1:A:1003:PRO:O | 1:A:1007:LEU:HD13 | 1.93 | 0.67 |
| 1:A:309:ILE:CG2 | 1:A:310:LEU:N | 2.55 | 0.67 |
| 1:A:915:TRP:CZ3 | 1:A:923:GLN:NE2 | 2.63 | 0.67 |
| 2:B:149:LYS:CD | 2:B:232:TYR:CD2 | 2.78 | 0.67 |
| 1:A:53:HIS:HB3 | 1:A:251:ILE:CD1 | 2.25 | 0.67 |
| 2:B:139:GLN:HG2 | 2:B:149:LYS:HB3 | 1.75 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:87:ASN:ND2 | 1:A:271:GLY:H | 1.91 | 0.67 |
| 1:A:661:VAL:HG23 | 1:A:662:ASP:N | 2.08 | 0.67 |
| 1:A:923:GLN:NE2 | 2:B:76:GLN:HG2 | 2.08 | 0.67 |
| 1:A:531:LEU:HD11 | 1:A:534:GLY:O | 1.93 | 0.67 |
| 1:A:693:THR:CG2 | 1:A:694:HIS:CE1 | 2.77 | 0.67 |
| 1:A:916:THR:CG2 | 1:A:919:GLN:H | 2.08 | 0.67 |
| 1:A:294:ALA:O | 1:A:297:ILE:HG12 | 1.93 | 0.67 |
| 1:A:487:CYS:SG | 1:A:580:PHE:CB | 2.81 | 0.67 |
| 1:A:793:ILE:HD12 | 1:A:793:ILE:H | 1.59 | 0.67 |
| 1:A:896:ARG:HB2 | 1:A:897:PRO:HD3 | 1.76 | 0.67 |
| 1:A:887:TRP:CH2 | 1:A:907:LEU:CD2 | 2.78 | 0.67 |
| 1:A:994:ARG:NH2 | 2:B:73:TYR:HB3 | 2.09 | 0.67 |
| 2:B:149:LYS:HD3 | 2:B:232:TYR:CD2 | 2.30 | 0.67 |
| 2:B:176:LYS:HB3 | 2:B:249:LEU:O | 1.94 | 0.67 |
| 2:B:178:CYS:SG | 2:B:248:LYS:HE3 | 2.34 | 0.67 |
| 1:A:171:LYS:C | 1:A:173:LEU:H | 1.98 | 0.67 |
| 1:A:412:THR:HG22 | 1:A:413:GLU:N | 2.10 | 0.67 |
| 1:A:903:HIS:CB | 2:B:88:VAL:O | 2.39 | 0.67 |
| 2:B:49:VAL:HG12 | 2:B:50:VAL:H | 1.59 | 0.67 |
| 1:A:115:VAL:O | 1:A:119:ILE:HG13 | 1.95 | 0.67 |
| 1:A:160:GLU:C | 1:A:162:LYS:H | 1.99 | 0.67 |
| 1:A:167:ILE:HG23 | 1:A:168:ALA:N | 2.10 | 0.67 |
| 1:A:56:SER:HB3 | 1:A:59:GLU:OE2 | 1.95 | 0.67 |
| 1:A:649:THR:HG23 | 1:A:652:ASP:H | 1.59 | 0.67 |
| 2:B:283:GLU:O | 2:B:284:PHE:CD1 | 2.47 | 0.67 |
| 1:A:48:MET:CE | 1:A:246:LEU:HG | 2.25 | 0.66 |
| 1:A:324:TYR:HD1 | 1:A:328:ARG:HG2 | 1.56 | 0.66 |
| 1:A:693:THR:HG21 | 1:A:694:HIS:CE1 | 2.31 | 0.66 |
| 1:A:877:ASP:OD1 | 1:A:930:VAL:HG23 | 1.95 | 0.66 |
| 1:A:785:ILE:O | 1:A:788:THR:HG22 | 1.95 | 0.66 |
| 1:A:811:LEU:HD11 | 1:A:815:THR:HG21 | 1.78 | 0.66 |
| 1:A:81:LEU:O | 1:A:81:LEU:HD23 | 1.93 | 0.66 |
| 1:A:901:ASN:CB | 1:A:904:LEU:HD12 | 2.06 | 0.66 |
| 1:A:923:GLN:CD | 2:B:76:GLN:HG2 | 2.14 | 0.66 |
| 1:A:315:PHE:HB2 | 1:A:336:ILE:HD13 | 1.77 | 0.66 |
| 1:A:855:ASN:HD22 | 1:A:857:PRO:HD2 | 1.58 | 0.66 |
| 1:A:880:THR:HG23 | 1:A:997:TRP:CZ3 | 2.30 | 0.66 |
| 1:A:947:LYS:CE | 1:A:964:LEU:HD22 | 2.24 | 0.66 |
| 1:A:443:LYS:HG3 | 1:A:455:ILE:CG2 | 2.16 | 0.66 |
| 1:A:657:LEU:O | 1:A:658:ARG:CB | 2.43 | 0.66 |
| 1:A:922:TYR:CZ | 2:B:275:HIS:CE1 | 2.84 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:78:LYS:HG2 | 2:B:79:SER:N | 2.09 | 0.66 |
| 1:A:726:ASP:OD1 | 1:A:743:MET:HG3 | 1.96 | 0.66 |
| 2:B:78:LYS:HD3 | 2:B:78:LYS:N | 2.11 | 0.66 |
| 1:A:399:HIS:CD2 | 1:A:408:SER:HB3 | 2.30 | 0.66 |
| 1:A:79:GLU:CA | 1:A:79:GLU:OE1 | 2.37 | 0.66 |
| 1:A:427:TRP:CH2 | 1:A:468:PHE:HE2 | 2.13 | 0.66 |
| 1:A:459:ASP:OD1 | 1:A:462:GLU:HB2 | 1.94 | 0.66 |
| 1:A:712:GLU:O | 1:A:716:ARG:HG3 | 1.95 | 0.66 |
| 2:B:261:VAL:HG13 | 2:B:282:VAL:O | 1.96 | 0.66 |
| 1:A:212:ILE:HD11 | 1:A:265:GLY:O | 1.96 | 0.66 |
| 1:A:442:PHE:CE1 | 1:A:466:LEU:HD13 | 2.31 | 0.66 |
| 2:B:77:LEU:HD21 | 2:B:186:ILE:HB | 1.78 | 0.66 |
| 1:A:291:THR:HG22 | 1:A:292:PRO:N | 2.11 | 0.65 |
| 1:A:315:PHE:CZ | 1:A:800:LEU:HD13 | 2.31 | 0.65 |
| 1:A:316:PHE:CE1 | 1:A:329:ALA:HB3 | 2.31 | 0.65 |
| 1:A:623:ILE:HG12 | 1:A:697:MET:CG | 2.26 | 0.65 |
| 1:A:791:LYS:CD | 1:A:819:ILE:CG2 | 2.74 | 0.65 |
| 1:A:786:ALA:HB1 | 1:A:946:ARG:CZ | 2.27 | 0.65 |
| 1:A:442:PHE:CE2 | 1:A:466:LEU:CD1 | 2.80 | 0.65 |
| 1:A:524:LEU:HD22 | 1:A:527:CYS:SG | 2.36 | 0.65 |
| 1:A:1014:ILE:HG23 | 1:A:1015:ARG:N | 2.12 | 0.65 |
| 1:A:360:LEU:HD13 | 1:A:363:LYS:CD | 2.19 | 0.65 |
| 1:A:966:ILE:HG23 | 1:A:970:PHE:CE2 | 2.32 | 0.65 |
| 1:A:452:PRO:HG2 | 1:A:453:LYS:HD2 | 1.76 | 0.65 |
| 1:A:794:PRO:HG3 | 1:A:870:GLN:HB2 | 1.76 | 0.65 |
| 1:A:903:HIS:CD2 | 1:A:904:LEU:HA | 2.32 | 0.65 |
| 1:A:522:ARG:O | 1:A:526:ARG:HG3 | 1.96 | 0.65 |
| 1:A:752:LYS:NZ | 1:A:758:ILE:HD12 | 2.10 | 0.65 |
| 1:A:1030:GLU:HB2 | 1:A:1031:LEU:HD12 | 1.78 | 0.65 |
| 1:A:491:PHE:CZ | 1:A:496:LYS:HE2 | 2.30 | 0.65 |
| 1:A:122:ILE:HD13 | 1:A:122:ILE:O | 1.96 | 0.65 |
| 1:A:200:VAL:HG12 | 1:A:202:MET:SD | 2.36 | 0.65 |
| 1:A:775:ARG:HH11 | 1:A:840:ILE:C | 1.96 | 0.65 |
| 1:A:876:THR:HG21 | 1:A:1004:PHE:CZ | 2.32 | 0.65 |
| 1:A:181:ILE:CG1 | 1:A:199:LEU:HD23 | 2.26 | 0.65 |
| 1:A:45:LYS:HZ2 | 1:A:281:SER:CB | 2.01 | 0.65 |
| 1:A:791:LYS:CD | 1:A:935:ILE:HG21 | 2.27 | 0.65 |
| 1:A:557:LEU:HD22 | 1:A:559:GLU:OE2 | 1.96 | 0.65 |
| 1:A:87:ASN:HA | 1:A:270:THR:CG2 | 2.26 | 0.65 |
| 1:A:1014:ILE:CG2 | 1:A:1015:ARG:N | 2.59 | 0.65 |
| 1:A:923:GLN:HG3 | 2:B:76:GLN:CG | 2.24 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:443:LYS:CG | 1:A:455:ILE:HG23 | 2.16 | 0.64 |
| 1:A:489:ILE:CG1 | 1:A:582:VAL:HG13 | 2.26 | 0.64 |
| 1:A:539:LEU:CD2 | 1:A:544:ARG:HG3 | 2.27 | 0.64 |
| 1:A:885:GLU:HG3 | 1:A:923:GLN:NE2 | 2.12 | 0.64 |
| 1:A:286:VAL:HG21 | 1:A:735:LYS:HG2 | 1.77 | 0.64 |
| 1:A:841:MET:HE1 | 1:A:841:MET:HA | 1.79 | 0.64 |
| 1:A:207:ARG:HG2 | 1:A:257:MET:HG2 | 1.72 | 0.64 |
| 1:A:338:VAL:HG23 | 1:A:343:GLU:OE2 | 1.98 | 0.64 |
| 2:B:213:LEU:HD21 | 2:B:249:LEU:HD22 | 1.80 | 0.64 |
| 1:A:116:ALA:HB3 | 1:A:145:LEU:HD13 | 1.79 | 0.64 |
| 1:A:124:PHE:CA | 1:A:127:GLN:HG2 | 2.26 | 0.64 |
| 1:A:775:ARG:HD3 | 1:A:840:ILE:HG23 | 1.77 | 0.64 |
| 1:A:903:HIS:CE1 | 2:B:87:ASP:HB2 | 2.33 | 0.64 |
| 1:A:227:LEU:HD21 | 1:A:275:ILE:HD11 | 1.78 | 0.64 |
| 2:B:181:ILE:HG22 | 2:B:224:TYR:OH | 1.97 | 0.64 |
| 1:A:923:GLN:HE21 | 2:B:76:GLN:HG2 | 1.62 | 0.64 |
| 1:A:284:SER:O | 1:A:286:VAL:N | 2.25 | 0.64 |
| 1:A:212:ILE:HD11 | 1:A:265:GLY:CA | 2.27 | 0.64 |
| 1:A:381:VAL:HG22 | 1:A:382:ILE:N | 2.10 | 0.64 |
| 1:A:559:GLU:CG | 1:A:600:MET:O | 2.34 | 0.64 |
| 2:B:54:ILE:O | 2:B:57:LEU:HB3 | 1.97 | 0.64 |
| 1:A:801:ILE:O | 1:A:805:VAL:HG12 | 1.98 | 0.64 |
| 2:B:77:LEU:CG | 2:B:186:ILE:HD12 | 2.26 | 0.64 |
| 1:A:308:ALA:HA | 1:A:340:TYR:CD2 | 2.32 | 0.64 |
| 1:A:312:GLY:C | 1:A:333:PHE:HD1 | 2.02 | 0.64 |
| 2:B:271:PHE:HB3 | 2:B:281:LYS:HE3 | 1.79 | 0.64 |
| 1:A:179:THR:O | 1:A:179:THR:HG23 | 1.98 | 0.63 |
| 1:A:903:HIS:CD2 | 1:A:904:LEU:CA | 2.78 | 0.63 |
| 2:B:130:ASN:OD1 | 2:B:153:LYS:HD2 | 1.97 | 0.63 |
| 1:A:442:PHE:CZ | 1:A:466:LEU:HD22 | 2.34 | 0.63 |
| 1:A:994:ARG:HH22 | 2:B:73:TYR:HB3 | 1.62 | 0.63 |
| 1:A:286:VAL:HG21 | 1:A:735:LYS:CG | 2.28 | 0.63 |
| 1:A:322:ILE:HG23 | 1:A:324:TYR:CE2 | 2.33 | 0.63 |
| 1:A:316:PHE:CE1 | 1:A:329:ALA:CB | 2.82 | 0.63 |
| 1:A:483:PHE:CZ | 1:A:505:GLU:HG2 | 2.34 | 0.63 |
| 1:A:791:LYS:HD2 | 1:A:819:ILE:HG23 | 1.80 | 0.63 |
| 2:B:148:THR:O | 2:B:148:THR:CG2 | 2.46 | 0.63 |
| 2:B:85:ARG:HB2 | 2:B:180:ILE:HD11 | 1.81 | 0.63 |
| 1:A:346:LEU:H | 1:A:346:LEU:HD23 | 1.62 | 0.63 |
| 1:A:473:LEU:HG | 1:A:479:TYR:CE1 | 2.34 | 0.63 |
| 1:A:120:CYS:CB | 1:A:142:ALA:HB2 | 2.29 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:786:ALA:CB | 1:A:858:LEU:HD21 | 2.21 | 0.63 |
| 2:B:129:ILE:HG13 | 2:B:130:ASN:N | 2.13 | 0.63 |
| 1:A:275:ILE:HG13 | 1:A:276:ILE:N | 2.13 | 0.63 |
| 1:A:503:THR:O | 1:A:503:THR:CG2 | 2.47 | 0.63 |
| 2:B:137:PHE:HD1 | 2:B:139:GLN:NE2 | 1.97 | 0.63 |
| 2:B:49:VAL:CG1 | 2:B:50:VAL:N | 2.61 | 0.63 |
| 1:A:134:THR:OG1 | 1:A:138:ASN:HB2 | 1.98 | 0.62 |
| 1:A:232:GLU:HB2 | 1:A:233:PRO:HD2 | 1.80 | 0.62 |
| 1:A:328:ARG:O | 1:A:331:VAL:HG22 | 1.99 | 0.62 |
| 1:A:300:PHE:CD1 | 1:A:854:VAL:HG21 | 2.34 | 0.62 |
| 2:B:84:LEU:HD11 | 2:B:282:VAL:HG21 | 1.79 | 0.62 |
| 2:B:69:TYR:HE1 | 2:B:235:LYS:HZ2 | 1.46 | 0.62 |
| 2:B:137:PHE:HD1 | 2:B:139:GLN:HE21 | 1.46 | 0.62 |
| 1:A:354:SER:N | 1:A:370:LEU:HD11 | 2.14 | 0.62 |
| 1:A:991:MET:CG | 1:A:992:PRO:HD2 | 2.29 | 0.62 |
| 1:A:298:GLU:O | 1:A:301:VAL:HG22 | 2.00 | 0.62 |
| 1:A:650:VAL:HG13 | 1:A:651:GLU:N | 2.13 | 0.62 |
| 1:A:787:TYR:CE1 | 1:A:943:VAL:HG22 | 2.35 | 0.62 |
| 1:A:830:SER:HB3 | 1:A:963:ILE:HG23 | 1.81 | 0.62 |
| 1:A:961:ASN:OD1 | 1:A:963:ILE:HG22 | 2.00 | 0.62 |
| 1:A:1015:ARG:CD | 1:A:1031:LEU:CD2 | 2.78 | 0.62 |
| 1:A:400:LEU:N | 1:A:400:LEU:HD12 | 2.15 | 0.62 |
| 1:A:64:TYR:C | 1:A:65:GLN:NE2 | 2.45 | 0.62 |
| 1:A:106:ALA:O | 1:A:110:GLN:HB2 | 1.99 | 0.62 |
| 1:A:399:HIS:CD2 | 1:A:408:SER:CB | 2.83 | 0.62 |
| 1:A:66:THR:OG1 | 1:A:72:LEU:HD12 | 2.00 | 0.62 |
| 1:A:791:LYS:HG3 | 1:A:935:ILE:CG2 | 2.28 | 0.62 |
| 1:A:398:SER:HB3 | 1:A:599:SER:O | 1.98 | 0.62 |
| 1:A:69:THR:CG2 | 1:A:70:LYS:H | 2.11 | 0.62 |
| 1:A:743:MET:CE | 1:A:762:ASP:HA | 2.29 | 0.62 |
| 1:A:801:ILE:HG21 | 1:A:875:PHE:HE2 | 1.63 | 0.62 |
| 1:A:360:LEU:O | 1:A:363:LYS:HB2 | 2.00 | 0.62 |
| 1:A:56:SER:HB2 | 1:A:59:GLU:OE2 | 1.99 | 0.62 |
| 1:A:392:GLN:HG3 | 1:A:604:PRO:O | 2.00 | 0.62 |
| 1:A:858:LEU:HD23 | 1:A:1033:TYR:CD2 | 2.35 | 0.62 |
| 1:A:70:LYS:O | 1:A:181:ILE:HG22 | 2.00 | 0.62 |
| 1:A:49:GLU:HG2 | 1:A:50:ILE:N | 2.15 | 0.62 |
| 1:A:807:VAL:CG2 | 1:A:808:PRO:HD2 | 2.30 | 0.62 |
| 1:A:815:THR:HG23 | 1:A:932:PHE:HB2 | 1.81 | 0.62 |
| 1:A:914:GLU:HB2 | 2:B:184:ASN:HA | 1.82 | 0.62 |
| 1:A:880:THR:HG21 | 1:A:1000:VAL:HG21 | 1.81 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:162:LYS:O | 1:A:163:SER:HB2 | 1.99 | 0.61 |
| 1:A:309:ILE:CG2 | 1:A:310:LEU:H | 2.13 | 0.61 |
| 1:A:775:ARG:HD2 | 1:A:840:ILE:HG21 | 1.75 | 0.61 |
| 1:A:807:VAL:HG22 | 1:A:808:PRO:CD | 2.30 | 0.61 |
| 1:A:885:GLU:OE2 | 2:B:76:GLN:HB2 | 2.00 | 0.61 |
| 2:B:84:LEU:CD1 | 2:B:282:VAL:HG21 | 2.29 | 0.61 |
| 1:A:1015:ARG:HE | 1:A:1031:LEU:HB3 | 1.64 | 0.61 |
| 1:A:254:PHE:O | 1:A:255:SER:HB3 | 2.00 | 0.61 |
| 1:A:901:ASN:O | 1:A:904:LEU:HD12 | 2.01 | 0.61 |
| 2:B:213:LEU:CD2 | 2:B:213:LEU:O | 2.48 | 0.61 |
| 1:A:537:LEU:HD12 | 1:A:538:PRO:CD | 2.25 | 0.61 |
| 1:A:873:ALA:HB2 | 1:A:1004:PHE:CB | 2.29 | 0.61 |
| 1:A:87:ASN:HA | 1:A:270:THR:HG22 | 1.82 | 0.61 |
| 2:B:81:GLY:HA2 | 2:B:280:GLY:H | 1.65 | 0.61 |
| 1:A:353:LEU:C | 1:A:370:LEU:HD11 | 2.20 | 0.61 |
| 1:A:345:LEU:HD13 | 1:A:788:THR:HG21 | 1.80 | 0.61 |
| 2:B:142:PHE:HE2 | 2:B:232:TYR:HA | 1.65 | 0.61 |
| 1:A:546:ALA:O | 1:A:549:THR:OG1 | 2.15 | 0.61 |
| 1:A:411:THR:HG21 | 1:A:601:ILE:HG21 | 1.82 | 0.61 |
| 1:A:312:GLY:C | 1:A:333:PHE:CD1 | 2.74 | 0.61 |
| 1:A:346:LEU:HD23 | 1:A:346:LEU:N | 2.16 | 0.61 |
| 1:A:400:LEU:HD22 | 1:A:427:TRP:HZ3 | 1.65 | 0.61 |
| 1:A:532:ILE:HG23 | 1:A:532:ILE:O | 1.99 | 0.61 |
| 1:A:79:GLU:OE2 | 1:A:79:GLU:O | 2.19 | 0.61 |
| 1:A:908:GLN:HA | 1:A:913:GLN:O | 2.00 | 0.61 |
| 2:B:177:PRO:HD3 | 2:B:288:ILE:HG13 | 1.82 | 0.61 |
| 2:B:85:ARG:O | 2:B:86:PRO:O | 2.19 | 0.61 |
| 1:A:775:ARG:HB3 | 1:A:840:ILE:HG21 | 1.82 | 0.61 |
| 1:A:872:PHE:O | 1:A:876:THR:HG23 | 2.01 | 0.61 |
| 1:A:939:GLN:OE1 | 1:A:939:GLN:HA | 1.99 | 0.61 |
| 1:A:674:ILE:HG21 | 1:A:699:PHE:CD2 | 2.36 | 0.60 |
| 1:A:163:SER:CB | 1:A:368:LYS:HD3 | 2.31 | 0.60 |
| 1:A:505:GLU:HG3 | 1:A:506:ASP:N | 2.14 | 0.60 |
| 1:A:567:LEU:HD12 | 1:A:592:LEU:HD22 | 1.83 | 0.60 |
| 1:A:827:PRO:CG | 1:A:967:ALA:HB1 | 2.31 | 0.60 |
| 1:A:511:ARG:CZ | 1:A:511:ARG:HB3 | 2.30 | 0.60 |
| 1:A:500:SER:O | 1:A:514:LEU:HD12 | 2.01 | 0.60 |
| 1:A:782:LYS:HG2 | 1:A:853:LEU:O | 2.01 | 0.60 |
| 1:A:801:ILE:HG21 | 1:A:875:PHE:CE2 | 2.36 | 0.60 |
| 1:A:166:ILE:CD1 | 1:A:753:ASN:HB3 | 2.31 | 0.60 |
| 1:A:794:PRO:HG3 | 1:A:870:GLN:CB | 2.32 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:178:ALA:HB2 | 1:A:194:LEU:HD11 | 1.82 | 0.60 |
| 1:A:760:LEU:CD2 | 1:A:760:LEU:H | 2.13 | 0.60 |
| 1:A:905:GLN:HG3 | 1:A:916:THR:OG1 | 2.02 | 0.60 |
| 2:B:88:VAL:HG21 | 2:B:284:PHE:CE1 | 2.35 | 0.60 |
| 1:A:1011:TYR:HE1 | 2:B:47:PHE:CE1 | 2.13 | 0.60 |
| 1:A:166:ILE:CA | 1:A:753:ASN:ND2 | 2.64 | 0.60 |
| 1:A:324:TYR:HB3 | 1:A:328:ARG:HB3 | 1.82 | 0.60 |
| 1:A:539:LEU:HD22 | 1:A:544:ARG:HG3 | 1.84 | 0.60 |
| 1:A:811:LEU:HD13 | 1:A:931:PHE:HB3 | 1.84 | 0.60 |
| 1:A:208:VAL:HG21 | 1:A:253:PHE:O | 2.01 | 0.60 |
| 1:A:313:ALA:O | 1:A:316:PHE:HB3 | 2.02 | 0.60 |
| 1:A:446:GLN:NE2 | 1:A:455:ILE:HG22 | 2.17 | 0.60 |
| 1:A:442:PHE:CD1 | 1:A:456:VAL:HG22 | 2.37 | 0.60 |
| 1:A:608:VAL:HB | 1:A:609:PRO:HD3 | 1.84 | 0.60 |
| 1:A:311:PHE:HA | 1:A:314:THR:HG22 | 1.83 | 0.60 |
| 1:A:399:HIS:CB | 1:A:407:HIS:O | 2.46 | 0.60 |
| 1:A:394:ARG:HH21 | 1:A:413:GLU:HB3 | 1.66 | 0.60 |
| 1:A:994:ARG:CZ | 2:B:73:TYR:HB3 | 2.32 | 0.60 |
| 1:A:70:LYS:HD3 | 1:A:184:GLY:HA3 | 1.82 | 0.60 |
| 1:A:307:LEU:N | 1:A:307:LEU:HD22 | 2.16 | 0.60 |
| 1:A:336:ILE:CG2 | 1:A:340:TYR:CE1 | 2.84 | 0.60 |
| 1:A:545:GLU:HA | 1:A:548:GLN:HB2 | 1.84 | 0.60 |
| 1:A:711:VAL:HG13 | 1:A:721:VAL:HG21 | 1.84 | 0.60 |
| 1:A:72:LEU:HD11 | 1:A:197:GLY:C | 2.23 | 0.60 |
| 2:B:179:PHE:HE1 | 2:B:249:LEU:HG | 1.67 | 0.60 |
| 1:A:163:SER:HB2 | 1:A:368:LYS:HB3 | 1.84 | 0.59 |
| 1:A:293:ILE:HD13 | 1:A:293:ILE:O | 2.02 | 0.59 |
| 1:A:351:VAL:O | 1:A:355:LEU:HG | 2.01 | 0.59 |
| 1:A:922:TYR:CZ | 1:A:991:MET:HE1 | 2.36 | 0.59 |
| 2:B:252:VAL:HB | 2:B:253:PRO:HD3 | 1.81 | 0.59 |
| 2:B:68:PRO:CD | 2:B:69:TYR:H | 2.13 | 0.59 |
| 1:A:254:PHE:CD2 | 1:A:276:ILE:CD1 | 2.84 | 0.59 |
| 1:A:653:ILE:O | 1:A:654:ALA:C | 2.40 | 0.59 |
| 1:A:1030:GLU:CD | 2:B:40:ILE:HD11 | 2.22 | 0.59 |
| 1:A:45:LYS:HZ1 | 1:A:281:SER:CB | 2.12 | 0.59 |
| 1:A:528:SER:OG | 1:A:591:GLY:HA2 | 2.02 | 0.59 |
| 1:A:640:VAL:HG23 | 1:A:642:ILE:HG13 | 1.84 | 0.59 |
| 2:B:83:THR:OG1 | 2:B:182:LYS:HD3 | 2.01 | 0.59 |
| 1:A:212:ILE:CD1 | 1:A:265:GLY:C | 2.69 | 0.59 |
| 1:A:255:SER:HB3 | 1:A:276:ILE:HG21 | 1.84 | 0.59 |
| 1:A:706:GLN:O | 1:A:710:ILE:HG12 | 2.01 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:166:ILE:CA | 1:A:753:ASN:HB3 | 2.32 | 0.59 |
| 1:A:923:GLN:HE21 | 2:B:76:GLN:CG | 2.16 | 0.59 |
| 1:A:117:ALA:CA | 1:A:145:LEU:HD12 | 2.30 | 0.59 |
| 1:A:314:THR:HG23 | 1:A:315:PHE:CD1 | 2.37 | 0.59 |
| 1:A:827:PRO:HG3 | 1:A:967:ALA:HB1 | 1.84 | 0.59 |
| 1:A:511:ARG:HD2 | 1:A:569:LEU:O | 2.02 | 0.59 |
| 1:A:764:PHE:CE1 | 1:A:767:ILE:HD12 | 2.37 | 0.59 |
| 2:B:32:ARG:NH1 | 2:B:32:ARG:HG2 | 2.18 | 0.59 |
| 1:A:127:GLN:HB2 | 1:A:132:ASP:OD2 | 2.01 | 0.59 |
| 1:A:165:ASN:O | 1:A:753:ASN:CB | 2.51 | 0.59 |
| 1:A:160:GLU:O | 1:A:162:LYS:N | 2.36 | 0.59 |
| 1:A:197:GLY:HA2 | 1:A:266:LEU:HD21 | 1.85 | 0.59 |
| 1:A:353:LEU:HB3 | 1:A:370:LEU:CD1 | 2.32 | 0.59 |
| 1:A:147:ALA:O | 1:A:150:VAL:CG1 | 2.51 | 0.59 |
| 1:A:53:HIS:HB2 | 1:A:250:ASN:HD21 | 1.68 | 0.59 |
| 1:A:427:TRP:CE2 | 1:A:431:CYS:SG | 2.96 | 0.59 |
| 1:A:451:VAL:CG1 | 1:A:471:LEU:HD13 | 2.33 | 0.59 |
| 1:A:114:TRP:CZ2 | 1:A:149:VAL:HG21 | 2.38 | 0.59 |
| 1:A:242:HIS:O | 1:A:248:THR:HG22 | 2.02 | 0.59 |
| 1:A:340:TYR:CZ | 1:A:796:LEU:CD2 | 2.85 | 0.59 |
| 1:A:60:LEU:HD22 | 1:A:213:ARG:HG2 | 1.85 | 0.59 |
| 1:A:684:PRO:O | 1:A:688:VAL:HG23 | 2.02 | 0.59 |
| 1:A:858:LEU:C | 1:A:858:LEU:HD13 | 2.24 | 0.59 |
| 1:A:906:ASP:HA | 2:B:83:THR:HG21 | 1.85 | 0.59 |
| 2:B:282:VAL:CG1 | 2:B:284:PHE:CE2 | 2.86 | 0.59 |
| 2:B:38:VAL:HG23 | 2:B:39:TRP:CD1 | 2.37 | 0.59 |
| 1:A:114:TRP:CH2 | 1:A:149:VAL:HG21 | 2.38 | 0.58 |
| 1:A:332:PHE:O | 1:A:335:ALA:HB3 | 2.03 | 0.58 |
| 1:A:443:LYS:HE2 | 1:A:457:ILE:HG13 | 1.85 | 0.58 |
| 1:A:661:VAL:HG22 | 1:A:662:ASP:N | 2.18 | 0.58 |
| 1:A:752:LYS:HZ2 | 1:A:758:ILE:HD12 | 1.68 | 0.58 |
| 1:A:124:PHE:CD1 | 1:A:134:THR:HG21 | 2.37 | 0.58 |
| 1:A:353:LEU:HB3 | 1:A:370:LEU:HG | 1.83 | 0.58 |
| 1:A:423:SER:O | 1:A:424:SER:O | 2.22 | 0.58 |
| 1:A:477:MET:HG3 | 1:A:478:GLY:H | 1.67 | 0.58 |
| 2:B:273:ASN:HB3 | 2:B:274:PRO:HD3 | 1.84 | 0.58 |
| 1:A:121:LEU:O | 1:A:121:LEU:HD23 | 2.03 | 0.58 |
| 1:A:174:VAL:O | 1:A:175:PRO:O | 2.21 | 0.58 |
| 1:A:220:ARG:HA | 1:A:261:GLY:HA3 | 1.84 | 0.58 |
| 1:A:793:ILE:HD12 | 1:A:793:ILE:N | 2.18 | 0.58 |
| 1:A:64:TYR:CE1 | 1:A:196:VAL:CG2 | 2.87 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:227:LEU:HD21 | 1:A:275:ILE:CD1 | 2.33 | 0.58 |
| 1:A:244:SER:O | 1:A:248:THR:HG23 | 2.04 | 0.58 |
| 1:A:864:PHE:HD1 | 1:A:865:GLN:CG | 2.13 | 0.58 |
| 1:A:87:ASN:CG | 1:A:270:THR:HG23 | 2.23 | 0.58 |
| 1:A:884:GLN:O | 2:B:71:PRO:HB2 | 2.04 | 0.58 |
| 2:B:84:LEU:CG | 2:B:181:ILE:HG12 | 2.33 | 0.58 |
| 2:B:209:ASP:O | 2:B:209:ASP:OD1 | 2.20 | 0.58 |
| 1:A:60:LEU:HD23 | 1:A:266:LEU:HD13 | 1.85 | 0.58 |
| 1:A:664:VAL:HG12 | 1:A:665:ASN:O | 2.02 | 0.58 |
| 1:A:906:ASP:OD1 | 2:B:83:THR:OG1 | 2.21 | 0.58 |
| 1:A:994:ARG:HH22 | 2:B:75:ASP:HB2 | 1.64 | 0.58 |
| 1:A:227:LEU:HD12 | 1:A:227:LEU:N | 2.18 | 0.58 |
| 1:A:524:LEU:HD21 | 1:A:539:LEU:HD11 | 1.84 | 0.58 |
| 1:A:922:TYR:HB3 | 2:B:76:GLN:HE22 | 1.69 | 0.58 |
| 2:B:78:LYS:HG2 | 2:B:79:SER:H | 1.67 | 0.58 |
| 1:A:567:LEU:HD23 | 1:A:568:TYR:N | 2.19 | 0.58 |
| 1:A:826:PHE:CB | 1:A:827:PRO:HD3 | 2.31 | 0.58 |
| 2:B:257:ASP:OD1 | 2:B:285:LYS:HB3 | 2.04 | 0.58 |
| 2:B:68:PRO:CD | 2:B:69:TYR:N | 2.66 | 0.58 |
| 1:A:911:TYR:CE2 | 2:B:71:PRO:HD3 | 2.39 | 0.58 |
| 1:A:149:VAL:HG23 | 1:A:150:VAL:N | 2.19 | 0.58 |
| 1:A:181:ILE:HB | 1:A:199:LEU:HB3 | 1.85 | 0.58 |
| 1:A:968:ILE:HG23 | 1:A:969:VAL:N | 2.19 | 0.58 |
| 1:A:994:ARG:HH21 | 2:B:75:ASP:CG | 2.06 | 0.58 |
| 1:A:791:LYS:HE2 | 1:A:935:ILE:HG22 | 1.84 | 0.58 |
| 2:B:186:ILE:HG23 | 2:B:189:PHE:CB | 2.32 | 0.58 |
| 1:A:1015:ARG:HD2 | 1:A:1031:LEU:HD22 | 1.85 | 0.57 |
| 2:B:264:ILE:HG12 | 2:B:265:LEU:N | 2.18 | 0.57 |
| 1:A:950:ARG:NH2 | 1:A:1020:ARG:HG3 | 2.19 | 0.57 |
| 1:A:164:THR:O | 1:A:165:ASN:HB2 | 2.04 | 0.57 |
| 1:A:253:PHE:O | 1:A:256:THR:HB | 2.04 | 0.57 |
| 1:A:707:LYS:NZ | 1:A:730:ASP:HB3 | 2.18 | 0.57 |
| 1:A:807:VAL:HG23 | 1:A:892:CYS:HB3 | 1.85 | 0.57 |
| 2:B:77:LEU:O | 2:B:77:LEU:HG | 2.04 | 0.57 |
| 1:A:212:ILE:CG1 | 1:A:265:GLY:C | 2.72 | 0.57 |
| 1:A:109:LEU:HD13 | 1:A:301:VAL:HG12 | 1.85 | 0.57 |
| 1:A:499:LEU:HB3 | 1:A:516:MET:HB3 | 1.87 | 0.57 |
| 1:A:922:TYR:HE2 | 1:A:991:MET:SD | 2.18 | 0.57 |
| 1:A:482:ARG:HG3 | 1:A:483:PHE:CD1 | 2.39 | 0.57 |
| 1:A:721:VAL:HG23 | 1:A:721:VAL:O | 2.03 | 0.57 |
| 1:A:827:PRO:HG2 | 1:A:971:GLN:HE21 | 1.70 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:394:ARG:HD2 | 1:A:452:PRO:O | 2.04 | 0.57 |
| 1:A:575:PRO:CB | 1:A:576:PRO:HD2 | 2.34 | 0.57 |
| 1:A:741:VAL:CG1 | 1:A:759:LEU:HD23 | 2.35 | 0.57 |
| 1:A:772:GLU:O | 1:A:772:GLU:HG2 | 2.04 | 0.57 |
| 1:A:237:SER:H | 1:A:249:ARG:HB3 | 1.69 | 0.57 |
| 1:A:791:LYS:HE3 | 1:A:824:ASP:OD2 | 2.04 | 0.57 |
| 1:A:276:ILE:HD12 | 1:A:277:GLY:N | 2.20 | 0.57 |
| 1:A:940:ILE:CD1 | 1:A:968:ILE:HD12 | 2.35 | 0.57 |
| 1:A:969:VAL:O | 1:A:972:VAL:HG12 | 2.05 | 0.57 |
| 1:A:221:LYS:HB2 | 1:A:260:GLU:HG2 | 1.86 | 0.57 |
| 1:A:356:THR:O | 1:A:360:LEU:HD23 | 2.04 | 0.57 |
| 1:A:723:VAL:CG1 | 1:A:734:LEU:HD23 | 2.34 | 0.57 |
| 1:A:966:ILE:HG23 | 1:A:970:PHE:CD2 | 2.40 | 0.57 |
| 1:A:293:ILE:HG23 | 1:A:294:ALA:N | 2.19 | 0.57 |
| 1:A:915:TRP:CH2 | 2:B:77:LEU:CB | 2.88 | 0.57 |
| 2:B:213:LEU:HD23 | 2:B:213:LEU:C | 2.25 | 0.57 |
| 1:A:918:GLY:CA | 2:B:276:ASP:HB3 | 2.35 | 0.57 |
| 1:A:483:PHE:HE2 | 1:A:504:LEU:CD1 | 2.04 | 0.56 |
| 1:A:929:THR:HG23 | 1:A:990:PHE:HD1 | 1.70 | 0.56 |
| 1:A:129:SER:O | 1:A:130:GLU:HG3 | 2.04 | 0.56 |
| 1:A:113:MET:SD | 1:A:346:LEU:HD11 | 2.45 | 0.56 |
| 2:B:259:VAL:CG2 | 2:B:259:VAL:O | 2.51 | 0.56 |
| 1:A:434:LEU:HD22 | 1:A:465:LEU:HD22 | 1.87 | 0.56 |
| 1:A:821:LEU:HD12 | 1:A:821:LEU:N | 2.20 | 0.56 |
| 1:A:922:TYR:CG | 1:A:991:MET:CE | 2.81 | 0.56 |
| 2:B:276:ASP:N | 2:B:276:ASP:OD1 | 2.36 | 0.56 |
| 1:A:235:THR:HG22 | 1:A:236:ARG:N | 2.20 | 0.56 |
| 1:A:242:HIS:CD2 | 1:A:244:SER:H | 2.19 | 0.56 |
| 1:A:336:ILE:HG22 | 1:A:340:TYR:CE1 | 2.41 | 0.56 |
| 1:A:376:LEU:HD22 | 1:A:770:GLY:CA | 2.35 | 0.56 |
| 1:A:784:SER:CA | 1:A:831:LEU:HD22 | 2.33 | 0.56 |
| 1:A:87:ASN:CB | 1:A:270:THR:HG23 | 2.36 | 0.56 |
| 1:A:322:ILE:HG23 | 1:A:324:TYR:HD2 | 1.69 | 0.56 |
| 1:A:466:LEU:O | 1:A:466:LEU:CD2 | 2.54 | 0.56 |
| 1:A:511:ARG:HH11 | 1:A:511:ARG:CB | 2.18 | 0.56 |
| 1:A:613:LEU:O | 1:A:613:LEU:HD13 | 2.05 | 0.56 |
| 1:A:792:ASN:O | 1:A:796:LEU:HD13 | 2.05 | 0.56 |
| 1:A:805:VAL:CG1 | 1:A:807:VAL:HB | 2.36 | 0.56 |
| 1:A:923:GLN:HG2 | 2:B:76:GLN:CD | 2.26 | 0.56 |
| 1:A:113:MET:HE2 | 1:A:145:LEU:O | 2.05 | 0.56 |
| 1:A:511:ARG:HG2 | 1:A:512:HIS:N | 2.17 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:811:LEU:HD11 | 1:A:815:THR:CG2 | 2.35 | 0.56 |
| 1:A:836:ALA:HB1 | 1:A:838:SER:O | 2.05 | 0.56 |
| 1:A:891:LEU:O | 1:A:895:LEU:HD21 | 2.05 | 0.56 |
| 1:A:351:VAL:HG11 | 1:A:829:VAL:HG22 | 1.87 | 0.56 |
| 1:A:885:GLU:CG | 1:A:923:GLN:NE2 | 2.68 | 0.56 |
| 1:A:113:MET:CE | 1:A:148:VAL:HB | 2.35 | 0.56 |
| 1:A:795:GLU:OE1 | 1:A:816:ILE:HG23 | 2.05 | 0.56 |
| 1:A:798:PRO:O | 1:A:801:ILE:HG22 | 2.06 | 0.56 |
| 1:A:922:TYR:CE2 | 1:A:991:MET:HE1 | 2.40 | 0.56 |
| 1:A:90:ARG:HG3 | 1:A:272:ASP:OD2 | 2.05 | 0.56 |
| 1:A:311:PHE:O | 1:A:315:PHE:HD1 | 1.88 | 0.56 |
| 1:A:399:HIS:CD2 | 1:A:408:SER:CA | 2.88 | 0.56 |
| 1:A:442:PHE:CG | 1:A:454:ARG:HD2 | 2.40 | 0.56 |
| 1:A:945:ILE:HB | 1:A:1012:ASP:OD2 | 2.05 | 0.56 |
| 1:A:376:LEU:HB3 | 1:A:771:VAL:HA | 1.88 | 0.56 |
| 1:A:557:LEU:HB2 | 1:A:559:GLU:CD | 2.25 | 0.56 |
| 1:A:872:PHE:HB3 | 2:B:55:PHE:CD1 | 2.41 | 0.56 |
| 1:A:631:ILE:HG23 | 1:A:632:THR:N | 2.21 | 0.55 |
| 1:A:690:ALA:CA | 1:A:693:THR:HG22 | 2.36 | 0.55 |
| 1:A:911:TYR:CZ | 2:B:71:PRO:HD3 | 2.41 | 0.55 |
| 1:A:922:TYR:CE1 | 2:B:275:HIS:CE1 | 2.94 | 0.55 |
| 1:A:189:ILE:HD12 | 1:A:193:GLN:HB2 | 1.87 | 0.55 |
| 1:A:599:SER:OG | 1:A:600:MET:N | 2.38 | 0.55 |
| 1:A:947:LYS:HE3 | 1:A:958:PHE:O | 2.06 | 0.55 |
| 1:A:940:ILE:HD13 | 1:A:968:ILE:CG1 | 2.35 | 0.55 |
| 1:A:903:HIS:CE1 | 2:B:87:ASP:HA | 2.41 | 0.55 |
| 1:A:124:PHE:HA | 1:A:127:GLN:CG | 2.35 | 0.55 |
| 1:A:207:ARG:HA | 1:A:257:MET:HG3 | 1.89 | 0.55 |
| 1:A:442:PHE:CD2 | 1:A:466:LEU:HD11 | 2.42 | 0.55 |
| 1:A:708:LEU:CD1 | 1:A:712:GLU:HG3 | 2.37 | 0.55 |
| 1:A:925:TYR:HD1 | 1:A:989:ASN:HD21 | 1.53 | 0.55 |
| 2:B:77:LEU:CD2 | 2:B:186:ILE:HD12 | 2.37 | 0.55 |
| 1:A:254:PHE:HD2 | 1:A:276:ILE:HD11 | 1.69 | 0.55 |
| 1:A:280:ALA:O | 1:A:281:SER:C | 2.45 | 0.55 |
| 1:A:442:PHE:CE2 | 1:A:466:LEU:HD21 | 2.41 | 0.55 |
| 1:A:530:ILE:HD11 | 1:A:539:LEU:HG | 1.88 | 0.55 |
| 1:A:57:VAL:HG12 | 1:A:58:ALA:N | 2.20 | 0.55 |
| 1:A:63:LYS:C | 1:A:65:GLN:NE2 | 2.60 | 0.55 |
| 2:B:84:LEU:HD11 | 2:B:181:ILE:HG12 | 1.87 | 0.55 |
| 1:A:169:SER:O | 1:A:172:ASN:HB2 | 2.06 | 0.55 |
| 1:A:442:PHE:CE2 | 1:A:466:LEU:CD2 | 2.90 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:557:LEU:CD2 | 1:A:559:GLU:OE2 | 2.54 | 0.55 |
| 1:A:708:LEU:C | 1:A:708:LEU:HD13 | 2.26 | 0.55 |
| 1:A:78:ALA:O | 1:A:79:GLU:C | 2.45 | 0.55 |
| 2:B:282:VAL:HG12 | 2:B:283:GLU:N | 2.22 | 0.55 |
| 1:A:341:VAL:HG23 | 1:A:341:VAL:O | 2.07 | 0.55 |
| 1:A:708:LEU:HD13 | 1:A:712:GLU:HG3 | 1.89 | 0.55 |
| 1:A:861:TYR:CE2 | 1:A:866:ILE:HG13 | 2.41 | 0.55 |
| 1:A:905:GLN:OE1 | 2:B:278:TYR:CD2 | 2.60 | 0.55 |
| 1:A:379:THR:O | 1:A:620:ILE:HG12 | 2.07 | 0.55 |
| 1:A:790:THR:HA | 1:A:862:SER:OG | 2.06 | 0.55 |
| 1:A:661:VAL:HG22 | 1:A:662:ASP:H | 1.72 | 0.54 |
| 2:B:227:HIS:NE2 | 2:B:228:TYR:CE1 | 2.76 | 0.54 |
| 2:B:87:ASP:CG | 2:B:87:ASP:O | 2.44 | 0.54 |
| 1:A:220:ARG:HH11 | 1:A:263:ALA:HB3 | 1.72 | 0.54 |
| 1:A:636:ILE:O | 1:A:640:VAL:HG22 | 2.08 | 0.54 |
| 1:A:806:SER:O | 1:A:896:ARG:HG3 | 2.07 | 0.54 |
| 1:A:143:LEU:O | 1:A:146:ILE:HG22 | 2.07 | 0.54 |
| 1:A:109:LEU:CD2 | 1:A:346:LEU:HD22 | 2.37 | 0.54 |
| 1:A:623:ILE:HG12 | 1:A:697:MET:HG2 | 1.87 | 0.54 |
| 1:A:1015:ARG:CD | 1:A:1031:LEU:HD22 | 2.37 | 0.54 |
| 1:A:251:ILE:N | 1:A:251:ILE:HD12 | 2.21 | 0.54 |
| 1:A:885:GLU:HG3 | 1:A:923:GLN:HE21 | 1.72 | 0.54 |
| 1:A:119:ILE:HG22 | 1:A:334:MET:HB3 | 1.89 | 0.54 |
| 1:A:401:TRP:CZ2 | 1:A:404:ASN:HA | 2.42 | 0.54 |
| 1:A:473:LEU:HD11 | 1:A:479:TYR:OH | 2.08 | 0.54 |
| 1:A:165:ASN:O | 1:A:753:ASN:OD1 | 2.25 | 0.54 |
| 1:A:784:SER:HA | 1:A:831:LEU:CD2 | 2.35 | 0.54 |
| 2:B:134:GLU:HG2 | 2:B:135:LYS:H | 1.73 | 0.54 |
| 2:B:47:PHE:O | 2:B:51:MET:HG2 | 2.07 | 0.54 |
| 2:B:85:ARG:HE | 2:B:86:PRO:N | 2.05 | 0.54 |
| 1:A:1015:ARG:CD | 1:A:1031:LEU:HD23 | 2.35 | 0.54 |
| 1:A:446:GLN:O | 1:A:448:ALA:N | 2.40 | 0.54 |
| 1:A:637:ALA:HB1 | 1:A:643:ILE:HG12 | 1.89 | 0.54 |
| 1:A:366:VAL:CG1 | 1:A:760:LEU:HD21 | 2.37 | 0.54 |
| 1:A:806:SER:HA | 1:A:896:ARG:NE | 2.23 | 0.54 |
| 1:A:856:GLU:H | 1:A:856:GLU:CD | 2.11 | 0.54 |
| 1:A:887:TRP:CH2 | 1:A:907:LEU:HD21 | 2.43 | 0.54 |
| 1:A:166:ILE:HG23 | 1:A:167:ILE:N | 2.22 | 0.54 |
| 1:A:112:LEU:CD2 | 1:A:341:VAL:HG12 | 2.35 | 0.54 |
| 1:A:587:PHE:HB2 | 1:A:588:PRO:CD | 2.33 | 0.54 |
| 1:A:991:MET:HG3 | 1:A:992:PRO:CD | 2.34 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:254:ARG:CD | 2:B:255:ASN:HD22 | 2.08 | 0.54 |
| 1:A:1013:GLU:O | 1:A:1017:LEU:HD13 | 2.08 | 0.54 |
| 1:A:788:THR:HG23 | 1:A:789:LEU:N | 2.22 | 0.54 |
| 1:A:146:ILE:CD1 | 1:A:146:ILE:C | 2.76 | 0.54 |
| 1:A:340:TYR:CZ | 1:A:796:LEU:HD21 | 2.43 | 0.54 |
| 1:A:48:MET:HE3 | 1:A:246:LEU:CG | 2.34 | 0.54 |
| 1:A:693:THR:HG23 | 1:A:694:HIS:CE1 | 2.40 | 0.54 |
| 1:A:999:LEU:HD12 | 1:A:999:LEU:N | 2.23 | 0.54 |
| 1:A:113:MET:HB2 | 1:A:149:VAL:CG1 | 2.38 | 0.53 |
| 1:A:147:ALA:HA | 1:A:150:VAL:HG12 | 1.89 | 0.53 |
| 1:A:44:MET:O | 1:A:44:MET:HG2 | 2.08 | 0.53 |
| 1:A:660:PRO:O | 1:A:663:GLN:HB2 | 2.08 | 0.53 |
| 1:A:282:LEU:CG | 1:A:282:LEU:O | 2.52 | 0.53 |
| 1:A:119:ILE:CG2 | 1:A:334:MET:HE1 | 2.28 | 0.53 |
| 1:A:334:MET:O | 1:A:337:VAL:HG23 | 2.08 | 0.53 |
| 1:A:940:ILE:CG1 | 1:A:968:ILE:HD12 | 2.36 | 0.53 |
| 1:A:925:TYR:CD1 | 1:A:989:ASN:ND2 | 2.75 | 0.53 |
| 1:A:180:VAL:CG1 | 1:A:194:LEU:CD2 | 2.86 | 0.53 |
| 1:A:398:SER:OG | 1:A:600:MET:O | 2.27 | 0.53 |
| 1:A:412:THR:HG22 | 1:A:414:ASP:H | 1.73 | 0.53 |
| 1:A:674:ILE:HG13 | 1:A:678:GLN:OE1 | 2.07 | 0.53 |
| 1:A:707:LYS:HZ3 | 1:A:730:ASP:HB3 | 1.73 | 0.53 |
| 1:A:332:PHE:HE1 | 1:A:799:TYR:HH | 1.49 | 0.53 |
| 2:B:85:ARG:HB2 | 2:B:180:ILE:CG1 | 2.38 | 0.53 |
| 1:A:391:THR:HA | 1:A:604:PRO:CA | 2.28 | 0.53 |
| 1:A:786:ALA:HA | 1:A:858:LEU:HD11 | 1.91 | 0.53 |
| 1:A:864:PHE:C | 1:A:864:PHE:CD1 | 2.82 | 0.53 |
| 1:A:905:GLN:HB3 | 2:B:83:THR:HG22 | 1.90 | 0.53 |
| 1:A:325:THR:OG1 | 1:A:327:LEU:HB2 | 2.08 | 0.53 |
| 1:A:450:PRO:HB2 | 1:A:453:LYS:HD3 | 1.88 | 0.53 |
| 1:A:554:LEU:HA | 1:A:557:LEU:HD13 | 1.91 | 0.53 |
| 1:A:679:LEU:CD2 | 1:A:679:LEU:C | 2.77 | 0.53 |
| 1:A:805:VAL:HG13 | 1:A:807:VAL:N | 2.24 | 0.53 |
| 1:A:856:GLU:CG | 1:A:857:PRO:HD3 | 2.35 | 0.53 |
| 2:B:231:TYR:CE2 | 2:B:233:GLY:HA2 | 2.43 | 0.53 |
| 1:A:1011:TYR:CZ | 2:B:47:PHE:CZ | 2.97 | 0.53 |
| 1:A:1015:ARG:HE | 1:A:1031:LEU:CB | 2.21 | 0.53 |
| 1:A:208:VAL:HG22 | 1:A:256:THR:O | 2.08 | 0.53 |
| 1:A:837:GLU:HB3 | 1:A:951:LEU:HG | 1.90 | 0.53 |
| 1:A:275:ILE:HG13 | 1:A:276:ILE:HG23 | 1.90 | 0.53 |
| 1:A:739:ILE:O | 1:A:739:ILE:HG23 | 2.09 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:126:GLU:CG | 2:B:127:GLY:N | 2.61 | 0.53 |
| 1:A:187:PHE:CD2 | 1:A:188:GLN:O | 2.62 | 0.53 |
| 1:A:469:SER:O | 1:A:473:LEU:HB3 | 2.09 | 0.53 |
| 1:A:674:ILE:O | 1:A:674:ILE:CG2 | 2.53 | 0.53 |
| 1:A:791:LYS:HD3 | 1:A:935:ILE:HG21 | 1.90 | 0.53 |
| 1:A:783:LYS:O | 1:A:946:ARG:HG2 | 2.09 | 0.53 |
| 1:A:400:LEU:CD2 | 1:A:427:TRP:HZ3 | 2.21 | 0.53 |
| 1:A:922:TYR:CD2 | 1:A:991:MET:SD | 2.94 | 0.53 |
| 2:B:84:LEU:CD1 | 2:B:282:VAL:CG2 | 2.86 | 0.53 |
| 1:A:150:VAL:HG13 | 1:A:151:VAL:N | 2.24 | 0.53 |
| 1:A:350:THR:HG23 | 1:A:351:VAL:N | 2.24 | 0.53 |
| 1:A:617:THR:CG2 | 1:A:618:ALA:N | 2.72 | 0.53 |
| 1:A:64:TYR:CE1 | 1:A:196:VAL:HG22 | 2.44 | 0.53 |
| 1:A:79:GLU:CG | 1:A:79:GLU:O | 2.57 | 0.53 |
| 1:A:850:ARG:HG2 | 1:A:850:ARG:O | 2.08 | 0.53 |
| 1:A:877:ASP:OD2 | 1:A:934:SER:HB3 | 2.08 | 0.53 |
| 1:A:327:LEU:O | 1:A:331:VAL:HG13 | 2.08 | 0.52 |
| 1:A:402:PHE:CZ | 1:A:407:HIS:CE1 | 2.97 | 0.52 |
| 1:A:781:LEU:O | 1:A:781:LEU:HD23 | 2.09 | 0.52 |
| 2:B:237:GLN:OE1 | 2:B:240:TYR:CD2 | 2.63 | 0.52 |
| 1:A:415:GLN:HE21 | 1:A:415:GLN:HA | 1.75 | 0.52 |
| 1:A:482:ARG:C | 1:A:484:PRO:HD3 | 2.28 | 0.52 |
| 1:A:482:ARG:O | 1:A:484:PRO:HD3 | 2.08 | 0.52 |
| 1:A:650:VAL:HG12 | 1:A:651:GLU:N | 2.21 | 0.52 |
| 1:A:173:LEU:HD12 | 1:A:173:LEU:H | 1.72 | 0.52 |
| 1:A:340:TYR:CZ | 1:A:796:LEU:HD23 | 2.45 | 0.52 |
| 1:A:377:GLY:C | 1:A:378:SER:OG | 2.47 | 0.52 |
| 1:A:381:VAL:CG2 | 1:A:382:ILE:N | 2.73 | 0.52 |
| 1:A:623:ILE:HG23 | 1:A:697:MET:HG2 | 1.91 | 0.52 |
| 1:A:814:ILE:HG23 | 1:A:815:THR:N | 2.24 | 0.52 |
| 1:A:847:ASN:HD22 | 1:A:849:LYS:N | 2.05 | 0.52 |
| 1:A:180:VAL:HG11 | 1:A:194:LEU:CD2 | 2.39 | 0.52 |
| 1:A:280:ALA:O | 1:A:282:LEU:N | 2.41 | 0.52 |
| 1:A:476:ALA:HB1 | 1:A:480:ARG:HH21 | 1.74 | 0.52 |
| 1:A:690:ALA:HA | 1:A:693:THR:CG2 | 2.39 | 0.52 |
| 1:A:1030:GLU:CB | 1:A:1031:LEU:HD12 | 2.39 | 0.52 |
| 1:A:442:PHE:CZ | 1:A:466:LEU:CD2 | 2.93 | 0.52 |
| 1:A:482:ARG:O | 1:A:484:PRO:CD | 2.58 | 0.52 |
| 1:A:491:PHE:HZ | 1:A:496:LYS:CE | 2.21 | 0.52 |
| 1:A:840:ILE:O | 1:A:840:ILE:HG22 | 2.09 | 0.52 |
| 2:B:84:LEU:HD23 | 2:B:179:PHE:CD2 | 2.44 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:264:ILE:HG12 | 2:B:265:LEU:H | 1.75 | 0.52 |
| 1:A:127:GLN:HG3 | 1:A:134:THR:HG21 | 1.91 | 0.52 |
| 1:A:915:TRP:CH2 | 2:B:77:LEU:CA | 2.93 | 0.52 |
| 1:A:115:VAL:CG1 | 1:A:116:ALA:N | 2.71 | 0.52 |
| 1:A:160:GLU:C | 1:A:162:LYS:N | 2.62 | 0.52 |
| 1:A:189:ILE:HB | 1:A:193:GLN:OE1 | 2.10 | 0.52 |
| 1:A:605:ARG:HB2 | 1:A:608:VAL:CG2 | 2.39 | 0.52 |
| 1:A:166:ILE:HD13 | 1:A:753:ASN:CB | 2.38 | 0.52 |
| 1:A:141:LEU:O | 1:A:141:LEU:HD23 | 2.10 | 0.52 |
| 1:A:699:PHE:CE2 | 1:A:710:ILE:HD12 | 2.45 | 0.52 |
| 1:A:984:MET:N | 1:A:985:PRO:HD2 | 2.25 | 0.52 |
| 1:A:158:TYR:O | 1:A:160:GLU:N | 2.42 | 0.52 |
| 1:A:527:CYS:SG | 1:A:594:PHE:HB2 | 2.50 | 0.52 |
| 1:A:65:GLN:H | 1:A:65:GLN:HE22 | 1.51 | 0.52 |
| 2:B:213:LEU:CD1 | 2:B:260:ILE:CD1 | 2.88 | 0.52 |
| 2:B:271:PHE:HB3 | 2:B:281:LYS:CE | 2.40 | 0.52 |
| 2:B:287:LYS:CE | 2:B:289:GLN:NE2 | 2.61 | 0.52 |
| 1:A:166:ILE:HA | 1:A:753:ASN:HD22 | 1.70 | 0.52 |
| 1:A:254:PHE:HD2 | 1:A:276:ILE:CG1 | 2.23 | 0.52 |
| 1:A:255:SER:CB | 1:A:276:ILE:HG12 | 2.37 | 0.52 |
| 1:A:808:PRO:O | 1:A:810:PRO:HD3 | 2.10 | 0.52 |
| 1:A:791:LYS:CE | 1:A:935:ILE:HG22 | 2.40 | 0.52 |
| 2:B:84:LEU:HD23 | 2:B:179:PHE:HD2 | 1.74 | 0.52 |
| 2:B:85:ARG:HB2 | 2:B:180:ILE:CD1 | 2.39 | 0.52 |
| 1:A:486:VAL:HG23 | 1:A:487:CYS:N | 2.25 | 0.51 |
| 1:A:648:GLU:HA | 1:A:652:ASP:OD2 | 2.10 | 0.51 |
| 1:A:675:ASN:O | 1:A:678:GLN:HG2 | 2.10 | 0.51 |
| 1:A:723:VAL:HG12 | 1:A:734:LEU:HD23 | 1.92 | 0.51 |
| 1:A:914:GLU:C | 2:B:184:ASN:HB3 | 2.28 | 0.51 |
| 2:B:142:PHE:CE2 | 2:B:232:TYR:HA | 2.44 | 0.51 |
| 1:A:1000:VAL:HB | 1:A:1001:PRO:HD3 | 1.91 | 0.51 |
| 1:A:166:ILE:HD13 | 1:A:754:ALA:N | 2.25 | 0.51 |
| 1:A:167:ILE:CG2 | 1:A:168:ALA:N | 2.72 | 0.51 |
| 1:A:215:LEU:HD13 | 1:A:215:LEU:C | 2.31 | 0.51 |
| 1:A:485:LYS:HA | 1:A:502:HIS:ND1 | 2.25 | 0.51 |
| 1:A:487:CYS:SG | 1:A:501:ILE:HD12 | 2.50 | 0.51 |
| 1:A:905:GLN:CG | 2:B:278:TYR:HB3 | 2.35 | 0.51 |
| 1:A:53:HIS:CD2 | 1:A:245:PRO:HG3 | 2.45 | 0.51 |
| 1:A:353:LEU:CB | 1:A:370:LEU:HG | 2.41 | 0.51 |
| 1:A:435:THR:HG23 | 1:A:436:LEU:N | 2.25 | 0.51 |
| 1:A:905:GLN:O | 2:B:83:THR:HG22 | 2.04 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:90:ARG:O | 1:A:91:PRO:C | 2.47 | 0.51 |
| 2:B:126:GLU:HA | 2:B:153:LYS:NZ | 2.24 | 0.51 |
| 1:A:212:ILE:CD1 | 1:A:265:GLY:CA | 2.89 | 0.51 |
| 1:A:212:ILE:HG21 | 1:A:252:ALA:HB3 | 1.91 | 0.51 |
| 1:A:780:ASN:ND2 | 1:A:834:GLU:O | 2.42 | 0.51 |
| 2:B:175:GLY:O | 2:B:176:LYS:O | 2.27 | 0.51 |
| 2:B:77:LEU:HD23 | 2:B:186:ILE:CD1 | 2.40 | 0.51 |
| 1:A:1016:LYS:C | 1:A:1019:VAL:HG22 | 2.29 | 0.51 |
| 1:A:124:PHE:HD1 | 1:A:134:THR:HG21 | 1.74 | 0.51 |
| 1:A:222:VAL:O | 1:A:233:PRO:HA | 2.10 | 0.51 |
| 1:A:523:VAL:HG13 | 1:A:524:LEU:N | 2.25 | 0.51 |
| 1:A:708:LEU:C | 1:A:708:LEU:CD1 | 2.79 | 0.51 |
| 1:A:987:ILE:HG22 | 1:A:988:PHE:CE2 | 2.45 | 0.51 |
| 1:A:181:ILE:HD13 | 1:A:186:LYS:HB3 | 1.90 | 0.51 |
| 1:A:348:THR:O | 1:A:351:VAL:HG12 | 2.11 | 0.51 |
| 1:A:351:VAL:HG11 | 1:A:829:VAL:CG2 | 2.40 | 0.51 |
| 1:A:601:ILE:CG1 | 1:A:602:ASP:N | 2.40 | 0.51 |
| 1:A:864:PHE:CD1 | 1:A:865:GLN:CG | 2.92 | 0.51 |
| 1:A:818:PHE:CE1 | 1:A:988:PHE:CD1 | 2.99 | 0.51 |
| 1:A:434:LEU:CD2 | 1:A:564:PHE:CE2 | 2.94 | 0.51 |
| 1:A:443:LYS:CE | 1:A:457:ILE:CG1 | 2.87 | 0.51 |
| 1:A:466:LEU:CD2 | 1:A:466:LEU:C | 2.79 | 0.51 |
| 1:A:545:GLU:O | 1:A:549:THR:N | 2.44 | 0.51 |
| 1:A:797:THR:N | 1:A:798:PRO:HD2 | 2.26 | 0.51 |
| 1:A:367:VAL:CG1 | 1:A:372:ALA:HB3 | 2.41 | 0.51 |
| 1:A:466:LEU:O | 1:A:466:LEU:HD22 | 2.11 | 0.51 |
| 1:A:978:LEU:CD2 | 1:A:990:PHE:CZ | 2.92 | 0.51 |
| 2:B:227:HIS:CE1 | 2:B:228:TYR:CE1 | 3.00 | 0.51 |
| 1:A:181:ILE:HD13 | 1:A:186:LYS:CB | 2.41 | 0.50 |
| 1:A:674:ILE:HG13 | 1:A:678:GLN:CG | 2.41 | 0.50 |
| 1:A:97:GLU:HB2 | 1:A:99:VAL:CG2 | 2.40 | 0.50 |
| 2:B:185:ARG:NH1 | 2:B:231:TYR:CZ | 2.78 | 0.50 |
| 1:A:1009:PHE:CD1 | 1:A:1009:PHE:C | 2.84 | 0.50 |
| 1:A:353:LEU:HB3 | 1:A:370:LEU:CG | 2.41 | 0.50 |
| 1:A:425:GLU:HG2 | 1:A:534:GLY:HA2 | 1.93 | 0.50 |
| 1:A:901:ASN:CG | 1:A:904:LEU:HD11 | 2.26 | 0.50 |
| 2:B:136:TYR:CG | 2:B:190:LEU:HD23 | 2.46 | 0.50 |
| 1:A:917:PHE:CB | 2:B:278:TYR:CE1 | 2.91 | 0.50 |
| 1:A:394:ARG:NH2 | 1:A:413:GLU:HB3 | 2.25 | 0.50 |
| 1:A:422:GLN:HG3 | 1:A:423:SER:N | 2.25 | 0.50 |
| 1:A:477:MET:HG3 | 1:A:478:GLY:N | 2.26 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:598:VAL:CG1 | 1:A:598:VAL:O | 2.55 | 0.50 |
| 1:A:64:TYR:HB3 | 1:A:197:GLY:HA2 | 1.92 | 0.50 |
| 1:A:314:THR:O | 1:A:318:VAL:HG13 | 2.12 | 0.50 |
| 1:A:398:SER:CB | 1:A:600:MET:O | 2.57 | 0.50 |
| 1:A:674:ILE:CG1 | 1:A:678:GLN:HG3 | 2.42 | 0.50 |
| 1:A:122:ILE:O | 1:A:126:ILE:HG12 | 2.11 | 0.50 |
| 1:A:674:ILE:CG2 | 1:A:699:PHE:CD2 | 2.95 | 0.50 |
| 1:A:799:TYR:O | 1:A:802:TYR:HB3 | 2.11 | 0.50 |
| 1:A:924:GLN:HG2 | 1:A:928:TYR:HE2 | 1.65 | 0.50 |
| 2:B:84:LEU:HD13 | 2:B:282:VAL:CG2 | 2.42 | 0.50 |
| 2:B:84:LEU:HG | 2:B:181:ILE:HG12 | 1.94 | 0.50 |
| 1:A:116:ALA:CB | 1:A:145:LEU:HD13 | 2.42 | 0.50 |
| 1:A:316:PHE:CD1 | 1:A:329:ALA:CB | 2.92 | 0.50 |
| 1:A:64:TYR:CE1 | 1:A:196:VAL:HG21 | 2.47 | 0.50 |
| 2:B:83:THR:O | 2:B:84:LEU:HD12 | 2.11 | 0.50 |
| 1:A:202:MET:HE2 | 1:A:220:ARG:HH12 | 1.76 | 0.50 |
| 1:A:276:ILE:HD12 | 1:A:276:ILE:C | 2.32 | 0.50 |
| 1:A:463:THR:CG2 | 1:A:464:ALA:N | 2.75 | 0.50 |
| 1:A:521:GLU:OE2 | 1:A:548:GLN:NE2 | 2.45 | 0.50 |
| 1:A:581:ASP:O | 1:A:587:PHE:HE1 | 1.95 | 0.50 |
| 1:A:914:GLU:O | 2:B:184:ASN:CG | 2.49 | 0.50 |
| 1:A:906:ASP:N | 2:B:83:THR:HG21 | 2.25 | 0.50 |
| 1:A:1011:TYR:OH | 2:B:47:PHE:CE1 | 2.63 | 0.50 |
| 1:A:157:TYR:CD2 | 1:A:157:TYR:O | 2.65 | 0.50 |
| 1:A:743:MET:HE3 | 1:A:762:ASP:CA | 2.41 | 0.50 |
| 1:A:741:VAL:HG13 | 1:A:759:LEU:HD23 | 1.93 | 0.50 |
| 1:A:905:GLN:OE1 | 2:B:278:TYR:HD2 | 1.91 | 0.50 |
| 1:A:114:TRP:CH2 | 1:A:146:ILE:HG12 | 2.42 | 0.50 |
| 1:A:914:GLU:O | 2:B:184:ASN:ND2 | 2.45 | 0.50 |
| 1:A:916:THR:HG22 | 1:A:919:GLN:CB | 2.42 | 0.50 |
| 1:A:976:CYS:O | 1:A:980:TYR:HD2 | 1.95 | 0.50 |
| 2:B:84:LEU:CD1 | 2:B:181:ILE:HG12 | 2.42 | 0.50 |
| 2:B:68:PRO:CG | 2:B:69:TYR:CE2 | 2.94 | 0.50 |
| 2:B:88:VAL:HG21 | 2:B:284:PHE:CG | 2.47 | 0.50 |
| 1:A:158:TYR:C | 1:A:160:GLU:H | 2.16 | 0.49 |
| 1:A:208:VAL:CG2 | 1:A:253:PHE:O | 2.59 | 0.49 |
| 1:A:119:ILE:CG2 | 1:A:334:MET:CE | 2.71 | 0.49 |
| 1:A:602:ASP:OD1 | 1:A:603:PRO:N | 2.45 | 0.49 |
| 1:A:811:LEU:HD23 | 1:A:816:ILE:CD1 | 2.39 | 0.49 |
| 2:B:68:PRO:CD | 2:B:69:TYR:CD2 | 2.94 | 0.49 |
| 1:A:70:LYS:HD3 | 1:A:184:GLY:HA2 | 1.93 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:415:GLN:NE2 | 1:A:415:GLN:HA | 2.27 | 0.49 |
| 1:A:507:PRO:O | 1:A:510:PRO:HD3 | 2.12 | 0.49 |
| 1:A:105:LEU:O | 1:A:110:GLN:HB3 | 2.12 | 0.49 |
| 1:A:45:LYS:HZ1 | 1:A:281:SER:HB2 | 1.64 | 0.49 |
| 1:A:300:PHE:HD1 | 1:A:854:VAL:HG21 | 1.77 | 0.49 |
| 1:A:353:LEU:CB | 1:A:370:LEU:HD11 | 2.42 | 0.49 |
| 1:A:564:PHE:CE1 | 1:A:598:VAL:HG11 | 2.47 | 0.49 |
| 1:A:629:HIS:HB3 | 1:A:630:PRO:HD2 | 1.94 | 0.49 |
| 1:A:786:ALA:CB | 1:A:946:ARG:CZ | 2.90 | 0.49 |
| 1:A:979:CYS:SG | 1:A:993:ILE:HD12 | 2.53 | 0.49 |
| 1:A:146:ILE:C | 1:A:149:VAL:HG22 | 2.32 | 0.49 |
| 1:A:489:ILE:HG12 | 1:A:582:VAL:CG1 | 2.36 | 0.49 |
| 1:A:940:ILE:HG12 | 1:A:968:ILE:CD1 | 2.41 | 0.49 |
| 2:B:277:PRO:O | 2:B:281:LYS:HG3 | 2.13 | 0.49 |
| 1:A:1000:VAL:HB | 1:A:1001:PRO:CD | 2.43 | 0.49 |
| 1:A:266:LEU:HD23 | 1:A:266:LEU:C | 2.33 | 0.49 |
| 1:A:60:LEU:CD2 | 1:A:266:LEU:HD13 | 2.43 | 0.49 |
| 1:A:923:GLN:CG | 2:B:76:GLN:CD | 2.81 | 0.49 |
| 1:A:870:GLN:HG2 | 1:A:938:CYS:HB3 | 1.95 | 0.49 |
| 2:B:46:ALA:HA | 2:B:49:VAL:CG1 | 2.42 | 0.49 |
| 2:B:78:LYS:CG | 2:B:79:SER:N | 2.76 | 0.49 |
| 1:A:208:VAL:CG2 | 1:A:256:THR:HB | 2.43 | 0.49 |
| 1:A:215:LEU:HD13 | 1:A:215:LEU:O | 2.13 | 0.49 |
| 1:A:283:ALA:O | 1:A:284:SER:C | 2.50 | 0.49 |
| 1:A:659:VAL:HG12 | 1:A:660:PRO:O | 2.13 | 0.49 |
| 1:A:463:THR:HG1 | 1:A:467:LYS:HE3 | 1.76 | 0.49 |
| 1:A:699:PHE:CE2 | 1:A:710:ILE:CD1 | 2.96 | 0.49 |
| 1:A:805:VAL:HG13 | 1:A:807:VAL:HB | 1.95 | 0.49 |
| 1:A:90:ARG:O | 1:A:91:PRO:O | 2.30 | 0.49 |
| 1:A:243:GLU:O | 1:A:245:PRO:HD3 | 2.13 | 0.49 |
| 1:A:63:LYS:C | 1:A:65:GLN:HE22 | 2.16 | 0.49 |
| 2:B:85:ARG:CB | 2:B:180:ILE:CG1 | 2.90 | 0.49 |
| 1:A:841:MET:CE | 1:A:841:MET:CA | 2.84 | 0.49 |
| 1:A:918:GLY:HA3 | 2:B:276:ASP:CB | 2.39 | 0.49 |
| 1:A:940:ILE:HG23 | 1:A:941:ALA:N | 2.25 | 0.49 |
| 1:A:158:TYR:C | 1:A:160:GLU:N | 2.66 | 0.49 |
| 1:A:994:ARG:NE | 2:B:73:TYR:CD1 | 2.81 | 0.49 |
| 1:A:787:TYR:OH | 1:A:827:PRO:HB2 | 2.13 | 0.48 |
| 1:A:795:GLU:HB3 | 1:A:816:ILE:CD1 | 2.39 | 0.48 |
| 1:A:785:ILE:HD13 | 1:A:854:VAL:CG2 | 2.43 | 0.48 |
| 1:A:987:ILE:HG22 | 1:A:988:PHE:CD2 | 2.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:399:HIS:C | 1:A:400:LEU:CD1 | 2.58 | 0.48 |
| 1:A:451:VAL:N | 1:A:452:PRO:HD2 | 2.28 | 0.48 |
| 1:A:380:SER:HB2 | 1:A:719:ALA:HB1 | 1.95 | 0.48 |
| 1:A:382:ILE:HG12 | 1:A:722:ALA:HB3 | 1.94 | 0.48 |
| 1:A:997:TRP:CE3 | 1:A:997:TRP:HA | 2.48 | 0.48 |
| 2:B:266:ALA:N | 2:B:269:VAL:HG22 | 2.28 | 0.48 |
| 1:A:253:PHE:CD1 | 1:A:275:ILE:CD1 | 2.96 | 0.48 |
| 1:A:412:THR:CG2 | 1:A:413:GLU:N | 2.75 | 0.48 |
| 1:A:207:ARG:O | 1:A:209:PRO:HD3 | 2.13 | 0.48 |
| 1:A:303:ILE:O | 1:A:307:LEU:CD2 | 2.59 | 0.48 |
| 1:A:61:GLU:OE2 | 1:A:68:ALA:HB2 | 2.13 | 0.48 |
| 1:A:752:LYS:CG | 1:A:758:ILE:HD11 | 2.32 | 0.48 |
| 2:B:37:TRP:O | 2:B:38:VAL:C | 2.50 | 0.48 |
| 1:A:220:ARG:HD2 | 1:A:263:ALA:HB2 | 1.95 | 0.48 |
| 1:A:481:GLU:O | 1:A:484:PRO:CD | 2.59 | 0.48 |
| 1:A:62:GLN:OE1 | 1:A:62:GLN:HA | 2.12 | 0.48 |
| 1:A:109:LEU:HG | 1:A:346:LEU:CD2 | 2.33 | 0.48 |
| 1:A:105:LEU:O | 1:A:110:GLN:CB | 2.62 | 0.48 |
| 1:A:259:LEU:HD22 | 1:A:259:LEU:O | 2.13 | 0.48 |
| 1:A:328:ARG:HG3 | 1:A:332:PHE:CZ | 2.47 | 0.48 |
| 1:A:336:ILE:HG23 | 1:A:340:TYR:CE1 | 2.48 | 0.48 |
| 1:A:497:PHE:CD1 | 1:A:497:PHE:C | 2.86 | 0.48 |
| 2:B:142:PHE:O | 2:B:143:LEU:HD23 | 2.14 | 0.48 |
| 2:B:139:GLN:HB2 | 2:B:232:TYR:CE1 | 2.48 | 0.48 |
| 1:A:340:TYR:CD1 | 1:A:340:TYR:N | 2.82 | 0.48 |
| 1:A:442:PHE:HZ | 1:A:466:LEU:HD22 | 1.77 | 0.48 |
| 1:A:477:MET:CG | 1:A:478:GLY:H | 2.26 | 0.48 |
| 1:A:524:LEU:C | 1:A:524:LEU:HD13 | 2.33 | 0.48 |
| 1:A:818:PHE:CE1 | 1:A:988:PHE:CE1 | 3.01 | 0.48 |
| 1:A:823:THR:HG21 | 1:A:932:PHE:CZ | 2.48 | 0.48 |
| 1:A:197:GLY:CA | 1:A:266:LEU:HD21 | 2.44 | 0.48 |
| 1:A:336:ILE:O | 1:A:340:TYR:CD1 | 2.67 | 0.48 |
| 1:A:394:ARG:HH22 | 1:A:413:GLU:HA | 1.77 | 0.48 |
| 1:A:662:ASP:O | 1:A:662:ASP:OD1 | 2.31 | 0.48 |
| 1:A:861:TYR:CE2 | 1:A:866:ILE:CG1 | 2.97 | 0.48 |
| 1:A:922:TYR:HA | 1:A:925:TYR:HD2 | 1.79 | 0.48 |
| 1:A:94:GLY:O | 1:A:95:THR:CG2 | 2.62 | 0.48 |
| 1:A:49:GLU:CG | 1:A:50:ILE:N | 2.76 | 0.48 |
| 1:A:787:TYR:CE1 | 1:A:939:GLN:HG3 | 2.49 | 0.48 |
| 1:A:922:TYR:CE1 | 1:A:991:MET:HE1 | 2.49 | 0.48 |
| 1:A:241:THR:OG1 | 1:A:249:ARG:HG3 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:492:ASN:HB2 | 1:A:495:ASN:OD1 | 2.14 | 0.48 |
| 1:A:791:LYS:CD | 1:A:819:ILE:HG23 | 2.43 | 0.48 |
| 1:A:827:PRO:CD | 1:A:967:ALA:HB1 | 2.43 | 0.48 |
| 1:A:981:CYS:HB3 | 1:A:984:MET:SD | 2.54 | 0.48 |
| 1:A:1027:TRP:O | 1:A:1031:LEU:HB2 | 2.14 | 0.47 |
| 1:A:316:PHE:CE1 | 1:A:329:ALA:HB1 | 2.48 | 0.47 |
| 1:A:360:LEU:HA | 1:A:363:LYS:HD2 | 1.96 | 0.47 |
| 1:A:567:LEU:CD1 | 1:A:592:LEU:CD2 | 2.75 | 0.47 |
| 1:A:787:TYR:CZ | 1:A:827:PRO:HB2 | 2.49 | 0.47 |
| 1:A:90:ARG:NH1 | 1:A:272:ASP:CG | 2.66 | 0.47 |
| 1:A:963:ILE:O | 1:A:963:ILE:HD13 | 2.14 | 0.47 |
| 1:A:113:MET:HE1 | 1:A:148:VAL:HB | 1.96 | 0.47 |
| 1:A:135:THR:HG23 | 1:A:136:ASP:N | 2.29 | 0.47 |
| 1:A:208:VAL:HG21 | 1:A:256:THR:HB | 1.96 | 0.47 |
| 1:A:427:TRP:CZ2 | 1:A:431:CYS:SG | 3.07 | 0.47 |
| 1:A:649:THR:CG2 | 1:A:651:GLU:HG2 | 2.44 | 0.47 |
| 1:A:824:ASP:OD1 | 1:A:939:GLN:HG2 | 2.14 | 0.47 |
| 2:B:129:ILE:HG23 | 2:B:152:CYS:HA | 1.96 | 0.47 |
| 1:A:110:GLN:H | 1:A:110:GLN:NE2 | 2.11 | 0.47 |
| 1:A:270:THR:HB | 1:A:273:ARG:HH21 | 1.79 | 0.47 |
| 1:A:827:PRO:O | 1:A:831:LEU:HD13 | 2.14 | 0.47 |
| 2:B:186:ILE:CG2 | 2:B:189:PHE:HB3 | 2.39 | 0.47 |
| 2:B:261:VAL:HG22 | 2:B:283:GLU:CD | 2.34 | 0.47 |
| 1:A:148:VAL:HA | 1:A:151:VAL:HG12 | 1.96 | 0.47 |
| 1:A:157:TYR:CG | 1:A:157:TYR:O | 2.67 | 0.47 |
| 1:A:367:VAL:HG12 | 1:A:369:ASN:O | 2.14 | 0.47 |
| 1:A:399:HIS:HD2 | 1:A:408:SER:HB3 | 1.75 | 0.47 |
| 1:A:463:THR:HG23 | 1:A:464:ALA:N | 2.29 | 0.47 |
| 1:A:587:PHE:CB | 1:A:588:PRO:CD | 2.91 | 0.47 |
| 1:A:90:ARG:CZ | 1:A:272:ASP:OD2 | 2.63 | 0.47 |
| 2:B:228:TYR:CD2 | 2:B:243:PRO:HD3 | 2.49 | 0.47 |
| 1:A:670:ARG:O | 1:A:694:HIS:HB3 | 2.14 | 0.47 |
| 1:A:73:SER:CB | 1:A:76:LEU:HD12 | 2.45 | 0.47 |
| 1:A:767:ILE:O | 1:A:771:VAL:HG13 | 2.14 | 0.47 |
| 1:A:115:VAL:HG13 | 1:A:116:ALA:N | 2.29 | 0.47 |
| 1:A:307:LEU:N | 1:A:307:LEU:CD2 | 2.76 | 0.47 |
| 1:A:823:THR:HG21 | 1:A:932:PHE:HZ | 1.80 | 0.47 |
| 2:B:213:LEU:HD11 | 2:B:260:ILE:HD13 | 1.96 | 0.47 |
| 1:A:311:PHE:C | 1:A:314:THR:HG22 | 2.35 | 0.47 |
| 1:A:348:THR:HG23 | 1:A:349:VAL:N | 2.30 | 0.47 |
| 1:A:363:LYS:O | 1:A:364:ASN:HB2 | 2.15 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:451:VAL:N | 1:A:452:PRO:CD | 2.78 | 0.47 |
| 1:A:483:PHE:HD2 | 1:A:504:LEU:HA | 1.79 | 0.47 |
| 1:A:581:ASP:O | 1:A:587:PHE:CE1 | 2.67 | 0.47 |
| 1:A:806:SER:HA | 1:A:896:ARG:HE | 1.80 | 0.47 |
| 1:A:913:GLN:HA | 2:B:185:ARG:HB2 | 1.97 | 0.47 |
| 1:A:930:VAL:HG23 | 1:A:931:PHE:N | 2.28 | 0.47 |
| 1:A:965:VAL:O | 1:A:968:ILE:CG2 | 2.57 | 0.47 |
| 1:A:450:PRO:C | 1:A:452:PRO:HD2 | 2.35 | 0.47 |
| 1:A:548:GLN:C | 1:A:552:LEU:HD21 | 2.32 | 0.47 |
| 1:A:501:ILE:HD13 | 1:A:580:PHE:CG | 2.49 | 0.47 |
| 1:A:612:VAL:HG12 | 1:A:612:VAL:O | 2.15 | 0.47 |
| 1:A:643:ILE:HD13 | 1:A:696:GLU:HB3 | 1.97 | 0.47 |
| 1:A:625:VAL:CG1 | 1:A:707:LYS:HG3 | 2.39 | 0.47 |
| 1:A:879:PHE:CD1 | 1:A:889:PRO:HB3 | 2.50 | 0.47 |
| 1:A:887:TRP:CH2 | 1:A:907:LEU:CG | 2.85 | 0.47 |
| 1:A:915:TRP:CH2 | 2:B:77:LEU:N | 2.82 | 0.47 |
| 1:A:254:PHE:CD2 | 1:A:276:ILE:CG1 | 2.98 | 0.47 |
| 1:A:580:PHE:HD2 | 1:A:587:PHE:CD1 | 2.33 | 0.47 |
| 1:A:165:ASN:O | 1:A:753:ASN:HB3 | 2.14 | 0.47 |
| 2:B:147:HIS:CG | 2:B:148:THR:H | 2.33 | 0.47 |
| 1:A:124:PHE:O | 1:A:127:GLN:HG2 | 2.14 | 0.47 |
| 1:A:179:THR:CG2 | 1:A:179:THR:O | 2.62 | 0.47 |
| 1:A:194:LEU:CD1 | 1:A:209:PRO:HB2 | 2.45 | 0.47 |
| 1:A:401:TRP:CD1 | 1:A:406:ILE:HD13 | 2.50 | 0.47 |
| 1:A:814:ILE:CD1 | 1:A:988:PHE:HD1 | 2.19 | 0.47 |
| 2:B:136:TYR:CD2 | 2:B:190:LEU:HD23 | 2.50 | 0.47 |
| 1:A:119:ILE:CG2 | 1:A:334:MET:HE2 | 2.42 | 0.46 |
| 1:A:524:LEU:CD2 | 1:A:539:LEU:HD11 | 2.44 | 0.46 |
| 2:B:85:ARG:HB2 | 2:B:180:ILE:HG13 | 1.96 | 0.46 |
| 2:B:77:LEU:CD2 | 2:B:186:ILE:HB | 2.43 | 0.46 |
| 1:A:239:GLU:O | 1:A:239:GLU:HG3 | 2.13 | 0.46 |
| 1:A:394:ARG:NH1 | 1:A:452:PRO:O | 2.46 | 0.46 |
| 1:A:640:VAL:CG2 | 1:A:642:ILE:HG13 | 2.45 | 0.46 |
| 1:A:381:VAL:HG12 | 1:A:721:VAL:HG12 | 1.93 | 0.46 |
| 1:A:788:THR:CG2 | 1:A:789:LEU:N | 2.78 | 0.46 |
| 1:A:794:PRO:CG | 1:A:870:GLN:HB2 | 2.44 | 0.46 |
| 1:A:985:PRO:O | 1:A:989:ASN:HA | 2.14 | 0.46 |
| 2:B:83:THR:O | 2:B:182:LYS:HD2 | 2.15 | 0.46 |
| 1:A:212:ILE:HG12 | 1:A:265:GLY:HA3 | 1.98 | 0.46 |
| 1:A:570:SER:O | 1:A:574:TYR:HD2 | 1.98 | 0.46 |
| 1:A:793:ILE:H | 1:A:793:ILE:CD1 | 2.26 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:77:LEU:HD23 | 2:B:186:ILE:HD12 | 1.98 | 0.46 |
| 1:A:120:CYS:HB2 | 1:A:142:ALA:CB | 2.34 | 0.46 |
| 1:A:962:ARG:O | 1:A:966:ILE:HG13 | 2.15 | 0.46 |
| 2:B:188:LYS:HA | 2:B:230:PRO:HB2 | 1.98 | 0.46 |
| 1:A:117:ALA:HB2 | 1:A:145:LEU:HB2 | 1.98 | 0.46 |
| 1:A:215:LEU:HD12 | 1:A:216:GLN:HE21 | 1.81 | 0.46 |
| 1:A:340:TYR:CE1 | 1:A:796:LEU:CD2 | 2.99 | 0.46 |
| 1:A:415:GLN:HE21 | 1:A:415:GLN:CA | 2.29 | 0.46 |
| 1:A:561:VAL:HG12 | 1:A:562:LEU:N | 2.31 | 0.46 |
| 1:A:689:GLU:O | 1:A:690:ALA:C | 2.51 | 0.46 |
| 1:A:731:SER:HB2 | 1:A:732:PRO:CD | 2.43 | 0.46 |
| 2:B:182:LYS:HD2 | 2:B:182:LYS:H | 1.80 | 0.46 |
| 2:B:80:PRO:HB2 | 2:B:183:MET:SD | 2.55 | 0.46 |
| 1:A:319:ALA:HA | 1:A:322:ILE:HG22 | 1.98 | 0.46 |
| 2:B:141:SER:OG | 2:B:142:PHE:N | 2.49 | 0.46 |
| 1:A:540:ASP:OD2 | 1:A:542:GLN:HB3 | 2.16 | 0.46 |
| 1:A:914:GLU:HB2 | 2:B:184:ASN:CB | 2.46 | 0.46 |
| 2:B:254:ARG:HD3 | 2:B:255:ASN:ND2 | 2.07 | 0.46 |
| 1:A:400:LEU:HD22 | 1:A:427:TRP:CZ3 | 2.49 | 0.46 |
| 1:A:496:LYS:HA | 1:A:496:LYS:HE2 | 1.97 | 0.46 |
| 1:A:166:ILE:CB | 1:A:753:ASN:HB3 | 2.46 | 0.46 |
| 1:A:978:LEU:HG | 1:A:990:PHE:CG | 2.50 | 0.46 |
| 2:B:265:LEU:O | 2:B:266:ALA:HB2 | 2.16 | 0.46 |
| 2:B:82:VAL:O | 2:B:82:VAL:HG23 | 2.16 | 0.46 |
| 2:B:84:LEU:HG | 2:B:181:ILE:CG1 | 2.46 | 0.46 |
| 1:A:311:PHE:CA | 1:A:314:THR:HG22 | 2.44 | 0.46 |
| 1:A:336:ILE:O | 1:A:336:ILE:HG22 | 2.15 | 0.46 |
| 1:A:412:THR:HG22 | 1:A:414:ASP:N | 2.31 | 0.46 |
| 1:A:410:ASP:HB3 | 1:A:415:GLN:CD | 2.36 | 0.46 |
| 1:A:981:CYS:SG | 1:A:982:PRO:HD2 | 2.56 | 0.46 |
| 1:A:993:ILE:N | 1:A:993:ILE:HD13 | 2.23 | 0.46 |
| 2:B:260:ILE:HG22 | 2:B:261:VAL:N | 2.30 | 0.46 |
| 1:A:127:GLN:OE1 | 1:A:138:ASN:HB2 | 2.16 | 0.46 |
| 1:A:524:LEU:HA | 1:A:527:CYS:SG | 2.56 | 0.46 |
| 1:A:712:GLU:HG2 | 1:A:736:LYS:HE3 | 1.98 | 0.46 |
| 1:A:752:LYS:HZ3 | 1:A:758:ILE:HD12 | 1.81 | 0.46 |
| 2:B:176:LYS:HE3 | 2:B:251:ASN:O | 2.16 | 0.46 |
| 1:A:66:THR:HG21 | 1:A:266:LEU:HD11 | 1.98 | 0.45 |
| 1:A:291:THR:CG2 | 1:A:292:PRO:N | 2.78 | 0.45 |
| 1:A:376:LEU:HD22 | 1:A:770:GLY:HA3 | 1.98 | 0.45 |
| 1:A:401:TRP:HD1 | 1:A:406:ILE:HD13 | 1.81 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:679:LEU:HD22 | 1:A:679:LEU:O | 2.14 | 0.45 |
| 1:A:805:VAL:CG1 | 1:A:807:VAL:HG12 | 2.46 | 0.45 |
| 1:A:951:LEU:HD22 | 1:A:955:GLN:OE1 | 2.16 | 0.45 |
| 1:A:674:ILE:HA | 1:A:678:GLN:OE1 | 2.17 | 0.45 |
| 1:A:690:ALA:HA | 1:A:693:THR:HG21 | 1.99 | 0.45 |
| 1:A:898:GLN:O | 1:A:904:LEU:CD1 | 2.63 | 0.45 |
| 1:A:869:ILE:HG21 | 1:A:1008:ILE:HG13 | 1.98 | 0.45 |
| 1:A:376:LEU:HD22 | 1:A:771:VAL:N | 2.31 | 0.45 |
| 1:A:46:LYS:NZ | 1:A:712:GLU:CD | 2.66 | 0.45 |
| 1:A:363:LYS:HE2 | 1:A:773:GLN:NE2 | 2.24 | 0.45 |
| 2:B:176:LYS:O | 2:B:177:PRO:O | 2.34 | 0.45 |
| 1:A:180:VAL:CG1 | 1:A:194:LEU:HD22 | 2.47 | 0.45 |
| 1:A:48:MET:CE | 1:A:246:LEU:CD1 | 2.94 | 0.45 |
| 1:A:602:ASP:HA | 1:A:603:PRO:HD3 | 1.69 | 0.45 |
| 1:A:657:LEU:O | 1:A:658:ARG:HB2 | 2.17 | 0.45 |
| 1:A:286:VAL:HG11 | 1:A:735:LYS:HE3 | 1.96 | 0.45 |
| 1:A:880:THR:HG23 | 1:A:881:ALA:N | 2.32 | 0.45 |
| 1:A:926:THR:O | 1:A:930:VAL:HG13 | 2.17 | 0.45 |
| 1:A:922:TYR:CE1 | 2:B:275:HIS:ND1 | 2.84 | 0.45 |
| 1:A:151:VAL:HG13 | 1:A:152:THR:N | 2.32 | 0.45 |
| 1:A:293:ILE:CG2 | 1:A:294:ALA:N | 2.79 | 0.45 |
| 1:A:451:VAL:CG1 | 1:A:452:PRO:HD3 | 2.46 | 0.45 |
| 1:A:649:THR:HG23 | 1:A:651:GLU:HG2 | 1.97 | 0.45 |
| 1:A:741:VAL:CG1 | 1:A:759:LEU:CD2 | 2.94 | 0.45 |
| 1:A:811:LEU:CD1 | 1:A:815:THR:HG21 | 2.46 | 0.45 |
| 1:A:92:PRO:C | 1:A:94:GLY:H | 2.20 | 0.45 |
| 1:A:235:THR:CG2 | 1:A:236:ARG:N | 2.80 | 0.45 |
| 1:A:456:VAL:HG21 | 1:A:467:LYS:HE3 | 1.98 | 0.45 |
| 1:A:653:ILE:C | 1:A:655:ALA:N | 2.69 | 0.45 |
| 1:A:807:VAL:C | 1:A:896:ARG:HG2 | 2.36 | 0.45 |
| 1:A:94:GLY:C | 1:A:95:THR:HG23 | 2.37 | 0.45 |
| 1:A:965:VAL:HG13 | 1:A:966:ILE:N | 2.32 | 0.45 |
| 2:B:140:GLU:HA | 2:B:140:GLU:OE1 | 2.17 | 0.45 |
| 1:A:100:LYS:HD3 | 1:A:103:ARG:HG3 | 1.99 | 0.45 |
| 1:A:219:GLY:O | 1:A:261:GLY:HA3 | 2.16 | 0.45 |
| 1:A:236:ARG:NH1 | 1:A:251:ILE:O | 2.49 | 0.45 |
| 1:A:544:ARG:O | 1:A:548:GLN:HG2 | 2.16 | 0.45 |
| 1:A:791:LYS:O | 1:A:795:GLU:HG3 | 2.17 | 0.45 |
| 1:A:872:PHE:HD2 | 2:B:55:PHE:CE1 | 2.34 | 0.45 |
| 1:A:917:PHE:HB3 | 2:B:278:TYR:CD1 | 2.51 | 0.45 |
| 2:B:82:VAL:CG2 | 2:B:281:LYS:N | 2.74 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:38:VAL:HG23 | 2:B:39:TRP:H | 1.82 | 0.45 |
| 1:A:162:LYS:HE2 | 1:A:162:LYS:HB2 | 1.73 | 0.45 |
| 1:A:173:LEU:CD1 | 1:A:173:LEU:O | 2.61 | 0.45 |
| 1:A:350:THR:CG2 | 1:A:351:VAL:N | 2.79 | 0.45 |
| 1:A:392:GLN:O | 1:A:393:ASN:HB3 | 2.17 | 0.45 |
| 1:A:407:HIS:HB3 | 1:A:420:PHE:CD2 | 2.52 | 0.45 |
| 1:A:594:PHE:CD1 | 1:A:594:PHE:C | 2.90 | 0.45 |
| 1:A:727:GLY:H | 1:A:730:ASP:CG | 2.18 | 0.45 |
| 1:A:881:ALA:HA | 1:A:997:TRP:CH2 | 2.52 | 0.45 |
| 1:A:318:VAL:HG23 | 1:A:319:ALA:N | 2.31 | 0.45 |
| 1:A:73:SER:HB3 | 1:A:76:LEU:HD12 | 1.98 | 0.45 |
| 1:A:763:ASN:ND2 | 1:A:765:ALA:H | 2.15 | 0.45 |
| 1:A:924:GLN:HG2 | 1:A:928:TYR:CZ | 2.51 | 0.45 |
| 1:A:913:GLN:HE21 | 2:B:77:LEU:CD2 | 2.07 | 0.45 |
| 1:A:251:ILE:CG2 | 1:A:252:ALA:N | 2.80 | 0.45 |
| 1:A:346:LEU:H | 1:A:346:LEU:CD2 | 2.26 | 0.45 |
| 1:A:483:PHE:CD2 | 1:A:504:LEU:HA | 2.52 | 0.45 |
| 1:A:791:LYS:HD2 | 1:A:824:ASP:OD2 | 2.17 | 0.45 |
| 1:A:916:THR:HG21 | 2:B:278:TYR:HB2 | 1.93 | 0.45 |
| 1:A:786:ALA:CB | 1:A:946:ARG:NH1 | 2.76 | 0.45 |
| 1:A:818:PHE:CZ | 1:A:988:PHE:CE1 | 3.04 | 0.45 |
| 1:A:914:GLU:OE1 | 2:B:182:LYS:HD3 | 2.17 | 0.45 |
| 2:B:84:LEU:HD13 | 2:B:282:VAL:HG22 | 1.98 | 0.45 |
| 1:A:92:PRO:CD | 1:A:171:LYS:HE3 | 2.42 | 0.44 |
| 1:A:196:VAL:HG23 | 1:A:267:VAL:O | 2.17 | 0.44 |
| 1:A:353:LEU:HB3 | 1:A:370:LEU:HD11 | 1.99 | 0.44 |
| 1:A:456:VAL:CG2 | 1:A:467:LYS:HE3 | 2.47 | 0.44 |
| 1:A:473:LEU:HG | 1:A:479:TYR:CZ | 2.51 | 0.44 |
| 1:A:823:THR:HB | 1:A:971:GLN:HG3 | 1.99 | 0.44 |
| 1:A:423:SER:O | 1:A:424:SER:C | 2.54 | 0.44 |
| 1:A:764:PHE:CZ | 1:A:767:ILE:HD12 | 2.53 | 0.44 |
| 1:A:947:LYS:HD2 | 1:A:964:LEU:HD21 | 1.98 | 0.44 |
| 1:A:830:SER:HB3 | 1:A:964:LEU:HA | 1.98 | 0.44 |
| 1:A:915:TRP:HH2 | 2:B:76:GLN:HB3 | 1.83 | 0.44 |
| 1:A:915:TRP:CE2 | 2:B:77:LEU:HD13 | 2.52 | 0.44 |
| 1:A:124:PHE:CE1 | 1:A:134:THR:CG2 | 3.00 | 0.44 |
| 1:A:147:ALA:CA | 1:A:150:VAL:HG12 | 2.47 | 0.44 |
| 1:A:473:LEU:CD1 | 1:A:479:TYR:OH | 2.65 | 0.44 |
| 1:A:480:ARG:HB2 | 1:A:480:ARG:HE | 1.63 | 0.44 |
| 1:A:790:THR:HG21 | 1:A:866:ILE:HG22 | 1.99 | 0.44 |
| 1:A:891:LEU:N | 1:A:891:LEU:HD22 | 2.32 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:179:PHE:HE1 | 2:B:249:LEU:CG | 2.30 | 0.44 |
| 2:B:78:LYS:HD3 | 2:B:78:LYS:H | 1.79 | 0.44 |
| 1:A:161:PHE:CG | 1:A:161:PHE:O | 2.71 | 0.44 |
| 1:A:220:ARG:HD2 | 1:A:263:ALA:CB | 2.46 | 0.44 |
| 1:A:339:ALA:O | 1:A:796:LEU:HD11 | 2.18 | 0.44 |
| 1:A:442:PHE:HE2 | 1:A:466:LEU:HD21 | 1.82 | 0.44 |
| 1:A:466:LEU:O | 1:A:466:LEU:HD23 | 2.18 | 0.44 |
| 1:A:643:ILE:HA | 1:A:696:GLU:OE1 | 2.18 | 0.44 |
| 1:A:794:PRO:CG | 1:A:870:GLN:CB | 2.96 | 0.44 |
| 2:B:136:TYR:CD1 | 2:B:190:LEU:HD23 | 2.53 | 0.44 |
| 1:A:805:VAL:HG11 | 1:A:807:VAL:HB | 1.99 | 0.44 |
| 1:A:940:ILE:CG2 | 1:A:941:ALA:N | 2.80 | 0.44 |
| 1:A:1015:ARG:NE | 1:A:1031:LEU:CD2 | 2.81 | 0.44 |
| 1:A:300:PHE:CZ | 1:A:304:ILE:HG13 | 2.52 | 0.44 |
| 1:A:385:ASP:HB2 | 1:A:707:LYS:HZ3 | 1.81 | 0.44 |
| 1:A:411:THR:HG21 | 1:A:601:ILE:HG23 | 1.99 | 0.44 |
| 1:A:446:GLN:O | 1:A:449:VAL:HG22 | 2.17 | 0.44 |
| 1:A:549:THR:O | 1:A:550:ALA:C | 2.55 | 0.44 |
| 1:A:381:VAL:O | 1:A:721:VAL:HA | 2.18 | 0.44 |
| 1:A:775:ARG:HH11 | 1:A:840:ILE:HG22 | 1.82 | 0.44 |
| 2:B:78:LYS:CG | 2:B:79:SER:H | 2.31 | 0.44 |
| 1:A:248:THR:HG1 | 1:A:251:ILE:HD13 | 1.83 | 0.44 |
| 1:A:466:LEU:HD22 | 1:A:466:LEU:C | 2.38 | 0.44 |
| 1:A:532:ILE:CG2 | 1:A:532:ILE:O | 2.64 | 0.44 |
| 1:A:743:MET:CE | 1:A:762:ASP:CA | 2.94 | 0.44 |
| 1:A:760:LEU:N | 1:A:760:LEU:CD2 | 2.77 | 0.44 |
| 1:A:807:VAL:CG2 | 1:A:808:PRO:CD | 2.95 | 0.44 |
| 1:A:858:LEU:C | 1:A:858:LEU:CD1 | 2.86 | 0.44 |
| 1:A:811:LEU:HA | 1:A:928:TYR:HD1 | 1.83 | 0.44 |
| 2:B:242:ASN:CG | 2:B:243:PRO:HD2 | 2.38 | 0.44 |
| 2:B:290:LYS:HG2 | 2:B:290:LYS:O | 2.17 | 0.44 |
| 1:A:1002:MET:O | 1:A:1003:PRO:C | 2.56 | 0.44 |
| 1:A:443:LYS:HD2 | 1:A:455:ILE:HD13 | 2.00 | 0.44 |
| 1:A:531:LEU:HG | 1:A:533:LYS:O | 2.18 | 0.44 |
| 1:A:545:GLU:O | 1:A:549:THR:HG23 | 2.18 | 0.44 |
| 1:A:433:VAL:HG11 | 1:A:564:PHE:HB3 | 1.99 | 0.44 |
| 1:A:806:SER:C | 1:A:896:ARG:HG3 | 2.38 | 0.44 |
| 1:A:940:ILE:HD11 | 1:A:968:ILE:HB | 1.99 | 0.44 |
| 1:A:864:PHE:CZ | 2:B:44:TYR:CD1 | 3.05 | 0.44 |
| 1:A:929:THR:O | 1:A:932:PHE:HB3 | 2.18 | 0.44 |
| 2:B:84:LEU:HD11 | 2:B:282:VAL:CG2 | 2.45 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:472:THR:HG23 | 1:A:473:LEU:N | 2.33 | 0.43 |
| 1:A:652:ASP:OD1 | 1:A:653:ILE:HG13 | 2.18 | 0.43 |
| 1:A:651:GLU:C | 1:A:654:ALA:CB | 2.84 | 0.43 |
| 1:A:669:ALA:O | 1:A:694:HIS:HD2 | 2.01 | 0.43 |
| 1:A:819:ILE:HG22 | 1:A:820:GLU:N | 2.28 | 0.43 |
| 1:A:978:LEU:CD2 | 1:A:990:PHE:CD2 | 2.96 | 0.43 |
| 2:B:185:ARG:NH1 | 2:B:231:TYR:OH | 2.51 | 0.43 |
| 2:B:57:LEU:HD23 | 2:B:57:LEU:C | 2.38 | 0.43 |
| 2:B:82:VAL:CG2 | 2:B:281:LYS:CA | 2.96 | 0.43 |
| 1:A:146:ILE:O | 1:A:149:VAL:HG23 | 2.16 | 0.43 |
| 1:A:322:ILE:CG2 | 1:A:324:TYR:CE2 | 3.02 | 0.43 |
| 1:A:565:CYS:HB3 | 1:A:594:PHE:HA | 2.00 | 0.43 |
| 1:A:693:THR:HG23 | 1:A:694:HIS:N | 2.32 | 0.43 |
| 2:B:182:LYS:HD2 | 2:B:182:LYS:N | 2.33 | 0.43 |
| 1:A:64:TYR:CD1 | 1:A:196:VAL:HG22 | 2.53 | 0.43 |
| 1:A:248:THR:OG1 | 1:A:251:ILE:HD13 | 2.19 | 0.43 |
| 1:A:254:PHE:O | 1:A:255:SER:CB | 2.63 | 0.43 |
| 1:A:315:PHE:CB | 1:A:336:ILE:CD1 | 2.94 | 0.43 |
| 2:B:81:GLY:O | 2:B:184:ASN:CG | 2.56 | 0.43 |
| 1:A:96:PRO:HB2 | 1:A:100:LYS:HG3 | 2.00 | 0.43 |
| 1:A:250:ASN:OD1 | 1:A:251:ILE:CD1 | 2.66 | 0.43 |
| 1:A:640:VAL:HG23 | 1:A:642:ILE:H | 1.84 | 0.43 |
| 1:A:634:LYS:HD2 | 1:A:673:VAL:HG21 | 2.00 | 0.43 |
| 1:A:791:LYS:CD | 1:A:935:ILE:CG2 | 2.96 | 0.43 |
| 1:A:922:TYR:HA | 1:A:925:TYR:CD2 | 2.54 | 0.43 |
| 1:A:94:GLY:O | 1:A:95:THR:HG23 | 2.18 | 0.43 |
| 1:A:827:PRO:HA | 1:A:967:ALA:CB | 2.48 | 0.43 |
| 1:A:378:SER:O | 1:A:720:ILE:HB | 2.19 | 0.43 |
| 1:A:846:ARG:HB2 | 1:A:851:ASP:CG | 2.39 | 0.43 |
| 2:B:149:LYS:HD3 | 2:B:232:TYR:CE2 | 2.53 | 0.43 |
| 2:B:282:VAL:HG13 | 2:B:284:PHE:CZ | 2.53 | 0.43 |
| 1:A:48:MET:HG3 | 1:A:49:GLU:N | 2.34 | 0.43 |
| 1:A:52:ASP:HB2 | 1:A:55:LEU:HD12 | 2.01 | 0.43 |
| 1:A:790:THR:CA | 1:A:862:SER:OG | 2.67 | 0.43 |
| 2:B:185:ARG:HB3 | 2:B:231:TYR:CD2 | 2.53 | 0.43 |
| 1:A:178:ALA:O | 1:A:188:GLN:HA | 2.18 | 0.43 |
| 1:A:222:VAL:HG23 | 1:A:222:VAL:O | 2.18 | 0.43 |
| 1:A:783:LYS:O | 1:A:946:ARG:CG | 2.66 | 0.43 |
| 1:A:254:PHE:CE2 | 1:A:276:ILE:CD1 | 2.87 | 0.43 |
| 1:A:45:LYS:HZ2 | 1:A:281:SER:HB3 | 1.83 | 0.43 |
| 1:A:475:ASN:HB3 | 1:A:477:MET:HG2 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:69:THR:HG23 | 1:A:70:LYS:HG2 | 2.00 | 0.43 |
| 2:B:237:GLN:HB3 | 2:B:240:TYR:HB2 | 2.00 | 0.43 |
| 2:B:251:ASN:ND2 | 2:B:253:PRO:O | 2.52 | 0.43 |
| 1:A:1002:MET:HB3 | 1:A:1003:PRO:CD | 2.43 | 0.43 |
| 1:A:398:SER:OG | 1:A:599:SER:OG | 2.36 | 0.43 |
| 1:A:693:THR:CG2 | 1:A:694:HIS:HD1 | 2.29 | 0.43 |
| 1:A:66:THR:OG1 | 1:A:72:LEU:CD1 | 2.64 | 0.43 |
| 1:A:783:LYS:C | 1:A:831:LEU:HD23 | 2.38 | 0.43 |
| 2:B:180:ILE:C | 2:B:180:ILE:HD12 | 2.39 | 0.43 |
| 1:A:230:GLU:CA | 1:A:230:GLU:OE1 | 2.48 | 0.43 |
| 1:A:451:VAL:HG11 | 1:A:471:LEU:HD13 | 2.00 | 0.43 |
| 1:A:582:VAL:O | 1:A:582:VAL:HG12 | 2.18 | 0.43 |
| 1:A:699:PHE:CZ | 1:A:710:ILE:HD12 | 2.53 | 0.43 |
| 1:A:339:ALA:CB | 1:A:796:LEU:CD1 | 2.85 | 0.43 |
| 1:A:188:GLN:HE21 | 1:A:188:GLN:HB3 | 1.58 | 0.42 |
| 1:A:87:ASN:HD22 | 1:A:271:GLY:H | 1.64 | 0.42 |
| 1:A:391:THR:HG21 | 1:A:636:ILE:HD13 | 2.01 | 0.42 |
| 1:A:402:PHE:O | 1:A:403:ASP:HB2 | 2.19 | 0.42 |
| 1:A:434:LEU:CD2 | 1:A:564:PHE:CZ | 3.02 | 0.42 |
| 1:A:391:THR:CA | 1:A:604:PRO:HA | 2.32 | 0.42 |
| 1:A:60:LEU:CD2 | 1:A:266:LEU:HB3 | 2.48 | 0.42 |
| 1:A:764:PHE:CE1 | 1:A:767:ILE:CD1 | 3.02 | 0.42 |
| 1:A:925:TYR:CG | 1:A:989:ASN:OD1 | 2.72 | 0.42 |
| 1:A:972:VAL:HG13 | 1:A:973:CYS:N | 2.33 | 0.42 |
| 2:B:185:ARG:HH11 | 2:B:185:ARG:HD2 | 1.74 | 0.42 |
| 2:B:48:TYR:HA | 2:B:48:TYR:HD1 | 1.61 | 0.42 |
| 1:A:122:ILE:CG2 | 1:A:123:ALA:N | 2.82 | 0.42 |
| 1:A:163:SER:OG | 1:A:164:THR:N | 2.52 | 0.42 |
| 1:A:311:PHE:HA | 1:A:314:THR:CG2 | 2.47 | 0.42 |
| 1:A:726:ASP:OD1 | 1:A:743:MET:CG | 2.65 | 0.42 |
| 1:A:799:TYR:CE2 | 1:A:803:ILE:HD11 | 2.54 | 0.42 |
| 1:A:861:TYR:CD1 | 1:A:865:GLN:NE2 | 2.87 | 0.42 |
| 2:B:66:ILE:HG22 | 2:B:67:ASP:O | 2.19 | 0.42 |
| 1:A:446:GLN:CB | 1:A:449:VAL:CG2 | 2.83 | 0.42 |
| 1:A:811:LEU:CA | 1:A:928:TYR:HD1 | 2.32 | 0.42 |
| 1:A:984:MET:N | 1:A:985:PRO:CD | 2.82 | 0.42 |
| 2:B:84:LEU:HG | 2:B:181:ILE:HA | 2.01 | 0.42 |
| 1:A:213:ARG:NH1 | 1:A:250:ASN:HB2 | 2.33 | 0.42 |
| 1:A:631:ILE:CG2 | 1:A:632:THR:N | 2.82 | 0.42 |
| 1:A:651:GLU:CA | 1:A:654:ALA:HB2 | 2.46 | 0.42 |
| 1:A:699:PHE:CD2 | 1:A:710:ILE:CD1 | 3.02 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:816:ILE:HG22 | 1:A:820:GLU:OE2 | 2.18 | 0.42 |
| 1:A:1007:LEU:HD21 | 2:B:54:ILE:HD13 | 2.01 | 0.42 |
| 2:B:82:VAL:HG13 | 2:B:280:GLY:CA | 2.42 | 0.42 |
| 1:A:124:PHE:HE1 | 1:A:134:THR:HG23 | 1.83 | 0.42 |
| 1:A:135:THR:CG2 | 1:A:136:ASP:N | 2.81 | 0.42 |
| 1:A:163:SER:C | 1:A:164:THR:OG1 | 2.58 | 0.42 |
| 1:A:422:GLN:CG | 1:A:423:SER:N | 2.82 | 0.42 |
| 1:A:587:PHE:CB | 1:A:588:PRO:HD2 | 2.30 | 0.42 |
| 1:A:805:VAL:O | 1:A:806:SER:HB2 | 2.19 | 0.42 |
| 1:A:811:LEU:CD2 | 1:A:816:ILE:CD1 | 2.97 | 0.42 |
| 1:A:875:PHE:O | 1:A:878:TYR:HB3 | 2.19 | 0.42 |
| 1:A:787:TYR:HB2 | 1:A:946:ARG:HG2 | 2.02 | 0.42 |
| 1:A:872:PHE:HD2 | 2:B:55:PHE:CZ | 2.37 | 0.42 |
| 2:B:75:ASP:O | 2:B:78:LYS:HB3 | 2.20 | 0.42 |
| 1:A:488:GLU:HB2 | 1:A:499:LEU:O | 2.20 | 0.42 |
| 1:A:535:GLN:HG2 | 1:A:536:GLU:N | 2.33 | 0.42 |
| 1:A:702:THR:HA | 1:A:706:GLN:HE22 | 1.80 | 0.42 |
| 1:A:793:ILE:HG22 | 1:A:871:SER:OG | 2.20 | 0.42 |
| 2:B:181:ILE:HG22 | 2:B:182:LYS:N | 2.35 | 0.42 |
| 1:A:182:ARG:NH2 | 1:A:189:ILE:HD13 | 2.35 | 0.42 |
| 1:A:307:LEU:CD2 | 1:A:307:LEU:H | 2.33 | 0.42 |
| 1:A:523:VAL:CG1 | 1:A:524:LEU:N | 2.81 | 0.42 |
| 1:A:46:LYS:O | 1:A:705:GLN:HB3 | 2.20 | 0.42 |
| 1:A:850:ARG:O | 1:A:850:ARG:CG | 2.67 | 0.42 |
| 1:A:994:ARG:H | 1:A:997:TRP:HD1 | 1.65 | 0.42 |
| 1:A:286:VAL:HG21 | 1:A:735:LYS:HG3 | 2.01 | 0.42 |
| 1:A:421:ASP:OD1 | 1:A:421:ASP:O | 2.37 | 0.42 |
| 1:A:504:LEU:HD23 | 1:A:509:ASP:HB2 | 2.02 | 0.42 |
| 1:A:921:LEU:HB3 | 1:A:925:TYR:CE2 | 2.55 | 0.42 |
| 2:B:272:ASP:OD2 | 2:B:275:HIS:HB2 | 2.20 | 0.42 |
| 2:B:40:ILE:HG22 | 2:B:41:SER:N | 2.34 | 0.42 |
| 2:B:82:VAL:HG22 | 2:B:281:LYS:CA | 2.49 | 0.42 |
| 1:A:166:ILE:O | 1:A:170:PHE:HD2 | 2.03 | 0.42 |
| 1:A:811:LEU:HD21 | 1:A:816:ILE:HD13 | 2.01 | 0.42 |
| 1:A:489:ILE:HA | 1:A:490:PRO:HD3 | 1.88 | 0.42 |
| 1:A:532:ILE:O | 1:A:533:LYS:CB | 2.67 | 0.42 |
| 2:B:192:GLY:N | 2:B:268:HIS:HD2 | 2.18 | 0.42 |
| 2:B:290:LYS:O | 2:B:290:LYS:CG | 2.68 | 0.42 |
| 1:A:196:VAL:HG13 | 1:A:196:VAL:O | 2.19 | 0.41 |
| 1:A:380:SER:C | 1:A:620:ILE:HG23 | 2.41 | 0.41 |
| 1:A:801:ILE:HG23 | 1:A:802:TYR:N | 2.35 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:921:LEU:HB3 | 1:A:925:TYR:CZ | 2.55 | 0.41 |
| 1:A:921:LEU:O | 1:A:925:TYR:CD2 | 2.73 | 0.41 |
| 1:A:823:THR:CG2 | 1:A:932:PHE:HZ | 2.33 | 0.41 |
| 2:B:33:THR:O | 2:B:34:LEU:HD23 | 2.20 | 0.41 |
| 1:A:122:ILE:HG23 | 1:A:123:ALA:N | 2.35 | 0.41 |
| 1:A:821:LEU:CD1 | 1:A:821:LEU:N | 2.83 | 0.41 |
| 2:B:213:LEU:HD12 | 2:B:260:ILE:CD1 | 2.50 | 0.41 |
| 1:A:916:THR:HG21 | 2:B:276:ASP:HB2 | 2.02 | 0.41 |
| 2:B:75:ASP:O | 2:B:78:LYS:HD2 | 2.20 | 0.41 |
| 1:A:314:THR:CG2 | 1:A:315:PHE:CD1 | 3.01 | 0.41 |
| 1:A:574:TYR:OH | 1:A:588:PRO:CD | 2.61 | 0.41 |
| 1:A:922:TYR:HB3 | 2:B:76:GLN:NE2 | 2.33 | 0.41 |
| 1:A:966:ILE:CG2 | 1:A:970:PHE:CD2 | 3.02 | 0.41 |
| 1:A:880:THR:CG2 | 1:A:997:TRP:CZ3 | 3.01 | 0.41 |
| 2:B:85:ARG:HB3 | 2:B:86:PRO:HD3 | 2.01 | 0.41 |
| 1:A:110:GLN:H | 1:A:110:GLN:CD | 2.22 | 0.41 |
| 1:A:124:PHE:C | 1:A:127:GLN:HG2 | 2.41 | 0.41 |
| 1:A:124:PHE:CE1 | 1:A:134:THR:HG23 | 2.56 | 0.41 |
| 1:A:207:ARG:CB | 1:A:257:MET:HG3 | 2.49 | 0.41 |
| 1:A:406:ILE:HD11 | 1:A:550:ALA:HB1 | 2.02 | 0.41 |
| 1:A:651:GLU:O | 1:A:652:ASP:O | 2.38 | 0.41 |
| 2:B:154:PHE:HD1 | 2:B:228:TYR:OH | 1.86 | 0.41 |
| 2:B:263:LYS:HD2 | 2:B:271:PHE:CZ | 2.55 | 0.41 |
| 2:B:36:ARG:O | 2:B:39:TRP:N | 2.50 | 0.41 |
| 1:A:669:ALA:O | 1:A:694:HIS:CD2 | 2.74 | 0.41 |
| 1:A:684:PRO:HB2 | 1:A:716:ARG:HH12 | 1.85 | 0.41 |
| 1:A:798:PRO:HA | 1:A:875:PHE:HZ | 1.85 | 0.41 |
| 1:A:927:CYS:HA | 1:A:930:VAL:HG22 | 2.03 | 0.41 |
| 2:B:54:ILE:C | 2:B:57:LEU:HB3 | 2.41 | 0.41 |
| 1:A:1019:VAL:HG23 | 1:A:1020:ARG:N | 2.36 | 0.41 |
| 1:A:210:ALA:HB1 | 1:A:269:ASN:O | 2.19 | 0.41 |
| 1:A:211:ASP:HB2 | 1:A:269:ASN:HB2 | 2.03 | 0.41 |
| 1:A:574:TYR:CE1 | 1:A:578:TYR:CE2 | 3.07 | 0.41 |
| 1:A:657:LEU:C | 1:A:658:ARG:HG3 | 2.33 | 0.41 |
| 1:A:791:LYS:HE2 | 1:A:935:ILE:CG2 | 2.50 | 0.41 |
| 1:A:793:ILE:HD11 | 1:A:863:TYR:HA | 2.01 | 0.41 |
| 1:A:967:ALA:O | 1:A:971:GLN:HB2 | 2.21 | 0.41 |
| 2:B:213:LEU:CD1 | 2:B:260:ILE:HD13 | 2.50 | 0.41 |
| 2:B:272:ASP:CG | 2:B:275:HIS:HB2 | 2.41 | 0.41 |
| 2:B:282:VAL:CG1 | 2:B:283:GLU:N | 2.83 | 0.41 |
| 1:A:1015:ARG:NE | 1:A:1031:LEU:HB3 | 2.32 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:220:ARG:HH21 | 1:A:222:VAL:HG12 | 1.85 | 0.41 |
| 1:A:227:LEU:N | 1:A:227:LEU:CD1 | 2.82 | 0.41 |
| 1:A:251:ILE:N | 1:A:251:ILE:CD1 | 2.83 | 0.41 |
| 1:A:353:LEU:CB | 1:A:370:LEU:CD1 | 2.99 | 0.41 |
| 1:A:353:LEU:HB2 | 1:A:370:LEU:HD21 | 2.02 | 0.41 |
| 1:A:446:GLN:C | 1:A:448:ALA:N | 2.74 | 0.41 |
| 1:A:581:ASP:HB3 | 1:A:584:ALA:O | 2.21 | 0.41 |
| 1:A:814:ILE:HD13 | 1:A:988:PHE:HA | 2.01 | 0.41 |
| 1:A:940:ILE:CD1 | 1:A:968:ILE:CG1 | 2.97 | 0.41 |
| 2:B:34:LEU:O | 2:B:36:ARG:HG3 | 2.20 | 0.41 |
| 1:A:885:GLU:HG3 | 2:B:76:GLN:HB3 | 2.03 | 0.41 |
| 1:A:104:GLN:OE1 | 1:A:104:GLN:HA | 2.21 | 0.41 |
| 1:A:315:PHE:CA | 1:A:318:VAL:HG22 | 2.44 | 0.41 |
| 1:A:341:VAL:HG23 | 1:A:343:GLU:OE2 | 2.20 | 0.41 |
| 1:A:479:TYR:HA | 1:A:482:ARG:CG | 2.48 | 0.41 |
| 1:A:479:TYR:HA | 1:A:482:ARG:HD2 | 1.95 | 0.41 |
| 1:A:351:VAL:CG1 | 1:A:829:VAL:HG22 | 2.49 | 0.41 |
| 1:A:905:GLN:CD | 2:B:278:TYR:CD2 | 2.83 | 0.41 |
| 2:B:254:ARG:C | 2:B:254:ARG:HD3 | 2.41 | 0.41 |
| 2:B:275:HIS:O | 2:B:277:PRO:HD3 | 2.20 | 0.41 |
| 1:A:200:VAL:CG1 | 1:A:202:MET:SD | 3.06 | 0.41 |
| 1:A:208:VAL:HG11 | 1:A:220:ARG:HH22 | 1.84 | 0.41 |
| 1:A:393:ASN:O | 1:A:393:ASN:OD1 | 2.38 | 0.41 |
| 1:A:446:GLN:OE1 | 1:A:454:ARG:CB | 2.63 | 0.41 |
| 1:A:653:ILE:O | 1:A:655:ALA:N | 2.54 | 0.41 |
| 1:A:692:ARG:HH11 | 1:A:692:ARG:HD2 | 1.54 | 0.41 |
| 1:A:171:LYS:C | 1:A:173:LEU:N | 2.61 | 0.41 |
| 1:A:353:LEU:CB | 1:A:370:LEU:CG | 2.98 | 0.41 |
| 1:A:64:TYR:O | 1:A:65:GLN:HB2 | 2.21 | 0.41 |
| 1:A:965:VAL:CG1 | 1:A:966:ILE:N | 2.84 | 0.41 |
| 1:A:814:ILE:CD1 | 1:A:988:PHE:HA | 2.51 | 0.41 |
| 2:B:190:LEU:N | 2:B:190:LEU:HD12 | 2.36 | 0.41 |
| 1:A:1016:LYS:HA | 1:A:1019:VAL:HG22 | 2.02 | 0.41 |
| 1:A:117:ALA:N | 1:A:145:LEU:HD12 | 2.36 | 0.41 |
| 1:A:315:PHE:CB | 1:A:336:ILE:HD11 | 2.51 | 0.41 |
| 1:A:356:THR:HG22 | 1:A:359:ARG:HH21 | 1.86 | 0.41 |
| 1:A:385:ASP:HB3 | 1:A:725:GLY:HA2 | 2.03 | 0.41 |
| 1:A:527:CYS:HB2 | 1:A:592:LEU:O | 2.20 | 0.41 |
| 1:A:60:LEU:HG | 1:A:64:TYR:CD2 | 2.56 | 0.41 |
| 1:A:691:LEU:HD11 | 1:A:713:SER:HB2 | 2.03 | 0.41 |
| 1:A:787:TYR:CZ | 1:A:939:GLN:HG3 | 2.56 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:915:TRP:CZ3 | 2:B:76:GLN:CG | 3.02 | 0.41 |
| 1:A:916:THR:HG22 | 1:A:919:GLN:HB2 | 2.02 | 0.41 |
| 1:A:254:PHE:HD2 | 1:A:276:ILE:CD1 | 2.29 | 0.40 |
| 1:A:527:CYS:CB | 1:A:592:LEU:O | 2.69 | 0.40 |
| 1:A:647:SER:OG | 1:A:671:ALA:HB2 | 2.20 | 0.40 |
| 1:A:699:PHE:CD2 | 1:A:710:ILE:HD11 | 2.56 | 0.40 |
| 1:A:72:LEU:HD13 | 1:A:198:ASP:N | 2.36 | 0.40 |
| 1:A:814:ILE:CG2 | 1:A:815:THR:N | 2.83 | 0.40 |
| 1:A:817:LEU:HA | 1:A:820:GLU:HG2 | 2.02 | 0.40 |
| 1:A:861:TYR:OH | 1:A:866:ILE:HD11 | 2.20 | 0.40 |
| 2:B:85:ARG:N | 2:B:86:PRO:CD | 2.85 | 0.40 |
| 1:A:1026:TRP:HH2 | 2:B:43:TYR:CD2 | 2.39 | 0.40 |
| 1:A:291:THR:CG2 | 1:A:292:PRO:HD2 | 2.52 | 0.40 |
| 1:A:339:ALA:C | 1:A:796:LEU:HD11 | 2.41 | 0.40 |
| 1:A:377:GLY:HA3 | 1:A:774:GLY:C | 2.34 | 0.40 |
| 1:A:473:LEU:HG | 1:A:473:LEU:O | 2.22 | 0.40 |
| 1:A:629:HIS:CB | 1:A:630:PRO:HD2 | 2.51 | 0.40 |
| 1:A:691:LEU:HD12 | 1:A:713:SER:HB3 | 2.02 | 0.40 |
| 1:A:783:LYS:HB3 | 1:A:831:LEU:HD23 | 2.03 | 0.40 |
| 1:A:855:ASN:HD22 | 1:A:857:PRO:CG | 2.32 | 0.40 |
| 2:B:229:PHE:N | 2:B:229:PHE:CD1 | 2.89 | 0.40 |
| 1:A:171:LYS:O | 1:A:174:VAL:HB | 2.20 | 0.40 |
| 1:A:322:ILE:CG2 | 1:A:324:TYR:CD2 | 2.99 | 0.40 |
| 1:A:340:TYR:CE1 | 1:A:796:LEU:HD21 | 2.57 | 0.40 |
| 1:A:428:ARG:HH11 | 1:A:428:ARG:HD3 | 1.70 | 0.40 |
| 1:A:741:VAL:HG13 | 1:A:759:LEU:CD2 | 2.51 | 0.40 |
| 1:A:877:ASP:HA | 1:A:1000:VAL:HG11 | 2.02 | 0.40 |
| 1:A:883:ALA:HA | 1:A:887:TRP:O | 2.22 | 0.40 |
| 1:A:547:PHE:CD1 | 1:A:547:PHE:C | 2.95 | 0.40 |
| 1:A:511:ARG:CZ | 1:A:568:TYR:CE2 | 3.04 | 0.40 |
| 1:A:787:TYR:HE1 | 1:A:943:VAL:CG2 | 2.35 | 0.40 |
| 1:A:884:GLN:HG3 | 2:B:72:ASP:HB3 | 2.04 | 0.40 |
| 1:A:947:LYS:HB3 | 1:A:947:LYS:NZ | 2.37 | 0.40 |
| 1:A:834:GLU:OE2 | 1:A:947:LYS:HE2 | 2.22 | 0.40 |
| 1:A:996:GLN:HA | 1:A:999:LEU:HD13 | 2.04 | 0.40 |
| 2:B:271:PHE:CD1 | 2:B:281:LYS:HE2 | 2.57 | 0.40 |
| 1:A:307:LEU:HD12 | 1:A:311:PHE:HE1 | 1.87 | 0.40 |
| 1:A:322:ILE:CG1 | 1:A:322:ILE:O | 2.60 | 0.40 |
| 1:A:856:GLU:N | 1:A:857:PRO:CD | 2.85 | 0.40 |
| 1:A:790:THR:N | 1:A:862:SER:OG | 2.55 | 0.40 |
| 2:B:213:LEU:HD12 | 2:B:260:ILE:HD11 | 2.02 | 0.40 |

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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 | 991/1034 (96%) | 904 (91%) | 60 (6%) | 27 (3%) | 5 | 38 |
| 2 | B | 163/290 (56%) | 133 (82%) | 17 (10%) | 13 (8%) | 1 | 16 |
| All | All | 1154/1324 (87%) | 1037 (90%) | 77 (7%) | 40 (4%) | 4 | 32 |

All (40) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 163 | SER |
| 1 | A | 172 | ASN |
| 1 | A | 175 | PRO |
| 1 | A | 283 | ALA |
| 1 | A | 378 | SER |
| 1 | A | 395 | MET |
| 1 | A | 423 | SER |
| 1 | A | 510 | PRO |
| 1 | A | 578 | TYR |
| 1 | A | 601 | ILE |
| 1 | A | 603 | PRO |
| 1 | A | 604 | PRO |
| 1 | A | 654 | ALA |
| 2 | B | 86 | PRO |
| 2 | B | 140 | GLU |
| 2 | B | 177 | PRO |
| 1 | A | 91 | PRO |
| 1 | A | 107 | GLY |
| 1 | A | 161 | PHE |
| 1 | A | 285 | GLY |
| 1 | A | 478 | GLY |
| 1 | A | 658 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 128 | SER |
| 2 | B | 255 | ASN |
| 2 | B | 279 | GLU |
| 1 | A | 159 | GLN |
| 1 | A | 424 | SER |
| 2 | B | 193 | ASN |
| 2 | B | 266 | ALA |
| 1 | A | 137 | ASP |
| 1 | A | 447 | ASP |
| 2 | B | 38 | VAL |
| 2 | B | 45 | VAL |
| 1 | A | 93 | ARG |
| 1 | A | 166 | ILE |
| 2 | B | 43 | TYR |
| 2 | B | 49 | VAL |
| 2 | B | 276 | ASP |
| 1 | A | 96 | PRO |
| 1 | A | 153 | GLY |

4.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|----------|-------------|----|
| 1 | A | 840/869 (97%) | 778 (93%) | 62 (7%) | 15 | 45 |
| 2 | B | 162/254 (64%) | 132 (82%) | 30 (18%) | 2 | 11 |
| All | All | 1002/1123 (89%) | 910 (91%) | 92 (9%) | 10 | 34 |

All (92) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 57 | VAL |
| 1 | A | 65 | GLN |
| 1 | A | 83 | ARG |
| 1 | A | 87 | ASN |
| 1 | A | 93 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 99 | VAL |
| 1 | A | 109 | LEU |
| 1 | A | 122 | ILE |
| 1 | A | 146 | ILE |
| 1 | A | 154 | CYS |
| 1 | A | 164 | THR |
| 1 | A | 173 | LEU |
| 1 | A | 174 | VAL |
| 1 | A | 203 | LYS |
| 1 | A | 208 | VAL |
| 1 | A | 293 | ILE |
| 1 | A | 307 | LEU |
| 1 | A | 309 | ILE |
| 1 | A | 346 | LEU |
| 1 | A | 376 | LEU |
| 1 | A | 378 | SER |
| 1 | A | 395 | MET |
| 1 | A | 421 | ASP |
| 1 | A | 443 | LYS |
| 1 | A | 446 | GLN |
| 1 | A | 453 | LYS |
| 1 | A | 466 | LEU |
| 1 | A | 467 | LYS |
| 1 | A | 480 | ARG |
| 1 | A | 532 | ILE |
| 1 | A | 533 | LYS |
| 1 | A | 539 | LEU |
| 1 | A | 552 | LEU |
| 1 | A | 599 | SER |
| 1 | A | 602 | ASP |
| 1 | A | 617 | THR |
| 1 | A | 650 | VAL |
| 1 | A | 657 | LEU |
| 1 | A | 665 | ASN |
| 1 | A | 666 | ARG |
| 1 | A | 667 | LYS |
| 1 | A | 679 | LEU |
| 1 | A | 683 | ASP |
| 1 | A | 697 | MET |
| 1 | A | 708 | LEU |
| 1 | A | 726 | ASP |
| 1 | A | 763 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 805 | VAL |
| 1 | A | 841 | MET |
| 1 | A | 847 | ASN |
| 1 | A | 856 | GLU |
| 1 | A | 884 | GLN |
| 1 | A | 885 | GLU |
| 1 | A | 903 | HIS |
| 1 | A | 904 | LEU |
| 1 | A | 913 | GLN |
| 1 | A | 922 | TYR |
| 1 | A | 963 | ILE |
| 1 | A | 984 | MET |
| 1 | A | 993 | ILE |
| 1 | A | 1006 | LEU |
| 1 | A | 1014 | ILE |
| 2 | B | 32 | ARG |
| 2 | B | 33 | THR |
| 2 | B | 35 | SER |
| 2 | B | 38 | VAL |
| 2 | B | 41 | SER |
| 2 | B | 42 | LEU |
| 2 | B | 48 | TYR |
| 2 | B | 49 | VAL |
| 2 | B | 60 | TYR |
| 2 | B | 61 | VAL |
| 2 | B | 72 | ASP |
| 2 | B | 78 | LYS |
| 2 | B | 85 | ARG |
| 2 | B | 87 | ASP |
| 2 | B | 125 | GLN |
| 2 | B | 126 | GLU |
| 2 | B | 139 | GLN |
| 2 | B | 178 | CYS |
| 2 | B | 182 | LYS |
| 2 | B | 188 | LYS |
| 2 | B | 234 | LYS |
| 2 | B | 235 | LYS |
| 2 | B | 240 | TYR |
| 2 | B | 254 | ARG |
| 2 | B | 262 | CYS |
| 2 | B | 276 | ASP |
| 2 | B | 281 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 287 | LYS |
| 2 | B | 288 | ILE |
| 2 | B | 290 | LYS |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 51 | ASN |
| 1 | A | 65 | GLN |
| 1 | A | 87 | ASN |
| 1 | A | 110 | GLN |
| 1 | A | 188 | GLN |
| 1 | A | 218 | GLN |
| 1 | A | 242 | HIS |
| 1 | A | 404 | ASN |
| 1 | A | 415 | GLN |
| 1 | A | 663 | GLN |
| 1 | A | 694 | HIS |
| 1 | A | 706 | GLN |
| 1 | A | 753 | ASN |
| 1 | A | 763 | ASN |
| 1 | A | 773 | GLN |
| 1 | A | 847 | ASN |
| 1 | A | 855 | ASN |
| 1 | A | 884 | GLN |
| 1 | A | 903 | HIS |
| 1 | A | 913 | GLN |
| 1 | A | 923 | GLN |
| 1 | A | 924 | GLN |
| 1 | A | 971 | GLN |
| 1 | A | 989 | ASN |
| 1 | A | 996 | GLN |
| 2 | B | 76 | GLN |
| 2 | B | 125 | GLN |
| 2 | B | 255 | ASN |
| 2 | B | 268 | HIS |
| 2 | B | 275 | HIS |
| 2 | B | 289 | GLN |

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.