



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:00 PM UTC

PDB ID : 3HFZ / pdb\_00003hfz  
Title : Crystal structure of Thermus thermophilus Phenylalanyl-tRNA synthetase complexed with m-tyrosine  
Authors : Klipcan, L.; Moor, N.; Kessler, N.; Safro, M.G.  
Deposited on : 2009-05-13  
Resolution : 2.90 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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

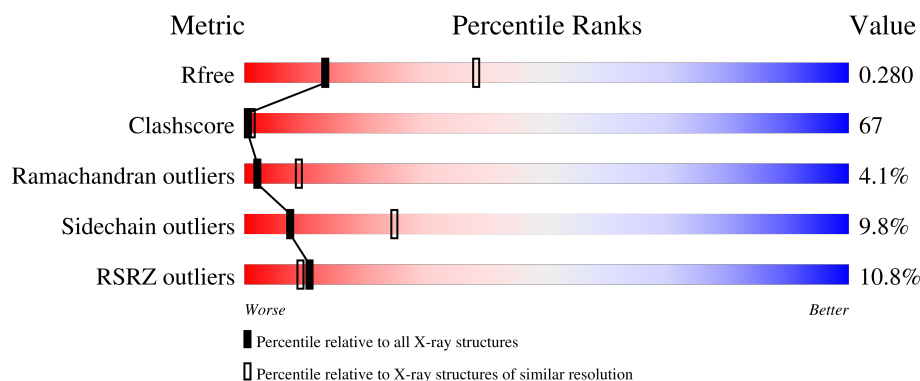
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 350    |                  |
| 2   | B     | 785    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | MTY  | A     | 351 | -         | -        | X       | -                |
| 3   | MTY  | B     | 786 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8517 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.

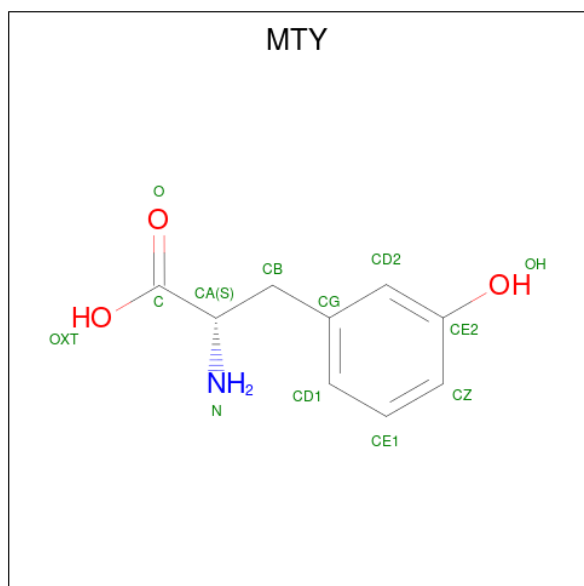
- Molecule 1 is a protein called Phenylalanyl-tRNA synthetase alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 266      | Total | C    | N   | O   | S | 11      | 0       | 0     |
|     |       |          | 2123  | 1388 | 363 | 365 | 7 |         |         |       |

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 785      | Total | C    | N    | O    | S  | 46      | 0       | 0     |
|     |       |          | 6127  | 3925 | 1091 | 1101 | 10 |         |         |       |

- Molecule 3 is META-TYROSINE (CCD ID: MTY) (formula:  $C_9H_{11}NO_3$ ).

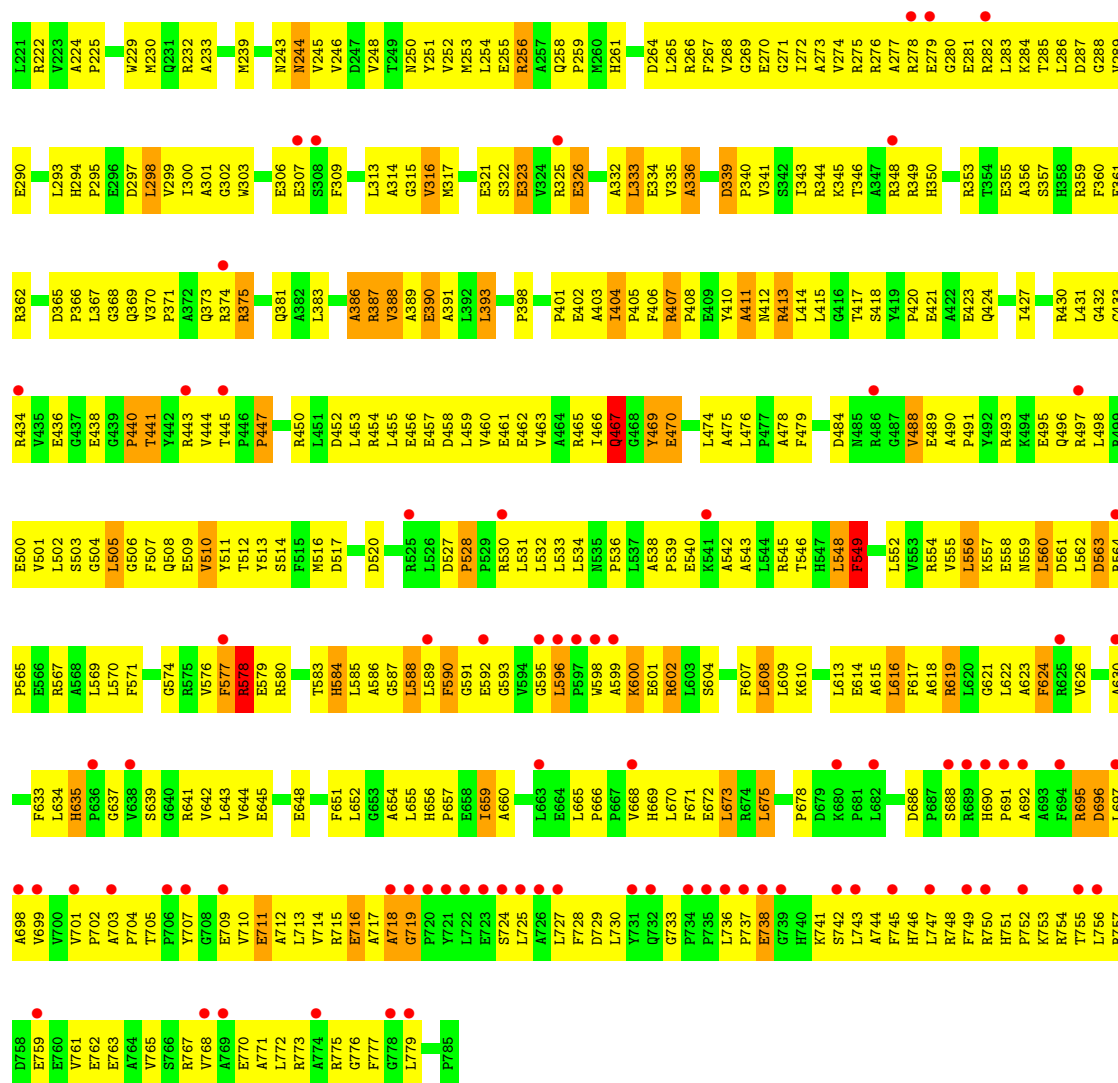


| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 13    | 9 | 1 | 3 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 13    | 9 | 1 | 3 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | A     | 64       | Total<br>64  | O<br>64  | 0       | 0       |
| 4   | B     | 177      | Total<br>177 | O<br>177 | 0       | 0       |





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 32 2 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 173.18Å 173.18Å 138.85Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 47.04 – 2.90<br>47.04 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (47.04-2.90)<br>99.2 (47.04-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.36 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.4.0067                                             | Depositor        |
| R, $R_{free}$                                                           | 0.269 , 0.282<br>0.267 , 0.280                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2688 reflections (5.02%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 69.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.295                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 45.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$ | Xtriage          |
| Estimated twinning fraction                                             | 0.005 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 8517                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 69.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.63         | 2/2191 (0.1%) | 1.06        | 10/2971 (0.3%)  |
| 2   | B     | 0.57         | 0/6280        | 1.07        | 43/8536 (0.5%)  |
| All | All   | 0.58         | 2/8471 (0.0%) | 1.07        | 53/11507 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 198 | VAL  | CA-CB | 6.88 | 1.59        | 1.54     |
| 1   | A     | 223 | VAL  | CA-CB | 5.33 | 1.61        | 1.54     |

All (53) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 387 | ARG  | N-CA-C | -9.31 | 95.18       | 110.17   |
| 2   | B     | 38  | VAL  | N-CA-C | 7.91  | 125.80      | 109.34   |
| 1   | A     | 329 | ILE  | CA-C-N | 7.81  | 127.36      | 118.85   |
| 1   | A     | 329 | ILE  | C-N-CA | 7.81  | 127.36      | 118.85   |
| 2   | B     | 37  | ARG  | N-CA-C | -7.79 | 96.55       | 109.24   |
| 2   | B     | 133 | LEU  | N-CA-C | -7.78 | 99.00       | 110.52   |
| 1   | A     | 151 | THR  | N-CA-C | 7.41  | 120.94      | 110.50   |
| 2   | B     | 463 | VAL  | N-CA-C | -7.06 | 103.89      | 110.53   |
| 2   | B     | 256 | ARG  | N-CA-C | 6.72  | 120.72      | 111.71   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 233 | LEU  | N-CA-C | -6.59 | 104.02      | 111.14   |
| 2   | B     | 549 | PHE  | CA-C-N | -6.32 | 112.49      | 119.19   |
| 2   | B     | 549 | PHE  | C-N-CA | -6.32 | 112.49      | 119.19   |
| 2   | B     | 411 | ALA  | N-CA-C | -6.29 | 103.35      | 111.02   |
| 2   | B     | 596 | LEU  | CA-C-N | 6.26  | 127.66      | 119.84   |
| 2   | B     | 596 | LEU  | C-N-CA | 6.26  | 127.66      | 119.84   |
| 2   | B     | 469 | TYR  | N-CA-C | -6.22 | 104.55      | 111.71   |
| 2   | B     | 467 | GLN  | N-CA-C | -6.18 | 103.86      | 112.45   |
| 2   | B     | 173 | LEU  | N-CA-C | -6.15 | 104.26      | 110.97   |
| 2   | B     | 118 | LEU  | N-CA-C | 6.02  | 118.85      | 109.52   |
| 2   | B     | 180 | LEU  | N-CA-C | -5.89 | 105.35      | 112.54   |
| 2   | B     | 528 | PRO  | N-CA-C | 5.88  | 117.87      | 110.70   |
| 2   | B     | 577 | PHE  | N-CA-C | 5.87  | 118.53      | 109.07   |
| 2   | B     | 453 | LEU  | N-CA-C | 5.84  | 118.97      | 107.98   |
| 2   | B     | 336 | ALA  | N-CA-C | 5.67  | 117.40      | 108.96   |
| 1   | A     | 90  | LEU  | CA-C-N | 5.67  | 125.59      | 119.76   |
| 1   | A     | 90  | LEU  | C-N-CA | 5.67  | 125.59      | 119.76   |
| 2   | B     | 528 | PRO  | CA-C-N | 5.55  | 125.83      | 119.83   |
| 2   | B     | 528 | PRO  | C-N-CA | 5.55  | 125.83      | 119.83   |
| 2   | B     | 332 | ALA  | N-CA-C | -5.52 | 99.42       | 108.41   |
| 2   | B     | 175 | ARG  | N-CA-C | -5.50 | 107.12      | 113.88   |
| 2   | B     | 326 | GLU  | N-CA-C | 5.45  | 117.65      | 111.11   |
| 1   | A     | 175 | LEU  | N-CA-C | -5.41 | 100.47      | 109.46   |
| 2   | B     | 388 | VAL  | N-CA-C | 5.38  | 116.42      | 108.45   |
| 2   | B     | 39  | PHE  | N-CA-C | 5.38  | 121.70      | 109.81   |
| 1   | A     | 89  | SER  | N-CA-C | -5.38 | 106.67      | 113.18   |
| 2   | B     | 56  | ILE  | CA-C-N | 5.34  | 126.51      | 119.84   |
| 2   | B     | 56  | ILE  | C-N-CA | 5.34  | 126.51      | 119.84   |
| 2   | B     | 563 | ASP  | N-CA-C | -5.32 | 101.28      | 109.52   |
| 2   | B     | 66  | LEU  | N-CA-C | 5.28  | 118.66      | 110.17   |
| 2   | B     | 608 | LEU  | N-CA-C | -5.22 | 105.28      | 110.97   |
| 1   | A     | 198 | VAL  | CA-C-O | 5.21  | 122.65      | 119.94   |
| 2   | B     | 406 | PHE  | N-CA-C | 5.17  | 116.81      | 108.34   |
| 1   | A     | 279 | GLU  | N-CA-C | -5.12 | 101.78      | 109.15   |
| 2   | B     | 675 | LEU  | N-CA-C | -5.12 | 103.70      | 110.40   |
| 2   | B     | 117 | ALA  | N-CA-C | -5.11 | 103.65      | 110.55   |
| 2   | B     | 158 | LEU  | N-CA-C | 5.08  | 117.23      | 110.53   |
| 2   | B     | 339 | ASP  | CA-C-N | 5.07  | 126.17      | 119.84   |
| 2   | B     | 339 | ASP  | C-N-CA | 5.07  | 126.17      | 119.84   |
| 2   | B     | 635 | HIS  | N-CA-C | -5.04 | 103.34      | 110.29   |
| 2   | B     | 314 | ALA  | N-CA-C | 5.03  | 117.64      | 110.24   |
| 2   | B     | 546 | THR  | N-CA-C | -5.01 | 107.55      | 113.97   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 2   | B     | 447 | PRO  | N-CA-C | -5.01 | 103.95                 | 111.57              |
| 2   | B     | 60  | ARG  | N-CA-C | -5.00 | 107.02                 | 112.72              |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 186 | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2123  | 0        | 2075     | 308     | 0            |
| 2   | B     | 6127  | 0        | 6180     | 803     | 1            |
| 3   | A     | 13    | 0        | 9        | 8       | 0            |
| 3   | B     | 13    | 0        | 9        | 11      | 0            |
| 4   | A     | 64    | 0        | 0        | 121     | 0            |
| 4   | B     | 177   | 0        | 0        | 256     | 1            |
| All | All   | 8517  | 0        | 8273     | 1096    | 1            |

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 67.

All (1096) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:284:GLY:HA3 | 4:A:391:HOH:O   | 1.16                     | 1.31              |
| 4:A:408:HOH:O   | 2:B:579:GLU:HB3 | 1.18                     | 1.31              |
| 2:B:9:LYS:HE2   | 4:B:951:HOH:O   | 1.22                     | 1.29              |
| 2:B:33:ASP:HB3  | 4:B:843:HOH:O   | 1.18                     | 1.27              |
| 1:A:112:GLU:HG2 | 4:A:377:HOH:O   | 1.15                     | 1.26              |
| 2:B:532:LEU:HA  | 4:B:933:HOH:O   | 1.19                     | 1.26              |
| 2:B:441:THR:HB  | 4:B:838:HOH:O   | 1.23                     | 1.25              |
| 1:A:154:LEU:HB2 | 4:A:414:HOH:O   | 1.34                     | 1.24              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:438:GLU:HB3  | 4:B:831:HOH:O    | 1.30                     | 1.24              |
| 2:B:528:PRO:HD2  | 4:B:892:HOH:O    | 1.35                     | 1.24              |
| 1:A:278:LEU:HB3  | 4:A:376:HOH:O    | 1.07                     | 1.23              |
| 1:A:240:LEU:HA   | 4:A:402:HOH:O    | 1.36                     | 1.23              |
| 2:B:388:VAL:HG12 | 4:B:954:HOH:O    | 1.39                     | 1.22              |
| 2:B:478:ALA:HA   | 4:B:841:HOH:O    | 1.38                     | 1.22              |
| 2:B:637:GLY:HA3  | 4:B:908:HOH:O    | 1.42                     | 1.19              |
| 2:B:643:LEU:HD12 | 4:B:791:HOH:O    | 1.38                     | 1.19              |
| 1:A:140:PRO:HD2  | 4:A:372:HOH:O    | 1.41                     | 1.17              |
| 1:A:254:GLN:HG2  | 4:A:406:HOH:O    | 1.41                     | 1.17              |
| 2:B:401:PRO:HA   | 4:B:803:HOH:O    | 1.45                     | 1.16              |
| 2:B:779:LEU:HG   | 4:B:916:HOH:O    | 1.42                     | 1.16              |
| 2:B:43:ARG:HD3   | 4:B:828:HOH:O    | 1.45                     | 1.15              |
| 1:A:272:PRO:HD2  | 4:A:366:HOH:O    | 1.44                     | 1.15              |
| 2:B:407:ARG:CG   | 4:B:838:HOH:O    | 1.95                     | 1.14              |
| 2:B:656:HIS:HB3  | 2:B:659:ILE:HD13 | 1.21                     | 1.11              |
| 2:B:211:PRO:HD3  | 4:B:879:HOH:O    | 1.51                     | 1.11              |
| 2:B:336:ALA:HB3  | 4:B:844:HOH:O    | 1.50                     | 1.10              |
| 1:A:206:GLU:HB2  | 4:A:398:HOH:O    | 1.46                     | 1.10              |
| 1:A:326:ARG:HD3  | 4:A:379:HOH:O    | 1.49                     | 1.10              |
| 2:B:445:THR:HG23 | 4:B:894:HOH:O    | 1.50                     | 1.10              |
| 2:B:635:HIS:HE1  | 4:B:908:HOH:O    | 1.34                     | 1.10              |
| 2:B:543:ALA:HA   | 4:B:933:HOH:O    | 1.51                     | 1.10              |
| 1:A:237:ILE:HG13 | 4:A:403:HOH:O    | 1.50                     | 1.09              |
| 2:B:95:GLU:HB2   | 4:B:911:HOH:O    | 1.52                     | 1.08              |
| 2:B:286:LEU:HD21 | 2:B:323:GLU:HG3  | 1.12                     | 1.08              |
| 2:B:2:ARG:HD2    | 4:B:794:HOH:O    | 1.54                     | 1.08              |
| 2:B:198:LEU:HD12 | 2:B:393:LEU:HD13 | 1.36                     | 1.08              |
| 2:B:100:GLY:HA2  | 4:B:830:HOH:O    | 1.54                     | 1.07              |
| 2:B:220:GLY:HA3  | 4:B:923:HOH:O    | 1.53                     | 1.07              |
| 2:B:467:GLN:HE21 | 2:B:467:GLN:HA   | 1.20                     | 1.06              |
| 2:B:303:TRP:HB3  | 4:B:922:HOH:O    | 1.56                     | 1.06              |
| 2:B:427:ILE:HG13 | 4:B:952:HOH:O    | 1.53                     | 1.06              |
| 2:B:736:LEU:HA   | 4:B:856:HOH:O    | 1.56                     | 1.05              |
| 1:A:243:ALA:HB3  | 4:A:402:HOH:O    | 1.53                     | 1.05              |
| 2:B:224:ALA:H    | 2:B:244:ASN:ND2  | 1.56                     | 1.04              |
| 2:B:456:GLU:HA   | 4:B:837:HOH:O    | 1.55                     | 1.04              |
| 1:A:237:ILE:HG23 | 4:A:403:HOH:O    | 1.57                     | 1.04              |
| 1:A:135:ASP:HA   | 4:A:397:HOH:O    | 1.58                     | 1.03              |
| 2:B:602:ARG:HH11 | 2:B:602:ARG:HB2  | 1.19                     | 1.03              |
| 1:A:251:VAL:HG23 | 4:A:368:HOH:O    | 1.57                     | 1.03              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:112:ARG:HG2  | 4:B:855:HOH:O    | 1.59                     | 1.02              |
| 2:B:239:MET:HE2  | 2:B:355:GLU:HG3  | 1.38                     | 1.02              |
| 1:A:298:ARG:HG2  | 4:A:362:HOH:O    | 1.58                     | 1.02              |
| 2:B:187:PRO:HG2  | 4:B:948:HOH:O    | 1.59                     | 1.02              |
| 2:B:205:GLU:HG3  | 4:B:812:HOH:O    | 1.60                     | 1.02              |
| 2:B:366:PRO:HD3  | 4:B:795:HOH:O    | 1.58                     | 1.02              |
| 2:B:407:ARG:HG3  | 4:B:838:HOH:O    | 1.53                     | 1.02              |
| 1:A:165:LEU:HD11 | 1:A:303:LEU:HD11 | 1.41                     | 1.01              |
| 2:B:511:TYR:HE1  | 4:B:865:HOH:O    | 1.40                     | 1.01              |
| 2:B:630:ALA:HB2  | 4:B:893:HOH:O    | 1.61                     | 1.00              |
| 1:A:173:LEU:HB3  | 4:A:414:HOH:O    | 1.64                     | 0.98              |
| 1:A:168:GLU:HG2  | 4:A:407:HOH:O    | 1.61                     | 0.98              |
| 2:B:286:LEU:HD21 | 2:B:323:GLU:CG   | 1.94                     | 0.98              |
| 1:A:190:HIS:HE1  | 4:A:355:HOH:O    | 1.44                     | 0.97              |
| 2:B:256:ARG:HD3  | 4:B:873:HOH:O    | 1.66                     | 0.96              |
| 2:B:306:GLU:HG3  | 4:B:941:HOH:O    | 1.66                     | 0.95              |
| 3:A:351:MTY:CB   | 4:A:381:HOH:O    | 2.13                     | 0.95              |
| 2:B:776:GLY:HA3  | 4:B:959:HOH:O    | 1.65                     | 0.95              |
| 2:B:532:LEU:HD23 | 4:B:933:HOH:O    | 1.66                     | 0.94              |
| 1:A:299:GLU:HB3  | 4:A:385:HOH:O    | 1.66                     | 0.94              |
| 2:B:56:ILE:CG1   | 4:B:842:HOH:O    | 2.16                     | 0.94              |
| 2:B:557:LYS:HG2  | 2:B:665:LEU:HD21 | 1.50                     | 0.94              |
| 2:B:199:PRO:HB2  | 4:B:924:HOH:O    | 1.68                     | 0.93              |
| 2:B:759:GLU:HB2  | 4:B:801:HOH:O    | 1.68                     | 0.93              |
| 2:B:775:ARG:HD2  | 4:B:874:HOH:O    | 1.67                     | 0.93              |
| 1:A:248:ASP:CB   | 4:A:399:HOH:O    | 2.17                     | 0.93              |
| 1:A:213:GLU:HG3  | 1:A:332:ILE:HD12 | 1.51                     | 0.93              |
| 2:B:80:ASN:H     | 2:B:80:ASN:HD22  | 1.14                     | 0.92              |
| 2:B:24:ARG:HD3   | 4:B:942:HOH:O    | 1.69                     | 0.92              |
| 2:B:589:LEU:HB2  | 2:B:609:LEU:HD12 | 1.50                     | 0.92              |
| 2:B:717:ALA:HB3  | 4:B:925:HOH:O    | 1.68                     | 0.91              |
| 1:A:279:GLU:CG   | 4:A:401:HOH:O    | 2.17                     | 0.90              |
| 2:B:643:LEU:HB3  | 4:B:791:HOH:O    | 1.69                     | 0.90              |
| 1:A:258:PHE:CE1  | 4:A:381:HOH:O    | 2.23                     | 0.90              |
| 2:B:455:LEU:HD23 | 4:B:961:HOH:O    | 1.70                     | 0.90              |
| 3:A:351:MTY:HD1  | 4:A:381:HOH:O    | 1.71                     | 0.89              |
| 2:B:635:HIS:CE1  | 4:B:908:HOH:O    | 2.13                     | 0.89              |
| 2:B:224:ALA:H    | 2:B:244:ASN:HD22 | 0.92                     | 0.89              |
| 1:A:237:ILE:HA   | 4:A:403:HOH:O    | 1.71                     | 0.88              |
| 3:A:351:MTY:HA   | 4:A:381:HOH:O    | 1.72                     | 0.88              |
| 2:B:763:GLU:HG2  | 4:B:816:HOH:O    | 1.71                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:296:ALA:HA   | 4:A:405:HOH:O    | 1.74                     | 0.88              |
| 2:B:211:PRO:CD   | 4:B:879:HOH:O    | 2.11                     | 0.88              |
| 1:A:190:HIS:CE1  | 4:A:355:HOH:O    | 2.22                     | 0.88              |
| 2:B:602:ARG:HB2  | 2:B:602:ARG:NH1  | 1.87                     | 0.88              |
| 2:B:527:ASP:HB3  | 4:B:892:HOH:O    | 1.74                     | 0.88              |
| 1:A:173:LEU:CB   | 4:A:414:HOH:O    | 2.19                     | 0.87              |
| 1:A:271:TRP:HA   | 4:A:366:HOH:O    | 1.74                     | 0.87              |
| 1:A:229:ALA:CB   | 4:B:869:HOH:O    | 2.23                     | 0.87              |
| 1:A:229:ALA:HB2  | 4:B:869:HOH:O    | 1.74                     | 0.87              |
| 1:A:98:GLY:HA2   | 4:B:958:HOH:O    | 1.73                     | 0.87              |
| 1:A:160:ARG:CZ   | 4:A:408:HOH:O    | 2.21                     | 0.87              |
| 1:A:155:THR:HB   | 2:B:534:LEU:HD21 | 1.56                     | 0.86              |
| 2:B:350:HIS:HD2  | 4:B:891:HOH:O    | 1.57                     | 0.86              |
| 1:A:237:ILE:CB   | 4:A:403:HOH:O    | 2.23                     | 0.86              |
| 2:B:642:VAL:C    | 2:B:643:LEU:HD22 | 2.01                     | 0.86              |
| 2:B:776:GLY:CA   | 4:B:959:HOH:O    | 2.19                     | 0.86              |
| 1:A:272:PRO:CD   | 4:A:366:HOH:O    | 2.10                     | 0.85              |
| 1:A:161:LEU:HD23 | 1:A:169:VAL:HG13 | 1.57                     | 0.85              |
| 1:A:321:ARG:HG2  | 4:A:380:HOH:O    | 1.75                     | 0.85              |
| 2:B:274:VAL:HG12 | 2:B:298:LEU:HD11 | 1.58                     | 0.85              |
| 2:B:600:LYS:HE2  | 4:B:860:HOH:O    | 1.74                     | 0.85              |
| 1:A:298:ARG:CG   | 4:A:362:HOH:O    | 2.19                     | 0.85              |
| 1:A:142:HIS:HE1  | 4:A:361:HOH:O    | 1.60                     | 0.85              |
| 3:A:351:MTY:CA   | 4:A:381:HOH:O    | 2.22                     | 0.84              |
| 2:B:55:PRO:HG2   | 4:B:937:HOH:O    | 1.76                     | 0.84              |
| 2:B:457:GLU:OE1  | 2:B:457:GLU:N    | 2.09                     | 0.84              |
| 2:B:759:GLU:CB   | 4:B:801:HOH:O    | 2.22                     | 0.84              |
| 2:B:707:TYR:OH   | 2:B:711:GLU:HG3  | 1.76                     | 0.84              |
| 3:A:351:MTY:HB2  | 4:A:381:HOH:O    | 1.77                     | 0.83              |
| 2:B:222:ARG:HG3  | 4:B:962:HOH:O    | 1.76                     | 0.83              |
| 2:B:578:ARG:HB3  | 4:B:870:HOH:O    | 1.76                     | 0.83              |
| 1:A:121:ALA:N    | 4:A:378:HOH:O    | 2.11                     | 0.83              |
| 2:B:1:MET:CE     | 4:B:834:HOH:O    | 2.25                     | 0.82              |
| 2:B:193:ALA:HB2  | 4:B:957:HOH:O    | 1.78                     | 0.82              |
| 1:A:261:VAL:HB   | 4:A:391:HOH:O    | 1.76                     | 0.82              |
| 2:B:56:ILE:HG13  | 4:B:842:HOH:O    | 1.77                     | 0.82              |
| 2:B:153:GLU:HB2  | 4:B:909:HOH:O    | 1.78                     | 0.82              |
| 1:A:154:LEU:HD12 | 4:A:414:HOH:O    | 1.80                     | 0.82              |
| 2:B:203:LYS:HG2  | 4:B:812:HOH:O    | 1.79                     | 0.82              |
| 1:A:194:PHE:HB2  | 4:A:363:HOH:O    | 1.79                     | 0.81              |
| 2:B:279:GLU:HB3  | 4:B:931:HOH:O    | 1.79                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:666:PRO:HD3  | 4:B:935:HOH:O    | 1.79                     | 0.81              |
| 2:B:325:ARG:HH11 | 2:B:325:ARG:HB2  | 1.45                     | 0.81              |
| 2:B:62:LYS:HD3   | 4:B:857:HOH:O    | 1.78                     | 0.81              |
| 1:A:279:GLU:HG3  | 4:A:401:HOH:O    | 1.78                     | 0.81              |
| 2:B:265:LEU:HD23 | 2:B:268:VAL:HG21 | 1.63                     | 0.81              |
| 2:B:224:ALA:N    | 2:B:244:ASN:ND2  | 2.29                     | 0.81              |
| 2:B:727:LEU:HB3  | 4:B:905:HOH:O    | 1.81                     | 0.81              |
| 2:B:28:LEU:HD13  | 2:B:176:ASP:HB3  | 1.63                     | 0.80              |
| 2:B:101:GLN:HB3  | 4:B:929:HOH:O    | 1.81                     | 0.80              |
| 2:B:695:ARG:HB3  | 2:B:747:LEU:HB2  | 1.64                     | 0.80              |
| 1:A:94:SER:CA    | 4:A:404:HOH:O    | 2.30                     | 0.80              |
| 1:A:324:MET:HA   | 1:A:329:ILE:HG13 | 1.63                     | 0.80              |
| 2:B:511:TYR:CE1  | 4:B:865:HOH:O    | 2.24                     | 0.79              |
| 2:B:193:ALA:CB   | 4:B:957:HOH:O    | 2.30                     | 0.79              |
| 2:B:718:ALA:HA   | 2:B:768:VAL:HG21 | 1.65                     | 0.79              |
| 3:B:786:MTY:CD2  | 4:B:876:HOH:O    | 2.29                     | 0.79              |
| 1:A:331:ASP:HB3  | 1:A:334:TYR:CE2  | 2.16                     | 0.79              |
| 2:B:224:ALA:N    | 2:B:244:ASN:HD22 | 1.76                     | 0.78              |
| 2:B:323:GLU:HG3  | 4:B:792:HOH:O    | 1.82                     | 0.78              |
| 3:A:351:MTY:CD1  | 4:A:381:HOH:O    | 2.30                     | 0.78              |
| 2:B:282:ARG:HH11 | 2:B:282:ARG:HB3  | 1.46                     | 0.78              |
| 2:B:516:MET:HE3  | 4:B:912:HOH:O    | 1.83                     | 0.78              |
| 2:B:737:PRO:HD3  | 4:B:856:HOH:O    | 1.83                     | 0.78              |
| 1:A:349:VAL:HG12 | 1:A:350:LEU:HD23 | 1.67                     | 0.77              |
| 2:B:691:PRO:HA   | 4:B:913:HOH:O    | 1.84                     | 0.77              |
| 1:A:86:VAL:CG1   | 4:A:384:HOH:O    | 2.32                     | 0.77              |
| 2:B:490:ALA:HB3  | 2:B:491:PRO:HD3  | 1.67                     | 0.77              |
| 2:B:600:LYS:CE   | 4:B:860:HOH:O    | 2.32                     | 0.77              |
| 2:B:350:HIS:CD2  | 4:B:891:HOH:O    | 2.34                     | 0.77              |
| 2:B:306:GLU:CB   | 4:B:941:HOH:O    | 2.32                     | 0.77              |
| 2:B:567:ARG:HA   | 2:B:591:GLY:HA3  | 1.67                     | 0.77              |
| 1:A:237:ILE:CG2  | 4:A:403:HOH:O    | 2.20                     | 0.76              |
| 2:B:190:ALA:CB   | 4:B:852:HOH:O    | 2.33                     | 0.76              |
| 1:A:264:GLY:HA2  | 4:A:391:HOH:O    | 1.84                     | 0.76              |
| 2:B:666:PRO:HG3  | 4:B:935:HOH:O    | 1.84                     | 0.76              |
| 2:B:80:ASN:HD22  | 2:B:80:ASN:N     | 1.84                     | 0.76              |
| 2:B:389:ALA:C    | 4:B:954:HOH:O    | 2.28                     | 0.76              |
| 1:A:119:TYR:CE1  | 4:A:373:HOH:O    | 2.38                     | 0.76              |
| 2:B:54:HIS:CD2   | 4:B:817:HOH:O    | 2.37                     | 0.76              |
| 2:B:656:HIS:CB   | 2:B:659:ILE:HD13 | 2.10                     | 0.75              |
| 1:A:115:ARG:HG2  | 1:A:115:ARG:HH11 | 1.50                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:290:VAL:O    | 1:A:294:VAL:HG23 | 1.85                     | 0.75              |
| 2:B:457:GLU:O    | 2:B:460:VAL:HG22 | 1.86                     | 0.75              |
| 2:B:775:ARG:HA   | 4:B:874:HOH:O    | 1.86                     | 0.75              |
| 1:A:349:VAL:CG1  | 4:A:409:HOH:O    | 2.35                     | 0.75              |
| 2:B:666:PRO:CG   | 4:B:935:HOH:O    | 2.34                     | 0.75              |
| 2:B:746:HIS:HE1  | 4:B:900:HOH:O    | 1.69                     | 0.75              |
| 2:B:158:LEU:HD22 | 2:B:159:GLU:H    | 1.52                     | 0.74              |
| 2:B:567:ARG:HD2  | 4:B:940:HOH:O    | 1.86                     | 0.74              |
| 2:B:55:PRO:CG    | 4:B:937:HOH:O    | 2.30                     | 0.74              |
| 2:B:317:MET:HA   | 3:B:786:MTY:N    | 2.02                     | 0.74              |
| 2:B:497:ARG:O    | 2:B:501:VAL:HG23 | 1.88                     | 0.74              |
| 2:B:516:MET:CE   | 4:B:912:HOH:O    | 2.33                     | 0.74              |
| 1:A:86:VAL:HG12  | 4:A:384:HOH:O    | 1.87                     | 0.74              |
| 2:B:99:LEU:HD12  | 2:B:101:GLN:H    | 1.52                     | 0.74              |
| 2:B:178:HIS:HE1  | 4:B:895:HOH:O    | 1.71                     | 0.74              |
| 2:B:729:ASP:H    | 2:B:744:ALA:HB3  | 1.50                     | 0.74              |
| 1:A:267:PHE:CE1  | 1:A:280:LEU:HB3  | 2.23                     | 0.74              |
| 2:B:70:ARG:HD2   | 4:B:943:HOH:O    | 1.87                     | 0.74              |
| 2:B:467:GLN:HA   | 2:B:467:GLN:NE2  | 2.01                     | 0.74              |
| 2:B:516:MET:HE3  | 2:B:545:ARG:HA   | 1.70                     | 0.73              |
| 1:A:195:ARG:HG2  | 1:A:223:VAL:HG13 | 1.70                     | 0.73              |
| 2:B:265:LEU:HA   | 2:B:268:VAL:HG23 | 1.68                     | 0.73              |
| 2:B:709:GLU:HA   | 4:B:956:HOH:O    | 1.87                     | 0.73              |
| 2:B:205:GLU:CG   | 4:B:812:HOH:O    | 2.24                     | 0.73              |
| 2:B:341:VAL:HG13 | 4:B:862:HOH:O    | 1.86                     | 0.73              |
| 2:B:307:GLU:HG2  | 4:B:938:HOH:O    | 1.89                     | 0.73              |
| 2:B:552:LEU:O    | 2:B:555:VAL:HG22 | 1.88                     | 0.73              |
| 2:B:730:LEU:HD13 | 2:B:743:LEU:CD2  | 2.18                     | 0.73              |
| 1:A:350:LEU:CD2  | 4:A:409:HOH:O    | 2.35                     | 0.73              |
| 2:B:261:HIS:HD2  | 3:B:786:MTY:HA   | 1.54                     | 0.73              |
| 2:B:282:ARG:HH12 | 2:B:290:GLU:HG3  | 1.53                     | 0.72              |
| 2:B:62:LYS:CD    | 4:B:857:HOH:O    | 2.35                     | 0.72              |
| 2:B:757:ARG:CG   | 4:B:848:HOH:O    | 2.36                     | 0.72              |
| 1:A:301:LEU:HB3  | 4:A:411:HOH:O    | 1.88                     | 0.72              |
| 2:B:193:ALA:HA   | 4:B:957:HOH:O    | 1.89                     | 0.72              |
| 1:A:279:GLU:HG2  | 4:A:401:HOH:O    | 1.86                     | 0.72              |
| 4:A:408:HOH:O    | 2:B:579:GLU:CB   | 1.94                     | 0.72              |
| 2:B:401:PRO:CA   | 4:B:803:HOH:O    | 2.16                     | 0.72              |
| 2:B:695:ARG:HH11 | 2:B:761:VAL:HG11 | 1.53                     | 0.72              |
| 2:B:159:GLU:HB3  | 4:B:811:HOH:O    | 1.88                     | 0.72              |
| 1:A:239:GLU:O    | 4:A:402:HOH:O    | 2.07                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:282:ARG:HB3  | 2:B:282:ARG:NH1  | 2.04                     | 0.72              |
| 1:A:265:ALA:HB2  | 2:B:469:TYR:HE2  | 1.55                     | 0.72              |
| 2:B:589:LEU:HG   | 2:B:590:PHE:H    | 1.54                     | 0.72              |
| 2:B:604:SER:HA   | 2:B:608:LEU:HD22 | 1.72                     | 0.72              |
| 1:A:142:HIS:CE1  | 4:A:361:HOH:O    | 2.37                     | 0.71              |
| 1:A:242:GLN:OE1  | 1:A:247:PRO:HA   | 1.90                     | 0.71              |
| 2:B:698:ALA:HA   | 2:B:743:LEU:O    | 1.89                     | 0.71              |
| 2:B:578:ARG:CB   | 4:B:870:HOH:O    | 2.35                     | 0.71              |
| 2:B:699:VAL:HG13 | 2:B:772:LEU:HD21 | 1.71                     | 0.71              |
| 1:A:128:GLU:OE2  | 1:A:132:PHE:HB2  | 1.89                     | 0.71              |
| 2:B:730:LEU:HD13 | 2:B:743:LEU:HD23 | 1.70                     | 0.71              |
| 2:B:44:GLY:HA3   | 2:B:94:THR:OG1   | 1.91                     | 0.70              |
| 2:B:176:ASP:OD2  | 2:B:465:ARG:NH2  | 2.24                     | 0.70              |
| 2:B:190:ALA:HB2  | 4:B:852:HOH:O    | 1.91                     | 0.70              |
| 1:A:334:TYR:HA   | 4:A:364:HOH:O    | 1.90                     | 0.70              |
| 2:B:596:LEU:HB2  | 2:B:599:ALA:HB3  | 1.72                     | 0.70              |
| 2:B:757:ARG:HG3  | 4:B:848:HOH:O    | 1.89                     | 0.70              |
| 2:B:176:ASP:CG   | 2:B:465:ARG:HH22 | 1.98                     | 0.70              |
| 2:B:757:ARG:HD2  | 4:B:827:HOH:O    | 1.90                     | 0.70              |
| 2:B:193:ALA:CA   | 4:B:957:HOH:O    | 2.38                     | 0.70              |
| 2:B:38:VAL:O     | 2:B:40:PRO:HD2   | 1.91                     | 0.70              |
| 2:B:564:ARG:HD2  | 2:B:564:ARG:N    | 2.06                     | 0.70              |
| 2:B:701:VAL:CG1  | 2:B:705:THR:HB   | 2.21                     | 0.70              |
| 2:B:70:ARG:CD    | 4:B:943:HOH:O    | 2.40                     | 0.70              |
| 2:B:696:ASP:OD1  | 2:B:746:HIS:HD2  | 1.75                     | 0.70              |
| 1:A:261:VAL:CG2  | 4:A:391:HOH:O    | 2.38                     | 0.69              |
| 2:B:90:ALA:HB2   | 2:B:118:LEU:HD11 | 1.72                     | 0.69              |
| 2:B:737:PRO:CD   | 4:B:856:HOH:O    | 2.40                     | 0.69              |
| 2:B:336:ALA:CB   | 4:B:844:HOH:O    | 2.22                     | 0.69              |
| 2:B:434:ARG:HH12 | 2:B:436:GLU:CD   | 2.01                     | 0.69              |
| 2:B:542:ALA:O    | 4:B:933:HOH:O    | 2.09                     | 0.69              |
| 1:A:237:ILE:CA   | 4:A:403:HOH:O    | 2.31                     | 0.69              |
| 2:B:770:GLU:HB3  | 4:B:822:HOH:O    | 1.92                     | 0.69              |
| 1:A:198:VAL:HG13 | 1:A:220:GLU:HB2  | 1.74                     | 0.69              |
| 1:A:287:HIS:ND1  | 1:A:288:PRO:HD2  | 2.08                     | 0.69              |
| 1:A:326:ARG:CD   | 4:A:379:HOH:O    | 2.20                     | 0.69              |
| 2:B:761:VAL:O    | 2:B:765:VAL:HG13 | 1.92                     | 0.69              |
| 2:B:153:GLU:CD   | 4:B:909:HOH:O    | 2.36                     | 0.68              |
| 2:B:279:GLU:CB   | 4:B:931:HOH:O    | 2.40                     | 0.68              |
| 1:A:340:LEU:HD21 | 2:B:570:LEU:HD21 | 1.75                     | 0.68              |
| 2:B:210:ALA:N    | 4:B:879:HOH:O    | 2.26                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:718:ALA:HA   | 2:B:768:VAL:CG2  | 2.22                     | 0.68              |
| 1:A:254:GLN:O    | 1:A:265:ALA:HB1  | 1.93                     | 0.68              |
| 2:B:725:LEU:HD21 | 2:B:745:PHE:HE1  | 1.57                     | 0.68              |
| 1:A:94:SER:HA    | 4:A:404:HOH:O    | 1.90                     | 0.68              |
| 1:A:165:LEU:CD1  | 1:A:303:LEU:HD11 | 2.21                     | 0.68              |
| 2:B:512:THR:CG2  | 4:B:820:HOH:O    | 2.41                     | 0.68              |
| 2:B:514:SER:HA   | 2:B:545:ARG:HD3  | 1.73                     | 0.68              |
| 2:B:695:ARG:HH11 | 2:B:761:VAL:CG1  | 2.05                     | 0.68              |
| 3:B:786:MTY:CG   | 4:B:876:HOH:O    | 2.41                     | 0.68              |
| 2:B:666:PRO:CD   | 4:B:935:HOH:O    | 2.36                     | 0.68              |
| 2:B:408:PRO:HD2  | 4:B:901:HOH:O    | 1.93                     | 0.68              |
| 1:A:254:GLN:CG   | 4:A:406:HOH:O    | 2.14                     | 0.67              |
| 2:B:33:ASP:O     | 2:B:34:ARG:HB3   | 1.94                     | 0.67              |
| 2:B:209:GLY:C    | 4:B:879:HOH:O    | 2.37                     | 0.67              |
| 2:B:82:ARG:HH22  | 2:B:134:GLU:CD   | 2.03                     | 0.67              |
| 2:B:583:THR:HG22 | 2:B:675:LEU:HD12 | 1.77                     | 0.67              |
| 2:B:270:GLU:HG3  | 4:B:799:HOH:O    | 1.94                     | 0.67              |
| 2:B:279:GLU:CA   | 4:B:931:HOH:O    | 2.42                     | 0.67              |
| 2:B:341:VAL:HG12 | 2:B:345:LYS:HE3  | 1.75                     | 0.67              |
| 2:B:52:GLU:HG3   | 2:B:54:HIS:CE1   | 2.29                     | 0.67              |
| 1:A:120:GLN:HG2  | 2:B:489:GLU:HB3  | 1.74                     | 0.67              |
| 2:B:153:GLU:CG   | 4:B:909:HOH:O    | 2.41                     | 0.67              |
| 2:B:253:MET:HE1  | 2:B:355:GLU:C    | 2.18                     | 0.67              |
| 2:B:407:ARG:HG2  | 4:B:838:HOH:O    | 1.73                     | 0.67              |
| 1:A:263:PRO:HG3  | 2:B:461:GLU:HB2  | 1.76                     | 0.67              |
| 1:A:332:ILE:HD13 | 1:A:335:PHE:HD2  | 1.58                     | 0.67              |
| 1:A:204:ARG:NH2  | 4:A:394:HOH:O    | 2.21                     | 0.67              |
| 1:A:260:PHE:N    | 1:A:260:PHE:CD1  | 2.63                     | 0.67              |
| 1:A:320:GLU:HG2  | 1:A:332:ILE:HD11 | 1.76                     | 0.67              |
| 2:B:607:PHE:HA   | 2:B:610:LYS:HB3  | 1.76                     | 0.67              |
| 1:A:161:LEU:CD2  | 1:A:169:VAL:HG13 | 2.25                     | 0.66              |
| 1:A:99:GLY:HA3   | 4:B:829:HOH:O    | 1.93                     | 0.66              |
| 2:B:287:ASP:H    | 2:B:317:MET:CE   | 2.08                     | 0.66              |
| 2:B:701:VAL:HG22 | 2:B:777:PHE:CD1  | 2.30                     | 0.66              |
| 2:B:198:LEU:HD12 | 2:B:393:LEU:CD1  | 2.22                     | 0.66              |
| 1:A:180:SER:O    | 1:A:183:GLN:HB3  | 1.95                     | 0.66              |
| 2:B:751:HIS:HB3  | 2:B:754:ARG:O    | 1.94                     | 0.66              |
| 2:B:62:LYS:CE    | 4:B:857:HOH:O    | 2.42                     | 0.66              |
| 2:B:713:LEU:HD23 | 4:B:836:HOH:O    | 1.95                     | 0.66              |
| 1:A:307:TYR:CD1  | 1:A:307:TYR:N    | 2.63                     | 0.66              |
| 2:B:120:PRO:HG3  | 2:B:133:LEU:HD13 | 1.78                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:701:VAL:HG22 | 2:B:777:PHE:CE1  | 2.31                     | 0.65              |
| 2:B:389:ALA:O    | 4:B:954:HOH:O    | 2.15                     | 0.65              |
| 2:B:589:LEU:CG   | 2:B:590:PHE:H    | 2.07                     | 0.65              |
| 1:A:251:VAL:CG2  | 4:A:368:HOH:O    | 2.30                     | 0.65              |
| 2:B:299:VAL:HG12 | 2:B:300:ILE:N    | 2.10                     | 0.65              |
| 2:B:712:ALA:O    | 2:B:716:GLU:HB2  | 1.96                     | 0.65              |
| 2:B:37:ARG:HH11  | 2:B:37:ARG:HB3   | 1.61                     | 0.65              |
| 2:B:610:LYS:O    | 2:B:614:GLU:HG3  | 1.97                     | 0.65              |
| 2:B:643:LEU:CB   | 4:B:791:HOH:O    | 2.36                     | 0.65              |
| 2:B:749:PHE:CE2  | 4:B:906:HOH:O    | 2.49                     | 0.65              |
| 1:A:229:ALA:N    | 1:A:232:HIS:HD2  | 1.95                     | 0.65              |
| 2:B:203:LYS:HE3  | 4:B:812:HOH:O    | 1.96                     | 0.65              |
| 2:B:220:GLY:CA   | 4:B:923:HOH:O    | 2.25                     | 0.65              |
| 2:B:467:GLN:HG2  | 4:B:952:HOH:O    | 1.96                     | 0.65              |
| 2:B:570:LEU:HD12 | 2:B:588:LEU:HD21 | 1.79                     | 0.65              |
| 2:B:688:SER:HB2  | 2:B:752:PRO:HA   | 1.78                     | 0.65              |
| 2:B:771:ALA:CB   | 4:B:839:HOH:O    | 2.44                     | 0.65              |
| 2:B:141:PRO:HD2  | 2:B:144:THR:HG21 | 1.79                     | 0.65              |
| 2:B:563:ASP:C    | 2:B:565:PRO:HD3  | 2.20                     | 0.65              |
| 1:A:128:GLU:O    | 1:A:174:LEU:HD12 | 1.97                     | 0.65              |
| 1:A:258:PHE:CZ   | 4:A:381:HOH:O    | 2.48                     | 0.65              |
| 2:B:14:GLU:HB2   | 4:B:789:HOH:O    | 1.95                     | 0.65              |
| 1:A:164:PRO:HG2  | 1:A:188:VAL:HG21 | 1.78                     | 0.65              |
| 1:A:340:LEU:C    | 1:A:342:PHE:H    | 2.03                     | 0.65              |
| 1:A:334:TYR:HD1  | 4:A:364:HOH:O    | 1.80                     | 0.64              |
| 2:B:776:GLY:C    | 4:B:959:HOH:O    | 2.39                     | 0.64              |
| 1:A:86:VAL:C     | 4:A:384:HOH:O    | 2.40                     | 0.64              |
| 2:B:341:VAL:CG1  | 2:B:345:LYS:HE3  | 2.26                     | 0.64              |
| 2:B:283:LEU:HD23 | 2:B:284:LYS:N    | 2.12                     | 0.64              |
| 1:A:267:PHE:HE1  | 1:A:280:LEU:HB3  | 1.63                     | 0.64              |
| 2:B:37:ARG:HB3   | 2:B:37:ARG:NH1   | 2.13                     | 0.64              |
| 2:B:549:PHE:CD1  | 2:B:549:PHE:C    | 2.75                     | 0.64              |
| 2:B:222:ARG:CG   | 4:B:962:HOH:O    | 2.38                     | 0.64              |
| 2:B:253:MET:HE2  | 2:B:359:ARG:HD2  | 1.78                     | 0.64              |
| 2:B:341:VAL:CG1  | 4:B:862:HOH:O    | 2.41                     | 0.64              |
| 1:A:155:THR:HG23 | 1:A:155:THR:O    | 1.98                     | 0.64              |
| 2:B:80:ASN:H     | 2:B:80:ASN:ND2   | 1.91                     | 0.64              |
| 1:A:319:VAL:O    | 1:A:321:ARG:N    | 2.30                     | 0.64              |
| 1:A:350:LEU:HD23 | 4:A:409:HOH:O    | 1.94                     | 0.64              |
| 2:B:727:LEU:HA   | 2:B:744:ALA:O    | 1.98                     | 0.64              |
| 1:A:209:ASP:O    | 1:A:333:ARG:HG3  | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:333:LEU:CD2  | 4:B:915:HOH:O    | 2.45                     | 0.64              |
| 2:B:210:ALA:CA   | 4:B:879:HOH:O    | 2.46                     | 0.64              |
| 2:B:210:ALA:HA   | 4:B:879:HOH:O    | 1.96                     | 0.64              |
| 2:B:585:LEU:O    | 2:B:673:LEU:HD12 | 1.98                     | 0.64              |
| 2:B:643:LEU:CD1  | 4:B:791:HOH:O    | 2.14                     | 0.64              |
| 1:A:119:TYR:HE1  | 4:A:373:HOH:O    | 1.77                     | 0.63              |
| 2:B:95:GLU:N     | 4:B:911:HOH:O    | 2.28                     | 0.63              |
| 2:B:669:HIS:HD2  | 4:B:823:HOH:O    | 1.81                     | 0.63              |
| 2:B:717:ALA:CB   | 4:B:925:HOH:O    | 2.38                     | 0.63              |
| 1:A:165:LEU:HD11 | 1:A:303:LEU:CD1  | 2.22                     | 0.63              |
| 2:B:256:ARG:NH2  | 4:B:948:HOH:O    | 2.31                     | 0.63              |
| 1:A:220:GLU:OE2  | 3:A:351:MTY:HD2  | 1.98                     | 0.63              |
| 2:B:256:ARG:NH2  | 2:B:375:ARG:HG3  | 2.12                     | 0.63              |
| 2:B:686:ASP:CB   | 4:B:953:HOH:O    | 2.45                     | 0.63              |
| 2:B:713:LEU:O    | 4:B:925:HOH:O    | 2.15                     | 0.63              |
| 2:B:754:ARG:NH2  | 4:B:854:HOH:O    | 2.29                     | 0.63              |
| 1:A:98:GLY:HA3   | 2:B:503:SER:O    | 1.98                     | 0.63              |
| 1:A:148:MET:HE1  | 1:A:257:TYR:HD2  | 1.63                     | 0.63              |
| 1:A:155:THR:CB   | 2:B:534:LEU:HD21 | 2.29                     | 0.63              |
| 2:B:49:ARG:HH21  | 2:B:51:LEU:CD2   | 2.10                     | 0.63              |
| 2:B:666:PRO:O    | 2:B:668:VAL:HG23 | 1.98                     | 0.63              |
| 2:B:35:ILE:N     | 2:B:35:ILE:HD12  | 2.13                     | 0.63              |
| 2:B:548:LEU:HD22 | 2:B:584:HIS:HB3  | 1.79                     | 0.63              |
| 2:B:595:GLY:HA3  | 4:B:904:HOH:O    | 1.99                     | 0.63              |
| 2:B:771:ALA:N    | 4:B:822:HOH:O    | 2.31                     | 0.63              |
| 1:A:87:ASP:OD1   | 1:A:88:VAL:N     | 2.32                     | 0.63              |
| 1:A:327:TYR:HE1  | 4:A:379:HOH:O    | 1.81                     | 0.63              |
| 2:B:36:GLU:O     | 2:B:154:VAL:HA   | 1.97                     | 0.63              |
| 2:B:207:PRO:HD2  | 4:B:853:HOH:O    | 1.98                     | 0.63              |
| 2:B:297:ASP:OD2  | 2:B:350:HIS:HE1  | 1.82                     | 0.63              |
| 2:B:536:PRO:HB3  | 2:B:542:ALA:HA   | 1.81                     | 0.63              |
| 2:B:121:ARG:HG3  | 2:B:121:ARG:HH11 | 1.62                     | 0.62              |
| 2:B:160:VAL:CG1  | 2:B:167:ALA:HB3  | 2.29                     | 0.62              |
| 2:B:434:ARG:HH12 | 2:B:436:GLU:CG   | 2.12                     | 0.62              |
| 2:B:635:HIS:O    | 2:B:639:SER:HB2  | 1.99                     | 0.62              |
| 1:A:161:LEU:HD23 | 1:A:169:VAL:CG1  | 2.29                     | 0.62              |
| 1:A:161:LEU:HD23 | 1:A:161:LEU:O    | 1.99                     | 0.62              |
| 2:B:729:ASP:N    | 2:B:744:ALA:HB3  | 2.13                     | 0.62              |
| 1:A:229:ALA:H    | 1:A:232:HIS:HD2  | 1.47                     | 0.62              |
| 2:B:747:LEU:O    | 2:B:748:ARG:HG3  | 1.99                     | 0.62              |
| 2:B:253:MET:HE1  | 2:B:355:GLU:CB   | 2.30                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:182:MET:HE3  | 1:A:182:MET:O    | 1.99                     | 0.62              |
| 1:A:202:VAL:HG22 | 1:A:216:PHE:O    | 1.99                     | 0.62              |
| 2:B:512:THR:HG21 | 4:B:820:HOH:O    | 1.98                     | 0.62              |
| 2:B:751:HIS:HB2  | 2:B:756:LEU:HD21 | 1.80                     | 0.62              |
| 2:B:325:ARG:HB2  | 2:B:325:ARG:NH1  | 2.14                     | 0.62              |
| 2:B:589:LEU:HD22 | 2:B:609:LEU:HB2  | 1.80                     | 0.62              |
| 2:B:701:VAL:HG11 | 2:B:705:THR:HB   | 1.82                     | 0.62              |
| 2:B:336:ALA:HA   | 2:B:369:GLN:HG2  | 1.81                     | 0.62              |
| 2:B:507:PHE:CD2  | 2:B:569:LEU:HG   | 2.34                     | 0.61              |
| 2:B:248:VAL:O    | 2:B:252:VAL:HG23 | 2.00                     | 0.61              |
| 2:B:346:THR:O    | 2:B:349:ARG:HB3  | 2.00                     | 0.61              |
| 1:A:246:GLY:HA3  | 4:A:353:HOH:O    | 2.00                     | 0.61              |
| 2:B:306:GLU:CG   | 4:B:941:HOH:O    | 2.30                     | 0.61              |
| 2:B:158:LEU:CD2  | 2:B:159:GLU:H    | 2.14                     | 0.61              |
| 2:B:198:LEU:CD1  | 2:B:393:LEU:HD13 | 2.24                     | 0.61              |
| 2:B:374:ARG:NE   | 4:B:851:HOH:O    | 2.29                     | 0.61              |
| 1:A:240:LEU:CA   | 4:A:402:HOH:O    | 2.15                     | 0.61              |
| 1:A:343:LEU:HD13 | 2:B:509:GLU:O    | 2.00                     | 0.61              |
| 2:B:255:GLU:OE2  | 2:B:375:ARG:HD2  | 2.01                     | 0.60              |
| 2:B:617:PHE:HD1  | 2:B:622:LEU:HB2  | 1.66                     | 0.60              |
| 1:A:139:ILE:HA   | 4:A:372:HOH:O    | 2.01                     | 0.60              |
| 2:B:118:LEU:O    | 2:B:133:LEU:HD23 | 1.99                     | 0.60              |
| 1:A:278:LEU:HD11 | 1:A:325:LEU:HD13 | 1.84                     | 0.60              |
| 2:B:267:PHE:CE1  | 2:B:321:GLU:HG2  | 2.36                     | 0.60              |
| 2:B:287:ASP:N    | 2:B:317:MET:CE   | 2.65                     | 0.60              |
| 2:B:602:ARG:HH11 | 2:B:602:ARG:CB   | 2.04                     | 0.60              |
| 2:B:578:ARG:O    | 2:B:579:GLU:HB2  | 2.01                     | 0.60              |
| 2:B:297:ASP:O    | 2:B:299:VAL:HG23 | 2.02                     | 0.60              |
| 2:B:370:VAL:HB   | 2:B:371:PRO:HD3  | 1.84                     | 0.60              |
| 2:B:539:PRO:HG2  | 2:B:540:GLU:OE2  | 2.02                     | 0.60              |
| 1:A:257:TYR:CD1  | 2:B:163:ASN:HB3  | 2.36                     | 0.60              |
| 1:A:332:ILE:HD13 | 1:A:332:ILE:O    | 2.00                     | 0.60              |
| 2:B:510:VAL:O    | 2:B:511:TYR:HD1  | 1.84                     | 0.60              |
| 2:B:749:PHE:CD2  | 4:B:906:HOH:O    | 2.55                     | 0.60              |
| 1:A:107:GLU:O    | 1:A:111:VAL:HG23 | 2.01                     | 0.60              |
| 2:B:455:LEU:HA   | 4:B:961:HOH:O    | 2.00                     | 0.60              |
| 2:B:609:LEU:HD23 | 2:B:609:LEU:O    | 2.02                     | 0.60              |
| 2:B:333:LEU:HD23 | 4:B:915:HOH:O    | 2.02                     | 0.59              |
| 2:B:334:GLU:OE1  | 3:B:786:MTY:HZ   | 2.02                     | 0.59              |
| 1:A:297:TYR:O    | 1:A:297:TYR:CD1  | 2.55                     | 0.59              |
| 2:B:176:ASP:CG   | 2:B:465:ARG:NH2  | 2.59                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:287:ASP:H    | 2:B:317:MET:HE2  | 1.66                     | 0.59              |
| 2:B:52:GLU:CG    | 2:B:54:HIS:CE1   | 2.85                     | 0.59              |
| 2:B:52:GLU:CG    | 2:B:54:HIS:HE1   | 2.15                     | 0.59              |
| 2:B:56:ILE:HG12  | 4:B:842:HOH:O    | 1.87                     | 0.59              |
| 2:B:549:PHE:HB3  | 2:B:672:GLU:OE1  | 2.03                     | 0.59              |
| 1:A:168:GLU:CA   | 4:A:407:HOH:O    | 2.49                     | 0.59              |
| 2:B:388:VAL:HB   | 4:B:957:HOH:O    | 2.01                     | 0.59              |
| 1:A:151:THR:HG22 | 1:A:152:PHE:N    | 2.18                     | 0.59              |
| 2:B:229:TRP:HD1  | 4:B:883:HOH:O    | 1.83                     | 0.59              |
| 2:B:243:ASN:O    | 2:B:244:ASN:C    | 2.46                     | 0.59              |
| 2:B:333:LEU:HD22 | 2:B:335:VAL:HG23 | 1.83                     | 0.59              |
| 2:B:443:ARG:HD2  | 4:B:833:HOH:O    | 2.02                     | 0.59              |
| 1:A:331:ASP:HB3  | 1:A:334:TYR:CD2  | 2.37                     | 0.59              |
| 2:B:1:MET:O      | 2:B:2:ARG:C      | 2.45                     | 0.59              |
| 2:B:302:GLY:C    | 4:B:922:HOH:O    | 2.45                     | 0.59              |
| 2:B:596:LEU:HD13 | 2:B:598:TRP:CH2  | 2.37                     | 0.59              |
| 1:A:128:GLU:OE1  | 1:A:185:ARG:NH1  | 2.36                     | 0.59              |
| 2:B:178:HIS:CD2  | 2:B:184:LEU:HB2  | 2.37                     | 0.59              |
| 2:B:702:PRO:C    | 2:B:704:PRO:HD2  | 2.28                     | 0.59              |
| 2:B:121:ARG:HG3  | 2:B:121:ARG:NH1  | 2.18                     | 0.58              |
| 2:B:323:GLU:CG   | 4:B:792:HOH:O    | 2.47                     | 0.58              |
| 2:B:659:ILE:N    | 2:B:659:ILE:HD12 | 2.18                     | 0.58              |
| 2:B:99:LEU:HD13  | 2:B:101:GLN:HB2  | 1.84                     | 0.58              |
| 2:B:556:LEU:HD12 | 2:B:556:LEU:O    | 2.04                     | 0.58              |
| 1:A:128:GLU:OE2  | 1:A:132:PHE:CB   | 2.51                     | 0.58              |
| 2:B:210:ALA:N    | 2:B:211:PRO:HD3  | 2.19                     | 0.58              |
| 2:B:418:SER:N    | 4:B:861:HOH:O    | 2.35                     | 0.58              |
| 2:B:763:GLU:CG   | 4:B:816:HOH:O    | 2.39                     | 0.58              |
| 2:B:212:HIS:ND1  | 2:B:398:PRO:HD3  | 2.19                     | 0.58              |
| 2:B:403:ALA:HB2  | 2:B:445:THR:HG22 | 1.84                     | 0.58              |
| 2:B:95:GLU:CB    | 4:B:911:HOH:O    | 2.25                     | 0.58              |
| 2:B:445:THR:CG2  | 4:B:894:HOH:O    | 2.28                     | 0.58              |
| 2:B:725:LEU:HD21 | 2:B:745:PHE:CE1  | 2.37                     | 0.58              |
| 2:B:768:VAL:O    | 2:B:772:LEU:HB2  | 2.04                     | 0.58              |
| 2:B:733:GLY:O    | 2:B:736:LEU:HB2  | 2.04                     | 0.58              |
| 1:A:296:ALA:CA   | 4:A:405:HOH:O    | 2.43                     | 0.58              |
| 2:B:243:ASN:OD1  | 2:B:246:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:140:PRO:HG2  | 1:A:143:HIS:HB2  | 1.84                     | 0.57              |
| 1:A:297:TYR:O    | 1:A:301:LEU:HD13 | 2.04                     | 0.57              |
| 2:B:505:LEU:O    | 2:B:505:LEU:HD23 | 2.03                     | 0.57              |
| 2:B:589:LEU:O    | 2:B:590:PHE:HB3  | 2.03                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:163:GLY:HA2  | 1:A:185:ARG:HH21 | 1.69                     | 0.57              |
| 1:A:248:ASP:CG   | 4:A:399:HOH:O    | 2.43                     | 0.57              |
| 2:B:265:LEU:HA   | 2:B:268:VAL:CG2  | 2.34                     | 0.57              |
| 2:B:715:ARG:NH1  | 2:B:725:LEU:HD13 | 2.18                     | 0.57              |
| 2:B:323:GLU:CB   | 4:B:792:HOH:O    | 2.52                     | 0.57              |
| 1:A:94:SER:HB3   | 4:A:404:HOH:O    | 2.03                     | 0.57              |
| 2:B:589:LEU:O    | 2:B:590:PHE:CB   | 2.53                     | 0.57              |
| 2:B:633:PHE:CD1  | 2:B:634:LEU:HG   | 2.40                     | 0.57              |
| 1:A:203:PHE:CD1  | 1:A:203:PHE:N    | 2.71                     | 0.57              |
| 1:A:142:HIS:CD2  | 4:A:382:HOH:O    | 2.58                     | 0.57              |
| 2:B:532:LEU:CA   | 4:B:933:HOH:O    | 2.03                     | 0.57              |
| 2:B:230:MET:HE2  | 2:B:251:TYR:CB   | 2.34                     | 0.57              |
| 2:B:258:GLN:NE2  | 4:B:797:HOH:O    | 2.37                     | 0.57              |
| 2:B:771:ALA:HB2  | 4:B:839:HOH:O    | 2.03                     | 0.57              |
| 2:B:158:LEU:HD12 | 2:B:173:LEU:HD21 | 1.87                     | 0.57              |
| 2:B:230:MET:HE2  | 2:B:251:TYR:HB2  | 1.87                     | 0.57              |
| 2:B:335:VAL:HB   | 2:B:373:GLN:NE2  | 2.20                     | 0.57              |
| 2:B:345:LYS:HE3  | 4:B:862:HOH:O    | 2.05                     | 0.57              |
| 2:B:413:ARG:O    | 4:B:869:HOH:O    | 2.17                     | 0.57              |
| 2:B:609:LEU:HD22 | 2:B:652:LEU:HD11 | 1.87                     | 0.57              |
| 1:A:94:SER:N     | 4:A:404:HOH:O    | 2.38                     | 0.57              |
| 2:B:403:ALA:CB   | 2:B:445:THR:HG22 | 2.35                     | 0.57              |
| 2:B:593:GLY:HA3  | 2:B:604:SER:HB3  | 1.87                     | 0.57              |
| 1:A:340:LEU:C    | 1:A:342:PHE:N    | 2.62                     | 0.56              |
| 2:B:62:LYS:HE2   | 4:B:857:HOH:O    | 2.05                     | 0.56              |
| 2:B:239:MET:CE   | 2:B:355:GLU:HG3  | 2.24                     | 0.56              |
| 2:B:699:VAL:CG1  | 2:B:772:LEU:HD21 | 2.35                     | 0.56              |
| 2:B:357:SER:O    | 2:B:361:GLU:HG3  | 2.05                     | 0.56              |
| 2:B:557:LYS:CG   | 2:B:665:LEU:HD21 | 2.32                     | 0.56              |
| 2:B:727:LEU:HD23 | 4:B:905:HOH:O    | 2.05                     | 0.56              |
| 2:B:6:SER:OG     | 2:B:153:GLU:OE2  | 2.16                     | 0.56              |
| 2:B:713:LEU:HA   | 4:B:836:HOH:O    | 2.05                     | 0.56              |
| 2:B:517:ASP:HB3  | 2:B:520:ASP:OD2  | 2.05                     | 0.56              |
| 1:A:92:GLY:O     | 4:A:404:HOH:O    | 2.17                     | 0.56              |
| 2:B:590:PHE:CG   | 2:B:591:GLY:N    | 2.74                     | 0.56              |
| 2:B:692:ALA:HB2  | 2:B:750:ARG:HD2  | 1.88                     | 0.56              |
| 2:B:333:LEU:HG   | 4:B:915:HOH:O    | 2.04                     | 0.56              |
| 2:B:440:PRO:HG2  | 2:B:441:THR:H    | 1.70                     | 0.56              |
| 2:B:532:LEU:CD2  | 4:B:933:HOH:O    | 2.35                     | 0.56              |
| 2:B:600:LYS:O    | 2:B:601:GLU:C    | 2.48                     | 0.56              |
| 1:A:163:GLY:HA2  | 1:A:185:ARG:NH2  | 2.21                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:LEU:HD12 | 1:A:301:LEU:HD23 | 1.88                     | 0.56              |
| 1:A:319:VAL:HG12 | 1:A:320:GLU:N    | 2.21                     | 0.56              |
| 2:B:8:LEU:O      | 2:B:8:LEU:HD12   | 2.05                     | 0.56              |
| 1:A:115:ARG:HG2  | 1:A:115:ARG:NH1  | 2.16                     | 0.56              |
| 2:B:538:ALA:HB1  | 2:B:539:PRO:HD2  | 1.87                     | 0.56              |
| 1:A:109:GLU:HG3  | 4:A:400:HOH:O    | 2.06                     | 0.55              |
| 2:B:479:PHE:N    | 4:B:841:HOH:O    | 2.24                     | 0.55              |
| 2:B:600:LYS:CD   | 4:B:860:HOH:O    | 2.54                     | 0.55              |
| 2:B:779:LEU:C    | 4:B:916:HOH:O    | 2.48                     | 0.55              |
| 1:A:283:ALA:HB2  | 1:A:315:PHE:CB   | 2.37                     | 0.55              |
| 2:B:160:VAL:HG13 | 2:B:167:ALA:HB3  | 1.88                     | 0.55              |
| 2:B:362:ARG:HH11 | 2:B:362:ARG:HG2  | 1.71                     | 0.55              |
| 1:A:300:ARG:CZ   | 4:A:389:HOH:O    | 2.54                     | 0.55              |
| 2:B:600:LYS:H    | 2:B:600:LYS:HD3  | 1.70                     | 0.55              |
| 1:A:106:MET:HG2  | 1:A:323:ALA:HB2  | 1.88                     | 0.55              |
| 2:B:554:ARG:O    | 2:B:558:GLU:HG3  | 2.06                     | 0.55              |
| 2:B:697:LEU:C    | 2:B:697:LEU:HD12 | 2.31                     | 0.55              |
| 2:B:220:GLY:C    | 4:B:923:HOH:O    | 2.48                     | 0.55              |
| 2:B:604:SER:HA   | 2:B:608:LEU:CD2  | 2.37                     | 0.55              |
| 1:A:233:LEU:O    | 1:A:237:ILE:HD13 | 2.07                     | 0.55              |
| 2:B:467:GLN:HE21 | 2:B:467:GLN:CA   | 2.06                     | 0.55              |
| 2:B:697:LEU:HD12 | 2:B:697:LEU:O    | 2.06                     | 0.55              |
| 2:B:427:ILE:HD12 | 2:B:466:ILE:CG2  | 2.37                     | 0.55              |
| 2:B:753:LYS:HB2  | 4:B:890:HOH:O    | 2.05                     | 0.55              |
| 2:B:634:LEU:HD11 | 2:B:651:PHE:CD1  | 2.42                     | 0.55              |
| 1:A:96:PHE:CZ    | 4:B:940:HOH:O    | 2.53                     | 0.54              |
| 1:A:320:GLU:O    | 1:A:324:MET:HG3  | 2.08                     | 0.54              |
| 1:A:197:VAL:HA   | 1:A:220:GLU:O    | 2.07                     | 0.54              |
| 1:A:350:LEU:HD21 | 4:A:409:HOH:O    | 2.05                     | 0.54              |
| 2:B:179:ALA:HB1  | 2:B:466:ILE:HD13 | 1.88                     | 0.54              |
| 2:B:287:ASP:CB   | 2:B:317:MET:HE1  | 2.37                     | 0.54              |
| 2:B:55:PRO:HD2   | 4:B:937:HOH:O    | 2.07                     | 0.54              |
| 2:B:557:LYS:HG2  | 2:B:665:LEU:CD2  | 2.32                     | 0.54              |
| 1:A:165:LEU:HD12 | 4:A:411:HOH:O    | 2.08                     | 0.54              |
| 2:B:206:ASP:CG   | 2:B:276:ARG:HH11 | 2.15                     | 0.54              |
| 2:B:623:ALA:HB3  | 2:B:645:GLU:HA   | 1.88                     | 0.54              |
| 1:A:127:VAL:HG23 | 2:B:577:PHE:CE2  | 2.43                     | 0.54              |
| 2:B:28:LEU:HD11  | 2:B:177:LEU:HD23 | 1.89                     | 0.54              |
| 2:B:299:VAL:CG1  | 2:B:300:ILE:N    | 2.71                     | 0.54              |
| 2:B:701:VAL:HG21 | 2:B:710:VAL:HG22 | 1.90                     | 0.54              |
| 1:A:96:PHE:HZ    | 4:B:940:HOH:O    | 1.90                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:600:LYS:HD3  | 2:B:600:LYS:N    | 2.23                     | 0.54              |
| 1:A:164:PRO:HG3  | 1:A:185:ARG:HA   | 1.90                     | 0.54              |
| 2:B:389:ALA:O    | 2:B:391:ALA:N    | 2.41                     | 0.54              |
| 2:B:567:ARG:CD   | 4:B:886:HOH:O    | 2.55                     | 0.54              |
| 1:A:201:ARG:NH1  | 1:A:336:PHE:CE1  | 2.76                     | 0.54              |
| 1:A:221:GLY:HA3  | 1:A:315:PHE:CZ   | 2.43                     | 0.54              |
| 1:A:321:ARG:O    | 1:A:324:MET:HB2  | 2.08                     | 0.54              |
| 2:B:412:ASN:O    | 2:B:414:LEU:N    | 2.41                     | 0.54              |
| 2:B:644:VAL:O    | 2:B:645:GLU:HB2  | 2.07                     | 0.54              |
| 2:B:763:GLU:O    | 2:B:767:ARG:HG2  | 2.08                     | 0.53              |
| 1:A:137:LEU:O    | 1:A:139:ILE:HG13 | 2.07                     | 0.53              |
| 1:A:199:PRO:HB3  | 1:A:219:LEU:HD12 | 1.90                     | 0.53              |
| 2:B:390:GLU:O    | 2:B:390:GLU:HG2  | 2.08                     | 0.53              |
| 2:B:427:ILE:HG23 | 2:B:466:ILE:HD12 | 1.89                     | 0.53              |
| 2:B:701:VAL:HG13 | 2:B:705:THR:HB   | 1.91                     | 0.53              |
| 1:A:322:LEU:O    | 1:A:324:MET:N    | 2.41                     | 0.53              |
| 2:B:724:SER:O    | 2:B:747:LEU:HA   | 2.09                     | 0.53              |
| 1:A:118:GLY:C    | 4:A:392:HOH:O    | 2.51                     | 0.53              |
| 1:A:194:PHE:CA   | 4:A:363:HOH:O    | 2.55                     | 0.53              |
| 1:A:229:ALA:HB1  | 4:B:869:HOH:O    | 1.97                     | 0.53              |
| 2:B:370:VAL:O    | 2:B:373:GLN:HB2  | 2.08                     | 0.53              |
| 2:B:513:TYR:CE1  | 4:B:796:HOH:O    | 2.54                     | 0.53              |
| 2:B:590:PHE:CD1  | 2:B:591:GLY:N    | 2.76                     | 0.53              |
| 2:B:607:PHE:N    | 4:B:934:HOH:O    | 2.41                     | 0.53              |
| 2:B:767:ARG:HE   | 2:B:767:ARG:N    | 2.06                     | 0.53              |
| 2:B:55:PRO:CD    | 4:B:937:HOH:O    | 2.57                     | 0.53              |
| 2:B:120:PRO:HG3  | 2:B:133:LEU:CD1  | 2.38                     | 0.53              |
| 2:B:532:LEU:CB   | 4:B:933:HOH:O    | 2.49                     | 0.53              |
| 2:B:619:ARG:HD2  | 2:B:619:ARG:O    | 2.08                     | 0.53              |
| 2:B:755:THR:HG22 | 2:B:756:LEU:N    | 2.24                     | 0.53              |
| 2:B:530:ARG:HG3  | 2:B:530:ARG:HH11 | 1.73                     | 0.53              |
| 1:A:164:PRO:HB3  | 1:A:188:VAL:HG23 | 1.91                     | 0.53              |
| 1:A:129:SER:O    | 1:A:131:PHE:N    | 2.41                     | 0.53              |
| 1:A:160:ARG:NH2  | 4:A:408:HOH:O    | 2.37                     | 0.53              |
| 2:B:19:GLU:H     | 2:B:19:GLU:CD    | 2.17                     | 0.53              |
| 2:B:140:LEU:HD21 | 2:B:149:ALA:HB2  | 1.91                     | 0.53              |
| 2:B:258:GLN:HE22 | 2:B:369:GLN:NE2  | 2.07                     | 0.53              |
| 1:A:298:ARG:NH1  | 1:A:304:PRO:O    | 2.41                     | 0.53              |
| 2:B:30:PHE:HB3   | 2:B:158:LEU:CD2  | 2.39                     | 0.52              |
| 2:B:206:ASP:OD2  | 2:B:276:ARG:HD3  | 2.09                     | 0.52              |
| 2:B:502:LEU:HD13 | 2:B:571:PHE:CE2  | 2.44                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:588:LEU:HD23 | 2:B:588:LEU:O    | 2.08                     | 0.52              |
| 2:B:699:VAL:HG22 | 2:B:772:LEU:HD21 | 1.91                     | 0.52              |
| 2:B:163:ASN:O    | 2:B:452:ASP:HB3  | 2.08                     | 0.52              |
| 2:B:258:GLN:HE22 | 2:B:369:GLN:HE21 | 1.57                     | 0.52              |
| 2:B:404:ILE:HD12 | 2:B:454:ARG:O    | 2.09                     | 0.52              |
| 2:B:770:GLU:CB   | 4:B:822:HOH:O    | 2.56                     | 0.52              |
| 1:A:103:ILE:HG23 | 1:A:319:VAL:HG11 | 1.92                     | 0.52              |
| 2:B:46:VAL:HB    | 2:B:143:GLY:O    | 2.08                     | 0.52              |
| 2:B:567:ARG:CA   | 2:B:591:GLY:HA3  | 2.39                     | 0.52              |
| 2:B:389:ALA:C    | 2:B:391:ALA:H    | 2.17                     | 0.52              |
| 2:B:715:ARG:NH1  | 2:B:715:ARG:HB2  | 2.24                     | 0.52              |
| 1:A:143:HIS:HA   | 4:A:383:HOH:O    | 2.10                     | 0.52              |
| 2:B:637:GLY:CA   | 4:B:908:HOH:O    | 2.22                     | 0.52              |
| 2:B:62:LYS:HB2   | 2:B:62:LYS:NZ    | 2.25                     | 0.52              |
| 2:B:275:ARG:HG3  | 2:B:275:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:349:VAL:O    | 1:A:350:LEU:HB2  | 2.10                     | 0.52              |
| 4:A:408:HOH:O    | 2:B:579:GLU:CA   | 2.40                     | 0.52              |
| 2:B:270:GLU:CG   | 4:B:799:HOH:O    | 2.57                     | 0.52              |
| 1:A:87:ASP:OD1   | 1:A:89:SER:N     | 2.39                     | 0.52              |
| 2:B:450:ARG:NH2  | 2:B:452:ASP:OD2  | 2.41                     | 0.52              |
| 2:B:517:ASP:OD1  | 2:B:540:GLU:HA   | 2.10                     | 0.52              |
| 2:B:729:ASP:HB3  | 2:B:744:ALA:HB2  | 1.92                     | 0.52              |
| 2:B:348:ARG:NH1  | 2:B:361:GLU:OE1  | 2.44                     | 0.51              |
| 1:A:101:HIS:CB   | 2:B:509:GLU:OE1  | 2.59                     | 0.51              |
| 2:B:600:LYS:HD3  | 4:B:860:HOH:O    | 2.10                     | 0.51              |
| 1:A:283:ALA:HB2  | 1:A:315:PHE:HA   | 1.91                     | 0.51              |
| 2:B:151:PRO:HG2  | 2:B:232:ARG:NH2  | 2.24                     | 0.51              |
| 1:A:168:GLU:N    | 4:A:407:HOH:O    | 2.44                     | 0.51              |
| 1:A:332:ILE:HD13 | 1:A:335:PHE:CD2  | 2.43                     | 0.51              |
| 2:B:652:LEU:HD13 | 2:B:671:PHE:HB3  | 1.92                     | 0.51              |
| 2:B:710:VAL:HG11 | 2:B:743:LEU:HD12 | 1.93                     | 0.51              |
| 2:B:728:PHE:CZ   | 2:B:744:ALA:HB1  | 2.44                     | 0.51              |
| 2:B:746:HIS:CE1  | 4:B:900:HOH:O    | 2.53                     | 0.51              |
| 1:A:114:PHE:HA   | 1:A:117:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:115:ARG:CZ   | 2:B:493:ARG:HH21 | 2.23                     | 0.51              |
| 1:A:180:SER:O    | 1:A:181:PRO:C    | 2.52                     | 0.51              |
| 1:A:182:MET:HG2  | 1:A:198:VAL:HG21 | 1.92                     | 0.51              |
| 2:B:530:ARG:NH1  | 4:B:870:HOH:O    | 2.43                     | 0.51              |
| 2:B:3:VAL:CG2    | 2:B:158:LEU:HB2  | 2.41                     | 0.51              |
| 2:B:141:PRO:O    | 2:B:144:THR:HG23 | 2.10                     | 0.51              |
| 2:B:261:HIS:CD2  | 3:B:786:MTY:HA   | 2.41                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:374:ARG:CD   | 4:B:851:HOH:O    | 2.59                     | 0.51              |
| 1:A:201:ARG:NH1  | 1:A:336:PHE:HE1  | 2.08                     | 0.51              |
| 2:B:9:LYS:HE3    | 4:B:947:HOH:O    | 2.11                     | 0.51              |
| 2:B:222:ARG:HG3  | 2:B:222:ARG:O    | 2.11                     | 0.51              |
| 2:B:250:ASN:O    | 2:B:253:MET:HB3  | 2.11                     | 0.51              |
| 1:A:197:VAL:HG21 | 1:A:219:LEU:HD21 | 1.93                     | 0.51              |
| 2:B:224:ALA:HB1  | 2:B:225:PRO:CD   | 2.41                     | 0.51              |
| 2:B:40:PRO:HG2   | 4:B:896:HOH:O    | 2.10                     | 0.51              |
| 2:B:567:ARG:HB3  | 2:B:591:GLY:HA3  | 1.93                     | 0.51              |
| 2:B:592:GLU:HG3  | 2:B:593:GLY:H    | 1.76                     | 0.51              |
| 1:A:175:LEU:HB3  | 1:A:203:PHE:CD1  | 2.46                     | 0.51              |
| 2:B:7:TRP:CE3    | 2:B:233:ALA:HB1  | 2.46                     | 0.51              |
| 2:B:407:ARG:HD3  | 2:B:456:GLU:OE2  | 2.10                     | 0.51              |
| 2:B:601:GLU:CD   | 2:B:601:GLU:H    | 2.19                     | 0.51              |
| 2:B:578:ARG:O    | 2:B:579:GLU:CB   | 2.59                     | 0.50              |
| 2:B:613:LEU:HD21 | 2:B:671:PHE:CE2  | 2.45                     | 0.50              |
| 2:B:686:ASP:HB2  | 4:B:953:HOH:O    | 2.10                     | 0.50              |
| 1:A:168:GLU:HA   | 4:A:407:HOH:O    | 2.11                     | 0.50              |
| 2:B:316:VAL:N    | 4:B:876:HOH:O    | 2.44                     | 0.50              |
| 2:B:624:PHE:C    | 2:B:624:PHE:CD2  | 2.88                     | 0.50              |
| 2:B:757:ARG:HG2  | 2:B:757:ARG:HH11 | 1.76                     | 0.50              |
| 1:A:248:ASP:HB3  | 4:A:399:HOH:O    | 1.92                     | 0.50              |
| 1:A:271:TRP:CA   | 4:A:366:HOH:O    | 2.45                     | 0.50              |
| 1:A:340:LEU:O    | 1:A:342:PHE:N    | 2.45                     | 0.50              |
| 2:B:360:PHE:HA   | 4:B:897:HOH:O    | 2.10                     | 0.50              |
| 2:B:548:LEU:HD22 | 2:B:584:HIS:CB   | 2.40                     | 0.50              |
| 2:B:287:ASP:H    | 2:B:317:MET:HE1  | 1.77                     | 0.50              |
| 2:B:353:ARG:C    | 2:B:353:ARG:HD3  | 2.36                     | 0.50              |
| 2:B:408:PRO:HB3  | 2:B:424:GLN:NE2  | 2.27                     | 0.50              |
| 2:B:644:VAL:HG11 | 2:B:678:PRO:HD2  | 1.94                     | 0.50              |
| 2:B:713:LEU:HD13 | 2:B:772:LEU:HD12 | 1.94                     | 0.50              |
| 2:B:710:VAL:O    | 2:B:714:VAL:HG23 | 2.11                     | 0.50              |
| 2:B:267:PHE:CD1  | 2:B:321:GLU:HG2  | 2.47                     | 0.50              |
| 2:B:403:ALA:HA   | 2:B:445:THR:HG22 | 1.92                     | 0.50              |
| 2:B:556:LEU:HD12 | 2:B:556:LEU:C    | 2.37                     | 0.50              |
| 2:B:659:ILE:HD12 | 2:B:659:ILE:H    | 1.76                     | 0.50              |
| 2:B:584:HIS:HD2  | 2:B:672:GLU:OE2  | 1.94                     | 0.50              |
| 2:B:753:LYS:N    | 4:B:890:HOH:O    | 2.45                     | 0.50              |
| 2:B:287:ASP:N    | 2:B:317:MET:HE2  | 2.27                     | 0.50              |
| 2:B:527:ASP:CB   | 4:B:892:HOH:O    | 2.47                     | 0.50              |
| 2:B:549:PHE:N    | 2:B:672:GLU:OE1  | 2.40                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:261:VAL:CB   | 4:A:391:HOH:O    | 2.40                     | 0.49              |
| 2:B:60:ARG:C     | 2:B:60:ARG:HD3   | 2.37                     | 0.49              |
| 2:B:145:PRO:HB3  | 4:B:826:HOH:O    | 2.11                     | 0.49              |
| 2:B:564:ARG:N    | 2:B:564:ARG:CD   | 2.75                     | 0.49              |
| 1:A:327:TYR:CE1  | 4:A:379:HOH:O    | 2.55                     | 0.49              |
| 2:B:224:ALA:HB3  | 2:B:244:ASN:HD21 | 1.77                     | 0.49              |
| 2:B:414:LEU:HD23 | 2:B:460:VAL:HG21 | 1.93                     | 0.49              |
| 2:B:563:ASP:C    | 2:B:564:ARG:HD2  | 2.35                     | 0.49              |
| 1:A:98:GLY:O     | 1:A:347:LYS:HE3  | 2.13                     | 0.49              |
| 1:A:210:ALA:HA   | 1:A:331:ASP:OD1  | 2.12                     | 0.49              |
| 1:A:264:GLY:O    | 1:A:265:ALA:HB2  | 2.11                     | 0.49              |
| 2:B:402:GLU:N    | 4:B:803:HOH:O    | 2.38                     | 0.49              |
| 2:B:17:SER:OG    | 2:B:20:VAL:HG23  | 2.12                     | 0.49              |
| 2:B:294:HIS:CE1  | 2:B:295:PRO:HG2  | 2.47                     | 0.49              |
| 2:B:751:HIS:HB2  | 2:B:756:LEU:CD2  | 2.43                     | 0.49              |
| 1:A:326:ARG:HG3  | 4:A:410:HOH:O    | 2.12                     | 0.49              |
| 2:B:461:GLU:O    | 2:B:465:ARG:HG2  | 2.12                     | 0.49              |
| 2:B:70:ARG:CB    | 4:B:943:HOH:O    | 2.60                     | 0.49              |
| 2:B:715:ARG:HB2  | 2:B:715:ARG:HH11 | 1.75                     | 0.49              |
| 1:A:94:SER:CB    | 4:A:404:HOH:O    | 2.56                     | 0.49              |
| 1:A:287:HIS:CE1  | 1:A:288:PRO:HD2  | 2.48                     | 0.49              |
| 1:A:319:VAL:O    | 1:A:320:GLU:C    | 2.55                     | 0.49              |
| 2:B:586:ALA:HB2  | 2:B:672:GLU:HA   | 1.95                     | 0.49              |
| 2:B:701:VAL:O    | 2:B:741:LYS:HG2  | 2.12                     | 0.49              |
| 1:A:307:TYR:N    | 1:A:307:TYR:HD1  | 2.06                     | 0.49              |
| 2:B:403:ALA:CA   | 2:B:445:THR:HG22 | 2.43                     | 0.49              |
| 2:B:230:MET:HE2  | 2:B:251:TYR:CG   | 2.48                     | 0.49              |
| 2:B:287:ASP:CG   | 2:B:317:MET:HE1  | 2.38                     | 0.49              |
| 2:B:335:VAL:HB   | 2:B:373:GLN:HE21 | 1.78                     | 0.49              |
| 2:B:500:GLU:HA   | 2:B:503:SER:OG   | 2.13                     | 0.49              |
| 2:B:297:ASP:OD2  | 2:B:350:HIS:CE1  | 2.64                     | 0.49              |
| 2:B:341:VAL:O    | 2:B:345:LYS:HG3  | 2.12                     | 0.49              |
| 2:B:548:LEU:HD21 | 2:B:574:GLY:H    | 1.78                     | 0.49              |
| 1:A:194:PHE:CB   | 4:A:363:HOH:O    | 2.47                     | 0.48              |
| 2:B:34:ARG:C     | 2:B:35:ILE:HD12  | 2.37                     | 0.48              |
| 2:B:51:LEU:HD11  | 2:B:67:ASP:HB2   | 1.93                     | 0.48              |
| 2:B:192:LYS:H    | 2:B:381:GLN:HE22 | 1.58                     | 0.48              |
| 2:B:287:ASP:N    | 2:B:317:MET:HE1  | 2.28                     | 0.48              |
| 2:B:539:PRO:HG2  | 2:B:540:GLU:CD   | 2.38                     | 0.48              |
| 1:A:183:GLN:O    | 1:A:187:MET:HG3  | 2.14                     | 0.48              |
| 2:B:592:GLU:HG3  | 2:B:593:GLY:N    | 2.27                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:115:ARG:NE   | 2:B:493:ARG:HH21 | 2.11                     | 0.48              |
| 1:A:185:ARG:C    | 4:A:386:HOH:O    | 2.56                     | 0.48              |
| 1:A:322:LEU:O    | 1:A:323:ALA:C    | 2.56                     | 0.48              |
| 1:A:348:GLY:O    | 1:A:349:VAL:C    | 2.56                     | 0.48              |
| 2:B:91:LEU:HB3   | 2:B:92:PRO:HD2   | 1.95                     | 0.48              |
| 2:B:214:THR:HA   | 2:B:393:LEU:O    | 2.14                     | 0.48              |
| 2:B:489:GLU:O    | 2:B:490:ALA:C    | 2.55                     | 0.48              |
| 1:A:113:ILE:O    | 1:A:117:LEU:HD12 | 2.14                     | 0.48              |
| 2:B:586:ALA:HB1  | 2:B:671:PHE:O    | 2.12                     | 0.48              |
| 2:B:754:ARG:NH1  | 2:B:756:LEU:HD23 | 2.29                     | 0.48              |
| 1:A:262:GLU:OE2  | 2:B:461:GLU:OE1  | 2.32                     | 0.48              |
| 1:A:280:LEU:CD1  | 1:A:317:LEU:HD22 | 2.43                     | 0.48              |
| 2:B:18:PRO:O     | 2:B:21:LEU:HB3   | 2.14                     | 0.48              |
| 2:B:527:ASP:CA   | 4:B:892:HOH:O    | 2.61                     | 0.48              |
| 2:B:316:VAL:HG22 | 2:B:357:SER:HB3  | 1.96                     | 0.48              |
| 2:B:703:ALA:N    | 2:B:704:PRO:HD2  | 2.28                     | 0.48              |
| 2:B:717:ALA:N    | 4:B:925:HOH:O    | 2.26                     | 0.48              |
| 1:A:101:HIS:CE1  | 1:A:103:ILE:HG12 | 2.48                     | 0.48              |
| 2:B:138:ASP:O    | 2:B:139:ALA:C    | 2.56                     | 0.48              |
| 2:B:213:PHE:HA   | 2:B:336:ALA:HB2  | 1.95                     | 0.48              |
| 2:B:243:ASN:O    | 2:B:244:ASN:O    | 2.30                     | 0.48              |
| 2:B:253:MET:HE3  | 2:B:259:PRO:HG3  | 1.95                     | 0.48              |
| 2:B:717:ALA:CB   | 4:B:839:HOH:O    | 2.62                     | 0.48              |
| 2:B:38:VAL:HG22  | 2:B:153:GLU:O    | 2.13                     | 0.48              |
| 2:B:286:LEU:C    | 2:B:288:GLY:H    | 2.21                     | 0.48              |
| 2:B:336:ALA:HA   | 2:B:369:GLN:CG   | 2.44                     | 0.48              |
| 2:B:99:LEU:O     | 2:B:101:GLN:HG2  | 2.14                     | 0.48              |
| 2:B:729:ASP:HB3  | 2:B:744:ALA:CB   | 2.44                     | 0.48              |
| 2:B:16:GLU:OE2   | 2:B:20:VAL:HG11  | 2.13                     | 0.48              |
| 2:B:326:GLU:CD   | 2:B:326:GLU:H    | 2.22                     | 0.48              |
| 2:B:530:ARG:HG3  | 2:B:530:ARG:NH1  | 2.29                     | 0.48              |
| 2:B:717:ALA:CA   | 4:B:925:HOH:O    | 2.62                     | 0.48              |
| 1:A:93:ALA:O     | 1:A:95:LEU:N     | 2.47                     | 0.47              |
| 1:A:182:MET:HE3  | 1:A:185:ARG:HB2  | 1.94                     | 0.47              |
| 2:B:39:PHE:HB2   | 2:B:152:GLU:HA   | 1.95                     | 0.47              |
| 2:B:635:HIS:ND1  | 2:B:637:GLY:N    | 2.62                     | 0.47              |
| 2:B:655:LEU:HG   | 2:B:656:HIS:N    | 2.29                     | 0.47              |
| 2:B:747:LEU:N    | 2:B:747:LEU:HD12 | 2.29                     | 0.47              |
| 1:A:114:PHE:HA   | 1:A:117:LEU:CD1  | 2.44                     | 0.47              |
| 1:A:219:LEU:O    | 1:A:316:GLY:HA2  | 2.14                     | 0.47              |
| 1:A:326:ARG:HG3  | 1:A:326:ARG:NH1  | 2.29                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:643:LEU:HD13 | 2:B:648:GLU:HA   | 1.95                     | 0.47              |
| 2:B:730:LEU:HD13 | 2:B:743:LEU:HD21 | 1.93                     | 0.47              |
| 2:B:753:LYS:CA   | 4:B:890:HOH:O    | 2.61                     | 0.47              |
| 1:A:240:LEU:O    | 1:A:244:LEU:HB2  | 2.14                     | 0.47              |
| 1:A:285:MET:SD   | 1:A:313:PHE:HB3  | 2.54                     | 0.47              |
| 2:B:277:ALA:O    | 2:B:295:PRO:HA   | 2.14                     | 0.47              |
| 2:B:509:GLU:HA   | 2:B:571:PHE:CE1  | 2.50                     | 0.47              |
| 2:B:190:ALA:HB3  | 4:B:852:HOH:O    | 2.07                     | 0.47              |
| 2:B:253:MET:HG3  | 2:B:259:PRO:HA   | 1.95                     | 0.47              |
| 2:B:495:GLU:O    | 2:B:498:LEU:HB3  | 2.15                     | 0.47              |
| 2:B:508:GLN:OE1  | 2:B:508:GLN:HA   | 2.14                     | 0.47              |
| 2:B:589:LEU:CD2  | 2:B:609:LEU:HB2  | 2.45                     | 0.47              |
| 2:B:688:SER:CB   | 2:B:752:PRO:HA   | 2.42                     | 0.47              |
| 1:A:229:ALA:H    | 1:A:232:HIS:CD2  | 2.29                     | 0.47              |
| 1:A:296:ALA:C    | 1:A:298:ARG:N    | 2.69                     | 0.47              |
| 2:B:30:PHE:HB3   | 2:B:158:LEU:HD21 | 1.97                     | 0.47              |
| 2:B:309:PHE:N    | 2:B:309:PHE:CD1  | 2.82                     | 0.47              |
| 2:B:387:ARG:HA   | 4:B:825:HOH:O    | 2.14                     | 0.47              |
| 2:B:516:MET:HG2  | 2:B:517:ASP:N    | 2.29                     | 0.47              |
| 1:A:86:VAL:CA    | 4:A:384:HOH:O    | 2.63                     | 0.47              |
| 1:A:210:ALA:CB   | 4:A:387:HOH:O    | 2.61                     | 0.47              |
| 2:B:3:VAL:HG23   | 2:B:158:LEU:HB2  | 1.96                     | 0.47              |
| 2:B:51:LEU:O     | 2:B:52:GLU:HB2   | 2.14                     | 0.47              |
| 2:B:161:THR:HB   | 2:B:162:PRO:HD2  | 1.96                     | 0.47              |
| 2:B:279:GLU:HA   | 4:B:931:HOH:O    | 2.08                     | 0.47              |
| 2:B:317:MET:HA   | 3:B:786:MTY:H2   | 1.77                     | 0.47              |
| 2:B:532:LEU:C    | 2:B:533:LEU:HD12 | 2.40                     | 0.47              |
| 2:B:555:VAL:HG23 | 2:B:556:LEU:N    | 2.29                     | 0.47              |
| 2:B:657:PRO:O    | 2:B:660:ALA:HB3  | 2.14                     | 0.47              |
| 3:B:786:MTY:CE2  | 4:B:876:HOH:O    | 2.57                     | 0.47              |
| 1:A:114:PHE:CE2  | 1:A:240:LEU:HD13 | 2.49                     | 0.47              |
| 1:A:278:LEU:HD11 | 1:A:325:LEU:CD1  | 2.44                     | 0.47              |
| 2:B:410:TYR:O    | 2:B:411:ALA:C    | 2.55                     | 0.47              |
| 1:A:108:ARG:O    | 1:A:109:GLU:C    | 2.57                     | 0.47              |
| 1:A:152:PHE:CD1  | 2:B:533:LEU:HD23 | 2.50                     | 0.47              |
| 1:A:194:PHE:HA   | 4:A:363:HOH:O    | 2.13                     | 0.47              |
| 2:B:368:GLY:O    | 2:B:371:PRO:HD2  | 2.15                     | 0.47              |
| 2:B:630:ALA:CB   | 4:B:893:HOH:O    | 2.41                     | 0.47              |
| 1:A:125:PRO:HG3  | 1:A:185:ARG:NH1  | 2.30                     | 0.46              |
| 1:A:148:MET:HE3  | 2:B:162:PRO:HG2  | 1.97                     | 0.46              |
| 1:A:208:THR:O    | 1:A:208:THR:HG22 | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:171:LEU:O    | 2:B:171:LEU:CD2  | 2.63                     | 0.46              |
| 2:B:212:HIS:ND1  | 2:B:398:PRO:CD   | 2.78                     | 0.46              |
| 2:B:580:ARG:HG2  | 2:B:580:ARG:HH11 | 1.78                     | 0.46              |
| 2:B:633:PHE:CE1  | 2:B:634:LEU:HG   | 2.50                     | 0.46              |
| 1:A:108:ARG:O    | 4:A:377:HOH:O    | 2.20                     | 0.46              |
| 1:A:164:PRO:C    | 1:A:166:GLY:H    | 2.23                     | 0.46              |
| 1:A:271:TRP:CE3  | 1:A:274:GLY:HA3  | 2.51                     | 0.46              |
| 1:A:288:PRO:CG   | 2:B:457:GLU:HG2  | 2.45                     | 0.46              |
| 2:B:564:ARG:O    | 2:B:565:PRO:C    | 2.59                     | 0.46              |
| 2:B:699:VAL:O    | 2:B:742:SER:HA   | 2.15                     | 0.46              |
| 1:A:271:TRP:C    | 4:A:366:HOH:O    | 2.58                     | 0.46              |
| 2:B:28:LEU:CD1   | 2:B:177:LEU:HD23 | 2.45                     | 0.46              |
| 2:B:369:GLN:CD   | 2:B:369:GLN:H    | 2.24                     | 0.46              |
| 1:A:271:TRP:CZ3  | 1:A:274:GLY:HA3  | 2.51                     | 0.46              |
| 1:A:301:LEU:HD23 | 4:A:411:HOH:O    | 2.14                     | 0.46              |
| 2:B:248:VAL:O    | 2:B:248:VAL:HG12 | 2.16                     | 0.46              |
| 2:B:626:VAL:HG13 | 2:B:641:ARG:O    | 2.15                     | 0.46              |
| 2:B:772:LEU:HG   | 2:B:777:PHE:HB2  | 1.97                     | 0.46              |
| 1:A:164:PRO:CB   | 1:A:188:VAL:CG2  | 2.94                     | 0.46              |
| 2:B:307:GLU:CG   | 4:B:938:HOH:O    | 2.58                     | 0.46              |
| 2:B:635:HIS:CE1  | 2:B:637:GLY:H    | 2.33                     | 0.46              |
| 2:B:517:ASP:HA   | 2:B:540:GLU:O    | 2.16                     | 0.46              |
| 2:B:587:GLY:N    | 2:B:671:PHE:CE1  | 2.84                     | 0.46              |
| 1:A:324:MET:HE3  | 1:A:332:ILE:N    | 2.30                     | 0.46              |
| 2:B:500:GLU:O    | 2:B:501:VAL:C    | 2.57                     | 0.46              |
| 2:B:759:GLU:HB3  | 4:B:801:HOH:O    | 2.02                     | 0.46              |
| 1:A:228:ILE:HG22 | 1:A:229:ALA:N    | 2.31                     | 0.46              |
| 2:B:211:PRO:HD2  | 4:B:879:HOH:O    | 1.98                     | 0.46              |
| 1:A:148:MET:HE1  | 1:A:257:TYR:CD2  | 2.47                     | 0.46              |
| 1:A:326:ARG:HG3  | 1:A:326:ARG:HH11 | 1.80                     | 0.46              |
| 2:B:420:PRO:HG2  | 2:B:423:GLU:HB2  | 1.97                     | 0.46              |
| 2:B:602:ARG:NH1  | 4:B:904:HOH:O    | 2.48                     | 0.46              |
| 2:B:609:LEU:HD22 | 2:B:652:LEU:CD1  | 2.46                     | 0.46              |
| 2:B:20:VAL:O     | 2:B:23:GLU:HB3   | 2.15                     | 0.46              |
| 2:B:178:HIS:CE1  | 4:B:895:HOH:O    | 2.54                     | 0.46              |
| 2:B:222:ARG:CG   | 2:B:222:ARG:O    | 2.64                     | 0.46              |
| 2:B:256:ARG:CZ   | 2:B:375:ARG:HG3  | 2.46                     | 0.46              |
| 2:B:701:VAL:HG12 | 2:B:702:PRO:O    | 2.16                     | 0.46              |
| 1:A:261:VAL:HG21 | 4:A:391:HOH:O    | 2.09                     | 0.45              |
| 2:B:212:HIS:O    | 2:B:336:ALA:HB1  | 2.15                     | 0.45              |
| 2:B:686:ASP:CG   | 4:B:953:HOH:O    | 2.59                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:344:GLU:O    | 1:A:347:LYS:HG3  | 2.17                     | 0.45              |
| 2:B:107:VAL:HG22 | 2:B:112:ARG:HB3  | 1.98                     | 0.45              |
| 2:B:404:ILE:HG12 | 2:B:444:VAL:O    | 2.16                     | 0.45              |
| 2:B:507:PHE:CE2  | 2:B:569:LEU:HD21 | 2.51                     | 0.45              |
| 1:A:331:ASP:O    | 1:A:334:TYR:CD2  | 2.69                     | 0.45              |
| 2:B:43:ARG:HG3   | 2:B:43:ARG:HH11  | 1.80                     | 0.45              |
| 2:B:176:ASP:N    | 4:B:871:HOH:O    | 2.50                     | 0.45              |
| 2:B:642:VAL:O    | 2:B:643:LEU:HD22 | 2.16                     | 0.45              |
| 2:B:14:GLU:CB    | 4:B:789:HOH:O    | 2.60                     | 0.45              |
| 2:B:461:GLU:O    | 2:B:461:GLU:HG2  | 2.16                     | 0.45              |
| 2:B:545:ARG:NH2  | 2:B:548:LEU:HD11 | 2.31                     | 0.45              |
| 2:B:80:ASN:HB2   | 2:B:82:ARG:HH12  | 1.81                     | 0.45              |
| 2:B:264:ASP:OD2  | 2:B:266:ARG:HD3  | 2.17                     | 0.45              |
| 2:B:459:LEU:O    | 2:B:462:GLU:HB2  | 2.17                     | 0.45              |
| 2:B:660:ALA:HB1  | 2:B:665:LEU:O    | 2.16                     | 0.45              |
| 1:A:283:ALA:HB1  | 1:A:314:ALA:O    | 2.17                     | 0.45              |
| 2:B:47:PHE:CE1   | 2:B:139:ALA:HB3  | 2.52                     | 0.45              |
| 2:B:669:HIS:CD2  | 4:B:823:HOH:O    | 2.63                     | 0.45              |
| 2:B:715:ARG:O    | 2:B:716:GLU:C    | 2.58                     | 0.45              |
| 1:A:179:THR:OG1  | 1:A:220:GLU:CG   | 2.65                     | 0.45              |
| 1:A:179:THR:OG1  | 1:A:220:GLU:HG2  | 2.16                     | 0.45              |
| 1:A:180:SER:O    | 1:A:183:GLN:N    | 2.36                     | 0.45              |
| 1:A:260:PHE:HD2  | 4:A:356:HOH:O    | 2.00                     | 0.45              |
| 2:B:297:ASP:O    | 2:B:298:LEU:C    | 2.60                     | 0.45              |
| 2:B:365:ASP:HA   | 2:B:366:PRO:HD2  | 1.74                     | 0.45              |
| 2:B:713:LEU:O    | 2:B:714:VAL:C    | 2.59                     | 0.45              |
| 2:B:512:THR:HG22 | 4:B:820:HOH:O    | 2.09                     | 0.45              |
| 2:B:557:LYS:HD3  | 2:B:561:ASP:OD2  | 2.16                     | 0.45              |
| 1:A:187:MET:SD   | 1:A:307:TYR:CE2  | 3.10                     | 0.45              |
| 2:B:277:ALA:HB2  | 2:B:299:VAL:HG21 | 1.98                     | 0.45              |
| 2:B:280:GLY:O    | 2:B:281:GLU:C    | 2.59                     | 0.45              |
| 2:B:559:ASN:O    | 2:B:561:ASP:N    | 2.50                     | 0.45              |
| 2:B:707:TYR:CZ   | 4:B:905:HOH:O    | 2.56                     | 0.45              |
| 1:A:280:LEU:HD11 | 1:A:322:LEU:HD21 | 1.99                     | 0.45              |
| 2:B:567:ARG:HA   | 2:B:591:GLY:CA   | 2.42                     | 0.45              |
| 2:B:593:GLY:CA   | 2:B:604:SER:HB3  | 2.47                     | 0.45              |
| 2:B:615:ALA:O    | 2:B:617:PHE:N    | 2.50                     | 0.45              |
| 2:B:43:ARG:HG3   | 2:B:43:ARG:NH1   | 2.32                     | 0.44              |
| 2:B:70:ARG:NE    | 4:B:943:HOH:O    | 2.47                     | 0.44              |
| 2:B:191:LEU:HD23 | 2:B:381:GLN:OE1  | 2.17                     | 0.44              |
| 2:B:265:LEU:HD23 | 2:B:268:VAL:CG2  | 2.39                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:655:LEU:HG   | 2:B:656:HIS:H    | 1.82                     | 0.44              |
| 2:B:659:ILE:H    | 2:B:659:ILE:CD1  | 2.30                     | 0.44              |
| 2:B:707:TYR:CE1  | 4:B:905:HOH:O    | 2.70                     | 0.44              |
| 2:B:754:ARG:HH11 | 2:B:756:LEU:HD23 | 1.82                     | 0.44              |
| 1:A:109:GLU:O    | 1:A:113:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:299:GLU:CB   | 4:A:385:HOH:O    | 2.42                     | 0.44              |
| 2:B:62:LYS:HB2   | 2:B:62:LYS:HZ3   | 1.82                     | 0.44              |
| 2:B:207:PRO:CD   | 4:B:853:HOH:O    | 2.59                     | 0.44              |
| 2:B:267:PHE:N    | 2:B:267:PHE:CD2  | 2.85                     | 0.44              |
| 2:B:589:LEU:CB   | 2:B:609:LEU:HD12 | 2.35                     | 0.44              |
| 1:A:101:HIS:HB2  | 2:B:509:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:193:PRO:HB2  | 2:B:479:PHE:CD1  | 2.52                     | 0.44              |
| 1:A:295:ASP:HA   | 1:A:298:ARG:HB2  | 1.99                     | 0.44              |
| 1:A:306:ALA:HB3  | 1:A:307:TYR:CE1  | 2.53                     | 0.44              |
| 2:B:153:GLU:OE1  | 2:B:154:VAL:N    | 2.46                     | 0.44              |
| 2:B:701:VAL:HG13 | 2:B:702:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:155:THR:O    | 1:A:155:THR:CG2  | 2.66                     | 0.44              |
| 1:A:156:GLY:HA3  | 2:B:531:LEU:HD23 | 2.00                     | 0.44              |
| 1:A:297:TYR:O    | 1:A:297:TYR:HD1  | 1.98                     | 0.44              |
| 2:B:588:LEU:CB   | 2:B:670:LEU:HB3  | 2.47                     | 0.44              |
| 1:A:86:VAL:HG13  | 4:A:384:HOH:O    | 2.11                     | 0.44              |
| 1:A:182:MET:CE   | 1:A:185:ARG:HB2  | 2.47                     | 0.44              |
| 1:A:296:ALA:C    | 1:A:298:ARG:H    | 2.25                     | 0.44              |
| 2:B:333:LEU:CG   | 4:B:915:HOH:O    | 2.63                     | 0.44              |
| 2:B:586:ALA:HB2  | 2:B:672:GLU:HG3  | 1.99                     | 0.44              |
| 2:B:609:LEU:HD23 | 2:B:609:LEU:C    | 2.43                     | 0.44              |
| 2:B:47:PHE:HB2   | 2:B:140:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:283:ALA:HA   | 3:A:351:MTY:CE1  | 2.47                     | 0.44              |
| 2:B:158:LEU:HD22 | 2:B:159:GLU:N    | 2.27                     | 0.44              |
| 2:B:198:LEU:O    | 2:B:200:PHE:N    | 2.44                     | 0.44              |
| 2:B:253:MET:HE1  | 2:B:355:GLU:HB3  | 2.00                     | 0.44              |
| 2:B:287:ASP:HB3  | 2:B:317:MET:HE1  | 1.99                     | 0.44              |
| 2:B:441:THR:CB   | 4:B:838:HOH:O    | 2.10                     | 0.44              |
| 2:B:587:GLY:O    | 2:B:671:PHE:CD1  | 2.71                     | 0.44              |
| 2:B:616:LEU:HD12 | 2:B:616:LEU:O    | 2.18                     | 0.44              |
| 2:B:89:LEU:C     | 2:B:89:LEU:CD2   | 2.90                     | 0.44              |
| 2:B:381:GLN:HG3  | 2:B:386:ALA:O    | 2.18                     | 0.44              |
| 2:B:507:PHE:C    | 4:B:958:HOH:O    | 2.61                     | 0.44              |
| 3:B:786:MTY:HA   | 3:B:786:MTY:HD2  | 1.67                     | 0.44              |
| 2:B:54:HIS:CD2   | 2:B:63:ARG:NH2   | 2.86                     | 0.44              |
| 2:B:198:LEU:HA   | 2:B:199:PRO:HD2  | 1.87                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:280:GLY:N    | 4:B:931:HOH:O    | 2.50                     | 0.44              |
| 2:B:315:GLY:H    | 3:B:786:MTY:HZ   | 1.82                     | 0.44              |
| 2:B:602:ARG:CZ   | 4:B:904:HOH:O    | 2.66                     | 0.44              |
| 2:B:759:GLU:O    | 2:B:763:GLU:HB3  | 2.18                     | 0.44              |
| 2:B:277:ALA:HB2  | 2:B:299:VAL:CG2  | 2.47                     | 0.43              |
| 2:B:389:ALA:C    | 2:B:391:ALA:N    | 2.76                     | 0.43              |
| 1:A:185:ARG:O    | 1:A:188:VAL:HG22 | 2.18                     | 0.43              |
| 2:B:276:ARG:HG3  | 2:B:295:PRO:O    | 2.18                     | 0.43              |
| 2:B:427:ILE:HD12 | 2:B:466:ILE:HG21 | 1.99                     | 0.43              |
| 2:B:711:GLU:HG2  | 2:B:725:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:164:PRO:HB3  | 1:A:188:VAL:CG2  | 2.48                     | 0.43              |
| 2:B:52:GLU:HG2   | 2:B:54:HIS:HE1   | 1.82                     | 0.43              |
| 2:B:115:GLY:O    | 2:B:116:MET:HB3  | 2.18                     | 0.43              |
| 2:B:615:ALA:O    | 2:B:616:LEU:C    | 2.61                     | 0.43              |
| 2:B:715:ARG:O    | 2:B:718:ALA:N    | 2.50                     | 0.43              |
| 1:A:117:LEU:HD21 | 1:A:239:GLU:HB3  | 1.99                     | 0.43              |
| 1:A:228:ILE:CG2  | 1:A:229:ALA:N    | 2.81                     | 0.43              |
| 2:B:164:ARG:O    | 2:B:167:ALA:HB3  | 2.19                     | 0.43              |
| 2:B:206:ASP:OD2  | 2:B:276:ARG:NH1  | 2.38                     | 0.43              |
| 2:B:273:ALA:N    | 2:B:301:ALA:O    | 2.43                     | 0.43              |
| 2:B:563:ASP:O    | 2:B:565:PRO:HD3  | 2.18                     | 0.43              |
| 1:A:115:ARG:NH2  | 2:B:493:ARG:HH21 | 2.17                     | 0.43              |
| 1:A:162:GLU:O    | 1:A:185:ARG:NH2  | 2.52                     | 0.43              |
| 1:A:300:ARG:C    | 1:A:301:LEU:HD12 | 2.43                     | 0.43              |
| 1:A:349:VAL:HG13 | 4:A:409:HOH:O    | 2.11                     | 0.43              |
| 2:B:197:PRO:HA   | 4:B:887:HOH:O    | 2.18                     | 0.43              |
| 2:B:294:HIS:CG   | 2:B:295:PRO:HD2  | 2.53                     | 0.43              |
| 2:B:556:LEU:O    | 2:B:560:LEU:HG   | 2.18                     | 0.43              |
| 1:A:154:LEU:CD1  | 4:A:414:HOH:O    | 2.47                     | 0.43              |
| 1:A:340:LEU:HB3  | 4:A:365:HOH:O    | 2.18                     | 0.43              |
| 2:B:45:VAL:HG11  | 2:B:123:LEU:HD11 | 2.01                     | 0.43              |
| 2:B:143:GLY:O    | 2:B:144:THR:C    | 2.59                     | 0.43              |
| 2:B:279:GLU:HG3  | 4:B:920:HOH:O    | 2.17                     | 0.43              |
| 2:B:287:ASP:OD1  | 2:B:289:VAL:HB   | 2.19                     | 0.43              |
| 2:B:497:ARG:HH22 | 2:B:619:ARG:HH12 | 1.66                     | 0.43              |
| 2:B:651:PHE:CE2  | 2:B:672:GLU:HB3  | 2.54                     | 0.43              |
| 2:B:652:LEU:HD12 | 2:B:670:LEU:O    | 2.19                     | 0.43              |
| 2:B:710:VAL:O    | 2:B:713:LEU:HB3  | 2.18                     | 0.43              |
| 1:A:331:ASP:O    | 1:A:334:TYR:HD2  | 2.02                     | 0.43              |
| 2:B:366:PRO:O    | 2:B:367:LEU:HD23 | 2.17                     | 0.43              |
| 2:B:408:PRO:HG2  | 2:B:421:GLU:HG2  | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:502:LEU:HD13 | 2:B:571:PHE:CD2  | 2.54                     | 0.43              |
| 2:B:613:LEU:CD1  | 2:B:652:LEU:HD22 | 2.48                     | 0.43              |
| 2:B:670:LEU:C    | 2:B:670:LEU:HD12 | 2.44                     | 0.43              |
| 2:B:695:ARG:O    | 2:B:696:ASP:OD1  | 2.37                     | 0.43              |
| 1:A:127:VAL:HG22 | 1:A:154:LEU:CD1  | 2.49                     | 0.43              |
| 1:A:162:GLU:H    | 1:A:162:GLU:HG2  | 1.70                     | 0.43              |
| 1:A:325:LEU:HD12 | 1:A:325:LEU:O    | 2.19                     | 0.43              |
| 2:B:49:ARG:HG2   | 2:B:137:GLU:HG3  | 2.01                     | 0.43              |
| 2:B:278:ARG:O    | 2:B:281:GLU:HB2  | 2.18                     | 0.43              |
| 2:B:690:HIS:CD2  | 2:B:754:ARG:HA   | 2.54                     | 0.43              |
| 1:A:283:ALA:CB   | 1:A:315:PHE:HA   | 2.49                     | 0.43              |
| 2:B:434:ARG:NH1  | 2:B:436:GLU:HG3  | 2.34                     | 0.43              |
| 2:B:617:PHE:O    | 2:B:618:ALA:C    | 2.61                     | 0.43              |
| 2:B:49:ARG:HH21  | 2:B:51:LEU:HD21  | 1.82                     | 0.43              |
| 2:B:344:ARG:O    | 2:B:348:ARG:HD3  | 2.19                     | 0.43              |
| 2:B:365:ASP:HB3  | 4:B:797:HOH:O    | 2.19                     | 0.43              |
| 2:B:697:LEU:HB2  | 2:B:779:LEU:HD11 | 2.01                     | 0.43              |
| 2:B:701:VAL:HG21 | 2:B:710:VAL:CG2  | 2.48                     | 0.43              |
| 1:A:207:GLN:OE1  | 1:A:207:GLN:HA   | 2.17                     | 0.42              |
| 2:B:528:PRO:CD   | 4:B:892:HOH:O    | 2.20                     | 0.42              |
| 1:A:122:VAL:O    | 1:A:122:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:140:PRO:HG2  | 1:A:143:HIS:CD2  | 2.53                     | 0.42              |
| 1:A:246:GLY:C    | 4:A:353:HOH:O    | 2.62                     | 0.42              |
| 2:B:147:SER:C    | 2:B:149:ALA:H    | 2.27                     | 0.42              |
| 2:B:412:ASN:C    | 2:B:414:LEU:N    | 2.76                     | 0.42              |
| 2:B:737:PRO:O    | 2:B:738:GLU:O    | 2.37                     | 0.42              |
| 2:B:62:LYS:NZ    | 2:B:81:ALA:HB3   | 2.34                     | 0.42              |
| 1:A:142:HIS:NE2  | 4:A:382:HOH:O    | 2.36                     | 0.42              |
| 1:A:271:TRP:HZ3  | 1:A:276:LYS:HE2  | 1.84                     | 0.42              |
| 2:B:145:PRO:HD2  | 2:B:148:GLU:OE2  | 2.19                     | 0.42              |
| 2:B:588:LEU:HD12 | 2:B:668:VAL:HG11 | 2.02                     | 0.42              |
| 1:A:191:THR:CG2  | 2:B:484:ASP:OD2  | 2.68                     | 0.42              |
| 2:B:213:PHE:HA   | 2:B:336:ALA:CB   | 2.49                     | 0.42              |
| 2:B:588:LEU:HB2  | 2:B:670:LEU:HB3  | 2.02                     | 0.42              |
| 2:B:637:GLY:N    | 4:B:908:HOH:O    | 2.48                     | 0.42              |
| 1:A:164:PRO:CG   | 1:A:188:VAL:HG21 | 2.46                     | 0.42              |
| 1:A:183:GLN:HG3  | 1:A:222:LEU:HD22 | 2.02                     | 0.42              |
| 1:A:287:HIS:ND1  | 1:A:288:PRO:CD   | 2.81                     | 0.42              |
| 1:A:306:ALA:HB3  | 1:A:307:TYR:CD1  | 2.55                     | 0.42              |
| 2:B:659:ILE:N    | 2:B:659:ILE:CD1  | 2.83                     | 0.42              |
| 1:A:280:LEU:HD12 | 1:A:317:LEU:HD22 | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:755:THR:HG22 | 2:B:756:LEU:H    | 1.85                     | 0.42              |
| 2:B:203:LYS:O    | 2:B:273:ALA:HA   | 2.19                     | 0.42              |
| 2:B:253:MET:HE1  | 2:B:355:GLU:HB2  | 2.01                     | 0.42              |
| 2:B:642:VAL:O    | 2:B:648:GLU:HA   | 2.19                     | 0.42              |
| 2:B:749:PHE:N    | 2:B:749:PHE:CD1  | 2.88                     | 0.42              |
| 1:A:151:THR:CG2  | 1:A:152:PHE:N    | 2.81                     | 0.42              |
| 1:A:191:THR:HG23 | 2:B:484:ASP:OD2  | 2.20                     | 0.42              |
| 1:A:322:LEU:C    | 1:A:324:MET:N    | 2.76                     | 0.42              |
| 2:B:707:TYR:CZ   | 2:B:711:GLU:HG3  | 2.54                     | 0.42              |
| 1:A:180:SER:N    | 1:A:181:PRO:HD2  | 2.35                     | 0.42              |
| 2:B:265:LEU:HD23 | 2:B:265:LEU:HA   | 1.93                     | 0.42              |
| 2:B:303:TRP:CD1  | 2:B:303:TRP:C    | 2.97                     | 0.42              |
| 2:B:366:PRO:C    | 2:B:367:LEU:HD23 | 2.44                     | 0.42              |
| 2:B:415:LEU:HB3  | 2:B:417:THR:HG23 | 2.01                     | 0.42              |
| 2:B:431:LEU:HD13 | 2:B:462:GLU:OE1  | 2.19                     | 0.42              |
| 2:B:456:GLU:CB   | 4:B:837:HOH:O    | 2.67                     | 0.42              |
| 2:B:630:ALA:CA   | 4:B:893:HOH:O    | 2.68                     | 0.42              |
| 2:B:634:LEU:HD11 | 2:B:651:PHE:HD1  | 1.84                     | 0.42              |
| 2:B:696:ASP:CG   | 2:B:746:HIS:HD2  | 2.28                     | 0.42              |
| 2:B:762:GLU:O    | 2:B:765:VAL:HG22 | 2.20                     | 0.42              |
| 2:B:177:LEU:O    | 2:B:180:LEU:HB2  | 2.20                     | 0.41              |
| 2:B:643:LEU:HD22 | 2:B:643:LEU:N    | 2.33                     | 0.41              |
| 2:B:743:LEU:O    | 2:B:745:PHE:HD2  | 2.03                     | 0.41              |
| 2:B:746:HIS:C    | 2:B:747:LEU:HD12 | 2.45                     | 0.41              |
| 2:B:751:HIS:CD2  | 2:B:754:ARG:CZ   | 3.03                     | 0.41              |
| 1:A:210:ALA:HB3  | 4:A:387:HOH:O    | 2.20                     | 0.41              |
| 2:B:224:ALA:O    | 2:B:244:ASN:ND2  | 2.53                     | 0.41              |
| 2:B:286:LEU:N    | 2:B:317:MET:HE2  | 2.35                     | 0.41              |
| 2:B:717:ALA:O    | 2:B:719:GLY:N    | 2.44                     | 0.41              |
| 2:B:173:LEU:O    | 2:B:175:ARG:N    | 2.53                     | 0.41              |
| 2:B:187:PRO:CG   | 4:B:948:HOH:O    | 2.38                     | 0.41              |
| 2:B:585:LEU:HB2  | 2:B:675:LEU:HD11 | 2.02                     | 0.41              |
| 1:A:127:VAL:HG22 | 1:A:154:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:349:VAL:CG1  | 1:A:350:LEU:HD23 | 2.44                     | 0.41              |
| 2:B:217:TYR:CE2  | 2:B:219:PHE:CD1  | 3.09                     | 0.41              |
| 2:B:432:GLY:C    | 2:B:447:PRO:HG3  | 2.44                     | 0.41              |
| 2:B:773:ARG:C    | 2:B:775:ARG:H    | 2.28                     | 0.41              |
| 2:B:779:LEU:CG   | 4:B:916:HOH:O    | 2.24                     | 0.41              |
| 2:B:17:SER:O     | 2:B:18:PRO:C     | 2.63                     | 0.41              |
| 2:B:99:LEU:O     | 2:B:101:GLN:N    | 2.54                     | 0.41              |
| 2:B:178:HIS:O    | 2:B:430:ARG:NH1  | 2.43                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:282:ARG:HH11 | 2:B:282:ARG:CB   | 2.25                     | 0.41              |
| 2:B:362:ARG:HG2  | 2:B:362:ARG:NH1  | 2.34                     | 0.41              |
| 2:B:404:ILE:HG22 | 2:B:405:PRO:HD2  | 2.02                     | 0.41              |
| 2:B:702:PRO:HD2  | 2:B:777:PHE:HE1  | 1.85                     | 0.41              |
| 2:B:120:PRO:HD3  | 2:B:133:LEU:HD22 | 2.01                     | 0.41              |
| 2:B:271:GLY:O    | 2:B:302:GLY:HA2  | 2.20                     | 0.41              |
| 2:B:315:GLY:O    | 2:B:316:VAL:HG23 | 2.21                     | 0.41              |
| 2:B:387:ARG:CA   | 4:B:825:HOH:O    | 2.69                     | 0.41              |
| 2:B:412:ASN:O    | 2:B:413:ARG:C    | 2.64                     | 0.41              |
| 2:B:434:ARG:NH1  | 2:B:436:GLU:CG   | 2.82                     | 0.41              |
| 2:B:690:HIS:HB3  | 2:B:691:PRO:HD2  | 2.02                     | 0.41              |
| 1:A:215:VAL:HG21 | 2:B:513:TYR:CD1  | 2.56                     | 0.41              |
| 2:B:101:GLN:HA   | 2:B:101:GLN:NE2  | 2.35                     | 0.41              |
| 2:B:243:ASN:ND2  | 4:B:880:HOH:O    | 2.18                     | 0.41              |
| 2:B:475:ALA:O    | 2:B:476:LEU:HD23 | 2.20                     | 0.41              |
| 2:B:504:GLY:O    | 2:B:506:GLY:N    | 2.54                     | 0.41              |
| 2:B:548:LEU:HD21 | 2:B:574:GLY:N    | 2.35                     | 0.41              |
| 2:B:699:VAL:CG2  | 2:B:772:LEU:HD21 | 2.50                     | 0.41              |
| 2:B:470:GLU:H    | 2:B:470:GLU:HG3  | 1.60                     | 0.41              |
| 2:B:587:GLY:O    | 2:B:671:PHE:HD1  | 2.02                     | 0.41              |
| 2:B:619:ARG:HD2  | 2:B:619:ARG:C    | 2.45                     | 0.41              |
| 1:A:115:ARG:HH21 | 2:B:493:ARG:HE   | 1.69                     | 0.41              |
| 1:A:140:PRO:CG   | 1:A:143:HIS:CD2  | 3.04                     | 0.41              |
| 1:A:143:HIS:CE1  | 1:A:145:ALA:HB2  | 2.56                     | 0.41              |
| 2:B:224:ALA:C    | 2:B:244:ASN:ND2  | 2.79                     | 0.41              |
| 2:B:232:ARG:CZ   | 4:B:909:HOH:O    | 2.69                     | 0.41              |
| 2:B:339:ASP:O    | 2:B:343:ILE:HG12 | 2.20                     | 0.41              |
| 2:B:533:LEU:HD12 | 2:B:533:LEU:N    | 2.35                     | 0.41              |
| 2:B:578:ARG:C    | 2:B:580:ARG:H    | 2.29                     | 0.41              |
| 2:B:613:LEU:HD12 | 2:B:652:LEU:HD22 | 2.03                     | 0.41              |
| 2:B:654:ALA:HA   | 2:B:669:HIS:HA   | 2.02                     | 0.41              |
| 2:B:770:GLU:CG   | 4:B:822:HOH:O    | 2.69                     | 0.41              |
| 2:B:93:GLY:N     | 2:B:103:VAL:O    | 2.32                     | 0.41              |
| 2:B:243:ASN:HB3  | 4:B:880:HOH:O    | 2.20                     | 0.41              |
| 2:B:253:MET:HE1  | 2:B:356:ALA:N    | 2.35                     | 0.41              |
| 2:B:504:GLY:O    | 2:B:505:LEU:C    | 2.63                     | 0.41              |
| 2:B:589:LEU:HB3  | 2:B:669:HIS:HB2  | 2.02                     | 0.41              |
| 2:B:592:GLU:C    | 2:B:602:ARG:HD3  | 2.46                     | 0.41              |
| 2:B:617:PHE:O    | 2:B:621:GLY:N    | 2.53                     | 0.41              |
| 2:B:736:LEU:O    | 2:B:738:GLU:N    | 2.54                     | 0.41              |
| 1:A:142:HIS:N    | 4:A:370:HOH:O    | 2.38                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:VAL:CG2  | 1:A:216:PHE:O    | 2.69                     | 0.40              |
| 2:B:169:GLY:HA2  | 2:B:254:LEU:O    | 2.22                     | 0.40              |
| 2:B:268:VAL:HG13 | 2:B:272:ILE:CD1  | 2.51                     | 0.40              |
| 2:B:315:GLY:H    | 3:B:786:MTY:CZ   | 2.34                     | 0.40              |
| 1:A:298:ARG:HG3  | 4:A:362:HOH:O    | 2.03                     | 0.40              |
| 2:B:160:VAL:HG13 | 2:B:167:ALA:CB   | 2.51                     | 0.40              |
| 2:B:269:GLY:HA2  | 4:B:885:HOH:O    | 2.21                     | 0.40              |
| 2:B:474:LEU:N    | 2:B:474:LEU:HD12 | 2.35                     | 0.40              |
| 1:A:201:ARG:HD2  | 1:A:215:VAL:CG1  | 2.52                     | 0.40              |
| 1:A:209:ASP:OD1  | 1:A:209:ASP:C    | 2.64                     | 0.40              |
| 2:B:691:PRO:CA   | 4:B:913:HOH:O    | 2.58                     | 0.40              |
| 2:B:709:GLU:CA   | 4:B:956:HOH:O    | 2.59                     | 0.40              |
| 1:A:173:LEU:HB2  | 4:A:414:HOH:O    | 2.01                     | 0.40              |
| 2:B:589:LEU:HG   | 4:B:823:HOH:O    | 2.21                     | 0.40              |
| 2:B:656:HIS:HA   | 2:B:657:PRO:HD3  | 1.95                     | 0.40              |
| 2:B:704:PRO:O    | 2:B:705:THR:C    | 2.64                     | 0.40              |
| 2:B:725:LEU:C    | 2:B:725:LEU:HD23 | 2.47                     | 0.40              |
| 1:A:197:VAL:CG2  | 1:A:219:LEU:HD21 | 2.51                     | 0.40              |
| 2:B:56:ILE:HB    | 2:B:59:THR:OG1   | 2.21                     | 0.40              |
| 2:B:192:LYS:N    | 2:B:381:GLN:HE22 | 2.19                     | 0.40              |
| 2:B:458:ASP:O    | 2:B:462:GLU:HG2  | 2.21                     | 0.40              |
| 2:B:496:GLN:O    | 2:B:497:ARG:C    | 2.64                     | 0.40              |

All (1) 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:B:110:GLY:O | 4:B:808:HOH:O[5_565] | 2.13                     | 0.07              |

## 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     | 264/350 (75%)   | 223 (84%) | 25 (10%)  | 16 (6%)  | 1           | 4  |
| 2   | B     | 783/785 (100%)  | 654 (84%) | 102 (13%) | 27 (3%)  | 3           | 12 |
| All | All   | 1047/1135 (92%) | 877 (84%) | 127 (12%) | 43 (4%)  | 2           | 9  |

All (43) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 93  | ALA  |
| 1   | A     | 94  | SER  |
| 1   | A     | 319 | VAL  |
| 1   | A     | 320 | GLU  |
| 1   | A     | 349 | VAL  |
| 2   | B     | 244 | ASN  |
| 2   | B     | 390 | GLU  |
| 2   | B     | 590 | PHE  |
| 2   | B     | 738 | GLU  |
| 1   | A     | 87  | ASP  |
| 1   | A     | 130 | GLU  |
| 1   | A     | 164 | PRO  |
| 1   | A     | 227 | GLY  |
| 1   | A     | 323 | ALA  |
| 2   | B     | 100 | GLY  |
| 2   | B     | 174 | ALA  |
| 2   | B     | 293 | LEU  |
| 2   | B     | 316 | VAL  |
| 2   | B     | 413 | ARG  |
| 2   | B     | 505 | LEU  |
| 2   | B     | 560 | LEU  |
| 2   | B     | 578 | ARG  |
| 2   | B     | 718 | ALA  |
| 2   | B     | 719 | GLY  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 322 | LEU  |
| 2   | B     | 488 | VAL  |
| 2   | B     | 616 | LEU  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 341 | LYS  |
| 2   | B     | 81  | ALA  |
| 2   | B     | 132 | LEU  |
| 2   | B     | 440 | PRO  |
| 2   | B     | 716 | GLU  |
| 2   | B     | 42  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 148 | GLU  |
| 2   | B     | 386 | ALA  |
| 2   | B     | 433 | CYS  |
| 1   | A     | 345 | GLN  |
| 2   | B     | 52  | GLU  |
| 1   | A     | 98  | GLY  |
| 2   | B     | 199 | PRO  |
| 2   | B     | 245 | VAL  |

### 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     | 214/277 (77%)  | 184 (86%) | 30 (14%) | 3           | 11 |
| 2   | B     | 630/630 (100%) | 577 (92%) | 53 (8%)  | 10          | 31 |
| All | All   | 844/907 (93%)  | 761 (90%) | 83 (10%) | 7           | 25 |

All (83) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 90  | LEU  |
| 1   | A     | 104 | THR  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 126 | GLU  |
| 1   | A     | 128 | GLU  |
| 1   | A     | 129 | SER  |
| 1   | A     | 161 | LEU  |
| 1   | A     | 162 | GLU  |
| 1   | A     | 169 | VAL  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 178 | HIS  |
| 1   | A     | 179 | THR  |
| 1   | A     | 191 | THR  |
| 1   | A     | 196 | ILE  |
| 1   | A     | 198 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 203 | PHE  |
| 1   | A     | 207 | GLN  |
| 1   | A     | 208 | THR  |
| 1   | A     | 213 | GLU  |
| 1   | A     | 219 | LEU  |
| 1   | A     | 256 | VAL  |
| 1   | A     | 260 | PHE  |
| 1   | A     | 280 | LEU  |
| 1   | A     | 307 | TYR  |
| 1   | A     | 308 | ARG  |
| 1   | A     | 311 | THR  |
| 1   | A     | 325 | LEU  |
| 1   | A     | 329 | ILE  |
| 1   | A     | 332 | ILE  |
| 1   | A     | 341 | LYS  |
| 2   | B     | 12  | VAL  |
| 2   | B     | 18  | PRO  |
| 2   | B     | 32  | THR  |
| 2   | B     | 62  | LYS  |
| 2   | B     | 80  | ASN  |
| 2   | B     | 87  | VAL  |
| 2   | B     | 89  | LEU  |
| 2   | B     | 111 | VAL  |
| 2   | B     | 118 | LEU  |
| 2   | B     | 136 | PRO  |
| 2   | B     | 147 | SER  |
| 2   | B     | 158 | LEU  |
| 2   | B     | 159 | GLU  |
| 2   | B     | 170 | LEU  |
| 2   | B     | 171 | LEU  |
| 2   | B     | 173 | LEU  |
| 2   | B     | 176 | ASP  |
| 2   | B     | 180 | LEU  |
| 2   | B     | 184 | LEU  |
| 2   | B     | 285 | THR  |
| 2   | B     | 298 | LEU  |
| 2   | B     | 313 | LEU  |
| 2   | B     | 322 | SER  |
| 2   | B     | 323 | GLU  |
| 2   | B     | 333 | LEU  |
| 2   | B     | 340 | PRO  |
| 2   | B     | 375 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 383 | LEU  |
| 2   | B     | 393 | LEU  |
| 2   | B     | 404 | ILE  |
| 2   | B     | 407 | ARG  |
| 2   | B     | 441 | THR  |
| 2   | B     | 467 | GLN  |
| 2   | B     | 470 | GLU  |
| 2   | B     | 488 | VAL  |
| 2   | B     | 510 | VAL  |
| 2   | B     | 548 | LEU  |
| 2   | B     | 549 | PHE  |
| 2   | B     | 556 | LEU  |
| 2   | B     | 562 | LEU  |
| 2   | B     | 576 | VAL  |
| 2   | B     | 578 | ARG  |
| 2   | B     | 584 | HIS  |
| 2   | B     | 588 | LEU  |
| 2   | B     | 600 | LYS  |
| 2   | B     | 602 | ARG  |
| 2   | B     | 619 | ARG  |
| 2   | B     | 624 | PHE  |
| 2   | B     | 659 | ILE  |
| 2   | B     | 673 | LEU  |
| 2   | B     | 695 | ARG  |
| 2   | B     | 696 | ASP  |
| 2   | B     | 711 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 142 | HIS  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 190 | HIS  |
| 1   | A     | 218 | GLN  |
| 1   | A     | 232 | HIS  |
| 2   | B     | 54  | HIS  |
| 2   | B     | 80  | ASN  |
| 2   | B     | 101 | GLN  |
| 2   | B     | 178 | HIS  |
| 2   | B     | 231 | GLN  |
| 2   | B     | 244 | ASN  |
| 2   | B     | 258 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 350 | HIS  |
| 2   | B     | 381 | GLN  |
| 2   | B     | 467 | GLN  |
| 2   | B     | 496 | GLN  |
| 2   | B     | 584 | HIS  |
| 2   | B     | 629 | GLN  |
| 2   | B     | 669 | HIS  |
| 2   | B     | 746 | HIS  |

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | MTY  | A     | 351 | -    | 12,13,13     | 0.45 | 0           | 13,17,17    | 0.92 | 1 (7%)      |
| 3   | MTY  | B     | 786 | -    | 12,13,13     | 0.62 | 0           | 13,17,17    | 0.83 | 1 (7%)      |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 3   | MTY  | A     | 351 | -    | -       | 0/8/8/8  | 0/1/1/1 |
| 3   | MTY  | B     | 786 | -    | -       | 6/8/8/8  | 0/1/1/1 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | B     | 786 | MTY  | CG-CB-CA | -2.56 | 108.89      | 114.13   |
| 3   | A     | 351 | MTY  | CG-CB-CA | -2.26 | 109.51      | 114.13   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 3   | B     | 786 | MTY  | CA-CB-CG-CD2 |
| 3   | B     | 786 | MTY  | CA-CB-CG-CD1 |
| 3   | B     | 786 | MTY  | N-CA-CB-CG   |
| 3   | B     | 786 | MTY  | OXT-C-CA-CB  |
| 3   | B     | 786 | MTY  | O-C-CA-CB    |
| 3   | B     | 786 | MTY  | C-CA-CB-CG   |

There are no ring outliers.

2 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 351 | MTY  | 8       | 0            |
| 3   | B     | 786 | MTY  | 11      | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 265/350 (75%)   | 0.73   | 23 (8%) 16 13  | 29, 61, 94, 104       | 0     |
| 2   | B     | 779/785 (99%)   | 0.83   | 90 (11%) 9 8   | 35, 66, 119, 120      | 0     |
| All | All   | 1044/1135 (91%) | 0.80   | 113 (10%) 11 9 | 29, 65, 115, 120      | 0     |

All (113) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 350 | LEU  | 6.4  |
| 1   | A     | 86  | VAL  | 5.5  |
| 2   | B     | 98  | GLY  | 5.4  |
| 1   | A     | 143 | HIS  | 5.0  |
| 2   | B     | 739 | GLY  | 4.7  |
| 1   | A     | 157 | GLU  | 4.5  |
| 2   | B     | 689 | ARG  | 4.5  |
| 2   | B     | 736 | LEU  | 4.2  |
| 2   | B     | 738 | GLU  | 4.2  |
| 2   | B     | 278 | ARG  | 4.1  |
| 2   | B     | 720 | PRO  | 4.1  |
| 2   | B     | 734 | PRO  | 3.9  |
| 2   | B     | 779 | LEU  | 3.9  |
| 2   | B     | 698 | ALA  | 3.9  |
| 2   | B     | 735 | PRO  | 3.9  |
| 2   | B     | 737 | PRO  | 3.8  |
| 1   | A     | 158 | GLY  | 3.7  |
| 2   | B     | 701 | VAL  | 3.6  |
| 2   | B     | 564 | ARG  | 3.6  |
| 2   | B     | 694 | PHE  | 3.5  |
| 2   | B     | 726 | ALA  | 3.5  |
| 1   | A     | 349 | VAL  | 3.4  |
| 1   | A     | 144 | PRO  | 3.4  |
| 2   | B     | 724 | SER  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 745 | PHE  | 3.3  |
| 2   | B     | 99  | LEU  | 3.2  |
| 2   | B     | 731 | TYR  | 3.2  |
| 2   | B     | 102 | LYS  | 3.2  |
| 2   | B     | 691 | PRO  | 3.1  |
| 2   | B     | 707 | TYR  | 3.0  |
| 2   | B     | 749 | PHE  | 3.0  |
| 2   | B     | 768 | VAL  | 3.0  |
| 2   | B     | 755 | THR  | 3.0  |
| 2   | B     | 598 | TRP  | 3.0  |
| 2   | B     | 722 | LEU  | 3.0  |
| 2   | B     | 759 | GLU  | 3.0  |
| 2   | B     | 577 | PHE  | 2.9  |
| 2   | B     | 769 | ALA  | 2.9  |
| 1   | A     | 339 | ARG  | 2.9  |
| 2   | B     | 774 | ALA  | 2.9  |
| 2   | B     | 308 | SER  | 2.8  |
| 2   | B     | 101 | GLN  | 2.8  |
| 2   | B     | 723 | GLU  | 2.8  |
| 2   | B     | 750 | ARG  | 2.8  |
| 2   | B     | 703 | ALA  | 2.8  |
| 2   | B     | 752 | PRO  | 2.8  |
| 2   | B     | 348 | ARG  | 2.7  |
| 2   | B     | 486 | ARG  | 2.7  |
| 2   | B     | 636 | PRO  | 2.7  |
| 2   | B     | 279 | GLU  | 2.7  |
| 2   | B     | 307 | GLU  | 2.7  |
| 2   | B     | 688 | SER  | 2.7  |
| 1   | A     | 208 | THR  | 2.6  |
| 1   | A     | 168 | GLU  | 2.6  |
| 2   | B     | 727 | LEU  | 2.6  |
| 2   | B     | 374 | ARG  | 2.6  |
| 2   | B     | 541 | LYS  | 2.6  |
| 2   | B     | 747 | LEU  | 2.6  |
| 2   | B     | 596 | LEU  | 2.5  |
| 2   | B     | 190 | ALA  | 2.5  |
| 2   | B     | 743 | LEU  | 2.5  |
| 2   | B     | 756 | LEU  | 2.5  |
| 1   | A     | 172 | ARG  | 2.5  |
| 1   | A     | 300 | ARG  | 2.5  |
| 1   | A     | 273 | GLU  | 2.4  |
| 2   | B     | 159 | GLU  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 718 | ALA  | 2.4  |
| 2   | B     | 443 | ARG  | 2.4  |
| 2   | B     | 208 | GLU  | 2.4  |
| 2   | B     | 595 | GLY  | 2.4  |
| 1   | A     | 141 | GLU  | 2.3  |
| 2   | B     | 732 | GLN  | 2.3  |
| 1   | A     | 308 | ARG  | 2.3  |
| 2   | B     | 325 | ARG  | 2.3  |
| 2   | B     | 668 | VAL  | 2.3  |
| 2   | B     | 592 | GLU  | 2.3  |
| 2   | B     | 697 | LEU  | 2.3  |
| 2   | B     | 690 | HIS  | 2.3  |
| 1   | A     | 321 | ARG  | 2.3  |
| 2   | B     | 625 | ARG  | 2.3  |
| 1   | A     | 334 | TYR  | 2.3  |
| 1   | A     | 299 | GLU  | 2.2  |
| 2   | B     | 630 | ALA  | 2.2  |
| 2   | B     | 709 | GLU  | 2.2  |
| 2   | B     | 682 | LEU  | 2.2  |
| 2   | B     | 97  | PRO  | 2.2  |
| 2   | B     | 778 | GLY  | 2.2  |
| 2   | B     | 680 | LYS  | 2.2  |
| 2   | B     | 725 | LEU  | 2.2  |
| 2   | B     | 692 | ALA  | 2.2  |
| 2   | B     | 60  | ARG  | 2.2  |
| 1   | A     | 142 | HIS  | 2.2  |
| 1   | A     | 148 | MET  | 2.2  |
| 2   | B     | 445 | THR  | 2.2  |
| 2   | B     | 663 | LEU  | 2.2  |
| 2   | B     | 497 | ARG  | 2.1  |
| 2   | B     | 530 | ARG  | 2.1  |
| 2   | B     | 719 | GLY  | 2.1  |
| 2   | B     | 721 | TYR  | 2.1  |
| 2   | B     | 742 | SER  | 2.1  |
| 2   | B     | 434 | ARG  | 2.1  |
| 2   | B     | 597 | PRO  | 2.1  |
| 2   | B     | 706 | PRO  | 2.1  |
| 2   | B     | 282 | ARG  | 2.1  |
| 1   | A     | 95  | LEU  | 2.1  |
| 1   | A     | 206 | GLU  | 2.1  |
| 2   | B     | 638 | VAL  | 2.1  |
| 2   | B     | 34  | ARG  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 525 | ARG  | 2.1  |
| 2   | B     | 699 | VAL  | 2.0  |
| 2   | B     | 599 | ALA  | 2.0  |
| 1   | A     | 169 | VAL  | 2.0  |
| 2   | B     | 589 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | MTY  | B     | 786 | 13/13 | 0.87 | 0.34 | 20,20,20,20                | 0     |
| 3   | MTY  | A     | 351 | 13/13 | 0.94 | 0.22 | 20,20,20,20                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.