



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:02 AM UTC

PDB ID : 7Y17 / pdb\_00007y17  
Title : Crystal structure of ribosomal ITS2 pre-rRNA processing complex from *Cyberlindnera jadinii*  
Authors : Chen, J.; Liu, L.  
Deposited on : 2022-06-07  
Resolution : 3.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

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

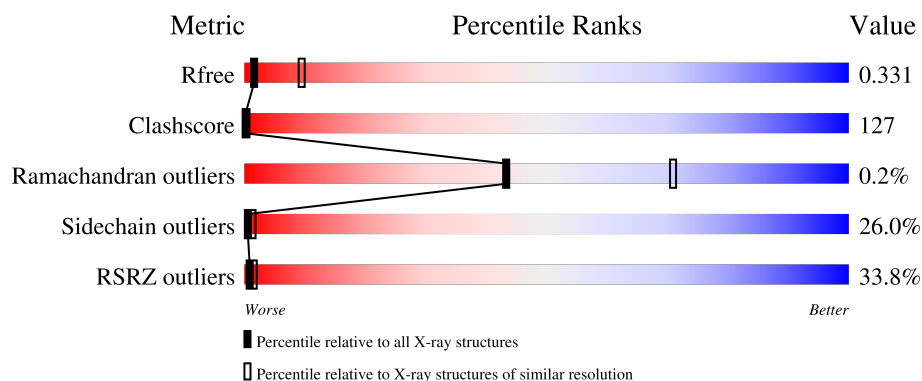
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1001 (3.44-3.36)                                      |
| Clashscore            | 190562                      | 1022 (3.44-3.36)                                      |
| Ramachandran outliers | 187476                      | 1012 (3.44-3.36)                                      |
| Sidechain outliers    | 187428                      | 1012 (3.44-3.36)                                      |
| RSRZ outliers         | 180081                      | 1001 (3.44-3.36)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 610    |                  |
| 1   | B     | 610    |                  |
| 1   | E     | 610    |                  |
| 2   | C     | 421    |                  |
| 2   | D     | 421    |                  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain               |
|-----|-------|--------|--------------------------------|
| 2   | F     | 421    | <p>25%<br/>29% 36% 15% 20%</p> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19118 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 Polynucleotide 5'-hydroxyl-kinase GRC3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | B     | 506      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3713  | 2387 | 619 | 695 | 12 |         |         |       |
| 1   | A     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3817  | 2451 | 636 | 718 | 12 |         |         |       |
| 1   | E     | 519      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3794  | 2429 | 633 | 720 | 12 |         |         |       |

- Molecule 2 is a protein called LAS1 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | C     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2551  | 1622 | 426 | 489 | 14 |         |         |       |
| 2   | D     | 325      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2323  | 1478 | 397 | 436 | 12 |         |         |       |
| 2   | F     | 338      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2534  | 1623 | 422 | 477 | 12 |         |         |       |

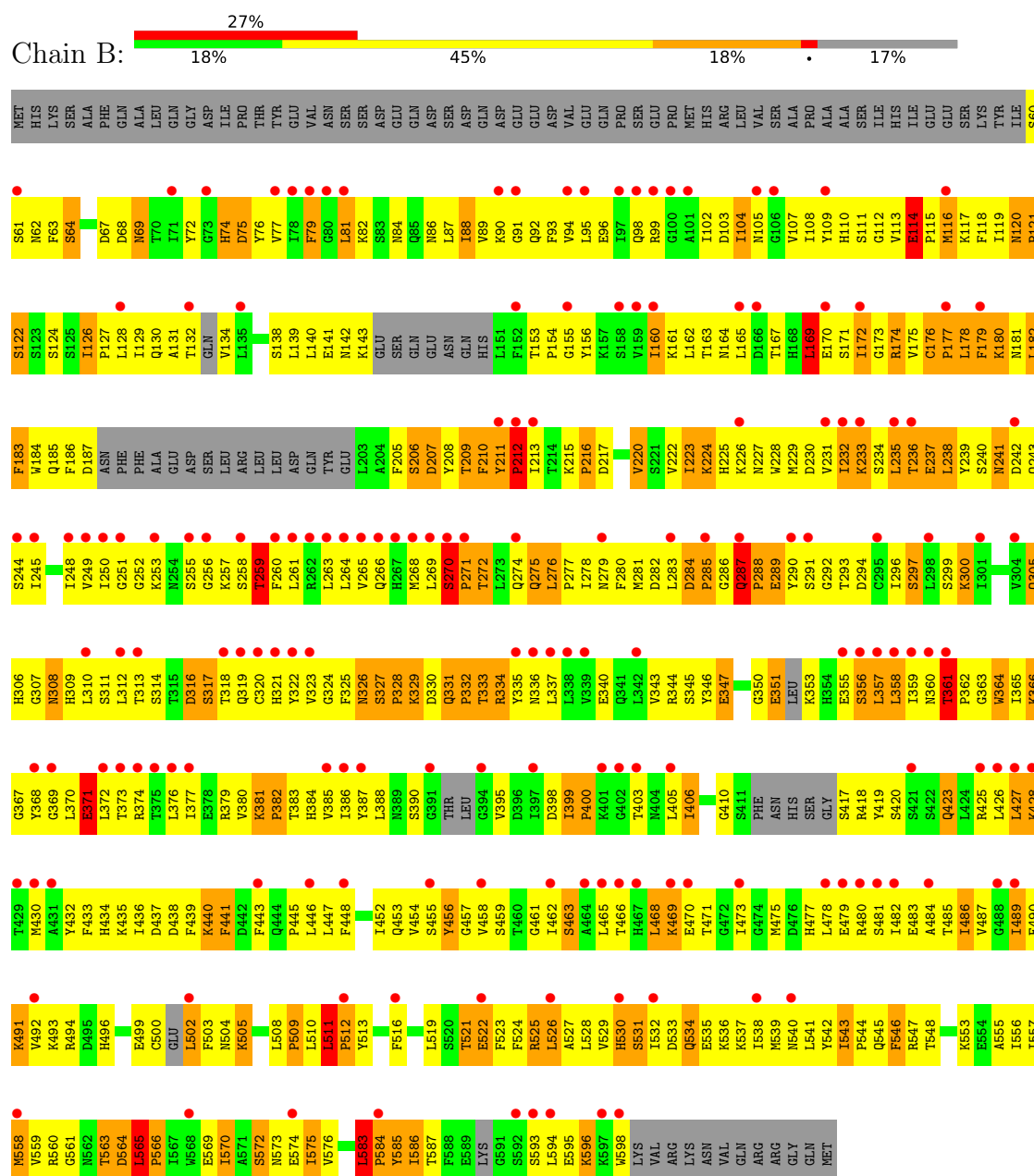
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | B     | 61       | Total | O  | 0       | 0       |
|     |       |          | 61    | 61 |         |         |
| 3   | C     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |
| 3   | D     | 60       | Total | O  | 0       | 0       |
|     |       |          | 60    | 60 |         |         |
| 3   | A     | 94       | Total | O  | 0       | 0       |
|     |       |          | 94    | 94 |         |         |
| 3   | E     | 79       | Total | O  | 0       | 0       |
|     |       |          | 79    | 79 |         |         |
| 3   | F     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |

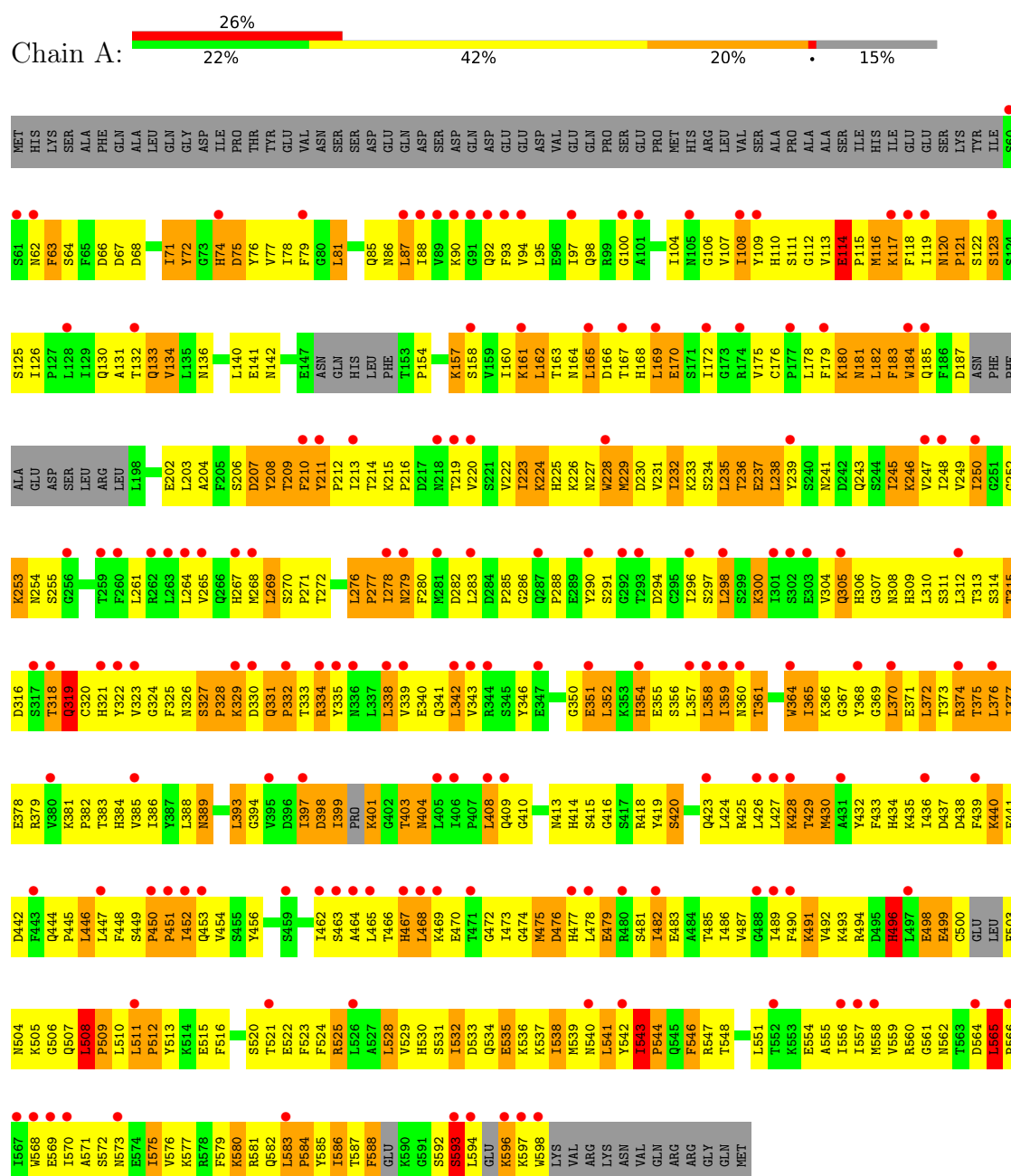
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

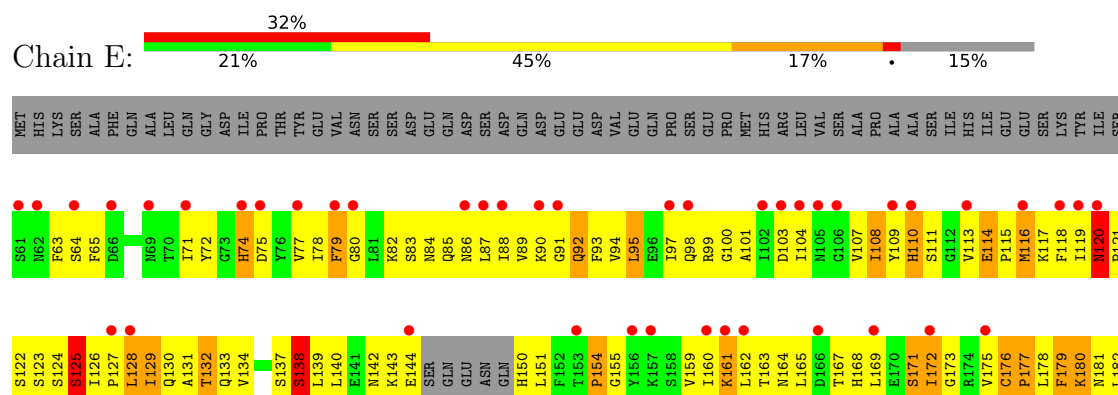
#### • Molecule 1: Polynucleotide 5'-hydroxyl-kinase GRC3

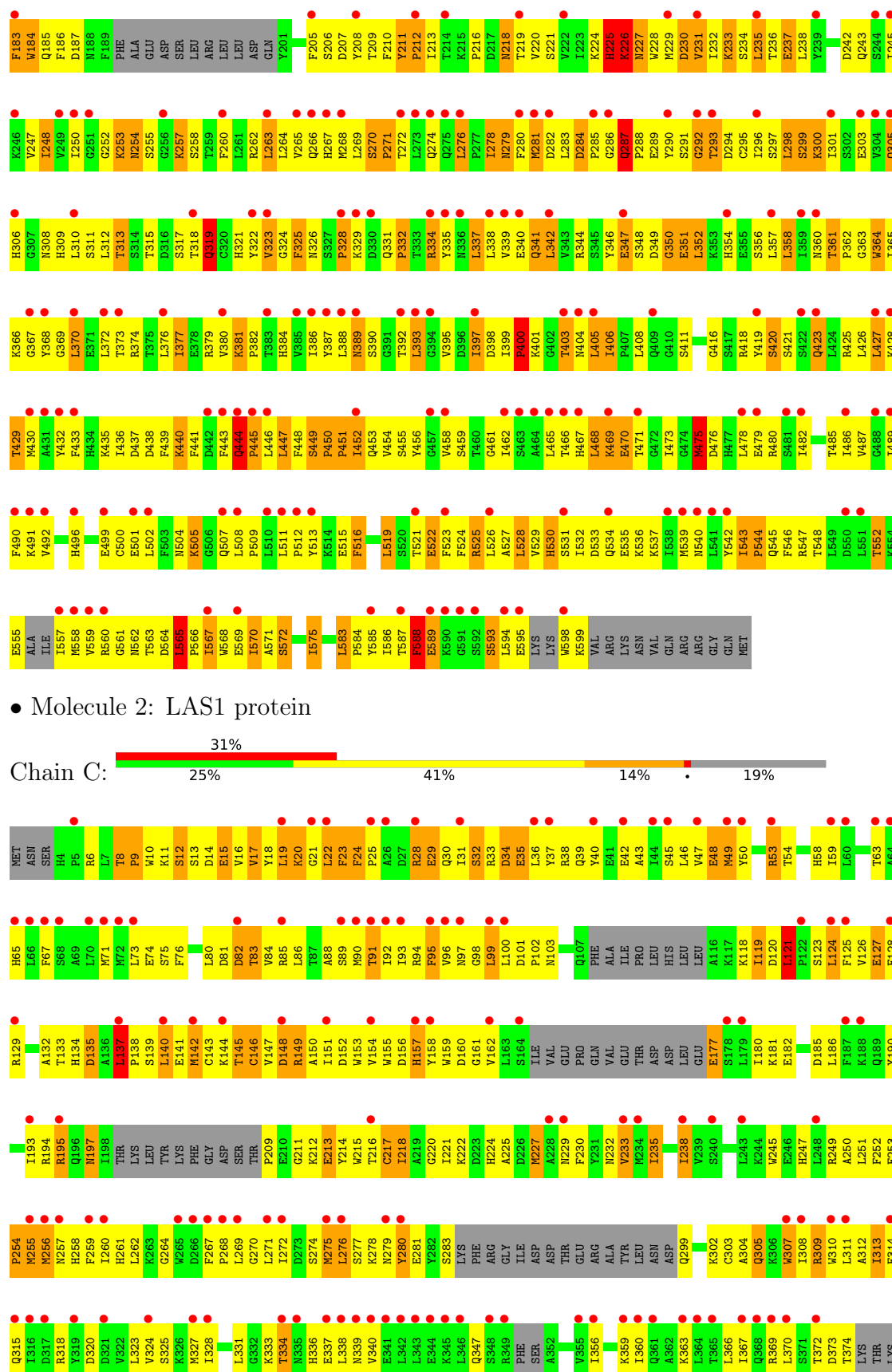


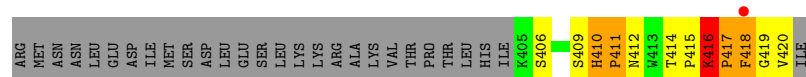
#### • Molecule 1: Polynucleotide 5'-hydroxyl-kinase GRC3



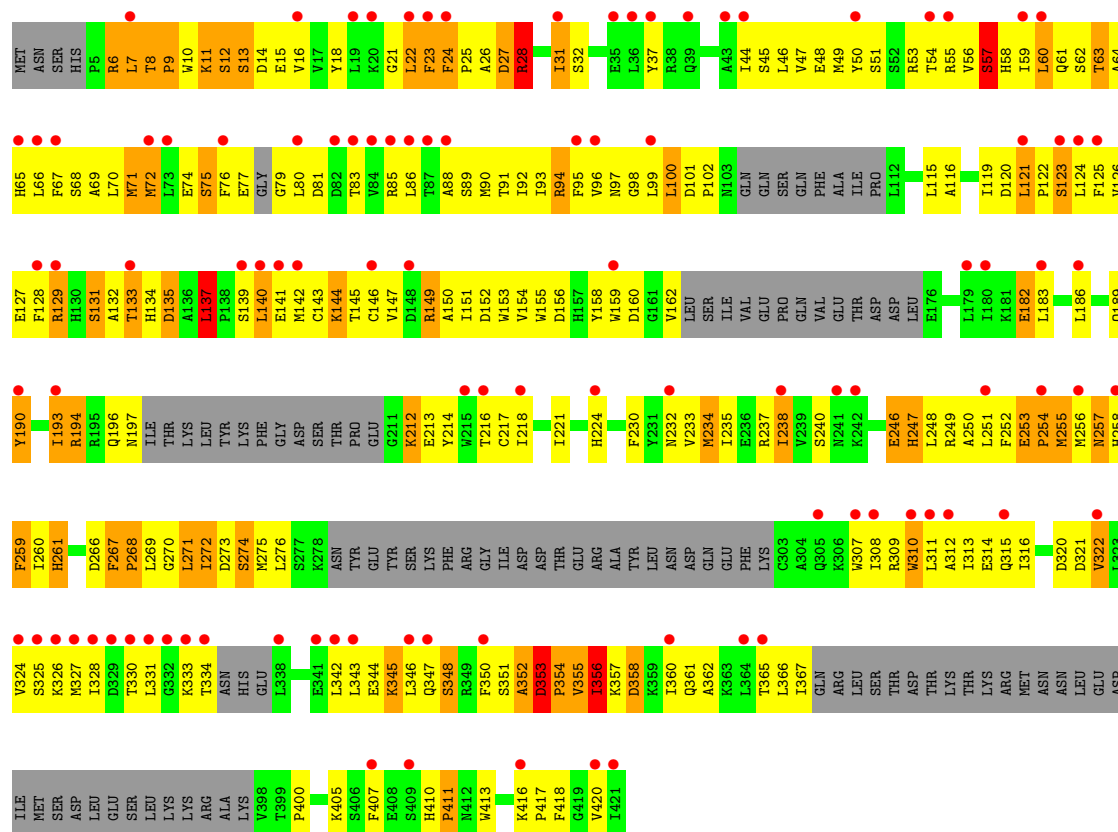
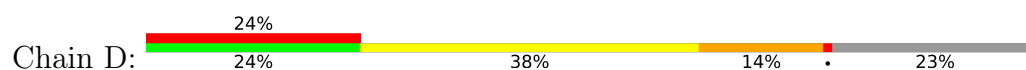
• Molecule 1: Polynucleotide 5'-hydroxyl-kinase GRC3



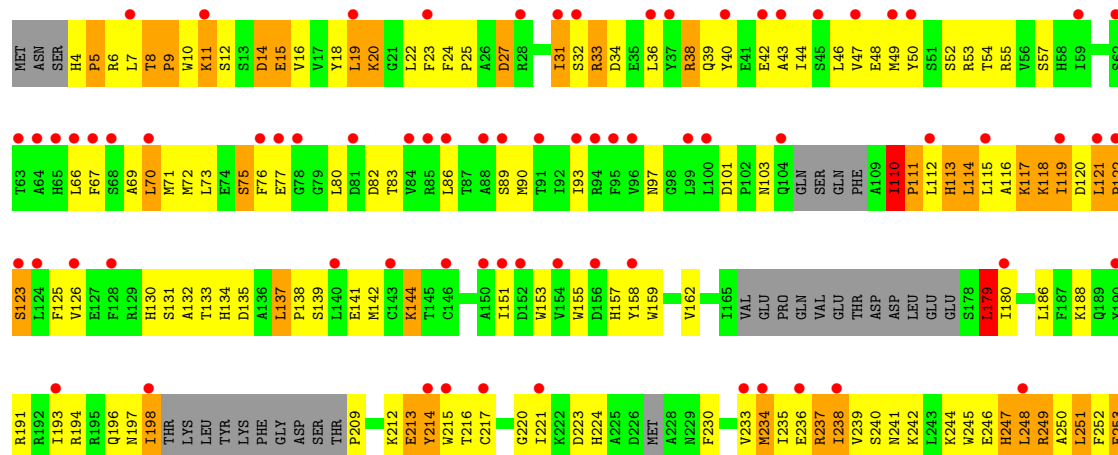
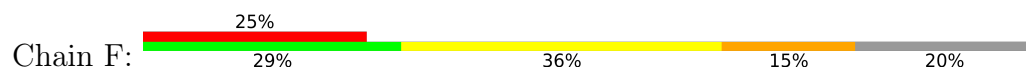


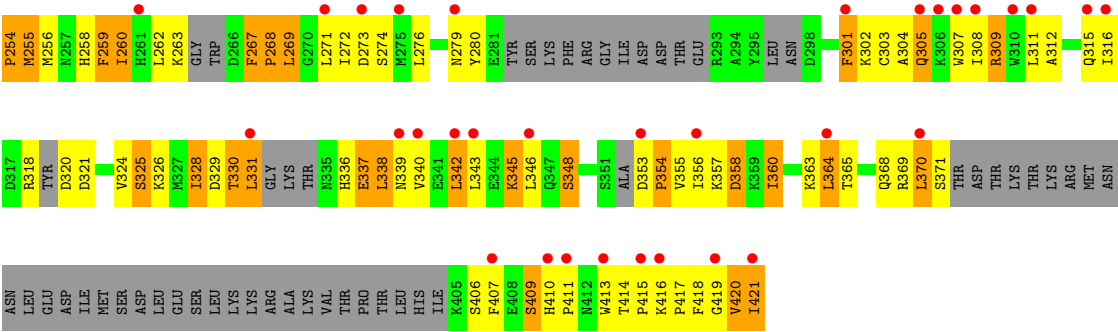


• Molecule 2: LAS1 protein



• Molecule 2: LAS1 protein





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 152.62Å 240.02Å 237.00Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 21.41 – 3.39<br>21.41 – 3.39                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 68.3 (21.41-3.39)<br>68.4 (21.41-3.39)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.26 (at 3.40Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17.1_3660                                          | Depositor        |
| R, $R_{free}$                                                           | 0.309 , 0.332<br>0.310 , 0.331                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2105 reflections (3.47%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 71.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.383                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.17 , 65.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.78                                                        | EDS              |
| Total number of atoms                                                   | 19118                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 124.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.78         | 19/3894 (0.5%)   | 1.19        | 46/5301 (0.9%)   |
| 1   | B     | 0.75         | 31/3787 (0.8%)   | 1.19        | 46/5155 (0.9%)   |
| 1   | E     | 0.84         | 28/3872 (0.7%)   | 1.28        | 54/5281 (1.0%)   |
| 2   | C     | 0.66         | 10/2601 (0.4%)   | 1.08        | 25/3540 (0.7%)   |
| 2   | D     | 0.76         | 9/2365 (0.4%)    | 1.12        | 25/3228 (0.8%)   |
| 2   | F     | 0.73         | 18/2577 (0.7%)   | 1.11        | 25/3501 (0.7%)   |
| All | All   | 0.76         | 115/19096 (0.6%) | 1.18        | 221/26006 (0.8%) |

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   | B     | 0                   | 3                   |
| 1   | E     | 0                   | 2                   |
| All | All   | 0                   | 5                   |

All (115) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 588 | PHE  | C-N   | 10.13 | 1.47        | 1.33     |
| 2   | F     | 416 | LYS  | C-N   | 9.19  | 1.40        | 1.33     |
| 1   | A     | 450 | PRO  | C-N   | 8.85  | 1.40        | 1.33     |
| 1   | A     | 449 | SER  | C-N   | 6.50  | 1.41        | 1.33     |
| 2   | F     | 4   | HIS  | C-N   | 6.17  | 1.41        | 1.33     |
| 2   | F     | 121 | LEU  | C-N   | 6.08  | 1.40        | 1.33     |
| 1   | E     | 565 | LEU  | C-N   | 6.07  | 1.40        | 1.33     |
| 1   | B     | 287 | GLN  | C-N   | 6.04  | 1.40        | 1.33     |
| 1   | E     | 449 | SER  | C-N   | 6.03  | 1.40        | 1.33     |
| 2   | C     | 416 | LYS  | C-N   | 5.92  | 1.40        | 1.33     |
| 1   | E     | 450 | PRO  | C-N   | 5.89  | 1.40        | 1.33     |
| 1   | B     | 583 | LEU  | C-N   | 5.84  | 1.41        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | E     | 211 | TYR  | C-N   | 5.82 | 1.41        | 1.34     |
| 1   | B     | 215 | LYS  | C-N   | 5.79 | 1.41        | 1.33     |
| 1   | E     | 444 | GLN  | C-N   | 5.77 | 1.40        | 1.33     |
| 1   | E     | 284 | ASP  | C-N   | 5.77 | 1.41        | 1.34     |
| 1   | A     | 114 | GLU  | C-N   | 5.76 | 1.40        | 1.33     |
| 2   | C     | 121 | LEU  | C-N   | 5.76 | 1.40        | 1.33     |
| 1   | A     | 565 | LEU  | C-N   | 5.72 | 1.41        | 1.33     |
| 1   | E     | 276 | LEU  | C-N   | 5.70 | 1.41        | 1.33     |
| 1   | E     | 212 | PRO  | N-CD  | 5.67 | 1.55        | 1.47     |
| 2   | D     | 24  | PHE  | C-N   | 5.63 | 1.40        | 1.34     |
| 1   | B     | 543 | ILE  | C-N   | 5.62 | 1.41        | 1.34     |
| 1   | E     | 287 | GLN  | C-N   | 5.61 | 1.40        | 1.34     |
| 2   | C     | 137 | LEU  | C-N   | 5.61 | 1.40        | 1.33     |
| 1   | B     | 284 | ASP  | C-N   | 5.61 | 1.40        | 1.34     |
| 1   | B     | 565 | LEU  | C-N   | 5.59 | 1.41        | 1.33     |
| 1   | E     | 381 | LYS  | C-N   | 5.56 | 1.40        | 1.33     |
| 1   | B     | 511 | LEU  | C-N   | 5.55 | 1.40        | 1.33     |
| 2   | F     | 414 | THR  | C-N   | 5.55 | 1.40        | 1.33     |
| 1   | B     | 381 | LYS  | C-N   | 5.51 | 1.40        | 1.33     |
| 2   | C     | 410 | HIS  | C-N   | 5.47 | 1.41        | 1.34     |
| 1   | E     | 126 | ILE  | C-N   | 5.46 | 1.41        | 1.33     |
| 1   | B     | 327 | SER  | C-N   | 5.45 | 1.40        | 1.33     |
| 1   | A     | 512 | PRO  | N-CD  | 5.44 | 1.55        | 1.47     |
| 1   | B     | 153 | THR  | C-N   | 5.43 | 1.41        | 1.34     |
| 2   | F     | 5   | PRO  | N-CD  | 5.43 | 1.55        | 1.47     |
| 1   | B     | 288 | PRO  | N-CD  | 5.42 | 1.55        | 1.47     |
| 1   | B     | 114 | GLU  | C-N   | 5.42 | 1.41        | 1.33     |
| 1   | A     | 450 | PRO  | N-CD  | 5.40 | 1.55        | 1.47     |
| 2   | D     | 267 | PHE  | C-N   | 5.39 | 1.41        | 1.34     |
| 1   | A     | 544 | PRO  | N-CD  | 5.37 | 1.55        | 1.47     |
| 1   | B     | 382 | PRO  | N-CD  | 5.36 | 1.55        | 1.47     |
| 1   | E     | 114 | GLU  | C-N   | 5.32 | 1.40        | 1.33     |
| 2   | F     | 110 | ILE  | C-N   | 5.32 | 1.40        | 1.33     |
| 1   | B     | 177 | PRO  | N-CD  | 5.31 | 1.55        | 1.47     |
| 1   | E     | 271 | PRO  | N-CD  | 5.29 | 1.55        | 1.47     |
| 2   | D     | 137 | LEU  | C-N   | 5.29 | 1.40        | 1.33     |
| 1   | A     | 583 | LEU  | C-N   | 5.29 | 1.41        | 1.34     |
| 1   | E     | 450 | PRO  | N-CD  | 5.29 | 1.55        | 1.47     |
| 1   | A     | 331 | GLN  | C-N   | 5.27 | 1.41        | 1.34     |
| 2   | C     | 253 | GLU  | C-N   | 5.26 | 1.41        | 1.34     |
| 1   | E     | 328 | PRO  | N-CD  | 5.26 | 1.55        | 1.47     |
| 1   | E     | 332 | PRO  | N-CD  | 5.25 | 1.55        | 1.47     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | F     | 411 | PRO  | N-CD  | 5.25 | 1.55        | 1.47     |
| 2   | F     | 8   | THR  | C-N   | 5.25 | 1.41        | 1.34     |
| 1   | A     | 270 | SER  | C-N   | 5.24 | 1.40        | 1.33     |
| 1   | B     | 328 | PRO  | N-CD  | 5.24 | 1.55        | 1.47     |
| 1   | E     | 177 | PRO  | N-CD  | 5.23 | 1.55        | 1.47     |
| 1   | B     | 271 | PRO  | N-CD  | 5.23 | 1.55        | 1.47     |
| 1   | B     | 512 | PRO  | N-CD  | 5.23 | 1.55        | 1.47     |
| 1   | B     | 361 | THR  | C-N   | 5.23 | 1.40        | 1.33     |
| 2   | C     | 411 | PRO  | N-CD  | 5.22 | 1.55        | 1.47     |
| 1   | B     | 176 | CYS  | C-N   | 5.22 | 1.41        | 1.34     |
| 1   | B     | 331 | GLN  | C-N   | 5.22 | 1.41        | 1.34     |
| 1   | A     | 508 | LEU  | C-N   | 5.22 | 1.41        | 1.34     |
| 1   | A     | 328 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | A     | 509 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | E     | 543 | ILE  | C-N   | 5.20 | 1.41        | 1.34     |
| 2   | F     | 415 | PRO  | N-CD  | 5.20 | 1.55        | 1.47     |
| 1   | B     | 285 | PRO  | N-CD  | 5.19 | 1.55        | 1.47     |
| 2   | D     | 253 | GLU  | C-N   | 5.19 | 1.41        | 1.34     |
| 2   | D     | 268 | PRO  | N-CD  | 5.18 | 1.55        | 1.47     |
| 2   | F     | 111 | PRO  | N-CD  | 5.18 | 1.55        | 1.47     |
| 1   | B     | 509 | PRO  | N-CD  | 5.18 | 1.55        | 1.47     |
| 2   | D     | 8   | THR  | C-N   | 5.18 | 1.41        | 1.34     |
| 1   | E     | 445 | PRO  | N-CD  | 5.18 | 1.55        | 1.47     |
| 2   | F     | 267 | PHE  | C-N   | 5.18 | 1.41        | 1.34     |
| 1   | E     | 583 | LEU  | C-N   | 5.17 | 1.41        | 1.34     |
| 2   | F     | 410 | HIS  | C-N   | 5.17 | 1.41        | 1.34     |
| 1   | A     | 277 | PRO  | N-CD  | 5.16 | 1.54        | 1.47     |
| 1   | B     | 115 | PRO  | N-CD  | 5.15 | 1.54        | 1.47     |
| 1   | B     | 212 | PRO  | N-CD  | 5.15 | 1.54        | 1.47     |
| 1   | B     | 154 | PRO  | N-CD  | 5.14 | 1.54        | 1.47     |
| 2   | F     | 9   | PRO  | N-CD  | 5.14 | 1.54        | 1.47     |
| 2   | F     | 25  | PRO  | N-CD  | 5.14 | 1.54        | 1.47     |
| 1   | B     | 362 | PRO  | N-CD  | 5.14 | 1.54        | 1.47     |
| 2   | F     | 254 | PRO  | N-CD  | 5.14 | 1.54        | 1.47     |
| 1   | A     | 584 | PRO  | N-CD  | 5.12 | 1.54        | 1.47     |
| 1   | B     | 566 | PRO  | N-CD  | 5.11 | 1.54        | 1.47     |
| 2   | C     | 9   | PRO  | N-CD  | 5.11 | 1.54        | 1.47     |
| 2   | D     | 254 | PRO  | N-CD  | 5.10 | 1.54        | 1.47     |
| 1   | A     | 271 | PRO  | N-CD  | 5.10 | 1.54        | 1.47     |
| 2   | F     | 268 | PRO  | N-CD  | 5.10 | 1.54        | 1.47     |
| 1   | E     | 285 | PRO  | N-CD  | 5.10 | 1.54        | 1.47     |
| 2   | F     | 253 | GLU  | C-N   | 5.10 | 1.41        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | E     | 544 | PRO  | N-CD  | 5.09 | 1.54        | 1.47     |
| 1   | E     | 331 | GLN  | C-N   | 5.08 | 1.40        | 1.34     |
| 1   | B     | 121 | PRO  | N-CD  | 5.07 | 1.54        | 1.47     |
| 1   | E     | 270 | SER  | C-N   | 5.07 | 1.40        | 1.34     |
| 2   | C     | 8   | THR  | C-N   | 5.06 | 1.40        | 1.34     |
| 1   | B     | 216 | PRO  | N-CD  | 5.06 | 1.54        | 1.47     |
| 1   | B     | 332 | PRO  | N-CD  | 5.05 | 1.54        | 1.47     |
| 1   | A     | 115 | PRO  | N-CD  | 5.04 | 1.54        | 1.47     |
| 1   | A     | 381 | LYS  | C-N   | 5.04 | 1.40        | 1.34     |
| 2   | D     | 411 | PRO  | N-CD  | 5.04 | 1.54        | 1.47     |
| 1   | A     | 332 | PRO  | N-CD  | 5.03 | 1.54        | 1.47     |
| 2   | C     | 254 | PRO  | N-CD  | 5.02 | 1.54        | 1.47     |
| 2   | D     | 9   | PRO  | N-CD  | 5.02 | 1.54        | 1.47     |
| 2   | C     | 417 | PRO  | N-CD  | 5.02 | 1.54        | 1.47     |
| 2   | F     | 122 | PRO  | N-CD  | 5.02 | 1.54        | 1.47     |
| 1   | E     | 115 | PRO  | N-CD  | 5.01 | 1.54        | 1.47     |
| 1   | E     | 127 | PRO  | N-CD  | 5.01 | 1.54        | 1.47     |
| 1   | E     | 451 | PRO  | N-CD  | 5.01 | 1.54        | 1.47     |
| 1   | B     | 584 | PRO  | N-CD  | 5.00 | 1.54        | 1.47     |

All (221) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | E     | 588 | PHE  | O-C-N   | -14.93 | 104.75      | 122.22   |
| 1   | E     | 588 | PHE  | CA-C-N  | 12.20  | 138.10      | 120.90   |
| 1   | E     | 588 | PHE  | C-N-CA  | 12.20  | 138.10      | 120.90   |
| 1   | B     | 169 | LEU  | N-CA-C  | -9.69  | 97.75       | 110.53   |
| 2   | F     | 354 | PRO  | CA-N-CD | -9.32  | 98.96       | 112.00   |
| 1   | E     | 449 | SER  | CA-C-N  | -8.95  | 113.21      | 119.66   |
| 1   | E     | 449 | SER  | C-N-CA  | -8.95  | 113.21      | 119.66   |
| 2   | D     | 102 | PRO  | N-CA-CB | 8.66   | 110.63      | 101.88   |
| 1   | A     | 547 | ARG  | N-CA-C  | -8.19  | 99.72       | 110.53   |
| 1   | E     | 82  | LYS  | N-CA-C  | -8.03  | 100.54      | 110.41   |
| 1   | B     | 287 | GLN  | CA-C-N  | -7.48  | 112.98      | 120.31   |
| 1   | B     | 287 | GLN  | C-N-CA  | -7.48  | 112.98      | 120.31   |
| 2   | C     | 416 | LYS  | CA-C-N  | -7.46  | 113.05      | 120.21   |
| 2   | C     | 416 | LYS  | C-N-CA  | -7.46  | 113.05      | 120.21   |
| 1   | E     | 292 | GLY  | N-CA-C  | -7.35  | 102.65      | 112.14   |
| 1   | E     | 450 | PRO  | CA-C-N  | -7.21  | 113.38      | 120.52   |
| 1   | E     | 450 | PRO  | C-N-CA  | -7.21  | 113.38      | 120.52   |
| 1   | B     | 185 | GLN  | N-CA-C  | -7.17  | 97.82       | 108.79   |
| 2   | C     | 121 | LEU  | CA-C-N  | -7.12  | 113.38      | 120.21   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 121 | LEU  | C-N-CA  | -7.12 | 113.38      | 120.21   |
| 2   | F     | 121 | LEU  | CA-C-N  | -7.05 | 113.05      | 120.03   |
| 2   | F     | 121 | LEU  | C-N-CA  | -7.05 | 113.05      | 120.03   |
| 1   | E     | 211 | TYR  | N-CA-C  | 7.05  | 119.66      | 108.23   |
| 1   | B     | 270 | SER  | CA-C-N  | -7.02 | 112.44      | 121.91   |
| 1   | B     | 270 | SER  | C-N-CA  | -7.02 | 112.44      | 121.91   |
| 1   | E     | 565 | LEU  | CA-C-N  | -6.98 | 113.12      | 120.03   |
| 1   | E     | 565 | LEU  | C-N-CA  | -6.98 | 113.12      | 120.03   |
| 1   | E     | 154 | PRO  | N-CA-CB | 6.97  | 110.56      | 103.25   |
| 1   | E     | 125 | SER  | N-CA-C  | -6.95 | 101.35      | 110.53   |
| 1   | B     | 361 | THR  | CA-C-N  | -6.94 | 112.63      | 119.78   |
| 1   | B     | 361 | THR  | C-N-CA  | -6.94 | 112.63      | 119.78   |
| 1   | B     | 511 | LEU  | CA-C-N  | -6.94 | 112.84      | 119.85   |
| 1   | B     | 511 | LEU  | C-N-CA  | -6.94 | 112.84      | 119.85   |
| 1   | E     | 552 | THR  | N-CA-C  | -6.93 | 101.38      | 110.53   |
| 1   | E     | 305 | GLN  | CA-C-N  | -6.91 | 111.17      | 122.65   |
| 1   | E     | 305 | GLN  | C-N-CA  | -6.91 | 111.17      | 122.65   |
| 2   | F     | 4   | HIS  | CA-C-N  | -6.90 | 113.20      | 120.03   |
| 2   | F     | 4   | HIS  | C-N-CA  | -6.90 | 113.20      | 120.03   |
| 1   | B     | 215 | LYS  | CA-C-N  | -6.89 | 112.66      | 119.76   |
| 1   | B     | 215 | LYS  | C-N-CA  | -6.89 | 112.66      | 119.76   |
| 1   | A     | 114 | GLU  | CA-C-N  | -6.81 | 113.67      | 120.21   |
| 1   | A     | 114 | GLU  | C-N-CA  | -6.81 | 113.67      | 120.21   |
| 1   | B     | 565 | LEU  | CA-C-N  | -6.80 | 112.96      | 119.76   |
| 1   | B     | 565 | LEU  | C-N-CA  | -6.80 | 112.96      | 119.76   |
| 1   | A     | 276 | LEU  | N-CA-C  | -6.79 | 101.20      | 109.83   |
| 1   | E     | 450 | PRO  | O-C-N   | 6.79  | 124.34      | 121.15   |
| 1   | E     | 400 | PRO  | N-CA-CB | 6.78  | 110.06      | 102.60   |
| 1   | A     | 154 | PRO  | N-CA-CB | 6.76  | 110.31      | 102.33   |
| 2   | F     | 414 | THR  | CA-C-N  | -6.76 | 112.80      | 119.76   |
| 2   | F     | 414 | THR  | C-N-CA  | -6.76 | 112.80      | 119.76   |
| 1   | A     | 565 | LEU  | CA-C-N  | -6.62 | 112.94      | 119.76   |
| 1   | A     | 565 | LEU  | C-N-CA  | -6.62 | 112.94      | 119.76   |
| 2   | F     | 110 | ILE  | CA-C-N  | -6.62 | 113.14      | 119.89   |
| 2   | F     | 110 | ILE  | C-N-CA  | -6.62 | 113.14      | 119.89   |
| 1   | B     | 381 | LYS  | CA-C-N  | -6.60 | 112.96      | 119.76   |
| 1   | B     | 381 | LYS  | C-N-CA  | -6.60 | 112.96      | 119.76   |
| 2   | D     | 137 | LEU  | CA-C-N  | -6.60 | 112.98      | 119.78   |
| 2   | D     | 137 | LEU  | C-N-CA  | -6.60 | 112.98      | 119.78   |
| 1   | A     | 449 | SER  | CA-C-N  | -6.54 | 113.64      | 120.38   |
| 1   | A     | 449 | SER  | C-N-CA  | -6.54 | 113.64      | 120.38   |
| 1   | A     | 157 | LYS  | CB-CA-C | -6.53 | 109.06      | 116.63   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 319 | GLN  | N-CA-C   | 6.53  | 118.78      | 108.79   |
| 2   | F     | 209 | PRO  | N-CA-CB  | 6.50  | 110.16      | 103.00   |
| 1   | E     | 444 | GLN  | CA-C-N   | -6.49 | 112.98      | 119.92   |
| 1   | E     | 444 | GLN  | C-N-CA   | -6.49 | 112.98      | 119.92   |
| 2   | F     | 337 | GLU  | N-CA-C   | -6.48 | 105.68      | 113.97   |
| 2   | D     | 354 | PRO  | N-CA-CB  | 6.47  | 110.54      | 103.23   |
| 1   | B     | 400 | PRO  | N-CA-CB  | 6.44  | 109.69      | 102.60   |
| 1   | E     | 505 | LYS  | N-CA-C   | -6.44 | 101.42      | 110.50   |
| 2   | F     | 416 | LYS  | CA-C-N   | -6.41 | 113.56      | 121.00   |
| 2   | F     | 416 | LYS  | C-N-CA   | -6.41 | 113.56      | 121.00   |
| 2   | D     | 12  | SER  | N-CA-C   | -6.40 | 101.91      | 110.55   |
| 2   | C     | 35  | GLU  | CB-CG-CD | -6.39 | 101.73      | 112.60   |
| 2   | D     | 400 | PRO  | N-CA-CB  | 6.38  | 109.95      | 103.25   |
| 1   | A     | 121 | PRO  | N-CA-CB  | 6.38  | 109.95      | 103.25   |
| 1   | B     | 114 | GLU  | CA-C-N   | -6.37 | 113.22      | 119.78   |
| 1   | B     | 114 | GLU  | C-N-CA   | -6.37 | 113.22      | 119.78   |
| 1   | E     | 475 | MET  | N-CA-C   | 6.36  | 118.22      | 111.28   |
| 1   | E     | 225 | HIS  | N-CA-C   | -6.36 | 100.62      | 110.10   |
| 1   | E     | 126 | ILE  | CA-C-N   | -6.35 | 113.24      | 119.78   |
| 1   | E     | 126 | ILE  | C-N-CA   | -6.35 | 113.24      | 119.78   |
| 2   | C     | 137 | LEU  | CA-C-N   | -6.35 | 113.44      | 119.85   |
| 2   | C     | 137 | LEU  | C-N-CA   | -6.35 | 113.44      | 119.85   |
| 1   | A     | 450 | PRO  | CA-C-N   | -6.35 | 113.70      | 120.94   |
| 1   | A     | 450 | PRO  | C-N-CA   | -6.35 | 113.70      | 120.94   |
| 1   | A     | 354 | HIS  | N-CA-C   | -6.33 | 104.38      | 111.28   |
| 1   | A     | 528 | LEU  | N-CA-C   | -6.30 | 101.16      | 110.48   |
| 2   | F     | 123 | SER  | N-CA-C   | -6.23 | 104.49      | 111.28   |
| 2   | C     | 313 | ILE  | N-CA-C   | 6.18  | 116.93      | 110.62   |
| 1   | E     | 381 | LYS  | CA-C-N   | -6.15 | 113.42      | 119.76   |
| 1   | E     | 381 | LYS  | C-N-CA   | -6.15 | 113.42      | 119.76   |
| 1   | B     | 570 | ILE  | N-CA-C   | 6.14  | 116.92      | 110.72   |
| 1   | B     | 371 | GLU  | N-CA-C   | -6.13 | 104.71      | 111.82   |
| 1   | E     | 276 | LEU  | CA-C-N   | -6.09 | 113.49      | 119.76   |
| 1   | E     | 276 | LEU  | C-N-CA   | -6.09 | 113.49      | 119.76   |
| 1   | E     | 114 | GLU  | CA-C-N   | -6.06 | 113.54      | 119.78   |
| 1   | E     | 114 | GLU  | C-N-CA   | -6.06 | 113.54      | 119.78   |
| 2   | D     | 345 | LYS  | N-CA-C   | -6.01 | 104.72      | 111.28   |
| 1   | B     | 357 | LEU  | N-CA-C   | 6.01  | 118.53      | 110.35   |
| 2   | C     | 222 | LYS  | N-CA-C   | 6.00  | 117.62      | 111.14   |
| 2   | D     | 135 | ASP  | N-CA-C   | 5.99  | 116.00      | 108.45   |
| 1   | B     | 543 | ILE  | CA-C-N   | -5.97 | 112.76      | 118.97   |
| 1   | B     | 543 | ILE  | C-N-CA   | -5.97 | 112.76      | 118.97   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 593 | SER  | CB-CA-C | -5.97 | 109.70      | 116.63   |
| 1   | A     | 331 | GLN  | CA-C-N  | -5.93 | 112.46      | 119.05   |
| 1   | A     | 331 | GLN  | C-N-CA  | -5.93 | 112.46      | 119.05   |
| 1   | B     | 583 | LEU  | CA-C-N  | -5.87 | 112.45      | 118.85   |
| 1   | B     | 583 | LEU  | C-N-CA  | -5.87 | 112.45      | 118.85   |
| 1   | A     | 276 | LEU  | CA-C-N  | -5.82 | 112.57      | 119.84   |
| 1   | A     | 276 | LEU  | C-N-CA  | -5.82 | 112.57      | 119.84   |
| 2   | F     | 8   | THR  | CA-C-N  | -5.80 | 112.61      | 119.05   |
| 2   | F     | 8   | THR  | C-N-CA  | -5.80 | 112.61      | 119.05   |
| 2   | D     | 355 | VAL  | N-CA-C  | -5.78 | 104.73      | 110.62   |
| 2   | C     | 410 | HIS  | CA-C-N  | -5.77 | 112.97      | 118.97   |
| 2   | C     | 410 | HIS  | C-N-CA  | -5.77 | 112.97      | 118.97   |
| 1   | E     | 331 | GLN  | CA-C-N  | -5.75 | 112.67      | 119.05   |
| 1   | E     | 331 | GLN  | C-N-CA  | -5.75 | 112.67      | 119.05   |
| 2   | D     | 27  | ASP  | N-CA-C  | -5.70 | 101.86      | 110.70   |
| 1   | A     | 496 | HIS  | N-CA-C  | -5.70 | 105.07      | 111.28   |
| 1   | A     | 87  | LEU  | N-CA-C  | 5.69  | 118.17      | 108.90   |
| 1   | A     | 157 | LYS  | N-CA-C  | 5.69  | 117.69      | 108.08   |
| 1   | E     | 583 | LEU  | CA-C-N  | -5.69 | 112.74      | 119.05   |
| 1   | E     | 583 | LEU  | C-N-CA  | -5.69 | 112.74      | 119.05   |
| 1   | B     | 499 | GLU  | CB-CA-C | -5.67 | 110.02      | 116.54   |
| 1   | E     | 377 | ILE  | CB-CA-C | -5.67 | 104.72      | 111.97   |
| 1   | B     | 331 | GLN  | CA-C-N  | -5.62 | 112.81      | 119.05   |
| 1   | B     | 331 | GLN  | C-N-CA  | -5.62 | 112.81      | 119.05   |
| 2   | C     | 34  | ASP  | N-CA-C  | -5.58 | 105.20      | 111.28   |
| 1   | B     | 345 | SER  | N-CA-C  | -5.57 | 105.21      | 111.28   |
| 1   | E     | 221 | SER  | N-CA-C  | -5.57 | 99.83       | 108.90   |
| 2   | C     | 146 | CYS  | N-CA-C  | 5.56  | 117.42      | 111.36   |
| 2   | C     | 253 | GLU  | CA-C-N  | -5.56 | 112.88      | 119.05   |
| 2   | C     | 253 | GLU  | C-N-CA  | -5.56 | 112.88      | 119.05   |
| 1   | E     | 543 | ILE  | CA-C-N  | -5.54 | 112.90      | 119.05   |
| 1   | E     | 543 | ILE  | C-N-CA  | -5.54 | 112.90      | 119.05   |
| 2   | F     | 253 | GLU  | CA-C-N  | -5.54 | 112.90      | 119.05   |
| 2   | F     | 253 | GLU  | C-N-CA  | -5.54 | 112.90      | 119.05   |
| 1   | B     | 220 | VAL  | N-CA-C  | 5.53  | 117.15      | 109.80   |
| 1   | A     | 359 | ILE  | N-CA-C  | 5.51  | 117.74      | 108.81   |
| 2   | F     | 267 | PHE  | CA-C-N  | -5.51 | 112.94      | 119.05   |
| 2   | F     | 267 | PHE  | C-N-CA  | -5.51 | 112.94      | 119.05   |
| 1   | A     | 583 | LEU  | CA-C-N  | -5.49 | 112.95      | 119.05   |
| 1   | A     | 583 | LEU  | C-N-CA  | -5.49 | 112.95      | 119.05   |
| 2   | D     | 267 | PHE  | CA-C-N  | -5.49 | 112.96      | 119.05   |
| 2   | D     | 267 | PHE  | C-N-CA  | -5.49 | 112.96      | 119.05   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | F     | 179 | LEU  | N-CA-C | 5.48  | 116.94      | 111.07   |
| 1   | E     | 319 | GLN  | N-CA-C | 5.47  | 116.84      | 108.42   |
| 2   | F     | 410 | HIS  | CA-C-N | -5.46 | 112.99      | 119.05   |
| 2   | F     | 410 | HIS  | C-N-CA | -5.46 | 112.99      | 119.05   |
| 2   | D     | 356 | ILE  | N-CA-C | -5.45 | 105.06      | 110.62   |
| 1   | E     | 237 | GLU  | N-CA-C | -5.44 | 105.35      | 111.28   |
| 2   | C     | 8   | THR  | CA-C-N | -5.44 | 113.01      | 119.05   |
| 2   | C     | 8   | THR  | C-N-CA | -5.44 | 113.01      | 119.05   |
| 1   | E     | 226 | LYS  | N-CA-C | -5.40 | 105.39      | 111.28   |
| 1   | B     | 89  | VAL  | N-CA-C | 5.40  | 115.90      | 108.12   |
| 1   | E     | 120 | ASN  | CA-C-N | -5.39 | 113.11      | 119.84   |
| 1   | E     | 120 | ASN  | C-N-CA | -5.39 | 113.11      | 119.84   |
| 1   | A     | 452 | ILE  | CA-C-N | 5.38  | 128.40      | 120.82   |
| 1   | A     | 452 | ILE  | C-N-CA | 5.38  | 128.40      | 120.82   |
| 2   | D     | 253 | GLU  | CA-C-N | -5.37 | 113.09      | 119.05   |
| 2   | D     | 253 | GLU  | C-N-CA | -5.37 | 113.09      | 119.05   |
| 2   | C     | 302 | LYS  | N-CA-C | 5.37  | 117.21      | 111.36   |
| 2   | D     | 310 | TRP  | N-CA-C | -5.36 | 105.52      | 111.36   |
| 1   | A     | 134 | VAL  | N-CA-C | -5.35 | 104.17      | 110.21   |
| 1   | A     | 342 | LEU  | N-CA-C | -5.35 | 105.45      | 111.28   |
| 1   | A     | 416 | GLY  | N-CA-C | -5.35 | 106.30      | 112.50   |
| 1   | A     | 372 | LEU  | N-CA-C | -5.35 | 105.45      | 111.28   |
| 1   | B     | 69  | ASN  | N-CA-C | -5.34 | 105.45      | 111.28   |
| 1   | A     | 341 | GLN  | N-CA-C | -5.34 | 105.46      | 111.28   |
| 1   | A     | 361 | THR  | CA-C-N | -5.33 | 113.17      | 119.84   |
| 1   | A     | 361 | THR  | C-N-CA | -5.33 | 113.17      | 119.84   |
| 2   | D     | 57  | SER  | N-CA-C | -5.33 | 102.51      | 110.23   |
| 1   | A     | 451 | PRO  | N-CA-C | 5.32  | 121.49      | 114.68   |
| 1   | E     | 350 | GLY  | N-CA-C | -5.31 | 106.36      | 112.73   |
| 1   | A     | 381 | LYS  | CA-C-N | -5.31 | 113.16      | 119.05   |
| 1   | A     | 381 | LYS  | C-N-CA | -5.31 | 113.16      | 119.05   |
| 2   | C     | 307 | TRP  | N-CA-C | -5.30 | 105.50      | 111.28   |
| 1   | B     | 259 | THR  | N-CA-C | -5.27 | 105.54      | 111.28   |
| 1   | B     | 176 | CYS  | CA-C-N | -5.26 | 113.21      | 119.05   |
| 1   | B     | 176 | CYS  | C-N-CA | -5.26 | 113.21      | 119.05   |
| 1   | A     | 508 | LEU  | CA-C-N | -5.26 | 113.21      | 119.05   |
| 1   | A     | 508 | LEU  | C-N-CA | -5.26 | 113.21      | 119.05   |
| 1   | A     | 327 | SER  | CA-C-N | -5.25 | 113.23      | 119.05   |
| 1   | A     | 327 | SER  | C-N-CA | -5.25 | 113.23      | 119.05   |
| 2   | D     | 24  | PHE  | CA-C-N | -5.22 | 113.16      | 118.85   |
| 2   | D     | 24  | PHE  | C-N-CA | -5.22 | 113.16      | 118.85   |
| 1   | B     | 153 | THR  | CA-C-N | -5.22 | 113.25      | 119.05   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 153 | THR  | C-N-CA  | -5.22 | 113.25      | 119.05   |
| 1   | B     | 406 | ILE  | CA-C-N  | 5.21  | 125.19      | 120.03   |
| 1   | B     | 406 | ILE  | C-N-CA  | 5.21  | 125.19      | 120.03   |
| 1   | E     | 287 | GLN  | CA-C-N  | -5.21 | 113.17      | 118.85   |
| 1   | E     | 287 | GLN  | C-N-CA  | -5.21 | 113.17      | 118.85   |
| 2   | D     | 144 | LYS  | N-CA-C  | -5.21 | 105.60      | 111.28   |
| 1   | B     | 505 | LYS  | N-CA-C  | 5.20  | 117.03      | 111.36   |
| 2   | D     | 8   | THR  | CA-C-N  | -5.20 | 113.27      | 119.05   |
| 2   | D     | 8   | THR  | C-N-CA  | -5.20 | 113.27      | 119.05   |
| 1   | E     | 476 | ASP  | N-CA-C  | 5.20  | 116.75      | 111.14   |
| 1   | B     | 327 | SER  | CA-C-N  | -5.19 | 113.57      | 119.28   |
| 1   | B     | 327 | SER  | C-N-CA  | -5.19 | 113.57      | 119.28   |
| 1   | E     | 284 | ASP  | CA-C-N  | -5.19 | 113.19      | 118.85   |
| 1   | E     | 284 | ASP  | C-N-CA  | -5.19 | 113.19      | 118.85   |
| 1   | B     | 211 | TYR  | CA-C-N  | -5.19 | 113.35      | 119.84   |
| 1   | B     | 211 | TYR  | C-N-CA  | -5.19 | 113.35      | 119.84   |
| 1   | E     | 176 | CYS  | CA-C-N  | -5.19 | 113.29      | 119.05   |
| 1   | E     | 176 | CYS  | C-N-CA  | -5.19 | 113.29      | 119.05   |
| 2   | C     | 48  | GLU  | N-CA-C  | -5.18 | 105.63      | 111.28   |
| 1   | A     | 543 | ILE  | CA-C-N  | -5.16 | 113.39      | 119.84   |
| 1   | A     | 543 | ILE  | C-N-CA  | -5.16 | 113.39      | 119.84   |
| 2   | D     | 28  | ARG  | N-CA-C  | -5.16 | 105.74      | 111.36   |
| 2   | C     | 305 | GLN  | N-CA-C  | -5.14 | 105.68      | 111.28   |
| 1   | A     | 451 | PRO  | CA-N-CD | -5.13 | 104.81      | 112.00   |
| 2   | C     | 309 | ARG  | N-CA-C  | -5.13 | 105.69      | 111.28   |
| 2   | C     | 148 | ASP  | N-CA-C  | -5.10 | 105.72      | 111.28   |
| 2   | D     | 352 | ALA  | N-CA-C  | 5.07  | 118.39      | 111.39   |
| 2   | F     | 249 | ARG  | N-CA-C  | -5.05 | 105.77      | 111.28   |
| 2   | C     | 149 | ARG  | N-CA-C  | -5.05 | 105.78      | 111.28   |
| 2   | F     | 302 | LYS  | N-CA-C  | -5.03 | 105.79      | 111.28   |
| 1   | B     | 74  | HIS  | N-CA-C  | 5.03  | 116.96      | 108.96   |
| 1   | E     | 418 | ARG  | N-CA-C  | -5.03 | 103.76      | 110.55   |
| 2   | C     | 118 | LYS  | N-CA-C  | -5.02 | 105.81      | 111.28   |
| 2   | D     | 248 | LEU  | N-CA-C  | -5.01 | 105.81      | 111.28   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 292 | GLY  | Peptide   |
| 1   | B     | 297 | SER  | Peptide   |
| 1   | B     | 371 | GLU  | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | E     | 138 | SER  | Peptide   |
| 1   | E     | 588 | PHE  | Mainchain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3817  | 0        | 3551     | 1107    | 0            |
| 1   | B     | 3713  | 0        | 3465     | 972     | 1            |
| 1   | E     | 3794  | 0        | 3501     | 991     | 3            |
| 2   | C     | 2551  | 0        | 2321     | 593     | 1            |
| 2   | D     | 2323  | 0        | 2023     | 537     | 0            |
| 2   | F     | 2534  | 0        | 2341     | 592     | 3            |
| 3   | A     | 94    | 0        | 0        | 14      | 0            |
| 3   | B     | 61    | 0        | 0        | 26      | 0            |
| 3   | C     | 46    | 0        | 0        | 6       | 0            |
| 3   | D     | 60    | 0        | 0        | 9       | 0            |
| 3   | E     | 79    | 0        | 0        | 24      | 0            |
| 3   | F     | 46    | 0        | 0        | 9       | 0            |
| All | All   | 19118 | 0        | 17202    | 4552    | 4            |

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 127.

All (4552) 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:B:454:VAL:HG11 | 2:D:407:PHE:CE1  | 1.23                     | 1.73              |
| 1:A:63:PHE:CE2   | 1:A:214:THR:HA   | 1.26                     | 1.69              |
| 2:F:252:PHE:HD1  | 2:F:307:TRP:CZ2  | 1.09                     | 1.66              |
| 2:F:252:PHE:CD1  | 2:F:307:TRP:CH2  | 1.75                     | 1.66              |
| 2:F:24:PHE:HD1   | 2:F:155:TRP:CE3  | 1.14                     | 1.64              |
| 2:F:331:LEU:CG   | 2:F:343:LEU:HD21 | 1.20                     | 1.63              |
| 2:F:110:ILE:HD11 | 2:F:115:LEU:CD1  | 1.26                     | 1.62              |
| 1:E:588:PHE:CA   | 2:F:5:PRO:HB3    | 1.15                     | 1.62              |
| 2:C:258:HIS:CD2  | 2:C:262:LEU:HD11 | 1.29                     | 1.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:238:ILE:HG21 | 2:F:307:TRP:CZ3  | 1.26                     | 1.61              |
| 2:C:11:LYS:HB2   | 1:A:585:TYR:CE2  | 1.11                     | 1.61              |
| 2:C:258:HIS:CD2  | 2:C:262:LEU:CD1  | 1.82                     | 1.60              |
| 1:A:169:LEU:CD2  | 1:A:441:PHE:CD1  | 1.86                     | 1.59              |
| 1:B:250:ILE:CD1  | 1:B:373:THR:HG21 | 1.22                     | 1.59              |
| 1:B:62:ASN:CB    | 1:B:216:PRO:HG3  | 1.26                     | 1.58              |
| 2:F:24:PHE:CD1   | 2:F:155:TRP:CE3  | 1.91                     | 1.57              |
| 1:B:118:PHE:CE1  | 1:B:306:HIS:HB3  | 1.05                     | 1.57              |
| 1:A:579:PHE:CD2  | 1:A:581:ARG:CB   | 1.87                     | 1.57              |
| 1:E:370:LEU:CG   | 1:E:397:ILE:HD11 | 1.32                     | 1.57              |
| 1:A:63:PHE:HE2   | 1:A:214:THR:CA   | 1.18                     | 1.56              |
| 1:B:468:LEU:CD1  | 1:B:561:GLY:HA2  | 1.28                     | 1.55              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:HG13 | 1.14                     | 1.55              |
| 1:E:125:SER:HA   | 1:E:220:VAL:CB   | 1.27                     | 1.55              |
| 2:D:259:PHE:CE1  | 2:D:268:PRO:HB3  | 1.40                     | 1.55              |
| 2:F:20:LYS:HA    | 2:F:159:TRP:CZ3  | 1.41                     | 1.54              |
| 1:B:118:PHE:CE1  | 1:B:306:HIS:CB   | 1.88                     | 1.54              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:CG1  | 1.82                     | 1.54              |
| 1:E:232:ILE:HD11 | 1:E:264:LEU:CB   | 1.38                     | 1.54              |
| 2:C:11:LYS:CB    | 1:A:585:TYR:HE2  | 0.95                     | 1.53              |
| 1:B:63:PHE:CB    | 1:B:88:ILE:HG12  | 1.35                     | 1.53              |
| 2:C:249:ARG:CB   | 2:C:307:TRP:CH2  | 1.93                     | 1.51              |
| 1:E:99:ARG:HA    | 1:E:142:ASN:CG   | 1.27                     | 1.51              |
| 2:D:24:PHE:HE2   | 2:D:155:TRP:CD1  | 1.27                     | 1.51              |
| 2:F:24:PHE:CD1   | 2:F:155:TRP:HE3  | 1.23                     | 1.51              |
| 1:B:250:ILE:HD11 | 1:B:373:THR:CG2  | 1.38                     | 1.51              |
| 1:A:325:PHE:CG   | 1:A:330:ASP:CB   | 1.94                     | 1.50              |
| 2:F:238:ILE:HG21 | 2:F:307:TRP:CH2  | 1.37                     | 1.50              |
| 2:D:24:PHE:CE2   | 2:D:155:TRP:CD1  | 2.00                     | 1.49              |
| 2:D:331:LEU:HD23 | 2:D:346:LEU:CD1  | 1.38                     | 1.49              |
| 1:B:118:PHE:CD1  | 1:B:306:HIS:HB3  | 1.46                     | 1.48              |
| 1:B:490:PHE:HB2  | 1:B:557:ILE:CG2  | 1.41                     | 1.48              |
| 1:A:325:PHE:CD1  | 1:A:330:ASP:CB   | 1.95                     | 1.48              |
| 2:C:235:ILE:CD1  | 2:C:278:LYS:HE2  | 1.39                     | 1.47              |
| 1:E:299:SER:HB3  | 1:E:317:SER:CB   | 1.03                     | 1.47              |
| 1:E:100:GLY:H    | 1:E:142:ASN:ND2  | 1.12                     | 1.47              |
| 1:A:63:PHE:CZ    | 1:A:212:PRO:HB2  | 1.48                     | 1.47              |
| 1:B:63:PHE:CB    | 1:B:88:ILE:CG1   | 1.91                     | 1.47              |
| 1:E:370:LEU:HD11 | 1:E:397:ILE:CD1  | 1.45                     | 1.47              |
| 1:B:63:PHE:CB    | 1:B:88:ILE:CD1   | 1.91                     | 1.46              |
| 1:E:299:SER:CB   | 1:E:317:SER:CB   | 1.94                     | 1.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:103:ASP:CB   | 1:B:108:ILE:HG12 | 1.45                     | 1.46              |
| 1:B:279:ASN:CG   | 1:B:300:LYS:HZ1  | 1.22                     | 1.46              |
| 1:E:588:PHE:HA   | 2:F:5:PRO:CB     | 1.42                     | 1.46              |
| 1:A:232:ILE:CD1  | 1:A:264:LEU:HB2  | 1.42                     | 1.45              |
| 1:A:466:THR:HB   | 1:A:511:LEU:CD2  | 1.43                     | 1.45              |
| 1:E:370:LEU:HD21 | 1:E:397:ILE:CD1  | 1.46                     | 1.45              |
| 1:A:172:ILE:CG2  | 1:A:179:PHE:HB3  | 1.43                     | 1.45              |
| 1:E:370:LEU:CD1  | 1:E:397:ILE:HD11 | 1.45                     | 1.44              |
| 1:B:455:SER:HB3  | 2:D:405:LYS:CB   | 1.45                     | 1.44              |
| 2:F:331:LEU:CD2  | 2:F:343:LEU:HD21 | 1.43                     | 1.44              |
| 1:A:172:ILE:HG21 | 1:A:179:PHE:CB   | 1.47                     | 1.43              |
| 2:D:62:SER:O     | 2:D:66:LEU:CD1   | 1.67                     | 1.43              |
| 1:E:184:TRP:CE3  | 1:E:211:TYR:HB2  | 1.54                     | 1.43              |
| 1:E:232:ILE:CD1  | 1:E:264:LEU:CB   | 1.97                     | 1.43              |
| 1:B:490:PHE:CB   | 1:B:557:ILE:CG2  | 1.94                     | 1.42              |
| 1:B:250:ILE:CD1  | 1:B:373:THR:CG2  | 1.93                     | 1.42              |
| 1:A:172:ILE:CG2  | 1:A:179:PHE:CB   | 1.95                     | 1.42              |
| 1:A:232:ILE:HD11 | 1:A:264:LEU:CB   | 1.45                     | 1.42              |
| 1:A:117:LYS:HD3  | 1:A:439:PHE:CE2  | 1.55                     | 1.42              |
| 1:E:100:GLY:N    | 1:E:142:ASN:HD21 | 1.07                     | 1.42              |
| 2:C:258:HIS:NE2  | 2:C:262:LEU:HD11 | 1.21                     | 1.41              |
| 2:F:331:LEU:HG   | 2:F:343:LEU:CD2  | 1.51                     | 1.41              |
| 1:B:454:VAL:CG1  | 2:D:407:PHE:CD1  | 2.04                     | 1.41              |
| 1:E:370:LEU:HD11 | 1:E:397:ILE:CG1  | 1.48                     | 1.41              |
| 2:F:110:ILE:CD1  | 2:F:115:LEU:HD11 | 1.47                     | 1.41              |
| 2:C:249:ARG:CB   | 2:C:307:TRP:CZ2  | 2.02                     | 1.40              |
| 2:D:183:LEU:CD2  | 2:D:224:HIS:HB3  | 1.47                     | 1.40              |
| 2:C:235:ILE:CD1  | 2:C:278:LYS:CE   | 1.98                     | 1.40              |
| 1:E:232:ILE:CD1  | 1:E:264:LEU:HD23 | 1.51                     | 1.39              |
| 1:B:111:SER:OG   | 1:B:142:ASN:CA   | 1.68                     | 1.39              |
| 2:C:65:HIS:ND1   | 2:C:94:ARG:NH2   | 1.69                     | 1.39              |
| 1:A:72:TYR:HE2   | 1:A:206:SER:CB   | 1.35                     | 1.39              |
| 2:D:276:LEU:HD22 | 2:D:333:LYS:CB   | 1.52                     | 1.38              |
| 1:E:184:TRP:CZ3  | 1:E:211:TYR:CB   | 2.06                     | 1.38              |
| 1:A:350:GLY:CA   | 1:A:357:LEU:HD11 | 1.50                     | 1.38              |
| 1:B:325:PHE:CD2  | 1:B:330:ASP:CB   | 2.06                     | 1.38              |
| 2:F:252:PHE:CE1  | 2:F:307:TRP:CH2  | 2.10                     | 1.38              |
| 2:D:125:PHE:CE2  | 2:D:150:ALA:HB2  | 1.58                     | 1.37              |
| 1:A:72:TYR:CE2   | 1:A:206:SER:HB3  | 1.59                     | 1.37              |
| 2:F:249:ARG:CB   | 2:F:307:TRP:HE1  | 1.38                     | 1.36              |
| 1:B:250:ILE:CG2  | 1:B:365:ILE:HD11 | 1.56                     | 1.35              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:64:SER:OG    | 1:B:86:ASN:N     | 1.60                     | 1.35              |
| 1:E:588:PHE:CA   | 2:F:5:PRO:CB     | 1.99                     | 1.35              |
| 1:A:72:TYR:CE2   | 1:A:206:SER:CB   | 2.09                     | 1.35              |
| 1:A:181:ASN:OD1  | 1:A:187:ASP:HB2  | 1.26                     | 1.35              |
| 2:C:82:ASP:OD1   | 2:D:65:HIS:NE2   | 1.57                     | 1.35              |
| 1:E:299:SER:CB   | 1:E:317:SER:HB3  | 1.54                     | 1.35              |
| 1:B:486:ILE:CD1  | 1:B:564:ASP:O    | 1.74                     | 1.34              |
| 1:A:276:LEU:HD13 | 1:A:354:HIS:O    | 1.26                     | 1.34              |
| 1:E:588:PHE:CB   | 2:F:5:PRO:HB3    | 1.56                     | 1.34              |
| 1:B:468:LEU:HD21 | 1:B:559:VAL:CG1  | 1.57                     | 1.34              |
| 1:E:169:LEU:CD1  | 1:E:183:PHE:CE1  | 2.11                     | 1.34              |
| 2:F:20:LYS:HZ1   | 2:F:162:VAL:CB   | 1.36                     | 1.33              |
| 1:A:184:TRP:CZ2  | 1:A:211:TYR:HB2  | 1.64                     | 1.33              |
| 1:B:127:PRO:HG3  | 3:B:710:HOH:O    | 1.22                     | 1.33              |
| 1:A:246:LYS:N    | 1:A:383:THR:CB   | 1.91                     | 1.32              |
| 2:C:11:LYS:CB    | 1:A:585:TYR:CE2  | 1.77                     | 1.32              |
| 1:E:500:CYS:HB2  | 1:E:515:GLU:OE2  | 1.23                     | 1.32              |
| 1:B:454:VAL:CG1  | 2:D:407:PHE:CE1  | 2.09                     | 1.32              |
| 1:E:454:VAL:HG22 | 1:E:539:MET:O    | 1.28                     | 1.32              |
| 2:F:238:ILE:CG2  | 2:F:307:TRP:CZ3  | 2.10                     | 1.32              |
| 2:D:58:HIS:CE1   | 2:D:98:GLY:HA3   | 1.64                     | 1.31              |
| 1:A:165:LEU:HD13 | 1:A:167:THR:N    | 1.44                     | 1.31              |
| 2:D:331:LEU:CD2  | 2:D:346:LEU:HB3  | 1.58                     | 1.31              |
| 1:A:463:SER:O    | 1:A:509:PRO:CG   | 1.78                     | 1.30              |
| 1:B:468:LEU:CD1  | 1:B:561:GLY:CA   | 2.08                     | 1.30              |
| 1:E:571:ALA:HB2  | 1:E:586:ILE:CD1  | 1.62                     | 1.30              |
| 2:F:330:THR:HG22 | 3:F:502:HOH:O    | 1.28                     | 1.30              |
| 2:F:331:LEU:CD2  | 2:F:343:LEU:CD2  | 2.08                     | 1.30              |
| 1:B:172:ILE:CD1  | 1:B:179:PHE:HB3  | 1.60                     | 1.29              |
| 2:F:111:PRO:CB   | 2:F:113:HIS:CE1  | 2.13                     | 1.29              |
| 2:D:331:LEU:CD2  | 2:D:346:LEU:CB   | 2.08                     | 1.29              |
| 2:D:326:LYS:C    | 2:D:330:THR:HG23 | 1.55                     | 1.29              |
| 1:E:531:SER:OG   | 2:F:418:PHE:HA   | 1.16                     | 1.29              |
| 2:F:20:LYS:CA    | 2:F:159:TRP:HZ3  | 1.44                     | 1.29              |
| 1:A:579:PHE:HD2  | 1:A:581:ARG:CB   | 1.28                     | 1.29              |
| 1:E:184:TRP:CZ3  | 1:E:211:TYR:CG   | 2.20                     | 1.28              |
| 1:A:117:LYS:HD3  | 1:A:439:PHE:CZ   | 1.68                     | 1.28              |
| 1:B:479:GLU:OE1  | 1:B:508:LEU:CB   | 1.81                     | 1.28              |
| 2:F:234:MET:CE   | 2:F:271:LEU:HD11 | 1.62                     | 1.28              |
| 1:A:223:ILE:HD11 | 3:A:726:HOH:O    | 1.18                     | 1.28              |
| 1:A:466:THR:CB   | 1:A:511:LEU:HD23 | 1.62                     | 1.28              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:36:LEU:CD2   | 2:C:40:TYR:HE1   | 1.47                     | 1.27              |
| 1:A:111:SER:HB3  | 1:A:141:GLU:O    | 1.22                     | 1.27              |
| 1:E:169:LEU:HD11 | 1:E:183:PHE:CZ   | 1.69                     | 1.27              |
| 1:E:370:LEU:CD2  | 1:E:397:ILE:HD11 | 1.64                     | 1.27              |
| 2:F:311:LEU:O    | 2:F:315:GLN:HG3  | 1.21                     | 1.27              |
| 1:E:169:LEU:CD1  | 1:E:183:PHE:CZ   | 2.18                     | 1.27              |
| 1:A:478:LEU:CD1  | 1:A:510:LEU:HD13 | 1.63                     | 1.27              |
| 1:E:103:ASP:OD1  | 1:E:130:GLN:HB2  | 1.34                     | 1.27              |
| 1:B:104:ILE:HG22 | 1:B:128:LEU:O    | 1.12                     | 1.26              |
| 2:C:11:LYS:HA    | 1:A:585:TYR:CD2  | 1.70                     | 1.26              |
| 2:C:258:HIS:NE2  | 2:C:262:LEU:HD21 | 1.47                     | 1.26              |
| 1:E:232:ILE:HD11 | 1:E:264:LEU:CA   | 1.64                     | 1.26              |
| 2:C:20:LYS:HE2   | 2:C:162:VAL:O    | 1.33                     | 1.26              |
| 2:D:62:SER:C     | 2:D:66:LEU:HD12  | 1.60                     | 1.26              |
| 1:A:225:HIS:HB2  | 1:A:227:ASN:OD1  | 1.16                     | 1.26              |
| 2:F:252:PHE:HD1  | 2:F:307:TRP:CH2  | 1.25                     | 1.26              |
| 2:C:258:HIS:CD2  | 2:C:262:LEU:CG   | 2.17                     | 1.26              |
| 1:A:165:LEU:CD1  | 1:A:167:THR:N    | 1.96                     | 1.26              |
| 2:F:234:MET:HE3  | 2:F:271:LEU:CD1  | 1.66                     | 1.26              |
| 1:B:279:ASN:CG   | 1:B:300:LYS:NZ   | 1.93                     | 1.25              |
| 1:A:399:ILE:O    | 1:A:401:LYS:HB3  | 1.31                     | 1.25              |
| 1:E:232:ILE:HD11 | 1:E:264:LEU:CD2  | 1.65                     | 1.25              |
| 1:B:172:ILE:HD11 | 1:B:179:PHE:O    | 1.33                     | 1.25              |
| 2:D:331:LEU:HD21 | 2:D:346:LEU:CB   | 1.66                     | 1.25              |
| 1:B:290:TYR:N    | 1:B:311:SER:OG   | 1.70                     | 1.25              |
| 1:A:169:LEU:HD21 | 1:A:441:PHE:CE1  | 1.72                     | 1.25              |
| 1:E:110:HIS:NE2  | 1:E:137:SER:O    | 1.70                     | 1.25              |
| 2:F:279:ASN:ND2  | 2:F:308:ILE:HD12 | 1.51                     | 1.25              |
| 2:F:336:HIS:CB   | 2:F:339:ASN:HD22 | 1.46                     | 1.25              |
| 1:B:87:LEU:CD1   | 1:B:160:ILE:HD13 | 1.65                     | 1.25              |
| 2:F:279:ASN:OD1  | 2:F:301:PHE:CE1  | 1.90                     | 1.25              |
| 1:A:224:LYS:HG3  | 1:A:228:TRP:CE3  | 1.71                     | 1.24              |
| 1:E:125:SER:CA   | 1:E:220:VAL:CB   | 2.14                     | 1.24              |
| 1:B:117:LYS:HD3  | 1:B:439:PHE:CE1  | 1.72                     | 1.24              |
| 2:D:276:LEU:CD2  | 2:D:333:LYS:CB   | 2.16                     | 1.24              |
| 1:A:385:VAL:CB   | 1:A:403:THR:HG23 | 1.64                     | 1.24              |
| 1:E:155:GLY:CA   | 3:E:713:HOH:O    | 1.72                     | 1.24              |
| 2:F:252:PHE:CD1  | 2:F:307:TRP:CZ2  | 2.02                     | 1.24              |
| 1:B:164:ASN:OD1  | 1:B:209:THR:HG22 | 1.28                     | 1.24              |
| 2:C:125:PHE:CZ   | 2:C:150:ALA:HB2  | 1.71                     | 1.24              |
| 1:A:490:PHE:CE1  | 1:A:523:PHE:HD1  | 1.53                     | 1.24              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:252:PHE:CD1  | 2:F:307:TRP:HH2  | 1.26                     | 1.24              |
| 2:C:235:ILE:HD13 | 2:C:278:LYS:CE   | 1.63                     | 1.24              |
| 1:B:502:LEU:CB   | 1:B:509:PRO:HB2  | 1.65                     | 1.23              |
| 1:B:62:ASN:CB    | 1:B:216:PRO:CG   | 2.16                     | 1.23              |
| 1:B:454:VAL:HG11 | 2:D:407:PHE:CD1  | 1.71                     | 1.23              |
| 2:D:327:MET:CA   | 2:D:330:THR:OG1  | 1.85                     | 1.23              |
| 1:E:232:ILE:CD1  | 1:E:264:LEU:CD2  | 2.16                     | 1.23              |
| 1:B:172:ILE:HD12 | 1:B:179:PHE:CB   | 1.68                     | 1.23              |
| 2:C:6:ARG:O      | 1:A:586:ILE:HG22 | 1.32                     | 1.23              |
| 2:D:326:LYS:O    | 2:D:330:THR:HG23 | 1.26                     | 1.23              |
| 2:F:273:ASP:OD1  | 2:F:330:THR:CG2  | 1.87                     | 1.23              |
| 2:C:88:ALA:HB2   | 3:C:502:HOH:O    | 1.36                     | 1.23              |
| 1:E:232:ILE:CD1  | 1:E:264:LEU:HB2  | 1.59                     | 1.23              |
| 1:E:531:SER:O    | 1:E:540:ASN:ND2  | 1.72                     | 1.23              |
| 2:F:238:ILE:CG2  | 2:F:307:TRP:CH2  | 2.20                     | 1.23              |
| 1:A:224:LYS:CG   | 1:A:228:TRP:CE3  | 2.20                     | 1.22              |
| 1:B:490:PHE:CB   | 1:B:557:ILE:HG21 | 1.63                     | 1.22              |
| 2:C:11:LYS:CG    | 1:A:585:TYR:CE2  | 2.21                     | 1.22              |
| 2:C:373:ASP:O    | 2:C:374:THR:HG22 | 1.13                     | 1.22              |
| 1:A:246:LYS:O    | 1:A:382:PRO:O    | 1.53                     | 1.22              |
| 1:E:100:GLY:N    | 1:E:142:ASN:ND2  | 1.74                     | 1.22              |
| 1:A:72:TYR:CZ    | 1:A:206:SER:HB3  | 1.74                     | 1.22              |
| 2:C:42:GLU:O     | 2:C:46:LEU:HD12  | 1.38                     | 1.22              |
| 1:A:165:LEU:CD1  | 1:A:167:THR:HB   | 1.68                     | 1.22              |
| 1:E:325:PHE:CE1  | 1:E:468:LEU:HD13 | 1.74                     | 1.22              |
| 1:A:170:GLU:CG   | 1:A:185:GLN:NE2  | 2.03                     | 1.21              |
| 1:A:334:ARG:HG3  | 1:A:513:TYR:OH   | 1.35                     | 1.21              |
| 1:A:184:TRP:CH2  | 1:A:211:TYR:HD2  | 1.58                     | 1.21              |
| 1:E:85:GLN:CB    | 1:E:131:ALA:CB   | 2.18                     | 1.21              |
| 1:E:482:ILE:O    | 1:E:485:THR:HG23 | 1.34                     | 1.21              |
| 1:A:110:HIS:HB3  | 1:A:140:LEU:CB   | 1.68                     | 1.21              |
| 1:E:370:LEU:CD2  | 1:E:397:ILE:CD1  | 2.14                     | 1.21              |
| 2:F:252:PHE:CE1  | 2:F:307:TRP:HH2  | 1.52                     | 1.21              |
| 1:A:451:PRO:O    | 1:A:541:LEU:O    | 1.53                     | 1.20              |
| 1:A:456:TYR:CB   | 1:A:537:LYS:CB   | 2.19                     | 1.20              |
| 2:F:279:ASN:ND2  | 2:F:308:ILE:CD1  | 2.03                     | 1.20              |
| 1:B:104:ILE:HD11 | 1:B:109:TYR:CD2  | 1.75                     | 1.20              |
| 1:A:133:GLN:NE2  | 1:A:134:VAL:O    | 1.73                     | 1.20              |
| 2:F:10:TRP:CA    | 2:F:50:TYR:HE2   | 1.54                     | 1.20              |
| 1:B:87:LEU:HD11  | 1:B:160:ILE:CD1  | 1.71                     | 1.20              |
| 2:F:110:ILE:CD1  | 2:F:115:LEU:CD1  | 2.11                     | 1.20              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:82:ASP:OD1   | 2:D:65:HIS:CD2   | 1.94                     | 1.20              |
| 1:E:169:LEU:HD12 | 1:E:183:PHE:CE1  | 1.71                     | 1.20              |
| 2:F:153:TRP:CZ2  | 2:F:157:HIS:HD2  | 1.58                     | 1.20              |
| 1:B:164:ASN:HA   | 1:B:210:PHE:CE1  | 1.75                     | 1.19              |
| 2:C:258:HIS:NE2  | 2:C:262:LEU:CD1  | 1.91                     | 1.19              |
| 2:D:259:PHE:CZ   | 2:D:268:PRO:HB3  | 1.76                     | 1.19              |
| 2:F:249:ARG:CB   | 2:F:307:TRP:NE1  | 2.05                     | 1.19              |
| 1:B:486:ILE:HD13 | 1:B:564:ASP:O    | 1.31                     | 1.19              |
| 1:A:63:PHE:CZ    | 1:A:212:PRO:CB   | 2.26                     | 1.19              |
| 1:E:446:LEU:HD13 | 1:E:528:LEU:HD23 | 1.22                     | 1.19              |
| 1:E:529:VAL:CG1  | 1:E:532:ILE:HD11 | 1.71                     | 1.19              |
| 1:E:530:HIS:NE2  | 1:E:570:ILE:CG2  | 2.05                     | 1.19              |
| 2:F:20:LYS:NZ    | 2:F:162:VAL:CB   | 2.03                     | 1.19              |
| 2:C:235:ILE:HD11 | 2:C:278:LYS:CE   | 1.62                     | 1.19              |
| 1:A:165:LEU:CD1  | 1:A:167:THR:CB   | 2.20                     | 1.19              |
| 1:B:462:ILE:HA   | 1:B:556:ILE:CB   | 1.71                     | 1.18              |
| 1:B:465:LEU:HD23 | 1:B:466:THR:N    | 1.56                     | 1.18              |
| 1:B:325:PHE:CG   | 1:B:330:ASP:CB   | 2.27                     | 1.18              |
| 1:A:494:ARG:O    | 3:A:702:HOH:O    | 1.60                     | 1.18              |
| 1:B:455:SER:CB   | 2:D:405:LYS:CB   | 2.22                     | 1.18              |
| 2:F:220:GLY:O    | 2:F:224:HIS:CD2  | 1.96                     | 1.18              |
| 2:C:42:GLU:O     | 2:C:46:LEU:CD1   | 1.89                     | 1.18              |
| 1:A:169:LEU:CD2  | 1:A:441:PHE:CE1  | 2.24                     | 1.18              |
| 2:F:273:ASP:OD1  | 2:F:330:THR:HG21 | 1.06                     | 1.18              |
| 1:B:110:HIS:HB3  | 1:B:140:LEU:CB   | 1.74                     | 1.18              |
| 1:B:182:LEU:HD13 | 1:B:183:PHE:CE2  | 1.77                     | 1.18              |
| 1:B:468:LEU:HD13 | 1:B:561:GLY:HA2  | 1.23                     | 1.18              |
| 1:E:262:ARG:NH1  | 1:E:308:ASN:OD1  | 1.77                     | 1.17              |
| 2:D:327:MET:HA   | 2:D:330:THR:OG1  | 1.02                     | 1.17              |
| 1:A:165:LEU:HD11 | 1:A:167:THR:HB   | 1.19                     | 1.17              |
| 1:B:180:LYS:HE2  | 1:B:181:ASN:HB2  | 1.22                     | 1.17              |
| 1:E:588:PHE:HA   | 2:F:5:PRO:CA     | 1.74                     | 1.17              |
| 1:B:223:ILE:CG2  | 3:B:721:HOH:O    | 1.89                     | 1.17              |
| 1:B:87:LEU:CD1   | 1:B:160:ILE:CD1  | 2.22                     | 1.17              |
| 2:C:36:LEU:HD21  | 2:C:40:TYR:HE1   | 1.09                     | 1.17              |
| 2:D:63:THR:HG21  | 2:D:159:TRP:HE1  | 1.02                     | 1.17              |
| 1:E:479:GLU:OE1  | 1:E:507:GLN:CB   | 1.92                     | 1.17              |
| 1:B:250:ILE:HD11 | 1:B:373:THR:HG23 | 1.24                     | 1.16              |
| 1:B:456:TYR:CE2  | 1:B:537:LYS:CA   | 2.24                     | 1.16              |
| 1:A:63:PHE:CE1   | 1:A:212:PRO:CB   | 2.28                     | 1.16              |
| 1:B:104:ILE:CG2  | 1:B:128:LEU:O    | 1.93                     | 1.16              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:164:ASN:OD1  | 1:B:209:THR:CG2  | 1.92                     | 1.16              |
| 2:D:259:PHE:CE1  | 2:D:268:PRO:CB   | 2.27                     | 1.16              |
| 1:E:530:HIS:O    | 2:F:418:PHE:CB   | 1.93                     | 1.16              |
| 2:F:353:ASP:HB3  | 2:F:354:PRO:HD3  | 1.19                     | 1.16              |
| 1:A:358:LEU:HD13 | 1:A:359:ILE:H    | 1.04                     | 1.16              |
| 1:B:585:TYR:HE1  | 2:D:9:PRO:O      | 1.29                     | 1.16              |
| 1:A:81:LEU:HD23  | 1:A:131:ALA:HB2  | 1.28                     | 1.16              |
| 2:F:10:TRP:HB3   | 2:F:50:TYR:CE2   | 1.81                     | 1.16              |
| 1:B:250:ILE:CG2  | 1:B:365:ILE:CD1  | 2.23                     | 1.15              |
| 2:C:177:GLU:OE1  | 2:C:180:ILE:CG2  | 1.94                     | 1.15              |
| 1:A:465:LEU:CD1  | 1:A:482:ILE:HG21 | 1.76                     | 1.15              |
| 1:E:340:GLU:HG2  | 1:E:379:ARG:HH11 | 1.11                     | 1.15              |
| 2:D:344:GLU:O    | 2:D:348:SER:OG   | 1.61                     | 1.15              |
| 1:A:169:LEU:HD22 | 1:A:441:PHE:CD1  | 1.64                     | 1.15              |
| 2:C:10:TRP:HB3   | 2:C:50:TYR:CE1   | 1.81                     | 1.15              |
| 2:F:280:TYR:CA   | 2:F:338:LEU:HD21 | 1.77                     | 1.15              |
| 1:B:456:TYR:CE2  | 1:B:537:LYS:HA   | 1.82                     | 1.15              |
| 2:F:20:LYS:HZ2   | 2:F:162:VAL:CG1  | 1.60                     | 1.15              |
| 1:A:94:VAL:O     | 1:A:162:LEU:HB2  | 1.43                     | 1.14              |
| 2:C:280:TYR:HB2  | 2:C:334:THR:CG2  | 1.78                     | 1.14              |
| 1:A:492:VAL:O    | 1:A:554:GLU:CB   | 1.94                     | 1.14              |
| 1:E:225:HIS:HB2  | 1:E:228:TRP:HB2  | 1.25                     | 1.14              |
| 1:B:232:ILE:CG1  | 1:B:264:LEU:HD23 | 1.71                     | 1.14              |
| 1:B:380:VAL:HB   | 1:B:382:PRO:HD3  | 1.20                     | 1.14              |
| 2:C:258:HIS:NE2  | 2:C:262:LEU:CD2  | 2.09                     | 1.14              |
| 1:A:165:LEU:CD1  | 1:A:167:THR:CA   | 2.24                     | 1.14              |
| 1:A:165:LEU:HD11 | 1:A:167:THR:CB   | 1.75                     | 1.14              |
| 1:E:370:LEU:HD11 | 1:E:397:ILE:HG13 | 1.27                     | 1.14              |
| 2:C:215:TRP:HA   | 2:C:218:ILE:HD12 | 1.25                     | 1.14              |
| 2:F:24:PHE:HD1   | 2:F:155:TRP:CZ3  | 1.65                     | 1.14              |
| 1:B:468:LEU:HD11 | 1:B:561:GLY:CA   | 1.77                     | 1.13              |
| 1:A:364:TRP:HB3  | 1:A:369:GLY:HA3  | 1.19                     | 1.13              |
| 2:F:20:LYS:NZ    | 2:F:162:VAL:HB   | 1.59                     | 1.13              |
| 2:D:357:LYS:HA   | 2:D:360:ILE:HD12 | 1.22                     | 1.13              |
| 1:A:170:GLU:CD   | 1:A:185:GLN:NE2  | 2.04                     | 1.13              |
| 1:A:175:VAL:O    | 1:A:568:TRP:HD1  | 1.31                     | 1.13              |
| 1:E:155:GLY:HA3  | 3:E:713:HOH:O    | 1.37                     | 1.13              |
| 1:E:451:PRO:HD3  | 2:F:413:TRP:CD2  | 1.84                     | 1.13              |
| 2:C:11:LYS:CG    | 1:A:585:TYR:HE2  | 1.60                     | 1.13              |
| 1:A:572:SER:O    | 1:A:575:ILE:CD1  | 1.96                     | 1.13              |
| 1:E:99:ARG:CA    | 1:E:142:ASN:CG   | 2.20                     | 1.13              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:531:SER:OG   | 2:F:418:PHE:CA   | 1.96                     | 1.13              |
| 2:F:10:TRP:CB    | 2:F:50:TYR:HE2   | 1.60                     | 1.13              |
| 1:B:104:ILE:HG23 | 1:B:129:ILE:HA   | 1.26                     | 1.13              |
| 2:C:418:PHE:CE2  | 1:A:447:LEU:HD21 | 1.84                     | 1.13              |
| 1:E:301:ILE:HG23 | 1:E:315:THR:HG23 | 1.28                     | 1.13              |
| 1:A:478:LEU:HD13 | 1:A:510:LEU:HD13 | 1.28                     | 1.12              |
| 1:B:87:LEU:HD13  | 1:B:160:ILE:HD13 | 1.16                     | 1.12              |
| 1:B:479:GLU:CD   | 1:B:508:LEU:CB   | 2.23                     | 1.12              |
| 2:C:36:LEU:HD21  | 2:C:40:TYR:CE1   | 1.84                     | 1.12              |
| 1:A:111:SER:H    | 1:A:140:LEU:CB   | 1.60                     | 1.12              |
| 1:A:181:ASN:OD1  | 1:A:187:ASP:CB   | 1.98                     | 1.12              |
| 1:A:483:GLU:CB   | 1:A:532:ILE:HD12 | 1.79                     | 1.12              |
| 1:B:111:SER:OG   | 1:B:142:ASN:HA   | 0.94                     | 1.12              |
| 1:A:463:SER:O    | 1:A:509:PRO:HG2  | 0.95                     | 1.12              |
| 1:A:464:ALA:CB   | 1:A:509:PRO:HB2  | 1.79                     | 1.12              |
| 2:F:24:PHE:CE1   | 2:F:155:TRP:HE3  | 1.67                     | 1.12              |
| 2:C:125:PHE:HZ   | 2:C:150:ALA:CA   | 1.63                     | 1.12              |
| 1:E:184:TRP:HZ3  | 1:E:211:TYR:CG   | 1.60                     | 1.12              |
| 1:E:287:GLN:HB3  | 3:E:719:HOH:O    | 1.48                     | 1.12              |
| 2:F:20:LYS:NZ    | 2:F:162:VAL:CG1  | 2.12                     | 1.12              |
| 1:B:279:ASN:HB2  | 1:B:300:LYS:HZ3  | 1.12                     | 1.11              |
| 2:C:418:PHE:HE2  | 1:A:447:LEU:HD21 | 0.99                     | 1.11              |
| 2:C:418:PHE:CZ   | 1:A:569:GLU:OE2  | 2.04                     | 1.11              |
| 2:D:183:LEU:CD2  | 2:D:224:HIS:CB   | 2.28                     | 1.11              |
| 1:E:248:ILE:HD11 | 1:E:382:PRO:CB   | 1.80                     | 1.11              |
| 1:E:294:ASP:OD1  | 1:E:325:PHE:O    | 1.67                     | 1.11              |
| 2:F:23:PHE:CE2   | 2:F:43:ALA:HB1   | 1.84                     | 1.11              |
| 2:F:111:PRO:HB3  | 2:F:113:HIS:CE1  | 1.83                     | 1.11              |
| 1:B:490:PHE:HB3  | 1:B:557:ILE:HG21 | 1.20                     | 1.11              |
| 1:A:245:ILE:O    | 1:A:356:SER:OG   | 1.68                     | 1.11              |
| 1:E:340:GLU:CG   | 1:E:379:ARG:HH11 | 1.64                     | 1.11              |
| 1:E:430:MET:HE1  | 1:E:568:TRP:CE3  | 1.85                     | 1.11              |
| 1:B:63:PHE:N     | 1:B:88:ILE:HD11  | 1.65                     | 1.11              |
| 1:B:99:ARG:HA    | 1:B:142:ASN:CB   | 1.81                     | 1.11              |
| 2:C:373:ASP:O    | 2:C:374:THR:CG2  | 1.99                     | 1.11              |
| 2:D:331:LEU:CD2  | 2:D:346:LEU:CD1  | 2.29                     | 1.11              |
| 1:E:172:ILE:HD13 | 1:E:183:PHE:HE2  | 1.11                     | 1.11              |
| 2:C:11:LYS:CA    | 1:A:585:TYR:CD2  | 2.34                     | 1.10              |
| 2:C:95:PHE:HE1   | 2:C:99:LEU:HD21  | 1.08                     | 1.10              |
| 1:B:164:ASN:ND2  | 1:B:208:TYR:HB3  | 1.64                     | 1.10              |
| 1:B:164:ASN:HD21 | 1:B:208:TYR:HB3  | 0.99                     | 1.10              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:328:PRO:HB3  | 1:B:335:TYR:CE2  | 1.86                     | 1.10              |
| 2:C:218:ILE:HG12 | 2:C:255:MET:HE1  | 1.17                     | 1.10              |
| 1:A:233:LYS:O    | 1:A:237:GLU:OE1  | 1.68                     | 1.10              |
| 1:E:184:TRP:CZ3  | 1:E:211:TYR:HB2  | 1.76                     | 1.10              |
| 1:E:299:SER:HB3  | 1:E:317:SER:HB2  | 1.23                     | 1.10              |
| 2:F:24:PHE:CE1   | 2:F:155:TRP:HB2  | 1.84                     | 1.10              |
| 1:B:107:VAL:HG21 | 1:B:266:GLN:NE2  | 1.65                     | 1.10              |
| 1:B:502:LEU:HB3  | 1:B:509:PRO:HB2  | 1.19                     | 1.10              |
| 1:A:350:GLY:HA3  | 1:A:357:LEU:HD11 | 1.33                     | 1.10              |
| 1:A:369:GLY:HA2  | 1:A:372:LEU:HD12 | 1.20                     | 1.10              |
| 1:E:225:HIS:CB   | 1:E:228:TRP:HB2  | 1.81                     | 1.10              |
| 1:E:487:VAL:O    | 1:E:526:LEU:HD23 | 1.47                     | 1.10              |
| 2:F:20:LYS:NZ    | 2:F:162:VAL:O    | 1.82                     | 1.10              |
| 2:F:24:PHE:HE1   | 2:F:155:TRP:HB2  | 1.03                     | 1.10              |
| 2:D:331:LEU:CD2  | 2:D:346:LEU:HD13 | 1.80                     | 1.10              |
| 1:B:87:LEU:HD11  | 1:B:160:ILE:HD11 | 1.22                     | 1.10              |
| 1:B:598:TRP:CE3  | 2:D:58:HIS:CE1   | 2.39                     | 1.10              |
| 2:C:414:THR:O    | 2:C:416:LYS:CD   | 2.00                     | 1.10              |
| 1:A:466:THR:CB   | 1:A:511:LEU:CD2  | 2.26                     | 1.10              |
| 1:E:232:ILE:HD11 | 1:E:264:LEU:CG   | 1.81                     | 1.10              |
| 1:A:170:GLU:HG3  | 1:A:185:GLN:HE22 | 1.01                     | 1.09              |
| 1:A:232:ILE:HD11 | 1:A:264:LEU:CG   | 1.80                     | 1.09              |
| 2:C:186:LEU:CB   | 2:C:221:ILE:HG12 | 1.80                     | 1.09              |
| 1:A:184:TRP:CZ2  | 1:A:211:TYR:CD2  | 2.40                     | 1.09              |
| 1:E:99:ARG:HA    | 1:E:142:ASN:ND2  | 1.66                     | 1.09              |
| 1:E:301:ILE:HG23 | 1:E:315:THR:CG2  | 1.81                     | 1.09              |
| 1:E:349:ASP:C    | 1:E:351:GLU:OE1  | 1.96                     | 1.09              |
| 1:B:104:ILE:O    | 1:B:107:VAL:HG22 | 1.53                     | 1.09              |
| 1:B:118:PHE:CD1  | 1:B:306:HIS:CB   | 2.22                     | 1.09              |
| 1:B:239:TYR:O    | 1:B:274:GLN:NE2  | 1.85                     | 1.09              |
| 1:A:385:VAL:HB   | 1:A:403:THR:CG2  | 1.81                     | 1.09              |
| 1:E:164:ASN:OD1  | 1:E:209:THR:HG22 | 1.51                     | 1.09              |
| 1:E:451:PRO:HG3  | 2:F:413:TRP:CZ2  | 1.86                     | 1.09              |
| 1:B:383:THR:HG22 | 1:B:384:HIS:CD2  | 1.88                     | 1.09              |
| 1:B:468:LEU:HD21 | 1:B:559:VAL:HG11 | 1.30                     | 1.09              |
| 1:A:232:ILE:HG13 | 1:A:264:LEU:HD23 | 1.29                     | 1.09              |
| 1:E:370:LEU:CD1  | 1:E:397:ILE:CD1  | 2.13                     | 1.09              |
| 1:E:446:LEU:CD1  | 1:E:528:LEU:HD23 | 1.83                     | 1.09              |
| 2:F:111:PRO:HB2  | 2:F:113:HIS:ND1  | 1.67                     | 1.09              |
| 1:A:350:GLY:HA2  | 1:A:357:LEU:HD11 | 1.33                     | 1.09              |
| 1:A:492:VAL:CG1  | 1:A:557:ILE:HD13 | 1.83                     | 1.09              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:91:GLY:O     | 1:E:120:ASN:OD1  | 1.70                     | 1.09              |
| 1:E:230:ASP:O    | 1:E:234:SER:N    | 1.83                     | 1.09              |
| 2:F:122:PRO:HG2  | 2:F:125:PHE:CE2  | 1.88                     | 1.09              |
| 2:D:160:ASP:OD2  | 3:D:501:HOH:O    | 1.70                     | 1.08              |
| 2:D:276:LEU:HD13 | 2:D:333:LYS:CB   | 1.83                     | 1.08              |
| 1:A:63:PHE:CE1   | 1:A:212:PRO:HB2  | 1.89                     | 1.08              |
| 1:A:374:ARG:O    | 1:A:377:ILE:HG12 | 1.35                     | 1.08              |
| 2:F:316:ILE:HD11 | 2:F:346:LEU:HD23 | 1.29                     | 1.08              |
| 2:C:36:LEU:CD2   | 2:C:40:TYR:CE1   | 2.36                     | 1.08              |
| 1:A:95:LEU:CB    | 1:A:162:LEU:HB3  | 1.84                     | 1.08              |
| 1:E:435:LYS:HE2  | 1:E:545:GLN:HE22 | 1.08                     | 1.08              |
| 1:E:529:VAL:HG13 | 1:E:532:ILE:HD11 | 1.29                     | 1.08              |
| 2:F:111:PRO:HB2  | 2:F:113:HIS:CE1  | 1.86                     | 1.08              |
| 2:F:272:ILE:CD1  | 2:F:315:GLN:NE2  | 2.15                     | 1.08              |
| 2:C:271:LEU:HD11 | 2:C:275:MET:HE2  | 1.28                     | 1.08              |
| 2:D:24:PHE:CE2   | 2:D:155:TRP:HD1  | 1.50                     | 1.08              |
| 1:A:389:ASN:ND2  | 1:A:408:LEU:HB3  | 1.68                     | 1.08              |
| 1:A:492:VAL:HG11 | 1:A:557:ILE:HD13 | 1.35                     | 1.08              |
| 1:E:430:MET:HE1  | 1:E:568:TRP:HE3  | 1.07                     | 1.08              |
| 2:C:125:PHE:CZ   | 2:C:150:ALA:CB   | 2.37                     | 1.08              |
| 1:A:117:LYS:CD   | 1:A:439:PHE:CE2  | 2.37                     | 1.08              |
| 1:A:483:GLU:CD   | 1:A:532:ILE:CD1  | 2.27                     | 1.08              |
| 2:D:190:TYR:HA   | 2:D:193:ILE:HD12 | 1.10                     | 1.07              |
| 1:A:111:SER:CB   | 1:A:141:GLU:O    | 2.02                     | 1.07              |
| 1:E:232:ILE:CD1  | 1:E:264:LEU:CG   | 2.32                     | 1.07              |
| 1:E:530:HIS:NE2  | 1:E:570:ILE:HG22 | 1.67                     | 1.07              |
| 2:F:40:TYR:CZ    | 2:F:67:PHE:HE2   | 1.72                     | 1.07              |
| 2:F:406:SER:HB2  | 3:F:504:HOH:O    | 1.52                     | 1.07              |
| 2:C:10:TRP:CA    | 2:C:50:TYR:HE1   | 1.67                     | 1.07              |
| 1:A:463:SER:OG   | 1:A:555:ALA:CB   | 2.02                     | 1.07              |
| 1:A:468:LEU:HD23 | 1:A:559:VAL:CG1  | 1.84                     | 1.07              |
| 2:D:58:HIS:HE1   | 2:D:98:GLY:CA    | 1.66                     | 1.07              |
| 2:D:259:PHE:HE1  | 2:D:268:PRO:CB   | 1.65                     | 1.07              |
| 1:A:565:LEU:HD13 | 1:A:570:ILE:HD11 | 1.29                     | 1.07              |
| 1:E:93:PHE:HB3   | 1:E:210:PHE:CD1  | 1.89                     | 1.07              |
| 1:E:524:PHE:HE2  | 1:E:543:ILE:HD11 | 1.16                     | 1.07              |
| 2:F:20:LYS:NZ    | 2:F:162:VAL:HG12 | 1.69                     | 1.07              |
| 2:F:272:ILE:HD13 | 2:F:315:GLN:NE2  | 1.69                     | 1.07              |
| 1:B:279:ASN:ND2  | 1:B:300:LYS:HZ1  | 1.51                     | 1.07              |
| 1:A:172:ILE:HD11 | 1:A:183:PHE:CE2  | 1.90                     | 1.07              |
| 1:A:358:LEU:HD13 | 1:A:359:ILE:N    | 1.69                     | 1.07              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:483:GLU:HB2  | 1:A:532:ILE:CD1  | 1.84                     | 1.07              |
| 1:E:504:ASN:O    | 1:E:509:PRO:HB3  | 1.55                     | 1.07              |
| 2:F:111:PRO:HG2  | 2:F:114:LEU:HB2  | 1.35                     | 1.07              |
| 2:F:262:LEU:HD13 | 2:F:263:LYS:HG3  | 1.32                     | 1.07              |
| 2:F:354:PRO:HD2  | 2:F:355:VAL:H    | 1.13                     | 1.07              |
| 1:B:468:LEU:HD11 | 1:B:561:GLY:N    | 1.69                     | 1.07              |
| 1:B:492:VAL:N    | 1:B:557:ILE:HD11 | 1.70                     | 1.07              |
| 2:C:414:THR:O    | 2:C:416:LYS:CE   | 2.03                     | 1.07              |
| 2:D:237:ARG:O    | 2:D:240:SER:OG   | 1.70                     | 1.07              |
| 1:A:206:SER:OG   | 1:A:211:TYR:OH   | 1.69                     | 1.07              |
| 1:E:370:LEU:CG   | 1:E:397:ILE:CD1  | 2.28                     | 1.07              |
| 1:B:72:TYR:OH    | 1:B:205:PHE:HA   | 1.54                     | 1.06              |
| 1:A:172:ILE:HG22 | 1:A:179:PHE:HB2  | 1.23                     | 1.06              |
| 1:B:81:LEU:HD22  | 1:B:160:ILE:HD11 | 1.36                     | 1.06              |
| 1:B:171:SER:O    | 1:B:174:ARG:HG3  | 1.55                     | 1.06              |
| 2:D:24:PHE:HE1   | 2:D:67:PHE:CZ    | 1.74                     | 1.06              |
| 1:A:230:ASP:O    | 1:A:234:SER:N    | 1.88                     | 1.06              |
| 1:A:232:ILE:CG1  | 1:A:264:LEU:HD23 | 1.83                     | 1.06              |
| 1:E:294:ASP:OD1  | 1:E:325:PHE:C    | 1.99                     | 1.06              |
| 1:E:364:TRP:HB3  | 1:E:369:GLY:HA3  | 1.12                     | 1.06              |
| 1:B:290:TYR:CA   | 1:B:311:SER:OG   | 2.02                     | 1.06              |
| 1:B:468:LEU:CD2  | 1:B:559:VAL:CG1  | 2.34                     | 1.06              |
| 1:B:468:LEU:HD12 | 1:B:561:GLY:HA2  | 1.32                     | 1.06              |
| 1:B:491:LYS:C    | 1:B:557:ILE:HD12 | 1.80                     | 1.06              |
| 1:E:248:ILE:HD11 | 1:E:382:PRO:HB3  | 1.11                     | 1.06              |
| 1:B:63:PHE:CB    | 1:B:88:ILE:HD11  | 1.76                     | 1.06              |
| 1:B:161:LYS:NZ   | 1:B:163:THR:OG1  | 1.88                     | 1.06              |
| 2:C:305:GLN:HA   | 2:C:308:ILE:CG1  | 1.85                     | 1.06              |
| 1:A:170:GLU:HG3  | 1:A:185:GLN:NE2  | 1.62                     | 1.06              |
| 1:E:85:GLN:CB    | 1:E:131:ALA:HB3  | 1.83                     | 1.06              |
| 1:E:226:LYS:O    | 1:E:230:ASP:N    | 1.89                     | 1.06              |
| 1:E:299:SER:CB   | 1:E:317:SER:HB2  | 1.72                     | 1.06              |
| 1:E:370:LEU:CD1  | 1:E:397:ILE:CG1  | 2.31                     | 1.06              |
| 2:F:12:SER:N     | 2:F:15:GLU:OE1   | 1.88                     | 1.06              |
| 2:F:20:LYS:HZ2   | 2:F:162:VAL:HG12 | 1.14                     | 1.06              |
| 2:C:177:GLU:OE1  | 2:C:180:ILE:HG23 | 1.50                     | 1.06              |
| 2:F:116:ALA:HA   | 2:F:119:ILE:HD11 | 1.38                     | 1.06              |
| 1:B:64:SER:OG    | 1:B:86:ASN:O     | 1.74                     | 1.05              |
| 1:B:223:ILE:HG21 | 3:B:721:HOH:O    | 1.48                     | 1.05              |
| 1:E:219:THR:O    | 3:E:702:HOH:O    | 1.73                     | 1.05              |
| 1:E:224:LYS:HG2  | 1:E:228:TRP:CZ3  | 1.89                     | 1.05              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:479:GLU:OE1  | 1:E:507:GLN:HB3  | 1.53                     | 1.05              |
| 1:E:504:ASN:ND2  | 1:E:505:LYS:O    | 1.88                     | 1.05              |
| 2:F:236:GLU:O    | 2:F:240:SER:N    | 1.88                     | 1.05              |
| 1:B:529:VAL:HG21 | 1:B:532:ILE:HD11 | 1.38                     | 1.05              |
| 2:C:128:PHE:CE2  | 2:C:138:PRO:HG2  | 1.91                     | 1.05              |
| 1:A:468:LEU:CD2  | 1:A:559:VAL:HG11 | 1.84                     | 1.05              |
| 1:E:172:ILE:HD13 | 1:E:183:PHE:CE2  | 1.89                     | 1.05              |
| 1:E:232:ILE:HD12 | 1:E:264:LEU:HD23 | 1.12                     | 1.05              |
| 1:E:499:GLU:O    | 1:E:515:GLU:CD   | 1.98                     | 1.05              |
| 2:F:256:MET:HA   | 2:F:259:PHE:HB3  | 1.36                     | 1.05              |
| 1:B:454:VAL:HG12 | 2:D:407:PHE:CD1  | 1.88                     | 1.05              |
| 1:B:491:LYS:C    | 1:B:557:ILE:CD1  | 2.29                     | 1.05              |
| 1:B:529:VAL:HG23 | 1:B:540:ASN:O    | 1.54                     | 1.05              |
| 2:C:186:LEU:HB3  | 2:C:221:ILE:CG1  | 1.87                     | 1.05              |
| 2:C:235:ILE:HD13 | 2:C:278:LYS:HE3  | 1.09                     | 1.05              |
| 2:C:258:HIS:CD2  | 2:C:262:LEU:HG   | 1.90                     | 1.05              |
| 1:A:184:TRP:CZ2  | 1:A:211:TYR:HD2  | 1.72                     | 1.05              |
| 1:E:224:LYS:CG   | 1:E:228:TRP:CE3  | 2.40                     | 1.05              |
| 1:A:377:ILE:H    | 1:A:377:ILE:HD13 | 1.19                     | 1.05              |
| 1:E:232:ILE:HD13 | 1:E:264:LEU:HB2  | 1.05                     | 1.05              |
| 2:C:418:PHE:HZ   | 1:A:569:GLU:OE2  | 1.37                     | 1.05              |
| 1:A:181:ASN:OD1  | 1:A:187:ASP:C    | 1.98                     | 1.05              |
| 1:A:408:LEU:H    | 1:A:408:LEU:HD13 | 1.17                     | 1.05              |
| 1:E:233:LYS:O    | 1:E:233:LYS:NZ   | 1.88                     | 1.05              |
| 1:E:284:ASP:OD1  | 1:E:287:GLN:N    | 1.88                     | 1.05              |
| 1:E:586:ILE:HG23 | 2:F:6:ARG:O      | 1.55                     | 1.05              |
| 2:F:345:LYS:O    | 2:F:348:SER:OG   | 1.75                     | 1.05              |
| 1:B:104:ILE:CD1  | 1:B:107:VAL:HG23 | 1.87                     | 1.04              |
| 1:B:250:ILE:HG23 | 1:B:365:ILE:CD1  | 1.84                     | 1.04              |
| 1:B:432:TYR:CE2  | 1:B:526:LEU:HB2  | 1.90                     | 1.04              |
| 2:C:299:GLN:O    | 2:C:303:CYS:N    | 1.88                     | 1.04              |
| 1:B:164:ASN:HA   | 1:B:210:PHE:HE1  | 0.89                     | 1.04              |
| 2:D:160:ASP:CG   | 3:D:501:HOH:O    | 1.98                     | 1.04              |
| 1:A:490:PHE:CE1  | 1:A:523:PHE:CD1  | 2.44                     | 1.04              |
| 1:E:99:ARG:CA    | 1:E:142:ASN:ND2  | 2.18                     | 1.04              |
| 1:B:207:ASP:O    | 3:B:701:HOH:O    | 1.74                     | 1.04              |
| 1:A:117:LYS:CD   | 1:A:439:PHE:HE2  | 1.69                     | 1.04              |
| 1:E:161:LYS:NZ   | 1:E:163:THR:OG1  | 1.88                     | 1.04              |
| 1:E:366:LYS:HD2  | 1:E:367:GLY:H    | 1.19                     | 1.04              |
| 1:E:433:PHE:HA   | 1:E:544:PRO:HB3  | 1.08                     | 1.04              |
| 2:F:237:ARG:HA   | 2:F:240:SER:HB2  | 1.39                     | 1.04              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:585:TYR:C    | 1:B:586:ILE:HD13 | 1.82                     | 1.04              |
| 1:B:594:LEU:O    | 2:D:59:ILE:HG13  | 1.58                     | 1.04              |
| 2:C:141:GLU:OE1  | 2:C:144:LYS:NZ   | 1.88                     | 1.04              |
| 2:D:183:LEU:HD21 | 2:D:224:HIS:HB3  | 1.06                     | 1.04              |
| 1:A:184:TRP:CH2  | 1:A:211:TYR:CD2  | 2.45                     | 1.04              |
| 2:F:10:TRP:CA    | 2:F:50:TYR:CE2   | 2.40                     | 1.04              |
| 2:C:258:HIS:CE1  | 2:C:262:LEU:HD21 | 1.91                     | 1.04              |
| 1:A:169:LEU:HD23 | 1:A:441:PHE:CD1  | 1.89                     | 1.04              |
| 2:F:345:LYS:C    | 2:F:348:SER:HG   | 1.66                     | 1.04              |
| 1:B:325:PHE:HZ   | 1:B:469:LYS:HB2  | 1.24                     | 1.03              |
| 2:C:133:THR:O    | 2:D:97:ASN:ND2   | 1.90                     | 1.03              |
| 2:D:268:PRO:HA   | 2:D:271:LEU:HD11 | 1.39                     | 1.03              |
| 2:F:312:ALA:HB1  | 2:F:342:LEU:HD21 | 1.36                     | 1.03              |
| 1:B:118:PHE:CE1  | 1:B:306:HIS:CG   | 2.46                     | 1.03              |
| 1:B:368:TYR:CE1  | 1:B:372:LEU:HG   | 1.92                     | 1.03              |
| 1:A:365:ILE:O    | 1:A:393:LEU:CD2  | 2.07                     | 1.03              |
| 1:E:181:ASN:O    | 3:E:703:HOH:O    | 1.74                     | 1.03              |
| 2:F:262:LEU:CD1  | 2:F:263:LYS:HG3  | 1.89                     | 1.03              |
| 1:B:171:SER:OG   | 1:B:174:ARG:HD2  | 1.59                     | 1.03              |
| 2:D:125:PHE:HZ   | 2:D:150:ALA:N    | 1.54                     | 1.03              |
| 1:A:165:LEU:HD11 | 1:A:167:THR:CA   | 1.87                     | 1.03              |
| 1:A:490:PHE:HB2  | 1:A:557:ILE:HG13 | 1.40                     | 1.03              |
| 1:E:103:ASP:O    | 1:E:130:GLN:OE1  | 1.76                     | 1.03              |
| 1:E:560:ARG:NH2  | 1:E:561:GLY:O    | 1.90                     | 1.03              |
| 2:F:345:LYS:HA   | 2:F:348:SER:OG   | 1.59                     | 1.03              |
| 2:F:353:ASP:HB3  | 2:F:354:PRO:CD   | 1.88                     | 1.03              |
| 1:B:103:ASP:HA   | 1:B:108:ILE:HA   | 1.39                     | 1.03              |
| 1:B:481:SER:O    | 3:B:702:HOH:O    | 1.75                     | 1.03              |
| 1:A:72:TYR:HE2   | 1:A:206:SER:HB2  | 1.21                     | 1.03              |
| 1:A:169:LEU:HD21 | 1:A:441:PHE:CD1  | 1.83                     | 1.03              |
| 1:E:299:SER:HA   | 1:E:317:SER:HA   | 1.41                     | 1.03              |
| 1:E:479:GLU:OE1  | 1:E:507:GLN:HB2  | 1.58                     | 1.03              |
| 2:D:58:HIS:HE1   | 2:D:98:GLY:HA3   | 0.87                     | 1.02              |
| 1:A:63:PHE:CE2   | 1:A:214:THR:CA   | 2.07                     | 1.02              |
| 2:F:40:TYR:CE1   | 2:F:67:PHE:HE2   | 1.76                     | 1.02              |
| 1:B:81:LEU:CD2   | 1:B:87:LEU:HD11  | 1.88                     | 1.02              |
| 1:B:111:SER:CB   | 1:B:142:ASN:HA   | 1.89                     | 1.02              |
| 1:E:466:THR:HG21 | 1:E:516:PHE:CD2  | 1.93                     | 1.02              |
| 2:F:280:TYR:CB   | 2:F:338:LEU:HD21 | 1.90                     | 1.02              |
| 2:D:24:PHE:CD2   | 2:D:155:TRP:CD1  | 2.47                     | 1.02              |
| 1:A:63:PHE:CE1   | 1:A:212:PRO:HB3  | 1.90                     | 1.02              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:425:ARG:O    | 1:E:429:THR:OG1  | 1.77                     | 1.02              |
| 2:F:328:ILE:H    | 2:F:328:ILE:HD12 | 1.25                     | 1.02              |
| 2:F:331:LEU:CG   | 2:F:343:LEU:CD2  | 2.10                     | 1.02              |
| 1:B:238:LEU:CD1  | 3:B:715:HOH:O    | 2.08                     | 1.01              |
| 2:C:15:GLU:N     | 2:C:15:GLU:OE1   | 1.92                     | 1.01              |
| 2:D:125:PHE:CE2  | 2:D:150:ALA:CB   | 2.43                     | 1.01              |
| 2:D:326:LYS:O    | 2:D:330:THR:N    | 1.91                     | 1.01              |
| 1:E:300:LYS:NZ   | 3:E:704:HOH:O    | 1.93                     | 1.01              |
| 2:C:90:MET:HE1   | 2:D:93:ILE:CD1   | 1.90                     | 1.01              |
| 2:D:149:ARG:HG3  | 3:D:506:HOH:O    | 1.59                     | 1.01              |
| 1:A:364:TRP:CZ3  | 1:A:368:TYR:HB3  | 1.94                     | 1.01              |
| 1:E:437:ASP:OD1  | 1:E:438:ASP:N    | 1.92                     | 1.01              |
| 1:E:502:LEU:CB   | 1:E:509:PRO:HB2  | 1.91                     | 1.01              |
| 1:B:380:VAL:CB   | 1:B:382:PRO:HD3  | 1.90                     | 1.01              |
| 2:C:11:LYS:HA    | 1:A:585:TYR:HD2  | 0.89                     | 1.01              |
| 2:C:125:PHE:HZ   | 2:C:150:ALA:CB   | 1.73                     | 1.01              |
| 2:C:418:PHE:CE2  | 1:A:447:LEU:CD2  | 2.42                     | 1.01              |
| 1:A:368:TYR:CE1  | 1:A:372:LEU:HD21 | 1.95                     | 1.01              |
| 1:B:103:ASP:CB   | 1:B:108:ILE:CG1  | 2.38                     | 1.01              |
| 1:A:165:LEU:CD1  | 1:A:167:THR:H    | 1.67                     | 1.01              |
| 1:A:170:GLU:CG   | 1:A:185:GLN:HE22 | 1.69                     | 1.01              |
| 1:A:172:ILE:HD11 | 1:A:183:PHE:HE2  | 1.19                     | 1.01              |
| 1:A:175:VAL:O    | 1:A:568:TRP:CD1  | 2.12                     | 1.01              |
| 1:A:383:THR:O    | 1:A:384:HIS:ND1  | 1.92                     | 1.01              |
| 2:D:246:GLU:O    | 2:D:250:ALA:N    | 1.93                     | 1.01              |
| 1:A:125:SER:CB   | 1:A:222:VAL:HG22 | 1.91                     | 1.01              |
| 1:A:225:HIS:CB   | 1:A:227:ASN:OD1  | 2.09                     | 1.01              |
| 1:A:226:LYS:O    | 1:A:230:ASP:CB   | 2.08                     | 1.01              |
| 1:A:364:TRP:CB   | 1:A:369:GLY:HA3  | 1.90                     | 1.01              |
| 1:E:571:ALA:HB2  | 1:E:586:ILE:HD12 | 1.40                     | 1.01              |
| 2:C:137:LEU:HD12 | 2:C:138:PRO:CD   | 1.90                     | 1.00              |
| 1:E:232:ILE:HD11 | 1:E:264:LEU:HA   | 1.38                     | 1.00              |
| 1:E:340:GLU:OE2  | 1:E:344:ARG:HD3  | 1.61                     | 1.00              |
| 2:C:148:ASP:HA   | 2:C:151:ILE:HG22 | 1.42                     | 1.00              |
| 1:A:408:LEU:HD22 | 1:A:409:GLN:H    | 1.26                     | 1.00              |
| 1:E:85:GLN:CB    | 1:E:131:ALA:H    | 1.74                     | 1.00              |
| 1:E:211:TYR:HD1  | 1:E:212:PRO:HD2  | 1.24                     | 1.00              |
| 1:E:335:TYR:O    | 1:E:339:VAL:HG23 | 1.61                     | 1.00              |
| 1:E:593:SER:HB3  | 1:E:594:LEU:HA   | 1.43                     | 1.00              |
| 2:F:331:LEU:HG   | 2:F:343:LEU:CG   | 1.92                     | 1.00              |
| 1:B:223:ILE:HD12 | 1:B:224:LYS:H    | 1.27                     | 1.00              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:274:SER:O    | 2:C:278:LYS:HG2  | 1.60                     | 1.00              |
| 1:A:246:LYS:H    | 1:A:383:THR:CB   | 1.72                     | 1.00              |
| 1:E:172:ILE:CD1  | 1:E:183:PHE:HE2  | 1.74                     | 1.00              |
| 1:E:276:LEU:HD13 | 1:E:354:HIS:CB   | 1.91                     | 1.00              |
| 2:F:247:HIS:O    | 2:F:250:ALA:N    | 1.95                     | 1.00              |
| 1:B:104:ILE:HD11 | 1:B:109:TYR:HD2  | 1.23                     | 0.99              |
| 1:B:490:PHE:CB   | 1:B:557:ILE:CB   | 2.39                     | 0.99              |
| 1:B:91:GLY:O     | 1:B:120:ASN:OD1  | 1.80                     | 0.99              |
| 2:D:276:LEU:CD1  | 2:D:333:LYS:CB   | 2.39                     | 0.99              |
| 2:F:311:LEU:O    | 2:F:315:GLN:CG   | 2.10                     | 0.99              |
| 1:A:125:SER:HB2  | 1:A:222:VAL:HG22 | 1.43                     | 0.99              |
| 1:A:368:TYR:CE1  | 1:A:372:LEU:CD2  | 2.45                     | 0.99              |
| 1:E:482:ILE:O    | 1:E:485:THR:CG2  | 2.09                     | 0.99              |
| 1:B:279:ASN:CB   | 1:B:300:LYS:NZ   | 2.24                     | 0.99              |
| 1:B:331:GLN:HB3  | 1:B:334:ARG:HB2  | 1.42                     | 0.99              |
| 2:C:271:LEU:CD1  | 2:C:275:MET:HE2  | 1.92                     | 0.99              |
| 1:A:162:LEU:HD21 | 1:A:210:PHE:CE2  | 1.97                     | 0.99              |
| 1:E:340:GLU:HG2  | 1:E:379:ARG:NH1  | 1.76                     | 0.99              |
| 1:E:433:PHE:CE1  | 1:E:526:LEU:O    | 2.16                     | 0.99              |
| 2:C:11:LYS:CB    | 1:A:585:TYR:CD2  | 2.45                     | 0.99              |
| 2:C:142:MET:HA   | 2:C:142:MET:HE3  | 1.42                     | 0.99              |
| 2:D:354:PRO:CB   | 2:D:356:ILE:HD12 | 1.93                     | 0.99              |
| 1:A:436:ILE:CG2  | 1:A:440:LYS:HB3  | 1.92                     | 0.99              |
| 1:B:122:SER:OG   | 1:B:182:LEU:O    | 1.79                     | 0.99              |
| 1:B:491:LYS:CA   | 1:B:557:ILE:HD12 | 1.91                     | 0.99              |
| 1:E:125:SER:OG   | 1:E:220:VAL:CB   | 2.11                     | 0.99              |
| 1:E:489:ILE:HD11 | 1:E:527:ALA:HB2  | 1.45                     | 0.99              |
| 1:A:414:HIS:O    | 1:A:418:ARG:N    | 1.95                     | 0.99              |
| 1:A:482:ILE:HD12 | 1:A:532:ILE:HG21 | 1.45                     | 0.99              |
| 1:E:479:GLU:CD   | 1:E:507:GLN:HB3  | 1.86                     | 0.99              |
| 2:F:158:TYR:HD1  | 2:F:159:TRP:CD1  | 1.80                     | 0.99              |
| 1:E:447:LEU:CD1  | 1:E:575:ILE:HG21 | 1.93                     | 0.98              |
| 2:F:406:SER:CB   | 3:F:504:HOH:O    | 2.09                     | 0.98              |
| 1:A:483:GLU:HB2  | 1:A:532:ILE:HD12 | 1.01                     | 0.98              |
| 1:B:350:GLY:HA2  | 1:B:357:LEU:HD13 | 1.46                     | 0.98              |
| 2:C:280:TYR:HB2  | 2:C:334:THR:HG23 | 1.45                     | 0.98              |
| 2:D:125:PHE:HE2  | 2:D:150:ALA:HB2  | 0.94                     | 0.98              |
| 1:E:121:PRO:O    | 1:E:182:LEU:O    | 1.79                     | 0.98              |
| 1:B:182:LEU:HD13 | 1:B:183:PHE:HE2  | 1.13                     | 0.98              |
| 2:C:95:PHE:CE1   | 2:C:99:LEU:HD21  | 1.97                     | 0.98              |
| 1:E:85:GLN:CB    | 1:E:131:ALA:N    | 2.27                     | 0.98              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:232:ILE:HG13 | 1:B:264:LEU:CD2  | 1.92                     | 0.98              |
| 1:A:162:LEU:CD2  | 1:A:210:PHE:CE2  | 2.46                     | 0.98              |
| 1:A:184:TRP:CZ2  | 1:A:211:TYR:CB   | 2.46                     | 0.98              |
| 1:A:565:LEU:CD1  | 1:A:570:ILE:HD11 | 1.92                     | 0.98              |
| 1:E:588:PHE:N    | 2:F:5:PRO:HB3    | 1.77                     | 0.98              |
| 2:F:153:TRP:CZ2  | 2:F:157:HIS:CD2  | 2.51                     | 0.98              |
| 1:B:388:LEU:HD13 | 1:B:406:ILE:HG13 | 1.45                     | 0.98              |
| 1:A:492:VAL:O    | 1:A:554:GLU:CA   | 2.11                     | 0.98              |
| 1:E:322:TYR:O    | 1:E:334:ARG:NH1  | 1.95                     | 0.98              |
| 1:B:121:PRO:HD3  | 1:B:308:ASN:HB3  | 1.45                     | 0.98              |
| 1:B:310:LEU:HD12 | 1:B:428:LYS:HD2  | 1.43                     | 0.98              |
| 1:B:483:GLU:O    | 3:B:702:HOH:O    | 1.78                     | 0.98              |
| 1:A:165:LEU:HD12 | 1:A:167:THR:CB   | 1.91                     | 0.98              |
| 1:B:490:PHE:HB2  | 1:B:557:ILE:HG22 | 0.99                     | 0.98              |
| 2:F:24:PHE:CE1   | 2:F:155:TRP:CE3  | 2.44                     | 0.98              |
| 2:D:190:TYR:CE2  | 2:D:218:ILE:HG23 | 1.98                     | 0.98              |
| 1:A:78:ILE:HA    | 1:A:161:LYS:HB3  | 1.45                     | 0.98              |
| 1:E:364:TRP:CZ3  | 1:E:368:TYR:HB3  | 1.97                     | 0.98              |
| 2:F:345:LYS:C    | 2:F:348:SER:OG   | 2.06                     | 0.98              |
| 1:E:530:HIS:O    | 2:F:418:PHE:O    | 1.80                     | 0.97              |
| 1:A:72:TYR:OH    | 1:A:206:SER:HB3  | 1.62                     | 0.97              |
| 1:B:164:ASN:CA   | 1:B:210:PHE:HE1  | 1.76                     | 0.97              |
| 2:C:249:ARG:CB   | 2:C:307:TRP:HH2  | 1.64                     | 0.97              |
| 1:B:530:HIS:ND1  | 1:B:531:SER:OG   | 1.96                     | 0.97              |
| 1:E:93:PHE:CB    | 1:E:210:PHE:CD1  | 2.47                     | 0.97              |
| 1:E:318:THR:HG22 | 1:E:319:GLN:HG3  | 1.44                     | 0.97              |
| 1:B:484:ALA:CB   | 1:B:585:TYR:CE2  | 2.47                     | 0.97              |
| 2:C:258:HIS:NE2  | 2:C:262:LEU:CG   | 2.21                     | 0.97              |
| 1:A:463:SER:C    | 1:A:509:PRO:HG2  | 1.88                     | 0.97              |
| 2:C:260:ILE:HG21 | 2:C:315:GLN:NE2  | 1.79                     | 0.97              |
| 2:D:127:GLU:OE1  | 1:A:367:GLY:HA3  | 1.65                     | 0.97              |
| 1:A:81:LEU:HD23  | 1:A:131:ALA:CB   | 1.94                     | 0.97              |
| 1:E:138:SER:HB3  | 1:E:140:LEU:CB   | 1.95                     | 0.97              |
| 1:E:232:ILE:CD1  | 1:E:264:LEU:HA   | 1.92                     | 0.97              |
| 1:B:456:TYR:CZ   | 1:B:537:LYS:HA   | 1.99                     | 0.97              |
| 2:D:24:PHE:CE1   | 2:D:67:PHE:HZ    | 1.82                     | 0.97              |
| 2:D:145:THR:HG22 | 3:D:506:HOH:O    | 1.64                     | 0.97              |
| 1:B:104:ILE:HD11 | 1:B:109:TYR:CE2  | 1.98                     | 0.97              |
| 1:B:238:LEU:HD12 | 3:B:715:HOH:O    | 1.63                     | 0.97              |
| 1:A:468:LEU:HD23 | 1:A:559:VAL:HG13 | 1.45                     | 0.97              |
| 1:E:184:TRP:CE3  | 1:E:211:TYR:CB   | 2.37                     | 0.97              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:279:ASN:HD22 | 2:F:308:ILE:CD1  | 1.68                     | 0.97              |
| 1:B:104:ILE:H    | 1:B:104:ILE:HD12 | 1.28                     | 0.96              |
| 1:B:126:ILE:HG12 | 1:B:220:VAL:O    | 1.65                     | 0.96              |
| 1:A:276:LEU:CD1  | 1:A:354:HIS:O    | 2.12                     | 0.96              |
| 2:F:336:HIS:CB   | 2:F:339:ASN:ND2  | 2.27                     | 0.96              |
| 1:E:370:LEU:HD21 | 1:E:397:ILE:HD13 | 0.97                     | 0.96              |
| 1:E:531:SER:HA   | 2:F:418:PHE:O    | 1.63                     | 0.96              |
| 1:B:63:PHE:N     | 1:B:88:ILE:CD1   | 2.27                     | 0.96              |
| 1:B:529:VAL:CG2  | 1:B:540:ASN:O    | 2.12                     | 0.96              |
| 1:E:99:ARG:HA    | 1:E:142:ASN:CB   | 1.94                     | 0.96              |
| 1:E:451:PRO:HG2  | 2:F:413:TRP:CH2  | 2.00                     | 0.96              |
| 1:B:328:PRO:HB3  | 1:B:335:TYR:CD2  | 2.01                     | 0.96              |
| 2:C:31:ILE:CG1   | 2:C:35:GLU:OE1   | 2.13                     | 0.96              |
| 1:E:499:GLU:O    | 1:E:515:GLU:OE2  | 1.83                     | 0.96              |
| 2:F:252:PHE:O    | 2:F:256:MET:HG2  | 1.66                     | 0.96              |
| 1:B:75:ASP:O     | 1:B:164:ASN:HB2  | 1.63                     | 0.96              |
| 2:D:331:LEU:O    | 2:D:343:LEU:HD21 | 1.64                     | 0.96              |
| 1:A:71:ILE:HD13  | 1:A:71:ILE:H     | 1.29                     | 0.96              |
| 2:F:153:TRP:CE2  | 2:F:157:HIS:CD2  | 2.52                     | 0.96              |
| 2:C:63:THR:HG21  | 2:C:159:TRP:HE1  | 1.27                     | 0.96              |
| 2:C:418:PHE:HE2  | 1:A:447:LEU:CD2  | 1.77                     | 0.96              |
| 1:E:254:ASN:O    | 1:E:254:ASN:ND2  | 1.99                     | 0.96              |
| 1:E:325:PHE:HE1  | 1:E:468:LEU:CD1  | 1.76                     | 0.96              |
| 1:B:279:ASN:CB   | 1:B:300:LYS:HZ3  | 1.79                     | 0.96              |
| 1:A:463:SER:OG   | 1:A:555:ALA:HB1  | 1.64                     | 0.96              |
| 2:F:280:TYR:HA   | 2:F:338:LEU:HD21 | 1.45                     | 0.96              |
| 1:B:347:GLU:OE1  | 1:B:379:ARG:NH2  | 1.99                     | 0.96              |
| 1:B:543:ILE:HD11 | 1:B:546:PHE:CD1  | 2.00                     | 0.96              |
| 1:E:248:ILE:CD1  | 1:E:382:PRO:HB3  | 1.95                     | 0.96              |
| 1:E:281:MET:CG   | 1:E:342:LEU:HD21 | 1.94                     | 0.96              |
| 1:E:321:HIS:NE2  | 1:E:341:GLN:NE2  | 2.13                     | 0.96              |
| 1:E:322:TYR:CE2  | 1:E:324:GLY:HA2  | 2.00                     | 0.96              |
| 2:F:186:LEU:HD12 | 2:F:224:HIS:NE2  | 1.80                     | 0.96              |
| 2:F:237:ARG:O    | 2:F:241:ASN:N    | 1.98                     | 0.96              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:HG12 | 1.91                     | 0.95              |
| 1:A:162:LEU:HD21 | 1:A:210:PHE:CD2  | 2.00                     | 0.95              |
| 2:F:345:LYS:CA   | 2:F:348:SER:OG   | 2.13                     | 0.95              |
| 1:E:570:ILE:H    | 1:E:570:ILE:HD13 | 1.31                     | 0.95              |
| 1:A:172:ILE:HG22 | 1:A:179:PHE:CB   | 1.76                     | 0.95              |
| 2:C:10:TRP:CB    | 2:C:50:TYR:HE1   | 1.79                     | 0.95              |
| 1:E:370:LEU:HG   | 1:E:397:ILE:HD11 | 1.48                     | 0.95              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:475:MET:O    | 1:B:478:LEU:HD22 | 1.66                     | 0.95              |
| 1:E:326:ASN:OD1  | 1:E:425:ARG:NH1  | 1.86                     | 0.95              |
| 2:F:20:LYS:HZ1   | 2:F:162:VAL:HB   | 0.79                     | 0.95              |
| 2:D:68:SER:HA    | 2:D:71:MET:HG3   | 1.49                     | 0.95              |
| 1:E:348:SER:O    | 1:E:351:GLU:OE2  | 1.84                     | 0.95              |
| 1:B:63:PHE:CA    | 1:B:88:ILE:CD1   | 2.45                     | 0.95              |
| 1:A:63:PHE:CD2   | 1:A:214:THR:HA   | 2.00                     | 0.95              |
| 1:B:468:LEU:HD21 | 1:B:559:VAL:HG12 | 1.48                     | 0.95              |
| 2:D:63:THR:HG21  | 2:D:159:TRP:NE1  | 1.80                     | 0.95              |
| 2:D:326:LYS:O    | 2:D:330:THR:CG2  | 2.15                     | 0.95              |
| 1:A:465:LEU:HD13 | 1:A:482:ILE:HG21 | 1.49                     | 0.95              |
| 2:F:153:TRP:CE2  | 2:F:157:HIS:HD2  | 1.82                     | 0.95              |
| 2:C:410:HIS:HA   | 1:A:453:GLN:OE1  | 1.64                     | 0.95              |
| 1:A:224:LYS:CG   | 1:A:228:TRP:HE3  | 1.69                     | 0.95              |
| 1:E:595:GLU:CB   | 2:F:55:ARG:CB    | 2.44                     | 0.95              |
| 2:F:325:SER:CA   | 2:F:328:ILE:HD13 | 1.96                     | 0.95              |
| 2:C:31:ILE:HG12  | 2:C:35:GLU:OE1   | 1.68                     | 0.94              |
| 2:F:279:ASN:OD1  | 2:F:301:PHE:CD1  | 2.21                     | 0.94              |
| 1:B:252:GLY:N    | 1:B:255:SER:OG   | 1.99                     | 0.94              |
| 1:E:433:PHE:HE1  | 1:E:526:LEU:O    | 1.49                     | 0.94              |
| 2:F:71:MET:O     | 2:F:75:SER:OG    | 1.85                     | 0.94              |
| 2:D:7:LEU:HD12   | 2:D:8:THR:N      | 1.81                     | 0.94              |
| 2:D:46:LEU:O     | 2:D:50:TYR:N     | 1.99                     | 0.94              |
| 2:D:134:HIS:C    | 2:D:135:ASP:OD1  | 2.10                     | 0.94              |
| 2:D:149:ARG:CG   | 3:D:506:HOH:O    | 2.14                     | 0.94              |
| 1:B:104:ILE:CD1  | 1:B:109:TYR:CE2  | 2.50                     | 0.94              |
| 2:D:125:PHE:HE2  | 2:D:150:ALA:CB   | 1.78                     | 0.94              |
| 1:B:530:HIS:N    | 3:B:704:HOH:O    | 1.99                     | 0.94              |
| 2:F:331:LEU:HD21 | 2:F:343:LEU:CD2  | 1.97                     | 0.94              |
| 2:C:125:PHE:CZ   | 2:C:150:ALA:CA   | 2.49                     | 0.94              |
| 1:B:164:ASN:HD21 | 1:B:208:TYR:CB   | 1.80                     | 0.94              |
| 1:B:180:LYS:HE2  | 1:B:181:ASN:CB   | 1.95                     | 0.94              |
| 1:B:351:GLU:O    | 1:B:353:LYS:CB   | 2.16                     | 0.94              |
| 1:E:232:ILE:CG1  | 1:E:264:LEU:HA   | 1.98                     | 0.94              |
| 2:F:110:ILE:HD11 | 2:F:115:LEU:HD12 | 1.49                     | 0.94              |
| 2:F:280:TYR:HA   | 2:F:338:LEU:CD2  | 1.98                     | 0.94              |
| 2:C:29:GLU:N     | 2:C:29:GLU:OE2   | 2.01                     | 0.94              |
| 2:C:227:MET:HG2  | 2:C:230:PHE:CB   | 1.98                     | 0.94              |
| 2:D:259:PHE:CZ   | 2:D:268:PRO:CB   | 2.48                     | 0.94              |
| 1:A:456:TYR:CB   | 1:A:537:LYS:CA   | 2.45                     | 0.94              |
| 1:E:109:TYR:CE1  | 1:E:271:PRO:HD3  | 2.02                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:588:PHE:HA   | 2:F:5:PRO:HB3    | 1.02                     | 0.94              |
| 2:F:11:LYS:N     | 2:F:15:GLU:OE1   | 2.00                     | 0.94              |
| 2:F:279:ASN:HD22 | 2:F:308:ILE:HD12 | 1.13                     | 0.94              |
| 2:D:99:LEU:HD12  | 2:D:121:LEU:HD11 | 1.50                     | 0.94              |
| 1:B:250:ILE:HG21 | 1:B:365:ILE:CD1  | 1.98                     | 0.94              |
| 1:B:585:TYR:CE1  | 2:D:9:PRO:O      | 2.21                     | 0.94              |
| 2:D:93:ILE:HD11  | 2:D:132:ALA:HB3  | 1.47                     | 0.94              |
| 1:A:385:VAL:CG1  | 1:A:403:THR:CG2  | 2.45                     | 0.94              |
| 1:E:233:LYS:O    | 1:E:236:THR:OG1  | 1.85                     | 0.94              |
| 1:A:540:ASN:C    | 1:A:541:LEU:HD23 | 1.92                     | 0.93              |
| 1:E:100:GLY:N    | 1:E:111:SER:OG   | 2.00                     | 0.93              |
| 1:E:281:MET:SD   | 1:E:283:LEU:HD21 | 2.08                     | 0.93              |
| 1:B:111:SER:OG   | 1:B:142:ASN:N    | 2.01                     | 0.93              |
| 2:C:59:ILE:HG12  | 1:A:596:LYS:HB3  | 1.47                     | 0.93              |
| 2:C:147:VAL:O    | 2:C:151:ILE:N    | 2.00                     | 0.93              |
| 2:D:62:SER:O     | 2:D:66:LEU:HD12  | 0.76                     | 0.93              |
| 1:E:447:LEU:HD11 | 1:E:575:ILE:HG21 | 1.50                     | 0.93              |
| 2:F:20:LYS:CA    | 2:F:159:TRP:CZ3  | 2.30                     | 0.93              |
| 2:D:190:TYR:HA   | 2:D:193:ILE:CD1  | 1.99                     | 0.93              |
| 2:F:238:ILE:HG21 | 2:F:307:TRP:HZ3  | 1.23                     | 0.93              |
| 2:F:365:THR:O    | 2:F:369:ARG:N    | 2.01                     | 0.93              |
| 2:C:141:GLU:O    | 2:C:145:THR:OG1  | 1.85                     | 0.93              |
| 1:A:492:VAL:CG1  | 1:A:557:ILE:CD1  | 2.46                     | 0.93              |
| 1:E:211:TYR:CD1  | 1:E:212:PRO:HD2  | 2.02                     | 0.93              |
| 2:C:15:GLU:O     | 2:C:18:TYR:N     | 2.00                     | 0.93              |
| 2:C:414:THR:O    | 2:C:416:LYS:HE3  | 1.68                     | 0.93              |
| 1:B:502:LEU:HB2  | 1:B:509:PRO:HB2  | 1.47                     | 0.93              |
| 2:C:186:LEU:HB3  | 2:C:221:ILE:HG12 | 0.94                     | 0.93              |
| 1:E:325:PHE:HE1  | 1:E:468:LEU:HD13 | 1.14                     | 0.93              |
| 2:F:121:LEU:HD12 | 2:F:122:PRO:HD3  | 1.47                     | 0.93              |
| 1:B:256:GLY:O    | 1:B:259:THR:OG1  | 1.85                     | 0.93              |
| 1:E:78:ILE:CD1   | 1:E:161:LYS:HG3  | 1.99                     | 0.93              |
| 1:E:232:ILE:CD1  | 1:E:264:LEU:CA   | 2.34                     | 0.93              |
| 1:E:588:PHE:N    | 2:F:5:PRO:CB     | 2.30                     | 0.93              |
| 2:F:252:PHE:HD1  | 2:F:307:TRP:HZ2  | 1.06                     | 0.93              |
| 1:B:169:LEU:HD12 | 1:B:183:PHE:CE1  | 2.03                     | 0.93              |
| 2:F:9:PRO:HG2    | 2:F:10:TRP:CE3   | 2.02                     | 0.93              |
| 1:B:494:ARG:CB   | 1:B:553:LYS:HG3  | 1.98                     | 0.93              |
| 2:C:10:TRP:CB    | 2:C:50:TYR:CE1   | 2.52                     | 0.93              |
| 2:D:183:LEU:HD22 | 2:D:224:HIS:HB3  | 1.47                     | 0.93              |
| 1:E:224:LYS:CG   | 1:E:228:TRP:CZ3  | 2.52                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:437:ASP:HB3  | 1:E:440:LYS:NZ   | 1.84                     | 0.93              |
| 1:A:169:LEU:HD22 | 1:A:441:PHE:HD1  | 1.14                     | 0.92              |
| 1:E:182:LEU:HB3  | 1:E:183:PHE:CE2  | 2.03                     | 0.92              |
| 1:E:461:GLY:HA3  | 3:F:504:HOH:O    | 1.69                     | 0.92              |
| 2:C:128:PHE:HZ   | 2:C:143:CYS:HG   | 1.05                     | 0.92              |
| 1:E:235:LEU:CD1  | 1:E:247:VAL:HG21 | 1.99                     | 0.92              |
| 2:F:420:VAL:C    | 2:F:421:ILE:HG12 | 1.93                     | 0.92              |
| 1:B:279:ASN:HB2  | 1:B:300:LYS:NZ   | 1.85                     | 0.92              |
| 1:B:351:GLU:O    | 1:B:353:LYS:O    | 1.86                     | 0.92              |
| 1:B:490:PHE:HB3  | 1:B:557:ILE:CG2  | 1.78                     | 0.92              |
| 2:C:137:LEU:HB2  | 2:D:94:ARG:NH2   | 1.85                     | 0.92              |
| 1:E:78:ILE:HD11  | 1:E:161:LYS:HG3  | 1.49                     | 0.92              |
| 1:E:318:THR:C    | 1:E:319:GLN:HG3  | 1.94                     | 0.92              |
| 2:D:96:VAL:HG12  | 2:D:100:LEU:HD11 | 1.48                     | 0.92              |
| 1:A:64:SER:OG    | 1:A:85:GLN:CB    | 2.18                     | 0.92              |
| 1:A:464:ALA:HB2  | 1:A:509:PRO:HB2  | 1.50                     | 0.92              |
| 2:C:182:GLU:O    | 2:C:186:LEU:N    | 2.02                     | 0.92              |
| 2:D:190:TYR:CA   | 2:D:193:ILE:HD12 | 1.98                     | 0.92              |
| 1:A:374:ARG:O    | 1:A:377:ILE:CG1  | 2.08                     | 0.92              |
| 1:A:420:SER:CB   | 1:A:423:GLN:HB3  | 1.99                     | 0.92              |
| 1:E:104:ILE:HG23 | 1:E:129:ILE:CD1  | 2.00                     | 0.92              |
| 2:F:336:HIS:O    | 2:F:340:VAL:HG23 | 1.69                     | 0.92              |
| 1:B:232:ILE:HG13 | 1:B:264:LEU:HD23 | 0.96                     | 0.92              |
| 1:B:595:GLU:CB   | 2:D:158:TYR:CE1  | 2.52                     | 0.92              |
| 2:D:271:LEU:O    | 2:D:274:SER:OG   | 1.85                     | 0.92              |
| 2:D:410:HIS:CD2  | 2:D:413:TRP:HD1  | 1.88                     | 0.92              |
| 1:A:579:PHE:CE2  | 1:A:581:ARG:CB   | 2.52                     | 0.92              |
| 1:E:85:GLN:CB    | 1:E:131:ALA:HB2  | 1.99                     | 0.92              |
| 1:E:416:GLY:HA3  | 3:E:723:HOH:O    | 1.70                     | 0.92              |
| 2:F:40:TYR:CE1   | 2:F:67:PHE:CE2   | 2.56                     | 0.92              |
| 1:E:531:SER:HG   | 2:F:418:PHE:HA   | 1.25                     | 0.92              |
| 2:C:65:HIS:ND1   | 2:C:94:ARG:CZ    | 2.32                     | 0.92              |
| 2:C:135:ASP:O    | 2:D:94:ARG:NH1   | 2.03                     | 0.92              |
| 1:A:95:LEU:HD21  | 1:A:116:MET:HE3  | 1.48                     | 0.92              |
| 1:E:444:GLN:NE2  | 1:E:445:PRO:O    | 2.03                     | 0.92              |
| 2:F:40:TYR:CZ    | 2:F:67:PHE:CE2   | 2.57                     | 0.92              |
| 1:B:104:ILE:N    | 1:B:107:VAL:O    | 2.02                     | 0.92              |
| 2:C:182:GLU:O    | 2:C:186:LEU:CB   | 2.18                     | 0.92              |
| 1:B:486:ILE:HD11 | 1:B:564:ASP:O    | 1.70                     | 0.92              |
| 1:E:224:LYS:HG3  | 1:E:228:TRP:CE3  | 2.05                     | 0.92              |
| 1:E:487:VAL:O    | 1:E:526:LEU:CD2  | 2.17                     | 0.92              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:250:ILE:HD13 | 1:B:373:THR:CG2  | 1.80                     | 0.91              |
| 1:B:528:LEU:HD12 | 3:B:704:HOH:O    | 1.70                     | 0.91              |
| 2:D:357:LYS:HA   | 2:D:360:ILE:CD1  | 2.00                     | 0.91              |
| 2:F:331:LEU:HD23 | 2:F:343:LEU:HD21 | 1.52                     | 0.91              |
| 2:C:305:GLN:HA   | 2:C:308:ILE:HD12 | 1.52                     | 0.91              |
| 1:A:492:VAL:O    | 1:A:554:GLU:HA   | 1.67                     | 0.91              |
| 1:A:570:ILE:CG2  | 3:A:734:HOH:O    | 2.17                     | 0.91              |
| 2:F:259:PHE:HZ   | 2:F:268:PRO:HA   | 1.33                     | 0.91              |
| 1:A:63:PHE:CZ    | 1:A:214:THR:HG23 | 2.05                     | 0.91              |
| 1:A:125:SER:HB2  | 1:A:222:VAL:CG2  | 1.99                     | 0.91              |
| 1:A:524:PHE:HD2  | 1:A:525:ARG:H    | 1.19                     | 0.91              |
| 2:F:325:SER:HA   | 2:F:328:ILE:HD13 | 1.52                     | 0.91              |
| 1:B:122:SER:OG   | 1:B:182:LEU:HD23 | 1.69                     | 0.91              |
| 1:B:257:LYS:O    | 1:B:260:PHE:N    | 2.02                     | 0.91              |
| 1:B:484:ALA:HB3  | 1:B:585:TYR:CE2  | 2.06                     | 0.91              |
| 2:D:154:VAL:HG23 | 2:D:159:TRP:HD1  | 1.34                     | 0.91              |
| 1:A:72:TYR:HD2   | 1:A:208:TYR:HH   | 1.08                     | 0.91              |
| 1:E:100:GLY:O    | 1:E:111:SER:OG   | 1.89                     | 0.91              |
| 2:F:10:TRP:HA    | 2:F:50:TYR:CE2   | 2.04                     | 0.91              |
| 2:C:305:GLN:HA   | 2:C:308:ILE:CD1  | 1.99                     | 0.91              |
| 2:D:125:PHE:CZ   | 2:D:150:ALA:HB2  | 2.05                     | 0.91              |
| 2:D:342:LEU:O    | 2:D:346:LEU:HG   | 1.71                     | 0.91              |
| 1:E:364:TRP:CB   | 1:E:369:GLY:HA3  | 1.99                     | 0.91              |
| 2:F:186:LEU:CD1  | 2:F:224:HIS:NE2  | 2.34                     | 0.91              |
| 2:D:60:LEU:O     | 2:D:63:THR:OG1   | 1.88                     | 0.91              |
| 2:D:93:ILE:HD11  | 2:D:132:ALA:CB   | 1.99                     | 0.91              |
| 1:B:368:TYR:HB2  | 2:C:124:LEU:CD2  | 2.01                     | 0.91              |
| 2:C:225:ALA:HA   | 2:C:227:MET:SD   | 2.10                     | 0.91              |
| 1:E:451:PRO:HG2  | 2:F:413:TRP:CZ3  | 2.06                     | 0.91              |
| 1:E:524:PHE:CD2  | 1:E:525:ARG:HB2  | 2.05                     | 0.91              |
| 1:B:167:THR:HA   | 1:B:439:PHE:O    | 1.70                     | 0.91              |
| 2:C:18:TYR:CE2   | 2:C:22:LEU:HD12  | 2.06                     | 0.91              |
| 2:C:137:LEU:HB2  | 2:D:94:ARG:HH21  | 1.35                     | 0.91              |
| 1:E:99:ARG:C     | 1:E:142:ASN:ND2  | 2.27                     | 0.91              |
| 1:E:435:LYS:HE2  | 1:E:545:GLN:NE2  | 1.84                     | 0.91              |
| 2:C:215:TRP:HA   | 2:C:218:ILE:CD1  | 2.00                     | 0.91              |
| 2:D:63:THR:CG2   | 2:D:159:TRP:HE1  | 1.83                     | 0.91              |
| 2:D:357:LYS:CA   | 2:D:360:ILE:HD12 | 2.00                     | 0.91              |
| 1:A:111:SER:N    | 1:A:140:LEU:CB   | 2.34                     | 0.91              |
| 1:B:81:LEU:HD22  | 1:B:87:LEU:HD11  | 1.51                     | 0.90              |
| 1:B:172:ILE:HD11 | 1:B:179:PHE:C    | 1.95                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:492:VAL:N    | 1:B:557:ILE:CD1  | 2.34                     | 0.90              |
| 1:A:388:LEU:C    | 1:A:389:ASN:OD1  | 2.15                     | 0.90              |
| 1:E:446:LEU:CD1  | 1:E:528:LEU:CD2  | 2.49                     | 0.90              |
| 1:B:119:ILE:H    | 1:B:307:GLY:HA3  | 1.34                     | 0.90              |
| 1:B:564:ASP:OD1  | 3:B:703:HOH:O    | 1.88                     | 0.90              |
| 1:A:368:TYR:HE1  | 1:A:372:LEU:CD2  | 1.83                     | 0.90              |
| 1:E:318:THR:HG22 | 1:E:319:GLN:CG   | 2.00                     | 0.90              |
| 2:F:23:PHE:CE2   | 2:F:43:ALA:CB    | 2.55                     | 0.90              |
| 1:E:253:LYS:HG2  | 3:E:708:HOH:O    | 1.72                     | 0.90              |
| 1:B:63:PHE:CB    | 1:B:88:ILE:HD13  | 1.98                     | 0.90              |
| 1:A:90:LYS:HD2   | 1:A:213:ILE:HD11 | 1.54                     | 0.90              |
| 1:A:182:LEU:HD13 | 1:A:183:PHE:CE2  | 2.06                     | 0.90              |
| 1:E:299:SER:HB3  | 1:E:317:SER:CA   | 2.00                     | 0.90              |
| 2:F:122:PRO:HG2  | 2:F:125:PHE:HE2  | 1.24                     | 0.90              |
| 2:D:125:PHE:CZ   | 2:D:150:ALA:CA   | 2.55                     | 0.90              |
| 1:A:224:LYS:HG2  | 1:A:228:TRP:CE3  | 2.02                     | 0.90              |
| 1:E:225:HIS:O    | 1:E:229:MET:N    | 2.04                     | 0.90              |
| 1:B:468:LEU:CD2  | 1:B:559:VAL:HG11 | 2.01                     | 0.90              |
| 1:A:119:ILE:HG12 | 1:A:309:HIS:CE1  | 2.06                     | 0.90              |
| 1:E:103:ASP:OD1  | 1:E:130:GLN:CB   | 2.18                     | 0.90              |
| 1:E:281:MET:CG   | 1:E:342:LEU:CD2  | 2.49                     | 0.90              |
| 2:F:197:ASN:OD1  | 2:F:198:ILE:N    | 2.04                     | 0.90              |
| 1:B:279:ASN:ND2  | 1:B:300:LYS:NZ   | 2.14                     | 0.90              |
| 2:C:213:GLU:O    | 2:C:217:CYS:SG   | 2.30                     | 0.90              |
| 2:F:245:TRP:O    | 2:F:248:LEU:HD21 | 1.70                     | 0.90              |
| 1:B:368:TYR:HB2  | 2:C:124:LEU:HD22 | 1.52                     | 0.90              |
| 2:D:331:LEU:HD23 | 2:D:346:LEU:CG   | 2.01                     | 0.90              |
| 2:D:331:LEU:CD2  | 2:D:346:LEU:HB2  | 2.00                     | 0.90              |
| 1:A:63:PHE:HZ    | 1:A:214:THR:HG23 | 1.36                     | 0.90              |
| 2:F:213:GLU:N    | 2:F:213:GLU:OE2  | 2.03                     | 0.90              |
| 1:B:68:ASP:HA    | 3:B:712:HOH:O    | 1.70                     | 0.90              |
| 1:B:117:LYS:CD   | 1:B:439:PHE:CE1  | 2.53                     | 0.90              |
| 2:C:36:LEU:CG    | 2:C:40:TYR:HE1   | 1.83                     | 0.90              |
| 1:A:465:LEU:HD13 | 1:A:482:ILE:CG2  | 2.01                     | 0.90              |
| 1:A:482:ILE:CD1  | 1:A:532:ILE:HG21 | 2.02                     | 0.90              |
| 2:C:260:ILE:HG21 | 2:C:315:GLN:HE22 | 1.35                     | 0.89              |
| 2:D:331:LEU:HB3  | 2:D:343:LEU:HD22 | 1.53                     | 0.89              |
| 1:A:312:LEU:HD13 | 1:A:441:PHE:HE1  | 1.35                     | 0.89              |
| 1:E:169:LEU:HD11 | 1:E:183:PHE:CE1  | 1.92                     | 0.89              |
| 1:E:232:ILE:HD12 | 1:E:264:LEU:CD2  | 1.93                     | 0.89              |
| 2:F:116:ALA:HA   | 2:F:119:ILE:CD1  | 2.02                     | 0.89              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:268:PRO:HA   | 2:D:271:LEU:CD1  | 2.02                     | 0.89              |
| 1:A:358:LEU:CD1  | 1:A:359:ILE:N    | 2.35                     | 0.89              |
| 1:E:281:MET:SD   | 1:E:342:LEU:CD2  | 2.61                     | 0.89              |
| 2:C:414:THR:O    | 2:C:416:LYS:HD2  | 1.73                     | 0.89              |
| 1:A:95:LEU:CD2   | 1:A:116:MET:HE3  | 2.02                     | 0.89              |
| 1:A:184:TRP:HH2  | 1:A:211:TYR:HD2  | 1.18                     | 0.89              |
| 1:A:325:PHE:CB   | 1:A:330:ASP:CB   | 2.50                     | 0.89              |
| 2:F:15:GLU:O     | 2:F:19:LEU:N     | 2.04                     | 0.89              |
| 2:F:112:LEU:O    | 2:F:116:ALA:HB2  | 1.72                     | 0.89              |
| 1:B:250:ILE:HG23 | 1:B:365:ILE:HD11 | 0.91                     | 0.89              |
| 1:B:250:ILE:HD13 | 1:B:373:THR:HG21 | 0.89                     | 0.89              |
| 1:B:468:LEU:HD11 | 1:B:560:ARG:C    | 1.97                     | 0.89              |
| 2:C:9:PRO:HG2    | 2:C:10:TRP:CE3   | 2.07                     | 0.89              |
| 1:A:475:MET:HE2  | 1:A:478:LEU:HD22 | 1.52                     | 0.89              |
| 1:A:420:SER:O    | 1:A:424:LEU:N    | 2.06                     | 0.89              |
| 2:F:235:ILE:HA   | 2:F:238:ILE:CD1  | 2.03                     | 0.89              |
| 2:C:271:LEU:HD11 | 2:C:275:MET:CE   | 2.03                     | 0.89              |
| 1:A:226:LYS:O    | 1:A:230:ASP:HB2  | 1.73                     | 0.89              |
| 1:A:368:TYR:HE1  | 1:A:372:LEU:HD21 | 1.37                     | 0.89              |
| 1:E:486:ILE:HD12 | 1:E:564:ASP:O    | 1.73                     | 0.89              |
| 2:F:111:PRO:CG   | 2:F:114:LEU:HG   | 2.02                     | 0.89              |
| 2:F:331:LEU:HG   | 2:F:343:LEU:HD21 | 0.89                     | 0.89              |
| 2:C:10:TRP:CD1   | 2:C:13:SER:HA    | 2.07                     | 0.89              |
| 2:C:148:ASP:HA   | 2:C:151:ILE:CG2  | 2.03                     | 0.89              |
| 1:E:225:HIS:O    | 1:E:228:TRP:HB3  | 1.73                     | 0.89              |
| 1:E:226:LYS:HA   | 1:E:229:MET:HB3  | 1.55                     | 0.89              |
| 1:B:490:PHE:CB   | 1:B:557:ILE:HB   | 2.01                     | 0.88              |
| 1:A:176:CYS:SG   | 1:A:179:PHE:HD1  | 1.96                     | 0.88              |
| 1:A:350:GLY:CA   | 1:A:357:LEU:CD1  | 2.46                     | 0.88              |
| 1:E:299:SER:CA   | 1:E:317:SER:HB2  | 2.01                     | 0.88              |
| 1:E:321:HIS:HE1  | 1:E:522:GLU:OE1  | 1.54                     | 0.88              |
| 1:E:524:PHE:HE2  | 1:E:543:ILE:CD1  | 1.85                     | 0.88              |
| 1:A:531:SER:OG   | 1:A:540:ASN:ND2  | 2.06                     | 0.88              |
| 2:F:24:PHE:HE1   | 2:F:155:TRP:CB   | 1.84                     | 0.88              |
| 1:B:308:ASN:O    | 1:B:308:ASN:ND2  | 2.05                     | 0.88              |
| 1:B:350:GLY:HA2  | 1:B:357:LEU:CD1  | 2.03                     | 0.88              |
| 1:B:454:VAL:HG11 | 2:D:407:PHE:HE1  | 1.07                     | 0.88              |
| 2:C:214:TYR:O    | 2:C:218:ILE:HG13 | 1.72                     | 0.88              |
| 2:C:258:HIS:HD2  | 2:C:262:LEU:HD12 | 1.37                     | 0.88              |
| 1:A:252:GLY:O    | 1:A:255:SER:OG   | 1.89                     | 0.88              |
| 1:A:365:ILE:O    | 1:A:393:LEU:HD22 | 1.70                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:483:GLU:OE1  | 1:A:531:SER:CA   | 2.21                     | 0.88              |
| 1:E:125:SER:CB   | 1:E:220:VAL:CB   | 2.51                     | 0.88              |
| 1:E:351:GLU:OE1  | 1:E:351:GLU:N    | 2.06                     | 0.88              |
| 1:B:334:ARG:HG3  | 1:B:513:TYR:OH   | 1.72                     | 0.88              |
| 1:B:466:THR:HB   | 1:B:511:LEU:HB3  | 1.53                     | 0.88              |
| 2:C:11:LYS:CA    | 1:A:585:TYR:CE2  | 2.53                     | 0.88              |
| 2:C:40:TYR:CE2   | 2:C:67:PHE:CD1   | 2.61                     | 0.88              |
| 1:A:464:ALA:HB2  | 1:A:509:PRO:CB   | 2.03                     | 0.88              |
| 1:E:363:GLY:CA   | 3:E:708:HOH:O    | 2.21                     | 0.88              |
| 1:E:451:PRO:CG   | 2:F:413:TRP:CZ2  | 2.55                     | 0.88              |
| 1:E:451:PRO:CG   | 2:F:413:TRP:CH2  | 2.57                     | 0.88              |
| 2:F:273:ASP:CG   | 2:F:330:THR:HG21 | 1.97                     | 0.88              |
| 2:D:322:VAL:O    | 2:D:325:SER:OG   | 1.91                     | 0.88              |
| 2:D:331:LEU:HB3  | 2:D:343:LEU:CD2  | 2.04                     | 0.88              |
| 1:A:465:LEU:CD1  | 1:A:482:ILE:CG2  | 2.51                     | 0.88              |
| 1:E:264:LEU:CD1  | 1:E:358:LEU:HD11 | 2.04                     | 0.88              |
| 1:B:186:PHE:HB2  | 1:B:207:ASP:OD1  | 1.74                     | 0.88              |
| 1:B:490:PHE:HB2  | 1:B:557:ILE:CB   | 2.01                     | 0.88              |
| 1:A:483:GLU:CD   | 1:A:532:ILE:HD13 | 1.98                     | 0.88              |
| 2:F:245:TRP:O    | 2:F:248:LEU:CD2  | 2.21                     | 0.88              |
| 2:F:279:ASN:ND2  | 2:F:308:ILE:HD11 | 1.87                     | 0.88              |
| 1:E:325:PHE:CE1  | 1:E:468:LEU:CD1  | 2.52                     | 0.88              |
| 2:F:280:TYR:CA   | 2:F:338:LEU:CD2  | 2.51                     | 0.88              |
| 1:A:184:TRP:HZ2  | 1:A:211:TYR:CD2  | 1.89                     | 0.88              |
| 1:A:226:LYS:O    | 1:A:230:ASP:N    | 2.06                     | 0.88              |
| 1:E:456:TYR:CB   | 1:E:537:LYS:O    | 2.22                     | 0.88              |
| 2:F:273:ASP:CG   | 3:F:502:HOH:O    | 2.17                     | 0.88              |
| 2:C:11:LYS:CA    | 1:A:585:TYR:HD2  | 1.75                     | 0.88              |
| 1:E:430:MET:CE   | 1:E:568:TRP:HE3  | 1.86                     | 0.88              |
| 1:E:546:PHE:CE2  | 1:E:548:THR:HA   | 2.08                     | 0.88              |
| 2:F:12:SER:HB3   | 2:F:14:ASP:OD1   | 1.74                     | 0.88              |
| 1:A:117:LYS:HD3  | 1:A:439:PHE:HE2  | 1.19                     | 0.87              |
| 1:E:588:PHE:HA   | 2:F:5:PRO:HA     | 1.57                     | 0.87              |
| 2:D:343:LEU:O    | 2:D:347:GLN:N    | 2.08                     | 0.87              |
| 1:A:172:ILE:HG21 | 1:A:179:PHE:CG   | 2.10                     | 0.87              |
| 1:E:86:ASN:O     | 1:E:87:LEU:HD23  | 1.74                     | 0.87              |
| 1:E:499:GLU:O    | 1:E:515:GLU:OE1  | 1.91                     | 0.87              |
| 1:A:468:LEU:CD2  | 1:A:559:VAL:CG1  | 2.48                     | 0.87              |
| 1:A:483:GLU:OE1  | 1:A:532:ILE:N    | 2.07                     | 0.87              |
| 2:F:111:PRO:CB   | 2:F:113:HIS:HE1  | 1.85                     | 0.87              |
| 2:F:272:ILE:HD13 | 2:F:315:GLN:CD   | 2.00                     | 0.87              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:42:GLU:O     | 2:C:46:LEU:HD11  | 1.75                     | 0.87              |
| 1:A:446:LEU:O    | 1:A:542:TYR:CE2  | 2.27                     | 0.87              |
| 2:C:32:SER:O     | 2:C:36:LEU:N     | 2.07                     | 0.87              |
| 2:F:141:GLU:HA   | 2:F:144:LYS:HG3  | 1.57                     | 0.87              |
| 1:A:170:GLU:CD   | 1:A:185:GLN:HE21 | 1.81                     | 0.87              |
| 1:A:232:ILE:HD13 | 1:A:264:LEU:HB2  | 1.55                     | 0.87              |
| 1:A:389:ASN:HD21 | 1:A:408:LEU:HB3  | 1.32                     | 0.87              |
| 2:C:148:ASP:CA   | 2:C:151:ILE:HG22 | 2.05                     | 0.87              |
| 2:C:258:HIS:HD2  | 2:C:262:LEU:CD1  | 1.50                     | 0.87              |
| 1:A:231:VAL:O    | 1:A:235:LEU:HD23 | 1.75                     | 0.87              |
| 1:A:296:ILE:HG22 | 1:A:342:LEU:HD21 | 1.55                     | 0.87              |
| 1:A:358:LEU:CD1  | 1:A:359:ILE:H    | 1.86                     | 0.87              |
| 1:E:92:GLN:O     | 1:E:209:THR:HG23 | 1.74                     | 0.87              |
| 1:E:281:MET:HG3  | 1:E:342:LEU:HD21 | 1.55                     | 0.87              |
| 1:B:223:ILE:HG22 | 3:B:721:HOH:O    | 1.61                     | 0.87              |
| 1:A:394:GLY:HA3  | 3:A:717:HOH:O    | 1.74                     | 0.87              |
| 1:A:466:THR:HB   | 1:A:511:LEU:HD23 | 0.87                     | 0.87              |
| 1:B:491:LYS:N    | 1:B:557:ILE:HD12 | 1.90                     | 0.87              |
| 2:C:215:TRP:CA   | 2:C:218:ILE:HD12 | 2.05                     | 0.87              |
| 2:D:49:MET:SD    | 2:D:53:ARG:NH1   | 2.46                     | 0.87              |
| 1:A:182:LEU:HD13 | 1:A:183:PHE:HE2  | 1.40                     | 0.87              |
| 1:A:213:ILE:HD13 | 1:A:219:THR:HG21 | 1.57                     | 0.87              |
| 1:E:184:TRP:CZ3  | 1:E:211:TYR:HB3  | 2.08                     | 0.87              |
| 1:E:440:LYS:NZ   | 1:E:440:LYS:HB2  | 1.88                     | 0.87              |
| 1:E:571:ALA:CB   | 1:E:586:ILE:CD1  | 2.50                     | 0.87              |
| 1:B:111:SER:CB   | 1:B:142:ASN:CA   | 2.49                     | 0.86              |
| 2:F:353:ASP:O    | 2:F:357:LYS:HG3  | 1.75                     | 0.86              |
| 1:B:486:ILE:HG23 | 1:B:565:LEU:HG   | 1.55                     | 0.86              |
| 2:C:232:ASN:O    | 2:C:235:ILE:HD12 | 1.75                     | 0.86              |
| 1:A:312:LEU:HD13 | 1:A:441:PHE:CE1  | 2.09                     | 0.86              |
| 1:B:104:ILE:HD12 | 1:B:107:VAL:HG23 | 1.54                     | 0.86              |
| 1:B:285:PRO:O    | 1:B:288:PRO:HD3  | 1.75                     | 0.86              |
| 2:F:122:PRO:HD2  | 2:F:125:PHE:CD2  | 2.09                     | 0.86              |
| 1:B:322:TYR:O    | 1:B:334:ARG:NH1  | 2.08                     | 0.86              |
| 1:B:465:LEU:CD1  | 1:B:482:ILE:HG21 | 2.05                     | 0.86              |
| 2:C:11:LYS:HG3   | 1:A:585:TYR:CE2  | 2.06                     | 0.86              |
| 1:E:524:PHE:HZ   | 1:E:546:PHE:HB2  | 1.39                     | 0.86              |
| 1:B:76:TYR:HB2   | 1:B:162:LEU:O    | 1.76                     | 0.86              |
| 1:B:232:ILE:CG1  | 1:B:264:LEU:CD2  | 2.52                     | 0.86              |
| 1:A:63:PHE:HE1   | 1:A:212:PRO:HB3  | 1.36                     | 0.86              |
| 1:E:184:TRP:CZ3  | 1:E:211:TYR:CD2  | 2.63                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:122:PRO:HD2  | 2:F:125:PHE:HD2  | 1.38                     | 0.86              |
| 1:B:118:PHE:O    | 1:B:119:ILE:HD13 | 1.74                     | 0.86              |
| 1:B:180:LYS:CE   | 1:B:181:ASN:HB2  | 2.05                     | 0.86              |
| 1:B:328:PRO:HB3  | 1:B:335:TYR:HE2  | 1.39                     | 0.86              |
| 2:C:96:VAL:O     | 2:C:99:LEU:HD12  | 1.74                     | 0.86              |
| 1:A:223:ILE:C    | 1:A:224:LYS:HD2  | 2.01                     | 0.86              |
| 1:B:383:THR:CG2  | 1:B:384:HIS:CD2  | 2.58                     | 0.86              |
| 1:A:401:LYS:HA   | 1:A:401:LYS:NZ   | 1.90                     | 0.86              |
| 1:E:370:LEU:CD2  | 1:E:397:ILE:HD13 | 1.91                     | 0.86              |
| 1:E:454:VAL:CG2  | 1:E:539:MET:O    | 2.19                     | 0.86              |
| 2:F:420:VAL:O    | 2:F:421:ILE:HG12 | 1.75                     | 0.86              |
| 1:B:63:PHE:CA    | 1:B:88:ILE:HD11  | 2.03                     | 0.86              |
| 1:B:240:SER:HA   | 1:B:274:GLN:HG3  | 1.56                     | 0.86              |
| 1:A:63:PHE:HZ    | 1:A:212:PRO:HB2  | 1.39                     | 0.86              |
| 1:B:531:SER:O    | 1:B:532:ILE:HD13 | 1.74                     | 0.85              |
| 2:C:53:ARG:HG2   | 2:C:53:ARG:HH11  | 1.40                     | 0.85              |
| 1:A:430:MET:HG2  | 1:A:566:PRO:HG3  | 1.55                     | 0.85              |
| 1:B:77:VAL:CG1   | 1:B:79:PHE:CZ    | 2.58                     | 0.85              |
| 2:C:8:THR:CG2    | 1:A:587:THR:HG23 | 2.05                     | 0.85              |
| 2:C:218:ILE:HG12 | 2:C:255:MET:CE   | 2.03                     | 0.85              |
| 2:C:275:MET:O    | 2:C:279:ASN:N    | 2.07                     | 0.85              |
| 1:E:437:ASP:HB3  | 1:E:440:LYS:HZ2  | 1.41                     | 0.85              |
| 2:F:111:PRO:HG2  | 2:F:114:LEU:CB   | 2.06                     | 0.85              |
| 1:B:118:PHE:HE1  | 1:B:306:HIS:HB3  | 1.04                     | 0.85              |
| 1:B:368:TYR:HE1  | 1:B:372:LEU:CG   | 1.89                     | 0.85              |
| 2:D:69:ALA:HA    | 2:D:72:MET:HG3   | 1.58                     | 0.85              |
| 1:E:250:ILE:HD12 | 1:E:373:THR:HG21 | 1.57                     | 0.85              |
| 1:B:346:TYR:O    | 1:B:350:GLY:N    | 2.08                     | 0.85              |
| 1:A:382:PRO:HB3  | 1:A:385:VAL:CG2  | 2.06                     | 0.85              |
| 1:B:290:TYR:HA   | 1:B:311:SER:OG   | 1.76                     | 0.85              |
| 1:B:455:SER:N    | 2:D:405:LYS:CB   | 2.39                     | 0.85              |
| 2:D:331:LEU:HD23 | 2:D:346:LEU:HD13 | 0.86                     | 0.85              |
| 1:A:172:ILE:CD1  | 1:A:183:PHE:HE2  | 1.89                     | 0.85              |
| 1:E:121:PRO:HB2  | 1:E:182:LEU:HD22 | 1.59                     | 0.85              |
| 1:E:411:SER:HB2  | 3:E:716:HOH:O    | 1.75                     | 0.85              |
| 1:B:598:TRP:CE2  | 2:D:98:GLY:HA2   | 2.12                     | 0.85              |
| 2:C:279:ASN:HD21 | 2:C:308:ILE:HD11 | 1.39                     | 0.85              |
| 2:D:326:LYS:C    | 2:D:330:THR:CG2  | 2.47                     | 0.85              |
| 1:E:337:LEU:HD12 | 1:E:337:LEU:O    | 1.77                     | 0.85              |
| 1:E:411:SER:CB   | 3:E:716:HOH:O    | 2.24                     | 0.85              |
| 2:C:177:GLU:OE1  | 2:C:180:ILE:HG21 | 1.75                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:258:HIS:CD2  | 2:C:262:LEU:HD12 | 2.09                     | 0.85              |
| 1:A:436:ILE:HG21 | 1:A:440:LYS:HB3  | 1.59                     | 0.85              |
| 1:E:103:ASP:OD1  | 1:E:132:THR:OG1  | 1.95                     | 0.85              |
| 2:F:331:LEU:HD23 | 2:F:343:LEU:CD2  | 2.01                     | 0.85              |
| 2:D:62:SER:C     | 2:D:66:LEU:CD1   | 2.34                     | 0.85              |
| 1:A:100:GLY:HA3  | 1:A:158:SER:HB3  | 1.57                     | 0.85              |
| 1:A:370:LEU:HD12 | 1:A:370:LEU:O    | 1.77                     | 0.85              |
| 1:B:288:PRO:HB2  | 1:B:291:SER:HB2  | 1.57                     | 0.85              |
| 2:D:273:ASP:O    | 2:D:276:LEU:HG   | 1.77                     | 0.85              |
| 1:A:117:LYS:CE   | 1:A:439:PHE:HE2  | 1.90                     | 0.85              |
| 1:A:213:ILE:CD1  | 1:A:219:THR:HG21 | 2.07                     | 0.85              |
| 1:A:388:LEU:O    | 1:A:389:ASN:OD1  | 1.95                     | 0.85              |
| 1:A:464:ALA:HB1  | 1:A:509:PRO:HB2  | 1.58                     | 0.85              |
| 1:B:81:LEU:CD2   | 1:B:160:ILE:HD11 | 2.06                     | 0.85              |
| 1:B:543:ILE:HD11 | 1:B:546:PHE:CG   | 2.12                     | 0.85              |
| 2:C:153:TRP:CZ2  | 2:C:157:HIS:CD2  | 2.65                     | 0.85              |
| 2:D:116:ALA:HA   | 2:D:119:ILE:CG2  | 2.04                     | 0.85              |
| 1:A:63:PHE:CZ    | 1:A:214:THR:CG2  | 2.60                     | 0.85              |
| 1:A:125:SER:CB   | 1:A:222:VAL:CG2  | 2.54                     | 0.85              |
| 1:A:165:LEU:HD12 | 1:A:167:THR:CG2  | 2.06                     | 0.85              |
| 2:F:235:ILE:O    | 2:F:239:VAL:HG23 | 1.77                     | 0.85              |
| 2:F:279:ASN:OD1  | 2:F:301:PHE:HE1  | 1.50                     | 0.85              |
| 2:C:40:TYR:CE2   | 2:C:67:PHE:HD1   | 1.93                     | 0.84              |
| 2:C:65:HIS:CG    | 2:C:94:ARG:HH21  | 1.93                     | 0.84              |
| 1:A:466:THR:HB   | 1:A:511:LEU:HD22 | 1.57                     | 0.84              |
| 1:A:539:MET:HG3  | 1:A:541:LEU:HD21 | 1.59                     | 0.84              |
| 1:B:490:PHE:C    | 1:B:557:ILE:HB   | 2.01                     | 0.84              |
| 1:B:504:ASN:O    | 1:B:509:PRO:HA   | 1.78                     | 0.84              |
| 1:B:547:ARG:O    | 1:B:548:THR:OG1  | 1.95                     | 0.84              |
| 2:C:410:HIS:CA   | 1:A:453:GLN:OE1  | 2.25                     | 0.84              |
| 1:A:479:GLU:O    | 1:A:482:ILE:HG13 | 1.77                     | 0.84              |
| 1:E:104:ILE:O    | 1:E:107:VAL:HG22 | 1.77                     | 0.84              |
| 2:F:259:PHE:HE1  | 2:F:267:PHE:HB2  | 1.40                     | 0.84              |
| 2:C:214:TYR:HA   | 2:C:217:CYS:SG   | 2.18                     | 0.84              |
| 2:D:28:ARG:O     | 2:D:31:ILE:HD11  | 1.77                     | 0.84              |
| 1:A:398:ASP:CG   | 1:A:401:LYS:HG2  | 2.03                     | 0.84              |
| 1:A:486:ILE:CD1  | 1:A:564:ASP:O    | 2.25                     | 0.84              |
| 2:D:58:HIS:CE1   | 2:D:98:GLY:CA    | 2.49                     | 0.84              |
| 1:B:325:PHE:CE2  | 1:B:330:ASP:CB   | 2.60                     | 0.84              |
| 1:A:95:LEU:HB3   | 1:A:162:LEU:HB3  | 1.56                     | 0.84              |
| 1:A:172:ILE:CD1  | 1:A:183:PHE:CE2  | 2.60                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:137:LEU:HD12 | 2:F:138:PRO:HD2  | 1.57                     | 0.84              |
| 2:C:98:GLY:O     | 2:C:102:PRO:HD3  | 1.78                     | 0.84              |
| 1:A:233:LYS:O    | 1:A:237:GLU:CD   | 2.20                     | 0.84              |
| 1:A:389:ASN:CG   | 1:A:408:LEU:HB3  | 2.02                     | 0.84              |
| 1:B:494:ARG:CB   | 1:B:553:LYS:O    | 2.26                     | 0.84              |
| 2:C:150:ALA:O    | 3:C:501:HOH:O    | 1.95                     | 0.84              |
| 2:D:155:TRP:HA   | 2:D:159:TRP:HB2  | 1.59                     | 0.84              |
| 1:E:453:GLN:O    | 2:F:407:PHE:N    | 2.10                     | 0.84              |
| 2:F:67:PHE:O     | 2:F:71:MET:HG3   | 1.76                     | 0.84              |
| 2:C:125:PHE:CZ   | 2:C:150:ALA:HA   | 2.11                     | 0.84              |
| 1:A:444:GLN:O    | 1:A:444:GLN:NE2  | 2.11                     | 0.84              |
| 2:F:116:ALA:O    | 2:F:119:ILE:HD12 | 1.77                     | 0.84              |
| 1:B:538:ILE:HG12 | 2:D:405:LYS:CB   | 2.07                     | 0.84              |
| 2:C:88:ALA:CB    | 3:C:502:HOH:O    | 2.02                     | 0.84              |
| 1:A:100:GLY:HA3  | 1:A:158:SER:CB   | 2.07                     | 0.84              |
| 1:B:110:HIS:O    | 1:B:113:VAL:HG12 | 1.76                     | 0.83              |
| 1:B:290:TYR:H    | 1:B:311:SER:HG   | 1.24                     | 0.83              |
| 2:C:128:PHE:HE2  | 2:C:138:PRO:HG2  | 1.37                     | 0.83              |
| 1:A:594:LEU:HD12 | 1:A:594:LEU:O    | 1.78                     | 0.83              |
| 1:E:184:TRP:HZ3  | 1:E:211:TYR:CD2  | 1.95                     | 0.83              |
| 1:E:228:TRP:HZ3  | 1:E:263:LEU:CD2  | 1.91                     | 0.83              |
| 2:F:268:PRO:O    | 2:F:272:ILE:HG13 | 1.77                     | 0.83              |
| 2:D:24:PHE:HE1   | 2:D:67:PHE:HZ    | 0.90                     | 0.83              |
| 1:E:325:PHE:CZ   | 1:E:468:LEU:HD13 | 2.13                     | 0.83              |
| 1:E:366:LYS:HB2  | 1:E:393:LEU:HD11 | 1.61                     | 0.83              |
| 2:F:110:ILE:CD1  | 2:F:115:LEU:HD12 | 2.05                     | 0.83              |
| 1:B:104:ILE:HD13 | 1:B:109:TYR:HE2  | 1.43                     | 0.83              |
| 2:D:350:PHE:O    | 2:D:351:SER:OG   | 1.96                     | 0.83              |
| 2:F:20:LYS:HZ3   | 2:F:162:VAL:C    | 1.86                     | 0.83              |
| 2:C:58:HIS:HB3   | 1:A:596:LYS:O    | 1.78                     | 0.83              |
| 1:A:468:LEU:HD21 | 1:A:559:VAL:HG11 | 1.60                     | 0.83              |
| 2:F:10:TRP:HA    | 2:F:50:TYR:HE2   | 1.39                     | 0.83              |
| 1:B:598:TRP:CZ3  | 2:D:98:GLY:HA3   | 2.13                     | 0.83              |
| 1:A:539:MET:O    | 1:A:541:LEU:CD2  | 2.26                     | 0.83              |
| 2:F:193:ILE:HA   | 2:F:196:GLN:OE1  | 1.78                     | 0.83              |
| 1:B:122:SER:H    | 1:B:182:LEU:CD2  | 1.91                     | 0.83              |
| 2:D:92:ILE:CD1   | 2:D:146:CYS:HB3  | 2.09                     | 0.83              |
| 1:E:279:ASN:HB2  | 1:E:356:SER:O    | 1.76                     | 0.83              |
| 1:B:104:ILE:HD12 | 1:B:107:VAL:O    | 1.79                     | 0.83              |
| 1:E:524:PHE:CE2  | 1:E:543:ILE:HD11 | 2.08                     | 0.83              |
| 2:F:27:ASP:O     | 2:F:31:ILE:HG22  | 1.79                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:90:MET:HA    | 2:F:93:ILE:HD12  | 1.61                     | 0.83              |
| 2:F:223:ASP:OD2  | 3:F:501:HOH:O    | 1.94                     | 0.83              |
| 1:B:104:ILE:CD1  | 1:B:109:TYR:HE2  | 1.90                     | 0.83              |
| 1:A:296:ILE:HG22 | 1:A:342:LEU:CD2  | 2.08                     | 0.83              |
| 1:A:454:VAL:O    | 1:A:538:ILE:HA   | 1.79                     | 0.83              |
| 1:E:77:VAL:CG1   | 1:E:79:PHE:CZ    | 2.62                     | 0.83              |
| 1:E:225:HIS:HB2  | 1:E:228:TRP:CB   | 2.08                     | 0.83              |
| 2:F:70:LEU:HD12  | 2:F:70:LEU:O     | 1.79                     | 0.83              |
| 1:B:379:ARG:O    | 1:B:379:ARG:HD3  | 1.79                     | 0.83              |
| 2:C:142:MET:HA   | 2:C:142:MET:CE   | 2.09                     | 0.83              |
| 2:D:268:PRO:O    | 2:D:271:LEU:HD12 | 1.78                     | 0.83              |
| 2:D:355:VAL:HA   | 2:D:358:ASP:OD2  | 1.79                     | 0.83              |
| 1:A:92:GLN:NE2   | 1:A:183:PHE:HB3  | 1.94                     | 0.83              |
| 1:A:478:LEU:HD12 | 1:A:510:LEU:HD13 | 1.57                     | 0.83              |
| 1:E:172:ILE:HD11 | 1:E:182:LEU:HB2  | 1.61                     | 0.83              |
| 1:A:224:LYS:HG3  | 1:A:228:TRP:CZ3  | 2.14                     | 0.83              |
| 1:E:588:PHE:CB   | 2:F:5:PRO:CB     | 2.46                     | 0.83              |
| 1:B:77:VAL:O     | 1:B:162:LEU:HB2  | 1.79                     | 0.82              |
| 1:A:95:LEU:CG    | 1:A:116:MET:HE3  | 2.09                     | 0.82              |
| 1:A:167:THR:HG23 | 1:A:169:LEU:H    | 1.43                     | 0.82              |
| 1:A:382:PRO:HB3  | 1:A:385:VAL:HG23 | 1.60                     | 0.82              |
| 1:A:94:VAL:O     | 1:A:162:LEU:CB   | 2.24                     | 0.82              |
| 1:A:210:PHE:HD1  | 1:A:210:PHE:H    | 1.27                     | 0.82              |
| 1:E:455:SER:OG   | 1:E:462:ILE:N    | 2.11                     | 0.82              |
| 1:E:466:THR:CG2  | 1:E:516:PHE:CD2  | 2.62                     | 0.82              |
| 2:F:237:ARG:HA   | 2:F:240:SER:CB   | 2.09                     | 0.82              |
| 1:A:224:LYS:CG   | 1:A:228:TRP:CZ3  | 2.63                     | 0.82              |
| 1:A:334:ARG:CG   | 1:A:513:TYR:OH   | 2.26                     | 0.82              |
| 1:A:483:GLU:OE1  | 1:A:532:ILE:HD13 | 1.79                     | 0.82              |
| 2:C:140:LEU:O    | 2:C:140:LEU:HD12 | 1.78                     | 0.82              |
| 2:C:305:GLN:O    | 2:C:308:ILE:HB   | 1.79                     | 0.82              |
| 1:A:382:PRO:HG2  | 1:A:401:LYS:HZ1  | 1.42                     | 0.82              |
| 1:A:399:ILE:O    | 1:A:401:LYS:CB   | 2.22                     | 0.82              |
| 1:A:507:GLN:O    | 1:A:508:LEU:HD22 | 1.77                     | 0.82              |
| 2:F:247:HIS:H    | 2:F:247:HIS:CD2  | 1.94                     | 0.82              |
| 1:B:77:VAL:HG12  | 1:B:79:PHE:CZ    | 2.14                     | 0.82              |
| 1:B:93:PHE:CD2   | 1:B:162:LEU:HD22 | 2.14                     | 0.82              |
| 1:B:117:LYS:HD3  | 1:B:439:PHE:HE1  | 1.42                     | 0.82              |
| 1:A:327:SER:OG   | 1:A:329:LYS:HE3  | 1.78                     | 0.82              |
| 2:F:316:ILE:CD1  | 2:F:346:LEU:HD23 | 2.09                     | 0.82              |
| 2:F:354:PRO:HD2  | 2:F:355:VAL:N    | 1.90                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:107:VAL:HG21 | 1:B:266:GLN:HE21 | 1.44                     | 0.82              |
| 1:B:595:GLU:CB   | 2:D:158:TYR:CZ   | 2.63                     | 0.82              |
| 1:A:165:LEU:HD12 | 1:A:167:THR:H    | 1.41                     | 0.82              |
| 1:A:524:PHE:CD2  | 1:A:525:ARG:HG2  | 2.14                     | 0.82              |
| 2:F:307:TRP:O    | 2:F:311:LEU:HG   | 1.79                     | 0.82              |
| 1:B:503:PHE:N    | 1:B:510:LEU:O    | 2.12                     | 0.82              |
| 2:C:81:ASP:O     | 2:C:85:ARG:HG3   | 1.80                     | 0.82              |
| 2:C:99:LEU:HD13  | 2:C:121:LEU:HD21 | 1.62                     | 0.82              |
| 1:A:305:GLN:OE1  | 1:A:313:THR:HB   | 1.79                     | 0.82              |
| 1:E:416:GLY:CA   | 3:E:723:HOH:O    | 2.26                     | 0.82              |
| 1:B:64:SER:OG    | 1:B:86:ASN:C     | 2.23                     | 0.82              |
| 2:C:40:TYR:CD2   | 2:C:67:PHE:HD1   | 1.97                     | 0.82              |
| 2:C:96:VAL:HA    | 2:C:99:LEU:CD1   | 2.09                     | 0.82              |
| 2:D:269:LEU:HA   | 2:D:272:ILE:CD1  | 2.10                     | 0.82              |
| 1:A:508:LEU:HD12 | 1:A:509:PRO:CD   | 2.09                     | 0.82              |
| 1:E:77:VAL:CG1   | 1:E:79:PHE:CE2   | 2.63                     | 0.82              |
| 1:E:321:HIS:HE1  | 1:E:522:GLU:CD   | 1.86                     | 0.82              |
| 2:F:252:PHE:CD1  | 2:F:307:TRP:HZ2  | 1.83                     | 0.82              |
| 2:C:417:PRO:O    | 2:C:419:GLY:N    | 2.12                     | 0.82              |
| 1:B:77:VAL:HG11  | 1:B:79:PHE:CE2   | 2.14                     | 0.82              |
| 1:B:383:THR:HG22 | 1:B:384:HIS:NE2  | 1.93                     | 0.82              |
| 1:A:433:PHE:CE1  | 1:A:528:LEU:HB2  | 2.15                     | 0.82              |
| 1:A:533:ASP:OD1  | 1:A:536:LYS:N    | 2.13                     | 0.82              |
| 1:E:433:PHE:HA   | 1:E:544:PRO:CB   | 2.03                     | 0.82              |
| 1:E:496:HIS:O    | 1:E:499:GLU:CB   | 2.27                     | 0.82              |
| 1:E:589:GLU:N    | 1:E:589:GLU:OE2  | 2.13                     | 0.82              |
| 2:F:356:ILE:O    | 2:F:360:ILE:HG13 | 1.80                     | 0.82              |
| 1:B:118:PHE:HD1  | 1:B:306:HIS:O    | 1.63                     | 0.81              |
| 2:C:182:GLU:O    | 2:C:186:LEU:HG   | 1.79                     | 0.81              |
| 2:D:249:ARG:O    | 2:D:253:GLU:N    | 2.13                     | 0.81              |
| 2:D:269:LEU:O    | 2:D:272:ILE:HD12 | 1.80                     | 0.81              |
| 1:A:165:LEU:HD12 | 1:A:167:THR:HG22 | 1.61                     | 0.81              |
| 2:C:53:ARG:HD3   | 1:A:485:THR:HG22 | 1.60                     | 0.81              |
| 1:E:299:SER:CA   | 1:E:317:SER:CB   | 2.59                     | 0.81              |
| 1:B:103:ASP:HA   | 1:B:107:VAL:O    | 1.80                     | 0.81              |
| 1:B:468:LEU:HD12 | 1:B:560:ARG:O    | 1.80                     | 0.81              |
| 1:A:104:ILE:O    | 1:A:107:VAL:HG22 | 1.79                     | 0.81              |
| 1:A:325:PHE:CE2  | 1:A:562:ASN:HB2  | 2.15                     | 0.81              |
| 1:A:511:LEU:HD23 | 1:A:511:LEU:O    | 1.80                     | 0.81              |
| 1:A:565:LEU:HD22 | 1:A:570:ILE:HG13 | 1.62                     | 0.81              |
| 2:C:235:ILE:CD1  | 2:C:278:LYS:HE3  | 1.84                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:170:GLU:OE1  | 1:A:185:GLN:NE2  | 2.12                     | 0.81              |
| 1:A:520:SER:O    | 1:A:521:THR:HG23 | 1.80                     | 0.81              |
| 1:E:593:SER:CB   | 1:E:594:LEU:HA   | 2.06                     | 0.81              |
| 1:B:110:HIS:CB   | 1:B:140:LEU:CB   | 2.58                     | 0.81              |
| 1:B:511:LEU:HD23 | 1:B:512:PRO:HD2  | 1.60                     | 0.81              |
| 1:A:172:ILE:CG2  | 1:A:179:PHE:CG   | 2.63                     | 0.81              |
| 2:F:237:ARG:HA   | 2:F:237:ARG:HE   | 1.44                     | 0.81              |
| 1:A:551:LEU:O    | 3:A:703:HOH:O    | 1.98                     | 0.81              |
| 1:E:225:HIS:CG   | 1:E:228:TRP:HB2  | 2.15                     | 0.81              |
| 2:F:23:PHE:HE2   | 2:F:43:ALA:HB1   | 1.44                     | 0.81              |
| 1:B:64:SER:OG    | 1:B:86:ASN:CA    | 2.27                     | 0.81              |
| 1:B:368:TYR:HE1  | 1:B:372:LEU:HG   | 1.42                     | 0.81              |
| 2:C:417:PRO:C    | 2:C:419:GLY:H    | 1.88                     | 0.81              |
| 1:A:63:PHE:HB3   | 1:A:88:ILE:HG12  | 1.62                     | 0.81              |
| 1:A:81:LEU:CD2   | 1:A:131:ALA:HB2  | 2.07                     | 0.81              |
| 1:A:184:TRP:CE2  | 1:A:211:TYR:HB2  | 2.15                     | 0.81              |
| 1:A:280:PHE:HE2  | 1:A:282:ASP:HB2  | 1.44                     | 0.81              |
| 1:A:368:TYR:CD1  | 1:A:372:LEU:HG   | 2.15                     | 0.81              |
| 1:A:483:GLU:CD   | 1:A:532:ILE:HD12 | 2.03                     | 0.81              |
| 1:A:487:VAL:HG21 | 1:A:558:MET:SD   | 2.20                     | 0.81              |
| 2:C:137:LEU:HD12 | 2:C:138:PRO:HD2  | 1.62                     | 0.81              |
| 2:C:153:TRP:CZ2  | 2:C:157:HIS:CE1  | 2.69                     | 0.81              |
| 1:A:63:PHE:CE2   | 1:A:214:THR:CG2  | 2.63                     | 0.81              |
| 1:A:297:SER:CB   | 1:A:319:GLN:O    | 2.28                     | 0.81              |
| 2:F:10:TRP:HB2   | 2:F:15:GLU:CD    | 2.06                     | 0.81              |
| 1:B:598:TRP:CE3  | 2:D:98:GLY:HA3   | 2.16                     | 0.81              |
| 2:C:10:TRP:CA    | 2:C:50:TYR:CE1   | 2.59                     | 0.81              |
| 1:E:347:GLU:O    | 1:E:351:GLU:HG3  | 1.81                     | 0.81              |
| 1:E:436:ILE:CG2  | 1:E:440:LYS:HB3  | 2.11                     | 0.81              |
| 2:F:122:PRO:CG   | 2:F:125:PHE:HE2  | 1.94                     | 0.81              |
| 1:B:84:ASN:CB    | 3:B:711:HOH:O    | 2.28                     | 0.81              |
| 1:A:350:GLY:HA2  | 1:A:357:LEU:CD1  | 2.10                     | 0.81              |
| 1:E:224:LYS:HG3  | 1:E:228:TRP:CD2  | 2.16                     | 0.81              |
| 1:E:530:HIS:C    | 2:F:418:PHE:CB   | 2.53                     | 0.81              |
| 1:B:103:ASP:O    | 1:B:130:GLN:NE2  | 2.14                     | 0.80              |
| 1:B:310:LEU:HB3  | 1:B:428:LYS:HG3  | 1.63                     | 0.80              |
| 1:B:326:ASN:HD22 | 1:B:326:ASN:H    | 1.29                     | 0.80              |
| 2:C:28:ARG:C     | 2:C:29:GLU:OE2   | 2.24                     | 0.80              |
| 2:D:190:TYR:CE2  | 2:D:218:ILE:CG2  | 2.63                     | 0.80              |
| 2:D:259:PHE:HE1  | 2:D:268:PRO:HB3  | 0.99                     | 0.80              |
| 1:A:93:PHE:CD2   | 1:A:162:LEU:HG   | 2.15                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:532:ILE:HG22 | 1:A:539:MET:HE3  | 1.61                     | 0.80              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:CB   | 2.59                     | 0.80              |
| 1:E:370:LEU:CD1  | 1:E:397:ILE:HG13 | 2.07                     | 0.80              |
| 1:E:530:HIS:O    | 2:F:418:PHE:CA   | 2.29                     | 0.80              |
| 2:C:271:LEU:O    | 2:C:275:MET:HG3  | 1.81                     | 0.80              |
| 2:C:304:ALA:O    | 2:C:307:TRP:HB2  | 1.79                     | 0.80              |
| 1:E:233:LYS:HZ1  | 1:E:237:GLU:CB   | 1.93                     | 0.80              |
| 2:C:230:PHE:HA   | 2:C:233:VAL:HG23 | 1.64                     | 0.80              |
| 2:C:417:PRO:HB2  | 1:A:584:PRO:CG   | 2.11                     | 0.80              |
| 2:D:90:MET:HE2   | 2:D:90:MET:HA    | 1.63                     | 0.80              |
| 1:A:176:CYS:SG   | 1:A:179:PHE:CD1  | 2.73                     | 0.80              |
| 1:E:169:LEU:HD13 | 1:E:183:PHE:CZ   | 2.17                     | 0.80              |
| 1:E:232:ILE:O    | 1:E:236:THR:HG23 | 1.81                     | 0.80              |
| 2:F:272:ILE:CG1  | 2:F:315:GLN:NE2  | 2.44                     | 0.80              |
| 1:B:368:TYR:CE1  | 1:B:372:LEU:CG   | 2.64                     | 0.80              |
| 1:B:432:TYR:HD2  | 1:B:526:LEU:HD13 | 1.45                     | 0.80              |
| 2:C:129:ARG:O    | 2:C:133:THR:OG1  | 1.99                     | 0.80              |
| 1:E:318:THR:O    | 1:E:319:GLN:HG3  | 1.81                     | 0.80              |
| 1:E:351:GLU:OE1  | 1:E:352:LEU:N    | 2.15                     | 0.80              |
| 2:D:331:LEU:HD21 | 2:D:346:LEU:HB3  | 0.83                     | 0.80              |
| 1:E:155:GLY:HA2  | 3:E:713:HOH:O    | 1.46                     | 0.80              |
| 1:E:324:GLY:C    | 1:E:325:PHE:CD1  | 2.60                     | 0.80              |
| 2:F:301:PHE:CD1  | 2:F:304:ALA:HB3  | 2.16                     | 0.80              |
| 1:B:432:TYR:HE2  | 1:B:526:LEU:HB2  | 1.46                     | 0.80              |
| 2:C:40:TYR:HE2   | 2:C:67:PHE:CE1   | 1.98                     | 0.80              |
| 2:D:13:SER:O     | 2:D:16:VAL:HG23  | 1.81                     | 0.80              |
| 1:E:253:LYS:N    | 3:E:708:HOH:O    | 2.14                     | 0.80              |
| 1:B:598:TRP:CZ2  | 2:D:98:GLY:HA2   | 2.17                     | 0.80              |
| 1:A:232:ILE:HD11 | 1:A:264:LEU:HB2  | 0.80                     | 0.80              |
| 1:A:394:GLY:CA   | 3:A:717:HOH:O    | 2.29                     | 0.80              |
| 1:A:408:LEU:HD22 | 1:A:409:GLN:N    | 1.97                     | 0.80              |
| 1:E:77:VAL:HG12  | 1:E:79:PHE:CZ    | 2.15                     | 0.80              |
| 1:E:318:THR:HB   | 1:E:319:GLN:OE1  | 1.80                     | 0.80              |
| 1:A:72:TYR:OH    | 1:A:206:SER:CB   | 2.30                     | 0.80              |
| 1:A:382:PRO:HG2  | 1:A:401:LYS:NZ   | 1.97                     | 0.80              |
| 1:E:435:LYS:CE   | 1:E:545:GLN:HE22 | 1.93                     | 0.80              |
| 1:E:521:THR:O    | 1:E:522:GLU:OE2  | 1.98                     | 0.80              |
| 2:C:249:ARG:CB   | 2:C:307:TRP:HZ2  | 1.84                     | 0.80              |
| 1:A:64:SER:CB    | 1:A:85:GLN:CB    | 2.60                     | 0.80              |
| 1:A:78:ILE:HA    | 1:A:161:LYS:CB   | 2.12                     | 0.80              |
| 1:E:487:VAL:CG2  | 1:E:527:ALA:HB3  | 2.12                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:LYS:HE2  | 1:B:233:LYS:O    | 1.82                     | 0.79              |
| 2:C:182:GLU:O    | 2:C:186:LEU:CG   | 2.31                     | 0.79              |
| 1:E:299:SER:HA   | 1:E:317:SER:CA   | 2.12                     | 0.79              |
| 1:A:454:VAL:HG21 | 1:A:462:ILE:HD12 | 1.64                     | 0.79              |
| 1:B:104:ILE:CG2  | 1:B:129:ILE:HA   | 2.11                     | 0.79              |
| 1:B:433:PHE:HA   | 1:B:544:PRO:HB3  | 1.64                     | 0.79              |
| 1:A:329:LYS:HD2  | 1:A:364:TRP:CH2  | 2.18                     | 0.79              |
| 1:A:490:PHE:CZ   | 1:A:523:PHE:CD1  | 2.70                     | 0.79              |
| 2:F:420:VAL:O    | 2:F:421:ILE:CG1  | 2.31                     | 0.79              |
| 1:B:231:VAL:O    | 1:B:235:LEU:HD23 | 1.83                     | 0.79              |
| 1:B:331:GLN:HB3  | 1:B:334:ARG:CB   | 2.12                     | 0.79              |
| 2:D:28:ARG:O     | 2:D:31:ILE:CD1   | 2.30                     | 0.79              |
| 1:A:385:VAL:HB   | 1:A:403:THR:HG23 | 0.86                     | 0.79              |
| 1:E:247:VAL:HG13 | 1:E:386:ILE:CD1  | 2.12                     | 0.79              |
| 1:E:264:LEU:HD12 | 1:E:358:LEU:HD11 | 1.64                     | 0.79              |
| 1:B:455:SER:CA   | 2:D:405:LYS:CB   | 2.60                     | 0.79              |
| 2:D:183:LEU:HD22 | 2:D:224:HIS:CB   | 2.05                     | 0.79              |
| 1:A:181:ASN:OD1  | 1:A:187:ASP:CA   | 2.29                     | 0.79              |
| 1:A:565:LEU:HD22 | 1:A:570:ILE:CG1  | 2.12                     | 0.79              |
| 1:E:104:ILE:O    | 1:E:266:GLN:NE2  | 2.14                     | 0.79              |
| 1:B:122:SER:H    | 1:B:182:LEU:HD23 | 1.46                     | 0.79              |
| 1:B:211:TYR:HD1  | 1:B:212:PRO:HD2  | 1.48                     | 0.79              |
| 1:B:511:LEU:HD23 | 1:B:512:PRO:CD   | 2.13                     | 0.79              |
| 2:D:256:MET:O    | 2:D:260:ILE:HG13 | 1.82                     | 0.79              |
| 1:A:483:GLU:OE1  | 1:A:531:SER:HA   | 1.81                     | 0.79              |
| 1:E:94:VAL:O     | 1:E:163:THR:N    | 2.13                     | 0.79              |
| 1:E:528:LEU:O    | 1:E:528:LEU:HD12 | 1.80                     | 0.79              |
| 1:B:77:VAL:CG1   | 1:B:79:PHE:CE2   | 2.65                     | 0.79              |
| 2:C:36:LEU:HG    | 2:C:40:TYR:CE1   | 2.18                     | 0.79              |
| 2:C:195:ARG:HG2  | 2:C:195:ARG:HH11 | 1.48                     | 0.79              |
| 1:A:223:ILE:O    | 1:A:224:LYS:HD2  | 1.83                     | 0.79              |
| 1:E:392:THR:O    | 1:E:393:LEU:HD12 | 1.83                     | 0.79              |
| 1:B:318:THR:HG22 | 1:B:319:GLN:HG3  | 1.63                     | 0.79              |
| 1:A:162:LEU:CD2  | 1:A:210:PHE:CD2  | 2.63                     | 0.79              |
| 1:E:373:THR:HG22 | 1:E:377:ILE:HD11 | 1.63                     | 0.79              |
| 2:F:11:LYS:HB3   | 2:F:11:LYS:HZ2   | 1.48                     | 0.79              |
| 1:B:211:TYR:HD1  | 1:B:212:PRO:CD   | 1.96                     | 0.79              |
| 1:A:331:GLN:O    | 1:A:335:TYR:N    | 2.12                     | 0.79              |
| 1:A:520:SER:O    | 1:A:521:THR:CG2  | 2.31                     | 0.79              |
| 1:E:98:GLN:O     | 1:E:142:ASN:HB3  | 1.83                     | 0.79              |
| 1:B:490:PHE:CA   | 1:B:557:ILE:HB   | 2.13                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:77:VAL:HG11  | 1:E:79:PHE:CE2   | 2.18                     | 0.78              |
| 2:F:111:PRO:HG2  | 2:F:114:LEU:HG   | 1.65                     | 0.78              |
| 2:F:279:ASN:HD21 | 2:F:308:ILE:CD1  | 1.96                     | 0.78              |
| 2:C:92:ILE:HD11  | 2:C:147:VAL:HG22 | 1.64                     | 0.78              |
| 2:C:370:LEU:HA   | 2:C:373:ASP:OD2  | 1.82                     | 0.78              |
| 2:D:238:ILE:HD12 | 2:D:238:ILE:O    | 1.83                     | 0.78              |
| 1:A:97:ILE:HG23  | 1:A:160:ILE:HG22 | 1.64                     | 0.78              |
| 1:A:119:ILE:CG1  | 1:A:309:HIS:CE1  | 2.66                     | 0.78              |
| 2:F:122:PRO:CG   | 2:F:125:PHE:CE2  | 2.65                     | 0.78              |
| 2:D:92:ILE:HD13  | 2:D:146:CYS:HB3  | 1.65                     | 0.78              |
| 2:D:116:ALA:HA   | 2:D:119:ILE:HG22 | 1.65                     | 0.78              |
| 2:F:10:TRP:HB2   | 2:F:15:GLU:OE2   | 1.83                     | 0.78              |
| 1:B:536:LYS:O    | 1:B:537:LYS:HB2  | 1.82                     | 0.78              |
| 2:C:6:ARG:O      | 1:A:586:ILE:CG2  | 2.26                     | 0.78              |
| 1:A:365:ILE:O    | 1:A:370:LEU:HB2  | 1.83                     | 0.78              |
| 1:A:385:VAL:HG12 | 1:A:403:THR:CG2  | 2.13                     | 0.78              |
| 2:C:182:GLU:O    | 2:C:186:LEU:HB2  | 1.84                     | 0.78              |
| 2:D:6:ARG:HH11   | 2:D:6:ARG:HG3    | 1.48                     | 0.78              |
| 2:D:230:PHE:CB   | 3:D:510:HOH:O    | 2.31                     | 0.78              |
| 1:A:237:GLU:CD   | 1:A:237:GLU:H    | 1.91                     | 0.78              |
| 2:F:235:ILE:HA   | 2:F:238:ILE:HD12 | 1.65                     | 0.78              |
| 1:B:93:PHE:HD2   | 1:B:162:LEU:HD22 | 1.47                     | 0.78              |
| 1:B:104:ILE:HD13 | 1:B:107:VAL:HG23 | 1.63                     | 0.78              |
| 2:C:86:LEU:HD23  | 2:D:90:MET:HG3   | 1.64                     | 0.78              |
| 2:F:179:LEU:HG   | 2:F:180:ILE:HG13 | 1.65                     | 0.78              |
| 2:F:259:PHE:CZ   | 2:F:268:PRO:HA   | 2.18                     | 0.78              |
| 1:B:465:LEU:CD1  | 1:B:482:ILE:CG2  | 2.62                     | 0.78              |
| 1:B:492:VAL:CB   | 1:B:557:ILE:HD11 | 2.14                     | 0.78              |
| 2:C:36:LEU:CG    | 2:C:40:TYR:CE1   | 2.63                     | 0.78              |
| 2:C:417:PRO:HB2  | 1:A:584:PRO:HG2  | 1.64                     | 0.78              |
| 2:D:134:HIS:O    | 2:D:135:ASP:OD1  | 2.02                     | 0.78              |
| 2:D:410:HIS:HD2  | 2:D:413:TRP:HD1  | 1.28                     | 0.78              |
| 1:A:71:ILE:HD11  | 1:A:78:ILE:HB    | 1.65                     | 0.78              |
| 1:A:78:ILE:HG13  | 1:A:161:LYS:CB   | 1.91                     | 0.78              |
| 1:A:93:PHE:HD2   | 1:A:162:LEU:HG   | 1.49                     | 0.78              |
| 1:A:227:ASN:O    | 1:A:231:VAL:N    | 2.10                     | 0.78              |
| 1:E:89:VAL:HG11  | 1:E:93:PHE:CE1   | 2.17                     | 0.78              |
| 1:E:461:GLY:CA   | 3:F:504:HOH:O    | 2.27                     | 0.78              |
| 2:F:10:TRP:CB    | 2:F:50:TYR:CE2   | 2.45                     | 0.78              |
| 2:F:33:ARG:CB    | 2:F:33:ARG:HH21  | 1.96                     | 0.78              |
| 1:E:93:PHE:HB3   | 1:E:210:PHE:HD1  | 1.43                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:9:PRO:HB3    | 2:C:54:THR:HG22  | 1.66                     | 0.78              |
| 2:C:212:LYS:O    | 2:C:216:THR:HG23 | 1.84                     | 0.78              |
| 2:D:154:VAL:HG23 | 2:D:159:TRP:CD1  | 2.19                     | 0.78              |
| 1:A:63:PHE:CE2   | 1:A:214:THR:N    | 2.51                     | 0.78              |
| 1:A:313:THR:O    | 1:A:315:THR:OG1  | 2.01                     | 0.78              |
| 1:A:483:GLU:HA   | 1:A:529:VAL:CG1  | 2.12                     | 0.78              |
| 1:E:110:HIS:CE1  | 1:E:137:SER:O    | 2.37                     | 0.78              |
| 2:F:20:LYS:HG3   | 2:F:159:TRP:HE3  | 1.49                     | 0.78              |
| 2:F:245:TRP:O    | 2:F:248:LEU:CG   | 2.32                     | 0.78              |
| 2:D:125:PHE:HZ   | 2:D:150:ALA:CA   | 1.91                     | 0.77              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:H    | 1.97                     | 0.77              |
| 1:E:451:PRO:HD3  | 2:F:413:TRP:CG   | 2.20                     | 0.77              |
| 1:E:451:PRO:CD   | 2:F:413:TRP:CD2  | 2.65                     | 0.77              |
| 1:B:598:TRP:CZ3  | 2:D:98:GLY:CA    | 2.67                     | 0.77              |
| 1:E:248:ILE:HD11 | 1:E:382:PRO:CG   | 2.13                     | 0.77              |
| 1:E:430:MET:CE   | 1:E:568:TRP:CE3  | 2.64                     | 0.77              |
| 1:B:164:ASN:ND2  | 1:B:208:TYR:CD1  | 2.52                     | 0.77              |
| 1:A:364:TRP:HB3  | 1:A:369:GLY:CA   | 2.09                     | 0.77              |
| 1:E:528:LEU:HD11 | 1:E:569:GLU:OE1  | 1.84                     | 0.77              |
| 2:F:279:ASN:HD21 | 2:F:308:ILE:HD12 | 1.50                     | 0.77              |
| 2:D:308:ILE:HA   | 2:D:311:LEU:HD12 | 1.64                     | 0.77              |
| 1:E:364:TRP:CH2  | 1:E:368:TYR:HB3  | 2.19                     | 0.77              |
| 1:B:104:ILE:HD13 | 1:B:107:VAL:CG2  | 2.13                     | 0.77              |
| 1:B:117:LYS:CD   | 1:B:439:PHE:HE1  | 1.93                     | 0.77              |
| 2:C:409:SER:HB3  | 1:A:450:PRO:HB2  | 1.65                     | 0.77              |
| 2:D:158:TYR:O    | 2:D:162:VAL:HG23 | 1.85                     | 0.77              |
| 1:A:579:PHE:HD2  | 1:A:581:ARG:CA   | 1.95                     | 0.77              |
| 1:B:104:ILE:CD1  | 1:B:109:TYR:CD2  | 2.64                     | 0.77              |
| 1:B:529:VAL:HA   | 1:B:541:LEU:HA   | 1.65                     | 0.77              |
| 2:C:9:PRO:HB2    | 2:C:50:TYR:HD1   | 1.47                     | 0.77              |
| 2:D:331:LEU:CD2  | 2:D:346:LEU:CG   | 2.61                     | 0.77              |
| 1:A:172:ILE:CG2  | 1:A:179:PHE:HB2  | 1.86                     | 0.77              |
| 1:E:334:ARG:O    | 1:E:338:LEU:HB2  | 1.85                     | 0.77              |
| 1:B:325:PHE:CZ   | 1:B:469:LYS:HB2  | 2.16                     | 0.77              |
| 1:B:598:TRP:HB2  | 2:D:58:HIS:HB2   | 1.67                     | 0.77              |
| 1:A:172:ILE:O    | 1:A:175:VAL:HG22 | 1.84                     | 0.77              |
| 1:A:298:LEU:H    | 1:A:298:LEU:HD23 | 1.50                     | 0.77              |
| 1:E:229:MET:O    | 1:E:232:ILE:HG22 | 1.84                     | 0.77              |
| 1:B:585:TYR:CD1  | 2:D:11:LYS:HA    | 2.20                     | 0.77              |
| 2:C:155:TRP:HA   | 2:C:159:TRP:HB2  | 1.65                     | 0.77              |
| 2:D:147:VAL:O    | 2:D:151:ILE:HG13 | 1.83                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:272:ILE:HG12 | 2:F:315:GLN:NE2  | 2.00                     | 0.77              |
| 1:B:490:PHE:CB   | 1:B:557:ILE:HG22 | 1.85                     | 0.77              |
| 1:A:346:TYR:O    | 1:A:357:LEU:HD21 | 1.84                     | 0.77              |
| 1:A:573:ASN:O    | 1:A:576:VAL:CG2  | 2.33                     | 0.77              |
| 1:E:132:THR:O    | 1:E:134:VAL:HG23 | 1.84                     | 0.77              |
| 1:E:248:ILE:CD1  | 1:E:382:PRO:CB   | 2.59                     | 0.77              |
| 1:E:490:PHE:HD1  | 1:E:521:THR:CG2  | 1.98                     | 0.77              |
| 1:B:164:ASN:CA   | 1:B:210:PHE:CE1  | 2.59                     | 0.77              |
| 1:B:586:ILE:HG23 | 2:D:6:ARG:O      | 1.84                     | 0.77              |
| 2:C:148:ASP:O    | 2:C:151:ILE:HG22 | 1.86                     | 0.77              |
| 2:D:351:SER:O    | 2:D:353:ASP:OD2  | 2.02                     | 0.77              |
| 1:E:164:ASN:HA   | 1:E:210:PHE:CE1  | 2.20                     | 0.77              |
| 1:E:479:GLU:OE2  | 1:E:507:GLN:HB3  | 1.83                     | 0.77              |
| 1:B:366:LYS:HE2  | 1:B:367:GLY:H    | 1.47                     | 0.76              |
| 2:C:258:HIS:O    | 2:C:262:LEU:HG   | 1.85                     | 0.76              |
| 2:D:122:PRO:HD2  | 2:D:125:PHE:HB2  | 1.67                     | 0.76              |
| 2:D:331:LEU:HD22 | 2:D:346:LEU:HB2  | 1.65                     | 0.76              |
| 1:A:454:VAL:C    | 1:A:538:ILE:HG23 | 2.10                     | 0.76              |
| 2:C:373:ASP:C    | 2:C:374:THR:HG22 | 2.09                     | 0.76              |
| 2:C:415:PRO:HG3  | 1:A:448:PHE:HA   | 1.67                     | 0.76              |
| 2:D:67:PHE:O     | 2:D:71:MET:HG2   | 1.84                     | 0.76              |
| 1:A:108:ILE:HG13 | 1:A:133:GLN:HG3  | 1.67                     | 0.76              |
| 1:A:294:ASP:CG   | 1:A:325:PHE:O    | 2.28                     | 0.76              |
| 1:E:555:GLU:O    | 3:E:705:HOH:O    | 2.02                     | 0.76              |
| 1:B:81:LEU:CD2   | 1:B:87:LEU:CD1   | 2.63                     | 0.76              |
| 2:C:309:ARG:HA   | 2:C:312:ALA:HB3  | 1.66                     | 0.76              |
| 1:A:385:VAL:CG1  | 1:A:403:THR:HG23 | 2.12                     | 0.76              |
| 1:E:366:LYS:HD2  | 1:E:367:GLY:N    | 1.98                     | 0.76              |
| 1:E:565:LEU:O    | 1:E:565:LEU:HD23 | 1.84                     | 0.76              |
| 1:B:468:LEU:CD1  | 1:B:560:ARG:C    | 2.58                     | 0.76              |
| 1:B:486:ILE:HD13 | 1:B:564:ASP:C    | 2.10                     | 0.76              |
| 2:C:20:LYS:CE    | 2:C:162:VAL:O    | 2.26                     | 0.76              |
| 2:C:76:PHE:CE2   | 2:C:84:VAL:HG21  | 2.19                     | 0.76              |
| 1:A:288:PRO:HB2  | 1:A:291:SER:HB2  | 1.65                     | 0.76              |
| 1:A:368:TYR:CD1  | 1:A:372:LEU:HD21 | 2.20                     | 0.76              |
| 1:E:451:PRO:HG3  | 2:F:413:TRP:CE2  | 2.21                     | 0.76              |
| 1:E:504:ASN:O    | 1:E:509:PRO:CB   | 2.33                     | 0.76              |
| 2:F:111:PRO:HG3  | 2:F:114:LEU:HG   | 1.65                     | 0.76              |
| 1:B:388:LEU:CD2  | 1:B:406:ILE:HD11 | 2.15                     | 0.76              |
| 1:A:346:TYR:O    | 1:A:350:GLY:HA3  | 1.86                     | 0.76              |
| 1:A:565:LEU:HD13 | 1:A:570:ILE:CD1  | 2.11                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:366:LYS:HE3  | 1:B:366:LYS:HA   | 1.66                     | 0.76              |
| 1:B:432:TYR:HD2  | 1:B:526:LEU:CD1  | 1.97                     | 0.76              |
| 1:B:572:SER:H    | 1:B:575:ILE:HD11 | 1.48                     | 0.76              |
| 1:A:78:ILE:HG13  | 1:A:161:LYS:HB3  | 1.66                     | 0.76              |
| 1:E:490:PHE:CD1  | 1:E:521:THR:CG2  | 2.69                     | 0.76              |
| 1:B:532:ILE:HD12 | 1:B:539:MET:HB2  | 1.67                     | 0.76              |
| 2:C:230:PHE:HA   | 2:C:233:VAL:CG2  | 2.16                     | 0.76              |
| 2:D:125:PHE:CZ   | 2:D:150:ALA:N    | 2.46                     | 0.76              |
| 2:D:194:ARG:HH11 | 2:D:194:ARG:HG3  | 1.47                     | 0.76              |
| 1:E:71:ILE:HD12  | 1:E:71:ILE:O     | 1.85                     | 0.76              |
| 1:E:299:SER:CA   | 1:E:317:SER:HA   | 2.14                     | 0.76              |
| 2:C:305:GLN:O    | 2:C:308:ILE:N    | 2.19                     | 0.76              |
| 1:A:265:VAL:HG13 | 1:A:278:ILE:HG21 | 1.68                     | 0.76              |
| 1:A:490:PHE:CB   | 1:A:557:ILE:HG13 | 2.16                     | 0.76              |
| 1:A:573:ASN:O    | 1:A:576:VAL:HG22 | 1.84                     | 0.76              |
| 1:E:480:ARG:O    | 3:E:706:HOH:O    | 2.03                     | 0.76              |
| 1:B:502:LEU:HB3  | 1:B:509:PRO:CB   | 2.09                     | 0.76              |
| 1:E:71:ILE:HD11  | 1:E:78:ILE:HB    | 1.67                     | 0.76              |
| 1:E:361:THR:HG22 | 1:E:362:PRO:HD2  | 1.67                     | 0.76              |
| 1:E:530:HIS:O    | 2:F:418:PHE:C    | 2.28                     | 0.76              |
| 2:F:38:ARG:HH21  | 2:F:38:ARG:HG3   | 1.50                     | 0.76              |
| 2:F:354:PRO:CD   | 2:F:355:VAL:H    | 1.96                     | 0.76              |
| 1:B:171:SER:HG   | 1:B:174:ARG:HD2  | 1.49                     | 0.76              |
| 2:C:10:TRP:HB3   | 2:C:50:TYR:CZ    | 2.21                     | 0.76              |
| 1:A:125:SER:HB3  | 1:A:222:VAL:HG22 | 1.68                     | 0.76              |
| 1:A:232:ILE:CD1  | 1:A:264:LEU:CB   | 2.26                     | 0.76              |
| 1:A:322:TYR:CE2  | 1:A:324:GLY:HA2  | 2.21                     | 0.76              |
| 1:A:432:TYR:OH   | 1:A:525:ARG:HB3  | 1.86                     | 0.76              |
| 1:A:466:THR:CB   | 1:A:511:LEU:O    | 2.33                     | 0.76              |
| 1:A:533:ASP:HB3  | 1:A:538:ILE:O    | 1.85                     | 0.76              |
| 1:E:169:LEU:HD13 | 1:E:169:LEU:O    | 1.86                     | 0.76              |
| 1:B:223:ILE:HD12 | 1:B:224:LYS:N    | 2.01                     | 0.75              |
| 2:C:277:SER:O    | 2:C:281:GLU:HG3  | 1.86                     | 0.75              |
| 2:D:28:ARG:O     | 2:D:31:ILE:CG1   | 2.34                     | 0.75              |
| 1:A:393:LEU:O    | 1:A:397:ILE:HD12 | 1.85                     | 0.75              |
| 1:E:294:ASP:OD2  | 1:E:563:THR:HB   | 1.86                     | 0.75              |
| 1:B:502:LEU:HD22 | 1:B:502:LEU:N    | 2.02                     | 0.75              |
| 2:C:153:TRP:HZ2  | 2:C:157:HIS:CE1  | 2.02                     | 0.75              |
| 1:A:63:PHE:HE2   | 1:A:214:THR:CB   | 1.99                     | 0.75              |
| 1:B:305:GLN:HG3  | 1:B:309:HIS:CD2  | 2.21                     | 0.75              |
| 1:B:327:SER:HB3  | 1:B:329:LYS:CE   | 2.17                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:28:ARG:O     | 2:D:31:ILE:HG12  | 1.86                     | 0.75              |
| 1:E:164:ASN:HA   | 1:E:210:PHE:HE1  | 1.51                     | 0.75              |
| 1:B:182:LEU:HB3  | 1:B:183:PHE:CD2  | 2.21                     | 0.75              |
| 2:C:22:LEU:HD23  | 2:C:43:ALA:N     | 2.01                     | 0.75              |
| 2:C:305:GLN:HA   | 2:C:308:ILE:CB   | 2.16                     | 0.75              |
| 2:D:25:PRO:HB2   | 2:D:28:ARG:HA    | 1.67                     | 0.75              |
| 2:D:183:LEU:HD21 | 2:D:224:HIS:CB   | 2.00                     | 0.75              |
| 2:F:251:LEU:O    | 2:F:254:PRO:HD2  | 1.87                     | 0.75              |
| 1:B:103:ASP:HA   | 1:B:108:ILE:CA   | 2.17                     | 0.75              |
| 1:B:244:SER:HA   | 1:B:356:SER:OG   | 1.87                     | 0.75              |
| 1:A:245:ILE:H    | 1:A:245:ILE:HD12 | 1.49                     | 0.75              |
| 1:A:420:SER:HB3  | 1:A:423:GLN:HB3  | 1.68                     | 0.75              |
| 1:A:433:PHE:HE1  | 1:A:528:LEU:HB2  | 1.50                     | 0.75              |
| 1:A:565:LEU:HD22 | 1:A:570:ILE:CD1  | 2.15                     | 0.75              |
| 1:E:338:LEU:HD23 | 1:E:338:LEU:O    | 1.86                     | 0.75              |
| 1:B:560:ARG:NH1  | 3:B:705:HOH:O    | 2.20                     | 0.75              |
| 2:D:327:MET:O    | 2:D:331:LEU:N    | 2.20                     | 0.75              |
| 1:A:236:THR:N    | 1:A:237:GLU:OE1  | 2.20                     | 0.75              |
| 1:A:335:TYR:O    | 1:A:339:VAL:HG23 | 1.85                     | 0.75              |
| 1:A:539:MET:O    | 1:A:541:LEU:HD23 | 1.85                     | 0.75              |
| 1:E:228:TRP:HZ3  | 1:E:263:LEU:HD23 | 1.50                     | 0.75              |
| 1:B:121:PRO:CD   | 1:B:124:SER:HB3  | 2.17                     | 0.75              |
| 1:B:368:TYR:HD2  | 2:C:124:LEU:HD21 | 1.51                     | 0.75              |
| 1:B:543:ILE:CD1  | 1:B:546:PHE:CG   | 2.70                     | 0.75              |
| 2:C:232:ASN:HA   | 2:C:278:LYS:NZ   | 2.02                     | 0.75              |
| 2:D:70:LEU:HD23  | 2:D:70:LEU:O     | 1.85                     | 0.75              |
| 1:A:464:ALA:HA   | 1:A:509:PRO:HD2  | 1.68                     | 0.75              |
| 1:A:465:LEU:HD11 | 1:A:482:ILE:HG21 | 1.68                     | 0.75              |
| 2:D:269:LEU:C    | 2:D:272:ILE:HD12 | 2.11                     | 0.75              |
| 1:E:269:LEU:HD11 | 1:E:278:ILE:CG2  | 2.17                     | 0.75              |
| 2:F:331:LEU:HD21 | 2:F:343:LEU:HD23 | 1.68                     | 0.75              |
| 1:B:63:PHE:CA    | 1:B:88:ILE:HD13  | 2.15                     | 0.75              |
| 1:A:117:LYS:HD3  | 1:A:439:PHE:HZ   | 1.46                     | 0.75              |
| 1:A:286:GLY:HA2  | 1:A:326:ASN:OD1  | 1.87                     | 0.75              |
| 1:A:398:ASP:OD1  | 1:A:401:LYS:HG2  | 1.86                     | 0.75              |
| 1:E:138:SER:HA   | 1:E:139:LEU:C    | 2.11                     | 0.75              |
| 1:E:290:TYR:CE1  | 1:E:301:ILE:CD1  | 2.70                     | 0.75              |
| 1:E:310:LEU:HD22 | 1:E:310:LEU:N    | 2.02                     | 0.75              |
| 1:E:438:ASP:OD2  | 1:E:439:PHE:N    | 2.19                     | 0.75              |
| 2:F:305:GLN:O    | 2:F:309:ARG:HG2  | 1.86                     | 0.75              |
| 1:B:104:ILE:CD1  | 1:B:107:VAL:CG2  | 2.65                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:153:TRP:CE2  | 2:C:157:HIS:CD2  | 2.75                     | 0.74              |
| 2:C:257:ASN:O    | 2:C:261:HIS:N    | 2.13                     | 0.74              |
| 2:C:304:ALA:O    | 2:C:308:ILE:N    | 2.20                     | 0.74              |
| 2:D:83:THR:HA    | 2:D:86:LEU:HD12  | 1.69                     | 0.74              |
| 1:A:454:VAL:O    | 1:A:538:ILE:HG23 | 1.87                     | 0.74              |
| 1:A:465:LEU:O    | 1:A:510:LEU:HA   | 1.87                     | 0.74              |
| 1:E:321:HIS:CE1  | 1:E:522:GLU:OE1  | 2.39                     | 0.74              |
| 1:B:465:LEU:HD13 | 1:B:482:ILE:HG21 | 1.66                     | 0.74              |
| 2:D:125:PHE:CZ   | 2:D:150:ALA:CB   | 2.68                     | 0.74              |
| 1:A:119:ILE:HG13 | 1:A:309:HIS:ND1  | 2.02                     | 0.74              |
| 1:A:478:LEU:CD1  | 1:A:510:LEU:CD1  | 2.57                     | 0.74              |
| 1:E:109:TYR:HE1  | 1:E:271:PRO:HD3  | 1.49                     | 0.74              |
| 1:B:490:PHE:HB3  | 1:B:557:ILE:CB   | 2.09                     | 0.74              |
| 1:A:436:ILE:HG22 | 1:A:440:LYS:O    | 1.87                     | 0.74              |
| 1:E:530:HIS:CE1  | 1:E:570:ILE:CG2  | 2.70                     | 0.74              |
| 1:E:588:PHE:N    | 2:F:5:PRO:HB2    | 2.01                     | 0.74              |
| 2:F:20:LYS:HA    | 2:F:159:TRP:CE3  | 2.19                     | 0.74              |
| 1:B:468:LEU:CD1  | 1:B:560:ARG:O    | 2.36                     | 0.74              |
| 1:A:369:GLY:CA   | 1:A:372:LEU:HD12 | 2.12                     | 0.74              |
| 1:E:452:ILE:HD12 | 1:E:543:ILE:HG22 | 1.68                     | 0.74              |
| 2:C:235:ILE:HD11 | 2:C:278:LYS:HE2  | 0.75                     | 0.74              |
| 1:A:95:LEU:CA    | 1:A:162:LEU:HB3  | 2.16                     | 0.74              |
| 1:A:162:LEU:H    | 1:A:162:LEU:HD13 | 1.52                     | 0.74              |
| 1:E:228:TRP:CZ3  | 1:E:263:LEU:CD2  | 2.71                     | 0.74              |
| 1:E:500:CYS:CB   | 1:E:515:GLU:OE2  | 2.19                     | 0.74              |
| 1:B:454:VAL:C    | 2:D:405:LYS:CB   | 2.60                     | 0.74              |
| 2:D:115:LEU:O    | 2:D:119:ILE:HG22 | 1.88                     | 0.74              |
| 1:A:184:TRP:CZ2  | 1:A:211:TYR:CG   | 2.75                     | 0.74              |
| 1:A:322:TYR:HB2  | 1:A:523:PHE:CE1  | 2.23                     | 0.74              |
| 1:B:172:ILE:O    | 1:B:175:VAL:HG22 | 1.86                     | 0.74              |
| 2:C:153:TRP:CZ2  | 2:C:157:HIS:CG   | 2.76                     | 0.74              |
| 2:C:195:ARG:HG2  | 2:C:195:ARG:NH1  | 2.01                     | 0.74              |
| 2:F:245:TRP:O    | 2:F:248:LEU:HG   | 1.87                     | 0.74              |
| 2:C:90:MET:HE1   | 2:D:93:ILE:HD13  | 1.68                     | 0.74              |
| 2:C:305:GLN:HA   | 2:C:308:ILE:HG13 | 1.68                     | 0.74              |
| 2:D:60:LEU:HD23  | 2:D:159:TRP:CZ2  | 2.23                     | 0.74              |
| 1:A:78:ILE:CG1   | 1:A:161:LYS:CB   | 2.57                     | 0.74              |
| 1:A:95:LEU:HA    | 1:A:162:LEU:HA   | 1.68                     | 0.74              |
| 2:F:256:MET:CA   | 2:F:259:PHE:HB3  | 2.16                     | 0.74              |
| 2:F:305:GLN:O    | 2:F:309:ARG:CG   | 2.36                     | 0.74              |
| 1:B:104:ILE:HD12 | 1:B:104:ILE:N    | 2.03                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:369:GLY:HA2  | 1:B:372:LEU:HB2  | 1.69                     | 0.74              |
| 1:B:583:LEU:HD13 | 1:B:583:LEU:N    | 2.03                     | 0.74              |
| 1:E:225:HIS:O    | 1:E:228:TRP:CB   | 2.35                     | 0.74              |
| 2:F:111:PRO:CG   | 2:F:113:HIS:CE1  | 2.71                     | 0.74              |
| 1:B:121:PRO:HD2  | 1:B:124:SER:HB3  | 1.67                     | 0.73              |
| 1:B:454:VAL:CG1  | 2:D:407:PHE:HD1  | 1.93                     | 0.73              |
| 1:B:529:VAL:HG21 | 1:B:532:ILE:CD1  | 2.15                     | 0.73              |
| 2:D:22:LEU:N     | 2:D:22:LEU:HD23  | 2.03                     | 0.73              |
| 1:A:110:HIS:CB   | 1:A:140:LEU:CB   | 2.60                     | 0.73              |
| 1:A:464:ALA:CB   | 1:A:509:PRO:CB   | 2.59                     | 0.73              |
| 1:E:397:ILE:N    | 1:E:397:ILE:HD12 | 2.03                     | 0.73              |
| 2:F:316:ILE:HD11 | 2:F:346:LEU:CD2  | 2.13                     | 0.73              |
| 2:C:8:THR:HG21   | 1:A:587:THR:HG23 | 1.69                     | 0.73              |
| 2:C:249:ARG:CA   | 2:C:307:TRP:CH2  | 2.70                     | 0.73              |
| 2:C:305:GLN:CA   | 2:C:308:ILE:HD12 | 2.18                     | 0.73              |
| 2:C:410:HIS:CB   | 1:A:451:PRO:HD3  | 2.19                     | 0.73              |
| 1:E:281:MET:HG3  | 1:E:342:LEU:CD2  | 2.17                     | 0.73              |
| 1:E:348:SER:O    | 1:E:351:GLU:CD   | 2.31                     | 0.73              |
| 1:E:584:PRO:O    | 2:F:11:LYS:O     | 2.06                     | 0.73              |
| 1:B:290:TYR:N    | 1:B:311:SER:HG   | 1.75                     | 0.73              |
| 1:B:583:LEU:HD13 | 1:B:583:LEU:H    | 1.52                     | 0.73              |
| 2:D:266:ASP:C    | 2:D:268:PRO:HD2  | 2.13                     | 0.73              |
| 2:D:327:MET:C    | 2:D:330:THR:OG1  | 2.31                     | 0.73              |
| 1:A:176:CYS:CB   | 1:A:179:PHE:HD1  | 2.01                     | 0.73              |
| 1:A:325:PHE:CD2  | 1:A:330:ASP:CB   | 2.70                     | 0.73              |
| 1:A:440:LYS:C    | 1:A:441:PHE:HD2  | 1.96                     | 0.73              |
| 1:A:451:PRO:C    | 1:A:541:LEU:O    | 2.29                     | 0.73              |
| 1:E:406:ILE:N    | 1:E:406:ILE:HD13 | 2.03                     | 0.73              |
| 2:F:115:LEU:O    | 2:F:119:ILE:HG13 | 1.87                     | 0.73              |
| 2:F:121:LEU:HD12 | 2:F:122:PRO:CD   | 2.18                     | 0.73              |
| 2:D:24:PHE:CE1   | 2:D:67:PHE:CZ    | 2.65                     | 0.73              |
| 2:D:276:LEU:CG   | 2:D:333:LYS:CB   | 2.66                     | 0.73              |
| 1:A:540:ASN:O    | 1:A:541:LEU:HD23 | 1.88                     | 0.73              |
| 1:E:107:VAL:CG2  | 1:E:266:GLN:HE21 | 2.01                     | 0.73              |
| 2:F:158:TYR:CD1  | 2:F:159:TRP:CD1  | 2.71                     | 0.73              |
| 2:F:248:LEU:O    | 2:F:252:PHE:N    | 2.21                     | 0.73              |
| 2:F:336:HIS:CB   | 2:F:339:ASN:HB2  | 2.19                     | 0.73              |
| 1:B:233:LYS:O    | 1:B:236:THR:OG1  | 2.06                     | 0.73              |
| 1:B:366:LYS:CE   | 1:B:367:GLY:H    | 2.01                     | 0.73              |
| 1:A:169:LEU:HD21 | 1:A:441:PHE:HE1  | 1.51                     | 0.73              |
| 1:A:232:ILE:HD11 | 1:A:264:LEU:HG   | 1.67                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:434:HIS:NE2  | 1:A:446:LEU:HD11 | 2.02                     | 0.73              |
| 1:A:304:VAL:HG23 | 1:A:306:HIS:HD2  | 1.51                     | 0.73              |
| 1:A:374:ARG:HG3  | 1:A:375:THR:N    | 2.03                     | 0.73              |
| 1:A:490:PHE:CZ   | 1:A:523:PHE:HD1  | 2.03                     | 0.73              |
| 1:E:572:SER:H    | 1:E:575:ILE:HG13 | 1.52                     | 0.73              |
| 2:F:262:LEU:HD13 | 2:F:262:LEU:O    | 1.89                     | 0.73              |
| 1:B:111:SER:OG   | 1:B:141:GLU:C    | 2.32                     | 0.73              |
| 1:A:107:VAL:HG21 | 1:A:109:TYR:OH   | 1.89                     | 0.73              |
| 1:A:427:LEU:O    | 1:A:427:LEU:HD23 | 1.88                     | 0.73              |
| 1:E:185:GLN:HG2  | 1:E:187:ASP:OD2  | 1.87                     | 0.73              |
| 1:E:365:ILE:CD1  | 1:E:393:LEU:CD1  | 2.67                     | 0.73              |
| 1:E:519:LEU:HD23 | 1:E:519:LEU:N    | 2.02                     | 0.73              |
| 2:F:248:LEU:HA   | 2:F:251:LEU:HB2  | 1.69                     | 0.73              |
| 1:B:126:ILE:N    | 1:B:126:ILE:HD13 | 2.04                     | 0.73              |
| 1:B:252:GLY:H    | 1:B:255:SER:HG   | 1.33                     | 0.73              |
| 1:A:296:ILE:CG2  | 1:A:342:LEU:CD2  | 2.66                     | 0.73              |
| 1:A:491:LYS:HB3  | 1:A:491:LYS:NZ   | 2.03                     | 0.73              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:CA   | 2.67                     | 0.73              |
| 1:E:447:LEU:CD1  | 1:E:575:ILE:CG2  | 2.66                     | 0.73              |
| 1:B:172:ILE:CD1  | 1:B:179:PHE:CB   | 2.46                     | 0.73              |
| 1:B:250:ILE:HG21 | 1:B:365:ILE:HD12 | 1.69                     | 0.73              |
| 1:B:328:PRO:CB   | 1:B:335:TYR:CE2  | 2.69                     | 0.73              |
| 1:A:245:ILE:HD12 | 1:A:245:ILE:N    | 2.04                     | 0.73              |
| 1:E:95:LEU:HD21  | 1:E:116:MET:HG3  | 1.70                     | 0.73              |
| 1:E:290:TYR:CD1  | 1:E:301:ILE:HD11 | 2.23                     | 0.73              |
| 1:E:341:GLN:HG3  | 1:E:342:LEU:N    | 2.04                     | 0.73              |
| 2:F:14:ASP:OD1   | 2:F:14:ASP:N     | 2.22                     | 0.73              |
| 2:F:328:ILE:HD12 | 2:F:328:ILE:N    | 2.03                     | 0.73              |
| 1:B:102:ILE:O    | 1:B:108:ILE:HA   | 1.89                     | 0.73              |
| 1:E:72:TYR:HE2   | 1:E:206:SER:OG   | 1.72                     | 0.73              |
| 1:E:95:LEU:O     | 1:E:95:LEU:HD23  | 1.88                     | 0.73              |
| 1:E:329:LYS:O    | 1:E:332:PRO:HD3  | 1.89                     | 0.73              |
| 1:E:531:SER:C    | 1:E:540:ASN:HD21 | 1.97                     | 0.73              |
| 1:B:182:LEU:CD1  | 1:B:183:PHE:HE2  | 1.99                     | 0.72              |
| 1:A:108:ILE:CG1  | 1:A:133:GLN:HG3  | 2.18                     | 0.72              |
| 1:B:92:GLN:HB3   | 1:B:119:ILE:HD12 | 1.71                     | 0.72              |
| 1:B:496:HIS:CB   | 1:B:519:LEU:CD2  | 2.68                     | 0.72              |
| 1:B:595:GLU:C    | 1:B:596:LYS:HD2  | 2.14                     | 0.72              |
| 1:A:72:TYR:CE2   | 1:A:206:SER:OG   | 2.42                     | 0.72              |
| 1:A:213:ILE:HD12 | 1:A:219:THR:OG1  | 1.89                     | 0.72              |
| 1:A:483:GLU:HA   | 1:A:529:VAL:HG11 | 1.70                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:346:TYR:O    | 1:E:350:GLY:N    | 2.22                     | 0.72              |
| 1:A:571:ALA:HA   | 1:A:575:ILE:HG13 | 1.70                     | 0.72              |
| 1:E:486:ILE:CD1  | 1:E:564:ASP:O    | 2.37                     | 0.72              |
| 2:F:20:LYS:NZ    | 2:F:162:VAL:C    | 2.46                     | 0.72              |
| 2:F:354:PRO:O    | 2:F:358:ASP:OD1  | 2.07                     | 0.72              |
| 1:B:533:ASP:OD1  | 1:B:535:GLU:N    | 2.23                     | 0.72              |
| 2:C:308:ILE:O    | 2:C:312:ALA:N    | 2.22                     | 0.72              |
| 1:A:310:LEU:HD22 | 1:A:310:LEU:N    | 2.04                     | 0.72              |
| 1:A:456:TYR:CB   | 1:A:537:LYS:C    | 2.62                     | 0.72              |
| 1:A:464:ALA:HA   | 1:A:509:PRO:CG   | 2.19                     | 0.72              |
| 1:E:571:ALA:HB2  | 1:E:586:ILE:HD13 | 1.65                     | 0.72              |
| 1:B:211:TYR:CD1  | 1:B:212:PRO:HD2  | 2.25                     | 0.72              |
| 1:B:305:GLN:CG   | 1:B:309:HIS:CD2  | 2.72                     | 0.72              |
| 2:C:22:LEU:HD22  | 2:C:43:ALA:HA    | 1.69                     | 0.72              |
| 2:C:186:LEU:HD13 | 2:C:224:HIS:CB   | 2.20                     | 0.72              |
| 1:A:304:VAL:HG23 | 1:A:306:HIS:CD2  | 2.24                     | 0.72              |
| 1:E:184:TRP:CH2  | 1:E:211:TYR:HB3  | 2.23                     | 0.72              |
| 1:E:252:GLY:O    | 1:E:255:SER:OG   | 2.05                     | 0.72              |
| 1:E:292:GLY:O    | 1:E:295:CYS:HB2  | 1.89                     | 0.72              |
| 1:E:364:TRP:HB3  | 1:E:369:GLY:CA   | 2.07                     | 0.72              |
| 1:E:453:GLN:O    | 2:F:407:PHE:CA   | 2.38                     | 0.72              |
| 2:F:20:LYS:HZ1   | 2:F:162:VAL:CA   | 2.02                     | 0.72              |
| 2:F:110:ILE:HD12 | 2:F:110:ILE:C    | 2.14                     | 0.72              |
| 2:F:118:LYS:HB2  | 2:F:118:LYS:HZ2  | 1.54                     | 0.72              |
| 2:D:186:LEU:HB3  | 2:D:221:ILE:HG12 | 1.72                     | 0.72              |
| 1:A:376:LEU:HD13 | 1:A:376:LEU:C    | 2.15                     | 0.72              |
| 1:A:434:HIS:NE2  | 1:A:446:LEU:CD1  | 2.53                     | 0.72              |
| 1:A:491:LYS:HB3  | 1:A:491:LYS:HZ2  | 1.54                     | 0.72              |
| 1:E:284:ASP:CG   | 1:E:287:GLN:H    | 1.93                     | 0.72              |
| 2:F:262:LEU:HD13 | 2:F:262:LEU:C    | 2.14                     | 0.72              |
| 1:B:510:LEU:C    | 1:B:510:LEU:HD23 | 2.15                     | 0.72              |
| 2:C:94:ARG:HG3   | 1:A:598:TRP:HH2  | 1.55                     | 0.72              |
| 2:D:331:LEU:HA   | 2:D:346:LEU:CD1  | 2.20                     | 0.72              |
| 1:A:283:LEU:HD22 | 1:A:339:VAL:HG13 | 1.72                     | 0.72              |
| 1:E:178:LEU:C    | 1:E:178:LEU:HD23 | 2.15                     | 0.72              |
| 1:E:364:TRP:CZ3  | 1:E:368:TYR:HD1  | 2.07                     | 0.72              |
| 1:B:320:CYS:O    | 1:B:321:HIS:ND1  | 2.22                     | 0.72              |
| 2:D:257:ASN:HD21 | 2:D:261:HIS:CD2  | 2.08                     | 0.72              |
| 1:E:110:HIS:CD2  | 1:E:137:SER:O    | 2.42                     | 0.72              |
| 1:E:269:LEU:HD11 | 1:E:278:ILE:HG22 | 1.70                     | 0.72              |
| 1:E:281:MET:SD   | 1:E:342:LEU:HD23 | 2.29                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:129:ARG:O    | 2:C:133:THR:N    | 2.20                     | 0.72              |
| 2:C:156:ASP:HA   | 2:C:160:ASP:OD1  | 1.90                     | 0.72              |
| 1:A:207:ASP:O    | 3:A:704:HOH:O    | 2.07                     | 0.72              |
| 1:A:368:TYR:CD1  | 1:A:372:LEU:CG   | 2.72                     | 0.72              |
| 1:A:493:LYS:O    | 1:A:496:HIS:HB2  | 1.90                     | 0.72              |
| 1:B:103:ASP:O    | 1:B:130:GLN:HB2  | 1.90                     | 0.71              |
| 2:D:361:GLN:O    | 2:D:365:THR:HG23 | 1.89                     | 0.71              |
| 1:A:365:ILE:O    | 1:A:393:LEU:HD21 | 1.90                     | 0.71              |
| 1:A:399:ILE:C    | 1:A:399:ILE:HD12 | 2.15                     | 0.71              |
| 1:E:182:LEU:HB3  | 1:E:183:PHE:CD2  | 2.25                     | 0.71              |
| 1:B:167:THR:CA   | 1:B:439:PHE:O    | 2.38                     | 0.71              |
| 1:B:475:MET:O    | 1:B:478:LEU:CD2  | 2.38                     | 0.71              |
| 2:C:10:TRP:HA    | 2:C:50:TYR:HE1   | 1.54                     | 0.71              |
| 2:D:70:LEU:HD23  | 2:D:70:LEU:C     | 2.15                     | 0.71              |
| 1:A:184:TRP:HH2  | 1:A:211:TYR:CD2  | 1.96                     | 0.71              |
| 1:E:405:LEU:HD23 | 1:E:405:LEU:C    | 2.15                     | 0.71              |
| 1:E:427:LEU:HD23 | 1:E:427:LEU:C    | 2.15                     | 0.71              |
| 1:B:104:ILE:HG22 | 1:B:128:LEU:C    | 2.12                     | 0.71              |
| 1:B:346:TYR:CB   | 1:B:357:LEU:HD21 | 2.20                     | 0.71              |
| 1:B:528:LEU:HD12 | 1:B:528:LEU:C    | 2.15                     | 0.71              |
| 1:B:586:ILE:HD13 | 1:B:586:ILE:N    | 2.03                     | 0.71              |
| 2:C:274:SER:O    | 2:C:278:LYS:CG   | 2.38                     | 0.71              |
| 1:A:169:LEU:HD23 | 1:A:441:PHE:CE1  | 2.15                     | 0.71              |
| 1:A:370:LEU:HD12 | 1:A:370:LEU:C    | 2.15                     | 0.71              |
| 1:E:466:THR:HG21 | 1:E:516:PHE:HD2  | 1.48                     | 0.71              |
| 1:B:182:LEU:HB3  | 1:B:183:PHE:HD2  | 1.55                     | 0.71              |
| 1:E:93:PHE:HB2   | 1:E:210:PHE:CD1  | 2.24                     | 0.71              |
| 1:E:567:ILE:O    | 1:E:570:ILE:HD13 | 1.90                     | 0.71              |
| 2:F:111:PRO:CG   | 2:F:113:HIS:HE1  | 2.03                     | 0.71              |
| 1:B:276:LEU:HD22 | 1:B:276:LEU:N    | 2.05                     | 0.71              |
| 1:B:331:GLN:HE22 | 1:B:468:LEU:HB3  | 1.54                     | 0.71              |
| 1:B:598:TRP:CH2  | 2:D:98:GLY:CA    | 2.74                     | 0.71              |
| 2:C:40:TYR:CD2   | 2:C:67:PHE:CD1   | 2.79                     | 0.71              |
| 1:A:328:PRO:HB3  | 1:A:335:TYR:CE2  | 2.25                     | 0.71              |
| 1:E:586:ILE:CG2  | 2:F:6:ARG:O      | 2.36                     | 0.71              |
| 1:B:343:VAL:O    | 1:B:347:GLU:N    | 2.21                     | 0.71              |
| 2:D:234:MET:O    | 2:D:237:ARG:N    | 2.23                     | 0.71              |
| 2:D:331:LEU:HD23 | 2:D:346:LEU:HD12 | 1.67                     | 0.71              |
| 1:E:232:ILE:HG12 | 1:E:264:LEU:HA   | 1.71                     | 0.71              |
| 1:E:366:LYS:CD   | 1:E:367:GLY:H    | 2.00                     | 0.71              |
| 1:B:373:THR:O    | 1:B:377:ILE:HG13 | 1.91                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:87:LEU:HD13  | 1:B:160:ILE:CD1  | 1.98                     | 0.71              |
| 1:B:594:LEU:O    | 2:D:59:ILE:CG1   | 2.37                     | 0.71              |
| 2:C:11:LYS:HB2   | 1:A:585:TYR:CZ   | 2.12                     | 0.71              |
| 1:E:164:ASN:OD1  | 1:E:209:THR:CG2  | 2.34                     | 0.71              |
| 2:F:22:LEU:HB3   | 2:F:43:ALA:HB2   | 1.72                     | 0.71              |
| 2:F:217:CYS:O    | 2:F:221:ILE:HG13 | 1.89                     | 0.71              |
| 1:B:531:SER:C    | 1:B:532:ILE:HD13 | 2.16                     | 0.71              |
| 2:C:36:LEU:O     | 2:C:40:TYR:CD1   | 2.44                     | 0.71              |
| 2:D:214:TYR:HA   | 2:D:217:CYS:SG   | 2.30                     | 0.71              |
| 2:F:117:LYS:C    | 2:F:117:LYS:HD3  | 2.15                     | 0.71              |
| 1:B:383:THR:CG2  | 1:B:384:HIS:NE2  | 2.54                     | 0.70              |
| 2:C:125:PHE:HE1  | 2:C:146:CYS:HG   | 1.39                     | 0.70              |
| 1:A:71:ILE:H     | 1:A:71:ILE:CD1   | 2.04                     | 0.70              |
| 1:A:383:THR:C    | 1:A:384:HIS:HD1  | 1.96                     | 0.70              |
| 1:B:224:LYS:HG3  | 1:B:228:TRP:CE3  | 2.26                     | 0.70              |
| 2:D:89:SER:OG    | 2:D:128:PHE:CE1  | 2.43                     | 0.70              |
| 1:A:160:ILE:C    | 1:A:160:ILE:HD12 | 2.17                     | 0.70              |
| 1:A:169:LEU:HD12 | 1:A:183:PHE:CZ   | 2.25                     | 0.70              |
| 1:E:432:TYR:OH   | 1:E:525:ARG:HG2  | 1.91                     | 0.70              |
| 1:B:81:LEU:HD21  | 1:B:87:LEU:HG    | 1.73                     | 0.70              |
| 1:B:172:ILE:CD1  | 1:B:179:PHE:C    | 2.65                     | 0.70              |
| 2:C:369:ARG:O    | 2:C:373:ASP:OD1  | 2.08                     | 0.70              |
| 1:A:331:GLN:CB   | 1:A:334:ARG:HB2  | 2.21                     | 0.70              |
| 1:E:172:ILE:CD1  | 1:E:183:PHE:CE2  | 2.62                     | 0.70              |
| 1:E:225:HIS:HB2  | 1:E:228:TRP:H    | 1.55                     | 0.70              |
| 1:E:235:LEU:HD13 | 1:E:247:VAL:HG21 | 1.73                     | 0.70              |
| 1:E:318:THR:HG22 | 1:E:319:GLN:CD   | 2.15                     | 0.70              |
| 1:E:363:GLY:HA2  | 3:E:708:HOH:O    | 1.87                     | 0.70              |
| 2:F:111:PRO:HG2  | 2:F:114:LEU:CG   | 2.21                     | 0.70              |
| 1:B:169:LEU:O    | 1:B:170:GLU:HB3  | 1.91                     | 0.70              |
| 2:C:310:TRP:CH2  | 2:C:314:GLU:OE1  | 2.44                     | 0.70              |
| 1:A:165:LEU:HD13 | 1:A:165:LEU:C    | 2.16                     | 0.70              |
| 1:A:175:VAL:C    | 1:A:568:TRP:HD1  | 1.97                     | 0.70              |
| 1:A:246:LYS:O    | 1:A:382:PRO:C    | 2.28                     | 0.70              |
| 1:E:78:ILE:CG1   | 1:E:161:LYS:HG3  | 2.20                     | 0.70              |
| 1:E:169:LEU:HD12 | 1:E:183:PHE:CD1  | 2.25                     | 0.70              |
| 1:E:364:TRP:HE3  | 1:E:369:GLY:HA2  | 1.56                     | 0.70              |
| 1:B:77:VAL:HG11  | 1:B:79:PHE:CZ    | 2.26                     | 0.70              |
| 2:C:48:GLU:OE2   | 2:D:80:LEU:CD2   | 2.39                     | 0.70              |
| 2:C:71:MET:O     | 2:C:75:SER:OG    | 2.07                     | 0.70              |
| 2:C:84:VAL:O     | 3:C:502:HOH:O    | 2.08                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:ILE:HG21 | 1:A:179:PHE:HB3  | 0.73                     | 0.70              |
| 1:A:525:ARG:HD3  | 1:A:544:PRO:HG2  | 1.72                     | 0.70              |
| 1:A:530:HIS:CD2  | 1:A:531:SER:HB3  | 2.26                     | 0.70              |
| 1:A:565:LEU:HD22 | 1:A:570:ILE:HD11 | 1.72                     | 0.70              |
| 1:E:365:ILE:C    | 1:E:365:ILE:HD12 | 2.16                     | 0.70              |
| 1:E:405:LEU:C    | 1:E:406:ILE:HD13 | 2.16                     | 0.70              |
| 2:F:273:ASP:CG   | 2:F:330:THR:CG2  | 2.60                     | 0.70              |
| 1:B:92:GLN:HB3   | 1:B:119:ILE:CD1  | 2.21                     | 0.70              |
| 1:E:490:PHE:HD1  | 1:E:521:THR:HG22 | 1.56                     | 0.70              |
| 2:D:6:ARG:HG3    | 2:D:6:ARG:NH1    | 2.05                     | 0.70              |
| 1:A:95:LEU:HA    | 1:A:162:LEU:CB   | 2.21                     | 0.70              |
| 1:A:162:LEU:HD13 | 1:A:162:LEU:N    | 2.05                     | 0.70              |
| 1:A:420:SER:O    | 1:A:423:GLN:N    | 2.24                     | 0.70              |
| 2:F:312:ALA:HB1  | 2:F:342:LEU:CD2  | 2.18                     | 0.70              |
| 1:B:598:TRP:HE3  | 2:D:58:HIS:CE1   | 2.09                     | 0.70              |
| 2:C:125:PHE:HE1  | 2:C:146:CYS:SG   | 2.15                     | 0.70              |
| 1:A:111:SER:HB2  | 1:A:141:GLU:N    | 2.07                     | 0.70              |
| 1:A:371:GLU:O    | 1:A:375:THR:OG1  | 2.10                     | 0.70              |
| 1:E:103:ASP:CG   | 1:E:132:THR:OG1  | 2.34                     | 0.70              |
| 1:E:360:ASN:OD1  | 1:E:361:THR:N    | 2.25                     | 0.70              |
| 2:F:328:ILE:H    | 2:F:328:ILE:CD1  | 2.00                     | 0.70              |
| 2:D:140:LEU:C    | 2:D:140:LEU:HD23 | 2.16                     | 0.70              |
| 1:E:435:LYS:HB3  | 1:E:441:PHE:CE1  | 2.27                     | 0.70              |
| 1:E:501:GLU:CB   | 1:E:502:LEU:HA   | 2.20                     | 0.70              |
| 1:E:571:ALA:HB2  | 1:E:586:ILE:HD11 | 1.70                     | 0.70              |
| 2:F:111:PRO:O    | 2:F:115:LEU:CD1  | 2.39                     | 0.70              |
| 2:C:65:HIS:CG    | 2:C:94:ARG:NH2   | 2.52                     | 0.70              |
| 1:A:322:TYR:CB   | 1:A:523:PHE:CE1  | 2.75                     | 0.70              |
| 1:A:389:ASN:HD21 | 1:A:408:LEU:CB   | 2.05                     | 0.70              |
| 1:E:364:TRP:CZ3  | 1:E:368:TYR:CD1  | 2.80                     | 0.70              |
| 1:E:451:PRO:CG   | 2:F:413:TRP:CE2  | 2.75                     | 0.70              |
| 2:F:22:LEU:HG    | 2:F:39:GLN:HB3   | 1.72                     | 0.70              |
| 2:F:38:ARG:HG3   | 2:F:38:ARG:NH2   | 2.04                     | 0.70              |
| 2:F:234:MET:CE   | 2:F:271:LEU:CD1  | 2.45                     | 0.70              |
| 1:B:420:SER:O    | 1:B:423:GLN:HG3  | 1.92                     | 0.69              |
| 1:B:456:TYR:OH   | 1:B:537:LYS:HA   | 1.90                     | 0.69              |
| 1:A:483:GLU:CG   | 1:A:532:ILE:HD12 | 2.22                     | 0.69              |
| 1:A:224:LYS:HG2  | 1:A:228:TRP:CZ3  | 2.26                     | 0.69              |
| 1:A:565:LEU:CD2  | 1:A:570:ILE:HD11 | 2.22                     | 0.69              |
| 1:E:438:ASP:CG   | 1:E:439:PHE:HD1  | 2.00                     | 0.69              |
| 2:F:237:ARG:CA   | 2:F:240:SER:HB2  | 2.18                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:481:SER:HA   | 2:D:53:ARG:HH11  | 1.56                     | 0.69              |
| 1:B:490:PHE:CG   | 1:B:557:ILE:HG21 | 2.27                     | 0.69              |
| 2:D:218:ILE:HA   | 2:D:221:ILE:HD12 | 1.74                     | 0.69              |
| 2:D:327:MET:HA   | 2:D:330:THR:CB   | 2.17                     | 0.69              |
| 1:A:165:LEU:HD13 | 1:A:166:ASP:C    | 2.16                     | 0.69              |
| 1:A:408:LEU:HD13 | 1:A:408:LEU:N    | 2.01                     | 0.69              |
| 1:A:454:VAL:HG21 | 1:A:541:LEU:HD11 | 1.74                     | 0.69              |
| 1:E:85:GLN:CB    | 1:E:131:ALA:CA   | 2.70                     | 0.69              |
| 1:E:230:ASP:OD1  | 1:E:234:SER:HB2  | 1.92                     | 0.69              |
| 1:B:432:TYR:CD2  | 1:B:526:LEU:CD1  | 2.76                     | 0.69              |
| 2:D:77:GLU:N     | 2:D:77:GLU:OE2   | 2.25                     | 0.69              |
| 2:D:125:PHE:CZ   | 2:D:150:ALA:HA   | 2.28                     | 0.69              |
| 1:A:81:LEU:O     | 1:A:157:LYS:CB   | 2.40                     | 0.69              |
| 1:A:278:ILE:HD13 | 1:A:278:ILE:C    | 2.16                     | 0.69              |
| 1:A:508:LEU:HD12 | 1:A:509:PRO:HD3  | 1.74                     | 0.69              |
| 2:F:234:MET:HE3  | 2:F:271:LEU:HD11 | 0.80                     | 0.69              |
| 1:B:72:TYR:OH    | 1:B:205:PHE:CA   | 2.38                     | 0.69              |
| 1:B:586:ILE:CG2  | 2:D:6:ARG:O      | 2.39                     | 0.69              |
| 2:C:153:TRP:CZ2  | 2:C:157:HIS:NE2  | 2.60                     | 0.69              |
| 2:C:181:LYS:O    | 2:C:185:ASP:N    | 2.24                     | 0.69              |
| 2:C:271:LEU:CD1  | 2:C:275:MET:CE   | 2.67                     | 0.69              |
| 2:D:149:ARG:NH1  | 2:D:149:ARG:HB3  | 2.08                     | 0.69              |
| 1:E:77:VAL:HG11  | 1:E:79:PHE:CZ    | 2.27                     | 0.69              |
| 1:E:451:PRO:HD3  | 2:F:413:TRP:CE2  | 2.27                     | 0.69              |
| 1:B:225:HIS:HD2  | 1:B:228:TRP:HE3  | 1.40                     | 0.69              |
| 1:B:380:VAL:CG1  | 1:B:382:PRO:HD3  | 2.23                     | 0.69              |
| 2:D:24:PHE:CD2   | 2:D:155:TRP:NE1  | 2.59                     | 0.69              |
| 1:E:233:LYS:HZ1  | 1:E:237:GLU:HB2  | 1.58                     | 0.69              |
| 1:E:301:ILE:HG12 | 1:E:315:THR:HG21 | 1.75                     | 0.69              |
| 1:B:326:ASN:HD22 | 1:B:326:ASN:N    | 1.91                     | 0.69              |
| 2:D:54:THR:HG22  | 2:D:55:ARG:N     | 2.08                     | 0.69              |
| 2:D:129:ARG:O    | 2:D:133:THR:OG1  | 2.06                     | 0.69              |
| 1:A:76:TYR:HD2   | 1:A:78:ILE:HD13  | 1.58                     | 0.69              |
| 1:A:95:LEU:HB2   | 1:A:162:LEU:HB3  | 1.72                     | 0.69              |
| 1:A:401:LYS:HA   | 1:A:401:LYS:HZ2  | 1.56                     | 0.69              |
| 1:A:525:ARG:HB3  | 1:A:525:ARG:HH21 | 1.57                     | 0.69              |
| 1:E:172:ILE:O    | 1:E:175:VAL:HG22 | 1.91                     | 0.69              |
| 1:E:440:LYS:HB2  | 1:E:440:LYS:HZ2  | 1.56                     | 0.69              |
| 1:B:366:LYS:HA   | 1:B:366:LYS:CE   | 2.19                     | 0.69              |
| 1:B:465:LEU:CD2  | 1:B:466:THR:N    | 2.48                     | 0.69              |
| 1:B:486:ILE:HD11 | 1:B:563:THR:C    | 2.17                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:529:VAL:CG2  | 1:B:532:ILE:HD11 | 2.18                     | 0.69              |
| 2:D:149:ARG:NE   | 2:D:149:ARG:HA   | 2.07                     | 0.69              |
| 1:A:130:GLN:HB3  | 1:A:132:THR:HG23 | 1.74                     | 0.69              |
| 1:E:524:PHE:CE2  | 1:E:543:ILE:CD1  | 2.72                     | 0.69              |
| 2:F:215:TRP:HA   | 2:F:215:TRP:CE3  | 2.26                     | 0.69              |
| 1:B:388:LEU:HD21 | 1:B:406:ILE:HD11 | 1.75                     | 0.69              |
| 2:C:90:MET:SD    | 2:D:93:ILE:HD12  | 2.31                     | 0.69              |
| 2:C:249:ARG:CA   | 2:C:307:TRP:HH2  | 2.04                     | 0.69              |
| 2:C:415:PRO:C    | 2:C:416:LYS:HD2  | 2.18                     | 0.69              |
| 2:F:7:LEU:HD23   | 2:F:7:LEU:O      | 1.93                     | 0.68              |
| 1:B:447:LEU:O    | 1:B:542:TYR:OH   | 2.10                     | 0.68              |
| 2:C:148:ASP:C    | 2:C:151:ILE:HG22 | 2.17                     | 0.68              |
| 2:D:81:ASP:OD2   | 2:D:85:ARG:NH2   | 2.27                     | 0.68              |
| 1:A:350:GLY:C    | 1:A:357:LEU:HD11 | 2.16                     | 0.68              |
| 1:E:92:GLN:OE1   | 1:E:167:THR:HG21 | 1.92                     | 0.68              |
| 1:E:322:TYR:HB3  | 1:E:490:PHE:HZ   | 1.57                     | 0.68              |
| 1:E:324:GLY:C    | 1:E:325:PHE:HD1  | 2.00                     | 0.68              |
| 1:B:76:TYR:HB3   | 1:B:163:THR:HA   | 1.76                     | 0.68              |
| 1:B:90:LYS:HE3   | 1:B:213:ILE:HD11 | 1.74                     | 0.68              |
| 2:C:409:SER:HB3  | 1:A:450:PRO:CB   | 2.22                     | 0.68              |
| 1:A:304:VAL:CG2  | 1:A:306:HIS:CD2  | 2.77                     | 0.68              |
| 1:A:456:TYR:CA   | 1:A:537:LYS:CB   | 2.70                     | 0.68              |
| 1:E:524:PHE:CE2  | 1:E:525:ARG:HB2  | 2.27                     | 0.68              |
| 1:E:567:ILE:CG2  | 1:E:571:ALA:HB3  | 2.23                     | 0.68              |
| 1:B:310:LEU:HB3  | 1:B:428:LYS:CG   | 2.22                     | 0.68              |
| 2:D:88:ALA:O     | 2:D:92:ILE:HG13  | 1.92                     | 0.68              |
| 1:B:276:LEU:HD22 | 1:B:276:LEU:H    | 1.57                     | 0.68              |
| 2:C:232:ASN:HA   | 2:C:235:ILE:HD11 | 1.75                     | 0.68              |
| 2:D:190:TYR:CD2  | 2:D:218:ILE:HG23 | 2.27                     | 0.68              |
| 2:D:194:ARG:HG3  | 2:D:194:ARG:NH1  | 2.06                     | 0.68              |
| 2:F:419:GLY:O    | 2:F:420:VAL:HG22 | 1.93                     | 0.68              |
| 1:B:366:LYS:HE2  | 1:B:367:GLY:N    | 2.09                     | 0.68              |
| 2:C:90:MET:CE    | 2:D:93:ILE:CD1   | 2.71                     | 0.68              |
| 2:C:260:ILE:HD12 | 2:C:268:PRO:HD3  | 1.75                     | 0.68              |
| 1:A:368:TYR:CD1  | 1:A:372:LEU:CD2  | 2.75                     | 0.68              |
| 1:E:366:LYS:HB2  | 1:E:393:LEU:CD1  | 2.24                     | 0.68              |
| 1:B:465:LEU:HD23 | 1:B:465:LEU:C    | 2.19                     | 0.68              |
| 1:B:595:GLU:O    | 1:B:596:LYS:HG3  | 1.94                     | 0.68              |
| 2:D:116:ALA:CA   | 2:D:119:ILE:HG22 | 2.23                     | 0.68              |
| 2:D:269:LEU:CA   | 2:D:272:ILE:HD12 | 2.24                     | 0.68              |
| 1:E:88:ILE:HG23  | 1:E:128:LEU:HD23 | 1.75                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:118:PHE:CD1  | 1:B:306:HIS:HB2  | 2.27                     | 0.68              |
| 1:A:269:LEU:HD23 | 1:A:278:ILE:HG22 | 1.76                     | 0.68              |
| 1:A:297:SER:HB3  | 1:A:319:GLN:O    | 1.94                     | 0.68              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:N    | 2.56                     | 0.68              |
| 2:F:251:LEU:O    | 2:F:255:MET:HE2  | 1.94                     | 0.68              |
| 2:C:28:ARG:CA    | 2:C:29:GLU:OE2   | 2.42                     | 0.68              |
| 2:C:86:LEU:HD22  | 2:D:91:THR:OG1   | 1.94                     | 0.68              |
| 2:C:153:TRP:HZ2  | 2:C:157:HIS:NE2  | 1.91                     | 0.68              |
| 1:A:170:GLU:HB2  | 1:A:185:GLN:CD   | 2.18                     | 0.68              |
| 1:A:350:GLY:HA3  | 1:A:357:LEU:CD1  | 2.20                     | 0.68              |
| 1:E:93:PHE:CB    | 1:E:210:PHE:HD1  | 2.00                     | 0.68              |
| 1:E:405:LEU:HD23 | 1:E:405:LEU:O    | 1.94                     | 0.68              |
| 1:E:565:LEU:HD23 | 1:E:565:LEU:C    | 2.17                     | 0.68              |
| 1:E:567:ILE:N    | 1:E:567:ILE:HD12 | 2.09                     | 0.68              |
| 1:B:358:LEU:C    | 1:B:359:ILE:HG13 | 2.19                     | 0.68              |
| 1:B:377:ILE:O    | 1:B:382:PRO:HD2  | 1.94                     | 0.68              |
| 1:B:584:PRO:HG3  | 2:D:417:PRO:O    | 1.93                     | 0.68              |
| 1:A:294:ASP:C    | 1:A:323:VAL:HG22 | 2.18                     | 0.68              |
| 1:A:486:ILE:HD12 | 1:A:564:ASP:O    | 1.93                     | 0.68              |
| 1:E:226:LYS:HA   | 1:E:229:MET:CB   | 2.23                     | 0.68              |
| 1:E:299:SER:CB   | 1:E:317:SER:CA   | 2.65                     | 0.68              |
| 2:F:220:GLY:O    | 2:F:224:HIS:HD2  | 1.71                     | 0.68              |
| 1:B:483:GLU:O    | 1:B:485:THR:HG23 | 1.92                     | 0.67              |
| 1:B:496:HIS:CB   | 1:B:519:LEU:HD22 | 2.24                     | 0.67              |
| 2:C:305:GLN:HA   | 2:C:308:ILE:HB   | 1.75                     | 0.67              |
| 2:D:362:ALA:O    | 2:D:365:THR:OG1  | 2.11                     | 0.67              |
| 1:A:175:VAL:C    | 1:A:568:TRP:CD1  | 2.72                     | 0.67              |
| 1:A:325:PHE:CD2  | 1:A:562:ASN:HB2  | 2.30                     | 0.67              |
| 1:A:539:MET:O    | 1:A:541:LEU:HD21 | 1.95                     | 0.67              |
| 2:F:237:ARG:NE   | 2:F:240:SER:HB2  | 2.09                     | 0.67              |
| 1:B:533:ASP:OD1  | 1:B:536:LYS:N    | 2.25                     | 0.67              |
| 2:C:271:LEU:O    | 2:C:275:MET:CG   | 2.42                     | 0.67              |
| 2:C:416:LYS:HD2  | 2:C:416:LYS:N    | 2.10                     | 0.67              |
| 1:A:169:LEU:CD2  | 1:A:441:PHE:HD1  | 1.69                     | 0.67              |
| 1:A:285:PRO:HB3  | 1:A:323:VAL:HG21 | 1.76                     | 0.67              |
| 1:E:290:TYR:HE1  | 1:E:301:ILE:CD1  | 2.07                     | 0.67              |
| 2:F:10:TRP:N     | 2:F:50:TYR:CE2   | 2.62                     | 0.67              |
| 1:B:523:PHE:CZ   | 1:B:525:ARG:C    | 2.72                     | 0.67              |
| 1:A:462:ILE:HG12 | 1:A:556:ILE:CB   | 2.24                     | 0.67              |
| 1:E:400:PRO:O    | 1:E:401:LYS:HG2  | 1.95                     | 0.67              |
| 1:E:453:GLN:O    | 2:F:407:PHE:HA   | 1.94                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:438:ASP:O    | 1:B:439:PHE:HB2  | 1.94                     | 0.67              |
| 2:D:122:PRO:HG2  | 2:D:125:PHE:CD1  | 2.30                     | 0.67              |
| 1:A:325:PHE:CE1  | 1:A:330:ASP:CB   | 2.72                     | 0.67              |
| 1:E:290:TYR:HD1  | 1:E:301:ILE:HD11 | 1.57                     | 0.67              |
| 1:E:390:SER:OG   | 3:E:707:HOH:O    | 2.11                     | 0.67              |
| 2:C:36:LEU:O     | 2:C:40:TYR:HD1   | 1.76                     | 0.67              |
| 2:D:7:LEU:HD12   | 2:D:8:THR:H      | 1.59                     | 0.67              |
| 2:D:123:SER:O    | 2:D:126:VAL:HB   | 1.95                     | 0.67              |
| 1:A:63:PHE:CD2   | 1:A:213:ILE:O    | 2.48                     | 0.67              |
| 1:A:162:LEU:CD2  | 1:A:210:PHE:HE2  | 2.04                     | 0.67              |
| 2:F:9:PRO:HD2    | 2:F:10:TRP:CZ3   | 2.30                     | 0.67              |
| 1:B:486:ILE:CD1  | 1:B:564:ASP:C    | 2.65                     | 0.67              |
| 2:C:305:GLN:CB   | 2:C:308:ILE:HD12 | 2.25                     | 0.67              |
| 1:A:596:LYS:HA   | 1:A:596:LYS:NZ   | 2.10                     | 0.67              |
| 2:F:247:HIS:O    | 2:F:251:LEU:N    | 2.27                     | 0.67              |
| 1:B:237:GLU:O    | 1:B:241:ASN:OD1  | 2.12                     | 0.67              |
| 1:A:253:LYS:O    | 1:A:254:ASN:HB3  | 1.92                     | 0.67              |
| 1:A:415:SER:HA   | 1:A:418:ARG:O    | 1.95                     | 0.67              |
| 1:A:486:ILE:HD11 | 1:A:564:ASP:O    | 1.95                     | 0.67              |
| 1:A:492:VAL:HG13 | 1:A:557:ILE:CD1  | 2.25                     | 0.67              |
| 1:E:281:MET:HE2  | 1:E:342:LEU:HD23 | 1.76                     | 0.67              |
| 1:E:365:ILE:HD12 | 1:E:366:LYS:HB2  | 1.76                     | 0.67              |
| 2:F:22:LEU:CD1   | 2:F:42:GLU:HB3   | 2.25                     | 0.67              |
| 1:A:120:ASN:HD22 | 1:A:120:ASN:C    | 2.02                     | 0.67              |
| 1:A:464:ALA:HA   | 1:A:509:PRO:CD   | 2.24                     | 0.67              |
| 1:E:184:TRP:CH2  | 1:E:211:TYR:CB   | 2.76                     | 0.67              |
| 1:E:224:LYS:HG2  | 1:E:228:TRP:CE3  | 2.14                     | 0.67              |
| 1:E:529:VAL:HG12 | 1:E:532:ILE:HD11 | 1.72                     | 0.67              |
| 2:D:269:LEU:HA   | 2:D:272:ILE:HD12 | 1.75                     | 0.67              |
| 1:A:72:TYR:HD2   | 1:A:208:TYR:OH   | 1.77                     | 0.67              |
| 1:A:305:GLN:OE1  | 1:A:313:THR:CB   | 2.43                     | 0.67              |
| 1:A:532:ILE:HD13 | 1:A:532:ILE:N    | 2.10                     | 0.67              |
| 1:E:487:VAL:HG22 | 1:E:527:ALA:HB3  | 1.76                     | 0.67              |
| 1:E:490:PHE:CD1  | 1:E:521:THR:HG21 | 2.29                     | 0.67              |
| 2:D:79:GLY:O     | 1:A:472:GLY:HA3  | 1.95                     | 0.67              |
| 1:E:72:TYR:CE2   | 1:E:206:SER:OG   | 2.47                     | 0.67              |
| 1:A:227:ASN:O    | 1:A:231:VAL:HG23 | 1.94                     | 0.66              |
| 1:E:312:LEU:O    | 1:E:435:LYS:NZ   | 2.27                     | 0.66              |
| 1:B:164:ASN:ND2  | 1:B:208:TYR:CB   | 2.48                     | 0.66              |
| 1:B:502:LEU:HA   | 1:B:510:LEU:O    | 1.95                     | 0.66              |
| 3:C:505:HOH:O    | 1:A:565:LEU:HB2  | 1.96                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:LEU:HD13 | 1:A:167:THR:H    | 1.34                     | 0.66              |
| 1:A:596:LYS:HA   | 1:A:596:LYS:HZ2  | 1.60                     | 0.66              |
| 1:E:167:THR:HA   | 1:E:439:PHE:O    | 1.94                     | 0.66              |
| 1:E:386:ILE:CG2  | 1:E:406:ILE:HD11 | 2.26                     | 0.66              |
| 2:F:259:PHE:HZ   | 2:F:268:PRO:CA   | 2.07                     | 0.66              |
| 1:B:107:VAL:HG11 | 1:B:266:GLN:HG2  | 1.77                     | 0.66              |
| 1:B:294:ASP:OD2  | 1:B:563:THR:HB   | 1.95                     | 0.66              |
| 2:C:96:VAL:C     | 2:C:99:LEU:HD12  | 2.20                     | 0.66              |
| 1:A:252:GLY:C    | 1:A:255:SER:HG   | 1.99                     | 0.66              |
| 1:E:225:HIS:CD2  | 1:E:228:TRP:HD1  | 2.13                     | 0.66              |
| 1:E:547:ARG:C    | 1:E:548:THR:HG23 | 2.21                     | 0.66              |
| 2:F:9:PRO:HG2    | 2:F:50:TYR:HD2   | 1.61                     | 0.66              |
| 2:F:237:ARG:O    | 2:F:237:ARG:HD3  | 1.95                     | 0.66              |
| 1:B:543:ILE:HD11 | 1:B:546:PHE:CE1  | 2.30                     | 0.66              |
| 2:D:190:TYR:HE2  | 2:D:218:ILE:CG2  | 2.06                     | 0.66              |
| 1:B:484:ALA:CB   | 1:B:585:TYR:HE2  | 2.08                     | 0.66              |
| 2:C:65:HIS:CE1   | 2:C:94:ARG:NH2   | 2.61                     | 0.66              |
| 2:D:85:ARG:HB2   | 2:D:137:LEU:HD13 | 1.78                     | 0.66              |
| 1:A:92:GLN:NE2   | 1:A:92:GLN:H     | 1.94                     | 0.66              |
| 1:A:165:LEU:HD11 | 1:A:167:THR:HA   | 1.76                     | 0.66              |
| 1:A:294:ASP:O    | 3:A:705:HOH:O    | 2.12                     | 0.66              |
| 1:A:516:PHE:HE2  | 1:A:521:THR:HG21 | 1.60                     | 0.66              |
| 1:E:447:LEU:HD12 | 1:E:575:ILE:CG2  | 2.26                     | 0.66              |
| 1:B:465:LEU:HD23 | 1:B:466:THR:CA   | 2.26                     | 0.66              |
| 2:D:24:PHE:HE2   | 2:D:155:TRP:HD1  | 0.78                     | 0.66              |
| 2:D:139:SER:HB3  | 1:A:469:LYS:HE3  | 1.76                     | 0.66              |
| 1:A:245:ILE:C    | 1:A:356:SER:OG   | 2.39                     | 0.66              |
| 1:A:261:LEU:HD11 | 1:A:359:ILE:O    | 1.95                     | 0.66              |
| 1:A:334:ARG:HG3  | 1:A:513:TYR:HH   | 1.56                     | 0.66              |
| 1:E:100:GLY:C    | 1:E:111:SER:HG   | 2.02                     | 0.66              |
| 1:E:570:ILE:HD13 | 1:E:570:ILE:N    | 2.08                     | 0.66              |
| 2:C:10:TRP:HA    | 2:C:50:TYR:CE1   | 2.29                     | 0.66              |
| 2:C:134:HIS:NE2  | 2:D:97:ASN:OD1   | 2.04                     | 0.66              |
| 1:A:430:MET:HG2  | 1:A:566:PRO:CG   | 2.25                     | 0.66              |
| 1:A:470:GLU:HA   | 1:A:470:GLU:OE1  | 1.95                     | 0.66              |
| 1:E:363:GLY:HA3  | 3:E:708:HOH:O    | 1.90                     | 0.66              |
| 1:E:469:LYS:HG3  | 1:E:470:GLU:HG2  | 1.77                     | 0.66              |
| 1:B:209:THR:HG23 | 1:B:210:PHE:CD1  | 2.31                     | 0.66              |
| 1:B:279:ASN:HA   | 1:B:300:LYS:HE3  | 1.78                     | 0.66              |
| 2:C:43:ALA:O     | 2:C:47:VAL:HG23  | 1.96                     | 0.66              |
| 2:C:125:PHE:CE1  | 2:C:146:CYS:SG   | 2.88                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:331:LEU:C    | 2:D:343:LEU:HD21 | 2.21                     | 0.66              |
| 1:A:456:TYR:CB   | 1:A:537:LYS:O    | 2.43                     | 0.66              |
| 1:E:349:ASP:O    | 1:E:351:GLU:OE1  | 2.12                     | 0.66              |
| 2:F:336:HIS:O    | 2:F:340:VAL:CG2  | 2.44                     | 0.66              |
| 1:B:172:ILE:HG22 | 1:B:443:PHE:CE2  | 2.31                     | 0.66              |
| 1:B:455:SER:HB3  | 2:D:405:LYS:CA   | 2.24                     | 0.66              |
| 2:C:14:ASP:O     | 2:C:17:VAL:HG23  | 1.96                     | 0.66              |
| 2:D:353:ASP:OD2  | 2:D:353:ASP:N    | 2.27                     | 0.66              |
| 2:D:410:HIS:HD2  | 2:D:413:TRP:CD1  | 2.11                     | 0.66              |
| 1:A:162:LEU:C    | 1:A:162:LEU:HD22 | 2.21                     | 0.66              |
| 1:A:162:LEU:HD22 | 1:A:162:LEU:O    | 1.96                     | 0.66              |
| 1:A:408:LEU:H    | 1:A:408:LEU:CD1  | 1.97                     | 0.66              |
| 2:F:235:ILE:CA   | 2:F:238:ILE:HD12 | 2.24                     | 0.66              |
| 2:F:420:VAL:C    | 2:F:421:ILE:CG1  | 2.69                     | 0.66              |
| 1:A:298:LEU:H    | 1:A:298:LEU:CD2  | 2.08                     | 0.66              |
| 2:F:111:PRO:HG3  | 2:F:113:HIS:HE1  | 1.60                     | 0.66              |
| 1:B:93:PHE:CD2   | 1:B:162:LEU:CD2  | 2.78                     | 0.65              |
| 1:B:118:PHE:HD1  | 1:B:306:HIS:C    | 2.04                     | 0.65              |
| 2:C:95:PHE:HE1   | 2:C:99:LEU:CD2   | 1.99                     | 0.65              |
| 1:A:226:LYS:O    | 1:A:230:ASP:HB3  | 1.95                     | 0.65              |
| 1:A:370:LEU:HD22 | 1:A:393:LEU:HD23 | 1.77                     | 0.65              |
| 1:A:377:ILE:HD13 | 1:A:377:ILE:N    | 2.04                     | 0.65              |
| 1:A:464:ALA:HA   | 1:A:509:PRO:HG2  | 1.76                     | 0.65              |
| 2:F:249:ARG:HA   | 2:F:307:TRP:HZ2  | 1.61                     | 0.65              |
| 1:B:276:LEU:O    | 1:B:276:LEU:HD23 | 1.96                     | 0.65              |
| 1:B:318:THR:HG22 | 1:B:319:GLN:CG   | 2.26                     | 0.65              |
| 2:C:186:LEU:CD1  | 2:C:224:HIS:CB   | 2.74                     | 0.65              |
| 2:C:305:GLN:O    | 2:C:309:ARG:N    | 2.29                     | 0.65              |
| 1:E:248:ILE:CD1  | 1:E:382:PRO:HG3  | 2.26                     | 0.65              |
| 1:E:299:SER:HB3  | 1:E:317:SER:HB3  | 0.66                     | 0.65              |
| 2:F:9:PRO:HG2    | 2:F:10:TRP:HE3   | 1.61                     | 0.65              |
| 1:B:81:LEU:C     | 1:B:156:TYR:CB   | 2.70                     | 0.65              |
| 2:D:308:ILE:O    | 2:D:311:LEU:HB2  | 1.96                     | 0.65              |
| 2:D:327:MET:C    | 2:D:330:THR:HG1  | 2.03                     | 0.65              |
| 2:D:331:LEU:HA   | 2:D:346:LEU:HD13 | 1.76                     | 0.65              |
| 1:A:463:SER:OG   | 1:A:555:ALA:HB2  | 1.96                     | 0.65              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:O    | 2.45                     | 0.65              |
| 2:F:194:ARG:CB   | 2:F:251:LEU:CD2  | 2.74                     | 0.65              |
| 1:B:82:LYS:HA    | 1:B:156:TYR:CB   | 2.27                     | 0.65              |
| 1:B:572:SER:OG   | 1:B:575:ILE:CG1  | 2.45                     | 0.65              |
| 1:E:78:ILE:HG21  | 1:E:98:GLN:HE22  | 1.61                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:235:LEU:HD12 | 1:E:247:VAL:HG21 | 1.75                     | 0.65              |
| 1:E:247:VAL:HG13 | 1:E:386:ILE:HD13 | 1.77                     | 0.65              |
| 1:E:340:GLU:OE2  | 1:E:379:ARG:NH1  | 2.28                     | 0.65              |
| 1:B:310:LEU:HD22 | 1:B:310:LEU:N    | 2.12                     | 0.65              |
| 1:B:379:ARG:HD3  | 1:B:379:ARG:C    | 2.22                     | 0.65              |
| 1:B:418:ARG:N    | 1:B:419:TYR:HA   | 2.11                     | 0.65              |
| 2:C:31:ILE:HG13  | 2:C:35:GLU:OE1   | 1.96                     | 0.65              |
| 2:D:331:LEU:O    | 2:D:343:LEU:CD2  | 2.42                     | 0.65              |
| 1:A:520:SER:C    | 1:A:521:THR:HG23 | 2.21                     | 0.65              |
| 1:B:252:GLY:O    | 1:B:255:SER:HB2  | 1.96                     | 0.65              |
| 1:B:340:GLU:O    | 1:B:344:ARG:HG2  | 1.96                     | 0.65              |
| 1:B:387:TYR:HD1  | 1:B:388:LEU:H    | 1.44                     | 0.65              |
| 2:C:220:GLY:O    | 2:C:224:HIS:CB   | 2.44                     | 0.65              |
| 2:D:267:PHE:O    | 2:D:271:LEU:HG   | 1.96                     | 0.65              |
| 1:A:322:TYR:HB2  | 1:A:523:PHE:CZ   | 2.30                     | 0.65              |
| 1:E:165:LEU:HD23 | 1:E:167:THR:HB   | 1.79                     | 0.65              |
| 1:E:543:ILE:HG13 | 1:E:544:PRO:HD2  | 1.76                     | 0.65              |
| 1:B:492:VAL:CA   | 1:B:557:ILE:HD11 | 2.26                     | 0.65              |
| 1:B:585:TYR:HD1  | 2:D:8:THR:O      | 1.80                     | 0.65              |
| 1:A:499:GLU:OE2  | 1:A:515:GLU:O    | 2.14                     | 0.65              |
| 1:B:63:PHE:H     | 1:B:88:ILE:HD11  | 1.57                     | 0.65              |
| 2:C:214:TYR:O    | 2:C:218:ILE:CG1  | 2.42                     | 0.65              |
| 2:D:334:THR:CB   | 2:D:342:LEU:HB3  | 2.26                     | 0.65              |
| 1:A:434:HIS:HB3  | 1:A:442:ASP:O    | 1.97                     | 0.65              |
| 1:A:490:PHE:CD1  | 1:A:523:PHE:HD1  | 2.12                     | 0.65              |
| 1:A:508:LEU:CD1  | 1:A:509:PRO:HD3  | 2.27                     | 0.65              |
| 1:E:337:LEU:HD12 | 1:E:337:LEU:C    | 2.20                     | 0.65              |
| 2:F:122:PRO:CD   | 2:F:125:PHE:CD2  | 2.79                     | 0.65              |
| 1:B:81:LEU:O     | 1:B:156:TYR:CB   | 2.44                     | 0.65              |
| 2:C:8:THR:HG23   | 1:A:587:THR:HG23 | 1.78                     | 0.65              |
| 2:D:28:ARG:HG3   | 2:D:28:ARG:HH11  | 1.62                     | 0.65              |
| 1:A:118:PHE:CE1  | 1:A:306:HIS:HB3  | 2.32                     | 0.65              |
| 1:A:250:ILE:HD13 | 1:A:373:THR:HG21 | 1.79                     | 0.65              |
| 1:A:508:LEU:HD12 | 1:A:509:PRO:HD2  | 1.78                     | 0.65              |
| 1:A:568:TRP:HA   | 1:A:571:ALA:O    | 1.96                     | 0.65              |
| 1:E:321:HIS:CE1  | 1:E:522:GLU:OE2  | 2.50                     | 0.65              |
| 1:B:529:VAL:HG22 | 1:B:540:ASN:O    | 1.97                     | 0.65              |
| 2:C:22:LEU:CD2   | 2:C:43:ALA:CA    | 2.74                     | 0.65              |
| 2:C:90:MET:HA    | 2:C:93:ILE:HD12  | 1.79                     | 0.65              |
| 2:D:85:ARG:HB2   | 2:D:137:LEU:CD1  | 2.27                     | 0.65              |
| 1:A:86:ASN:CB    | 1:A:130:GLN:HA   | 2.27                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:376:LEU:O    | 1:A:376:LEU:HD22 | 1.97                     | 0.65              |
| 1:A:385:VAL:CG1  | 1:A:403:THR:HG21 | 2.27                     | 0.65              |
| 2:F:70:LEU:HA    | 2:F:73:LEU:HD12  | 1.78                     | 0.65              |
| 1:B:161:LYS:NZ   | 1:B:163:THR:HG1  | 1.91                     | 0.64              |
| 1:B:598:TRP:CE3  | 2:D:98:GLY:CA    | 2.80                     | 0.64              |
| 2:C:30:GLN:OE1   | 2:C:30:GLN:HA    | 1.95                     | 0.64              |
| 1:A:92:GLN:HE22  | 1:A:183:PHE:HB3  | 1.61                     | 0.64              |
| 1:A:170:GLU:CB   | 1:A:185:GLN:CD   | 2.70                     | 0.64              |
| 1:A:233:LYS:O    | 1:A:236:THR:OG1  | 2.15                     | 0.64              |
| 1:A:483:GLU:OE1  | 1:A:532:ILE:CD1  | 2.43                     | 0.64              |
| 1:A:575:ILE:HG12 | 1:A:576:VAL:N    | 2.12                     | 0.64              |
| 1:E:78:ILE:HD11  | 1:E:161:LYS:CG   | 2.24                     | 0.64              |
| 1:E:288:PRO:HB3  | 1:E:291:SER:HB2  | 1.79                     | 0.64              |
| 1:E:289:GLU:O    | 1:E:290:TYR:HD2  | 1.80                     | 0.64              |
| 1:E:365:ILE:HD12 | 1:E:393:LEU:CD1  | 2.27                     | 0.64              |
| 2:F:11:LYS:HB3   | 2:F:11:LYS:NZ    | 2.11                     | 0.64              |
| 1:B:332:PRO:HD2  | 2:C:141:GLU:HB2  | 1.78                     | 0.64              |
| 1:B:465:LEU:HD23 | 1:B:466:THR:H    | 1.55                     | 0.64              |
| 2:C:11:LYS:CD    | 1:A:585:TYR:CE2  | 2.79                     | 0.64              |
| 1:A:206:SER:O    | 1:A:211:TYR:HE2  | 1.80                     | 0.64              |
| 1:E:78:ILE:HG13  | 1:E:161:LYS:HG3  | 1.79                     | 0.64              |
| 1:E:169:LEU:HD11 | 1:E:183:PHE:HZ   | 1.53                     | 0.64              |
| 1:B:364:TRP:O    | 1:B:365:ILE:HD13 | 1.96                     | 0.64              |
| 1:B:478:LEU:HD23 | 1:B:479:GLU:HG2  | 1.78                     | 0.64              |
| 2:C:11:LYS:HD2   | 1:A:585:TYR:OH   | 1.97                     | 0.64              |
| 2:C:22:LEU:CD2   | 2:C:43:ALA:N     | 2.61                     | 0.64              |
| 1:E:108:ILE:CG2  | 1:E:133:GLN:CB   | 2.75                     | 0.64              |
| 1:E:325:PHE:HA   | 1:E:562:ASN:HB3  | 1.78                     | 0.64              |
| 1:E:392:THR:C    | 1:E:393:LEU:HD12 | 2.22                     | 0.64              |
| 1:B:230:ASP:O    | 1:B:234:SER:N    | 2.30                     | 0.64              |
| 1:B:479:GLU:OE2  | 1:B:508:LEU:CB   | 2.45                     | 0.64              |
| 2:C:9:PRO:CB     | 2:C:50:TYR:HD1   | 2.11                     | 0.64              |
| 2:C:43:ALA:HA    | 2:C:46:LEU:HD13  | 1.80                     | 0.64              |
| 2:D:267:PHE:O    | 2:D:271:LEU:N    | 2.28                     | 0.64              |
| 1:A:165:LEU:O    | 1:A:165:LEU:HD22 | 1.96                     | 0.64              |
| 1:A:269:LEU:CD2  | 1:A:278:ILE:HG22 | 2.28                     | 0.64              |
| 1:E:228:TRP:CZ3  | 1:E:263:LEU:HD22 | 2.32                     | 0.64              |
| 1:E:235:LEU:HD13 | 1:E:247:VAL:CG2  | 2.27                     | 0.64              |
| 1:B:468:LEU:HD13 | 1:B:561:GLY:CA   | 2.04                     | 0.64              |
| 2:C:10:TRP:CZ2   | 2:C:16:VAL:HG21  | 2.32                     | 0.64              |
| 2:C:40:TYR:HE2   | 2:C:67:PHE:CD1   | 2.10                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:46:LEU:HD12  | 2:C:46:LEU:H     | 1.62                     | 0.64              |
| 2:D:154:VAL:CG2  | 2:D:159:TRP:HD1  | 2.10                     | 0.64              |
| 1:E:233:LYS:HZ3  | 1:E:236:THR:HG1  | 1.44                     | 0.64              |
| 1:E:344:ARG:NH2  | 1:E:379:ARG:HH22 | 1.94                     | 0.64              |
| 1:E:570:ILE:HA   | 1:E:575:ILE:HD12 | 1.79                     | 0.64              |
| 1:E:586:ILE:C    | 2:F:8:THR:HG23   | 2.23                     | 0.64              |
| 1:B:486:ILE:CG2  | 1:B:565:LEU:HG   | 2.27                     | 0.64              |
| 2:C:218:ILE:HG23 | 2:C:255:MET:CE   | 2.28                     | 0.64              |
| 2:D:24:PHE:HE2   | 2:D:155:TRP:CG   | 2.05                     | 0.64              |
| 1:A:224:LYS:CB   | 1:A:228:TRP:HE3  | 2.10                     | 0.64              |
| 1:E:98:GLN:O     | 1:E:142:ASN:CB   | 2.46                     | 0.64              |
| 1:E:103:ASP:CG   | 1:E:132:THR:HG1  | 2.05                     | 0.64              |
| 1:E:433:PHE:CD1  | 1:E:544:PRO:HD3  | 2.33                     | 0.64              |
| 1:E:522:GLU:OE2  | 1:E:522:GLU:HA   | 1.97                     | 0.64              |
| 1:A:162:LEU:HD21 | 1:A:210:PHE:HE2  | 1.56                     | 0.64              |
| 1:A:239:TYR:OH   | 1:A:276:LEU:HD12 | 1.97                     | 0.64              |
| 1:A:382:PRO:CB   | 1:A:385:VAL:HG23 | 2.27                     | 0.64              |
| 1:B:452:ILE:HD12 | 1:B:543:ILE:HG12 | 1.79                     | 0.64              |
| 1:A:232:ILE:CG1  | 1:A:264:LEU:CD2  | 2.71                     | 0.64              |
| 1:A:427:LEU:HD23 | 1:A:427:LEU:C    | 2.23                     | 0.64              |
| 1:A:568:TRP:HE3  | 1:A:568:TRP:H    | 1.44                     | 0.64              |
| 1:E:248:ILE:CD1  | 1:E:382:PRO:CG   | 2.76                     | 0.64              |
| 2:F:22:LEU:HD11  | 2:F:42:GLU:HB3   | 1.78                     | 0.64              |
| 2:F:111:PRO:O    | 2:F:115:LEU:HD12 | 1.98                     | 0.64              |
| 1:B:454:VAL:HG13 | 2:D:407:PHE:CD1  | 2.27                     | 0.64              |
| 1:B:529:VAL:HG23 | 1:B:540:ASN:C    | 2.22                     | 0.64              |
| 1:A:76:TYR:CD2   | 1:A:78:ILE:HD13  | 2.32                     | 0.64              |
| 1:A:322:TYR:CD1  | 1:A:523:PHE:CE1  | 2.85                     | 0.64              |
| 1:A:398:ASP:OD2  | 1:A:398:ASP:N    | 2.25                     | 0.64              |
| 1:A:446:LEU:O    | 1:A:542:TYR:HE2  | 1.80                     | 0.64              |
| 1:E:530:HIS:CE1  | 1:E:570:ILE:HG22 | 2.30                     | 0.64              |
| 2:F:259:PHE:CE1  | 2:F:267:PHE:HB2  | 2.29                     | 0.64              |
| 1:B:175:VAL:HG23 | 1:B:176:CYS:N    | 2.13                     | 0.64              |
| 1:B:484:ALA:CB   | 1:B:585:TYR:CD2  | 2.81                     | 0.64              |
| 1:A:63:PHE:HZ    | 1:A:212:PRO:CB   | 1.99                     | 0.64              |
| 1:A:454:VAL:O    | 1:A:538:ILE:CG2  | 2.45                     | 0.64              |
| 1:E:118:PHE:CD1  | 1:E:306:HIS:HB3  | 2.33                     | 0.64              |
| 1:E:282:ASP:HA   | 1:E:360:ASN:HB3  | 1.80                     | 0.64              |
| 1:B:528:LEU:CD1  | 3:B:704:HOH:O    | 2.38                     | 0.63              |
| 2:C:31:ILE:HD11  | 2:C:35:GLU:OE2   | 1.98                     | 0.63              |
| 2:C:247:HIS:O    | 2:C:250:ALA:HB3  | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:16:VAL:HA    | 2:F:19:LEU:HB2   | 1.79                     | 0.63              |
| 2:C:89:SER:O     | 2:C:93:ILE:HG13  | 1.97                     | 0.63              |
| 1:A:239:TYR:CD2  | 1:A:268:MET:HE2  | 2.33                     | 0.63              |
| 1:A:440:LYS:O    | 1:A:441:PHE:HD2  | 1.80                     | 0.63              |
| 1:A:478:LEU:HD13 | 1:A:510:LEU:CD1  | 2.17                     | 0.63              |
| 1:E:530:HIS:CE1  | 1:E:570:ILE:HG23 | 2.32                     | 0.63              |
| 2:F:38:ARG:HH21  | 2:F:38:ARG:CG    | 2.12                     | 0.63              |
| 2:F:40:TYR:CG    | 2:F:67:PHE:HD2   | 2.16                     | 0.63              |
| 2:C:65:HIS:CE1   | 2:C:94:ARG:CZ    | 2.81                     | 0.63              |
| 1:A:224:LYS:HB3  | 1:A:228:TRP:HB3  | 1.81                     | 0.63              |
| 1:A:385:VAL:CB   | 1:A:403:THR:CG2  | 2.46                     | 0.63              |
| 1:A:464:ALA:CA   | 1:A:509:PRO:HG2  | 2.28                     | 0.63              |
| 1:E:236:THR:HG21 | 1:E:267:HIS:HB3  | 1.81                     | 0.63              |
| 1:E:530:HIS:NE2  | 1:E:570:ILE:HG23 | 2.08                     | 0.63              |
| 1:B:532:ILE:HD12 | 1:B:539:MET:CB   | 2.28                     | 0.63              |
| 2:D:259:PHE:CE1  | 2:D:268:PRO:CA   | 2.81                     | 0.63              |
| 2:D:266:ASP:O    | 2:D:270:GLY:N    | 2.32                     | 0.63              |
| 1:A:420:SER:CA   | 1:A:423:GLN:HB3  | 2.28                     | 0.63              |
| 1:E:438:ASP:OD2  | 1:E:439:PHE:HD1  | 1.80                     | 0.63              |
| 1:E:486:ILE:HG22 | 1:E:526:LEU:HD22 | 1.81                     | 0.63              |
| 1:E:598:TRP:HD1  | 1:E:599:LYS:H    | 1.43                     | 0.63              |
| 2:D:307:TRP:O    | 2:D:311:LEU:HG   | 1.98                     | 0.63              |
| 1:A:117:LYS:CD   | 1:A:439:PHE:CZ   | 2.64                     | 0.63              |
| 1:E:310:LEU:HD22 | 1:E:310:LEU:H    | 1.62                     | 0.63              |
| 2:C:99:LEU:O     | 2:C:102:PRO:HD2  | 1.98                     | 0.63              |
| 2:C:304:ALA:O    | 2:C:307:TRP:N    | 2.32                     | 0.63              |
| 2:D:320:ASP:OD1  | 2:D:321:ASP:N    | 2.31                     | 0.63              |
| 1:A:569:GLU:OE1  | 1:A:570:ILE:N    | 2.32                     | 0.63              |
| 1:E:100:GLY:CA   | 1:E:111:SER:OG   | 2.46                     | 0.63              |
| 1:E:279:ASN:CB   | 1:E:356:SER:O    | 2.46                     | 0.63              |
| 2:F:417:PRO:HD2  | 2:F:419:GLY:O    | 1.98                     | 0.63              |
| 1:B:234:SER:HA   | 1:B:237:GLU:OE2  | 1.98                     | 0.63              |
| 1:B:388:LEU:HD13 | 1:B:406:ILE:CG1  | 2.24                     | 0.63              |
| 1:B:598:TRP:CD1  | 3:D:502:HOH:O    | 2.51                     | 0.63              |
| 2:C:128:PHE:HD2  | 2:C:128:PHE:O    | 1.81                     | 0.63              |
| 2:C:280:TYR:HB2  | 2:C:334:THR:HG22 | 1.76                     | 0.63              |
| 1:E:123:SER:HB2  | 1:E:182:LEU:HD21 | 1.79                     | 0.63              |
| 1:B:103:ASP:CA   | 1:B:108:ILE:HA   | 2.23                     | 0.63              |
| 1:B:481:SER:O    | 1:B:485:THR:HG21 | 1.98                     | 0.63              |
| 1:E:318:THR:CG2  | 1:E:319:GLN:OE1  | 2.46                     | 0.63              |
| 2:F:249:ARG:HA   | 2:F:252:PHE:HB2  | 1.81                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:164:ASN:OD1  | 1:B:209:THR:HG23 | 1.95                     | 0.63              |
| 1:B:180:LYS:HD3  | 1:B:181:ASN:H    | 1.64                     | 0.63              |
| 1:B:227:ASN:O    | 1:B:231:VAL:HG23 | 1.99                     | 0.63              |
| 1:B:258:SER:OG   | 1:B:289:GLU:OE1  | 2.15                     | 0.63              |
| 2:C:9:PRO:HB2    | 2:C:50:TYR:CD1   | 2.31                     | 0.63              |
| 2:C:99:LEU:HD13  | 2:C:121:LEU:CD2  | 2.29                     | 0.63              |
| 2:D:24:PHE:HD2   | 2:D:155:TRP:NE1  | 1.95                     | 0.63              |
| 1:A:112:GLY:H    | 1:A:140:LEU:HA   | 1.64                     | 0.63              |
| 1:A:117:LYS:CE   | 1:A:439:PHE:CE2  | 2.78                     | 0.63              |
| 1:A:167:THR:O    | 1:A:168:HIS:HB2  | 1.97                     | 0.63              |
| 1:A:572:SER:OG   | 1:A:575:ILE:HD12 | 1.99                     | 0.63              |
| 2:F:354:PRO:CD   | 2:F:355:VAL:N    | 2.59                     | 0.63              |
| 1:B:81:LEU:HD23  | 1:B:87:LEU:HD11  | 1.81                     | 0.62              |
| 1:A:63:PHE:CE2   | 1:A:214:THR:HG22 | 2.33                     | 0.62              |
| 1:A:368:TYR:CE1  | 1:A:372:LEU:HD23 | 2.32                     | 0.62              |
| 1:E:475:MET:O    | 1:E:478:LEU:HD22 | 1.98                     | 0.62              |
| 2:F:20:LYS:NZ    | 2:F:162:VAL:CA   | 2.61                     | 0.62              |
| 2:F:247:HIS:O    | 2:F:250:ALA:HB3  | 1.98                     | 0.62              |
| 1:B:452:ILE:CD1  | 1:B:543:ILE:HG12 | 2.28                     | 0.62              |
| 1:B:598:TRP:HB2  | 2:D:58:HIS:CB    | 2.29                     | 0.62              |
| 2:C:197:ASN:ND2  | 2:C:197:ASN:O    | 2.33                     | 0.62              |
| 2:D:85:ARG:O     | 2:D:89:SER:HB2   | 1.98                     | 0.62              |
| 2:D:95:PHE:O     | 2:D:99:LEU:HG    | 1.97                     | 0.62              |
| 1:E:324:GLY:O    | 1:E:562:ASN:N    | 2.25                     | 0.62              |
| 2:F:247:HIS:O    | 2:F:250:ALA:CA   | 2.47                     | 0.62              |
| 1:A:104:ILE:HD12 | 1:A:109:TYR:HD2  | 1.63                     | 0.62              |
| 1:A:107:VAL:HG23 | 1:A:109:TYR:CE2  | 2.34                     | 0.62              |
| 1:A:125:SER:HB3  | 1:A:222:VAL:CG2  | 2.25                     | 0.62              |
| 1:A:167:THR:OG1  | 1:A:169:LEU:HB2  | 2.00                     | 0.62              |
| 1:A:594:LEU:HD12 | 1:A:594:LEU:C    | 2.24                     | 0.62              |
| 1:E:104:ILE:HG23 | 1:E:129:ILE:HD11 | 1.81                     | 0.62              |
| 1:E:104:ILE:HG23 | 1:E:129:ILE:HD12 | 1.79                     | 0.62              |
| 1:E:281:MET:SD   | 1:E:342:LEU:HD22 | 2.38                     | 0.62              |
| 1:E:322:TYR:HB3  | 1:E:490:PHE:CZ   | 2.34                     | 0.62              |
| 1:E:364:TRP:CE3  | 1:E:369:GLY:HA2  | 2.34                     | 0.62              |
| 2:F:10:TRP:CB    | 2:F:15:GLU:OE2   | 2.48                     | 0.62              |
| 2:F:259:PHE:CZ   | 2:F:268:PRO:CA   | 2.82                     | 0.62              |
| 1:B:248:ILE:HD11 | 1:B:359:ILE:HD13 | 1.81                     | 0.62              |
| 1:B:380:VAL:HG11 | 1:B:382:PRO:HB3  | 1.81                     | 0.62              |
| 2:C:325:SER:OG   | 2:C:359:LYS:HE3  | 1.99                     | 0.62              |
| 1:A:475:MET:HE2  | 1:A:475:MET:O    | 1.99                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:224:LYS:CB   | 1:E:228:TRP:CE3  | 2.82                     | 0.62              |
| 1:E:288:PRO:O    | 1:E:289:GLU:HB2  | 1.98                     | 0.62              |
| 2:F:23:PHE:CD2   | 2:F:43:ALA:HB1   | 2.34                     | 0.62              |
| 1:B:318:THR:HG22 | 1:B:319:GLN:CD   | 2.24                     | 0.62              |
| 2:D:9:PRO:HD2    | 2:D:10:TRP:CZ3   | 2.35                     | 0.62              |
| 1:A:465:LEU:HG   | 1:A:558:MET:HB3  | 1.81                     | 0.62              |
| 1:E:118:PHE:CE1  | 1:E:306:HIS:HB3  | 2.35                     | 0.62              |
| 1:E:301:ILE:CG2  | 1:E:315:THR:CG2  | 2.68                     | 0.62              |
| 1:E:318:THR:CB   | 1:E:319:GLN:OE1  | 2.47                     | 0.62              |
| 2:F:10:TRP:HE3   | 2:F:50:TYR:CD2   | 2.18                     | 0.62              |
| 2:F:328:ILE:HA   | 2:F:331:LEU:HD22 | 1.82                     | 0.62              |
| 2:F:420:VAL:O    | 2:F:420:VAL:HG23 | 2.00                     | 0.62              |
| 1:B:482:ILE:C    | 3:B:702:HOH:O    | 2.43                     | 0.62              |
| 2:C:59:ILE:HG12  | 1:A:596:LYS:CB   | 2.26                     | 0.62              |
| 1:A:211:TYR:CD1  | 1:A:212:PRO:HD2  | 2.34                     | 0.62              |
| 1:A:569:GLU:OE1  | 1:A:570:ILE:HG12 | 1.99                     | 0.62              |
| 1:A:583:LEU:CB   | 1:A:586:ILE:C    | 2.73                     | 0.62              |
| 2:F:139:SER:OG   | 2:F:142:MET:HB2  | 1.99                     | 0.62              |
| 1:B:462:ILE:CA   | 1:B:556:ILE:CB   | 2.65                     | 0.62              |
| 1:B:479:GLU:OE2  | 1:B:508:LEU:N    | 2.32                     | 0.62              |
| 1:B:484:ALA:HB2  | 1:B:585:TYR:CE2  | 2.32                     | 0.62              |
| 2:C:125:PHE:HZ   | 2:C:150:ALA:N    | 1.96                     | 0.62              |
| 2:D:77:GLU:O     | 2:D:77:GLU:HG2   | 1.98                     | 0.62              |
| 2:D:189:GLN:O    | 2:D:193:ILE:HG13 | 1.99                     | 0.62              |
| 1:A:87:LEU:HD22  | 1:A:212:PRO:HB3  | 1.81                     | 0.62              |
| 1:E:225:HIS:CB   | 1:E:228:TRP:CB   | 2.70                     | 0.62              |
| 1:E:321:HIS:CD2  | 1:E:341:GLN:NE2  | 2.68                     | 0.62              |
| 1:E:338:LEU:HD23 | 1:E:338:LEU:C    | 2.24                     | 0.62              |
| 1:B:249:VAL:O    | 1:B:361:THR:OG1  | 2.18                     | 0.62              |
| 1:B:521:THR:O    | 1:B:522:GLU:OE2  | 2.17                     | 0.62              |
| 2:C:49:MET:HE3   | 1:A:477:HIS:HB3  | 1.81                     | 0.62              |
| 2:C:218:ILE:CG1  | 2:C:255:MET:HE1  | 2.11                     | 0.62              |
| 2:C:305:GLN:C    | 2:C:308:ILE:H    | 2.08                     | 0.62              |
| 2:D:131:SER:O    | 2:D:135:ASP:HB2  | 2.00                     | 0.62              |
| 2:F:280:TYR:N    | 2:F:338:LEU:CD2  | 2.63                     | 0.62              |
| 1:B:511:LEU:HD23 | 1:B:512:PRO:N    | 2.15                     | 0.62              |
| 2:C:90:MET:HE1   | 2:D:93:ILE:HD11  | 1.80                     | 0.62              |
| 1:B:334:ARG:CG   | 1:B:513:TYR:OH   | 2.47                     | 0.62              |
| 2:C:8:THR:HG21   | 1:A:587:THR:CG2  | 2.29                     | 0.62              |
| 1:A:278:ILE:HD13 | 1:A:279:ASN:C    | 2.25                     | 0.62              |
| 1:A:510:LEU:HG   | 1:A:510:LEU:O    | 1.98                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:97:ILE:HD13  | 1:E:110:HIS:O    | 2.00                     | 0.62              |
| 1:E:373:THR:O    | 1:E:377:ILE:HG12 | 2.00                     | 0.62              |
| 1:E:533:ASP:OD1  | 1:E:535:GLU:N    | 2.33                     | 0.62              |
| 1:B:316:ASP:OD1  | 1:B:316:ASP:N    | 2.31                     | 0.61              |
| 2:C:213:GLU:O    | 2:C:216:THR:OG1  | 2.14                     | 0.61              |
| 2:C:277:SER:O    | 2:C:280:TYR:HD2  | 1.83                     | 0.61              |
| 2:D:320:ASP:O    | 2:D:324:VAL:HG23 | 2.00                     | 0.61              |
| 1:A:119:ILE:HG22 | 1:A:119:ILE:O    | 2.00                     | 0.61              |
| 1:A:176:CYS:SG   | 1:A:178:LEU:HB2  | 2.40                     | 0.61              |
| 1:E:257:LYS:HG3  | 1:E:258:SER:N    | 2.13                     | 0.61              |
| 1:E:283:LEU:HD13 | 1:E:339:VAL:CG1  | 2.30                     | 0.61              |
| 1:E:524:PHE:HD2  | 1:E:525:ARG:HB2  | 1.59                     | 0.61              |
| 2:F:133:THR:HG22 | 2:F:134:HIS:CD2  | 2.35                     | 0.61              |
| 1:B:62:ASN:CB    | 1:B:216:PRO:CB   | 2.78                     | 0.61              |
| 2:C:22:LEU:HD23  | 2:C:43:ALA:CA    | 2.30                     | 0.61              |
| 2:D:28:ARG:HH11  | 2:D:28:ARG:CG    | 2.13                     | 0.61              |
| 2:F:82:ASP:O     | 2:F:86:LEU:HD12  | 2.00                     | 0.61              |
| 1:B:134:VAL:O    | 1:B:134:VAL:HG12 | 2.00                     | 0.61              |
| 1:B:236:THR:O    | 1:B:239:TYR:HB3  | 2.00                     | 0.61              |
| 2:C:214:TYR:O    | 2:C:218:ILE:CD1  | 2.48                     | 0.61              |
| 2:D:47:VAL:HG11  | 2:D:64:ALA:HB2   | 1.82                     | 0.61              |
| 1:A:297:SER:HB2  | 1:A:319:GLN:O    | 2.00                     | 0.61              |
| 1:E:184:TRP:CE3  | 1:E:211:TYR:CD2  | 2.87                     | 0.61              |
| 1:E:247:VAL:CG1  | 1:E:386:ILE:HD13 | 2.30                     | 0.61              |
| 1:B:492:VAL:HB   | 1:B:557:ILE:HD11 | 1.82                     | 0.61              |
| 2:D:122:PRO:HD2  | 2:D:125:PHE:CG   | 2.36                     | 0.61              |
| 1:A:379:ARG:O    | 1:A:379:ARG:HD3  | 2.00                     | 0.61              |
| 1:A:438:ASP:OD2  | 1:A:439:PHE:N    | 2.34                     | 0.61              |
| 1:E:128:LEU:HD22 | 1:E:129:ILE:H    | 1.66                     | 0.61              |
| 1:B:118:PHE:CZ   | 1:B:306:HIS:CG   | 2.88                     | 0.61              |
| 1:A:94:VAL:C     | 1:A:162:LEU:HB2  | 2.24                     | 0.61              |
| 1:A:175:VAL:HG23 | 1:A:176:CYS:HB2  | 1.81                     | 0.61              |
| 1:A:184:TRP:HZ2  | 1:A:211:TYR:CG   | 2.18                     | 0.61              |
| 1:E:227:ASN:O    | 1:E:231:VAL:HG23 | 2.00                     | 0.61              |
| 1:E:235:LEU:N    | 1:E:235:LEU:HD23 | 2.16                     | 0.61              |
| 2:F:24:PHE:CD1   | 2:F:155:TRP:CZ3  | 2.56                     | 0.61              |
| 2:F:356:ILE:O    | 2:F:360:ILE:CG1  | 2.48                     | 0.61              |
| 1:B:257:LYS:C    | 1:B:260:PHE:H    | 2.08                     | 0.61              |
| 1:B:468:LEU:CD2  | 1:B:559:VAL:HG13 | 2.29                     | 0.61              |
| 2:C:418:PHE:CE2  | 1:A:447:LEU:HD23 | 2.35                     | 0.61              |
| 2:D:149:ARG:CG   | 2:D:149:ARG:HH11 | 2.13                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:356:ILE:O    | 2:F:360:ILE:CD1  | 2.48                     | 0.61              |
| 1:B:164:ASN:CG   | 1:B:208:TYR:HB3  | 2.25                     | 0.61              |
| 1:B:572:SER:OG   | 1:B:575:ILE:HD11 | 2.00                     | 0.61              |
| 1:E:94:VAL:HG23  | 1:E:165:LEU:HD13 | 1.83                     | 0.61              |
| 1:E:235:LEU:CD1  | 1:E:247:VAL:CG2  | 2.77                     | 0.61              |
| 1:E:264:LEU:HD12 | 1:E:358:LEU:CD1  | 2.31                     | 0.61              |
| 1:E:335:TYR:O    | 1:E:339:VAL:CG2  | 2.44                     | 0.61              |
| 1:E:370:LEU:O    | 1:E:370:LEU:HD13 | 1.99                     | 0.61              |
| 2:F:33:ARG:HA    | 2:F:36:LEU:HB2   | 1.82                     | 0.61              |
| 1:B:368:TYR:CD2  | 2:C:124:LEU:HD21 | 2.32                     | 0.61              |
| 1:A:72:TYR:CZ    | 1:A:206:SER:CB   | 2.53                     | 0.61              |
| 1:A:466:THR:OG1  | 1:A:511:LEU:O    | 2.17                     | 0.61              |
| 1:E:224:LYS:HB3  | 1:E:228:TRP:CE3  | 2.36                     | 0.61              |
| 2:F:158:TYR:HD1  | 2:F:159:TRP:NE1  | 1.99                     | 0.61              |
| 1:B:598:TRP:CD2  | 2:D:98:GLY:HA2   | 2.35                     | 0.61              |
| 1:A:95:LEU:HG    | 1:A:116:MET:HE3  | 1.83                     | 0.61              |
| 1:A:451:PRO:HB2  | 1:A:540:ASN:HB3  | 1.82                     | 0.61              |
| 1:A:528:LEU:HD21 | 1:A:569:GLU:OE2  | 2.01                     | 0.61              |
| 1:E:248:ILE:HD12 | 1:E:382:PRO:HG3  | 1.83                     | 0.61              |
| 2:F:40:TYR:CD2   | 2:F:67:PHE:HD2   | 2.19                     | 0.61              |
| 1:B:81:LEU:HD22  | 1:B:87:LEU:HD21  | 1.82                     | 0.61              |
| 1:B:92:GLN:HE22  | 1:B:184:TRP:H    | 1.47                     | 0.61              |
| 1:B:598:TRP:HB2  | 2:D:58:HIS:CG    | 2.36                     | 0.61              |
| 2:D:122:PRO:HD2  | 2:D:125:PHE:CB   | 2.30                     | 0.61              |
| 1:A:95:LEU:HA    | 1:A:162:LEU:CA   | 2.30                     | 0.61              |
| 1:E:232:ILE:HG23 | 1:E:233:LYS:N    | 2.15                     | 0.61              |
| 2:F:43:ALA:O     | 2:F:47:VAL:HG23  | 2.00                     | 0.61              |
| 2:F:215:TRP:HA   | 2:F:215:TRP:HE3  | 1.66                     | 0.61              |
| 1:B:81:LEU:HD21  | 1:B:87:LEU:CG    | 2.31                     | 0.60              |
| 1:B:432:TYR:CD2  | 1:B:526:LEU:HD13 | 2.33                     | 0.60              |
| 2:C:22:LEU:HB3   | 2:C:43:ALA:HB2   | 1.82                     | 0.60              |
| 1:E:77:VAL:HG12  | 1:E:79:PHE:CE2   | 2.34                     | 0.60              |
| 1:E:364:TRP:HZ3  | 1:E:368:TYR:CD1  | 2.19                     | 0.60              |
| 1:E:451:PRO:CG   | 2:F:413:TRP:CZ3  | 2.82                     | 0.60              |
| 1:E:572:SER:OG   | 1:E:575:ILE:HD11 | 2.00                     | 0.60              |
| 2:F:103:ASN:OD1  | 2:F:115:LEU:HD21 | 2.01                     | 0.60              |
| 1:B:76:TYR:CB    | 1:B:163:THR:HA   | 2.31                     | 0.60              |
| 1:B:359:ILE:HG22 | 1:B:360:ASN:N    | 2.16                     | 0.60              |
| 2:C:11:LYS:HD2   | 1:A:585:TYR:CZ   | 2.37                     | 0.60              |
| 2:C:195:ARG:HH11 | 2:C:195:ARG:CG   | 2.14                     | 0.60              |
| 2:C:230:PHE:CA   | 2:C:233:VAL:HG23 | 2.30                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:267:PHE:C    | 2:D:270:GLY:H    | 2.08                     | 0.60              |
| 1:A:66:ASP:HA    | 1:A:67:ASP:CB    | 2.29                     | 0.60              |
| 1:A:232:ILE:HG12 | 1:A:264:LEU:HD23 | 1.80                     | 0.60              |
| 1:E:99:ARG:HA    | 1:E:142:ASN:HB3  | 1.83                     | 0.60              |
| 1:E:233:LYS:HD2  | 1:E:236:THR:OG1  | 2.01                     | 0.60              |
| 2:F:70:LEU:HD12  | 2:F:70:LEU:C     | 2.26                     | 0.60              |
| 1:B:111:SER:CB   | 1:B:142:ASN:CB   | 2.79                     | 0.60              |
| 1:B:156:TYR:N    | 3:B:708:HOH:O    | 2.34                     | 0.60              |
| 1:B:211:TYR:HD1  | 1:B:212:PRO:N    | 1.99                     | 0.60              |
| 1:A:78:ILE:CG1   | 1:A:161:LYS:HB3  | 2.28                     | 0.60              |
| 1:A:452:ILE:HG22 | 1:A:452:ILE:O    | 2.00                     | 0.60              |
| 1:A:572:SER:O    | 1:A:575:ILE:HD13 | 1.59                     | 0.60              |
| 1:E:63:PHE:CB    | 1:E:86:ASN:O     | 2.49                     | 0.60              |
| 1:E:444:GLN:NE2  | 1:E:444:GLN:O    | 2.27                     | 0.60              |
| 1:E:586:ILE:HA   | 2:F:6:ARG:O      | 2.01                     | 0.60              |
| 2:F:113:HIS:HA   | 2:F:116:ALA:HB3  | 1.83                     | 0.60              |
| 1:B:209:THR:HG23 | 1:B:210:PHE:HD1  | 1.65                     | 0.60              |
| 1:B:473:ILE:HD11 | 2:D:49:MET:HA    | 1.83                     | 0.60              |
| 2:C:305:GLN:CA   | 2:C:308:ILE:HB   | 2.30                     | 0.60              |
| 1:A:93:PHE:HB3   | 1:A:210:PHE:HB3  | 1.82                     | 0.60              |
| 1:A:97:ILE:HD11  | 1:A:116:MET:HE1  | 1.84                     | 0.60              |
| 1:E:180:LYS:HE2  | 1:E:187:ASP:HB3  | 1.83                     | 0.60              |
| 1:E:308:ASN:O    | 1:E:310:LEU:HD22 | 2.01                     | 0.60              |
| 1:B:164:ASN:ND2  | 1:B:208:TYR:HD1  | 1.97                     | 0.60              |
| 1:B:465:LEU:HD13 | 1:B:482:ILE:CG2  | 2.28                     | 0.60              |
| 2:D:217:CYS:O    | 2:D:221:ILE:HD12 | 2.02                     | 0.60              |
| 1:A:95:LEU:HG    | 1:A:116:MET:CE   | 2.31                     | 0.60              |
| 1:A:107:VAL:HG21 | 1:A:109:TYR:CZ   | 2.36                     | 0.60              |
| 1:A:232:ILE:CD1  | 1:A:264:LEU:CG   | 2.67                     | 0.60              |
| 1:A:453:GLN:HG2  | 1:A:540:ASN:OD1  | 2.00                     | 0.60              |
| 1:A:456:TYR:CB   | 1:A:537:LYS:HA   | 2.31                     | 0.60              |
| 1:A:483:GLU:HA   | 1:A:529:VAL:HG12 | 1.83                     | 0.60              |
| 2:F:89:SER:O     | 2:F:93:ILE:HG13  | 2.00                     | 0.60              |
| 2:F:249:ARG:HA   | 2:F:307:TRP:CZ2  | 2.36                     | 0.60              |
| 1:B:230:ASP:HA   | 1:B:233:LYS:HB3  | 1.83                     | 0.60              |
| 2:D:267:PHE:N    | 2:D:268:PRO:HD2  | 2.17                     | 0.60              |
| 1:A:297:SER:HB3  | 1:A:320:CYS:HA   | 1.84                     | 0.60              |
| 1:E:281:MET:HG2  | 1:E:342:LEU:HD21 | 1.79                     | 0.60              |
| 1:E:299:SER:CA   | 1:E:317:SER:CA   | 2.77                     | 0.60              |
| 1:E:447:LEU:HD12 | 1:E:575:ILE:HG21 | 1.76                     | 0.60              |
| 2:F:353:ASP:CB   | 2:F:354:PRO:CD   | 2.69                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:60:SER:O     | 1:B:216:PRO:HB3  | 2.02                     | 0.60              |
| 1:B:103:ASP:CA   | 1:B:107:VAL:O    | 2.48                     | 0.60              |
| 1:B:528:LEU:HD12 | 1:B:528:LEU:O    | 2.01                     | 0.60              |
| 2:C:96:VAL:HA    | 2:C:99:LEU:HD12  | 1.81                     | 0.60              |
| 2:C:232:ASN:HA   | 2:C:235:ILE:CD1  | 2.31                     | 0.60              |
| 1:A:483:GLU:OE1  | 1:A:531:SER:C    | 2.45                     | 0.60              |
| 1:E:107:VAL:HG21 | 1:E:266:GLN:HE21 | 1.66                     | 0.60              |
| 1:E:438:ASP:O    | 1:E:441:PHE:HE2  | 1.85                     | 0.60              |
| 2:F:117:LYS:HE2  | 2:F:117:LYS:O    | 2.01                     | 0.60              |
| 1:B:165:LEU:H    | 1:B:209:THR:HG21 | 1.66                     | 0.60              |
| 1:B:225:HIS:HD2  | 1:B:228:TRP:CE3  | 2.20                     | 0.60              |
| 1:B:465:LEU:HD11 | 1:B:482:ILE:HG22 | 1.84                     | 0.60              |
| 2:C:177:GLU:OE1  | 2:C:180:ILE:HD13 | 2.01                     | 0.60              |
| 2:D:327:MET:O    | 2:D:331:LEU:HG   | 2.02                     | 0.60              |
| 1:A:596:LYS:HB2  | 1:A:596:LYS:HZ3  | 1.67                     | 0.60              |
| 1:E:529:VAL:HG12 | 1:E:529:VAL:O    | 2.02                     | 0.60              |
| 2:F:237:ARG:HE   | 2:F:240:SER:HB2  | 1.66                     | 0.60              |
| 1:B:268:MET:SD   | 1:B:278:ILE:HD12 | 2.42                     | 0.60              |
| 1:B:598:TRP:CZ3  | 2:D:58:HIS:CE1   | 2.89                     | 0.60              |
| 2:C:125:PHE:CE2  | 2:C:150:ALA:HA   | 2.36                     | 0.60              |
| 1:A:327:SER:OG   | 1:A:329:LYS:CE   | 2.48                     | 0.60              |
| 2:F:69:ALA:O     | 2:F:73:LEU:HD12  | 2.02                     | 0.60              |
| 1:B:469:LYS:HG3  | 1:B:470:GLU:N    | 2.17                     | 0.60              |
| 2:C:254:PRO:HA   | 2:C:257:ASN:ND2  | 2.16                     | 0.60              |
| 2:C:276:LEU:HD11 | 2:C:331:LEU:CD2  | 2.31                     | 0.60              |
| 2:D:7:LEU:HD12   | 2:D:7:LEU:C      | 2.27                     | 0.60              |
| 1:E:103:ASP:HA   | 1:E:107:VAL:O    | 2.00                     | 0.60              |
| 1:E:294:ASP:HB3  | 1:E:322:TYR:HE2  | 1.65                     | 0.60              |
| 1:B:350:GLY:CA   | 1:B:357:LEU:HD13 | 2.27                     | 0.59              |
| 2:C:96:VAL:CA    | 2:C:99:LEU:HD12  | 2.32                     | 0.59              |
| 2:D:149:ARG:HG3  | 2:D:149:ARG:HH11 | 1.66                     | 0.59              |
| 1:A:162:LEU:HD21 | 1:A:210:PHE:HD2  | 1.64                     | 0.59              |
| 1:A:226:LYS:O    | 1:A:230:ASP:CA   | 2.49                     | 0.59              |
| 2:D:352:ALA:C    | 2:D:353:ASP:OD2  | 2.45                     | 0.59              |
| 1:A:95:LEU:HA    | 1:A:162:LEU:HB3  | 1.82                     | 0.59              |
| 1:B:171:SER:O    | 1:B:174:ARG:CG   | 2.43                     | 0.59              |
| 2:D:89:SER:HA    | 2:D:128:PHE:CZ   | 2.37                     | 0.59              |
| 2:D:190:TYR:O    | 2:D:190:TYR:HD1  | 1.84                     | 0.59              |
| 2:D:252:PHE:CB   | 2:D:307:TRP:HH2  | 2.15                     | 0.59              |
| 1:A:63:PHE:CE2   | 1:A:213:ILE:C    | 2.79                     | 0.59              |
| 1:A:120:ASN:O    | 1:A:120:ASN:ND2  | 2.22                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:SER:HB2  | 1:A:208:TYR:HE2  | 1.67                     | 0.59              |
| 1:E:89:VAL:CG1   | 1:E:93:PHE:CE1   | 2.86                     | 0.59              |
| 1:E:107:VAL:HG22 | 1:E:266:GLN:HE21 | 1.66                     | 0.59              |
| 1:E:213:ILE:HG22 | 1:E:213:ILE:O    | 2.01                     | 0.59              |
| 1:E:226:LYS:CA   | 1:E:229:MET:HB3  | 2.28                     | 0.59              |
| 1:E:571:ALA:CB   | 1:E:586:ILE:HD13 | 2.28                     | 0.59              |
| 2:F:83:THR:HA    | 2:F:86:LEU:HD12  | 1.83                     | 0.59              |
| 1:B:368:TYR:HB2  | 2:C:124:LEU:HD21 | 1.84                     | 0.59              |
| 1:A:473:ILE:HG22 | 1:A:474:GLY:N    | 2.16                     | 0.59              |
| 1:A:479:GLU:O    | 1:A:482:ILE:CG1  | 2.49                     | 0.59              |
| 1:A:483:GLU:OE1  | 1:A:531:SER:N    | 2.35                     | 0.59              |
| 1:A:530:HIS:CD2  | 1:A:531:SER:CB   | 2.85                     | 0.59              |
| 1:A:530:HIS:O    | 1:A:540:ASN:HB2  | 2.03                     | 0.59              |
| 1:A:596:LYS:CB   | 1:A:596:LYS:HZ3  | 2.16                     | 0.59              |
| 1:E:445:PRO:CG   | 1:E:448:PHE:CZ   | 2.85                     | 0.59              |
| 2:F:9:PRO:HG2    | 2:F:10:TRP:CZ3   | 2.36                     | 0.59              |
| 2:F:301:PHE:CE1  | 2:F:304:ALA:CB   | 2.86                     | 0.59              |
| 1:B:511:LEU:HD22 | 1:B:512:PRO:O    | 2.02                     | 0.59              |
| 1:B:544:PRO:HG2  | 1:B:545:GLN:H    | 1.66                     | 0.59              |
| 2:D:12:SER:OG    | 2:D:14:ASP:HB2   | 2.03                     | 0.59              |
| 2:D:230:PHE:O    | 2:D:233:VAL:HB   | 2.03                     | 0.59              |
| 1:A:322:TYR:HB2  | 1:A:523:PHE:CD1  | 2.37                     | 0.59              |
| 1:E:173:GLY:HA2  | 1:E:176:CYS:O    | 2.01                     | 0.59              |
| 1:E:264:LEU:HD11 | 1:E:358:LEU:HD11 | 1.81                     | 0.59              |
| 1:E:322:TYR:CZ   | 1:E:324:GLY:HA2  | 2.36                     | 0.59              |
| 2:F:212:LYS:O    | 2:F:216:THR:HG23 | 2.03                     | 0.59              |
| 2:C:11:LYS:HG3   | 1:A:585:TYR:CD2  | 2.38                     | 0.59              |
| 2:C:232:ASN:HA   | 2:C:278:LYS:HZ3  | 1.67                     | 0.59              |
| 1:A:385:VAL:O    | 1:A:404:ASN:OD1  | 2.20                     | 0.59              |
| 1:A:524:PHE:CE2  | 1:A:525:ARG:HG2  | 2.37                     | 0.59              |
| 2:F:122:PRO:CD   | 2:F:125:PHE:CE2  | 2.85                     | 0.59              |
| 2:F:197:ASN:C    | 2:F:198:ILE:HD12 | 2.27                     | 0.59              |
| 2:F:245:TRP:CB   | 2:F:247:HIS:CD2  | 2.86                     | 0.59              |
| 1:B:107:VAL:HG23 | 1:B:109:TYR:CE2  | 2.37                     | 0.59              |
| 1:B:226:LYS:O    | 1:B:230:ASP:N    | 2.31                     | 0.59              |
| 1:B:310:LEU:O    | 1:B:311:SER:HB2  | 2.02                     | 0.59              |
| 2:C:80:LEU:HD23  | 2:D:48:GLU:OE1   | 2.03                     | 0.59              |
| 2:C:230:PHE:C    | 2:C:233:VAL:HG23 | 2.28                     | 0.59              |
| 2:C:245:TRP:CE2  | 2:C:247:HIS:CB   | 2.85                     | 0.59              |
| 1:A:95:LEU:CD2   | 1:A:118:PHE:HE2  | 2.16                     | 0.59              |
| 1:A:389:ASN:OD1  | 1:A:408:LEU:HA   | 2.02                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:94:VAL:CG2   | 1:E:165:LEU:HD13 | 2.33                     | 0.59              |
| 1:E:283:LEU:CD1  | 1:E:339:VAL:CG1  | 2.81                     | 0.59              |
| 1:E:466:THR:HG21 | 1:E:516:PHE:CG   | 2.37                     | 0.59              |
| 2:F:301:PHE:CD1  | 2:F:304:ALA:CB   | 2.86                     | 0.59              |
| 1:B:112:GLY:H    | 1:B:140:LEU:CB   | 2.15                     | 0.59              |
| 1:B:223:ILE:CD1  | 1:B:224:LYS:H    | 2.09                     | 0.59              |
| 2:D:37:TYR:HB3   | 2:D:71:MET:HE1   | 1.85                     | 0.59              |
| 2:D:328:ILE:HD11 | 2:D:356:ILE:HG22 | 1.85                     | 0.59              |
| 1:A:133:GLN:HE21 | 1:A:134:VAL:N    | 2.00                     | 0.59              |
| 1:A:250:ILE:CD1  | 1:A:373:THR:HG21 | 2.32                     | 0.59              |
| 1:A:325:PHE:CD2  | 1:A:562:ASN:CB   | 2.86                     | 0.59              |
| 1:A:346:TYR:O    | 1:A:350:GLY:CA   | 2.50                     | 0.59              |
| 1:A:525:ARG:CD   | 1:A:544:PRO:HG2  | 2.31                     | 0.59              |
| 1:E:281:MET:CE   | 1:E:342:LEU:HD23 | 2.32                     | 0.59              |
| 1:E:321:HIS:HE1  | 1:E:522:GLU:OE2  | 1.85                     | 0.59              |
| 1:E:340:GLU:CD   | 1:E:379:ARG:HH11 | 2.10                     | 0.59              |
| 1:E:364:TRP:CE3  | 1:E:369:GLY:CA   | 2.85                     | 0.59              |
| 2:F:23:PHE:O     | 2:F:24:PHE:HD2   | 1.86                     | 0.59              |
| 1:B:248:ILE:HB   | 1:B:385:VAL:HG22 | 1.84                     | 0.59              |
| 1:B:433:PHE:HB3  | 1:B:446:LEU:HD11 | 1.84                     | 0.59              |
| 2:C:100:LEU:O    | 2:C:103:ASN:CB   | 2.51                     | 0.59              |
| 2:C:251:LEU:O    | 2:C:254:PRO:HD2  | 2.02                     | 0.59              |
| 2:C:304:ALA:O    | 2:C:307:TRP:CB   | 2.51                     | 0.59              |
| 1:A:63:PHE:HZ    | 1:A:212:PRO:CG   | 2.15                     | 0.59              |
| 1:A:334:ARG:HG3  | 1:A:513:TYR:CZ   | 2.34                     | 0.59              |
| 1:A:368:TYR:HE1  | 1:A:372:LEU:HD23 | 1.64                     | 0.59              |
| 1:A:533:ASP:OD1  | 1:A:535:GLU:N    | 2.35                     | 0.59              |
| 1:E:128:LEU:C    | 1:E:129:ILE:HD12 | 2.27                     | 0.59              |
| 1:E:283:LEU:HD13 | 1:E:339:VAL:HG13 | 1.85                     | 0.59              |
| 2:F:110:ILE:CG1  | 2:F:115:LEU:HD11 | 2.27                     | 0.59              |
| 2:F:325:SER:C    | 2:F:328:ILE:HD13 | 2.28                     | 0.59              |
| 1:B:118:PHE:CD1  | 1:B:306:HIS:O    | 2.51                     | 0.59              |
| 1:B:225:HIS:HB2  | 1:B:227:ASN:ND2  | 2.18                     | 0.59              |
| 1:A:63:PHE:CZ    | 1:A:212:PRO:CG   | 2.86                     | 0.59              |
| 1:A:170:GLU:CG   | 1:A:185:GLN:CD   | 2.76                     | 0.59              |
| 1:A:238:LEU:HD12 | 1:A:238:LEU:O    | 2.02                     | 0.59              |
| 1:A:286:GLY:CA   | 1:A:326:ASN:OD1  | 2.51                     | 0.59              |
| 1:E:301:ILE:HG12 | 1:E:315:THR:CG2  | 2.33                     | 0.59              |
| 1:E:468:LEU:HD23 | 1:E:469:LYS:H    | 1.68                     | 0.59              |
| 2:F:118:LYS:HB2  | 2:F:118:LYS:NZ   | 2.13                     | 0.59              |
| 1:B:327:SER:HB3  | 1:B:329:LYS:HE2  | 1.84                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:487:VAL:O    | 1:B:527:ALA:O    | 2.21                     | 0.58              |
| 2:C:137:LEU:HD12 | 2:C:138:PRO:HD3  | 1.84                     | 0.58              |
| 2:C:227:MET:SD   | 2:C:227:MET:N    | 2.60                     | 0.58              |
| 2:C:334:THR:OG1  | 2:C:339:ASN:OD1  | 2.20                     | 0.58              |
| 2:D:246:GLU:OE1  | 2:D:246:GLU:HA   | 2.01                     | 0.58              |
| 1:A:107:VAL:CG2  | 1:A:109:TYR:CZ   | 2.86                     | 0.58              |
| 1:E:93:PHE:HB3   | 1:E:210:PHE:CG   | 2.37                     | 0.58              |
| 1:E:228:TRP:HZ3  | 1:E:263:LEU:HD22 | 1.66                     | 0.58              |
| 1:E:547:ARG:O    | 1:E:548:THR:HG23 | 2.02                     | 0.58              |
| 1:B:239:TYR:OH   | 1:B:276:LEU:HD23 | 2.03                     | 0.58              |
| 1:B:529:VAL:HG13 | 1:B:529:VAL:O    | 2.03                     | 0.58              |
| 1:B:598:TRP:CB   | 2:D:58:HIS:HB2   | 2.33                     | 0.58              |
| 2:C:10:TRP:N     | 2:C:50:TYR:HE1   | 2.00                     | 0.58              |
| 2:C:230:PHE:O    | 2:C:233:VAL:HG23 | 2.02                     | 0.58              |
| 2:C:271:LEU:HG   | 2:C:275:MET:HE3  | 1.85                     | 0.58              |
| 1:E:328:PRO:HB3  | 1:E:335:TYR:CE2  | 2.38                     | 0.58              |
| 1:E:583:LEU:CB   | 1:E:586:ILE:HB   | 2.33                     | 0.58              |
| 1:B:90:LYS:CE    | 1:B:213:ILE:HD11 | 2.33                     | 0.58              |
| 1:B:351:GLU:N    | 1:B:351:GLU:OE1  | 2.35                     | 0.58              |
| 2:C:11:LYS:HG3   | 1:A:584:PRO:O    | 2.04                     | 0.58              |
| 1:A:237:GLU:OE1  | 1:A:237:GLU:N    | 2.33                     | 0.58              |
| 1:A:572:SER:OG   | 1:A:575:ILE:CD1  | 2.51                     | 0.58              |
| 1:E:289:GLU:C    | 1:E:290:TYR:HD2  | 2.12                     | 0.58              |
| 2:F:33:ARG:HH21  | 2:F:33:ARG:HB3   | 1.68                     | 0.58              |
| 2:F:312:ALA:O    | 2:F:316:ILE:HG13 | 2.04                     | 0.58              |
| 1:B:257:LYS:O    | 1:B:260:PHE:HB3  | 2.02                     | 0.58              |
| 1:B:532:ILE:HG23 | 1:B:539:MET:HB3  | 1.85                     | 0.58              |
| 2:C:417:PRO:C    | 2:C:419:GLY:N    | 2.56                     | 0.58              |
| 2:D:24:PHE:CE2   | 2:D:155:TRP:CG   | 2.85                     | 0.58              |
| 2:D:345:LYS:HA   | 2:D:348:SER:OG   | 2.03                     | 0.58              |
| 1:A:170:GLU:CB   | 1:A:185:GLN:NE2  | 2.67                     | 0.58              |
| 1:E:117:LYS:HD2  | 1:E:439:PHE:CE2  | 2.38                     | 0.58              |
| 1:E:288:PRO:HB2  | 1:E:291:SER:O    | 2.03                     | 0.58              |
| 1:E:290:TYR:CD1  | 1:E:301:ILE:CD1  | 2.86                     | 0.58              |
| 1:E:365:ILE:CD1  | 1:E:393:LEU:HD11 | 2.33                     | 0.58              |
| 1:E:373:THR:CG2  | 1:E:377:ILE:HD11 | 2.31                     | 0.58              |
| 1:E:530:HIS:NE2  | 1:E:570:ILE:HG21 | 2.13                     | 0.58              |
| 2:F:22:LEU:HD13  | 2:F:43:ALA:N     | 2.19                     | 0.58              |
| 2:F:130:HIS:HB2  | 3:F:509:HOH:O    | 2.02                     | 0.58              |
| 1:B:121:PRO:CG   | 1:B:124:SER:HB3  | 2.33                     | 0.58              |
| 1:B:225:HIS:H    | 1:B:225:HIS:CD2  | 2.22                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:598:TRP:CH2  | 2:D:98:GLY:N     | 2.71                     | 0.58              |
| 2:D:246:GLU:H    | 2:D:310:TRP:HH2  | 1.51                     | 0.58              |
| 1:A:358:LEU:O    | 1:A:359:ILE:HG12 | 2.03                     | 0.58              |
| 1:A:385:VAL:O    | 1:A:404:ASN:CG   | 2.46                     | 0.58              |
| 1:E:104:ILE:CG2  | 1:E:129:ILE:HD11 | 2.33                     | 0.58              |
| 1:B:250:ILE:CG2  | 1:B:365:ILE:CG1  | 2.81                     | 0.58              |
| 2:C:15:GLU:O     | 2:C:16:VAL:C     | 2.46                     | 0.58              |
| 2:C:18:TYR:CE2   | 2:C:22:LEU:CD1   | 2.86                     | 0.58              |
| 2:C:119:ILE:O    | 2:C:120:ASP:HB2  | 2.02                     | 0.58              |
| 1:E:100:GLY:C    | 1:E:111:SER:OG   | 2.45                     | 0.58              |
| 1:E:445:PRO:HG2  | 1:E:448:PHE:CZ   | 2.38                     | 0.58              |
| 1:B:121:PRO:HB2  | 1:B:182:LEU:HD21 | 1.86                     | 0.58              |
| 1:B:257:LYS:O    | 1:B:260:PHE:CA   | 2.52                     | 0.58              |
| 1:B:328:PRO:CB   | 1:B:335:TYR:HE2  | 2.11                     | 0.58              |
| 1:B:572:SER:H    | 1:B:575:ILE:CD1  | 2.15                     | 0.58              |
| 1:B:598:TRP:CH2  | 2:D:98:GLY:HA2   | 2.38                     | 0.58              |
| 2:C:90:MET:CE    | 2:D:132:ALA:HB1  | 2.33                     | 0.58              |
| 2:C:95:PHE:CE1   | 2:C:99:LEU:HD11  | 2.39                     | 0.58              |
| 1:A:63:PHE:HB3   | 1:A:88:ILE:CG1   | 2.32                     | 0.58              |
| 1:A:382:PRO:CD   | 1:A:401:LYS:HZ3  | 2.17                     | 0.58              |
| 1:A:436:ILE:HG23 | 1:A:437:ASP:N    | 2.17                     | 0.58              |
| 1:A:472:GLY:O    | 1:A:473:ILE:HG12 | 2.04                     | 0.58              |
| 1:A:572:SER:O    | 1:A:575:ILE:CG1  | 2.52                     | 0.58              |
| 1:E:282:ASP:OD2  | 1:E:360:ASN:ND2  | 2.36                     | 0.58              |
| 1:B:102:ILE:O    | 1:B:109:TYR:N    | 2.33                     | 0.58              |
| 1:B:357:LEU:O    | 1:B:358:LEU:HD22 | 2.03                     | 0.58              |
| 1:B:585:TYR:CD1  | 2:D:8:THR:O      | 2.57                     | 0.58              |
| 2:C:256:MET:O    | 2:C:260:ILE:HG12 | 2.03                     | 0.58              |
| 2:C:416:LYS:HZ3  | 2:C:416:LYS:HB3  | 1.69                     | 0.58              |
| 2:D:249:ARG:O    | 2:D:253:GLU:CB   | 2.52                     | 0.58              |
| 1:A:232:ILE:HG12 | 1:A:264:LEU:HA   | 1.84                     | 0.58              |
| 1:E:111:SER:OG   | 1:E:142:ASN:ND2  | 2.29                     | 0.58              |
| 1:E:364:TRP:CH2  | 1:E:368:TYR:HD1  | 2.22                     | 0.58              |
| 1:E:586:ILE:HG12 | 2:F:7:LEU:HA     | 1.84                     | 0.58              |
| 2:F:321:ASP:O    | 2:F:325:SER:OG   | 2.19                     | 0.58              |
| 1:B:138:SER:HA   | 1:B:139:LEU:CB   | 2.33                     | 0.58              |
| 1:B:427:LEU:HD23 | 1:B:427:LEU:O    | 2.03                     | 0.58              |
| 1:B:510:LEU:HD23 | 1:B:511:LEU:N    | 2.19                     | 0.58              |
| 1:B:583:LEU:HB2  | 1:B:586:ILE:N    | 2.19                     | 0.58              |
| 2:C:22:LEU:CD2   | 2:C:43:ALA:HA    | 2.33                     | 0.58              |
| 2:C:229:ASN:ND2  | 2:C:229:ASN:O    | 2.37                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:145:THR:CG2  | 3:D:506:HOH:O    | 2.34                     | 0.58              |
| 2:D:312:ALA:O    | 2:D:316:ILE:HG13 | 2.03                     | 0.58              |
| 1:A:269:LEU:HD23 | 1:A:278:ILE:CG2  | 2.33                     | 0.58              |
| 1:A:492:VAL:HG13 | 1:A:557:ILE:HG12 | 1.86                     | 0.58              |
| 1:E:228:TRP:CZ3  | 1:E:263:LEU:HD23 | 2.35                     | 0.58              |
| 1:E:340:GLU:CG   | 1:E:379:ARG:NH1  | 2.45                     | 0.58              |
| 1:E:524:PHE:CZ   | 1:E:546:PHE:HB2  | 2.30                     | 0.58              |
| 1:B:118:PHE:CD1  | 1:B:306:HIS:C    | 2.82                     | 0.57              |
| 2:D:259:PHE:CZ   | 2:D:268:PRO:CA   | 2.87                     | 0.57              |
| 1:E:225:HIS:CD2  | 1:E:228:TRP:CD1  | 2.92                     | 0.57              |
| 2:F:20:LYS:CB    | 2:F:159:TRP:CE3  | 2.87                     | 0.57              |
| 2:F:20:LYS:CB    | 2:F:159:TRP:CZ3  | 2.87                     | 0.57              |
| 2:F:53:ARG:O     | 2:F:54:THR:HG23  | 2.04                     | 0.57              |
| 2:F:120:ASP:HB3  | 2:F:157:HIS:NE2  | 2.19                     | 0.57              |
| 2:D:93:ILE:HG12  | 2:D:129:ARG:HA   | 1.85                     | 0.57              |
| 1:A:98:GLN:O     | 1:A:142:ASN:CB   | 2.52                     | 0.57              |
| 1:A:420:SER:C    | 1:A:423:GLN:H    | 2.12                     | 0.57              |
| 1:A:451:PRO:O    | 1:A:541:LEU:C    | 2.44                     | 0.57              |
| 1:E:72:TYR:HE2   | 1:E:206:SER:HG   | 1.53                     | 0.57              |
| 1:E:225:HIS:N    | 1:E:228:TRP:HB3  | 2.19                     | 0.57              |
| 2:F:72:MET:HA    | 2:F:75:SER:OG    | 2.04                     | 0.57              |
| 2:C:10:TRP:HD1   | 2:C:13:SER:HA    | 1.65                     | 0.57              |
| 2:D:350:PHE:C    | 2:D:351:SER:HG   | 2.06                     | 0.57              |
| 1:A:298:LEU:HD23 | 1:A:298:LEU:O    | 2.05                     | 0.57              |
| 1:E:78:ILE:CD1   | 1:E:161:LYS:CG   | 2.78                     | 0.57              |
| 1:E:245:ILE:HG13 | 1:E:245:ILE:O    | 2.03                     | 0.57              |
| 1:E:365:ILE:CD1  | 1:E:366:LYS:HB2  | 2.34                     | 0.57              |
| 1:E:397:ILE:O    | 1:E:397:ILE:HG22 | 2.04                     | 0.57              |
| 1:B:490:PHE:C    | 1:B:557:ILE:HD12 | 2.28                     | 0.57              |
| 2:C:28:ARG:N     | 2:C:29:GLU:OE2   | 2.37                     | 0.57              |
| 2:D:89:SER:O     | 2:D:93:ILE:HG13  | 2.04                     | 0.57              |
| 1:E:490:PHE:CD1  | 1:E:521:THR:HG22 | 2.36                     | 0.57              |
| 1:E:523:PHE:CD1  | 1:E:524:PHE:N    | 2.73                     | 0.57              |
| 1:E:525:ARG:HH21 | 1:E:525:ARG:CG   | 2.16                     | 0.57              |
| 2:C:53:ARG:HH11  | 2:C:53:ARG:CG    | 2.13                     | 0.57              |
| 2:C:96:VAL:HA    | 2:C:99:LEU:HD11  | 1.87                     | 0.57              |
| 2:D:58:HIS:CE1   | 2:D:98:GLY:C     | 2.82                     | 0.57              |
| 2:D:127:GLU:OE1  | 1:A:366:LYS:O    | 2.22                     | 0.57              |
| 1:E:436:ILE:HG21 | 1:E:440:LYS:HB3  | 1.86                     | 0.57              |
| 2:F:52:SER:OG    | 2:F:57:SER:OG    | 2.17                     | 0.57              |
| 2:F:249:ARG:CB   | 2:F:307:TRP:CE2  | 2.87                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:235:ILE:HA   | 2:C:238:ILE:HD12 | 1.86                     | 0.57              |
| 2:C:249:ARG:CA   | 2:C:307:TRP:CZ2  | 2.85                     | 0.57              |
| 2:C:269:LEU:HD22 | 2:C:323:LEU:HG   | 1.85                     | 0.57              |
| 2:C:305:GLN:O    | 2:C:308:ILE:CB   | 2.50                     | 0.57              |
| 2:D:310:TRP:HD1  | 2:D:313:ILE:HD12 | 1.69                     | 0.57              |
| 1:A:451:PRO:O    | 1:A:541:LEU:N    | 2.37                     | 0.57              |
| 1:E:74:HIS:CD2   | 1:E:75:ASP:N     | 2.73                     | 0.57              |
| 1:E:182:LEU:HG   | 1:E:419:TYR:HE1  | 1.70                     | 0.57              |
| 1:E:183:PHE:CD2  | 1:E:183:PHE:N    | 2.73                     | 0.57              |
| 2:F:328:ILE:HA   | 2:F:331:LEU:CD2  | 2.35                     | 0.57              |
| 1:B:64:SER:N     | 1:B:86:ASN:O     | 2.37                     | 0.57              |
| 1:B:468:LEU:CD1  | 1:B:561:GLY:N    | 2.46                     | 0.57              |
| 2:C:419:GLY:O    | 2:C:420:VAL:HB   | 2.05                     | 0.57              |
| 2:D:356:ILE:O    | 2:D:360:ILE:HG13 | 2.04                     | 0.57              |
| 1:A:588:PHE:N    | 1:A:588:PHE:CD2  | 2.73                     | 0.57              |
| 1:E:92:GLN:OE1   | 1:E:167:THR:CG2  | 2.53                     | 0.57              |
| 2:C:53:ARG:HG2   | 2:C:53:ARG:NH1   | 2.16                     | 0.57              |
| 2:C:141:GLU:OE1  | 2:C:141:GLU:HA   | 2.05                     | 0.57              |
| 2:C:218:ILE:CG2  | 2:C:255:MET:CE   | 2.83                     | 0.57              |
| 2:D:27:ASP:O     | 2:D:31:ILE:HD13  | 2.05                     | 0.57              |
| 2:D:140:LEU:HD23 | 2:D:141:GLU:N    | 2.19                     | 0.57              |
| 1:A:183:PHE:CD2  | 1:A:183:PHE:N    | 2.73                     | 0.57              |
| 1:A:524:PHE:HD2  | 1:A:525:ARG:N    | 1.96                     | 0.57              |
| 1:E:468:LEU:O    | 1:E:469:LYS:HB3  | 2.04                     | 0.57              |
| 2:F:9:PRO:CG     | 2:F:10:TRP:CZ3   | 2.88                     | 0.57              |
| 1:B:469:LYS:CG   | 1:B:470:GLU:H    | 2.16                     | 0.57              |
| 2:C:276:LEU:HD11 | 2:C:331:LEU:HD23 | 1.86                     | 0.57              |
| 2:D:259:PHE:CZ   | 2:D:268:PRO:HA   | 2.40                     | 0.57              |
| 2:D:266:ASP:C    | 2:D:268:PRO:CD   | 2.78                     | 0.57              |
| 1:E:436:ILE:HG23 | 1:E:437:ASP:N    | 2.20                     | 0.57              |
| 2:F:254:PRO:HG2  | 2:F:255:MET:SD   | 2.45                     | 0.57              |
| 2:F:305:GLN:O    | 2:F:309:ARG:HG3  | 2.04                     | 0.57              |
| 1:B:437:ASP:HB3  | 1:B:440:LYS:HZ2  | 1.69                     | 0.57              |
| 2:C:24:PHE:HE2   | 2:C:67:PHE:HZ    | 1.52                     | 0.57              |
| 2:C:280:TYR:CD2  | 2:C:281:GLU:N    | 2.73                     | 0.57              |
| 2:D:51:SER:HA    | 2:D:56:VAL:HG13  | 1.87                     | 0.57              |
| 2:D:79:GLY:C     | 1:A:472:GLY:HA3  | 2.30                     | 0.57              |
| 1:A:294:ASP:OD1  | 1:A:325:PHE:O    | 2.23                     | 0.57              |
| 1:E:104:ILE:CG2  | 1:E:129:ILE:CD1  | 2.80                     | 0.57              |
| 1:E:225:HIS:O    | 1:E:228:TRP:N    | 2.38                     | 0.57              |
| 1:B:211:TYR:CD1  | 1:B:212:PRO:N    | 2.73                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:244:SER:HA   | 1:B:356:SER:CB   | 2.35                     | 0.56              |
| 1:B:368:TYR:CB   | 2:C:124:LEU:CD2  | 2.81                     | 0.56              |
| 1:B:502:LEU:HB2  | 1:B:509:PRO:CB   | 2.29                     | 0.56              |
| 2:D:154:VAL:CG2  | 2:D:159:TRP:CD1  | 2.86                     | 0.56              |
| 2:D:276:LEU:HD21 | 2:D:333:LYS:CB   | 2.31                     | 0.56              |
| 1:A:111:SER:CB   | 1:A:141:GLU:C    | 2.78                     | 0.56              |
| 1:E:172:ILE:HD12 | 1:E:182:LEU:HD12 | 1.87                     | 0.56              |
| 1:E:173:GLY:HA3  | 1:E:180:LYS:HB2  | 1.86                     | 0.56              |
| 1:E:400:PRO:O    | 1:E:401:LYS:CG   | 2.53                     | 0.56              |
| 1:B:280:PHE:HB3  | 1:B:299:SER:O    | 2.05                     | 0.56              |
| 1:B:432:TYR:CD2  | 1:B:526:LEU:HD12 | 2.39                     | 0.56              |
| 2:C:9:PRO:CG     | 2:C:10:TRP:CE3   | 2.86                     | 0.56              |
| 2:C:18:TYR:HD2   | 2:C:18:TYR:O     | 1.88                     | 0.56              |
| 1:A:294:ASP:CG   | 1:A:325:PHE:C    | 2.73                     | 0.56              |
| 1:E:298:LEU:HD23 | 1:E:318:THR:HB   | 1.87                     | 0.56              |
| 1:E:451:PRO:O    | 2:F:409:SER:HA   | 2.05                     | 0.56              |
| 2:F:364:LEU:O    | 2:F:368:GLN:CB   | 2.52                     | 0.56              |
| 1:B:102:ILE:C    | 1:B:108:ILE:HG23 | 2.30                     | 0.56              |
| 1:B:327:SER:CB   | 1:B:329:LYS:HE2  | 2.35                     | 0.56              |
| 1:B:368:TYR:HE1  | 1:B:372:LEU:CD1  | 2.18                     | 0.56              |
| 2:D:21:GLY:O     | 2:D:24:PHE:O     | 2.21                     | 0.56              |
| 1:A:63:PHE:CE2   | 1:A:213:ILE:O    | 2.59                     | 0.56              |
| 1:A:119:ILE:HG13 | 1:A:309:HIS:CE1  | 2.40                     | 0.56              |
| 1:A:304:VAL:HG21 | 1:A:306:HIS:NE2  | 2.21                     | 0.56              |
| 1:A:359:ILE:HG22 | 1:A:360:ASN:N    | 2.20                     | 0.56              |
| 1:A:466:THR:OG1  | 1:A:511:LEU:HD23 | 2.02                     | 0.56              |
| 1:A:489:ILE:HG22 | 1:A:524:PHE:HB3  | 1.87                     | 0.56              |
| 1:E:184:TRP:CD2  | 1:E:211:TYR:HB2  | 2.33                     | 0.56              |
| 1:E:490:PHE:O    | 1:E:557:ILE:N    | 2.38                     | 0.56              |
| 2:F:251:LEU:C    | 2:F:254:PRO:HD2  | 2.30                     | 0.56              |
| 1:B:441:PHE:CD2  | 1:B:441:PHE:N    | 2.73                     | 0.56              |
| 2:C:140:LEU:HD12 | 2:C:140:LEU:C    | 2.28                     | 0.56              |
| 2:D:37:TYR:OH    | 2:D:74:GLU:HG3   | 2.05                     | 0.56              |
| 2:D:235:ILE:O    | 2:D:238:ILE:HG22 | 2.06                     | 0.56              |
| 1:A:95:LEU:CA    | 1:A:162:LEU:CB   | 2.81                     | 0.56              |
| 1:A:224:LYS:CB   | 1:A:228:TRP:CE3  | 2.88                     | 0.56              |
| 2:F:253:GLU:HA   | 2:F:256:MET:HG3  | 1.87                     | 0.56              |
| 1:B:239:TYR:CD1  | 1:B:268:MET:HB3  | 2.41                     | 0.56              |
| 1:B:384:HIS:O    | 1:B:385:VAL:HG23 | 2.06                     | 0.56              |
| 2:C:94:ARG:HG3   | 1:A:598:TRP:CH2  | 2.39                     | 0.56              |
| 2:C:218:ILE:CG2  | 2:C:255:MET:HE2  | 2.35                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:76:PHE:CD2   | 2:D:77:GLU:N     | 2.74                     | 0.56              |
| 2:D:410:HIS:CD2  | 2:D:413:TRP:CD1  | 2.80                     | 0.56              |
| 1:E:290:TYR:CE1  | 1:E:301:ILE:HD13 | 2.40                     | 0.56              |
| 1:B:293:THR:HG21 | 1:B:425:ARG:HH11 | 1.71                     | 0.56              |
| 1:B:484:ALA:HB3  | 1:B:585:TYR:HE2  | 1.67                     | 0.56              |
| 2:C:63:THR:HG21  | 2:C:159:TRP:NE1  | 2.09                     | 0.56              |
| 2:C:90:MET:HE2   | 2:D:132:ALA:HB1  | 1.88                     | 0.56              |
| 2:C:252:PHE:O    | 2:C:256:MET:N    | 2.35                     | 0.56              |
| 1:E:567:ILE:HG22 | 1:E:571:ALA:HB3  | 1.87                     | 0.56              |
| 1:E:587:THR:N    | 2:F:8:THR:HG23   | 2.21                     | 0.56              |
| 1:B:331:GLN:CB   | 1:B:334:ARG:HB2  | 2.26                     | 0.56              |
| 1:B:432:TYR:CE1  | 1:B:544:PRO:HG3  | 2.41                     | 0.56              |
| 2:C:53:ARG:HD3   | 1:A:485:THR:CG2  | 2.35                     | 0.56              |
| 2:D:74:GLU:OE2   | 2:D:144:LYS:CE   | 2.54                     | 0.56              |
| 1:A:110:HIS:O    | 1:A:113:VAL:HG12 | 2.06                     | 0.56              |
| 1:A:364:TRP:CE3  | 1:A:369:GLY:N    | 2.73                     | 0.56              |
| 1:E:451:PRO:CD   | 2:F:413:TRP:CE2  | 2.88                     | 0.56              |
| 2:F:239:VAL:O    | 2:F:242:LYS:CB   | 2.54                     | 0.56              |
| 1:B:107:VAL:CG2  | 1:B:266:GLN:NE2  | 2.55                     | 0.56              |
| 1:B:167:THR:CB   | 1:B:439:PHE:O    | 2.53                     | 0.56              |
| 1:B:227:ASN:HA   | 1:B:230:ASP:HB3  | 1.88                     | 0.56              |
| 1:B:387:TYR:HD1  | 1:B:388:LEU:N    | 2.03                     | 0.56              |
| 2:C:299:GLN:CB   | 2:C:303:CYS:SG   | 2.94                     | 0.56              |
| 2:D:95:PHE:CE1   | 2:D:99:LEU:HD11  | 2.41                     | 0.56              |
| 2:D:259:PHE:HZ   | 2:D:268:PRO:CB   | 2.10                     | 0.56              |
| 1:A:475:MET:HE2  | 1:A:478:LEU:CD2  | 2.31                     | 0.56              |
| 1:E:165:LEU:O    | 1:E:209:THR:HG21 | 2.06                     | 0.56              |
| 1:E:269:LEU:HD21 | 1:E:278:ILE:HG22 | 1.88                     | 0.56              |
| 1:B:81:LEU:CD2   | 1:B:87:LEU:CG    | 2.84                     | 0.56              |
| 1:B:121:PRO:HD3  | 1:B:308:ASN:CB   | 2.27                     | 0.56              |
| 1:B:132:THR:C    | 1:B:134:VAL:HG22 | 2.31                     | 0.56              |
| 1:B:260:PHE:HE2  | 1:B:386:ILE:HG21 | 1.70                     | 0.56              |
| 2:C:232:ASN:CB   | 2:C:278:LYS:NZ   | 2.69                     | 0.56              |
| 2:C:406:SER:O    | 2:C:406:SER:OG   | 2.22                     | 0.56              |
| 2:C:420:VAL:C    | 1:A:531:SER:HB2  | 2.31                     | 0.56              |
| 2:D:96:VAL:HG13  | 2:D:121:LEU:HD22 | 1.88                     | 0.56              |
| 1:A:203:LEU:O    | 1:A:204:ALA:HB3  | 2.06                     | 0.56              |
| 1:A:211:TYR:HD1  | 1:A:212:PRO:HD2  | 1.71                     | 0.56              |
| 1:A:329:LYS:O    | 1:A:332:PRO:HD3  | 2.06                     | 0.56              |
| 1:A:451:PRO:CB   | 1:A:540:ASN:HB3  | 2.36                     | 0.56              |
| 1:E:351:GLU:CD   | 1:E:352:LEU:H    | 2.11                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:437:ASP:HB3  | 1:E:440:LYS:HZ1  | 1.64                     | 0.56              |
| 1:E:448:PHE:N    | 1:E:448:PHE:CD2  | 2.73                     | 0.56              |
| 2:F:188:LYS:O    | 2:F:191:ARG:HB3  | 2.06                     | 0.56              |
| 2:F:272:ILE:CG1  | 2:F:315:GLN:HE22 | 2.18                     | 0.56              |
| 1:B:172:ILE:HD12 | 1:B:179:PHE:HB3  | 0.72                     | 0.56              |
| 1:B:179:PHE:CE1  | 1:B:427:LEU:HD12 | 2.41                     | 0.56              |
| 1:B:387:TYR:CD1  | 1:B:388:LEU:N    | 2.73                     | 0.56              |
| 2:C:24:PHE:HE2   | 2:C:67:PHE:CZ    | 2.24                     | 0.56              |
| 2:D:44:ILE:HD13  | 2:D:68:SER:HB2   | 1.88                     | 0.56              |
| 2:D:266:ASP:O    | 2:D:269:LEU:N    | 2.39                     | 0.56              |
| 1:A:236:THR:HG21 | 1:A:267:HIS:HB3  | 1.88                     | 0.56              |
| 1:A:399:ILE:O    | 1:A:401:LYS:C    | 2.48                     | 0.56              |
| 1:E:219:THR:HG22 | 1:E:220:VAL:N    | 2.20                     | 0.56              |
| 1:E:386:ILE:HG23 | 1:E:406:ILE:HD11 | 1.87                     | 0.56              |
| 1:E:426:LEU:HA   | 1:E:429:THR:OG1  | 2.05                     | 0.56              |
| 1:E:454:VAL:CG2  | 1:E:539:MET:HG3  | 2.36                     | 0.56              |
| 1:E:567:ILE:HD12 | 1:E:567:ILE:H    | 1.70                     | 0.56              |
| 1:B:81:LEU:HD22  | 1:B:87:LEU:CD1   | 2.31                     | 0.55              |
| 1:B:111:SER:HB2  | 1:B:142:ASN:CB   | 2.36                     | 0.55              |
| 1:B:388:LEU:HD22 | 1:B:406:ILE:HD11 | 1.88                     | 0.55              |
| 1:B:492:VAL:HG12 | 1:B:557:ILE:HD11 | 1.89                     | 0.55              |
| 2:C:25:PRO:HG3   | 2:C:36:LEU:HD12  | 1.88                     | 0.55              |
| 2:C:76:PHE:CE2   | 2:C:84:VAL:CG2   | 2.88                     | 0.55              |
| 2:C:305:GLN:C    | 2:C:308:ILE:HB   | 2.29                     | 0.55              |
| 1:E:74:HIS:HD2   | 1:E:75:ASP:N     | 2.03                     | 0.55              |
| 1:E:265:VAL:HG22 | 1:E:278:ILE:CD1  | 2.36                     | 0.55              |
| 1:E:530:HIS:CE1  | 1:E:569:GLU:HB3  | 2.41                     | 0.55              |
| 2:F:112:LEU:O    | 2:F:116:ALA:CB   | 2.50                     | 0.55              |
| 2:F:194:ARG:CB   | 2:F:251:LEU:HD21 | 2.36                     | 0.55              |
| 1:B:79:PHE:N     | 1:B:79:PHE:CD1   | 2.73                     | 0.55              |
| 1:B:530:HIS:CE1  | 1:B:531:SER:HG   | 2.14                     | 0.55              |
| 2:C:22:LEU:HD23  | 2:C:43:ALA:HB2   | 1.87                     | 0.55              |
| 2:C:40:TYR:HE2   | 2:C:67:PHE:HE1   | 1.50                     | 0.55              |
| 2:D:22:LEU:HD23  | 2:D:22:LEU:H     | 1.71                     | 0.55              |
| 1:A:63:PHE:CZ    | 1:A:214:THR:HG22 | 2.41                     | 0.55              |
| 1:A:446:LEU:O    | 1:A:542:TYR:CZ   | 2.59                     | 0.55              |
| 1:A:465:LEU:HD11 | 1:A:482:ILE:CG2  | 2.31                     | 0.55              |
| 1:E:465:LEU:CD2  | 1:E:467:HIS:CD2  | 2.89                     | 0.55              |
| 2:F:110:ILE:HD11 | 2:F:115:LEU:HD11 | 0.58                     | 0.55              |
| 2:F:331:LEU:HG   | 2:F:343:LEU:HG   | 1.87                     | 0.55              |
| 1:B:279:ASN:CB   | 1:B:300:LYS:CE   | 2.84                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:276:LEU:HD11 | 2:C:331:LEU:HG   | 1.88                     | 0.55              |
| 1:A:167:THR:HA   | 1:A:439:PHE:O    | 2.06                     | 0.55              |
| 1:A:328:PRO:HB3  | 1:A:335:TYR:CD2  | 2.41                     | 0.55              |
| 1:A:487:VAL:CG2  | 1:A:558:MET:SD   | 2.94                     | 0.55              |
| 2:F:121:LEU:CD1  | 2:F:122:PRO:HD3  | 2.30                     | 0.55              |
| 2:F:238:ILE:CG2  | 2:F:307:TRP:HZ3  | 1.89                     | 0.55              |
| 2:F:324:VAL:HG12 | 2:F:328:ILE:HD11 | 1.89                     | 0.55              |
| 2:C:232:ASN:CB   | 2:C:278:LYS:HZ1  | 2.19                     | 0.55              |
| 1:A:294:ASP:C    | 1:A:323:VAL:CG2  | 2.79                     | 0.55              |
| 2:F:20:LYS:CG    | 2:F:159:TRP:HE3  | 2.19                     | 0.55              |
| 2:F:111:PRO:O    | 2:F:115:LEU:HD13 | 2.06                     | 0.55              |
| 1:B:170:GLU:HB2  | 1:B:183:PHE:HB2  | 1.88                     | 0.55              |
| 1:B:279:ASN:O    | 1:B:358:LEU:HB2  | 2.06                     | 0.55              |
| 1:A:71:ILE:HD13  | 1:A:71:ILE:N     | 2.09                     | 0.55              |
| 1:A:382:PRO:CG   | 1:A:401:LYS:NZ   | 2.69                     | 0.55              |
| 1:A:452:ILE:O    | 1:A:454:VAL:HG13 | 2.06                     | 0.55              |
| 1:A:466:THR:CG2  | 1:A:511:LEU:CD2  | 2.83                     | 0.55              |
| 1:E:92:GLN:NE2   | 1:E:92:GLN:H     | 2.05                     | 0.55              |
| 1:E:252:GLY:C    | 1:E:255:SER:HG   | 2.13                     | 0.55              |
| 1:E:334:ARG:O    | 1:E:338:LEU:CB   | 2.54                     | 0.55              |
| 1:E:389:ASN:ND2  | 1:E:408:LEU:CB   | 2.70                     | 0.55              |
| 2:F:9:PRO:CG     | 2:F:10:TRP:CE3   | 2.85                     | 0.55              |
| 2:F:23:PHE:C     | 2:F:24:PHE:HD2   | 2.14                     | 0.55              |
| 1:B:118:PHE:CE1  | 1:B:306:HIS:HB2  | 2.23                     | 0.55              |
| 1:B:368:TYR:CD1  | 1:B:372:LEU:HG   | 2.39                     | 0.55              |
| 2:C:24:PHE:CD2   | 2:C:24:PHE:N     | 2.73                     | 0.55              |
| 2:C:82:ASP:O     | 2:C:86:LEU:HD12  | 2.06                     | 0.55              |
| 1:E:349:ASP:CA   | 1:E:351:GLU:OE1  | 2.55                     | 0.55              |
| 2:F:358:ASP:OD1  | 2:F:358:ASP:N    | 2.34                     | 0.55              |
| 1:B:183:PHE:CD2  | 1:B:183:PHE:N    | 2.73                     | 0.55              |
| 2:C:305:GLN:O    | 2:C:308:ILE:CA   | 2.54                     | 0.55              |
| 2:D:119:ILE:O    | 2:D:120:ASP:HB3  | 2.06                     | 0.55              |
| 2:D:149:ARG:HG2  | 3:D:506:HOH:O    | 1.94                     | 0.55              |
| 1:A:308:ASN:O    | 1:A:310:LEU:HD22 | 2.07                     | 0.55              |
| 1:A:312:LEU:CD1  | 1:A:441:PHE:HE1  | 2.13                     | 0.55              |
| 1:A:340:GLU:O    | 1:A:343:VAL:HB   | 2.06                     | 0.55              |
| 1:A:542:TYR:O    | 1:A:543:ILE:HG22 | 2.06                     | 0.55              |
| 1:E:224:LYS:HG2  | 1:E:263:LEU:CD2  | 2.37                     | 0.55              |
| 1:B:445:PRO:HD2  | 3:B:714:HOH:O    | 2.07                     | 0.55              |
| 2:D:142:MET:O    | 2:D:145:THR:HB   | 2.07                     | 0.55              |
| 1:A:160:ILE:HD12 | 1:A:160:ILE:O    | 2.06                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:230:ASP:HA   | 1:A:233:LYS:HB3  | 1.89                     | 0.55              |
| 1:A:288:PRO:CB   | 1:A:291:SER:HB2  | 2.33                     | 0.55              |
| 1:A:382:PRO:HB3  | 1:A:385:VAL:HG22 | 1.88                     | 0.55              |
| 1:A:447:LEU:O    | 1:A:542:TYR:OH   | 2.24                     | 0.55              |
| 1:E:276:LEU:HD13 | 1:E:354:HIS:CA   | 2.36                     | 0.55              |
| 1:E:570:ILE:CA   | 1:E:575:ILE:HD12 | 2.36                     | 0.55              |
| 2:F:247:HIS:O    | 2:F:250:ALA:CB   | 2.55                     | 0.55              |
| 2:F:280:TYR:N    | 2:F:338:LEU:HD22 | 2.22                     | 0.55              |
| 2:C:95:PHE:CD1   | 2:C:95:PHE:C     | 2.85                     | 0.55              |
| 1:A:170:GLU:HB2  | 1:A:185:GLN:OE1  | 2.07                     | 0.55              |
| 1:E:225:HIS:HB2  | 1:E:228:TRP:N    | 2.22                     | 0.55              |
| 1:E:325:PHE:CD1  | 1:E:325:PHE:N    | 2.73                     | 0.55              |
| 2:F:246:GLU:O    | 2:F:246:GLU:HG3  | 2.07                     | 0.55              |
| 2:F:318:ARG:O    | 2:F:320:ASP:CB   | 2.54                     | 0.55              |
| 1:B:426:LEU:HD13 | 1:B:566:PRO:HA   | 1.87                     | 0.55              |
| 2:C:22:LEU:HD21  | 2:C:42:GLU:HB3   | 1.89                     | 0.55              |
| 2:D:25:PRO:O     | 2:D:26:ALA:HB3   | 2.06                     | 0.55              |
| 2:D:54:THR:CG2   | 2:D:55:ARG:N     | 2.70                     | 0.55              |
| 2:D:190:TYR:HD1  | 2:D:190:TYR:C    | 2.15                     | 0.55              |
| 1:A:108:ILE:HD12 | 1:A:108:ILE:N    | 2.21                     | 0.55              |
| 1:A:490:PHE:CZ   | 1:A:523:PHE:CE1  | 2.95                     | 0.55              |
| 1:E:182:LEU:CB   | 1:E:183:PHE:CE2  | 2.85                     | 0.55              |
| 1:E:253:LYS:O    | 1:E:254:ASN:HB3  | 2.06                     | 0.55              |
| 1:E:451:PRO:CD   | 2:F:413:TRP:CE3  | 2.90                     | 0.55              |
| 2:F:331:LEU:HD23 | 2:F:343:LEU:HD22 | 1.88                     | 0.55              |
| 1:B:155:GLY:CA   | 3:B:708:HOH:O    | 2.55                     | 0.54              |
| 1:B:180:LYS:HE2  | 1:B:181:ASN:CA   | 2.37                     | 0.54              |
| 1:B:182:LEU:CD1  | 1:B:183:PHE:CE2  | 2.71                     | 0.54              |
| 2:C:11:LYS:HD2   | 1:A:585:TYR:CE2  | 2.42                     | 0.54              |
| 2:C:181:LYS:O    | 2:C:185:ASP:HB2  | 2.07                     | 0.54              |
| 2:C:258:HIS:CD2  | 2:C:258:HIS:C    | 2.86                     | 0.54              |
| 1:A:300:LYS:O    | 1:A:316:ASP:O    | 2.24                     | 0.54              |
| 1:A:454:VAL:CG2  | 1:A:541:LEU:HD11 | 2.37                     | 0.54              |
| 2:F:259:PHE:CD1  | 2:F:259:PHE:C    | 2.86                     | 0.54              |
| 1:B:77:VAL:HG12  | 1:B:79:PHE:CE2   | 2.38                     | 0.54              |
| 1:B:299:SER:HA   | 1:B:317:SER:HB3  | 1.89                     | 0.54              |
| 1:B:522:GLU:OE2  | 1:B:522:GLU:HA   | 2.06                     | 0.54              |
| 2:C:10:TRP:CD2   | 2:C:16:VAL:HG23  | 2.42                     | 0.54              |
| 2:D:190:TYR:HE2  | 2:D:218:ILE:HG23 | 1.56                     | 0.54              |
| 2:D:344:GLU:O    | 2:D:348:SER:N    | 2.36                     | 0.54              |
| 1:A:420:SER:HB3  | 1:A:423:GLN:CB   | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:364:TRP:HZ3  | 1:E:368:TYR:HD1  | 1.54                     | 0.54              |
| 1:E:516:PHE:C    | 1:E:516:PHE:CD1  | 2.86                     | 0.54              |
| 1:E:524:PHE:CD2  | 1:E:524:PHE:C    | 2.85                     | 0.54              |
| 1:B:107:VAL:CG2  | 1:B:109:TYR:CE2  | 2.90                     | 0.54              |
| 1:B:491:LYS:HB2  | 1:B:522:GLU:O    | 2.07                     | 0.54              |
| 2:D:56:VAL:CG2   | 2:D:61:GLN:HB2   | 2.37                     | 0.54              |
| 2:D:76:PHE:CD2   | 2:D:76:PHE:C     | 2.86                     | 0.54              |
| 2:D:259:PHE:CD1  | 2:D:259:PHE:C    | 2.86                     | 0.54              |
| 1:A:210:PHE:CD1  | 1:A:210:PHE:N    | 2.74                     | 0.54              |
| 1:A:359:ILE:HG22 | 1:A:360:ASN:O    | 2.07                     | 0.54              |
| 1:E:134:VAL:O    | 1:E:134:VAL:HG12 | 2.08                     | 0.54              |
| 1:E:310:LEU:HB3  | 1:E:428:LYS:HG2  | 1.89                     | 0.54              |
| 1:E:567:ILE:H    | 1:E:567:ILE:CD1  | 2.20                     | 0.54              |
| 1:E:570:ILE:H    | 1:E:570:ILE:CD1  | 2.12                     | 0.54              |
| 2:F:121:LEU:CD1  | 2:F:122:PRO:CD   | 2.86                     | 0.54              |
| 2:F:237:ARG:HA   | 2:F:237:ARG:NE   | 2.17                     | 0.54              |
| 1:B:453:GLN:HB3  | 1:B:538:ILE:CG2  | 2.36                     | 0.54              |
| 2:C:73:LEU:HD23  | 2:C:84:VAL:HG12  | 1.89                     | 0.54              |
| 2:C:160:ASP:OD2  | 2:C:161:GLY:N    | 2.40                     | 0.54              |
| 2:C:214:TYR:CA   | 2:C:217:CYS:SG   | 2.93                     | 0.54              |
| 2:C:224:HIS:O    | 2:C:227:MET:SD   | 2.65                     | 0.54              |
| 1:A:119:ILE:CG1  | 1:A:309:HIS:ND1  | 2.70                     | 0.54              |
| 1:A:232:ILE:HG13 | 1:A:264:LEU:CD2  | 2.21                     | 0.54              |
| 1:E:344:ARG:HH21 | 1:E:379:ARG:HH12 | 1.54                     | 0.54              |
| 2:F:10:TRP:HE3   | 2:F:50:TYR:HD2   | 1.55                     | 0.54              |
| 1:B:98:GLN:HA    | 1:B:143:LYS:C    | 2.32                     | 0.54              |
| 1:B:583:LEU:O    | 1:B:583:LEU:HD22 | 2.07                     | 0.54              |
| 2:C:418:PHE:N    | 2:C:418:PHE:CD2  | 2.73                     | 0.54              |
| 2:D:95:PHE:CZ    | 2:D:99:LEU:HD11  | 2.42                     | 0.54              |
| 2:D:190:TYR:C    | 2:D:190:TYR:CD1  | 2.86                     | 0.54              |
| 1:A:78:ILE:CA    | 1:A:161:LYS:HB3  | 2.27                     | 0.54              |
| 1:A:116:MET:HG3  | 1:A:118:PHE:CE2  | 2.43                     | 0.54              |
| 1:A:207:ASP:C    | 1:A:208:TYR:CD2  | 2.85                     | 0.54              |
| 1:A:516:PHE:CE2  | 1:A:521:THR:HG21 | 2.42                     | 0.54              |
| 1:E:85:GLN:O     | 1:E:130:GLN:HA   | 2.05                     | 0.54              |
| 1:B:440:LYS:C    | 1:B:441:PHE:CD2  | 2.86                     | 0.54              |
| 2:C:10:TRP:CE2   | 2:C:16:VAL:HG21  | 2.42                     | 0.54              |
| 2:C:90:MET:HB2   | 2:D:90:MET:HB2   | 1.89                     | 0.54              |
| 2:D:93:ILE:CD1   | 2:D:132:ALA:HB3  | 2.29                     | 0.54              |
| 1:A:162:LEU:HD22 | 1:A:210:PHE:CE2  | 2.42                     | 0.54              |
| 1:E:365:ILE:HD12 | 1:E:393:LEU:HD13 | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:426:LEU:O    | 1:E:430:MET:N    | 2.30                     | 0.54              |
| 1:E:466:THR:OG1  | 1:E:511:LEU:O    | 2.21                     | 0.54              |
| 1:E:513:TYR:C    | 1:E:513:TYR:CD2  | 2.85                     | 0.54              |
| 2:F:234:MET:O    | 2:F:238:ILE:HD12 | 2.08                     | 0.54              |
| 2:F:360:ILE:HD12 | 2:F:360:ILE:H    | 1.72                     | 0.54              |
| 1:A:62:ASN:CB    | 1:A:216:PRO:HG3  | 2.38                     | 0.54              |
| 1:A:246:LYS:CB   | 1:A:383:THR:CB   | 2.74                     | 0.54              |
| 1:A:434:HIS:CD2  | 1:A:446:LEU:HD11 | 2.42                     | 0.54              |
| 1:E:471:THR:O    | 1:E:471:THR:HG22 | 2.07                     | 0.54              |
| 2:F:10:TRP:N     | 2:F:50:TYR:CD2   | 2.76                     | 0.54              |
| 2:C:299:GLN:O    | 2:C:303:CYS:SG   | 2.66                     | 0.54              |
| 2:D:267:PHE:HA   | 2:D:270:GLY:HA3  | 1.89                     | 0.54              |
| 1:E:232:ILE:CG1  | 1:E:264:LEU:CA   | 2.77                     | 0.54              |
| 1:E:318:THR:CG2  | 1:E:319:GLN:CD   | 2.81                     | 0.54              |
| 1:E:524:PHE:O    | 1:E:525:ARG:HG3  | 2.08                     | 0.54              |
| 2:F:316:ILE:CD1  | 2:F:346:LEU:CD2  | 2.80                     | 0.54              |
| 1:B:217:ASP:CB   | 3:B:725:HOH:O    | 2.56                     | 0.54              |
| 2:C:158:TYR:CD1  | 2:C:158:TYR:C    | 2.85                     | 0.54              |
| 1:E:436:ILE:CG2  | 1:E:440:LYS:CB   | 2.86                     | 0.54              |
| 1:E:468:LEU:CD2  | 1:E:469:LYS:H    | 2.21                     | 0.54              |
| 2:F:89:SER:OG    | 2:F:137:LEU:HD11 | 2.08                     | 0.54              |
| 2:F:234:MET:HG3  | 2:F:235:ILE:N    | 2.23                     | 0.54              |
| 2:F:312:ALA:CB   | 2:F:342:LEU:HD21 | 2.24                     | 0.54              |
| 1:B:368:TYR:CE1  | 1:B:372:LEU:CD1  | 2.91                     | 0.54              |
| 2:D:232:ASN:OD1  | 2:D:271:LEU:HA   | 2.08                     | 0.54              |
| 1:A:213:ILE:CD1  | 1:A:219:THR:CG2  | 2.82                     | 0.54              |
| 1:A:463:SER:O    | 1:A:509:PRO:HG3  | 1.96                     | 0.54              |
| 1:E:74:HIS:CD2   | 1:E:75:ASP:CG    | 2.86                     | 0.54              |
| 1:E:260:PHE:C    | 1:E:260:PHE:CD2  | 2.86                     | 0.54              |
| 1:E:466:THR:HG21 | 1:E:516:PHE:HB2  | 1.90                     | 0.54              |
| 1:E:530:HIS:HE1  | 1:E:569:GLU:HB3  | 1.73                     | 0.54              |
| 1:B:138:SER:HA   | 1:B:139:LEU:C    | 2.33                     | 0.53              |
| 1:B:175:VAL:CG2  | 1:B:176:CYS:N    | 2.72                     | 0.53              |
| 2:C:73:LEU:HD21  | 3:C:502:HOH:O    | 2.08                     | 0.53              |
| 2:D:89:SER:HA    | 2:D:128:PHE:CE1  | 2.43                     | 0.53              |
| 1:A:434:HIS:NE2  | 1:A:446:LEU:HD12 | 2.22                     | 0.53              |
| 1:E:93:PHE:C     | 1:E:93:PHE:CD2   | 2.85                     | 0.53              |
| 1:E:99:ARG:HA    | 1:E:142:ASN:OD1  | 1.95                     | 0.53              |
| 1:E:108:ILE:HG23 | 1:E:133:GLN:CB   | 2.38                     | 0.53              |
| 1:B:182:LEU:O    | 1:B:182:LEU:HD23 | 2.08                     | 0.53              |
| 1:B:261:LEU:HD12 | 1:B:360:ASN:ND2  | 2.23                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:310:TRP:CZ3  | 2:C:314:GLU:OE1  | 2.61                     | 0.53              |
| 2:D:155:TRP:O    | 2:D:160:ASP:HB2  | 2.08                     | 0.53              |
| 1:A:87:LEU:CD2   | 1:A:212:PRO:HB3  | 2.35                     | 0.53              |
| 1:A:280:PHE:C    | 1:A:280:PHE:CD2  | 2.86                     | 0.53              |
| 1:A:335:TYR:CD1  | 1:A:335:TYR:C    | 2.85                     | 0.53              |
| 1:A:472:GLY:C    | 1:A:473:ILE:HG12 | 2.34                     | 0.53              |
| 1:A:565:LEU:CD2  | 1:A:570:ILE:CG1  | 2.86                     | 0.53              |
| 2:F:262:LEU:HD13 | 2:F:263:LYS:CG   | 2.23                     | 0.53              |
| 1:B:127:PRO:HA   | 1:B:222:VAL:HG21 | 1.90                     | 0.53              |
| 1:B:318:THR:CG2  | 1:B:319:GLN:CD   | 2.81                     | 0.53              |
| 1:B:327:SER:CB   | 1:B:329:LYS:CE   | 2.86                     | 0.53              |
| 1:B:492:VAL:CG1  | 1:B:557:ILE:HD11 | 2.38                     | 0.53              |
| 1:B:596:LYS:HD2  | 1:B:596:LYS:N    | 2.24                     | 0.53              |
| 1:A:246:LYS:HB2  | 1:A:383:THR:CB   | 2.38                     | 0.53              |
| 1:A:329:LYS:HD2  | 1:A:364:TRP:CZ2  | 2.42                     | 0.53              |
| 1:A:466:THR:HB   | 1:A:511:LEU:O    | 2.08                     | 0.53              |
| 1:E:71:ILE:HD12  | 1:E:71:ILE:C     | 2.33                     | 0.53              |
| 1:E:231:VAL:O    | 1:E:235:LEU:HG   | 2.09                     | 0.53              |
| 1:E:587:THR:C    | 2:F:5:PRO:HB2    | 2.32                     | 0.53              |
| 1:E:598:TRP:CD1  | 1:E:599:LYS:H    | 2.24                     | 0.53              |
| 2:F:251:LEU:O    | 2:F:254:PRO:CD   | 2.55                     | 0.53              |
| 1:B:177:PRO:O    | 1:B:180:LYS:HD2  | 2.08                     | 0.53              |
| 2:D:99:LEU:N     | 2:D:99:LEU:HD23  | 2.23                     | 0.53              |
| 2:D:128:PHE:CD1  | 2:D:128:PHE:C    | 2.85                     | 0.53              |
| 1:E:74:HIS:CD2   | 1:E:74:HIS:C     | 2.85                     | 0.53              |
| 2:F:238:ILE:HG22 | 2:F:307:TRP:CZ3  | 2.31                     | 0.53              |
| 2:C:224:HIS:O    | 2:C:227:MET:HE1  | 2.09                     | 0.53              |
| 2:C:420:VAL:O    | 2:C:420:VAL:HG12 | 2.08                     | 0.53              |
| 2:D:9:PRO:HD2    | 2:D:10:TRP:CE3   | 2.42                     | 0.53              |
| 2:D:183:LEU:HD22 | 2:D:224:HIS:HB2  | 1.87                     | 0.53              |
| 1:A:436:ILE:HG22 | 1:A:440:LYS:HB3  | 1.85                     | 0.53              |
| 1:A:475:MET:O    | 1:A:478:LEU:HD22 | 2.08                     | 0.53              |
| 1:A:494:ARG:C    | 3:A:702:HOH:O    | 2.28                     | 0.53              |
| 1:E:293:THR:HG21 | 1:E:425:ARG:HD2  | 1.90                     | 0.53              |
| 2:F:214:TYR:C    | 2:F:214:TYR:CD2  | 2.85                     | 0.53              |
| 1:B:570:ILE:C    | 1:B:575:ILE:CD1  | 2.82                     | 0.53              |
| 2:C:137:LEU:CB   | 2:D:94:ARG:NH2   | 2.68                     | 0.53              |
| 2:C:182:GLU:O    | 2:C:186:LEU:CA   | 2.56                     | 0.53              |
| 1:A:456:TYR:H    | 1:A:537:LYS:CB   | 2.22                     | 0.53              |
| 1:E:455:SER:HB2  | 1:E:459:SER:OG   | 2.08                     | 0.53              |
| 1:E:468:LEU:HD23 | 1:E:513:TYR:CE1  | 2.44                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:492:VAL:HG11 | 1:E:496:HIS:CB   | 2.38                     | 0.53              |
| 2:F:33:ARG:O     | 2:F:34:ASP:C     | 2.51                     | 0.53              |
| 1:B:61:SER:O     | 1:B:216:PRO:HA   | 2.08                     | 0.53              |
| 1:B:62:ASN:C     | 1:B:88:ILE:CD1   | 2.82                     | 0.53              |
| 1:E:321:HIS:CE1  | 1:E:522:GLU:CD   | 2.76                     | 0.53              |
| 1:E:499:GLU:O    | 1:E:500:CYS:HB2  | 2.08                     | 0.53              |
| 1:E:528:LEU:HD12 | 1:E:528:LEU:C    | 2.34                     | 0.53              |
| 1:B:279:ASN:CG   | 1:B:300:LYS:CE   | 2.79                     | 0.53              |
| 1:B:325:PHE:CD1  | 1:B:330:ASP:CB   | 2.91                     | 0.53              |
| 2:D:28:ARG:C     | 2:D:31:ILE:HD11  | 2.33                     | 0.53              |
| 1:A:63:PHE:CE2   | 1:A:214:THR:CB   | 2.83                     | 0.53              |
| 1:A:503:PHE:N    | 1:A:509:PRO:O    | 2.41                     | 0.53              |
| 1:A:524:PHE:CD2  | 1:A:525:ARG:N    | 2.73                     | 0.53              |
| 1:B:180:LYS:HD3  | 1:B:181:ASN:N    | 2.23                     | 0.53              |
| 1:B:368:TYR:CD1  | 1:B:368:TYR:C    | 2.87                     | 0.53              |
| 1:B:380:VAL:CG1  | 1:B:382:PRO:HB3  | 2.39                     | 0.53              |
| 1:B:395:VAL:HA   | 1:B:398:ASP:HB2  | 1.91                     | 0.53              |
| 1:B:598:TRP:CZ2  | 2:C:134:HIS:O    | 2.62                     | 0.53              |
| 2:C:48:GLU:OE2   | 2:D:80:LEU:HD22  | 2.09                     | 0.53              |
| 2:C:153:TRP:NE1  | 2:C:157:HIS:CD2  | 2.76                     | 0.53              |
| 1:A:532:ILE:CD1  | 1:A:532:ILE:H    | 2.22                     | 0.53              |
| 1:E:169:LEU:O    | 1:E:172:ILE:HG23 | 2.08                     | 0.53              |
| 2:F:76:PHE:HE2   | 2:F:80:LEU:O     | 1.92                     | 0.53              |
| 1:B:180:LYS:HD3  | 1:B:180:LYS:N    | 2.23                     | 0.53              |
| 1:A:368:TYR:O    | 1:A:372:LEU:N    | 2.32                     | 0.53              |
| 1:E:172:ILE:HG13 | 1:E:179:PHE:HB3  | 1.91                     | 0.53              |
| 1:E:467:HIS:O    | 1:E:513:TYR:HB2  | 2.08                     | 0.53              |
| 2:F:7:LEU:H      | 2:F:7:LEU:CD2    | 2.22                     | 0.53              |
| 1:B:368:TYR:HD2  | 2:C:124:LEU:CD2  | 2.19                     | 0.52              |
| 1:B:490:PHE:CG   | 1:B:557:ILE:CG2  | 2.83                     | 0.52              |
| 2:C:88:ALA:O     | 2:C:91:THR:OG1   | 2.27                     | 0.52              |
| 1:A:532:ILE:HD13 | 1:A:532:ILE:H    | 1.73                     | 0.52              |
| 1:E:104:ILE:HG23 | 1:E:129:ILE:CG1  | 2.39                     | 0.52              |
| 1:E:164:ASN:CA   | 1:E:210:PHE:HE1  | 2.22                     | 0.52              |
| 2:F:22:LEU:HD11  | 2:F:39:GLN:HA    | 1.90                     | 0.52              |
| 2:F:46:LEU:HD23  | 2:F:49:MET:HE2   | 1.91                     | 0.52              |
| 2:C:418:PHE:N    | 2:C:418:PHE:HD2  | 2.06                     | 0.52              |
| 2:D:230:PHE:HA   | 2:D:233:VAL:HG23 | 1.91                     | 0.52              |
| 2:D:251:LEU:O    | 2:D:254:PRO:HD2  | 2.09                     | 0.52              |
| 2:D:268:PRO:C    | 2:D:271:LEU:HD12 | 2.34                     | 0.52              |
| 1:E:432:TYR:CE1  | 1:E:544:PRO:HG3  | 2.44                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:585:TYR:HE2  | 2:F:11:LYS:HG2   | 1.74                     | 0.52              |
| 2:F:20:LYS:CE    | 2:F:159:TRP:O    | 2.58                     | 0.52              |
| 1:B:92:GLN:NE2   | 1:B:183:PHE:HB3  | 2.24                     | 0.52              |
| 1:B:368:TYR:CB   | 2:C:124:LEU:HD22 | 2.33                     | 0.52              |
| 2:C:97:ASN:O     | 2:C:101:ASP:HB2  | 2.10                     | 0.52              |
| 2:D:186:LEU:HB3  | 2:D:221:ILE:CG1  | 2.40                     | 0.52              |
| 1:A:164:ASN:CB   | 1:A:209:THR:CG2  | 2.87                     | 0.52              |
| 1:A:184:TRP:HE1  | 1:A:210:PHE:C    | 2.17                     | 0.52              |
| 1:A:532:ILE:CG2  | 1:A:539:MET:HE3  | 2.36                     | 0.52              |
| 1:E:225:HIS:O    | 1:E:228:TRP:CA   | 2.56                     | 0.52              |
| 1:E:420:SER:O    | 1:E:423:GLN:N    | 2.42                     | 0.52              |
| 1:E:475:MET:O    | 1:E:478:LEU:CD2  | 2.57                     | 0.52              |
| 2:F:123:SER:O    | 2:F:126:VAL:HB   | 2.10                     | 0.52              |
| 1:B:239:TYR:O    | 1:B:274:GLN:CD   | 2.50                     | 0.52              |
| 1:B:248:ILE:CD1  | 1:B:359:ILE:HD13 | 2.38                     | 0.52              |
| 2:C:258:HIS:O    | 2:C:261:HIS:HB3  | 2.09                     | 0.52              |
| 1:A:247:VAL:HG12 | 1:A:248:ILE:O    | 2.09                     | 0.52              |
| 1:E:341:GLN:O    | 1:E:344:ARG:HG2  | 2.08                     | 0.52              |
| 2:F:40:TYR:CG    | 2:F:67:PHE:CD2   | 2.96                     | 0.52              |
| 2:F:328:ILE:O    | 2:F:331:LEU:HD22 | 2.10                     | 0.52              |
| 1:B:310:LEU:N    | 1:B:310:LEU:CD2  | 2.73                     | 0.52              |
| 1:B:463:SER:O    | 1:B:509:PRO:HG3  | 2.09                     | 0.52              |
| 1:B:480:ARG:HH21 | 2:D:49:MET:HE1   | 1.75                     | 0.52              |
| 1:B:583:LEU:HB2  | 1:B:586:ILE:H    | 1.72                     | 0.52              |
| 2:C:48:GLU:CD    | 2:D:80:LEU:CD2   | 2.83                     | 0.52              |
| 2:C:245:TRP:NE1  | 2:C:247:HIS:CB   | 2.73                     | 0.52              |
| 1:A:66:ASP:CB    | 1:A:68:ASP:CB    | 2.87                     | 0.52              |
| 1:E:370:LEU:CD1  | 1:E:397:ILE:HG12 | 2.36                     | 0.52              |
| 2:F:10:TRP:C     | 2:F:15:GLU:OE1   | 2.52                     | 0.52              |
| 2:F:269:LEU:HD11 | 2:F:326:LYS:CB   | 2.40                     | 0.52              |
| 2:F:280:TYR:N    | 2:F:338:LEU:HD21 | 2.23                     | 0.52              |
| 1:B:418:ARG:N    | 1:B:419:TYR:CA   | 2.72                     | 0.52              |
| 2:C:15:GLU:O     | 2:C:18:TYR:CA    | 2.57                     | 0.52              |
| 2:C:21:GLY:O     | 2:C:24:PHE:O     | 2.26                     | 0.52              |
| 2:D:182:GLU:O    | 2:D:186:LEU:HG   | 2.10                     | 0.52              |
| 2:D:267:PHE:O    | 2:D:270:GLY:N    | 2.43                     | 0.52              |
| 1:E:229:MET:O    | 1:E:232:ILE:CG2  | 2.56                     | 0.52              |
| 1:E:318:THR:C    | 1:E:319:GLN:CG   | 2.73                     | 0.52              |
| 1:E:445:PRO:HG2  | 1:E:448:PHE:CE1  | 2.45                     | 0.52              |
| 1:E:468:LEU:CD2  | 1:E:469:LYS:N    | 2.73                     | 0.52              |
| 1:E:567:ILE:N    | 1:E:567:ILE:CD1  | 2.73                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:570:ILE:N    | 1:E:570:ILE:CD1  | 2.73                     | 0.52              |
| 2:F:245:TRP:CB   | 2:F:247:HIS:NE2  | 2.73                     | 0.52              |
| 1:B:225:HIS:CB   | 1:B:227:ASN:ND2  | 2.73                     | 0.52              |
| 1:B:235:LEU:N    | 1:B:235:LEU:CD2  | 2.73                     | 0.52              |
| 1:B:260:PHE:CE2  | 1:B:386:ILE:HG21 | 2.45                     | 0.52              |
| 1:B:528:LEU:CD2  | 1:B:569:GLU:OE2  | 2.58                     | 0.52              |
| 2:C:10:TRP:N     | 2:C:50:TYR:CE1   | 2.76                     | 0.52              |
| 2:D:96:VAL:O     | 2:D:100:LEU:CD1  | 2.57                     | 0.52              |
| 2:D:345:LYS:CA   | 2:D:348:SER:OG   | 2.57                     | 0.52              |
| 2:D:354:PRO:N    | 2:D:357:LYS:CB   | 2.73                     | 0.52              |
| 1:A:276:LEU:HB3  | 1:A:354:HIS:O    | 2.10                     | 0.52              |
| 1:A:322:TYR:CD1  | 1:A:523:PHE:CZ   | 2.98                     | 0.52              |
| 1:A:464:ALA:CA   | 1:A:509:PRO:CG   | 2.88                     | 0.52              |
| 1:E:79:PHE:HE1   | 1:E:162:LEU:HG   | 1.75                     | 0.52              |
| 1:E:89:VAL:HG11  | 1:E:93:PHE:CD1   | 2.45                     | 0.52              |
| 1:B:490:PHE:O    | 1:B:557:ILE:HB   | 2.09                     | 0.52              |
| 2:C:153:TRP:CZ2  | 2:C:157:HIS:ND1  | 2.77                     | 0.52              |
| 2:C:182:GLU:C    | 2:C:186:LEU:HG   | 2.35                     | 0.52              |
| 2:D:89:SER:OG    | 2:D:128:PHE:HE1  | 1.93                     | 0.52              |
| 2:D:327:MET:CA   | 2:D:330:THR:HG1  | 2.14                     | 0.52              |
| 1:A:108:ILE:N    | 1:A:108:ILE:CD1  | 2.73                     | 0.52              |
| 1:A:373:THR:O    | 1:A:377:ILE:N    | 2.38                     | 0.52              |
| 1:A:444:GLN:NE2  | 1:A:445:PRO:O    | 2.42                     | 0.52              |
| 1:A:532:ILE:CD1  | 1:A:532:ILE:N    | 2.73                     | 0.52              |
| 1:E:78:ILE:HG21  | 1:E:98:GLN:NE2   | 2.24                     | 0.52              |
| 1:E:529:VAL:HG13 | 1:E:532:ILE:CD1  | 2.20                     | 0.52              |
| 2:F:194:ARG:CB   | 2:F:251:LEU:HD22 | 2.40                     | 0.52              |
| 1:B:63:PHE:N     | 1:B:88:ILE:HD13  | 2.18                     | 0.52              |
| 1:B:455:SER:HB3  | 2:D:405:LYS:N    | 2.24                     | 0.52              |
| 1:A:246:LYS:C    | 1:A:382:PRO:O    | 2.44                     | 0.52              |
| 2:F:15:GLU:OE2   | 2:F:50:TYR:OH    | 2.23                     | 0.52              |
| 2:F:33:ARG:HH21  | 2:F:33:ARG:HB2   | 1.73                     | 0.52              |
| 1:B:112:GLY:HA3  | 1:B:140:LEU:HA   | 1.92                     | 0.52              |
| 1:B:164:ASN:ND2  | 1:B:208:TYR:CG   | 2.77                     | 0.52              |
| 1:B:169:LEU:O    | 1:B:170:GLU:CB   | 2.58                     | 0.52              |
| 1:B:322:TYR:CE2  | 1:B:324:GLY:HA2  | 2.45                     | 0.52              |
| 2:C:232:ASN:CA   | 2:C:278:LYS:NZ   | 2.72                     | 0.52              |
| 2:D:145:THR:O    | 2:D:149:ARG:HB2  | 2.09                     | 0.52              |
| 1:A:570:ILE:HG22 | 3:A:734:HOH:O    | 1.97                     | 0.52              |
| 2:F:198:ILE:N    | 2:F:198:ILE:CD1  | 2.73                     | 0.52              |
| 1:B:328:PRO:HB3  | 1:B:335:TYR:HD2  | 1.69                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:15:GLU:H     | 2:C:15:GLU:CD    | 2.02                     | 0.51              |
| 2:C:46:LEU:O     | 2:C:50:TYR:HD2   | 1.93                     | 0.51              |
| 2:C:324:VAL:O    | 2:C:328:ILE:HG12 | 2.10                     | 0.51              |
| 2:D:149:ARG:NH1  | 2:D:149:ARG:CB   | 2.73                     | 0.51              |
| 1:A:181:ASN:CG   | 1:A:187:ASP:C    | 2.76                     | 0.51              |
| 1:A:239:TYR:CE1  | 1:A:276:LEU:HD12 | 2.44                     | 0.51              |
| 1:E:129:ILE:CD1  | 1:E:129:ILE:N    | 2.73                     | 0.51              |
| 2:F:82:ASP:O     | 2:F:86:LEU:CD1   | 2.58                     | 0.51              |
| 2:F:82:ASP:C     | 2:F:86:LEU:HD12  | 2.36                     | 0.51              |
| 1:B:93:PHE:HD2   | 1:B:162:LEU:CD2  | 2.20                     | 0.51              |
| 1:B:119:ILE:N    | 1:B:307:GLY:HA3  | 2.16                     | 0.51              |
| 2:C:218:ILE:HG21 | 2:C:255:MET:HE2  | 1.92                     | 0.51              |
| 2:D:24:PHE:HD2   | 2:D:155:TRP:HE1  | 1.58                     | 0.51              |
| 2:D:234:MET:C    | 2:D:234:MET:SD   | 2.94                     | 0.51              |
| 2:D:272:ILE:O    | 2:D:275:MET:N    | 2.43                     | 0.51              |
| 1:A:546:PHE:N    | 1:A:546:PHE:HD1  | 2.09                     | 0.51              |
| 1:A:584:PRO:O    | 1:A:585:TYR:CD2  | 2.63                     | 0.51              |
| 1:E:265:VAL:HG13 | 1:E:278:ILE:CD1  | 2.40                     | 0.51              |
| 1:E:533:ASP:CG   | 1:E:536:LYS:H    | 2.18                     | 0.51              |
| 2:F:118:LYS:NZ   | 2:F:118:LYS:CB   | 2.73                     | 0.51              |
| 1:B:180:LYS:CD   | 1:B:181:ASN:N    | 2.73                     | 0.51              |
| 1:B:327:SER:CB   | 1:B:329:LYS:NZ   | 2.73                     | 0.51              |
| 1:B:446:LEU:HD13 | 1:B:528:LEU:HD21 | 1.92                     | 0.51              |
| 1:B:509:PRO:HG2  | 1:B:509:PRO:O    | 2.10                     | 0.51              |
| 1:B:528:LEU:HD22 | 1:B:569:GLU:OE2  | 2.09                     | 0.51              |
| 1:B:529:VAL:CG2  | 1:B:532:ILE:CD1  | 2.86                     | 0.51              |
| 1:B:598:TRP:CE3  | 2:D:58:HIS:ND1   | 2.78                     | 0.51              |
| 2:C:9:PRO:O      | 2:C:53:ARG:NH1   | 2.42                     | 0.51              |
| 2:C:254:PRO:HA   | 2:C:257:ASN:HD21 | 1.75                     | 0.51              |
| 1:A:248:ILE:O    | 1:A:249:VAL:CG2  | 2.58                     | 0.51              |
| 1:A:389:ASN:OD1  | 1:A:408:LEU:HB3  | 2.11                     | 0.51              |
| 1:E:138:SER:CB   | 1:E:140:LEU:N    | 2.73                     | 0.51              |
| 2:F:338:LEU:CD1  | 2:F:339:ASN:ND2  | 2.73                     | 0.51              |
| 1:B:104:ILE:HG23 | 1:B:129:ILE:CA   | 2.18                     | 0.51              |
| 1:B:248:ILE:HD13 | 1:B:359:ILE:HB   | 1.92                     | 0.51              |
| 1:B:305:GLN:CD   | 1:B:309:HIS:CD2  | 2.89                     | 0.51              |
| 1:B:465:LEU:HD23 | 1:B:466:THR:C    | 2.35                     | 0.51              |
| 2:C:49:MET:HG3   | 2:C:50:TYR:N     | 2.25                     | 0.51              |
| 2:D:74:GLU:C     | 2:D:76:PHE:N     | 2.64                     | 0.51              |
| 2:D:259:PHE:HE1  | 2:D:268:PRO:CD   | 2.22                     | 0.51              |
| 2:D:267:PHE:N    | 2:D:268:PRO:CD   | 2.74                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:66:ASP:CB    | 1:A:68:ASP:N     | 2.73                     | 0.51              |
| 1:A:420:SER:CB   | 1:A:423:GLN:CB   | 2.82                     | 0.51              |
| 1:A:565:LEU:CG   | 1:A:570:ILE:HD11 | 2.40                     | 0.51              |
| 1:E:99:ARG:CA    | 1:E:142:ASN:CB   | 2.78                     | 0.51              |
| 1:E:121:PRO:HG2  | 1:E:123:SER:HB3  | 1.92                     | 0.51              |
| 1:E:283:LEU:CD1  | 1:E:339:VAL:HG13 | 2.40                     | 0.51              |
| 1:E:334:ARG:O    | 1:E:338:LEU:N    | 2.38                     | 0.51              |
| 2:F:40:TYR:CD2   | 2:F:67:PHE:CD2   | 2.98                     | 0.51              |
| 1:B:93:PHE:CE2   | 1:B:162:LEU:HD21 | 2.46                     | 0.51              |
| 1:B:332:PRO:HD2  | 2:C:141:GLU:CB   | 2.40                     | 0.51              |
| 1:B:583:LEU:N    | 1:B:583:LEU:CD1  | 2.73                     | 0.51              |
| 2:C:251:LEU:C    | 2:C:254:PRO:HD2  | 2.35                     | 0.51              |
| 2:D:149:ARG:CG   | 2:D:149:ARG:NH1  | 2.73                     | 0.51              |
| 1:A:181:ASN:ND2  | 1:A:187:ASP:O    | 2.44                     | 0.51              |
| 1:E:455:SER:HG   | 1:E:462:ILE:H    | 1.55                     | 0.51              |
| 2:F:316:ILE:CG1  | 2:F:346:LEU:CD2  | 2.88                     | 0.51              |
| 2:C:10:TRP:CE2   | 2:C:16:VAL:CG2   | 2.93                     | 0.51              |
| 2:C:10:TRP:NE1   | 2:C:13:SER:HA    | 2.25                     | 0.51              |
| 2:C:65:HIS:ND1   | 2:C:94:ARG:NE    | 2.59                     | 0.51              |
| 2:C:83:THR:HA    | 2:C:86:LEU:HD12  | 1.92                     | 0.51              |
| 2:D:85:ARG:CB    | 2:D:137:LEU:HD13 | 2.39                     | 0.51              |
| 2:D:116:ALA:C    | 2:D:119:ILE:HG22 | 2.36                     | 0.51              |
| 1:A:310:LEU:N    | 1:A:310:LEU:CD2  | 2.73                     | 0.51              |
| 1:E:482:ILE:C    | 1:E:485:THR:HG23 | 2.24                     | 0.51              |
| 1:B:210:PHE:CD1  | 1:B:210:PHE:N    | 2.78                     | 0.51              |
| 1:A:282:ASP:HA   | 1:A:360:ASN:HB3  | 1.92                     | 0.51              |
| 1:A:310:LEU:HD12 | 1:A:428:LYS:HE2  | 1.93                     | 0.51              |
| 1:A:511:LEU:HD23 | 1:A:511:LEU:C    | 2.34                     | 0.51              |
| 1:A:541:LEU:HD23 | 1:A:541:LEU:N    | 2.26                     | 0.51              |
| 1:E:265:VAL:HG13 | 1:E:278:ILE:HD13 | 1.92                     | 0.51              |
| 2:F:66:LEU:O     | 2:F:69:ALA:N     | 2.44                     | 0.51              |
| 2:F:316:ILE:HG12 | 2:F:346:LEU:CD2  | 2.41                     | 0.51              |
| 2:C:101:ASP:C    | 2:C:103:ASN:H    | 2.18                     | 0.51              |
| 2:C:259:PHE:HB3  | 2:C:267:PHE:CD2  | 2.46                     | 0.51              |
| 1:A:95:LEU:HD21  | 1:A:116:MET:CE   | 2.33                     | 0.51              |
| 1:A:323:VAL:HG23 | 1:A:324:GLY:N    | 2.26                     | 0.51              |
| 1:A:489:ILE:HG22 | 1:A:524:PHE:CB   | 2.40                     | 0.51              |
| 1:E:466:THR:CB   | 1:E:511:LEU:HD23 | 2.40                     | 0.51              |
| 1:B:211:TYR:CD1  | 1:B:212:PRO:CD   | 2.85                     | 0.51              |
| 1:B:368:TYR:CD2  | 2:C:124:LEU:CD2  | 2.94                     | 0.51              |
| 2:C:33:ARG:NH2   | 2:C:33:ARG:HG2   | 2.26                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:167:THR:HG23 | 1:A:168:HIS:N    | 2.25                     | 0.51              |
| 1:A:475:MET:SD   | 1:A:475:MET:C    | 2.94                     | 0.51              |
| 1:A:483:GLU:CB   | 1:A:532:ILE:CD1  | 2.64                     | 0.51              |
| 1:A:483:GLU:OE2  | 1:A:532:ILE:CD1  | 2.59                     | 0.51              |
| 1:E:218:ASN:O    | 1:E:219:THR:OG1  | 2.29                     | 0.51              |
| 1:E:305:GLN:HG3  | 1:E:309:HIS:CG   | 2.46                     | 0.51              |
| 1:E:416:GLY:HA2  | 3:E:723:HOH:O    | 2.02                     | 0.51              |
| 1:E:558:MET:HG2  | 1:E:559:VAL:H    | 1.76                     | 0.51              |
| 2:F:330:THR:CG2  | 3:F:502:HOH:O    | 2.11                     | 0.51              |
| 1:B:257:LYS:O    | 1:B:261:LEU:N    | 2.43                     | 0.51              |
| 1:B:276:LEU:N    | 1:B:276:LEU:CD2  | 2.73                     | 0.51              |
| 2:C:59:ILE:O     | 2:C:63:THR:OG1   | 2.24                     | 0.51              |
| 2:D:60:LEU:CD2   | 2:D:159:TRP:CZ2  | 2.92                     | 0.51              |
| 2:D:230:PHE:CB   | 2:D:233:VAL:CG2  | 2.89                     | 0.51              |
| 2:D:343:LEU:O    | 2:D:346:LEU:HB2  | 2.10                     | 0.51              |
| 1:A:72:TYR:OH    | 1:A:204:ALA:O    | 2.23                     | 0.51              |
| 1:E:168:HIS:O    | 1:E:441:PHE:HB2  | 2.11                     | 0.51              |
| 1:E:454:VAL:HG21 | 1:E:539:MET:HG3  | 1.92                     | 0.51              |
| 1:B:103:ASP:CA   | 1:B:108:ILE:HG12 | 2.30                     | 0.50              |
| 1:B:183:PHE:HD2  | 1:B:183:PHE:N    | 2.08                     | 0.50              |
| 1:B:437:ASP:HB3  | 1:B:440:LYS:NZ   | 2.26                     | 0.50              |
| 1:B:478:LEU:CD2  | 1:B:479:GLU:HG2  | 2.41                     | 0.50              |
| 2:C:186:LEU:HD13 | 2:C:221:ILE:HA   | 1.93                     | 0.50              |
| 2:C:209:PRO:N    | 2:C:212:LYS:CB   | 2.73                     | 0.50              |
| 2:D:122:PRO:CG   | 2:D:125:PHE:CD1  | 2.94                     | 0.50              |
| 2:D:331:LEU:CD1  | 2:D:360:ILE:CG2  | 2.88                     | 0.50              |
| 1:A:368:TYR:O    | 1:A:371:GLU:N    | 2.44                     | 0.50              |
| 1:A:436:ILE:CG2  | 1:A:437:ASP:N    | 2.74                     | 0.50              |
| 1:A:505:LYS:N    | 1:A:506:GLY:HA3  | 2.26                     | 0.50              |
| 1:A:570:ILE:HG21 | 3:A:734:HOH:O    | 1.96                     | 0.50              |
| 1:A:596:LYS:NZ   | 1:A:596:LYS:CA   | 2.73                     | 0.50              |
| 1:E:99:ARG:CA    | 1:E:142:ASN:HB3  | 2.41                     | 0.50              |
| 1:E:267:HIS:HA   | 1:E:270:SER:OG   | 2.11                     | 0.50              |
| 1:E:531:SER:OG   | 2:F:418:PHE:C    | 2.54                     | 0.50              |
| 1:E:545:GLN:O    | 1:E:546:PHE:HB3  | 2.11                     | 0.50              |
| 1:B:279:ASN:HA   | 1:B:300:LYS:CE   | 2.41                     | 0.50              |
| 1:B:461:GLY:O    | 1:B:556:ILE:CB   | 2.58                     | 0.50              |
| 2:C:15:GLU:O     | 2:C:19:LEU:N     | 2.43                     | 0.50              |
| 2:D:149:ARG:CB   | 2:D:149:ARG:CZ   | 2.89                     | 0.50              |
| 1:A:169:LEU:CD2  | 1:A:441:PHE:CG   | 2.80                     | 0.50              |
| 1:A:224:LYS:HG2  | 1:A:228:TRP:HE3  | 1.46                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:TRP:HZ3  | 1:A:368:TYR:HB3  | 1.70                     | 0.50              |
| 1:E:88:ILE:CG2   | 1:E:128:LEU:HD23 | 2.40                     | 0.50              |
| 1:E:232:ILE:HG12 | 1:E:264:LEU:CA   | 2.41                     | 0.50              |
| 1:E:301:ILE:CG1  | 1:E:315:THR:HG21 | 2.39                     | 0.50              |
| 1:B:118:PHE:C    | 1:B:119:ILE:HD13 | 2.36                     | 0.50              |
| 1:B:223:ILE:O    | 1:B:224:LYS:HD2  | 2.11                     | 0.50              |
| 2:C:125:PHE:CE1  | 2:C:150:ALA:HB2  | 2.35                     | 0.50              |
| 2:C:177:GLU:O    | 2:C:180:ILE:HG12 | 2.11                     | 0.50              |
| 2:D:247:HIS:O    | 2:D:251:LEU:HG   | 2.11                     | 0.50              |
| 1:A:175:VAL:HG23 | 1:A:176:CYS:N    | 2.26                     | 0.50              |
| 1:A:440:LYS:C    | 1:A:441:PHE:CD2  | 2.85                     | 0.50              |
| 1:A:466:THR:O    | 1:A:466:THR:HG23 | 2.11                     | 0.50              |
| 1:E:128:LEU:HD22 | 1:E:129:ILE:N    | 2.26                     | 0.50              |
| 1:E:466:THR:HB   | 1:E:511:LEU:HD23 | 1.92                     | 0.50              |
| 1:B:122:SER:OG   | 1:B:182:LEU:C    | 2.52                     | 0.50              |
| 1:B:122:SER:OG   | 1:B:182:LEU:HA   | 2.12                     | 0.50              |
| 1:B:206:SER:HB3  | 1:B:208:TYR:CE2  | 2.47                     | 0.50              |
| 2:D:11:LYS:HG3   | 2:D:12:SER:N     | 2.26                     | 0.50              |
| 2:D:246:GLU:N    | 2:D:310:TRP:HH2  | 2.09                     | 0.50              |
| 1:A:170:GLU:HG3  | 1:A:185:GLN:CD   | 2.32                     | 0.50              |
| 1:A:184:TRP:CD1  | 1:A:209:THR:O    | 2.64                     | 0.50              |
| 1:A:370:LEU:HD22 | 1:A:393:LEU:CD2  | 2.40                     | 0.50              |
| 1:A:560:ARG:NH2  | 1:A:561:GLY:O    | 2.45                     | 0.50              |
| 1:E:224:LYS:HG3  | 1:E:228:TRP:CZ3  | 2.31                     | 0.50              |
| 2:C:132:ALA:O    | 2:D:94:ARG:HD3   | 2.12                     | 0.50              |
| 1:A:228:TRP:CZ2  | 1:A:409:GLN:CB   | 2.95                     | 0.50              |
| 1:A:252:GLY:N    | 1:A:255:SER:OG   | 2.45                     | 0.50              |
| 1:A:466:THR:OG1  | 1:A:512:PRO:C    | 2.55                     | 0.50              |
| 1:A:492:VAL:HG13 | 1:A:557:ILE:CG1  | 2.41                     | 0.50              |
| 1:A:520:SER:C    | 1:A:521:THR:CG2  | 2.84                     | 0.50              |
| 1:A:546:PHE:N    | 1:A:546:PHE:CD1  | 2.79                     | 0.50              |
| 1:A:576:VAL:HG23 | 1:A:577:LYS:N    | 2.25                     | 0.50              |
| 2:F:259:PHE:HE1  | 2:F:267:PHE:CB   | 2.18                     | 0.50              |
| 1:B:117:LYS:HD2  | 1:B:439:PHE:HE1  | 1.72                     | 0.50              |
| 2:C:232:ASN:HA   | 2:C:278:LYS:CE   | 2.42                     | 0.50              |
| 2:D:230:PHE:CA   | 2:D:233:VAL:HG23 | 2.42                     | 0.50              |
| 1:A:298:LEU:CD2  | 1:A:298:LEU:N    | 2.73                     | 0.50              |
| 1:A:298:LEU:HD22 | 1:A:342:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:426:LEU:O    | 1:A:430:MET:HB2  | 2.12                     | 0.50              |
| 1:A:456:TYR:N    | 1:A:537:LYS:CB   | 2.74                     | 0.50              |
| 1:E:113:VAL:HG22 | 1:E:114:GLU:N    | 2.26                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:531:SER:CA   | 2:F:418:PHE:O    | 2.50                     | 0.50              |
| 2:F:110:ILE:HD12 | 2:F:115:LEU:CD1  | 2.29                     | 0.50              |
| 2:F:117:LYS:HD3  | 2:F:117:LYS:O    | 2.12                     | 0.50              |
| 2:F:251:LEU:O    | 2:F:254:PRO:CG   | 2.60                     | 0.50              |
| 2:F:301:PHE:CE1  | 2:F:304:ALA:HB3  | 2.47                     | 0.50              |
| 2:C:126:VAL:O    | 2:C:129:ARG:HG2  | 2.12                     | 0.50              |
| 2:C:280:TYR:CE2  | 2:C:281:GLU:HG2  | 2.46                     | 0.50              |
| 1:A:432:TYR:OH   | 1:A:525:ARG:CB   | 2.59                     | 0.50              |
| 1:A:454:VAL:O    | 1:A:538:ILE:CA   | 2.57                     | 0.50              |
| 1:A:499:GLU:HG3  | 1:A:499:GLU:O    | 2.10                     | 0.50              |
| 1:E:248:ILE:CG1  | 1:E:382:PRO:HB3  | 2.41                     | 0.50              |
| 2:F:236:GLU:O    | 2:F:240:SER:OG   | 2.27                     | 0.50              |
| 1:B:118:PHE:HE1  | 1:B:306:HIS:CG   | 2.08                     | 0.50              |
| 1:B:213:ILE:HG23 | 3:B:725:HOH:O    | 2.11                     | 0.50              |
| 1:B:250:ILE:CD1  | 1:B:373:THR:HG23 | 2.02                     | 0.50              |
| 1:B:395:VAL:O    | 1:B:398:ASP:CB   | 2.59                     | 0.50              |
| 1:B:456:TYR:H    | 1:B:456:TYR:HD2  | 1.60                     | 0.50              |
| 2:C:40:TYR:CE2   | 2:C:67:PHE:CE1   | 2.83                     | 0.50              |
| 2:D:60:LEU:HD23  | 2:D:159:TRP:HZ2  | 1.75                     | 0.50              |
| 2:D:308:ILE:O    | 2:D:312:ALA:N    | 2.38                     | 0.50              |
| 1:A:276:LEU:CG   | 1:A:354:HIS:O    | 2.60                     | 0.50              |
| 1:E:427:LEU:C    | 1:E:427:LEU:CD2  | 2.85                     | 0.50              |
| 1:E:435:LYS:HB3  | 1:E:441:PHE:CD1  | 2.47                     | 0.50              |
| 1:E:438:ASP:CG   | 1:E:439:PHE:CD1  | 2.85                     | 0.50              |
| 1:E:465:LEU:HB2  | 1:E:508:LEU:HD21 | 1.94                     | 0.50              |
| 2:F:9:PRO:HB2    | 2:F:50:TYR:HA    | 1.93                     | 0.50              |
| 2:F:103:ASN:HB3  | 2:F:115:LEU:CD2  | 2.42                     | 0.50              |
| 1:B:334:ARG:HG3  | 1:B:513:TYR:HH   | 1.76                     | 0.50              |
| 1:B:530:HIS:NE2  | 2:D:416:LYS:O    | 2.30                     | 0.50              |
| 2:C:9:PRO:CG     | 2:C:50:TYR:HD1   | 2.24                     | 0.50              |
| 2:D:272:ILE:O    | 2:D:276:LEU:HD23 | 2.11                     | 0.50              |
| 1:A:182:LEU:HB3  | 1:A:183:PHE:CD2  | 2.46                     | 0.50              |
| 1:A:430:MET:HG3  | 1:A:566:PRO:CB   | 2.41                     | 0.50              |
| 1:E:444:GLN:HE21 | 1:E:444:GLN:C    | 2.18                     | 0.50              |
| 2:F:256:MET:O    | 2:F:259:PHE:HB3  | 2.12                     | 0.50              |
| 1:B:270:SER:C    | 1:B:272:THR:H    | 2.19                     | 0.49              |
| 1:B:457:GLY:C    | 1:B:459:SER:N    | 2.69                     | 0.49              |
| 1:A:76:TYR:HD2   | 1:A:78:ILE:CD1   | 2.25                     | 0.49              |
| 1:E:364:TRP:CE3  | 1:E:369:GLY:N    | 2.80                     | 0.49              |
| 1:E:468:LEU:CD2  | 1:E:513:TYR:HE1  | 2.25                     | 0.49              |
| 1:E:598:TRP:CD1  | 1:E:599:LYS:N    | 2.80                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:744:HOH:O    | 2:F:10:TRP:HH2   | 1.92                     | 0.49              |
| 2:F:116:ALA:CA   | 2:F:119:ILE:CD1  | 2.85                     | 0.49              |
| 1:B:232:ILE:HG21 | 1:B:263:LEU:HD12 | 1.94                     | 0.49              |
| 1:B:325:PHE:CZ   | 1:B:469:LYS:HD3  | 2.47                     | 0.49              |
| 1:B:418:ARG:CB   | 1:B:419:TYR:C    | 2.86                     | 0.49              |
| 1:B:572:SER:OG   | 1:B:575:ILE:CD1  | 2.60                     | 0.49              |
| 1:A:74:HIS:ND1   | 1:A:74:HIS:N     | 2.60                     | 0.49              |
| 1:E:338:LEU:C    | 1:E:338:LEU:CD2  | 2.85                     | 0.49              |
| 1:E:523:PHE:HE1  | 1:E:525:ARG:O    | 1.94                     | 0.49              |
| 2:F:20:LYS:HE3   | 2:F:159:TRP:O    | 2.13                     | 0.49              |
| 2:F:103:ASN:HB3  | 2:F:115:LEU:HD21 | 1.94                     | 0.49              |
| 2:C:124:LEU:CD1  | 2:C:124:LEU:C    | 2.85                     | 0.49              |
| 2:C:142:MET:CE   | 2:C:142:MET:CA   | 2.86                     | 0.49              |
| 1:A:296:ILE:CG2  | 1:A:342:LEU:HD23 | 2.41                     | 0.49              |
| 1:A:296:ILE:HD12 | 1:A:338:LEU:CD2  | 2.41                     | 0.49              |
| 1:A:389:ASN:OD1  | 1:A:389:ASN:N    | 2.46                     | 0.49              |
| 1:B:239:TYR:C    | 1:B:274:GLN:NE2  | 2.68                     | 0.49              |
| 2:C:8:THR:N      | 1:A:585:TYR:O    | 2.40                     | 0.49              |
| 2:C:15:GLU:O     | 2:C:18:TYR:HB3   | 2.13                     | 0.49              |
| 2:C:94:ARG:CG    | 1:A:598:TRP:CH2  | 2.94                     | 0.49              |
| 2:D:122:PRO:HD2  | 2:D:125:PHE:CD1  | 2.48                     | 0.49              |
| 1:A:169:LEU:HD12 | 1:A:183:PHE:CE1  | 2.47                     | 0.49              |
| 1:E:323:VAL:HA   | 1:E:334:ARG:NH1  | 2.27                     | 0.49              |
| 1:E:525:ARG:CG   | 1:E:525:ARG:NH2  | 2.73                     | 0.49              |
| 1:B:447:LEU:CD1  | 1:B:575:ILE:HG21 | 2.43                     | 0.49              |
| 1:B:595:GLU:C    | 1:B:596:LYS:CD   | 2.86                     | 0.49              |
| 2:C:230:PHE:HA   | 2:C:233:VAL:HG21 | 1.95                     | 0.49              |
| 2:C:260:ILE:HD13 | 2:C:260:ILE:N    | 2.27                     | 0.49              |
| 2:C:260:ILE:CG2  | 2:C:315:GLN:HE22 | 2.17                     | 0.49              |
| 2:D:149:ARG:NE   | 2:D:149:ARG:CA   | 2.72                     | 0.49              |
| 1:A:239:TYR:OH   | 1:A:276:LEU:HB2  | 2.13                     | 0.49              |
| 1:A:329:LYS:CD   | 1:A:364:TRP:CH2  | 2.94                     | 0.49              |
| 1:A:476:ASP:O    | 1:A:479:GLU:OE1  | 2.30                     | 0.49              |
| 1:E:180:LYS:O    | 1:E:181:ASN:HB2  | 2.11                     | 0.49              |
| 1:E:297:SER:HA   | 1:E:319:GLN:O    | 2.12                     | 0.49              |
| 2:F:316:ILE:HG12 | 2:F:346:LEU:HD22 | 1.93                     | 0.49              |
| 1:B:326:ASN:N    | 1:B:326:ASN:ND2  | 2.60                     | 0.49              |
| 1:B:331:GLN:HE22 | 1:B:468:LEU:CB   | 2.25                     | 0.49              |
| 1:B:395:VAL:O    | 1:B:398:ASP:HB2  | 2.11                     | 0.49              |
| 2:C:417:PRO:HB2  | 1:A:584:PRO:HG3  | 1.94                     | 0.49              |
| 1:A:100:GLY:HA3  | 1:A:158:SER:HB2  | 1.93                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:290:TYR:CD1  | 1:A:315:THR:HG21 | 2.48                     | 0.49              |
| 1:A:358:LEU:CD1  | 1:A:358:LEU:C    | 2.86                     | 0.49              |
| 1:A:427:LEU:C    | 1:A:427:LEU:CD2  | 2.85                     | 0.49              |
| 1:A:572:SER:O    | 1:A:575:ILE:HD11 | 1.85                     | 0.49              |
| 1:E:225:HIS:N    | 1:E:228:TRP:CB   | 2.76                     | 0.49              |
| 1:E:322:TYR:CE2  | 1:E:324:GLY:CA   | 2.85                     | 0.49              |
| 1:E:482:ILE:HD13 | 1:E:508:LEU:HD12 | 1.95                     | 0.49              |
| 2:F:40:TYR:O     | 2:F:44:ILE:HD12  | 2.13                     | 0.49              |
| 2:F:158:TYR:CD1  | 2:F:159:TRP:NE1  | 2.80                     | 0.49              |
| 1:B:284:ASP:CG   | 1:B:287:GLN:H    | 2.21                     | 0.49              |
| 1:B:418:ARG:CB   | 1:B:420:SER:C    | 2.86                     | 0.49              |
| 1:B:486:ILE:HD11 | 1:B:563:THR:O    | 2.13                     | 0.49              |
| 2:C:48:GLU:CD    | 2:D:80:LEU:HD23  | 2.38                     | 0.49              |
| 2:C:180:ILE:HG13 | 2:C:181:LYS:N    | 2.26                     | 0.49              |
| 2:C:280:TYR:CB   | 2:C:334:THR:HG23 | 2.31                     | 0.49              |
| 2:C:323:LEU:O    | 2:C:327:MET:HG3  | 2.12                     | 0.49              |
| 1:A:325:PHE:HB2  | 1:A:330:ASP:CB   | 2.39                     | 0.49              |
| 1:E:294:ASP:HB3  | 1:E:322:TYR:CE2  | 2.47                     | 0.49              |
| 1:E:568:TRP:O    | 1:E:575:ILE:HD11 | 2.11                     | 0.49              |
| 2:F:262:LEU:CD1  | 2:F:262:LEU:C    | 2.85                     | 0.49              |
| 2:C:10:TRP:CD2   | 2:C:16:VAL:CG2   | 2.96                     | 0.49              |
| 2:C:65:HIS:HB3   | 2:C:91:THR:HG22  | 1.93                     | 0.49              |
| 2:C:279:ASN:HD21 | 2:C:308:ILE:CD1  | 2.17                     | 0.49              |
| 2:D:230:PHE:CB   | 2:D:233:VAL:HG21 | 2.42                     | 0.49              |
| 1:A:176:CYS:HB3  | 1:A:179:PHE:HD1  | 1.77                     | 0.49              |
| 1:A:346:TYR:O    | 1:A:350:GLY:N    | 2.46                     | 0.49              |
| 1:E:109:TYR:CE1  | 1:E:271:PRO:CD   | 2.86                     | 0.49              |
| 1:E:128:LEU:C    | 1:E:129:ILE:CD1  | 2.86                     | 0.49              |
| 1:E:486:ILE:O    | 1:E:526:LEU:HD22 | 2.13                     | 0.49              |
| 1:E:528:LEU:HD21 | 1:E:569:GLU:CD   | 2.37                     | 0.49              |
| 2:F:252:PHE:O    | 2:F:255:MET:HG2  | 2.12                     | 0.49              |
| 2:F:311:LEU:C    | 2:F:315:GLN:HG3  | 2.19                     | 0.49              |
| 2:C:133:THR:HG22 | 2:D:97:ASN:ND2   | 2.27                     | 0.49              |
| 2:C:314:GLU:HG2  | 2:C:318:ARG:HH12 | 1.78                     | 0.49              |
| 2:D:28:ARG:HA    | 2:D:31:ILE:HD11  | 1.95                     | 0.49              |
| 2:D:344:GLU:C    | 2:D:348:SER:OG   | 2.50                     | 0.49              |
| 1:E:446:LEU:HD13 | 1:E:528:LEU:CD2  | 2.10                     | 0.49              |
| 2:F:9:PRO:CD     | 2:F:10:TRP:CZ3   | 2.96                     | 0.49              |
| 1:B:432:TYR:OH   | 1:B:525:ARG:HD2  | 2.13                     | 0.49              |
| 2:C:268:PRO:HA   | 2:C:271:LEU:HB3  | 1.93                     | 0.49              |
| 2:C:304:ALA:O    | 2:C:307:TRP:CA   | 2.61                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:92:ILE:O     | 2:D:96:VAL:HG23  | 2.13                     | 0.49              |
| 1:A:375:THR:O    | 1:A:379:ARG:HB2  | 2.12                     | 0.49              |
| 1:A:440:LYS:HB2  | 1:A:440:LYS:NZ   | 2.27                     | 0.49              |
| 1:A:504:ASN:C    | 1:A:506:GLY:HA3  | 2.38                     | 0.49              |
| 1:E:560:ARG:HD3  | 1:E:561:GLY:N    | 2.28                     | 0.49              |
| 2:F:269:LEU:CD1  | 2:F:326:LYS:CB   | 2.90                     | 0.49              |
| 1:B:127:PRO:CA   | 1:B:222:VAL:HG21 | 2.40                     | 0.48              |
| 1:B:465:LEU:CD2  | 1:B:465:LEU:C    | 2.85                     | 0.48              |
| 2:D:28:ARG:CG    | 2:D:28:ARG:NH1   | 2.73                     | 0.48              |
| 2:D:145:THR:O    | 2:D:149:ARG:HG2  | 2.13                     | 0.48              |
| 2:D:331:LEU:C    | 2:D:343:LEU:CD2  | 2.86                     | 0.48              |
| 2:D:334:THR:CB   | 2:D:342:LEU:CB   | 2.91                     | 0.48              |
| 1:E:178:LEU:C    | 1:E:178:LEU:CD2  | 2.85                     | 0.48              |
| 1:E:485:THR:OG1  | 1:E:487:VAL:CG1  | 2.61                     | 0.48              |
| 1:B:248:ILE:HD12 | 1:B:376:LEU:HD11 | 1.94                     | 0.48              |
| 1:B:305:GLN:CG   | 1:B:309:HIS:CG   | 2.96                     | 0.48              |
| 1:B:366:LYS:CE   | 1:B:366:LYS:CA   | 2.89                     | 0.48              |
| 1:B:469:LYS:HG3  | 1:B:470:GLU:H    | 1.76                     | 0.48              |
| 2:C:124:LEU:O    | 2:C:124:LEU:HD13 | 2.12                     | 0.48              |
| 2:D:125:PHE:HE1  | 2:D:149:ARG:HB3  | 1.78                     | 0.48              |
| 1:A:310:LEU:HB3  | 1:A:428:LYS:CD   | 2.43                     | 0.48              |
| 1:A:358:LEU:HD12 | 1:A:359:ILE:N    | 2.25                     | 0.48              |
| 1:E:370:LEU:CD1  | 1:E:370:LEU:C    | 2.85                     | 0.48              |
| 1:E:445:PRO:CG   | 1:E:448:PHE:CE1  | 2.96                     | 0.48              |
| 1:E:455:SER:HG   | 1:E:462:ILE:N    | 2.08                     | 0.48              |
| 2:F:20:LYS:HA    | 2:F:159:TRP:HZ3  | 0.63                     | 0.48              |
| 2:F:103:ASN:CG   | 2:F:115:LEU:HD21 | 2.38                     | 0.48              |
| 2:F:116:ALA:C    | 2:F:119:ILE:HD12 | 2.38                     | 0.48              |
| 2:F:272:ILE:HG12 | 2:F:315:GLN:HE21 | 1.77                     | 0.48              |
| 1:B:122:SER:N    | 1:B:182:LEU:CD2  | 2.69                     | 0.48              |
| 1:B:213:ILE:CG2  | 3:B:725:HOH:O    | 2.60                     | 0.48              |
| 2:D:46:LEU:HD22  | 2:D:49:MET:HE3   | 1.95                     | 0.48              |
| 2:D:99:LEU:CD1   | 2:D:121:LEU:HD11 | 2.33                     | 0.48              |
| 2:D:321:ASP:O    | 2:D:325:SER:N    | 2.42                     | 0.48              |
| 1:A:290:TYR:CE1  | 1:A:315:THR:HG21 | 2.48                     | 0.48              |
| 1:A:305:GLN:CD   | 1:A:313:THR:HB   | 2.39                     | 0.48              |
| 1:A:542:TYR:C    | 1:A:543:ILE:CG2  | 2.85                     | 0.48              |
| 1:E:104:ILE:HG23 | 1:E:129:ILE:HG13 | 1.95                     | 0.48              |
| 1:E:264:LEU:CD1  | 1:E:358:LEU:CD1  | 2.86                     | 0.48              |
| 1:E:361:THR:HG22 | 1:E:362:PRO:CD   | 2.39                     | 0.48              |
| 1:E:502:LEU:CB   | 1:E:509:PRO:CB   | 2.77                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:121:PRO:HG2  | 1:B:124:SER:HB3  | 1.94                     | 0.48              |
| 1:B:235:LEU:N    | 1:B:235:LEU:HD22 | 2.28                     | 0.48              |
| 1:B:456:TYR:HE2  | 1:B:537:LYS:CA   | 1.76                     | 0.48              |
| 2:C:89:SER:O     | 2:C:93:ILE:CG1   | 2.61                     | 0.48              |
| 1:E:328:PRO:HB3  | 1:E:335:TYR:CD2  | 2.49                     | 0.48              |
| 2:F:119:ILE:O    | 2:F:120:ASP:HB3  | 2.13                     | 0.48              |
| 1:B:523:PHE:CZ   | 1:B:525:ARG:O    | 2.66                     | 0.48              |
| 1:B:598:TRP:CE3  | 2:D:58:HIS:NE2   | 2.80                     | 0.48              |
| 2:C:18:TYR:C     | 2:C:18:TYR:CD2   | 2.91                     | 0.48              |
| 2:D:354:PRO:O    | 2:D:358:ASP:N    | 2.42                     | 0.48              |
| 1:A:71:ILE:O     | 1:A:71:ILE:HG12  | 2.12                     | 0.48              |
| 1:A:107:VAL:CG2  | 1:A:109:TYR:CE2  | 2.97                     | 0.48              |
| 1:A:165:LEU:HD12 | 1:A:167:THR:HB   | 1.59                     | 0.48              |
| 1:A:310:LEU:HB3  | 1:A:428:LYS:HD2  | 1.95                     | 0.48              |
| 1:A:359:ILE:CG2  | 1:A:360:ASN:N    | 2.76                     | 0.48              |
| 1:E:294:ASP:OD2  | 1:E:563:THR:CB   | 2.60                     | 0.48              |
| 1:E:310:LEU:HB3  | 1:E:428:LYS:CG   | 2.43                     | 0.48              |
| 1:E:325:PHE:HD1  | 1:E:325:PHE:N    | 2.11                     | 0.48              |
| 1:E:399:ILE:HG13 | 1:E:399:ILE:O    | 2.11                     | 0.48              |
| 1:E:598:TRP:O    | 1:E:599:LYS:HG3  | 2.14                     | 0.48              |
| 1:B:238:LEU:HD11 | 3:B:715:HOH:O    | 1.90                     | 0.48              |
| 1:B:257:LYS:O    | 1:B:260:PHE:CB   | 2.61                     | 0.48              |
| 1:B:511:LEU:C    | 1:B:511:LEU:CD2  | 2.86                     | 0.48              |
| 2:C:95:PHE:CD1   | 2:C:99:LEU:HD11  | 2.49                     | 0.48              |
| 2:C:272:ILE:HD12 | 2:C:327:MET:HE1  | 1.94                     | 0.48              |
| 2:D:74:GLU:OE2   | 2:D:144:LYS:HE2  | 2.14                     | 0.48              |
| 1:A:63:PHE:O     | 1:A:64:SER:C     | 2.57                     | 0.48              |
| 1:A:225:HIS:O    | 1:A:228:TRP:N    | 2.47                     | 0.48              |
| 1:A:351:GLU:OE1  | 1:A:352:LEU:N    | 2.45                     | 0.48              |
| 1:A:576:VAL:O    | 1:A:580:LYS:N    | 2.47                     | 0.48              |
| 1:E:232:ILE:CG2  | 1:E:233:LYS:N    | 2.75                     | 0.48              |
| 1:E:340:GLU:CD   | 1:E:379:ARG:NH1  | 2.70                     | 0.48              |
| 1:E:454:VAL:HA   | 2:F:407:PHE:H    | 1.78                     | 0.48              |
| 1:B:68:ASP:CA    | 3:B:712:HOH:O    | 2.44                     | 0.48              |
| 1:B:94:VAL:HG23  | 1:B:165:LEU:HD13 | 1.96                     | 0.48              |
| 2:C:24:PHE:CE2   | 2:C:67:PHE:HZ    | 2.30                     | 0.48              |
| 1:A:162:LEU:N    | 1:A:162:LEU:CD1  | 2.73                     | 0.48              |
| 1:A:298:LEU:HD21 | 1:A:319:GLN:OE1  | 2.14                     | 0.48              |
| 1:A:489:ILE:CG2  | 1:A:524:PHE:HB3  | 2.44                     | 0.48              |
| 1:E:150:HIS:CA   | 1:E:151:LEU:C    | 2.87                     | 0.48              |
| 1:E:233:LYS:NZ   | 1:E:237:GLU:CB   | 2.73                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:F:256:MET:O   | 2:F:259:PHE:N    | 2.46                     | 0.48              |
| 2:D:139:SER:HB3 | 1:A:469:LYS:CE   | 2.44                     | 0.48              |
| 2:D:327:MET:HA  | 2:D:330:THR:CG2  | 2.44                     | 0.48              |
| 1:A:466:THR:HA  | 1:A:511:LEU:O    | 2.13                     | 0.48              |
| 1:A:473:ILE:CG2 | 1:A:474:GLY:N    | 2.76                     | 0.48              |
| 1:A:503:PHE:HB3 | 3:A:736:HOH:O    | 2.14                     | 0.48              |
| 1:E:364:TRP:CZ3 | 1:E:368:TYR:CB   | 2.86                     | 0.48              |
| 1:E:400:PRO:O   | 1:E:401:LYS:CD   | 2.62                     | 0.48              |
| 1:B:104:ILE:CG2 | 1:B:128:LEU:C    | 2.79                     | 0.48              |
| 1:B:490:PHE:HB3 | 1:B:557:ILE:CD1  | 2.44                     | 0.48              |
| 1:B:598:TRP:CD2 | 2:D:98:GLY:CA    | 2.97                     | 0.48              |
| 2:C:11:LYS:CG   | 1:A:585:TYR:CD2  | 2.86                     | 0.48              |
| 2:C:186:LEU:CA  | 2:C:221:ILE:HG12 | 2.34                     | 0.48              |
| 1:A:175:VAL:HB  | 1:A:568:TRP:HB3  | 1.96                     | 0.48              |
| 1:A:280:PHE:CE2 | 1:A:282:ASP:HB2  | 2.35                     | 0.48              |
| 1:E:430:MET:HB2 | 1:E:566:PRO:HG3  | 1.95                     | 0.48              |
| 2:F:237:ARG:CA  | 2:F:237:ARG:NE   | 2.73                     | 0.48              |
| 2:F:331:LEU:HB3 | 2:F:343:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:103:ASP:HA  | 1:B:107:VAL:C    | 2.39                     | 0.48              |
| 1:B:170:GLU:OE2 | 1:B:180:LYS:O    | 2.32                     | 0.48              |
| 1:B:469:LYS:CG  | 1:B:470:GLU:N    | 2.73                     | 0.48              |
| 2:C:12:SER:N    | 1:A:584:PRO:O    | 2.46                     | 0.48              |
| 1:A:162:LEU:CD2 | 1:A:162:LEU:C    | 2.86                     | 0.48              |
| 1:A:277:PRO:O   | 1:A:277:PRO:HG2  | 2.14                     | 0.48              |
| 1:A:277:PRO:O   | 1:A:355:GLU:CB   | 2.62                     | 0.48              |
| 1:A:370:LEU:O   | 1:A:373:THR:HB   | 2.13                     | 0.48              |
| 1:A:573:ASN:C   | 1:A:576:VAL:HG22 | 2.39                     | 0.48              |
| 1:E:99:ARG:CB   | 1:E:142:ASN:ND2  | 2.75                     | 0.48              |
| 1:E:227:ASN:ND2 | 1:E:228:TRP:N    | 2.62                     | 0.48              |
| 1:E:451:PRO:HD3 | 2:F:413:TRP:CE3  | 2.43                     | 0.48              |
| 1:B:327:SER:OG  | 1:B:329:LYS:HE2  | 2.13                     | 0.47              |
| 1:B:358:LEU:O   | 1:B:359:ILE:HG13 | 2.13                     | 0.47              |
| 1:B:432:TYR:O   | 1:B:435:LYS:HG2  | 2.14                     | 0.47              |
| 2:C:249:ARG:C   | 2:C:307:TRP:HH2  | 2.22                     | 0.47              |
| 2:D:56:VAL:HG23 | 2:D:61:GLN:HB2   | 1.94                     | 0.47              |
| 2:D:268:PRO:CA  | 2:D:271:LEU:CD1  | 2.85                     | 0.47              |
| 1:A:224:LYS:O   | 1:A:225:HIS:C    | 2.56                     | 0.47              |
| 1:A:239:TYR:CZ  | 1:A:276:LEU:HD12 | 2.48                     | 0.47              |
| 1:A:305:GLN:OE1 | 1:A:315:THR:HG23 | 2.14                     | 0.47              |
| 1:E:65:PHE:HB2  | 3:E:728:HOH:O    | 2.13                     | 0.47              |
| 1:E:86:ASN:C    | 1:E:87:LEU:HD23  | 2.37                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:170:GLU:OE1  | 1:B:183:PHE:C    | 2.57                     | 0.47              |
| 1:B:290:TYR:HA   | 1:B:311:SER:CB   | 2.44                     | 0.47              |
| 1:B:491:LYS:NZ   | 1:B:491:LYS:HB3  | 2.30                     | 0.47              |
| 1:B:502:LEU:HD23 | 1:B:502:LEU:O    | 2.13                     | 0.47              |
| 1:B:553:LYS:HG3  | 1:B:553:LYS:O    | 2.13                     | 0.47              |
| 1:B:570:ILE:O    | 1:B:575:ILE:HD12 | 2.14                     | 0.47              |
| 1:B:598:TRP:HB2  | 2:D:58:HIS:ND1   | 2.28                     | 0.47              |
| 2:D:6:ARG:HH11   | 2:D:6:ARG:CG     | 2.21                     | 0.47              |
| 1:E:466:THR:HB   | 1:E:511:LEU:HB3  | 1.96                     | 0.47              |
| 1:B:510:LEU:HD23 | 1:B:511:LEU:C    | 2.39                     | 0.47              |
| 2:C:43:ALA:HA    | 2:C:46:LEU:CD1   | 2.44                     | 0.47              |
| 1:A:294:ASP:HB3  | 1:A:323:VAL:HG23 | 1.96                     | 0.47              |
| 1:E:377:ILE:HG23 | 1:E:382:PRO:HG3  | 1.95                     | 0.47              |
| 1:E:458:VAL:O    | 1:E:458:VAL:HG12 | 2.13                     | 0.47              |
| 1:E:473:ILE:HD13 | 2:F:48:GLU:OE2   | 2.14                     | 0.47              |
| 2:F:247:HIS:CD2  | 2:F:247:HIS:N    | 2.73                     | 0.47              |
| 2:F:258:HIS:C    | 2:F:258:HIS:ND1  | 2.73                     | 0.47              |
| 2:F:420:VAL:O    | 2:F:421:ILE:HG13 | 2.11                     | 0.47              |
| 1:B:456:TYR:CE1  | 1:B:479:GLU:OE2  | 2.67                     | 0.47              |
| 1:B:492:VAL:HG22 | 1:B:493:LYS:N    | 2.29                     | 0.47              |
| 2:C:13:SER:O     | 2:C:13:SER:OG    | 2.31                     | 0.47              |
| 1:A:213:ILE:CD1  | 1:A:219:THR:OG1  | 2.59                     | 0.47              |
| 1:E:235:LEU:O    | 1:E:238:LEU:HB3  | 2.13                     | 0.47              |
| 2:F:20:LYS:HB2   | 2:F:159:TRP:CE3  | 2.48                     | 0.47              |
| 2:F:186:LEU:HD13 | 2:F:224:HIS:NE2  | 2.27                     | 0.47              |
| 2:F:238:ILE:HA   | 2:F:252:PHE:HZ   | 1.79                     | 0.47              |
| 1:B:87:LEU:O     | 1:B:128:LEU:CD2  | 2.63                     | 0.47              |
| 1:B:229:MET:O    | 1:B:233:LYS:HB2  | 2.14                     | 0.47              |
| 1:B:327:SER:HB3  | 1:B:329:LYS:NZ   | 2.30                     | 0.47              |
| 1:B:380:VAL:HG12 | 1:B:382:PRO:N    | 2.29                     | 0.47              |
| 1:B:456:TYR:CE2  | 1:B:537:LYS:CB   | 2.96                     | 0.47              |
| 2:C:8:THR:O      | 1:A:585:TYR:HB3  | 2.13                     | 0.47              |
| 2:C:276:LEU:HD11 | 2:C:331:LEU:CG   | 2.44                     | 0.47              |
| 1:E:95:LEU:HD23  | 1:E:95:LEU:C     | 2.38                     | 0.47              |
| 1:E:400:PRO:O    | 1:E:401:LYS:HD3  | 2.14                     | 0.47              |
| 2:F:113:HIS:ND1  | 2:F:114:LEU:N    | 2.62                     | 0.47              |
| 1:B:155:GLY:C    | 3:B:708:HOH:O    | 2.58                     | 0.47              |
| 1:B:530:HIS:HA   | 2:D:418:PHE:CE1  | 2.49                     | 0.47              |
| 2:C:247:HIS:O    | 2:C:250:ALA:N    | 2.47                     | 0.47              |
| 1:E:88:ILE:HG23  | 1:E:128:LEU:CD2  | 2.42                     | 0.47              |
| 2:F:82:ASP:O     | 2:F:86:LEU:HG    | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:313:THR:HG22 | 1:B:314:SER:N    | 2.29                     | 0.47              |
| 1:B:423:GLN:NE2  | 1:B:423:GLN:C    | 2.73                     | 0.47              |
| 1:B:482:ILE:O    | 1:B:485:THR:HG23 | 2.15                     | 0.47              |
| 2:C:53:ARG:CG    | 2:C:53:ARG:NH1   | 2.73                     | 0.47              |
| 2:C:416:LYS:CD   | 2:C:416:LYS:N    | 2.73                     | 0.47              |
| 2:D:18:TYR:O     | 2:D:22:LEU:HD21  | 2.15                     | 0.47              |
| 2:D:238:ILE:HD12 | 2:D:238:ILE:C    | 2.36                     | 0.47              |
| 2:D:257:ASN:ND2  | 2:D:257:ASN:C    | 2.73                     | 0.47              |
| 2:D:310:TRP:CD1  | 2:D:313:ILE:HD12 | 2.48                     | 0.47              |
| 1:A:401:LYS:HA   | 1:A:401:LYS:CE   | 2.44                     | 0.47              |
| 1:A:408:LEU:HD12 | 3:A:731:HOH:O    | 2.15                     | 0.47              |
| 1:E:167:THR:HG22 | 3:E:711:HOH:O    | 2.14                     | 0.47              |
| 1:E:233:LYS:HZ3  | 1:E:233:LYS:C    | 2.00                     | 0.47              |
| 1:E:397:ILE:CD1  | 1:E:397:ILE:N    | 2.73                     | 0.47              |
| 1:E:444:GLN:NE2  | 1:E:444:GLN:C    | 2.73                     | 0.47              |
| 2:F:22:LEU:HD13  | 2:F:43:ALA:H     | 1.78                     | 0.47              |
| 2:F:89:SER:OG    | 2:F:137:LEU:CD1  | 2.62                     | 0.47              |
| 2:F:120:ASP:OD2  | 2:F:157:HIS:CE1  | 2.68                     | 0.47              |
| 2:F:238:ILE:CB   | 2:F:307:TRP:HZ3  | 2.28                     | 0.47              |
| 2:F:247:HIS:O    | 2:F:248:LEU:C    | 2.57                     | 0.47              |
| 1:B:325:PHE:CE2  | 1:B:469:LYS:HD3  | 2.50                     | 0.47              |
| 1:B:388:LEU:HA   | 1:B:406:ILE:HG13 | 1.96                     | 0.47              |
| 2:C:252:PHE:O    | 2:C:255:MET:HB2  | 2.15                     | 0.47              |
| 2:D:18:TYR:O     | 2:D:22:LEU:CD2   | 2.63                     | 0.47              |
| 2:D:273:ASP:C    | 2:D:276:LEU:HG   | 2.40                     | 0.47              |
| 1:A:328:PRO:HB3  | 1:A:335:TYR:HE2  | 1.78                     | 0.47              |
| 1:A:420:SER:HB2  | 1:A:423:GLN:HB3  | 1.94                     | 0.47              |
| 2:F:40:TYR:CD1   | 2:F:67:PHE:CE2   | 3.03                     | 0.47              |
| 2:F:40:TYR:CE2   | 2:F:67:PHE:CE2   | 3.02                     | 0.47              |
| 1:B:328:PRO:CB   | 1:B:335:TYR:CD2  | 2.86                     | 0.47              |
| 1:B:343:VAL:HA   | 1:B:346:TYR:CB   | 2.45                     | 0.47              |
| 1:B:359:ILE:CG2  | 1:B:360:ASN:N    | 2.77                     | 0.47              |
| 2:C:15:GLU:C     | 2:C:18:TYR:H     | 2.22                     | 0.47              |
| 2:C:86:LEU:HD22  | 2:D:91:THR:HG1   | 1.79                     | 0.47              |
| 2:C:119:ILE:H    | 2:C:119:ILE:HG12 | 1.57                     | 0.47              |
| 2:C:320:ASP:OD1  | 2:C:320:ASP:N    | 2.41                     | 0.47              |
| 1:B:543:ILE:CD1  | 1:B:546:PHE:CD2  | 2.98                     | 0.47              |
| 2:C:85:ARG:HE    | 2:C:137:LEU:HG   | 1.80                     | 0.47              |
| 2:C:177:GLU:CD   | 2:C:177:GLU:N    | 2.73                     | 0.47              |
| 2:C:177:GLU:CD   | 2:C:180:ILE:HG21 | 2.39                     | 0.47              |
| 2:D:74:GLU:O     | 2:D:76:PHE:N     | 2.48                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:LEU:CD2   | 1:A:116:MET:CE   | 2.86                     | 0.47              |
| 1:A:296:ILE:HG21 | 1:A:342:LEU:CD2  | 2.44                     | 0.47              |
| 1:E:340:GLU:O    | 1:E:344:ARG:HG2  | 2.14                     | 0.47              |
| 1:E:388:LEU:HD12 | 1:E:408:LEU:HA   | 1.97                     | 0.47              |
| 1:E:468:LEU:HD22 | 1:E:469:LYS:N    | 2.30                     | 0.47              |
| 2:F:179:LEU:HG   | 2:F:180:ILE:N    | 2.30                     | 0.47              |
| 1:B:87:LEU:O     | 1:B:128:LEU:HD23 | 2.16                     | 0.46              |
| 1:B:271:PRO:HA   | 1:B:275:GLN:HE21 | 1.80                     | 0.46              |
| 2:C:159:TRP:HA   | 2:C:159:TRP:CE3  | 2.50                     | 0.46              |
| 2:C:418:PHE:HD2  | 2:C:418:PHE:H    | 1.63                     | 0.46              |
| 2:D:95:PHE:CE2   | 2:D:150:ALA:HB1  | 2.50                     | 0.46              |
| 1:A:133:GLN:OE1  | 1:A:136:ASN:CB   | 2.63                     | 0.46              |
| 1:A:420:SER:O    | 1:A:423:GLN:CA   | 2.63                     | 0.46              |
| 1:E:172:ILE:CD1  | 1:E:182:LEU:HB2  | 2.41                     | 0.46              |
| 1:E:207:ASP:OD1  | 1:E:207:ASP:N    | 2.48                     | 0.46              |
| 1:B:492:VAL:HG12 | 1:B:557:ILE:CG1  | 2.45                     | 0.46              |
| 1:B:528:LEU:O    | 1:B:542:TYR:N    | 2.46                     | 0.46              |
| 2:C:22:LEU:HD23  | 2:C:43:ALA:CB    | 2.44                     | 0.46              |
| 1:A:307:GLY:O    | 1:A:309:HIS:HD2  | 1.98                     | 0.46              |
| 1:A:313:THR:HG22 | 1:A:314:SER:N    | 2.30                     | 0.46              |
| 1:A:530:HIS:HD2  | 1:A:531:SER:OG   | 1.97                     | 0.46              |
| 2:F:122:PRO:CG   | 2:F:125:PHE:CD2  | 2.98                     | 0.46              |
| 2:F:131:SER:O    | 2:F:135:ASP:N    | 2.49                     | 0.46              |
| 2:F:336:HIS:CB   | 2:F:339:ASN:CB   | 2.92                     | 0.46              |
| 1:B:104:ILE:CD1  | 1:B:104:ILE:H    | 2.13                     | 0.46              |
| 1:B:180:LYS:CD   | 1:B:181:ASN:H    | 2.29                     | 0.46              |
| 1:B:530:HIS:ND1  | 1:B:530:HIS:C    | 2.73                     | 0.46              |
| 2:C:225:ALA:CA   | 2:C:227:MET:SD   | 2.94                     | 0.46              |
| 2:D:269:LEU:CA   | 2:D:272:ILE:CD1  | 2.86                     | 0.46              |
| 1:A:118:PHE:CD1  | 1:A:306:HIS:HB3  | 2.51                     | 0.46              |
| 1:E:110:HIS:HE2  | 1:E:137:SER:H    | 1.64                     | 0.46              |
| 1:E:161:LYS:NZ   | 1:E:163:THR:HG1  | 2.08                     | 0.46              |
| 1:E:504:ASN:O    | 1:E:509:PRO:CA   | 2.63                     | 0.46              |
| 1:E:525:ARG:HD2  | 1:E:543:ILE:HD11 | 1.96                     | 0.46              |
| 2:F:252:PHE:O    | 2:F:256:MET:CG   | 2.51                     | 0.46              |
| 1:B:171:SER:OG   | 1:B:174:ARG:CD   | 2.48                     | 0.46              |
| 1:B:293:THR:CG2  | 1:B:425:ARG:HD2  | 2.45                     | 0.46              |
| 1:B:543:ILE:HD11 | 1:B:546:PHE:CD2  | 2.48                     | 0.46              |
| 2:D:194:ARG:HH11 | 2:D:194:ARG:CG   | 2.21                     | 0.46              |
| 2:D:331:LEU:CB   | 2:D:343:LEU:CD2  | 2.84                     | 0.46              |
| 1:A:176:CYS:HB3  | 1:A:179:PHE:HB2  | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:456:TYR:O    | 1:A:537:LYS:CB   | 2.63                     | 0.46              |
| 1:A:489:ILE:O    | 1:A:524:PHE:CB   | 2.64                     | 0.46              |
| 1:A:546:PHE:HD1  | 1:A:546:PHE:H    | 1.63                     | 0.46              |
| 1:A:579:PHE:O    | 1:A:580:LYS:HB2  | 2.14                     | 0.46              |
| 1:E:225:HIS:N    | 1:E:225:HIS:ND1  | 2.60                     | 0.46              |
| 1:E:335:TYR:OH   | 1:E:362:PRO:HG2  | 2.15                     | 0.46              |
| 1:E:403:THR:C    | 1:E:404:ASN:ND2  | 2.73                     | 0.46              |
| 2:F:331:LEU:HG   | 2:F:343:LEU:CD1  | 2.45                     | 0.46              |
| 1:B:287:GLN:OE1  | 1:B:287:GLN:HA   | 2.15                     | 0.46              |
| 1:B:446:LEU:O    | 1:B:542:TYR:CZ   | 2.69                     | 0.46              |
| 1:B:463:SER:OG   | 1:B:555:ALA:HB1  | 2.14                     | 0.46              |
| 1:B:502:LEU:N    | 1:B:502:LEU:CD2  | 2.73                     | 0.46              |
| 2:C:151:ILE:HG23 | 2:C:152:ASP:N    | 2.30                     | 0.46              |
| 1:A:322:TYR:HB2  | 1:A:523:PHE:CE2  | 2.50                     | 0.46              |
| 1:E:364:TRP:CH2  | 1:E:368:TYR:CD1  | 3.02                     | 0.46              |
| 1:E:492:VAL:HG21 | 1:E:496:HIS:CB   | 2.46                     | 0.46              |
| 2:F:33:ARG:CB    | 2:F:33:ARG:NH2   | 2.73                     | 0.46              |
| 2:F:33:ARG:HB3   | 2:F:33:ARG:NH2   | 2.30                     | 0.46              |
| 2:F:256:MET:C    | 2:F:259:PHE:HB3  | 2.39                     | 0.46              |
| 1:B:186:PHE:HD2  | 1:B:187:ASP:N    | 2.13                     | 0.46              |
| 1:B:447:LEU:HD12 | 1:B:575:ILE:HG21 | 1.98                     | 0.46              |
| 2:C:143:CYS:O    | 2:C:147:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:93:PHE:HB3   | 1:A:210:PHE:CB   | 2.45                     | 0.46              |
| 1:A:322:TYR:CG   | 1:A:523:PHE:CZ   | 3.03                     | 0.46              |
| 1:E:296:ILE:HD11 | 1:E:335:TYR:CE1  | 2.51                     | 0.46              |
| 1:E:525:ARG:HG3  | 1:E:525:ARG:NH2  | 2.31                     | 0.46              |
| 1:B:178:LEU:HD13 | 1:B:178:LEU:HA   | 1.72                     | 0.46              |
| 1:B:381:LYS:N    | 1:B:382:PRO:CD   | 2.78                     | 0.46              |
| 1:B:417:SER:N    | 1:B:419:TYR:HA   | 2.30                     | 0.46              |
| 1:B:445:PRO:HG2  | 1:B:448:PHE:CE1  | 2.51                     | 0.46              |
| 1:B:528:LEU:HG   | 1:B:542:TYR:HB2  | 1.97                     | 0.46              |
| 2:C:280:TYR:CB   | 2:C:334:THR:CG2  | 2.72                     | 0.46              |
| 1:A:322:TYR:CB   | 1:A:523:PHE:CD1  | 2.98                     | 0.46              |
| 1:E:95:LEU:HB2   | 1:E:161:LYS:O    | 2.16                     | 0.46              |
| 1:E:233:LYS:NZ   | 1:E:236:THR:OG1  | 2.48                     | 0.46              |
| 1:E:346:TYR:O    | 1:E:350:GLY:CA   | 2.63                     | 0.46              |
| 2:F:272:ILE:O    | 2:F:276:LEU:HG   | 2.15                     | 0.46              |
| 1:B:81:LEU:CD2   | 1:B:87:LEU:HD21  | 2.44                     | 0.46              |
| 1:B:436:ILE:HG23 | 1:B:437:ASP:N    | 2.31                     | 0.46              |
| 1:B:525:ARG:HA   | 1:B:525:ARG:HD3  | 1.69                     | 0.46              |
| 2:C:307:TRP:O    | 2:C:310:TRP:N    | 2.49                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:96:VAL:O     | 2:D:100:LEU:HD12 | 2.16                     | 0.46              |
| 2:D:255:MET:SD   | 2:D:259:PHE:HB3  | 2.55                     | 0.46              |
| 1:A:123:SER:HG   | 1:A:419:TYR:HE1  | 1.61                     | 0.46              |
| 1:A:227:ASN:CG   | 1:A:228:TRP:N    | 2.73                     | 0.46              |
| 1:A:451:PRO:HG2  | 1:A:540:ASN:OD1  | 2.15                     | 0.46              |
| 1:E:227:ASN:ND2  | 1:E:227:ASN:C    | 2.73                     | 0.46              |
| 1:E:283:LEU:CD1  | 1:E:339:VAL:HG11 | 2.45                     | 0.46              |
| 1:E:372:LEU:HD23 | 1:E:372:LEU:HA   | 1.76                     | 0.46              |
| 1:E:420:SER:O    | 1:E:423:GLN:HB3  | 2.15                     | 0.46              |
| 2:F:110:ILE:HD12 | 2:F:111:PRO:O    | 2.16                     | 0.46              |
| 1:B:180:LYS:HE2  | 1:B:181:ASN:N    | 2.30                     | 0.46              |
| 1:B:256:GLY:C    | 1:B:259:THR:HG1  | 2.02                     | 0.46              |
| 1:B:257:LYS:HA   | 1:B:260:PHE:CB   | 2.46                     | 0.46              |
| 1:B:432:TYR:CD2  | 1:B:526:LEU:HB2  | 2.47                     | 0.46              |
| 1:B:490:PHE:CE2  | 1:B:559:VAL:HG21 | 2.51                     | 0.46              |
| 2:C:146:CYS:O    | 2:C:149:ARG:HB3  | 2.15                     | 0.46              |
| 2:D:259:PHE:HE1  | 2:D:268:PRO:CG   | 2.22                     | 0.46              |
| 2:D:342:LEU:O    | 2:D:346:LEU:CG   | 2.55                     | 0.46              |
| 1:A:175:VAL:HG21 | 1:A:430:MET:HE1  | 1.97                     | 0.46              |
| 1:A:568:TRP:O    | 1:A:572:SER:HB3  | 2.16                     | 0.46              |
| 1:E:121:PRO:O    | 1:E:122:SER:OG   | 2.32                     | 0.46              |
| 1:E:138:SER:HB3  | 1:E:140:LEU:N    | 2.30                     | 0.46              |
| 2:F:237:ARG:HE   | 2:F:237:ARG:CA   | 2.13                     | 0.46              |
| 1:B:257:LYS:O    | 1:B:258:SER:C    | 2.59                     | 0.46              |
| 2:C:53:ARG:HH21  | 1:A:481:SER:HA   | 1.81                     | 0.46              |
| 2:D:139:SER:CB   | 1:A:469:LYS:HE3  | 2.44                     | 0.46              |
| 2:D:151:ILE:O    | 2:D:154:VAL:HG22 | 2.16                     | 0.46              |
| 1:A:126:ILE:N    | 1:A:220:VAL:O    | 2.38                     | 0.46              |
| 1:A:498:GLU:HG3  | 1:A:498:GLU:O    | 2.16                     | 0.46              |
| 1:E:284:ASP:OD1  | 1:E:286:GLY:N    | 2.49                     | 0.46              |
| 1:E:450:PRO:HA   | 2:F:413:TRP:CD1  | 2.51                     | 0.46              |
| 1:E:466:THR:HG21 | 1:E:516:PHE:CB   | 2.46                     | 0.46              |
| 2:F:117:LYS:C    | 2:F:117:LYS:CD   | 2.87                     | 0.46              |
| 2:F:214:TYR:C    | 2:F:214:TYR:HD2  | 2.22                     | 0.46              |
| 1:B:67:ASP:O     | 1:B:69:ASN:N     | 2.43                     | 0.45              |
| 1:B:116:MET:HE2  | 1:B:116:MET:HB3  | 1.80                     | 0.45              |
| 1:B:138:SER:HB3  | 1:B:140:LEU:O    | 2.16                     | 0.45              |
| 1:B:308:ASN:ND2  | 1:B:308:ASN:C    | 2.73                     | 0.45              |
| 2:C:260:ILE:O    | 2:C:264:GLY:CA   | 2.65                     | 0.45              |
| 1:E:351:GLU:CD   | 1:E:352:LEU:N    | 2.73                     | 0.45              |
| 1:E:445:PRO:HG3  | 1:E:448:PHE:CZ   | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:232:ASN:CA   | 2:C:278:LYS:HZ3  | 2.29                     | 0.45              |
| 2:D:68:SER:O     | 2:D:71:MET:HB2   | 2.16                     | 0.45              |
| 1:E:219:THR:HG22 | 1:E:220:VAL:H    | 1.80                     | 0.45              |
| 1:E:269:LEU:HD21 | 1:E:278:ILE:CG2  | 2.45                     | 0.45              |
| 1:E:309:HIS:CD2  | 1:E:313:THR:OG1  | 2.68                     | 0.45              |
| 1:E:377:ILE:HD13 | 1:E:377:ILE:N    | 2.31                     | 0.45              |
| 1:E:468:LEU:HG   | 1:E:513:TYR:HE1  | 1.80                     | 0.45              |
| 1:E:586:ILE:CA   | 2:F:6:ARG:O      | 2.64                     | 0.45              |
| 2:F:40:TYR:CD1   | 2:F:67:PHE:CD2   | 3.04                     | 0.45              |
| 2:F:235:ILE:HD11 | 2:F:271:LEU:CD2  | 2.47                     | 0.45              |
| 2:F:237:ARG:O    | 2:F:240:SER:HB2  | 2.16                     | 0.45              |
| 2:F:342:LEU:CD2  | 2:F:342:LEU:C    | 2.89                     | 0.45              |
| 1:B:107:VAL:CG2  | 1:B:109:TYR:HE2  | 2.29                     | 0.45              |
| 1:B:121:PRO:HG2  | 1:B:124:SER:H    | 1.81                     | 0.45              |
| 1:B:122:SER:H    | 1:B:182:LEU:HD21 | 1.78                     | 0.45              |
| 2:C:49:MET:HE2   | 1:A:481:SER:HB2  | 1.99                     | 0.45              |
| 2:D:93:ILE:HD11  | 2:D:132:ALA:HB1  | 1.91                     | 0.45              |
| 2:D:232:ASN:CG   | 2:D:274:SER:OG   | 2.59                     | 0.45              |
| 1:A:108:ILE:HG12 | 1:A:133:GLN:HG3  | 1.97                     | 0.45              |
| 1:A:342:LEU:HD12 | 1:A:342:LEU:HA   | 1.80                     | 0.45              |
| 1:E:77:VAL:C     | 1:E:78:ILE:HD12  | 2.41                     | 0.45              |
| 1:E:224:LYS:HG3  | 1:E:228:TRP:CE2  | 2.51                     | 0.45              |
| 1:E:294:ASP:O    | 1:E:322:TYR:HD2  | 1.99                     | 0.45              |
| 1:E:446:LEU:HD12 | 1:E:528:LEU:HD21 | 1.98                     | 0.45              |
| 2:F:237:ARG:HD3  | 2:F:237:ARG:C    | 2.40                     | 0.45              |
| 1:B:399:ILE:CG2  | 1:B:400:PRO:HA   | 2.47                     | 0.45              |
| 1:B:572:SER:N    | 1:B:575:ILE:CD1  | 2.79                     | 0.45              |
| 2:C:49:MET:CE    | 1:A:481:SER:HB2  | 2.46                     | 0.45              |
| 2:D:230:PHE:O    | 2:D:233:VAL:N    | 2.49                     | 0.45              |
| 2:D:309:ARG:O    | 2:D:313:ILE:N    | 2.42                     | 0.45              |
| 2:D:331:LEU:CD2  | 2:D:346:LEU:HD12 | 2.33                     | 0.45              |
| 1:A:250:ILE:HG22 | 1:A:386:ILE:O    | 2.15                     | 0.45              |
| 1:A:516:PHE:CD2  | 1:A:516:PHE:O    | 2.70                     | 0.45              |
| 1:E:226:LYS:O    | 1:E:229:MET:HB3  | 2.15                     | 0.45              |
| 1:E:242:ASP:HA   | 1:E:243:GLN:HA   | 1.74                     | 0.45              |
| 1:E:298:LEU:CD2  | 1:E:319:GLN:OE1  | 2.65                     | 0.45              |
| 1:E:507:GLN:NE2  | 1:E:534:GLN:HB3  | 2.32                     | 0.45              |
| 2:F:338:LEU:HD12 | 2:F:339:ASN:ND2  | 2.31                     | 0.45              |
| 1:B:167:THR:OG1  | 1:B:439:PHE:O    | 2.33                     | 0.45              |
| 1:B:223:ILE:CD1  | 1:B:224:LYS:N    | 2.73                     | 0.45              |
| 1:B:281:MET:HE1  | 1:B:343:VAL:HG22 | 1.97                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:305:GLN:HG2  | 1:B:309:HIS:CG   | 2.52                     | 0.45              |
| 1:B:572:SER:OG   | 1:B:575:ILE:HG13 | 2.16                     | 0.45              |
| 2:C:370:LEU:HA   | 2:C:373:ASP:CG   | 2.42                     | 0.45              |
| 2:D:153:TRP:O    | 2:D:156:ASP:HB2  | 2.17                     | 0.45              |
| 1:A:92:GLN:NE2   | 1:A:92:GLN:N     | 2.63                     | 0.45              |
| 1:A:399:ILE:C    | 1:A:399:ILE:CD1  | 2.86                     | 0.45              |
| 1:A:572:SER:O    | 1:A:575:ILE:HG12 | 2.16                     | 0.45              |
| 2:F:15:GLU:O     | 2:F:18:TYR:HB3   | 2.15                     | 0.45              |
| 1:B:72:TYR:HE2   | 1:B:206:SER:H    | 1.62                     | 0.45              |
| 1:B:277:PRO:O    | 1:B:355:GLU:CB   | 2.65                     | 0.45              |
| 1:B:283:LEU:HA   | 1:B:296:ILE:HG12 | 1.99                     | 0.45              |
| 1:B:358:LEU:HD13 | 1:B:358:LEU:HA   | 1.73                     | 0.45              |
| 2:C:124:LEU:O    | 2:C:127:GLU:HB3  | 2.17                     | 0.45              |
| 1:A:322:TYR:HD1  | 1:A:523:PHE:CE1  | 2.32                     | 0.45              |
| 1:A:593:SER:HB2  | 1:A:594:LEU:H    | 1.48                     | 0.45              |
| 1:E:178:LEU:HD23 | 1:E:178:LEU:O    | 2.15                     | 0.45              |
| 1:E:365:ILE:CD1  | 1:E:365:ILE:C    | 2.85                     | 0.45              |
| 2:F:320:ASP:O    | 2:F:324:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:293:THR:HG21 | 1:B:425:ARG:HD2  | 1.98                     | 0.45              |
| 1:B:307:GLY:O    | 1:B:309:HIS:N    | 2.47                     | 0.45              |
| 1:B:370:LEU:O    | 1:B:374:ARG:N    | 2.42                     | 0.45              |
| 1:B:380:VAL:HG12 | 1:B:382:PRO:CA   | 2.47                     | 0.45              |
| 2:C:31:ILE:HG12  | 2:C:35:GLU:CD    | 2.40                     | 0.45              |
| 1:A:133:GLN:NE2  | 1:A:134:VAL:N    | 2.64                     | 0.45              |
| 1:A:278:ILE:C    | 1:A:278:ILE:CD1  | 2.85                     | 0.45              |
| 1:E:72:TYR:O     | 1:E:77:VAL:HG22  | 2.16                     | 0.45              |
| 1:B:176:CYS:HB2  | 1:B:179:PHE:HB2  | 1.99                     | 0.45              |
| 1:B:211:TYR:CD1  | 1:B:211:TYR:C    | 2.94                     | 0.45              |
| 1:B:456:TYR:HE1  | 1:B:479:GLU:OE2  | 1.99                     | 0.45              |
| 2:C:337:GLU:O    | 2:C:338:LEU:C    | 2.60                     | 0.45              |
| 2:D:68:SER:HA    | 2:D:71:MET:CG    | 2.33                     | 0.45              |
| 2:D:343:LEU:HA   | 2:D:346:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:93:PHE:HD2   | 1:A:162:LEU:CG   | 2.25                     | 0.45              |
| 1:E:99:ARG:CB    | 1:E:142:ASN:HB3  | 2.46                     | 0.45              |
| 1:E:341:GLN:HA   | 1:E:344:ARG:HG2  | 1.99                     | 0.45              |
| 1:E:382:PRO:HB2  | 1:E:384:HIS:O    | 2.17                     | 0.45              |
| 2:F:24:PHE:CE1   | 2:F:155:TRP:CD2  | 3.02                     | 0.45              |
| 2:F:271:LEU:HD23 | 2:F:271:LEU:HA   | 1.79                     | 0.45              |
| 1:B:225:HIS:CB   | 1:B:227:ASN:HD21 | 2.29                     | 0.45              |
| 1:B:241:ASN:C    | 1:B:274:GLN:HE22 | 2.25                     | 0.45              |
| 1:B:528:LEU:C    | 1:B:528:LEU:CD1  | 2.85                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:250:ALA:O    | 2:C:254:PRO:HD2  | 2.17                     | 0.45              |
| 2:C:310:TRP:CE3  | 2:C:310:TRP:O    | 2.70                     | 0.45              |
| 2:D:410:HIS:ND1  | 2:D:411:PRO:CD   | 2.80                     | 0.45              |
| 1:A:523:PHE:CE2  | 1:A:524:PHE:O    | 2.70                     | 0.45              |
| 1:E:207:ASP:O    | 1:E:208:TYR:CG   | 2.70                     | 0.45              |
| 1:E:310:LEU:N    | 1:E:310:LEU:CD2  | 2.73                     | 0.45              |
| 1:E:486:ILE:HD11 | 1:E:565:LEU:HA   | 1.99                     | 0.45              |
| 1:E:489:ILE:CD1  | 1:E:527:ALA:HB2  | 2.31                     | 0.45              |
| 2:F:237:ARG:C    | 2:F:237:ARG:CD   | 2.88                     | 0.45              |
| 2:C:8:THR:CG2    | 1:A:587:THR:CG2  | 2.85                     | 0.45              |
| 2:C:36:LEU:HD23  | 2:C:40:TYR:CE1   | 2.44                     | 0.45              |
| 2:C:137:LEU:H    | 2:D:94:ARG:HH22  | 1.64                     | 0.45              |
| 2:C:211:GLY:O    | 2:C:215:TRP:CD1  | 2.70                     | 0.45              |
| 2:C:269:LEU:HD22 | 2:C:323:LEU:CG   | 2.47                     | 0.45              |
| 2:C:280:TYR:CD2  | 2:C:280:TYR:C    | 2.94                     | 0.45              |
| 2:C:356:ILE:O    | 2:C:360:ILE:HG12 | 2.17                     | 0.45              |
| 1:A:72:TYR:CE2   | 1:A:206:SER:HB2  | 2.13                     | 0.45              |
| 1:A:107:VAL:HG23 | 1:A:109:TYR:CZ   | 2.50                     | 0.45              |
| 1:A:166:ASP:OD1  | 1:A:168:HIS:CD2  | 2.70                     | 0.45              |
| 1:A:184:TRP:HE1  | 1:A:210:PHE:CA   | 2.29                     | 0.45              |
| 1:A:278:ILE:HD13 | 1:A:279:ASN:N    | 2.32                     | 0.45              |
| 1:A:413:ASN:CB   | 1:A:418:ARG:CB   | 2.95                     | 0.45              |
| 1:A:452:ILE:HD13 | 1:A:546:PHE:CZ   | 2.52                     | 0.45              |
| 1:A:478:LEU:HD21 | 1:A:508:LEU:HB2  | 1.99                     | 0.45              |
| 1:A:523:PHE:CD2  | 1:A:524:PHE:O    | 2.70                     | 0.45              |
| 1:E:169:LEU:HD13 | 1:E:169:LEU:C    | 2.42                     | 0.45              |
| 1:E:210:PHE:CD2  | 1:E:210:PHE:O    | 2.70                     | 0.45              |
| 1:E:283:LEU:HD13 | 1:E:339:VAL:HG11 | 1.98                     | 0.45              |
| 1:E:298:LEU:CD2  | 1:E:318:THR:HB   | 2.47                     | 0.45              |
| 1:E:485:THR:OG1  | 1:E:487:VAL:HG12 | 2.17                     | 0.45              |
| 2:F:111:PRO:HB3  | 2:F:113:HIS:HE1  | 1.56                     | 0.45              |
| 1:B:169:LEU:HD12 | 1:B:183:PHE:HE1  | 1.72                     | 0.44              |
| 1:B:239:TYR:CE1  | 1:B:268:MET:HB3  | 2.50                     | 0.44              |
| 1:B:368:TYR:O    | 1:B:371:GLU:N    | 2.50                     | 0.44              |
| 1:B:595:GLU:C    | 1:B:596:LYS:CG   | 2.89                     | 0.44              |
| 2:C:137:LEU:N    | 2:D:94:ARG:NH2   | 2.66                     | 0.44              |
| 2:D:190:TYR:CE2  | 2:D:218:ILE:HG21 | 2.48                     | 0.44              |
| 2:D:257:ASN:O    | 2:D:260:ILE:HB   | 2.16                     | 0.44              |
| 2:D:266:ASP:O    | 2:D:269:LEU:CB   | 2.65                     | 0.44              |
| 1:A:184:TRP:CD1  | 1:A:184:TRP:O    | 2.70                     | 0.44              |
| 1:A:239:TYR:CD1  | 1:A:239:TYR:O    | 2.70                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:442:ASP:OD1  | 1:A:442:ASP:N    | 2.50                     | 0.44              |
| 1:A:524:PHE:HE2  | 1:A:525:ARG:NE   | 2.15                     | 0.44              |
| 1:E:83:SER:O     | 1:E:84:ASN:C     | 2.60                     | 0.44              |
| 1:E:247:VAL:HG13 | 1:E:386:ILE:HD12 | 1.93                     | 0.44              |
| 1:E:523:PHE:CE1  | 1:E:525:ARG:O    | 2.70                     | 0.44              |
| 1:E:524:PHE:HD2  | 1:E:525:ARG:N    | 2.15                     | 0.44              |
| 2:F:11:LYS:NZ    | 2:F:11:LYS:CB    | 2.73                     | 0.44              |
| 2:F:235:ILE:HA   | 2:F:238:ILE:HD13 | 1.96                     | 0.44              |
| 2:F:238:ILE:CG1  | 2:F:252:PHE:CZ   | 3.00                     | 0.44              |
| 1:B:72:TYR:HE2   | 1:B:206:SER:N    | 2.15                     | 0.44              |
| 1:B:211:TYR:CE1  | 1:B:212:PRO:O    | 2.70                     | 0.44              |
| 1:B:278:ILE:HD11 | 1:B:358:LEU:HG   | 1.99                     | 0.44              |
| 1:B:572:SER:O    | 1:B:575:ILE:N    | 2.46                     | 0.44              |
| 2:C:10:TRP:CD1   | 2:C:10:TRP:O     | 2.70                     | 0.44              |
| 2:C:101:ASP:C    | 2:C:103:ASN:N    | 2.74                     | 0.44              |
| 2:C:190:TYR:O    | 2:C:193:ILE:N    | 2.50                     | 0.44              |
| 2:C:215:TRP:CA   | 2:C:218:ILE:CD1  | 2.82                     | 0.44              |
| 2:D:10:TRP:O     | 2:D:10:TRP:CD1   | 2.70                     | 0.44              |
| 2:D:12:SER:OG    | 2:D:14:ASP:CB    | 2.65                     | 0.44              |
| 2:D:128:PHE:CD1  | 2:D:128:PHE:O    | 2.70                     | 0.44              |
| 2:D:213:GLU:O    | 2:D:216:THR:CB   | 2.65                     | 0.44              |
| 1:A:81:LEU:HD21  | 1:A:85:GLN:O     | 2.17                     | 0.44              |
| 1:A:92:GLN:H     | 1:A:92:GLN:CD    | 2.24                     | 0.44              |
| 1:A:283:LEU:CD2  | 1:A:339:VAL:HG13 | 2.45                     | 0.44              |
| 1:A:385:VAL:HG12 | 1:A:403:THR:HG22 | 1.94                     | 0.44              |
| 1:A:401:LYS:HA   | 1:A:401:LYS:HZ1  | 1.78                     | 0.44              |
| 1:E:299:SER:HA   | 1:E:317:SER:HB2  | 1.89                     | 0.44              |
| 2:F:272:ILE:HG23 | 2:F:315:GLN:HE22 | 1.81                     | 0.44              |
| 2:F:345:LYS:HA   | 2:F:345:LYS:HD3  | 1.77                     | 0.44              |
| 1:B:74:HIS:ND1   | 1:B:75:ASP:N     | 2.65                     | 0.44              |
| 1:B:225:HIS:HB2  | 1:B:227:ASN:HD21 | 1.81                     | 0.44              |
| 1:B:553:LYS:HA   | 1:B:553:LYS:HD2  | 1.69                     | 0.44              |
| 2:C:89:SER:O     | 2:C:93:ILE:CD1   | 2.66                     | 0.44              |
| 2:C:340:VAL:HG22 | 2:C:367:ILE:HG22 | 1.98                     | 0.44              |
| 2:C:411:PRO:HG2  | 2:C:412:ASN:H    | 1.82                     | 0.44              |
| 2:D:256:MET:O    | 2:D:259:PHE:CD2  | 2.70                     | 0.44              |
| 2:D:310:TRP:O    | 2:D:314:GLU:N    | 2.30                     | 0.44              |
| 1:A:63:PHE:CD2   | 1:A:63:PHE:O     | 2.70                     | 0.44              |
| 1:A:71:ILE:HD11  | 1:A:78:ILE:CB    | 2.42                     | 0.44              |
| 1:A:309:HIS:ND1  | 1:A:313:THR:OG1  | 2.50                     | 0.44              |
| 1:A:327:SER:HB3  | 3:A:718:HOH:O    | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:572:SER:HG   | 1:A:575:ILE:HD12 | 1.81                     | 0.44              |
| 1:E:305:GLN:NE2  | 1:E:313:THR:OG1  | 2.51                     | 0.44              |
| 1:E:530:HIS:C    | 2:F:418:PHE:CA   | 2.85                     | 0.44              |
| 1:B:94:VAL:CG2   | 1:B:165:LEU:HD13 | 2.47                     | 0.44              |
| 1:B:455:SER:CB   | 2:D:405:LYS:N    | 2.80                     | 0.44              |
| 2:C:139:SER:O    | 2:C:142:MET:HB3  | 2.16                     | 0.44              |
| 1:A:479:GLU:H    | 1:A:479:GLU:HG3  | 1.46                     | 0.44              |
| 1:A:569:GLU:CD   | 1:A:569:GLU:C    | 2.85                     | 0.44              |
| 1:E:210:PHE:O    | 1:E:211:TYR:CD2  | 2.70                     | 0.44              |
| 1:E:344:ARG:HH21 | 1:E:379:ARG:HH22 | 1.63                     | 0.44              |
| 1:E:435:LYS:HA   | 1:E:441:PHE:HA   | 1.98                     | 0.44              |
| 2:F:18:TYR:CD2   | 2:F:18:TYR:O     | 2.70                     | 0.44              |
| 2:F:214:TYR:CD2  | 2:F:214:TYR:O    | 2.70                     | 0.44              |
| 2:F:308:ILE:O    | 2:F:311:LEU:HB2  | 2.18                     | 0.44              |
| 1:B:269:LEU:HA   | 1:B:269:LEU:HD23 | 1.74                     | 0.44              |
| 1:B:477:HIS:HB3  | 2:D:49:MET:HE2   | 1.99                     | 0.44              |
| 2:D:58:HIS:CD2   | 2:D:62:SER:OG    | 2.70                     | 0.44              |
| 2:D:63:THR:HA    | 2:D:66:LEU:HD13  | 1.98                     | 0.44              |
| 2:D:267:PHE:C    | 2:D:270:GLY:N    | 2.73                     | 0.44              |
| 1:A:331:GLN:CB   | 1:A:334:ARG:CB   | 2.92                     | 0.44              |
| 1:E:150:HIS:HA   | 1:E:151:LEU:C    | 2.42                     | 0.44              |
| 1:E:370:LEU:HD13 | 1:E:370:LEU:C    | 2.41                     | 0.44              |
| 1:E:524:PHE:CD2  | 1:E:525:ARG:N    | 2.85                     | 0.44              |
| 2:F:31:ILE:HG12  | 2:F:32:SER:N     | 2.33                     | 0.44              |
| 2:F:312:ALA:CB   | 2:F:342:LEU:CD2  | 2.91                     | 0.44              |
| 1:B:74:HIS:ND1   | 1:B:74:HIS:C     | 2.74                     | 0.44              |
| 1:B:516:PHE:CD2  | 1:B:516:PHE:O    | 2.70                     | 0.44              |
| 1:B:543:ILE:CD1  | 1:B:546:PHE:CD1  | 2.85                     | 0.44              |
| 1:B:546:PHE:CD1  | 1:B:546:PHE:N    | 2.86                     | 0.44              |
| 1:B:586:ILE:HG22 | 2:D:6:ARG:O      | 2.16                     | 0.44              |
| 2:D:150:ALA:O    | 2:D:153:TRP:HB3  | 2.18                     | 0.44              |
| 2:D:268:PRO:HA   | 2:D:271:LEU:HD12 | 1.94                     | 0.44              |
| 1:A:162:LEU:HD23 | 1:A:210:PHE:CD2  | 2.51                     | 0.44              |
| 1:A:335:TYR:O    | 1:A:335:TYR:CD1  | 2.70                     | 0.44              |
| 1:A:401:LYS:HZ2  | 1:A:401:LYS:CA   | 2.27                     | 0.44              |
| 1:A:447:LEU:C    | 1:A:542:TYR:OH   | 2.61                     | 0.44              |
| 1:A:596:LYS:HD3  | 1:A:596:LYS:C    | 2.42                     | 0.44              |
| 1:E:124:SER:OG   | 1:E:125:SER:N    | 2.50                     | 0.44              |
| 1:E:177:PRO:O    | 1:E:180:LYS:HB3  | 2.18                     | 0.44              |
| 1:E:280:PHE:O    | 1:E:298:LEU:HA   | 2.18                     | 0.44              |
| 1:E:403:THR:O    | 1:E:404:ASN:ND2  | 2.50                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:256:MET:O    | 2:F:260:ILE:HG13 | 2.16                     | 0.44              |
| 2:F:272:ILE:HG12 | 2:F:315:GLN:HE22 | 1.76                     | 0.44              |
| 1:B:107:VAL:HG23 | 1:B:107:VAL:O    | 2.18                     | 0.44              |
| 1:B:120:ASN:OD1  | 1:B:120:ASN:N    | 2.41                     | 0.44              |
| 1:B:130:GLN:HB3  | 1:B:132:THR:OG1  | 2.18                     | 0.44              |
| 1:B:491:LYS:C    | 1:B:557:ILE:HD11 | 2.11                     | 0.44              |
| 2:C:9:PRO:HB3    | 2:C:54:THR:CG2   | 2.44                     | 0.44              |
| 2:C:46:LEU:O     | 2:C:50:TYR:CD2   | 2.70                     | 0.44              |
| 2:C:229:ASN:ND2  | 2:C:229:ASN:C    | 2.73                     | 0.44              |
| 2:C:314:GLU:O    | 2:C:318:ARG:NH1  | 2.51                     | 0.44              |
| 2:D:74:GLU:C     | 2:D:76:PHE:H     | 2.25                     | 0.44              |
| 2:D:85:ARG:HB2   | 2:D:137:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:78:ILE:HD12  | 1:A:161:LYS:HB2  | 1.55                     | 0.44              |
| 1:A:255:SER:O    | 1:A:410:GLY:HA2  | 2.17                     | 0.44              |
| 1:A:568:TRP:CE3  | 1:A:568:TRP:N    | 2.82                     | 0.44              |
| 1:E:75:ASP:O     | 1:E:208:TYR:CE1  | 2.71                     | 0.44              |
| 1:E:433:PHE:CZ   | 1:E:526:LEU:O    | 2.69                     | 0.44              |
| 1:E:452:ILE:HD12 | 1:E:543:ILE:CG2  | 2.44                     | 0.44              |
| 1:E:456:TYR:CB   | 1:E:537:LYS:C    | 2.89                     | 0.44              |
| 2:F:22:LEU:HG    | 2:F:39:GLN:CB    | 2.43                     | 0.44              |
| 1:B:107:VAL:HG23 | 1:B:109:TYR:HE2  | 1.82                     | 0.44              |
| 1:B:380:VAL:HG12 | 1:B:382:PRO:CD   | 2.48                     | 0.44              |
| 2:C:129:ARG:C    | 2:C:133:THR:HG1  | 2.12                     | 0.44              |
| 2:D:89:SER:CB    | 2:D:128:PHE:CZ   | 3.01                     | 0.44              |
| 2:D:90:MET:HE2   | 2:D:90:MET:CA    | 2.35                     | 0.44              |
| 2:D:183:LEU:CD2  | 2:D:224:HIS:CG   | 2.98                     | 0.44              |
| 1:A:210:PHE:CD1  | 1:A:210:PHE:O    | 2.70                     | 0.44              |
| 1:A:368:TYR:HD1  | 1:A:372:LEU:CG   | 2.27                     | 0.44              |
| 1:E:449:SER:O    | 1:E:542:TYR:OH   | 2.24                     | 0.44              |
| 1:E:598:TRP:HD1  | 1:E:599:LYS:N    | 2.13                     | 0.44              |
| 2:F:82:ASP:O     | 2:F:86:LEU:CG    | 2.66                     | 0.44              |
| 2:F:212:LYS:C    | 2:F:213:GLU:OE2  | 2.60                     | 0.44              |
| 1:B:111:SER:CB   | 1:B:142:ASN:N    | 2.78                     | 0.44              |
| 1:B:293:THR:CG2  | 1:B:425:ARG:HH11 | 2.30                     | 0.44              |
| 1:B:310:LEU:HB2  | 1:B:312:LEU:HG   | 1.99                     | 0.44              |
| 1:B:388:LEU:CD1  | 1:B:406:ILE:CD1  | 2.96                     | 0.44              |
| 1:B:570:ILE:O    | 1:B:575:ILE:CD1  | 2.66                     | 0.44              |
| 2:C:197:ASN:ND2  | 2:C:197:ASN:C    | 2.73                     | 0.44              |
| 2:D:196:GLN:O    | 2:D:197:ASN:HB3  | 2.18                     | 0.44              |
| 1:A:283:LEU:O    | 1:A:285:PRO:HD3  | 2.18                     | 0.44              |
| 1:A:408:LEU:CD2  | 1:A:409:GLN:N    | 2.74                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:254:ASN:ND2  | 1:E:254:ASN:C    | 2.74                     | 0.44              |
| 1:E:487:VAL:HG23 | 1:E:527:ALA:HB3  | 1.95                     | 0.44              |
| 2:F:11:LYS:CA    | 2:F:15:GLU:OE1   | 2.66                     | 0.44              |
| 1:B:82:LYS:CA    | 1:B:156:TYR:CB   | 2.94                     | 0.43              |
| 1:B:240:SER:HA   | 1:B:274:GLN:CG   | 2.39                     | 0.43              |
| 1:B:426:LEU:O    | 1:B:430:MET:N    | 2.41                     | 0.43              |
| 1:B:523:PHE:HZ   | 1:B:525:ARG:C    | 2.22                     | 0.43              |
| 2:C:232:ASN:C    | 2:C:235:ILE:HD12 | 2.41                     | 0.43              |
| 1:A:169:LEU:HD21 | 1:A:312:LEU:HD13 | 1.99                     | 0.43              |
| 1:A:206:SER:CB   | 1:A:208:TYR:HE2  | 2.31                     | 0.43              |
| 1:E:90:LYS:HE3   | 1:E:122:SER:HB3  | 2.00                     | 0.43              |
| 1:E:233:LYS:O    | 1:E:233:LYS:HD2  | 2.18                     | 0.43              |
| 1:E:335:TYR:O    | 1:E:335:TYR:CD1  | 2.70                     | 0.43              |
| 1:E:425:ARG:C    | 1:E:429:THR:OG1  | 2.58                     | 0.43              |
| 1:E:560:ARG:HD3  | 1:E:560:ARG:C    | 2.43                     | 0.43              |
| 2:F:97:ASN:HB3   | 2:F:101:ASP:OD1  | 2.18                     | 0.43              |
| 2:F:197:ASN:CG   | 2:F:198:ILE:N    | 2.73                     | 0.43              |
| 1:B:182:LEU:CD2  | 1:B:182:LEU:C    | 2.92                     | 0.43              |
| 1:B:228:TRP:HH2  | 1:B:410:GLY:H    | 1.66                     | 0.43              |
| 1:B:333:THR:O    | 1:B:337:LEU:HB3  | 2.18                     | 0.43              |
| 2:C:305:GLN:CA   | 2:C:308:ILE:HG13 | 2.43                     | 0.43              |
| 2:C:363:LYS:O    | 2:C:367:ILE:HG12 | 2.18                     | 0.43              |
| 2:D:353:ASP:N    | 2:D:357:LYS:CB   | 2.81                     | 0.43              |
| 1:A:245:ILE:N    | 1:A:245:ILE:CD1  | 2.73                     | 0.43              |
| 1:A:318:THR:C    | 1:A:319:GLN:HG3  | 2.42                     | 0.43              |
| 1:E:138:SER:HA   | 1:E:140:LEU:N    | 2.33                     | 0.43              |
| 1:E:310:LEU:H    | 1:E:310:LEU:CD2  | 2.29                     | 0.43              |
| 2:F:255:MET:SD   | 2:F:255:MET:N    | 2.91                     | 0.43              |
| 1:B:103:ASP:C    | 1:B:107:VAL:O    | 2.59                     | 0.43              |
| 1:B:227:ASN:CG   | 1:B:228:TRP:N    | 2.76                     | 0.43              |
| 1:B:256:GLY:C    | 1:B:259:THR:OG1  | 2.58                     | 0.43              |
| 1:B:456:TYR:CE1  | 1:B:537:LYS:HD2  | 2.53                     | 0.43              |
| 1:B:598:TRP:H    | 2:D:58:HIS:HB2   | 1.83                     | 0.43              |
| 2:C:137:LEU:N    | 2:D:94:ARG:HH22  | 2.16                     | 0.43              |
| 2:D:247:HIS:ND1  | 2:D:247:HIS:N    | 2.64                     | 0.43              |
| 1:A:280:PHE:HA   | 1:A:358:LEU:HB3  | 1.99                     | 0.43              |
| 1:A:430:MET:CG   | 1:A:566:PRO:CB   | 2.95                     | 0.43              |
| 1:A:530:HIS:CD2  | 1:A:531:SER:OG   | 2.70                     | 0.43              |
| 1:E:79:PHE:CD1   | 1:E:79:PHE:N     | 2.85                     | 0.43              |
| 1:E:124:SER:HB2  | 1:E:308:ASN:ND2  | 2.34                     | 0.43              |
| 1:E:130:GLN:HB3  | 1:E:132:THR:OG1  | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:164:ASN:OD1  | 1:E:165:LEU:N    | 2.51                     | 0.43              |
| 1:E:454:VAL:CG2  | 1:E:539:MET:CG   | 2.96                     | 0.43              |
| 2:F:10:TRP:HD1   | 2:F:12:SER:O     | 2.01                     | 0.43              |
| 2:F:116:ALA:HA   | 2:F:119:ILE:HD12 | 1.95                     | 0.43              |
| 2:F:153:TRP:NE1  | 2:F:157:HIS:CD2  | 2.85                     | 0.43              |
| 2:F:235:ILE:C    | 2:F:238:ILE:HD12 | 2.42                     | 0.43              |
| 1:B:284:ASP:OD1  | 1:B:286:GLY:N    | 2.52                     | 0.43              |
| 2:C:369:ARG:HA   | 2:C:372:THR:HG22 | 1.99                     | 0.43              |
| 2:D:26:ALA:C     | 2:D:28:ARG:N     | 2.76                     | 0.43              |
| 1:A:184:TRP:O    | 1:A:184:TRP:CG   | 2.71                     | 0.43              |
| 1:E:465:LEU:HD13 | 1:E:482:ILE:HG21 | 2.00                     | 0.43              |
| 1:E:489:ILE:HD11 | 1:E:527:ALA:CB   | 2.32                     | 0.43              |
| 1:E:570:ILE:C    | 1:E:575:ILE:HD12 | 2.43                     | 0.43              |
| 2:F:279:ASN:CG   | 2:F:305:GLN:HE21 | 2.25                     | 0.43              |
| 1:B:282:ASP:HB3  | 1:B:297:SER:OG   | 2.18                     | 0.43              |
| 1:B:452:ILE:HB   | 1:B:541:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:454:VAL:HG13 | 2:D:407:PHE:HD1  | 1.73                     | 0.43              |
| 2:C:299:GLN:C    | 2:C:303:CYS:SG   | 3.01                     | 0.43              |
| 2:D:13:SER:O     | 2:D:16:VAL:CG2   | 2.60                     | 0.43              |
| 2:D:149:ARG:HB3  | 2:D:149:ARG:CZ   | 2.48                     | 0.43              |
| 1:A:175:VAL:CG2  | 1:A:176:CYS:N    | 2.82                     | 0.43              |
| 1:A:232:ILE:CG1  | 1:A:264:LEU:CB   | 2.94                     | 0.43              |
| 1:A:368:TYR:HD1  | 1:A:372:LEU:HD11 | 1.84                     | 0.43              |
| 1:A:594:LEU:C    | 1:A:594:LEU:CD1  | 2.91                     | 0.43              |
| 1:E:205:PHE:O    | 1:E:206:SER:OG   | 2.28                     | 0.43              |
| 1:E:230:ASP:HA   | 1:E:233:LYS:HB3  | 2.00                     | 0.43              |
| 1:E:280:PHE:O    | 1:E:299:SER:N    | 2.51                     | 0.43              |
| 1:E:490:PHE:HB2  | 1:E:557:ILE:O    | 2.18                     | 0.43              |
| 2:F:18:TYR:CD2   | 2:F:18:TYR:C     | 2.94                     | 0.43              |
| 2:F:111:PRO:HG3  | 2:F:113:HIS:CE1  | 2.42                     | 0.43              |
| 2:F:370:LEU:O    | 2:F:371:SER:C    | 2.62                     | 0.43              |
| 1:B:126:ILE:N    | 1:B:126:ILE:CD1  | 2.73                     | 0.43              |
| 1:B:182:LEU:HB3  | 1:B:183:PHE:CE2  | 2.52                     | 0.43              |
| 1:B:546:PHE:N    | 1:B:546:PHE:HD1  | 2.16                     | 0.43              |
| 1:B:598:TRP:CD1  | 1:B:598:TRP:C    | 2.95                     | 0.43              |
| 2:C:15:GLU:O     | 2:C:18:TYR:CB    | 2.67                     | 0.43              |
| 2:D:74:GLU:OE2   | 2:D:144:LYS:HE3  | 2.19                     | 0.43              |
| 1:A:283:LEU:HD23 | 1:A:296:ILE:HG23 | 2.00                     | 0.43              |
| 1:A:298:LEU:CD2  | 1:A:319:GLN:OE1  | 2.67                     | 0.43              |
| 1:A:364:TRP:CE3  | 1:A:368:TYR:HB3  | 2.47                     | 0.43              |
| 1:A:508:LEU:CD1  | 1:A:509:PRO:CD   | 2.85                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:341:GLN:HG3  | 1:E:342:LEU:H    | 1.81                     | 0.43              |
| 1:E:365:ILE:HD12 | 1:E:366:LYS:N    | 2.33                     | 0.43              |
| 1:E:531:SER:HA   | 2:F:418:PHE:C    | 2.37                     | 0.43              |
| 1:E:565:LEU:C    | 1:E:565:LEU:CD2  | 2.87                     | 0.43              |
| 1:B:239:TYR:OH   | 1:B:276:LEU:CD2  | 2.65                     | 0.43              |
| 1:B:261:LEU:O    | 1:B:265:VAL:HG23 | 2.18                     | 0.43              |
| 2:C:308:ILE:O    | 2:C:312:ALA:HB2  | 2.18                     | 0.43              |
| 2:C:409:SER:HB3  | 1:A:450:PRO:CG   | 2.47                     | 0.43              |
| 2:D:23:PHE:O     | 2:D:24:PHE:HD1   | 2.01                     | 0.43              |
| 1:A:596:LYS:NZ   | 1:A:596:LYS:CB   | 2.81                     | 0.43              |
| 2:F:120:ASP:OD2  | 2:F:157:HIS:NE2  | 2.51                     | 0.43              |
| 2:F:256:MET:HA   | 2:F:259:PHE:CB   | 2.25                     | 0.43              |
| 2:F:303:CYS:SG   | 2:F:304:ALA:N    | 2.91                     | 0.43              |
| 1:B:251:GLY:O    | 1:B:363:GLY:O    | 2.36                     | 0.43              |
| 1:B:485:THR:HB   | 1:B:560:ARG:HE   | 1.84                     | 0.43              |
| 2:C:258:HIS:CD2  | 2:C:258:HIS:O    | 2.72                     | 0.43              |
| 2:C:416:LYS:HB3  | 2:C:416:LYS:NZ   | 2.31                     | 0.43              |
| 2:D:56:VAL:O     | 2:D:57:SER:C     | 2.60                     | 0.43              |
| 1:A:172:ILE:HD12 | 1:A:183:PHE:CD2  | 2.54                     | 0.43              |
| 1:A:224:LYS:HB3  | 1:A:228:TRP:CB   | 2.48                     | 0.43              |
| 1:A:340:GLU:O    | 1:A:343:VAL:N    | 2.52                     | 0.43              |
| 1:A:520:SER:O    | 1:A:521:THR:HG22 | 2.16                     | 0.43              |
| 1:A:565:LEU:CD2  | 1:A:570:ILE:HG13 | 2.40                     | 0.43              |
| 1:E:109:TYR:CD1  | 1:E:271:PRO:HD3  | 2.51                     | 0.43              |
| 1:E:138:SER:CA   | 1:E:139:LEU:C    | 2.86                     | 0.43              |
| 1:E:229:MET:HB2  | 1:E:229:MET:HE2  | 1.81                     | 0.43              |
| 1:E:248:ILE:CG1  | 1:E:382:PRO:CB   | 2.97                     | 0.43              |
| 1:E:283:LEU:HD11 | 1:E:339:VAL:CG1  | 2.47                     | 0.43              |
| 1:E:398:ASP:OD2  | 1:E:399:ILE:HG22 | 2.18                     | 0.43              |
| 1:E:586:ILE:CB   | 2:F:6:ARG:O      | 2.66                     | 0.43              |
| 2:F:198:ILE:N    | 2:F:198:ILE:HD12 | 2.32                     | 0.43              |
| 2:F:233:VAL:O    | 2:F:236:GLU:HG3  | 2.18                     | 0.43              |
| 2:F:342:LEU:O    | 2:F:346:LEU:HG   | 2.18                     | 0.43              |
| 1:B:278:ILE:HG13 | 1:B:358:LEU:HD23 | 2.00                     | 0.43              |
| 1:B:351:GLU:O    | 1:B:353:LYS:C    | 2.59                     | 0.43              |
| 1:B:583:LEU:HD21 | 2:D:13:SER:OG    | 2.19                     | 0.43              |
| 2:C:128:PHE:HD2  | 2:C:128:PHE:C    | 2.27                     | 0.43              |
| 2:D:11:LYS:HG3   | 2:D:12:SER:H     | 1.84                     | 0.43              |
| 2:D:235:ILE:HA   | 2:D:238:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:165:LEU:CD1  | 1:A:165:LEU:C    | 2.85                     | 0.43              |
| 1:A:248:ILE:HD12 | 1:A:376:LEU:HD11 | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:466:THR:CA   | 1:A:511:LEU:O    | 2.66                     | 0.43              |
| 1:A:573:ASN:O    | 1:A:576:VAL:HG23 | 2.18                     | 0.43              |
| 1:E:74:HIS:NE2   | 1:E:75:ASP:OD2   | 2.52                     | 0.43              |
| 1:E:171:SER:HB3  | 1:E:443:PHE:HB2  | 2.01                     | 0.43              |
| 2:F:328:ILE:CA   | 2:F:331:LEU:HD22 | 2.48                     | 0.43              |
| 1:B:114:GLU:H    | 1:B:114:GLU:HG2  | 1.52                     | 0.43              |
| 1:B:329:LYS:HG2  | 1:B:330:ASP:N    | 2.33                     | 0.43              |
| 1:B:379:ARG:C    | 1:B:379:ARG:CD   | 2.90                     | 0.43              |
| 1:B:390:SER:HB3  | 1:B:405:LEU:HD11 | 2.01                     | 0.43              |
| 1:B:432:TYR:CE2  | 1:B:526:LEU:HD12 | 2.53                     | 0.43              |
| 1:B:575:ILE:HG13 | 1:B:575:ILE:H    | 1.60                     | 0.43              |
| 2:D:45:SER:O     | 2:D:49:MET:HB2   | 2.18                     | 0.43              |
| 2:D:74:GLU:O     | 2:D:75:SER:C     | 2.62                     | 0.43              |
| 1:A:236:THR:OG1  | 1:A:237:GLU:OE1  | 2.31                     | 0.43              |
| 1:A:482:ILE:HD13 | 1:A:532:ILE:HG21 | 1.95                     | 0.43              |
| 1:E:176:CYS:HB2  | 1:E:568:TRP:CE2  | 2.54                     | 0.43              |
| 1:E:323:VAL:CA   | 1:E:334:ARG:NH1  | 2.81                     | 0.43              |
| 1:E:377:ILE:O    | 1:E:382:PRO:HD2  | 2.18                     | 0.43              |
| 1:E:399:ILE:HA   | 1:E:400:PRO:HA   | 1.52                     | 0.43              |
| 1:E:511:LEU:HD23 | 1:E:516:PHE:HB2  | 2.01                     | 0.43              |
| 1:B:118:PHE:HE1  | 1:B:306:HIS:CB   | 1.74                     | 0.42              |
| 1:B:489:ILE:HA   | 1:B:557:ILE:O    | 2.19                     | 0.42              |
| 2:C:65:HIS:CB    | 2:C:94:ARG:HH21  | 2.29                     | 0.42              |
| 2:C:128:PHE:C    | 2:C:128:PHE:CD2  | 2.96                     | 0.42              |
| 2:C:257:ASN:HA   | 2:C:260:ILE:HG12 | 2.00                     | 0.42              |
| 2:D:71:MET:HE3   | 2:D:71:MET:HB3   | 1.68                     | 0.42              |
| 2:D:212:LYS:HE3  | 2:D:212:LYS:HB3  | 1.79                     | 0.42              |
| 1:A:358:LEU:C    | 1:A:359:ILE:CG1  | 2.91                     | 0.42              |
| 1:E:264:LEU:HD22 | 1:E:268:MET:HG3  | 2.01                     | 0.42              |
| 2:F:235:ILE:HD11 | 2:F:274:SER:OG   | 2.18                     | 0.42              |
| 1:B:376:LEU:O    | 1:B:380:VAL:HG23 | 2.19                     | 0.42              |
| 2:D:37:TYR:CD1   | 2:D:71:MET:SD    | 3.11                     | 0.42              |
| 2:D:62:SER:O     | 2:D:66:LEU:CG    | 2.57                     | 0.42              |
| 2:D:257:ASN:C    | 2:D:257:ASN:HD22 | 2.26                     | 0.42              |
| 1:A:111:SER:HB2  | 1:A:140:LEU:C    | 2.44                     | 0.42              |
| 1:A:279:ASN:HB3  | 1:A:357:LEU:HA   | 2.00                     | 0.42              |
| 1:A:385:VAL:HG11 | 1:A:403:THR:HG21 | 2.00                     | 0.42              |
| 1:A:467:HIS:CE1  | 1:A:560:ARG:HB3  | 2.54                     | 0.42              |
| 1:E:523:PHE:CE1  | 1:E:525:ARG:C    | 2.97                     | 0.42              |
| 1:B:67:ASP:C     | 1:B:69:ASN:N     | 2.77                     | 0.42              |
| 1:B:81:LEU:HD22  | 1:B:160:ILE:CD1  | 2.27                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:328:PRO:CG   | 1:B:335:TYR:HE2  | 2.32                     | 0.42              |
| 1:B:524:PHE:CD2  | 1:B:524:PHE:C    | 2.95                     | 0.42              |
| 1:B:593:SER:HA   | 1:B:594:LEU:HA   | 1.52                     | 0.42              |
| 2:C:366:LEU:O    | 2:C:370:LEU:HG   | 2.19                     | 0.42              |
| 2:C:373:ASP:C    | 2:C:374:THR:CG2  | 2.80                     | 0.42              |
| 2:C:410:HIS:CB   | 1:A:453:GLN:OE1  | 2.68                     | 0.42              |
| 2:D:309:ARG:O    | 2:D:312:ALA:HB3  | 2.20                     | 0.42              |
| 2:D:320:ASP:O    | 2:D:324:VAL:N    | 2.37                     | 0.42              |
| 1:A:213:ILE:CD1  | 1:A:219:THR:CB   | 2.98                     | 0.42              |
| 1:E:387:TYR:O    | 1:E:405:LEU:HA   | 2.18                     | 0.42              |
| 2:F:247:HIS:H    | 2:F:247:HIS:HD2  | 1.59                     | 0.42              |
| 2:F:304:ALA:O    | 2:F:308:ILE:HG13 | 2.20                     | 0.42              |
| 2:F:338:LEU:HD11 | 2:F:339:ASN:ND2  | 2.34                     | 0.42              |
| 2:F:365:THR:O    | 2:F:369:ARG:CA   | 2.66                     | 0.42              |
| 1:B:162:LEU:HD23 | 1:B:162:LEU:HA   | 1.81                     | 0.42              |
| 1:B:167:THR:C    | 1:B:169:LEU:H    | 2.27                     | 0.42              |
| 1:B:232:ILE:HG21 | 1:B:263:LEU:CD1  | 2.49                     | 0.42              |
| 1:B:572:SER:O    | 1:B:573:ASN:C    | 2.63                     | 0.42              |
| 2:C:23:PHE:HD1   | 2:C:23:PHE:HA    | 1.73                     | 0.42              |
| 2:C:151:ILE:CG2  | 2:C:152:ASP:N    | 2.83                     | 0.42              |
| 2:C:410:HIS:CB   | 1:A:451:PRO:CD   | 2.95                     | 0.42              |
| 2:D:60:LEU:O     | 2:D:60:LEU:HD22  | 2.18                     | 0.42              |
| 1:A:248:ILE:O    | 1:A:249:VAL:HG22 | 2.18                     | 0.42              |
| 1:A:305:GLN:HG3  | 1:A:309:HIS:CD2  | 2.55                     | 0.42              |
| 1:A:322:TYR:CB   | 1:A:523:PHE:CZ   | 3.00                     | 0.42              |
| 1:E:216:PRO:HD3  | 3:E:745:HOH:O    | 2.19                     | 0.42              |
| 1:E:300:LYS:HB3  | 1:E:300:LYS:HE2  | 1.59                     | 0.42              |
| 1:E:370:LEU:O    | 1:E:374:ARG:N    | 2.45                     | 0.42              |
| 1:E:504:ASN:ND2  | 1:E:505:LYS:C    | 2.73                     | 0.42              |
| 2:F:16:VAL:O     | 2:F:20:LYS:N     | 2.38                     | 0.42              |
| 2:F:249:ARG:O    | 2:F:252:PHE:HB2  | 2.19                     | 0.42              |
| 1:A:98:GLN:O     | 1:A:142:ASN:CA   | 2.67                     | 0.42              |
| 1:A:239:TYR:O    | 1:A:239:TYR:HD1  | 2.02                     | 0.42              |
| 1:A:446:LEU:HD13 | 1:A:569:GLU:HG3  | 2.01                     | 0.42              |
| 1:E:293:THR:OG1  | 1:E:429:THR:HG23 | 2.19                     | 0.42              |
| 1:E:444:GLN:NE2  | 1:E:445:PRO:C    | 2.74                     | 0.42              |
| 1:E:466:THR:CG2  | 1:E:516:PHE:HD2  | 2.21                     | 0.42              |
| 2:F:43:ALA:HA    | 2:F:46:LEU:HD12  | 2.01                     | 0.42              |
| 2:F:155:TRP:CD1  | 2:F:155:TRP:C    | 2.96                     | 0.42              |
| 2:C:31:ILE:HD11  | 2:C:35:GLU:CD    | 2.45                     | 0.42              |
| 2:C:101:ASP:O    | 2:C:103:ASN:N    | 2.48                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:268:PRO:O    | 2:D:272:ILE:HD11 | 2.19                     | 0.42              |
| 1:A:75:ASP:OD1   | 1:A:75:ASP:N     | 2.50                     | 0.42              |
| 1:A:296:ILE:HG21 | 1:A:342:LEU:HD23 | 2.02                     | 0.42              |
| 1:E:93:PHE:HB2   | 1:E:210:PHE:CE1  | 2.55                     | 0.42              |
| 1:E:232:ILE:HD11 | 1:E:264:LEU:HD22 | 1.84                     | 0.42              |
| 1:E:324:GLY:O    | 1:E:325:PHE:CD1  | 2.72                     | 0.42              |
| 1:E:361:THR:HA   | 1:E:362:PRO:HD3  | 1.83                     | 0.42              |
| 1:E:482:ILE:C    | 1:E:485:THR:CG2  | 2.86                     | 0.42              |
| 1:E:512:PRO:HG2  | 1:E:515:GLU:HB2  | 2.01                     | 0.42              |
| 2:F:23:PHE:CE2   | 2:F:43:ALA:HB3   | 2.48                     | 0.42              |
| 1:B:103:ASP:CB   | 1:B:108:ILE:CD1  | 2.98                     | 0.42              |
| 1:B:227:ASN:OD1  | 1:B:228:TRP:N    | 2.52                     | 0.42              |
| 1:B:368:TYR:HE1  | 1:B:372:LEU:HD11 | 1.84                     | 0.42              |
| 1:B:486:ILE:HG13 | 1:B:486:ILE:O    | 2.18                     | 0.42              |
| 2:C:90:MET:HE1   | 2:D:132:ALA:HB1  | 2.00                     | 0.42              |
| 2:C:146:CYS:O    | 2:C:150:ALA:N    | 2.43                     | 0.42              |
| 2:C:275:MET:HE3  | 2:C:311:LEU:HD11 | 2.01                     | 0.42              |
| 2:C:309:ARG:O    | 2:C:313:ILE:HG13 | 2.19                     | 0.42              |
| 2:D:308:ILE:HA   | 2:D:311:LEU:CD1  | 2.44                     | 0.42              |
| 2:D:331:LEU:HD12 | 2:D:360:ILE:HG23 | 2.01                     | 0.42              |
| 1:A:308:ASN:HD22 | 1:A:310:LEU:HD11 | 1.85                     | 0.42              |
| 1:A:512:PRO:HG2  | 1:A:515:GLU:CB   | 2.50                     | 0.42              |
| 1:A:525:ARG:HB3  | 1:A:525:ARG:NH2  | 2.30                     | 0.42              |
| 1:E:248:ILE:HG13 | 1:E:384:HIS:O    | 2.20                     | 0.42              |
| 1:E:269:LEU:HD11 | 1:E:278:ILE:HG21 | 1.99                     | 0.42              |
| 1:B:242:ASP:HA   | 1:B:243:GLN:HA   | 1.74                     | 0.42              |
| 1:B:368:TYR:O    | 1:B:371:GLU:HB3  | 2.20                     | 0.42              |
| 1:B:380:VAL:CG1  | 1:B:382:PRO:CD   | 2.94                     | 0.42              |
| 1:B:486:ILE:HD11 | 1:B:564:ASP:C    | 2.39                     | 0.42              |
| 2:C:125:PHE:CZ   | 2:C:150:ALA:N    | 2.83                     | 0.42              |
| 2:C:227:MET:CG   | 2:C:230:PHE:CB   | 2.86                     | 0.42              |
| 2:C:310:TRP:CE3  | 2:C:310:TRP:C    | 2.98                     | 0.42              |
| 2:D:276:LEU:HD23 | 2:D:276:LEU:N    | 2.33                     | 0.42              |
| 1:A:120:ASN:C    | 1:A:120:ASN:ND2  | 2.73                     | 0.42              |
| 1:A:245:ILE:N    | 1:A:356:SER:OG   | 2.53                     | 0.42              |
| 1:A:368:TYR:HA   | 1:A:371:GLU:HB3  | 2.00                     | 0.42              |
| 1:E:101:ALA:CB   | 1:E:133:GLN:CB   | 2.98                     | 0.42              |
| 1:E:169:LEU:HD13 | 1:E:183:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:299:SER:HA   | 1:E:317:SER:CB   | 2.34                     | 0.42              |
| 1:E:432:TYR:CD1  | 1:E:432:TYR:C    | 2.95                     | 0.42              |
| 2:F:224:HIS:O    | 2:F:230:PHE:CB   | 2.67                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:64:SER:CB    | 1:B:86:ASN:O     | 2.66                     | 0.42              |
| 1:B:368:TYR:CE1  | 1:B:372:LEU:HD11 | 2.55                     | 0.42              |
| 1:B:468:LEU:HD12 | 1:B:561:GLY:CA   | 2.14                     | 0.42              |
| 2:C:15:GLU:C     | 2:C:17:VAL:N     | 2.77                     | 0.42              |
| 2:C:128:PHE:CE1  | 2:C:143:CYS:HA   | 2.55                     | 0.42              |
| 1:E:138:SER:CA   | 1:E:140:LEU:N    | 2.82                     | 0.42              |
| 1:E:397:ILE:HD12 | 1:E:397:ILE:H    | 1.80                     | 0.42              |
| 1:B:172:ILE:HG13 | 1:B:173:GLY:N    | 2.34                     | 0.42              |
| 1:B:250:ILE:HG22 | 1:B:365:ILE:HG13 | 2.02                     | 0.42              |
| 1:B:584:PRO:HG2  | 1:B:585:TYR:H    | 1.83                     | 0.42              |
| 2:C:85:ARG:HD2   | 2:C:138:PRO:O    | 2.20                     | 0.42              |
| 2:D:89:SER:CB    | 2:D:128:PHE:HZ   | 2.32                     | 0.42              |
| 2:D:256:MET:HA   | 2:D:259:PHE:HD2  | 1.84                     | 0.42              |
| 1:A:463:SER:HG   | 1:A:555:ALA:HB1  | 1.80                     | 0.42              |
| 1:A:478:LEU:HD11 | 1:A:510:LEU:HB2  | 2.01                     | 0.42              |
| 1:E:341:GLN:C    | 1:E:344:ARG:HG2  | 2.45                     | 0.42              |
| 1:E:381:LYS:HA   | 1:E:401:LYS:NZ   | 2.35                     | 0.42              |
| 2:C:86:LEU:CD2   | 2:D:91:THR:OG1   | 2.66                     | 0.41              |
| 2:C:418:PHE:CE1  | 1:A:569:GLU:OE2  | 2.68                     | 0.41              |
| 2:D:190:TYR:O    | 2:D:190:TYR:CD1  | 2.70                     | 0.41              |
| 1:A:490:PHE:CD1  | 1:A:523:PHE:CD1  | 2.98                     | 0.41              |
| 1:E:95:LEU:CD2   | 1:E:116:MET:O    | 2.68                     | 0.41              |
| 1:E:164:ASN:CA   | 1:E:210:PHE:CE1  | 2.98                     | 0.41              |
| 1:E:377:ILE:HG22 | 1:E:401:LYS:HG3  | 2.01                     | 0.41              |
| 2:F:67:PHE:CE1   | 2:F:151:ILE:HD13 | 2.55                     | 0.41              |
| 2:C:37:TYR:OH    | 2:C:74:GLU:OE1   | 2.36                     | 0.41              |
| 2:C:96:VAL:CA    | 2:C:99:LEU:CD1   | 2.86                     | 0.41              |
| 2:C:128:PHE:CE2  | 2:C:138:PRO:CG   | 2.83                     | 0.41              |
| 2:D:70:LEU:C     | 2:D:70:LEU:CD2   | 2.85                     | 0.41              |
| 2:D:127:GLU:CD   | 1:A:367:GLY:HA3  | 2.41                     | 0.41              |
| 2:D:343:LEU:HA   | 2:D:346:LEU:HB2  | 2.03                     | 0.41              |
| 1:A:169:LEU:O    | 1:A:169:LEU:HD13 | 2.21                     | 0.41              |
| 1:A:401:LYS:O    | 1:A:403:THR:OG1  | 2.38                     | 0.41              |
| 1:A:473:ILE:HG22 | 1:A:474:GLY:O    | 2.20                     | 0.41              |
| 1:E:365:ILE:HD12 | 1:E:366:LYS:CB   | 2.47                     | 0.41              |
| 1:E:567:ILE:HG23 | 1:E:571:ALA:HB3  | 2.00                     | 0.41              |
| 2:F:23:PHE:CD2   | 2:F:43:ALA:CB    | 3.00                     | 0.41              |
| 1:B:111:SER:OG   | 1:B:141:GLU:O    | 2.37                     | 0.41              |
| 1:B:131:ALA:O    | 1:B:134:VAL:CG2  | 2.68                     | 0.41              |
| 1:B:257:LYS:HA   | 1:B:260:PHE:HB3  | 2.02                     | 0.41              |
| 1:B:435:LYS:HB3  | 1:B:441:PHE:CE1  | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:468:LEU:O    | 1:B:469:LYS:HB3  | 2.21                     | 0.41              |
| 2:C:190:TYR:O    | 2:C:194:ARG:N    | 2.48                     | 0.41              |
| 2:D:22:LEU:N     | 2:D:22:LEU:CD2   | 2.73                     | 0.41              |
| 2:D:50:TYR:CD1   | 2:D:53:ARG:NH2   | 2.88                     | 0.41              |
| 2:D:96:VAL:HG13  | 2:D:121:LEU:CD2  | 2.50                     | 0.41              |
| 2:D:140:LEU:C    | 2:D:140:LEU:CD2  | 2.85                     | 0.41              |
| 1:A:508:LEU:HA   | 1:A:508:LEU:HD13 | 1.77                     | 0.41              |
| 1:E:107:VAL:HG23 | 1:E:109:TYR:CE2  | 2.54                     | 0.41              |
| 1:E:238:LEU:O    | 1:E:238:LEU:HD12 | 2.20                     | 0.41              |
| 1:E:364:TRP:CH2  | 1:E:368:TYR:CB   | 2.99                     | 0.41              |
| 2:F:141:GLU:HA   | 2:F:144:LYS:CG   | 2.41                     | 0.41              |
| 2:F:308:ILE:HA   | 2:F:311:LEU:HD12 | 2.02                     | 0.41              |
| 1:B:530:HIS:HA   | 2:D:418:PHE:CD1  | 2.55                     | 0.41              |
| 2:D:125:PHE:CE1  | 2:D:149:ARG:HB3  | 2.55                     | 0.41              |
| 1:A:64:SER:HB3   | 1:A:85:GLN:CB    | 2.50                     | 0.41              |
| 1:A:309:HIS:CD2  | 1:A:309:HIS:H    | 2.38                     | 0.41              |
| 1:E:585:TYR:HA   | 2:F:8:THR:O      | 2.20                     | 0.41              |
| 2:F:103:ASN:CB   | 2:F:115:LEU:HD21 | 2.51                     | 0.41              |
| 2:F:236:GLU:C    | 2:F:240:SER:HG   | 2.23                     | 0.41              |
| 2:F:353:ASP:CB   | 2:F:354:PRO:HD3  | 2.12                     | 0.41              |
| 1:B:293:THR:HG21 | 1:B:425:ARG:NH1  | 2.35                     | 0.41              |
| 1:B:293:THR:HG22 | 1:B:294:ASP:N    | 2.36                     | 0.41              |
| 1:B:586:ILE:HD12 | 2:D:7:LEU:HD13   | 2.01                     | 0.41              |
| 2:C:138:PRO:HB3  | 2:C:142:MET:HG2  | 2.03                     | 0.41              |
| 2:C:414:THR:O    | 2:C:416:LYS:HD3  | 2.10                     | 0.41              |
| 2:C:417:PRO:CB   | 1:A:584:PRO:HG2  | 2.43                     | 0.41              |
| 2:D:10:TRP:O     | 2:D:12:SER:O     | 2.39                     | 0.41              |
| 2:D:25:PRO:HD2   | 2:D:28:ARG:HD3   | 2.02                     | 0.41              |
| 1:A:97:ILE:HD11  | 1:A:116:MET:CE   | 2.50                     | 0.41              |
| 1:A:235:LEU:CD1  | 1:A:384:HIS:CD2  | 3.04                     | 0.41              |
| 1:A:483:GLU:O    | 1:A:485:THR:HG23 | 2.20                     | 0.41              |
| 1:E:218:ASN:ND2  | 1:E:218:ASN:N    | 2.68                     | 0.41              |
| 1:E:233:LYS:NZ   | 1:E:237:GLU:HB2  | 2.30                     | 0.41              |
| 1:E:341:GLN:O    | 1:E:344:ARG:HB2  | 2.20                     | 0.41              |
| 1:E:365:ILE:HD13 | 1:E:393:LEU:CD1  | 2.50                     | 0.41              |
| 1:E:439:PHE:N    | 1:E:439:PHE:CD1  | 2.88                     | 0.41              |
| 1:E:468:LEU:HA   | 1:E:513:TYR:CD1  | 2.55                     | 0.41              |
| 2:F:122:PRO:HG2  | 2:F:125:PHE:CD2  | 2.44                     | 0.41              |
| 1:B:250:ILE:CG2  | 1:B:365:ILE:HG13 | 2.49                     | 0.41              |
| 1:B:457:GLY:O    | 1:B:463:SER:HA   | 2.20                     | 0.41              |
| 1:B:539:MET:HB2  | 1:B:539:MET:HE3  | 1.73                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:558:MET:HE2  | 1:B:558:MET:HB2  | 1.74                     | 0.41              |
| 2:C:11:LYS:HD2   | 1:A:585:TYR:HH   | 1.85                     | 0.41              |
| 2:C:23:PHE:CE2   | 2:C:63:THR:HB    | 2.56                     | 0.41              |
| 2:C:254:PRO:O    | 2:C:257:ASN:ND2  | 2.54                     | 0.41              |
| 2:D:255:MET:SD   | 2:D:255:MET:O    | 2.78                     | 0.41              |
| 1:A:106:GLY:HA3  | 1:A:229:MET:HE2  | 2.02                     | 0.41              |
| 1:A:107:VAL:C    | 1:A:108:ILE:HD12 | 2.46                     | 0.41              |
| 1:A:180:LYS:O    | 1:A:181:ASN:HB2  | 2.19                     | 0.41              |
| 1:A:248:ILE:CD1  | 1:A:376:LEU:HD11 | 2.51                     | 0.41              |
| 1:A:436:ILE:HG22 | 1:A:440:LYS:C    | 2.45                     | 0.41              |
| 1:E:107:VAL:HG22 | 1:E:266:GLN:NE2  | 2.33                     | 0.41              |
| 1:E:468:LEU:HA   | 1:E:513:TYR:HD1  | 1.85                     | 0.41              |
| 1:B:96:GLU:O     | 1:B:161:LYS:HB3  | 2.20                     | 0.41              |
| 1:B:161:LYS:HZ1  | 1:B:163:THR:HG1  | 1.60                     | 0.41              |
| 1:B:399:ILE:HA   | 1:B:400:PRO:HA   | 1.71                     | 0.41              |
| 1:B:434:HIS:O    | 1:B:441:PHE:HA   | 2.19                     | 0.41              |
| 1:B:480:ARG:O    | 1:B:480:ARG:HG2  | 2.20                     | 0.41              |
| 1:B:516:PHE:HE2  | 1:B:521:THR:HG21 | 1.86                     | 0.41              |
| 1:B:534:GLN:HE21 | 1:B:534:GLN:HB2  | 1.60                     | 0.41              |
| 2:C:46:LEU:C     | 2:C:50:TYR:HD2   | 2.29                     | 0.41              |
| 1:A:385:VAL:C    | 1:A:386:ILE:HD12 | 2.46                     | 0.41              |
| 1:A:529:VAL:CG1  | 1:A:532:ILE:CG2  | 2.98                     | 0.41              |
| 1:E:92:GLN:NE2   | 1:E:92:GLN:N     | 2.68                     | 0.41              |
| 1:E:451:PRO:CG   | 2:F:413:TRP:CD2  | 3.01                     | 0.41              |
| 2:F:89:SER:CB    | 2:F:137:LEU:HD11 | 2.50                     | 0.41              |
| 2:F:364:LEU:HD22 | 2:F:368:GLN:CB   | 2.51                     | 0.41              |
| 1:B:280:PHE:CD2  | 1:B:280:PHE:C    | 2.98                     | 0.41              |
| 1:B:318:THR:CG2  | 1:B:319:GLN:NE2  | 2.84                     | 0.41              |
| 1:B:337:LEU:O    | 1:B:337:LEU:HD12 | 2.21                     | 0.41              |
| 1:B:441:PHE:N    | 1:B:441:PHE:HD2  | 2.17                     | 0.41              |
| 1:B:510:LEU:C    | 1:B:510:LEU:CD2  | 2.86                     | 0.41              |
| 1:B:583:LEU:HG   | 1:B:587:THR:HA   | 2.02                     | 0.41              |
| 2:C:181:LYS:O    | 2:C:185:ASP:CB   | 2.68                     | 0.41              |
| 2:C:279:ASN:ND2  | 2:C:308:ILE:HD11 | 2.21                     | 0.41              |
| 2:D:150:ALA:O    | 2:D:153:TRP:N    | 2.54                     | 0.41              |
| 2:D:272:ILE:C    | 2:D:275:MET:H    | 2.29                     | 0.41              |
| 2:D:410:HIS:ND1  | 2:D:411:PRO:HD2  | 2.36                     | 0.41              |
| 1:A:94:VAL:O     | 1:A:162:LEU:CA   | 2.67                     | 0.41              |
| 1:A:172:ILE:HD12 | 1:A:183:PHE:CE2  | 2.52                     | 0.41              |
| 1:A:176:CYS:CB   | 1:A:179:PHE:CD1  | 2.93                     | 0.41              |
| 1:A:466:THR:HG21 | 1:A:511:LEU:HD21 | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:143:LYS:HA   | 1:E:144:GLU:HA   | 1.77                     | 0.41              |
| 1:E:233:LYS:HZ1  | 1:E:237:GLU:N    | 2.19                     | 0.41              |
| 1:E:366:LYS:CD   | 1:E:367:GLY:N    | 2.73                     | 0.41              |
| 2:F:22:LEU:HD22  | 2:F:40:TYR:HA    | 1.77                     | 0.41              |
| 2:F:253:GLU:HA   | 2:F:256:MET:CG   | 2.50                     | 0.41              |
| 1:B:122:SER:N    | 1:B:182:LEU:HD21 | 2.36                     | 0.41              |
| 1:B:170:GLU:CB   | 1:B:183:PHE:HB2  | 2.51                     | 0.41              |
| 1:B:173:GLY:HA2  | 1:B:180:LYS:HB3  | 2.02                     | 0.41              |
| 1:B:238:LEU:HD12 | 1:B:238:LEU:O    | 2.20                     | 0.41              |
| 1:B:335:TYR:CD1  | 1:B:335:TYR:C    | 2.99                     | 0.41              |
| 1:B:445:PRO:HD3  | 1:B:574:GLU:OE1  | 2.21                     | 0.41              |
| 1:B:483:GLU:C    | 1:B:485:THR:HG23 | 2.45                     | 0.41              |
| 2:C:180:ILE:CG1  | 2:C:181:LYS:N    | 2.84                     | 0.41              |
| 2:C:257:ASN:O    | 2:C:258:HIS:C    | 2.61                     | 0.41              |
| 2:C:347:GLN:OE1  | 2:C:360:ILE:HB   | 2.21                     | 0.41              |
| 2:D:23:PHE:C     | 2:D:24:PHE:HD1   | 2.29                     | 0.41              |
| 2:D:47:VAL:O     | 2:D:51:SER:CB    | 2.69                     | 0.41              |
| 2:D:58:HIS:CD2   | 2:D:58:HIS:O     | 2.74                     | 0.41              |
| 2:D:60:LEU:CD2   | 2:D:159:TRP:CH2  | 3.04                     | 0.41              |
| 2:D:149:ARG:NH2  | 2:D:149:ARG:O    | 2.53                     | 0.41              |
| 2:D:255:MET:SD   | 2:D:255:MET:C    | 3.04                     | 0.41              |
| 1:A:72:TYR:CD2   | 1:A:208:TYR:OH   | 2.60                     | 0.41              |
| 1:A:104:ILE:CD1  | 1:A:109:TYR:HD2  | 2.31                     | 0.41              |
| 1:A:172:ILE:HG21 | 1:A:179:PHE:CD2  | 2.54                     | 0.41              |
| 1:A:224:LYS:HB3  | 1:A:228:TRP:CE3  | 2.56                     | 0.41              |
| 1:A:261:LEU:HD23 | 1:A:261:LEU:HA   | 1.74                     | 0.41              |
| 1:A:305:GLN:OE1  | 1:A:313:THR:CG2  | 2.69                     | 0.41              |
| 1:A:492:VAL:CG1  | 1:A:557:ILE:HD11 | 2.46                     | 0.41              |
| 1:E:78:ILE:CG2   | 1:E:98:GLN:NE2   | 2.83                     | 0.41              |
| 1:E:218:ASN:ND2  | 1:E:218:ASN:H    | 2.18                     | 0.41              |
| 1:E:294:ASP:O    | 1:E:322:TYR:CD2  | 2.74                     | 0.41              |
| 1:E:309:HIS:HD2  | 1:E:313:THR:OG1  | 2.03                     | 0.41              |
| 1:E:323:VAL:O    | 1:E:334:ARG:NH1  | 2.54                     | 0.41              |
| 1:E:346:TYR:O    | 1:E:350:GLY:HA3  | 2.20                     | 0.41              |
| 1:E:401:LYS:O    | 1:E:403:THR:HG23 | 2.20                     | 0.41              |
| 1:E:426:LEU:CD2  | 1:E:564:ASP:OD2  | 2.68                     | 0.41              |
| 2:F:118:LYS:HZ2  | 2:F:118:LYS:CB   | 2.25                     | 0.41              |
| 2:F:342:LEU:C    | 2:F:342:LEU:HD22 | 2.46                     | 0.41              |
| 1:B:128:LEU:HB3  | 1:B:130:GLN:OE1  | 2.21                     | 0.41              |
| 1:B:164:ASN:HD22 | 1:B:208:TYR:HD1  | 1.65                     | 0.41              |
| 1:B:516:PHE:CD2  | 1:B:516:PHE:C    | 2.95                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:88:ALA:HA    | 2:C:91:THR:OG1   | 2.21                     | 0.41              |
| 2:D:246:GLU:HA   | 2:D:249:ARG:CB   | 2.51                     | 0.41              |
| 2:D:366:LEU:O    | 2:D:367:ILE:HB   | 2.21                     | 0.41              |
| 1:A:215:LYS:HA   | 1:A:216:PRO:HD3  | 1.97                     | 0.41              |
| 1:A:247:VAL:HG12 | 1:A:248:ILE:N    | 2.36                     | 0.41              |
| 1:A:435:LYS:HG3  | 1:A:435:LYS:O    | 2.21                     | 0.41              |
| 1:A:489:ILE:O    | 1:A:524:PHE:N    | 2.54                     | 0.41              |
| 1:A:525:ARG:H    | 1:A:525:ARG:HG2  | 1.58                     | 0.41              |
| 1:E:80:GLY:HA2   | 1:E:159:VAL:HA   | 2.02                     | 0.41              |
| 1:E:182:LEU:CB   | 1:E:183:PHE:CD2  | 3.00                     | 0.41              |
| 1:E:376:LEU:HD13 | 1:E:376:LEU:C    | 2.46                     | 0.41              |
| 2:F:162:VAL:O    | 2:F:162:VAL:HG12 | 2.21                     | 0.41              |
| 2:F:248:LEU:CA   | 2:F:251:LEU:HB2  | 2.45                     | 0.41              |
| 2:F:364:LEU:C    | 2:F:364:LEU:CD2  | 2.94                     | 0.41              |
| 1:B:62:ASN:C     | 1:B:88:ILE:HD13  | 2.46                     | 0.40              |
| 1:B:122:SER:N    | 1:B:182:LEU:HD23 | 2.26                     | 0.40              |
| 1:B:585:TYR:HB3  | 1:B:586:ILE:HD13 | 2.03                     | 0.40              |
| 2:C:24:PHE:CZ    | 2:C:159:TRP:CD1  | 3.09                     | 0.40              |
| 2:C:247:HIS:C    | 2:C:250:ALA:H    | 2.30                     | 0.40              |
| 2:D:276:LEU:HD13 | 2:D:333:LYS:CA   | 2.45                     | 0.40              |
| 1:A:72:TYR:CZ    | 1:A:206:SER:OG   | 2.72                     | 0.40              |
| 1:A:248:ILE:C    | 1:A:249:VAL:HG23 | 2.46                     | 0.40              |
| 1:A:294:ASP:OD2  | 1:A:325:PHE:C    | 2.65                     | 0.40              |
| 1:A:464:ALA:CA   | 1:A:509:PRO:HB2  | 2.48                     | 0.40              |
| 1:A:596:LYS:HZ3  | 1:A:596:LYS:CA   | 2.33                     | 0.40              |
| 1:E:78:ILE:HG12  | 1:E:98:GLN:NE2   | 2.36                     | 0.40              |
| 1:E:100:GLY:O    | 1:E:111:SER:N    | 2.54                     | 0.40              |
| 2:F:180:ILE:O    | 2:F:180:ILE:HG22 | 2.19                     | 0.40              |
| 2:F:235:ILE:CD1  | 2:F:274:SER:OG   | 2.69                     | 0.40              |
| 1:B:103:ASP:N    | 1:B:108:ILE:HG23 | 2.37                     | 0.40              |
| 1:B:119:ILE:O    | 1:B:119:ILE:HG22 | 2.21                     | 0.40              |
| 1:B:336:ASN:HD21 | 1:B:372:LEU:HD21 | 1.86                     | 0.40              |
| 2:C:31:ILE:CD1   | 2:C:35:GLU:OE2   | 2.68                     | 0.40              |
| 2:D:28:ARG:C     | 2:D:31:ILE:CD1   | 2.92                     | 0.40              |
| 2:D:81:ASP:OD1   | 2:D:81:ASP:N     | 2.46                     | 0.40              |
| 1:A:165:LEU:HD12 | 1:A:167:THR:N    | 2.00                     | 0.40              |
| 1:A:213:ILE:HD11 | 1:A:219:THR:HG21 | 1.95                     | 0.40              |
| 1:A:382:PRO:CB   | 1:A:385:VAL:CG2  | 2.88                     | 0.40              |
| 1:E:436:ILE:HG23 | 1:E:437:ASP:H    | 1.85                     | 0.40              |
| 1:E:466:THR:HA   | 1:E:511:LEU:O    | 2.21                     | 0.40              |
| 1:E:594:LEU:O    | 1:E:595:GLU:CB   | 2.70                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:214:TYR:HD2  | 2:F:214:TYR:O    | 2.04                     | 0.40              |
| 2:F:237:ARG:C    | 2:F:240:SER:HB2  | 2.45                     | 0.40              |
| 2:F:312:ALA:CB   | 2:F:342:LEU:HG   | 2.52                     | 0.40              |
| 1:B:77:VAL:HG12  | 1:B:79:PHE:CE1   | 2.53                     | 0.40              |
| 1:B:223:ILE:CG1  | 1:B:224:LYS:N    | 2.84                     | 0.40              |
| 1:B:368:TYR:HE1  | 1:B:372:LEU:CD2  | 2.33                     | 0.40              |
| 2:D:246:GLU:N    | 2:D:310:TRP:CH2  | 2.86                     | 0.40              |
| 1:A:114:GLU:H    | 1:A:114:GLU:HG2  | 1.61                     | 0.40              |
| 1:A:454:VAL:HG22 | 1:A:541:LEU:HD21 | 2.03                     | 0.40              |
| 1:E:366:LYS:CG   | 1:E:367:GLY:N    | 2.84                     | 0.40              |
| 1:E:588:PHE:CB   | 2:F:5:PRO:CG     | 2.99                     | 0.40              |
| 1:B:285:PRO:HG3  | 1:B:323:VAL:HG21 | 2.04                     | 0.40              |
| 1:B:366:LYS:HE3  | 1:B:367:GLY:H    | 1.81                     | 0.40              |
| 2:C:323:LEU:HD11 | 2:C:327:MET:HE3  | 2.03                     | 0.40              |
| 1:A:77:VAL:C     | 1:A:78:ILE:HD12  | 2.46                     | 0.40              |
| 1:A:231:VAL:O    | 1:A:234:SER:HB3  | 2.21                     | 0.40              |
| 1:A:516:PHE:CD2  | 1:A:516:PHE:C    | 2.95                     | 0.40              |
| 1:E:78:ILE:CG1   | 1:E:98:GLN:NE2   | 2.84                     | 0.40              |
| 2:F:259:PHE:CE1  | 2:F:267:PHE:CB   | 3.01                     | 0.40              |
| 1:B:92:GLN:NE2   | 1:B:184:TRP:H    | 2.17                     | 0.40              |
| 1:B:95:LEU:O     | 1:B:95:LEU:HD23  | 2.21                     | 0.40              |
| 1:B:223:ILE:O    | 1:B:224:LYS:HE3  | 2.20                     | 0.40              |
| 1:B:366:LYS:CE   | 1:B:367:GLY:N    | 2.73                     | 0.40              |
| 1:B:585:TYR:CE1  | 2:D:11:LYS:HA    | 2.55                     | 0.40              |
| 2:C:258:HIS:HA   | 2:C:261:HIS:CB   | 2.52                     | 0.40              |
| 2:C:270:GLY:O    | 2:C:274:SER:OG   | 2.27                     | 0.40              |
| 2:D:15:GLU:H     | 2:D:15:GLU:HG3   | 1.61                     | 0.40              |
| 1:A:77:VAL:HG12  | 1:A:79:PHE:CE2   | 2.57                     | 0.40              |
| 1:A:425:ARG:O    | 1:A:429:THR:OG1  | 2.38                     | 0.40              |
| 1:A:512:PRO:HG2  | 1:A:515:GLU:H    | 1.87                     | 0.40              |
| 2:F:119:ILE:HG13 | 2:F:119:ILE:H    | 1.57                     | 0.40              |
| 2:F:131:SER:O    | 2:F:132:ALA:C    | 2.63                     | 0.40              |
| 2:F:256:MET:C    | 2:F:259:PHE:H    | 2.30                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 2:C:195:ARG:NH2 | 1:E:207:ASP:OD2[1_655] | 1.73                     | 0.47              |
| 1:B:503:PHE:O   | 2:F:371:SER:O[5_545]   | 1.97                     | 0.23              |

*Continued on next page...*

Continued from previous page...

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:E:366:LYS:NZ | 2:F:123:SER:CB[3_554] | 2.02                     | 0.18              |
| 1:E:366:LYS:CE | 2:F:123:SER:CB[3_554] | 2.17                     | 0.03              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 505/610 (83%)   | 481 (95%)  | 23 (5%)  | 1 (0%)   | 43          | 71  |
| 1   | B     | 488/610 (80%)   | 462 (95%)  | 26 (5%)  | 0        | 100         | 100 |
| 1   | E     | 509/610 (83%)   | 483 (95%)  | 24 (5%)  | 2 (0%)   | 30          | 59  |
| 2   | C     | 326/421 (77%)   | 315 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 2   | D     | 309/421 (73%)   | 296 (96%)  | 11 (4%)  | 2 (1%)   | 21          | 50  |
| 2   | F     | 314/421 (75%)   | 301 (96%)  | 12 (4%)  | 1 (0%)   | 36          | 65  |
| All | All   | 2451/3093 (79%) | 2338 (95%) | 107 (4%) | 6 (0%)   | 43          | 71  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 101 | ASP  |
| 1   | E     | 154 | PRO  |
| 1   | A     | 121 | PRO  |
| 2   | F     | 244 | LYS  |
| 1   | E     | 400 | PRO  |
| 2   | D     | 353 | ASP  |

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

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |   |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1   | A     | 386/561 (69%)   | 264 (68%)  | 122 (32%) | 0           | 0 |
| 1   | B     | 377/561 (67%)   | 278 (74%)  | 99 (26%)  | 0           | 1 |
| 1   | E     | 383/561 (68%)   | 282 (74%)  | 101 (26%) | 0           | 1 |
| 2   | C     | 254/388 (66%)   | 199 (78%)  | 55 (22%)  | 1           | 3 |
| 2   | D     | 211/388 (54%)   | 159 (75%)  | 52 (25%)  | 1           | 2 |
| 2   | F     | 254/388 (66%)   | 199 (78%)  | 55 (22%)  | 1           | 3 |
| All | All   | 1865/2847 (66%) | 1381 (74%) | 484 (26%) | 0           | 1 |

All (484) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 64  | SER  |
| 1   | B     | 75  | ASP  |
| 1   | B     | 79  | PHE  |
| 1   | B     | 81  | LEU  |
| 1   | B     | 88  | ILE  |
| 1   | B     | 104 | ILE  |
| 1   | B     | 105 | ASN  |
| 1   | B     | 114 | GLU  |
| 1   | B     | 116 | MET  |
| 1   | B     | 120 | ASN  |
| 1   | B     | 122 | SER  |
| 1   | B     | 126 | ILE  |
| 1   | B     | 160 | ILE  |
| 1   | B     | 169 | LEU  |
| 1   | B     | 172 | ILE  |
| 1   | B     | 174 | ARG  |
| 1   | B     | 178 | LEU  |
| 1   | B     | 179 | PHE  |
| 1   | B     | 180 | LYS  |
| 1   | B     | 182 | LEU  |
| 1   | B     | 183 | PHE  |
| 1   | B     | 206 | SER  |
| 1   | B     | 207 | ASP  |
| 1   | B     | 209 | THR  |
| 1   | B     | 210 | PHE  |
| 1   | B     | 212 | PRO  |
| 1   | B     | 223 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 224 | LYS  |
| 1   | B     | 232 | ILE  |
| 1   | B     | 233 | LYS  |
| 1   | B     | 235 | LEU  |
| 1   | B     | 236 | THR  |
| 1   | B     | 237 | GLU  |
| 1   | B     | 238 | LEU  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 245 | ILE  |
| 1   | B     | 253 | LYS  |
| 1   | B     | 259 | THR  |
| 1   | B     | 270 | SER  |
| 1   | B     | 272 | THR  |
| 1   | B     | 275 | GLN  |
| 1   | B     | 276 | LEU  |
| 1   | B     | 287 | GLN  |
| 1   | B     | 289 | GLU  |
| 1   | B     | 300 | LYS  |
| 1   | B     | 305 | GLN  |
| 1   | B     | 308 | ASN  |
| 1   | B     | 316 | ASP  |
| 1   | B     | 317 | SER  |
| 1   | B     | 326 | ASN  |
| 1   | B     | 329 | LYS  |
| 1   | B     | 333 | THR  |
| 1   | B     | 334 | ARG  |
| 1   | B     | 347 | GLU  |
| 1   | B     | 351 | GLU  |
| 1   | B     | 356 | SER  |
| 1   | B     | 358 | LEU  |
| 1   | B     | 361 | THR  |
| 1   | B     | 364 | TRP  |
| 1   | B     | 366 | LYS  |
| 1   | B     | 399 | ILE  |
| 1   | B     | 403 | THR  |
| 1   | B     | 423 | GLN  |
| 1   | B     | 427 | LEU  |
| 1   | B     | 428 | LYS  |
| 1   | B     | 440 | LYS  |
| 1   | B     | 441 | PHE  |
| 1   | B     | 456 | TYR  |
| 1   | B     | 458 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 463 | SER  |
| 1   | B     | 468 | LEU  |
| 1   | B     | 469 | LYS  |
| 1   | B     | 471 | THR  |
| 1   | B     | 486 | ILE  |
| 1   | B     | 489 | ILE  |
| 1   | B     | 491 | LYS  |
| 1   | B     | 500 | CYS  |
| 1   | B     | 502 | LEU  |
| 1   | B     | 505 | LYS  |
| 1   | B     | 511 | LEU  |
| 1   | B     | 521 | THR  |
| 1   | B     | 522 | GLU  |
| 1   | B     | 525 | ARG  |
| 1   | B     | 526 | LEU  |
| 1   | B     | 530 | HIS  |
| 1   | B     | 531 | SER  |
| 1   | B     | 534 | GLN  |
| 1   | B     | 546 | PHE  |
| 1   | B     | 558 | MET  |
| 1   | B     | 563 | THR  |
| 1   | B     | 564 | ASP  |
| 1   | B     | 565 | LEU  |
| 1   | B     | 572 | SER  |
| 1   | B     | 575 | ILE  |
| 1   | B     | 576 | VAL  |
| 1   | B     | 583 | LEU  |
| 1   | B     | 585 | TYR  |
| 1   | B     | 586 | ILE  |
| 1   | B     | 596 | LYS  |
| 2   | C     | 12  | SER  |
| 2   | C     | 15  | GLU  |
| 2   | C     | 17  | VAL  |
| 2   | C     | 19  | LEU  |
| 2   | C     | 20  | LYS  |
| 2   | C     | 22  | LEU  |
| 2   | C     | 23  | PHE  |
| 2   | C     | 24  | PHE  |
| 2   | C     | 28  | ARG  |
| 2   | C     | 29  | GLU  |
| 2   | C     | 32  | SER  |
| 2   | C     | 34  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 38  | ARG  |
| 2   | C     | 39  | GLN  |
| 2   | C     | 45  | SER  |
| 2   | C     | 49  | MET  |
| 2   | C     | 53  | ARG  |
| 2   | C     | 82  | ASP  |
| 2   | C     | 83  | THR  |
| 2   | C     | 91  | THR  |
| 2   | C     | 95  | PHE  |
| 2   | C     | 99  | LEU  |
| 2   | C     | 119 | ILE  |
| 2   | C     | 121 | LEU  |
| 2   | C     | 123 | SER  |
| 2   | C     | 124 | LEU  |
| 2   | C     | 127 | GLU  |
| 2   | C     | 135 | ASP  |
| 2   | C     | 137 | LEU  |
| 2   | C     | 140 | LEU  |
| 2   | C     | 142 | MET  |
| 2   | C     | 145 | THR  |
| 2   | C     | 154 | VAL  |
| 2   | C     | 157 | HIS  |
| 2   | C     | 177 | GLU  |
| 2   | C     | 195 | ARG  |
| 2   | C     | 197 | ASN  |
| 2   | C     | 213 | GLU  |
| 2   | C     | 217 | CYS  |
| 2   | C     | 218 | ILE  |
| 2   | C     | 227 | MET  |
| 2   | C     | 233 | VAL  |
| 2   | C     | 235 | ILE  |
| 2   | C     | 238 | ILE  |
| 2   | C     | 255 | MET  |
| 2   | C     | 256 | MET  |
| 2   | C     | 275 | MET  |
| 2   | C     | 276 | LEU  |
| 2   | C     | 280 | TYR  |
| 2   | C     | 283 | SER  |
| 2   | C     | 333 | LYS  |
| 2   | C     | 334 | THR  |
| 2   | C     | 336 | HIS  |
| 2   | C     | 416 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 418 | PHE  |
| 2   | D     | 6   | ARG  |
| 2   | D     | 7   | LEU  |
| 2   | D     | 11  | LYS  |
| 2   | D     | 13  | SER  |
| 2   | D     | 22  | LEU  |
| 2   | D     | 23  | PHE  |
| 2   | D     | 28  | ARG  |
| 2   | D     | 31  | ILE  |
| 2   | D     | 32  | SER  |
| 2   | D     | 57  | SER  |
| 2   | D     | 60  | LEU  |
| 2   | D     | 63  | THR  |
| 2   | D     | 71  | MET  |
| 2   | D     | 72  | MET  |
| 2   | D     | 75  | SER  |
| 2   | D     | 94  | ARG  |
| 2   | D     | 100 | LEU  |
| 2   | D     | 121 | LEU  |
| 2   | D     | 123 | SER  |
| 2   | D     | 124 | LEU  |
| 2   | D     | 129 | ARG  |
| 2   | D     | 131 | SER  |
| 2   | D     | 133 | THR  |
| 2   | D     | 137 | LEU  |
| 2   | D     | 140 | LEU  |
| 2   | D     | 143 | CYS  |
| 2   | D     | 149 | ARG  |
| 2   | D     | 152 | ASP  |
| 2   | D     | 182 | GLU  |
| 2   | D     | 190 | TYR  |
| 2   | D     | 193 | ILE  |
| 2   | D     | 194 | ARG  |
| 2   | D     | 212 | LYS  |
| 2   | D     | 234 | MET  |
| 2   | D     | 238 | ILE  |
| 2   | D     | 246 | GLU  |
| 2   | D     | 247 | HIS  |
| 2   | D     | 255 | MET  |
| 2   | D     | 257 | ASN  |
| 2   | D     | 258 | HIS  |
| 2   | D     | 259 | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 261 | HIS  |
| 2   | D     | 271 | LEU  |
| 2   | D     | 272 | ILE  |
| 2   | D     | 274 | SER  |
| 2   | D     | 315 | GLN  |
| 2   | D     | 322 | VAL  |
| 2   | D     | 348 | SER  |
| 2   | D     | 353 | ASP  |
| 2   | D     | 356 | ILE  |
| 2   | D     | 358 | ASP  |
| 2   | D     | 420 | VAL  |
| 1   | A     | 63  | PHE  |
| 1   | A     | 71  | ILE  |
| 1   | A     | 72  | TYR  |
| 1   | A     | 74  | HIS  |
| 1   | A     | 75  | ASP  |
| 1   | A     | 81  | LEU  |
| 1   | A     | 108 | ILE  |
| 1   | A     | 114 | GLU  |
| 1   | A     | 116 | MET  |
| 1   | A     | 117 | LYS  |
| 1   | A     | 120 | ASN  |
| 1   | A     | 122 | SER  |
| 1   | A     | 123 | SER  |
| 1   | A     | 133 | GLN  |
| 1   | A     | 161 | LYS  |
| 1   | A     | 162 | LEU  |
| 1   | A     | 163 | THR  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 169 | LEU  |
| 1   | A     | 170 | GLU  |
| 1   | A     | 180 | LYS  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 182 | LEU  |
| 1   | A     | 183 | PHE  |
| 1   | A     | 184 | TRP  |
| 1   | A     | 202 | GLU  |
| 1   | A     | 207 | ASP  |
| 1   | A     | 208 | TYR  |
| 1   | A     | 209 | THR  |
| 1   | A     | 210 | PHE  |
| 1   | A     | 211 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 223 | ILE  |
| 1   | A     | 224 | LYS  |
| 1   | A     | 228 | TRP  |
| 1   | A     | 229 | MET  |
| 1   | A     | 232 | ILE  |
| 1   | A     | 235 | LEU  |
| 1   | A     | 236 | THR  |
| 1   | A     | 237 | GLU  |
| 1   | A     | 238 | LEU  |
| 1   | A     | 241 | ASN  |
| 1   | A     | 243 | GLN  |
| 1   | A     | 245 | ILE  |
| 1   | A     | 246 | LYS  |
| 1   | A     | 250 | ILE  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 272 | THR  |
| 1   | A     | 278 | ILE  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 298 | LEU  |
| 1   | A     | 300 | LYS  |
| 1   | A     | 305 | GLN  |
| 1   | A     | 311 | SER  |
| 1   | A     | 315 | THR  |
| 1   | A     | 318 | THR  |
| 1   | A     | 319 | GLN  |
| 1   | A     | 321 | HIS  |
| 1   | A     | 329 | LYS  |
| 1   | A     | 333 | THR  |
| 1   | A     | 334 | ARG  |
| 1   | A     | 338 | LEU  |
| 1   | A     | 351 | GLU  |
| 1   | A     | 352 | LEU  |
| 1   | A     | 358 | LEU  |
| 1   | A     | 361 | THR  |
| 1   | A     | 364 | TRP  |
| 1   | A     | 365 | ILE  |
| 1   | A     | 370 | LEU  |
| 1   | A     | 374 | ARG  |
| 1   | A     | 375 | THR  |
| 1   | A     | 376 | LEU  |
| 1   | A     | 377 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 378 | GLU  |
| 1   | A     | 389 | ASN  |
| 1   | A     | 393 | LEU  |
| 1   | A     | 397 | ILE  |
| 1   | A     | 398 | ASP  |
| 1   | A     | 399 | ILE  |
| 1   | A     | 401 | LYS  |
| 1   | A     | 403 | THR  |
| 1   | A     | 404 | ASN  |
| 1   | A     | 408 | LEU  |
| 1   | A     | 420 | SER  |
| 1   | A     | 428 | LYS  |
| 1   | A     | 429 | THR  |
| 1   | A     | 430 | MET  |
| 1   | A     | 440 | LYS  |
| 1   | A     | 446 | LEU  |
| 1   | A     | 467 | HIS  |
| 1   | A     | 468 | LEU  |
| 1   | A     | 475 | MET  |
| 1   | A     | 476 | ASP  |
| 1   | A     | 479 | GLU  |
| 1   | A     | 482 | ILE  |
| 1   | A     | 491 | LYS  |
| 1   | A     | 496 | HIS  |
| 1   | A     | 498 | GLU  |
| 1   | A     | 499 | GLU  |
| 1   | A     | 500 | CYS  |
| 1   | A     | 508 | LEU  |
| 1   | A     | 511 | LEU  |
| 1   | A     | 522 | GLU  |
| 1   | A     | 525 | ARG  |
| 1   | A     | 532 | ILE  |
| 1   | A     | 534 | GLN  |
| 1   | A     | 535 | GLU  |
| 1   | A     | 538 | ILE  |
| 1   | A     | 541 | LEU  |
| 1   | A     | 543 | ILE  |
| 1   | A     | 546 | PHE  |
| 1   | A     | 548 | THR  |
| 1   | A     | 565 | LEU  |
| 1   | A     | 575 | ILE  |
| 1   | A     | 580 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 582 | GLN  |
| 1   | A     | 586 | ILE  |
| 1   | A     | 588 | PHE  |
| 1   | A     | 592 | SER  |
| 1   | A     | 593 | SER  |
| 1   | A     | 596 | LYS  |
| 1   | A     | 597 | LYS  |
| 1   | E     | 64  | SER  |
| 1   | E     | 74  | HIS  |
| 1   | E     | 79  | PHE  |
| 1   | E     | 92  | GLN  |
| 1   | E     | 95  | LEU  |
| 1   | E     | 108 | ILE  |
| 1   | E     | 110 | HIS  |
| 1   | E     | 116 | MET  |
| 1   | E     | 119 | ILE  |
| 1   | E     | 120 | ASN  |
| 1   | E     | 125 | SER  |
| 1   | E     | 128 | LEU  |
| 1   | E     | 129 | ILE  |
| 1   | E     | 132 | THR  |
| 1   | E     | 138 | SER  |
| 1   | E     | 160 | ILE  |
| 1   | E     | 161 | LYS  |
| 1   | E     | 171 | SER  |
| 1   | E     | 172 | ILE  |
| 1   | E     | 179 | PHE  |
| 1   | E     | 180 | LYS  |
| 1   | E     | 183 | PHE  |
| 1   | E     | 184 | TRP  |
| 1   | E     | 186 | PHE  |
| 1   | E     | 218 | ASN  |
| 1   | E     | 225 | HIS  |
| 1   | E     | 226 | LYS  |
| 1   | E     | 227 | ASN  |
| 1   | E     | 230 | ASP  |
| 1   | E     | 231 | VAL  |
| 1   | E     | 233 | LYS  |
| 1   | E     | 235 | LEU  |
| 1   | E     | 248 | ILE  |
| 1   | E     | 253 | LYS  |
| 1   | E     | 254 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 257 | LYS  |
| 1   | E     | 263 | LEU  |
| 1   | E     | 272 | THR  |
| 1   | E     | 274 | GLN  |
| 1   | E     | 278 | ILE  |
| 1   | E     | 279 | ASN  |
| 1   | E     | 281 | MET  |
| 1   | E     | 287 | GLN  |
| 1   | E     | 293 | THR  |
| 1   | E     | 298 | LEU  |
| 1   | E     | 299 | SER  |
| 1   | E     | 300 | LYS  |
| 1   | E     | 303 | GLU  |
| 1   | E     | 311 | SER  |
| 1   | E     | 313 | THR  |
| 1   | E     | 319 | GLN  |
| 1   | E     | 323 | VAL  |
| 1   | E     | 325 | PHE  |
| 1   | E     | 334 | ARG  |
| 1   | E     | 337 | LEU  |
| 1   | E     | 341 | GLN  |
| 1   | E     | 342 | LEU  |
| 1   | E     | 347 | GLU  |
| 1   | E     | 351 | GLU  |
| 1   | E     | 352 | LEU  |
| 1   | E     | 357 | LEU  |
| 1   | E     | 358 | LEU  |
| 1   | E     | 361 | THR  |
| 1   | E     | 364 | TRP  |
| 1   | E     | 370 | LEU  |
| 1   | E     | 380 | VAL  |
| 1   | E     | 389 | ASN  |
| 1   | E     | 393 | LEU  |
| 1   | E     | 395 | VAL  |
| 1   | E     | 397 | ILE  |
| 1   | E     | 403 | THR  |
| 1   | E     | 405 | LEU  |
| 1   | E     | 406 | ILE  |
| 1   | E     | 420 | SER  |
| 1   | E     | 421 | SER  |
| 1   | E     | 423 | GLN  |
| 1   | E     | 427 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 429 | THR  |
| 1   | E     | 440 | LYS  |
| 1   | E     | 444 | GLN  |
| 1   | E     | 447 | LEU  |
| 1   | E     | 452 | ILE  |
| 1   | E     | 468 | LEU  |
| 1   | E     | 469 | LYS  |
| 1   | E     | 470 | GLU  |
| 1   | E     | 475 | MET  |
| 1   | E     | 491 | LYS  |
| 1   | E     | 516 | PHE  |
| 1   | E     | 519 | LEU  |
| 1   | E     | 522 | GLU  |
| 1   | E     | 525 | ARG  |
| 1   | E     | 528 | LEU  |
| 1   | E     | 530 | HIS  |
| 1   | E     | 552 | THR  |
| 1   | E     | 565 | LEU  |
| 1   | E     | 567 | ILE  |
| 1   | E     | 570 | ILE  |
| 1   | E     | 572 | SER  |
| 1   | E     | 575 | ILE  |
| 1   | E     | 589 | GLU  |
| 1   | E     | 593 | SER  |
| 2   | F     | 11  | LYS  |
| 2   | F     | 14  | ASP  |
| 2   | F     | 15  | GLU  |
| 2   | F     | 19  | LEU  |
| 2   | F     | 20  | LYS  |
| 2   | F     | 27  | ASP  |
| 2   | F     | 31  | ILE  |
| 2   | F     | 33  | ARG  |
| 2   | F     | 38  | ARG  |
| 2   | F     | 70  | LEU  |
| 2   | F     | 75  | SER  |
| 2   | F     | 77  | GLU  |
| 2   | F     | 110 | ILE  |
| 2   | F     | 113 | HIS  |
| 2   | F     | 114 | LEU  |
| 2   | F     | 117 | LYS  |
| 2   | F     | 118 | LYS  |
| 2   | F     | 119 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 137 | LEU  |
| 2   | F     | 144 | LYS  |
| 2   | F     | 179 | LEU  |
| 2   | F     | 198 | ILE  |
| 2   | F     | 213 | GLU  |
| 2   | F     | 214 | TYR  |
| 2   | F     | 234 | MET  |
| 2   | F     | 237 | ARG  |
| 2   | F     | 238 | ILE  |
| 2   | F     | 247 | HIS  |
| 2   | F     | 248 | LEU  |
| 2   | F     | 251 | LEU  |
| 2   | F     | 255 | MET  |
| 2   | F     | 259 | PHE  |
| 2   | F     | 260 | ILE  |
| 2   | F     | 269 | LEU  |
| 2   | F     | 301 | PHE  |
| 2   | F     | 305 | GLN  |
| 2   | F     | 309 | ARG  |
| 2   | F     | 325 | SER  |
| 2   | F     | 328 | ILE  |
| 2   | F     | 329 | ASP  |
| 2   | F     | 330 | THR  |
| 2   | F     | 331 | LEU  |
| 2   | F     | 337 | GLU  |
| 2   | F     | 338 | LEU  |
| 2   | F     | 342 | LEU  |
| 2   | F     | 345 | LYS  |
| 2   | F     | 348 | SER  |
| 2   | F     | 358 | ASP  |
| 2   | F     | 360 | ILE  |
| 2   | F     | 363 | LYS  |
| 2   | F     | 364 | LEU  |
| 2   | F     | 370 | LEU  |
| 2   | F     | 409 | SER  |
| 2   | F     | 420 | VAL  |
| 2   | F     | 421 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 92  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 105 | ASN  |
| 1   | B     | 225 | HIS  |
| 1   | B     | 227 | ASN  |
| 1   | B     | 266 | GLN  |
| 1   | B     | 275 | GLN  |
| 1   | B     | 305 | GLN  |
| 1   | B     | 326 | ASN  |
| 1   | B     | 423 | GLN  |
| 1   | B     | 434 | HIS  |
| 1   | B     | 467 | HIS  |
| 1   | B     | 534 | GLN  |
| 1   | B     | 540 | ASN  |
| 2   | C     | 134 | HIS  |
| 2   | C     | 197 | ASN  |
| 2   | C     | 229 | ASN  |
| 2   | C     | 257 | ASN  |
| 2   | C     | 258 | HIS  |
| 2   | C     | 279 | ASN  |
| 2   | C     | 336 | HIS  |
| 2   | C     | 361 | GLN  |
| 2   | D     | 39  | GLN  |
| 2   | D     | 58  | HIS  |
| 2   | D     | 61  | GLN  |
| 2   | D     | 224 | HIS  |
| 2   | D     | 257 | ASN  |
| 2   | D     | 261 | HIS  |
| 1   | A     | 92  | GLN  |
| 1   | A     | 130 | GLN  |
| 1   | A     | 185 | GLN  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 308 | ASN  |
| 1   | A     | 496 | HIS  |
| 1   | A     | 530 | HIS  |
| 1   | A     | 534 | GLN  |
| 1   | A     | 545 | GLN  |
| 1   | A     | 582 | GLN  |
| 1   | E     | 74  | HIS  |
| 1   | E     | 98  | GLN  |
| 1   | E     | 105 | ASN  |
| 1   | E     | 142 | ASN  |
| 1   | E     | 185 | GLN  |
| 1   | E     | 218 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 266 | GLN  |
| 1   | E     | 274 | GLN  |
| 1   | E     | 305 | GLN  |
| 1   | E     | 309 | HIS  |
| 1   | E     | 341 | GLN  |
| 1   | E     | 504 | ASN  |
| 1   | E     | 507 | GLN  |
| 1   | E     | 545 | GLN  |
| 1   | E     | 562 | ASN  |
| 2   | F     | 134 | HIS  |
| 2   | F     | 157 | HIS  |
| 2   | F     | 247 | HIS  |
| 2   | F     | 279 | ASN  |
| 2   | F     | 305 | GLN  |
| 2   | F     | 315 | GLN  |
| 2   | F     | 339 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   |   |   | OWAB(Å²)          | Q<0.9 |
|-----|-------|-----------------|--------|-----------|---|---|-------------------|-------|
| 1   | A     | 519/610 (85%)   | 1.56   | 159 (30%) | 1 | 2 | 76, 119, 148, 236 | 0     |
| 1   | B     | 506/610 (82%)   | 1.58   | 166 (32%) | 1 | 1 | 42, 125, 156, 187 | 0     |
| 1   | E     | 519/610 (85%)   | 1.82   | 198 (38%) | 1 | 1 | 68, 113, 156, 201 | 0     |
| 2   | C     | 340/421 (80%)   | 1.88   | 130 (38%) | 1 | 1 | 84, 149, 223, 243 | 0     |
| 2   | D     | 325/421 (77%)   | 1.60   | 102 (31%) | 1 | 2 | 77, 123, 169, 180 | 0     |
| 2   | F     | 338/421 (80%)   | 1.53   | 105 (31%) | 1 | 2 | 75, 123, 158, 191 | 0     |
| All | All   | 2547/3093 (82%) | 1.66   | 860 (33%) | 1 | 1 | 42, 123, 175, 243 | 0     |

All (860) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 387 | TYR  | 12.3 |
| 2   | F     | 279 | ASN  | 11.0 |
| 2   | C     | 316 | ILE  | 10.6 |
| 2   | F     | 104 | GLN  | 10.3 |
| 1   | A     | 596 | LYS  | 10.1 |
| 1   | A     | 409 | GLN  | 9.4  |
| 1   | B     | 90  | LYS  | 8.8  |
| 2   | D     | 330 | THR  | 8.7  |
| 1   | E     | 80  | GLY  | 8.7  |
| 2   | D     | 218 | ILE  | 8.7  |
| 1   | E     | 172 | ILE  | 8.4  |
| 1   | E     | 392 | THR  | 8.3  |
| 1   | E     | 598 | TRP  | 8.1  |
| 2   | F     | 31  | ILE  | 8.1  |
| 1   | E     | 393 | LEU  | 8.0  |
| 1   | E     | 322 | TYR  | 8.0  |
| 2   | C     | 359 | LYS  | 7.9  |
| 2   | C     | 346 | LEU  | 7.8  |
| 1   | E     | 594 | LEU  | 7.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 61  | SER  | 7.6  |
| 2   | F     | 32  | SER  | 7.5  |
| 2   | D     | 39  | GLN  | 7.4  |
| 2   | F     | 316 | ILE  | 7.3  |
| 2   | F     | 112 | LEU  | 7.3  |
| 1   | A     | 598 | TRP  | 7.2  |
| 1   | B     | 368 | TYR  | 7.2  |
| 1   | E     | 491 | LYS  | 7.2  |
| 1   | B     | 262 | ARG  | 7.2  |
| 1   | A     | 88  | ILE  | 7.1  |
| 1   | E     | 88  | ILE  | 7.1  |
| 1   | A     | 267 | HIS  | 7.0  |
| 1   | B     | 320 | CYS  | 7.0  |
| 1   | A     | 323 | VAL  | 6.9  |
| 1   | B     | 598 | TRP  | 6.9  |
| 1   | E     | 250 | ILE  | 6.9  |
| 1   | E     | 507 | GLN  | 6.8  |
| 2   | C     | 343 | LEU  | 6.8  |
| 1   | E     | 557 | ILE  | 6.8  |
| 2   | F     | 306 | LYS  | 6.7  |
| 2   | C     | 360 | ILE  | 6.6  |
| 2   | D     | 84  | VAL  | 6.6  |
| 2   | C     | 128 | PHE  | 6.5  |
| 1   | B     | 385 | VAL  | 6.5  |
| 2   | D     | 331 | LEU  | 6.5  |
| 2   | D     | 333 | LYS  | 6.4  |
| 1   | B     | 592 | SER  | 6.4  |
| 1   | B     | 235 | LEU  | 6.4  |
| 2   | C     | 369 | ARG  | 6.4  |
| 1   | B     | 492 | VAL  | 6.3  |
| 1   | A     | 303 | GLU  | 6.3  |
| 2   | F     | 84  | VAL  | 6.3  |
| 1   | B     | 387 | TYR  | 6.1  |
| 1   | B     | 401 | LYS  | 6.1  |
| 2   | D     | 35  | GLU  | 6.0  |
| 2   | C     | 328 | ILE  | 6.0  |
| 2   | F     | 261 | HIS  | 6.0  |
| 2   | D     | 346 | LEU  | 6.0  |
| 1   | B     | 80  | GLY  | 5.8  |
| 2   | C     | 367 | ILE  | 5.7  |
| 1   | E     | 479 | GLU  | 5.7  |
| 2   | D     | 305 | GLN  | 5.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 42  | GLU  | 5.6  |
| 2   | C     | 280 | TYR  | 5.5  |
| 2   | D     | 308 | ILE  | 5.5  |
| 1   | A     | 177 | PRO  | 5.5  |
| 1   | A     | 293 | THR  | 5.5  |
| 1   | A     | 385 | VAL  | 5.4  |
| 2   | C     | 140 | LEU  | 5.4  |
| 2   | C     | 73  | LEU  | 5.4  |
| 1   | B     | 360 | ASN  | 5.4  |
| 1   | A     | 540 | ASN  | 5.4  |
| 2   | D     | 315 | GLN  | 5.4  |
| 1   | B     | 338 | LEU  | 5.4  |
| 2   | C     | 31  | ILE  | 5.4  |
| 1   | A     | 298 | LEU  | 5.3  |
| 1   | E     | 304 | VAL  | 5.3  |
| 1   | A     | 570 | ILE  | 5.3  |
| 2   | D     | 19  | LEU  | 5.3  |
| 1   | E     | 116 | MET  | 5.3  |
| 2   | F     | 156 | ASP  | 5.3  |
| 2   | D     | 23  | PHE  | 5.3  |
| 1   | E     | 478 | LEU  | 5.3  |
| 2   | C     | 44  | ILE  | 5.3  |
| 1   | A     | 268 | MET  | 5.2  |
| 1   | A     | 228 | TRP  | 5.2  |
| 2   | D     | 216 | THR  | 5.2  |
| 2   | C     | 60  | LEU  | 5.1  |
| 2   | C     | 356 | ILE  | 5.1  |
| 1   | E     | 446 | LEU  | 5.1  |
| 1   | B     | 318 | THR  | 5.1  |
| 1   | B     | 397 | ILE  | 5.1  |
| 1   | E     | 482 | ILE  | 5.0  |
| 1   | B     | 61  | SER  | 5.0  |
| 1   | A     | 265 | VAL  | 5.0  |
| 2   | D     | 124 | LEU  | 5.0  |
| 2   | C     | 71  | MET  | 5.0  |
| 2   | F     | 95  | PHE  | 4.9  |
| 1   | A     | 239 | TYR  | 4.9  |
| 2   | D     | 67  | PHE  | 4.9  |
| 1   | B     | 260 | PHE  | 4.9  |
| 1   | A     | 477 | HIS  | 4.9  |
| 2   | C     | 259 | PHE  | 4.9  |
| 2   | C     | 68  | SER  | 4.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 140 | LEU  | 4.9  |
| 2   | D     | 256 | MET  | 4.9  |
| 2   | D     | 159 | TRP  | 4.9  |
| 1   | E     | 105 | ASN  | 4.9  |
| 2   | C     | 256 | MET  | 4.9  |
| 2   | F     | 343 | LEU  | 4.9  |
| 1   | E     | 245 | ILE  | 4.8  |
| 1   | B     | 231 | VAL  | 4.8  |
| 1   | E     | 244 | SER  | 4.8  |
| 2   | D     | 343 | LEU  | 4.8  |
| 1   | E     | 569 | GLU  | 4.8  |
| 1   | E     | 274 | GLN  | 4.8  |
| 1   | B     | 372 | LEU  | 4.7  |
| 1   | E     | 306 | HIS  | 4.7  |
| 1   | B     | 301 | ILE  | 4.7  |
| 2   | C     | 59  | ILE  | 4.7  |
| 2   | F     | 100 | LEU  | 4.7  |
| 2   | C     | 85  | ARG  | 4.7  |
| 1   | E     | 385 | VAL  | 4.7  |
| 1   | A     | 497 | LEU  | 4.7  |
| 1   | B     | 467 | HIS  | 4.6  |
| 1   | A     | 368 | TYR  | 4.6  |
| 2   | C     | 178 | SER  | 4.6  |
| 2   | C     | 129 | ARG  | 4.6  |
| 1   | B     | 322 | TYR  | 4.6  |
| 1   | B     | 158 | SER  | 4.6  |
| 2   | F     | 308 | ILE  | 4.6  |
| 1   | A     | 467 | HIS  | 4.6  |
| 1   | A     | 567 | ILE  | 4.5  |
| 1   | E     | 539 | MET  | 4.5  |
| 2   | C     | 363 | LYS  | 4.5  |
| 1   | A     | 344 | ARG  | 4.5  |
| 1   | B     | 81  | LEU  | 4.5  |
| 1   | A     | 338 | LEU  | 4.5  |
| 2   | C     | 342 | LEU  | 4.5  |
| 2   | D     | 215 | TRP  | 4.5  |
| 2   | C     | 319 | TYR  | 4.5  |
| 1   | A     | 263 | LEU  | 4.5  |
| 1   | A     | 61  | SER  | 4.5  |
| 1   | A     | 260 | PHE  | 4.5  |
| 1   | A     | 443 | PHE  | 4.5  |
| 2   | D     | 329 | ASP  | 4.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 64  | ALA  | 4.4  |
| 2   | D     | 328 | ILE  | 4.4  |
| 2   | C     | 267 | PHE  | 4.4  |
| 2   | C     | 164 | SER  | 4.4  |
| 1   | E     | 558 | MET  | 4.4  |
| 2   | F     | 88  | ALA  | 4.4  |
| 1   | B     | 100 | GLY  | 4.3  |
| 1   | E     | 273 | LEU  | 4.3  |
| 2   | D     | 60  | LEU  | 4.3  |
| 1   | B     | 267 | HIS  | 4.3  |
| 2   | D     | 241 | ASN  | 4.3  |
| 2   | C     | 372 | THR  | 4.3  |
| 2   | F     | 23  | PHE  | 4.3  |
| 1   | B     | 109 | TYR  | 4.3  |
| 1   | E     | 62  | ASN  | 4.3  |
| 2   | D     | 342 | LEU  | 4.3  |
| 1   | E     | 354 | HIS  | 4.2  |
| 1   | E     | 212 | PRO  | 4.2  |
| 2   | C     | 93  | ILE  | 4.2  |
| 1   | E     | 323 | VAL  | 4.2  |
| 2   | F     | 356 | ILE  | 4.2  |
| 1   | A     | 281 | MET  | 4.2  |
| 1   | B     | 358 | LEU  | 4.2  |
| 1   | A     | 278 | ILE  | 4.2  |
| 2   | C     | 365 | THR  | 4.2  |
| 2   | D     | 360 | ILE  | 4.2  |
| 1   | E     | 464 | ALA  | 4.1  |
| 2   | C     | 324 | VAL  | 4.1  |
| 2   | D     | 258 | HIS  | 4.1  |
| 2   | D     | 190 | TYR  | 4.1  |
| 2   | C     | 315 | GLN  | 4.1  |
| 2   | C     | 66  | LEU  | 4.0  |
| 1   | B     | 356 | SER  | 4.0  |
| 2   | C     | 338 | LEU  | 4.0  |
| 2   | C     | 345 | LYS  | 4.0  |
| 1   | A     | 573 | ASN  | 4.0  |
| 1   | A     | 478 | LEU  | 4.0  |
| 1   | A     | 594 | LEU  | 4.0  |
| 2   | F     | 416 | LYS  | 4.0  |
| 1   | B     | 473 | ILE  | 4.0  |
| 1   | B     | 298 | LEU  | 4.0  |
| 1   | E     | 590 | LYS  | 4.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 310 | TRP  | 4.0  |
| 1   | A     | 359 | ILE  | 4.0  |
| 1   | A     | 557 | ILE  | 4.0  |
| 2   | C     | 272 | ILE  | 4.0  |
| 1   | A     | 351 | GLU  | 4.0  |
| 2   | D     | 183 | LEU  | 4.0  |
| 1   | B     | 295 | CYS  | 3.9  |
| 1   | E     | 534 | GLN  | 3.9  |
| 1   | B     | 269 | LEU  | 3.9  |
| 2   | C     | 195 | ARG  | 3.9  |
| 1   | A     | 90  | LYS  | 3.9  |
| 2   | C     | 100 | LEU  | 3.9  |
| 1   | E     | 219 | THR  | 3.9  |
| 1   | A     | 480 | ARG  | 3.9  |
| 1   | E     | 510 | LEU  | 3.9  |
| 2   | C     | 179 | LEU  | 3.9  |
| 1   | E     | 389 | ASN  | 3.9  |
| 1   | A     | 395 | VAL  | 3.9  |
| 2   | D     | 347 | GLN  | 3.9  |
| 1   | E     | 265 | VAL  | 3.8  |
| 2   | F     | 67  | PHE  | 3.8  |
| 2   | F     | 301 | PHE  | 3.8  |
| 1   | A     | 526 | LEU  | 3.8  |
| 1   | A     | 569 | GLU  | 3.8  |
| 2   | C     | 334 | THR  | 3.8  |
| 2   | D     | 407 | PHE  | 3.8  |
| 2   | F     | 143 | CYS  | 3.8  |
| 1   | B     | 159 | VAL  | 3.8  |
| 1   | E     | 458 | VAL  | 3.8  |
| 1   | A     | 91  | GLY  | 3.8  |
| 1   | A     | 100 | GLY  | 3.8  |
| 1   | A     | 322 | TYR  | 3.8  |
| 1   | E     | 87  | LEU  | 3.8  |
| 1   | B     | 261 | LEU  | 3.7  |
| 1   | E     | 526 | LEU  | 3.7  |
| 1   | E     | 383 | THR  | 3.7  |
| 1   | A     | 453 | GLN  | 3.7  |
| 1   | E     | 423 | GLN  | 3.7  |
| 2   | C     | 158 | TYR  | 3.7  |
| 2   | C     | 234 | MET  | 3.7  |
| 1   | E     | 370 | LEU  | 3.7  |
| 1   | E     | 457 | GLY  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 270 | SER  | 3.7  |
| 1   | A     | 219 | THR  | 3.7  |
| 2   | C     | 340 | VAL  | 3.7  |
| 1   | A     | 158 | SER  | 3.6  |
| 1   | B     | 166 | ASP  | 3.6  |
| 2   | C     | 341 | GLU  | 3.6  |
| 1   | A     | 287 | GLN  | 3.6  |
| 1   | E     | 109 | TYR  | 3.6  |
| 1   | E     | 156 | TYR  | 3.6  |
| 1   | E     | 463 | SER  | 3.6  |
| 1   | E     | 492 | VAL  | 3.6  |
| 2   | C     | 275 | MET  | 3.6  |
| 1   | E     | 508 | LEU  | 3.6  |
| 2   | C     | 22  | LEU  | 3.6  |
| 1   | E     | 98  | GLN  | 3.6  |
| 2   | D     | 76  | PHE  | 3.6  |
| 1   | B     | 251 | GLY  | 3.6  |
| 1   | E     | 268 | MET  | 3.6  |
| 1   | B     | 97  | ILE  | 3.6  |
| 1   | B     | 342 | LEU  | 3.6  |
| 2   | C     | 276 | LEU  | 3.6  |
| 1   | A     | 423 | GLN  | 3.6  |
| 2   | C     | 339 | ASN  | 3.6  |
| 1   | E     | 465 | LEU  | 3.6  |
| 2   | F     | 311 | LEU  | 3.6  |
| 1   | B     | 339 | VAL  | 3.6  |
| 1   | E     | 376 | LEU  | 3.6  |
| 2   | C     | 271 | LEU  | 3.6  |
| 1   | E     | 272 | THR  | 3.6  |
| 1   | E     | 106 | GLY  | 3.5  |
| 2   | C     | 19  | LEU  | 3.5  |
| 1   | B     | 279 | ASN  | 3.5  |
| 1   | E     | 359 | ILE  | 3.5  |
| 1   | B     | 99  | ARG  | 3.5  |
| 2   | D     | 125 | PHE  | 3.5  |
| 1   | A     | 213 | ILE  | 3.5  |
| 2   | F     | 151 | ILE  | 3.5  |
| 2   | C     | 348 | SER  | 3.5  |
| 2   | C     | 355 | VAL  | 3.5  |
| 1   | A     | 357 | LEU  | 3.5  |
| 2   | D     | 121 | LEU  | 3.5  |
| 2   | C     | 50  | TYR  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 421 | SER  | 3.5  |
| 2   | D     | 332 | GLY  | 3.5  |
| 2   | D     | 88  | ALA  | 3.5  |
| 1   | E     | 511 | LEU  | 3.5  |
| 1   | A     | 556 | ILE  | 3.5  |
| 1   | B     | 79  | PHE  | 3.5  |
| 1   | E     | 433 | PHE  | 3.5  |
| 1   | A     | 101 | ALA  | 3.5  |
| 1   | E     | 567 | ILE  | 3.5  |
| 1   | E     | 144 | GLU  | 3.4  |
| 1   | A     | 220 | VAL  | 3.4  |
| 2   | F     | 99  | LEU  | 3.4  |
| 1   | E     | 120 | ASN  | 3.4  |
| 2   | F     | 19  | LEU  | 3.4  |
| 1   | B     | 481 | SER  | 3.4  |
| 1   | B     | 446 | LEU  | 3.4  |
| 2   | C     | 349 | ARG  | 3.4  |
| 1   | A     | 259 | THR  | 3.4  |
| 1   | E     | 445 | PRO  | 3.4  |
| 2   | F     | 128 | PHE  | 3.4  |
| 1   | E     | 231 | VAL  | 3.4  |
| 1   | E     | 357 | LEU  | 3.4  |
| 1   | E     | 428 | LYS  | 3.4  |
| 2   | C     | 268 | PRO  | 3.4  |
| 2   | C     | 307 | TRP  | 3.4  |
| 1   | A     | 593 | SER  | 3.4  |
| 1   | E     | 79  | PHE  | 3.4  |
| 2   | D     | 409 | SER  | 3.4  |
| 1   | B     | 312 | LEU  | 3.4  |
| 2   | F     | 121 | LEU  | 3.4  |
| 1   | E     | 290 | TYR  | 3.4  |
| 1   | B     | 160 | ILE  | 3.4  |
| 1   | B     | 597 | LYS  | 3.4  |
| 1   | E     | 523 | PHE  | 3.3  |
| 1   | A     | 165 | LEU  | 3.3  |
| 1   | E     | 276 | LEU  | 3.3  |
| 2   | C     | 344 | GLU  | 3.3  |
| 1   | A     | 119 | ILE  | 3.3  |
| 1   | B     | 266 | GLN  | 3.3  |
| 1   | B     | 172 | ILE  | 3.3  |
| 1   | B     | 359 | ILE  | 3.3  |
| 2   | C     | 317 | ASP  | 3.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 374 | ARG  | 3.3  |
| 2   | D     | 141 | GLU  | 3.3  |
| 1   | E     | 229 | MET  | 3.3  |
| 1   | A     | 552 | THR  | 3.3  |
| 2   | C     | 67  | PHE  | 3.3  |
| 1   | B     | 253 | LYS  | 3.3  |
| 2   | C     | 63  | THR  | 3.3  |
| 2   | C     | 91  | THR  | 3.3  |
| 1   | E     | 157 | LYS  | 3.3  |
| 1   | B     | 268 | MET  | 3.3  |
| 2   | F     | 180 | ILE  | 3.3  |
| 1   | E     | 239 | TYR  | 3.2  |
| 1   | E     | 162 | LEU  | 3.2  |
| 1   | B     | 323 | VAL  | 3.2  |
| 1   | B     | 430 | MET  | 3.2  |
| 1   | E     | 394 | GLY  | 3.2  |
| 1   | E     | 427 | LEU  | 3.2  |
| 1   | E     | 260 | PHE  | 3.2  |
| 2   | C     | 96  | VAL  | 3.2  |
| 2   | C     | 265 | TRP  | 3.2  |
| 1   | E     | 347 | GLU  | 3.2  |
| 2   | F     | 77  | GLU  | 3.2  |
| 1   | B     | 263 | LEU  | 3.2  |
| 2   | C     | 36  | LEU  | 3.2  |
| 2   | F     | 124 | LEU  | 3.2  |
| 2   | C     | 25  | PRO  | 3.2  |
| 1   | A     | 92  | GLN  | 3.2  |
| 2   | D     | 365 | THR  | 3.2  |
| 2   | C     | 49  | MET  | 3.2  |
| 2   | D     | 421 | ILE  | 3.2  |
| 2   | F     | 411 | PRO  | 3.2  |
| 1   | A     | 296 | ILE  | 3.2  |
| 2   | C     | 28  | ARG  | 3.2  |
| 2   | D     | 334 | THR  | 3.2  |
| 2   | F     | 221 | ILE  | 3.2  |
| 1   | A     | 342 | LEU  | 3.2  |
| 1   | B     | 94  | VAL  | 3.2  |
| 1   | E     | 110 | HIS  | 3.2  |
| 1   | E     | 496 | HIS  | 3.2  |
| 1   | A     | 185 | GLN  | 3.2  |
| 2   | D     | 31  | ILE  | 3.2  |
| 2   | D     | 325 | SER  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 426 | LEU  | 3.1  |
| 2   | C     | 311 | LEU  | 3.1  |
| 2   | D     | 186 | LEU  | 3.1  |
| 1   | A     | 566 | PRO  | 3.1  |
| 1   | A     | 462 | ILE  | 3.1  |
| 2   | F     | 234 | MET  | 3.1  |
| 1   | E     | 488 | GLY  | 3.1  |
| 2   | D     | 364 | LEU  | 3.1  |
| 1   | A     | 172 | ILE  | 3.1  |
| 1   | B     | 287 | GLN  | 3.1  |
| 1   | E     | 66  | ASP  | 3.1  |
| 1   | E     | 499 | GLU  | 3.1  |
| 1   | E     | 595 | GLU  | 3.1  |
| 1   | E     | 380 | VAL  | 3.1  |
| 2   | F     | 146 | CYS  | 3.1  |
| 2   | F     | 94  | ARG  | 3.1  |
| 1   | A     | 451 | PRO  | 3.1  |
| 1   | A     | 62  | ASN  | 3.1  |
| 2   | F     | 198 | ILE  | 3.1  |
| 1   | B     | 427 | LEU  | 3.1  |
| 1   | E     | 118 | PHE  | 3.1  |
| 2   | D     | 16  | VAL  | 3.1  |
| 1   | E     | 462 | ILE  | 3.1  |
| 1   | B     | 376 | LEU  | 3.1  |
| 1   | A     | 376 | LEU  | 3.1  |
| 2   | F     | 419 | GLY  | 3.1  |
| 1   | B     | 265 | VAL  | 3.1  |
| 1   | B     | 170 | GLU  | 3.1  |
| 1   | A     | 397 | ILE  | 3.1  |
| 1   | E     | 296 | ILE  | 3.1  |
| 1   | B     | 357 | LEU  | 3.0  |
| 1   | A     | 312 | LEU  | 3.0  |
| 2   | C     | 157 | HIS  | 3.0  |
| 2   | F     | 410 | HIS  | 3.0  |
| 1   | B     | 319 | GLN  | 3.0  |
| 1   | A     | 292 | GLY  | 3.0  |
| 1   | A     | 488 | GLY  | 3.0  |
| 1   | E     | 292 | GLY  | 3.0  |
| 1   | B     | 179 | PHE  | 3.0  |
| 2   | F     | 275 | MET  | 3.0  |
| 2   | C     | 26  | ALA  | 3.0  |
| 2   | C     | 243 | LEU  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 360 | ASN  | 3.0  |
| 1   | E     | 467 | HIS  | 3.0  |
| 1   | B     | 394 | GLY  | 3.0  |
| 1   | E     | 161 | LYS  | 3.0  |
| 2   | C     | 337 | GLU  | 3.0  |
| 2   | F     | 42  | GLU  | 3.0  |
| 1   | E     | 486 | ILE  | 3.0  |
| 1   | E     | 409 | GLN  | 3.0  |
| 1   | A     | 247 | VAL  | 3.0  |
| 2   | C     | 154 | VAL  | 3.0  |
| 1   | B     | 443 | PHE  | 3.0  |
| 1   | E     | 104 | ILE  | 3.0  |
| 1   | A     | 279 | ASN  | 3.0  |
| 2   | D     | 238 | ILE  | 3.0  |
| 1   | A     | 211 | TYR  | 3.0  |
| 1   | A     | 597 | LYS  | 3.0  |
| 1   | E     | 208 | TYR  | 3.0  |
| 2   | F     | 158 | TYR  | 3.0  |
| 1   | A     | 339 | VAL  | 3.0  |
| 1   | A     | 380 | VAL  | 3.0  |
| 1   | E     | 74  | HIS  | 3.0  |
| 1   | E     | 77  | VAL  | 3.0  |
| 1   | B     | 98  | GLN  | 3.0  |
| 2   | C     | 335 | ASN  | 3.0  |
| 1   | B     | 248 | ILE  | 3.0  |
| 1   | B     | 482 | ILE  | 3.0  |
| 2   | C     | 137 | LEU  | 2.9  |
| 2   | F     | 346 | LEU  | 2.9  |
| 1   | E     | 329 | LYS  | 2.9  |
| 1   | E     | 469 | LYS  | 2.9  |
| 2   | F     | 62  | SER  | 2.9  |
| 2   | F     | 315 | GLN  | 2.9  |
| 2   | F     | 421 | ILE  | 2.9  |
| 1   | A     | 583 | LEU  | 2.9  |
| 2   | F     | 217 | CYS  | 2.9  |
| 1   | E     | 328 | PRO  | 2.9  |
| 1   | B     | 464 | ALA  | 2.9  |
| 2   | D     | 420 | VAL  | 2.9  |
| 1   | E     | 267 | HIS  | 2.9  |
| 1   | A     | 408 | LEU  | 2.9  |
| 1   | A     | 468 | LEU  | 2.9  |
| 2   | F     | 150 | ALA  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 290 | TYR  | 2.9  |
| 1   | B     | 213 | ILE  | 2.9  |
| 1   | B     | 377 | ILE  | 2.9  |
| 1   | A     | 250 | ILE  | 2.9  |
| 1   | A     | 406 | ILE  | 2.9  |
| 1   | A     | 436 | ILE  | 2.9  |
| 1   | A     | 482 | ILE  | 2.9  |
| 1   | A     | 489 | ILE  | 2.9  |
| 1   | E     | 386 | ILE  | 2.9  |
| 1   | B     | 264 | LEU  | 2.9  |
| 1   | A     | 447 | LEU  | 2.9  |
| 2   | C     | 364 | LEU  | 2.9  |
| 2   | D     | 326 | LYS  | 2.9  |
| 2   | F     | 11  | LYS  | 2.9  |
| 2   | D     | 54  | THR  | 2.9  |
| 2   | D     | 87  | THR  | 2.9  |
| 2   | C     | 122 | PRO  | 2.9  |
| 2   | C     | 418 | PHE  | 2.9  |
| 1   | B     | 250 | ILE  | 2.9  |
| 2   | C     | 193 | ILE  | 2.9  |
| 2   | F     | 66  | LEU  | 2.9  |
| 1   | B     | 177 | PRO  | 2.9  |
| 2   | D     | 83  | THR  | 2.9  |
| 2   | F     | 37  | TYR  | 2.9  |
| 1   | A     | 511 | LEU  | 2.9  |
| 1   | E     | 160 | ILE  | 2.9  |
| 2   | C     | 188 | LYS  | 2.9  |
| 2   | F     | 273 | ASP  | 2.8  |
| 1   | B     | 271 | PRO  | 2.8  |
| 1   | E     | 559 | VAL  | 2.8  |
| 2   | D     | 20  | LYS  | 2.8  |
| 1   | A     | 169 | LEU  | 2.8  |
| 2   | F     | 122 | PRO  | 2.8  |
| 1   | A     | 330 | ASP  | 2.8  |
| 1   | B     | 425 | ARG  | 2.8  |
| 1   | A     | 89  | VAL  | 2.8  |
| 1   | A     | 262 | ARG  | 2.8  |
| 2   | F     | 310 | TRP  | 2.8  |
| 1   | E     | 538 | ILE  | 2.8  |
| 2   | D     | 66  | LEU  | 2.8  |
| 1   | E     | 64  | SER  | 2.8  |
| 1   | B     | 77  | VAL  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 429 | THR  | 2.8  |
| 1   | B     | 466 | THR  | 2.8  |
| 1   | A     | 117 | LYS  | 2.8  |
| 1   | E     | 466 | THR  | 2.8  |
| 2   | D     | 148 | ASP  | 2.8  |
| 1   | A     | 358 | LEU  | 2.8  |
| 1   | E     | 251 | GLY  | 2.8  |
| 1   | A     | 334 | ARG  | 2.8  |
| 2   | F     | 85  | ARG  | 2.8  |
| 1   | B     | 512 | PRO  | 2.8  |
| 1   | E     | 175 | VAL  | 2.8  |
| 2   | D     | 133 | THR  | 2.8  |
| 1   | E     | 442 | ASP  | 2.8  |
| 2   | C     | 327 | MET  | 2.8  |
| 2   | D     | 327 | MET  | 2.8  |
| 1   | B     | 540 | ASN  | 2.8  |
| 1   | E     | 404 | ASN  | 2.8  |
| 2   | F     | 50  | TYR  | 2.8  |
| 1   | A     | 74  | HIS  | 2.8  |
| 1   | B     | 516 | PHE  | 2.7  |
| 1   | A     | 364 | TRP  | 2.7  |
| 2   | F     | 152 | ASP  | 2.7  |
| 1   | E     | 560 | ARG  | 2.7  |
| 1   | B     | 101 | ALA  | 2.7  |
| 1   | E     | 305 | GLN  | 2.7  |
| 2   | D     | 179 | LEU  | 2.7  |
| 1   | B     | 489 | ILE  | 2.7  |
| 2   | C     | 45  | SER  | 2.7  |
| 1   | B     | 403 | THR  | 2.7  |
| 2   | F     | 413 | TRP  | 2.7  |
| 2   | F     | 353 | ASP  | 2.7  |
| 1   | E     | 431 | ALA  | 2.7  |
| 2   | C     | 228 | ALA  | 2.7  |
| 1   | B     | 458 | VAL  | 2.7  |
| 1   | E     | 275 | GLN  | 2.7  |
| 1   | E     | 127 | PRO  | 2.7  |
| 1   | E     | 372 | LEU  | 2.7  |
| 1   | E     | 541 | LEU  | 2.7  |
| 1   | A     | 439 | PHE  | 2.7  |
| 2   | C     | 255 | MET  | 2.7  |
| 2   | D     | 142 | MET  | 2.7  |
| 2   | F     | 407 | PHE  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 314 | GLU  | 2.7  |
| 1   | E     | 481 | SER  | 2.7  |
| 1   | E     | 419 | TYR  | 2.7  |
| 1   | B     | 321 | HIS  | 2.7  |
| 1   | A     | 360 | ASN  | 2.7  |
| 1   | E     | 222 | VAL  | 2.7  |
| 1   | B     | 212 | PRO  | 2.7  |
| 2   | F     | 305 | GLN  | 2.7  |
| 1   | B     | 291 | SER  | 2.7  |
| 1   | B     | 593 | SER  | 2.7  |
| 2   | C     | 89  | SER  | 2.7  |
| 1   | A     | 128 | LEU  | 2.7  |
| 1   | B     | 431 | ALA  | 2.7  |
| 2   | D     | 312 | ALA  | 2.7  |
| 1   | E     | 368 | TYR  | 2.7  |
| 1   | E     | 513 | TYR  | 2.7  |
| 2   | D     | 50  | TYR  | 2.7  |
| 2   | D     | 251 | LEU  | 2.7  |
| 1   | A     | 321 | HIS  | 2.7  |
| 1   | E     | 281 | MET  | 2.6  |
| 1   | E     | 430 | MET  | 2.6  |
| 1   | A     | 426 | LEU  | 2.6  |
| 2   | F     | 7   | LEU  | 2.6  |
| 2   | F     | 364 | LEU  | 2.6  |
| 1   | E     | 585 | TYR  | 2.6  |
| 2   | C     | 361 | GLN  | 2.6  |
| 2   | C     | 368 | GLN  | 2.6  |
| 1   | B     | 522 | GLU  | 2.6  |
| 2   | D     | 73  | LEU  | 2.6  |
| 2   | F     | 307 | TRP  | 2.6  |
| 1   | A     | 301 | ILE  | 2.6  |
| 1   | A     | 374 | ARG  | 2.6  |
| 1   | E     | 90  | LYS  | 2.6  |
| 2   | D     | 85  | ARG  | 2.6  |
| 2   | F     | 49  | MET  | 2.6  |
| 1   | E     | 367 | GLY  | 2.6  |
| 1   | A     | 370 | LEU  | 2.6  |
| 1   | B     | 335 | TYR  | 2.6  |
| 1   | B     | 386 | ILE  | 2.6  |
| 1   | A     | 335 | TYR  | 2.6  |
| 2   | C     | 92  | ILE  | 2.6  |
| 2   | C     | 308 | ILE  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 65  | HIS  | 2.6  |
| 2   | D     | 82  | ASP  | 2.6  |
| 1   | B     | 402 | GLY  | 2.6  |
| 1   | E     | 86  | ASN  | 2.6  |
| 2   | C     | 279 | ASN  | 2.6  |
| 1   | E     | 303 | GLU  | 2.6  |
| 2   | F     | 248 | LEU  | 2.6  |
| 1   | A     | 521 | THR  | 2.6  |
| 1   | A     | 248 | ILE  | 2.6  |
| 2   | F     | 119 | ILE  | 2.6  |
| 2   | F     | 190 | TYR  | 2.6  |
| 1   | E     | 512 | PRO  | 2.6  |
| 1   | B     | 336 | ASN  | 2.6  |
| 2   | C     | 321 | ASP  | 2.6  |
| 1   | B     | 310 | LEU  | 2.6  |
| 1   | E     | 169 | LEU  | 2.6  |
| 2   | D     | 44  | ILE  | 2.5  |
| 1   | E     | 285 | PRO  | 2.5  |
| 2   | C     | 5   | PRO  | 2.5  |
| 1   | B     | 244 | SER  | 2.5  |
| 1   | E     | 592 | SER  | 2.5  |
| 2   | C     | 70  | LEU  | 2.5  |
| 1   | E     | 113 | VAL  | 2.5  |
| 1   | E     | 282 | ASP  | 2.5  |
| 2   | F     | 96  | VAL  | 2.5  |
| 2   | F     | 64  | ALA  | 2.5  |
| 1   | A     | 167 | THR  | 2.5  |
| 1   | A     | 471 | THR  | 2.5  |
| 2   | F     | 193 | ILE  | 2.5  |
| 1   | B     | 448 | PHE  | 2.5  |
| 2   | D     | 36  | LEU  | 2.5  |
| 1   | B     | 480 | ARG  | 2.5  |
| 1   | E     | 246 | LYS  | 2.5  |
| 1   | B     | 242 | ASP  | 2.5  |
| 1   | B     | 245 | ILE  | 2.5  |
| 1   | B     | 375 | THR  | 2.5  |
| 2   | D     | 350 | PHE  | 2.5  |
| 2   | D     | 65  | HIS  | 2.5  |
| 2   | C     | 370 | LEU  | 2.5  |
| 1   | E     | 69  | ASN  | 2.5  |
| 2   | D     | 193 | ILE  | 2.5  |
| 1   | E     | 443 | PHE  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 226 | LYS  | 2.5  |
| 1   | A     | 542 | TYR  | 2.5  |
| 2   | F     | 214 | TYR  | 2.5  |
| 2   | D     | 146 | CYS  | 2.5  |
| 1   | B     | 538 | ILE  | 2.5  |
| 1   | A     | 105 | ASN  | 2.5  |
| 1   | A     | 336 | ASN  | 2.5  |
| 2   | C     | 125 | PHE  | 2.5  |
| 2   | C     | 229 | ASN  | 2.5  |
| 1   | A     | 132 | THR  | 2.5  |
| 2   | F     | 28  | ARG  | 2.5  |
| 1   | A     | 109 | TYR  | 2.5  |
| 2   | D     | 322 | VAL  | 2.5  |
| 1   | E     | 397 | ILE  | 2.4  |
| 1   | B     | 479 | GLU  | 2.4  |
| 2   | D     | 95  | PHE  | 2.4  |
| 1   | E     | 403 | THR  | 2.4  |
| 1   | E     | 405 | LEU  | 2.4  |
| 1   | E     | 97  | ILE  | 2.4  |
| 1   | E     | 452 | ILE  | 2.4  |
| 1   | A     | 428 | LYS  | 2.4  |
| 1   | B     | 165 | LEU  | 2.4  |
| 1   | A     | 256 | GLY  | 2.4  |
| 2   | D     | 224 | HIS  | 2.4  |
| 1   | A     | 431 | ALA  | 2.4  |
| 1   | E     | 266 | GLN  | 2.4  |
| 2   | D     | 59  | ILE  | 2.4  |
| 1   | B     | 428 | LYS  | 2.4  |
| 1   | A     | 174 | ARG  | 2.4  |
| 1   | E     | 589 | GLU  | 2.4  |
| 1   | A     | 317 | SER  | 2.4  |
| 1   | B     | 478 | LEU  | 2.4  |
| 1   | E     | 214 | THR  | 2.4  |
| 2   | D     | 307 | TRP  | 2.4  |
| 2   | D     | 324 | VAL  | 2.4  |
| 2   | F     | 233 | VAL  | 2.4  |
| 2   | D     | 55  | ARG  | 2.4  |
| 1   | E     | 280 | PHE  | 2.4  |
| 2   | D     | 24  | PHE  | 2.4  |
| 1   | B     | 283 | LEU  | 2.4  |
| 1   | A     | 283 | LEU  | 2.4  |
| 1   | E     | 501 | GLU  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 551 | LEU  | 2.4  |
| 1   | B     | 361 | THR  | 2.4  |
| 2   | F     | 91  | THR  | 2.4  |
| 1   | E     | 336 | ASN  | 2.4  |
| 1   | E     | 103 | ASP  | 2.4  |
| 1   | E     | 432 | TYR  | 2.4  |
| 2   | F     | 93  | ILE  | 2.4  |
| 2   | F     | 238 | ILE  | 2.4  |
| 1   | A     | 93  | PHE  | 2.4  |
| 2   | C     | 269 | LEU  | 2.4  |
| 2   | D     | 80  | LEU  | 2.4  |
| 2   | F     | 70  | LEU  | 2.4  |
| 1   | E     | 91  | GLY  | 2.3  |
| 2   | C     | 216 | THR  | 2.3  |
| 1   | B     | 290 | TYR  | 2.3  |
| 2   | C     | 37  | TYR  | 2.3  |
| 2   | C     | 260 | ILE  | 2.3  |
| 1   | B     | 274 | GLN  | 2.3  |
| 2   | D     | 128 | PHE  | 2.3  |
| 2   | D     | 254 | PRO  | 2.3  |
| 2   | F     | 89  | SER  | 2.3  |
| 1   | E     | 540 | ASN  | 2.3  |
| 1   | B     | 152 | PHE  | 2.3  |
| 1   | B     | 502 | LEU  | 2.3  |
| 2   | D     | 311 | LEU  | 2.3  |
| 2   | F     | 115 | LEU  | 2.3  |
| 1   | B     | 73  | GLY  | 2.3  |
| 1   | B     | 78  | ILE  | 2.3  |
| 1   | A     | 405 | LEU  | 2.3  |
| 1   | E     | 166 | ASP  | 2.3  |
| 2   | C     | 266 | ASP  | 2.3  |
| 1   | E     | 339 | VAL  | 2.3  |
| 2   | C     | 162 | VAL  | 2.3  |
| 1   | B     | 106 | GLY  | 2.3  |
| 1   | E     | 256 | GLY  | 2.3  |
| 1   | E     | 591 | GLY  | 2.3  |
| 1   | B     | 116 | MET  | 2.3  |
| 1   | B     | 373 | THR  | 2.3  |
| 1   | A     | 558 | MET  | 2.3  |
| 2   | C     | 65  | HIS  | 2.3  |
| 2   | F     | 45  | SER  | 2.3  |
| 1   | B     | 465 | LEU  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 124 | LEU  | 2.3  |
| 2   | F     | 339 | ASN  | 2.3  |
| 1   | A     | 329 | LYS  | 2.3  |
| 1   | E     | 249 | VAL  | 2.3  |
| 2   | C     | 47  | VAL  | 2.3  |
| 1   | B     | 232 | ILE  | 2.3  |
| 1   | A     | 332 | PRO  | 2.3  |
| 1   | A     | 184 | TRP  | 2.3  |
| 1   | E     | 153 | THR  | 2.3  |
| 2   | F     | 36  | LEU  | 2.3  |
| 2   | F     | 123 | SER  | 2.3  |
| 2   | F     | 40  | TYR  | 2.3  |
| 2   | D     | 242 | LYS  | 2.3  |
| 2   | D     | 416 | LYS  | 2.3  |
| 1   | B     | 462 | ILE  | 2.2  |
| 1   | A     | 97  | ILE  | 2.2  |
| 1   | A     | 465 | LEU  | 2.2  |
| 1   | E     | 338 | LEU  | 2.2  |
| 1   | B     | 313 | THR  | 2.2  |
| 1   | E     | 293 | THR  | 2.2  |
| 2   | C     | 187 | PHE  | 2.2  |
| 1   | B     | 469 | LYS  | 2.2  |
| 1   | B     | 304 | VAL  | 2.2  |
| 2   | C     | 233 | VAL  | 2.2  |
| 2   | D     | 232 | ASN  | 2.2  |
| 1   | E     | 330 | ASP  | 2.2  |
| 2   | C     | 82  | ASP  | 2.2  |
| 1   | B     | 71  | ILE  | 2.2  |
| 1   | E     | 119 | ILE  | 2.2  |
| 2   | C     | 238 | ILE  | 2.2  |
| 1   | B     | 155 | GLY  | 2.2  |
| 1   | B     | 391 | GLY  | 2.2  |
| 1   | B     | 526 | LEU  | 2.2  |
| 1   | A     | 427 | LEU  | 2.2  |
| 1   | E     | 128 | LEU  | 2.2  |
| 1   | E     | 342 | LEU  | 2.2  |
| 1   | A     | 469 | LYS  | 2.2  |
| 1   | E     | 490 | PHE  | 2.2  |
| 1   | A     | 60  | SER  | 2.2  |
| 1   | A     | 94  | VAL  | 2.2  |
| 1   | B     | 105 | ASN  | 2.2  |
| 1   | B     | 574 | GLU  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 558 | MET  | 2.2  |
| 1   | A     | 450 | PRO  | 2.2  |
| 2   | F     | 43  | ALA  | 2.2  |
| 1   | A     | 490 | PHE  | 2.2  |
| 2   | C     | 310 | TRP  | 2.2  |
| 1   | B     | 236 | THR  | 2.2  |
| 1   | E     | 531 | SER  | 2.2  |
| 2   | C     | 257 | ASN  | 2.2  |
| 1   | E     | 388 | LEU  | 2.2  |
| 2   | F     | 370 | LEU  | 2.2  |
| 1   | B     | 285 | PRO  | 2.2  |
| 2   | C     | 21  | GLY  | 2.2  |
| 2   | F     | 415 | PRO  | 2.2  |
| 1   | E     | 183 | PHE  | 2.2  |
| 1   | E     | 318 | THR  | 2.2  |
| 1   | E     | 521 | THR  | 2.2  |
| 1   | B     | 258 | SER  | 2.2  |
| 1   | A     | 459 | SER  | 2.2  |
| 1   | A     | 564 | ASP  | 2.2  |
| 1   | E     | 542 | TYR  | 2.1  |
| 1   | A     | 452 | ILE  | 2.1  |
| 1   | E     | 489 | ILE  | 2.1  |
| 1   | A     | 264 | LEU  | 2.1  |
| 1   | B     | 455 | SER  | 2.1  |
| 2   | C     | 90  | MET  | 2.1  |
| 2   | D     | 123 | SER  | 2.1  |
| 1   | E     | 340 | GLU  | 2.1  |
| 2   | D     | 341 | GLU  | 2.1  |
| 1   | B     | 488 | GLY  | 2.1  |
| 1   | A     | 79  | PHE  | 2.1  |
| 1   | E     | 550 | ASP  | 2.1  |
| 1   | B     | 249 | VAL  | 2.1  |
| 1   | A     | 354 | HIS  | 2.1  |
| 2   | F     | 126 | VAL  | 2.1  |
| 1   | E     | 471 | THR  | 2.1  |
| 1   | E     | 102 | ILE  | 2.1  |
| 2   | C     | 40  | TYR  | 2.1  |
| 1   | A     | 87  | LEU  | 2.1  |
| 2   | D     | 7   | LEU  | 2.1  |
| 2   | D     | 99  | LEU  | 2.1  |
| 2   | D     | 72  | MET  | 2.1  |
| 1   | A     | 464 | ALA  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 53  | ARG  | 2.1  |
| 2   | D     | 43  | ALA  | 2.1  |
| 1   | B     | 369 | GLY  | 2.1  |
| 2   | C     | 148 | ASP  | 2.1  |
| 2   | F     | 47  | VAL  | 2.1  |
| 1   | B     | 95  | LEU  | 2.1  |
| 1   | B     | 128 | LEU  | 2.1  |
| 1   | B     | 594 | LEU  | 2.1  |
| 2   | C     | 99  | LEU  | 2.1  |
| 2   | D     | 22  | LEU  | 2.1  |
| 2   | F     | 140 | LEU  | 2.1  |
| 1   | E     | 444 | GLN  | 2.1  |
| 2   | C     | 240 | SER  | 2.1  |
| 2   | D     | 139 | SER  | 2.1  |
| 2   | D     | 96  | VAL  | 2.1  |
| 2   | F     | 154 | VAL  | 2.1  |
| 2   | F     | 340 | VAL  | 2.1  |
| 1   | E     | 263 | LEU  | 2.1  |
| 1   | E     | 301 | ILE  | 2.1  |
| 2   | C     | 248 | LEU  | 2.1  |
| 2   | D     | 86  | LEU  | 2.1  |
| 2   | D     | 129 | ARG  | 2.1  |
| 2   | F     | 63  | THR  | 2.1  |
| 1   | B     | 484 | ALA  | 2.1  |
| 2   | F     | 78  | GLY  | 2.1  |
| 1   | B     | 584 | PRO  | 2.1  |
| 1   | A     | 118 | PHE  | 2.1  |
| 2   | F     | 76  | PHE  | 2.1  |
| 1   | B     | 255 | SER  | 2.1  |
| 1   | A     | 463 | SER  | 2.1  |
| 1   | E     | 422 | SER  | 2.1  |
| 1   | A     | 343 | VAL  | 2.1  |
| 1   | A     | 218 | ASN  | 2.1  |
| 1   | A     | 108 | ILE  | 2.1  |
| 2   | D     | 338 | LEU  | 2.1  |
| 1   | E     | 75  | ASP  | 2.1  |
| 2   | D     | 37  | TYR  | 2.1  |
| 1   | B     | 91  | GLY  | 2.1  |
| 1   | B     | 470 | GLU  | 2.1  |
| 1   | A     | 179 | PHE  | 2.1  |
| 1   | A     | 347 | GLU  | 2.1  |
| 1   | E     | 205 | PHE  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 95  | PHE  | 2.1  |
| 1   | B     | 233 | LYS  | 2.0  |
| 1   | A     | 161 | LYS  | 2.0  |
| 1   | A     | 123 | SER  | 2.0  |
| 1   | A     | 302 | SER  | 2.0  |
| 1   | E     | 71  | ILE  | 2.0  |
| 1   | E     | 310 | LEU  | 2.0  |
| 2   | C     | 97  | ASN  | 2.0  |
| 2   | D     | 180 | ILE  | 2.0  |
| 1   | B     | 530 | HIS  | 2.0  |
| 1   | A     | 568 | TRP  | 2.0  |
| 2   | C     | 72  | MET  | 2.0  |
| 2   | C     | 142 | MET  | 2.0  |
| 1   | E     | 587 | THR  | 2.0  |
| 2   | F     | 81  | ASP  | 2.0  |
| 1   | B     | 256 | GLY  | 2.0  |
| 1   | A     | 210 | PHE  | 2.0  |
| 1   | E     | 286 | GLY  | 2.0  |
| 1   | B     | 355 | GLU  | 2.0  |
| 2   | C     | 144 | LYS  | 2.0  |
| 1   | B     | 135 | LEU  | 2.0  |
| 1   | E     | 235 | LEU  | 2.0  |
| 2   | F     | 86  | LEU  | 2.0  |
| 2   | F     | 331 | LEU  | 2.0  |
| 2   | F     | 68  | SER  | 2.0  |
| 1   | B     | 568 | TRP  | 2.0  |
| 2   | F     | 215 | TRP  | 2.0  |
| 1   | B     | 132 | THR  | 2.0  |
| 1   | B     | 211 | TYR  | 2.0  |
| 1   | A     | 318 | THR  | 2.0  |
| 1   | E     | 335 | TYR  | 2.0  |
| 1   | E     | 373 | THR  | 2.0  |
| 1   | A     | 305 | GLN  | 2.0  |
| 2   | F     | 236 | GLU  | 2.0  |
| 1   | E     | 334 | ARG  | 2.0  |
| 1   | B     | 337 | LEU  | 2.0  |
| 1   | B     | 405 | LEU  | 2.0  |
| 1   | E     | 502 | LEU  | 2.0  |
| 2   | F     | 271 | LEU  | 2.0  |
| 2   | F     | 342 | LEU  | 2.0  |
| 1   | B     | 532 | ILE  | 2.0  |
| 2   | C     | 151 | ILE  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 59  | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.