



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 PM UTC

PDB ID : 1Z3H / pdb\_00001z3h  
Title : The exportin Cse1 in its cargo-free, cytoplasmic state  
Authors : Cook, A.; Fernandez, E.; Lindner, D.; Ebert, J.; Schlenstedt, G.; Conti, E.  
Deposited on : 2005-03-12  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

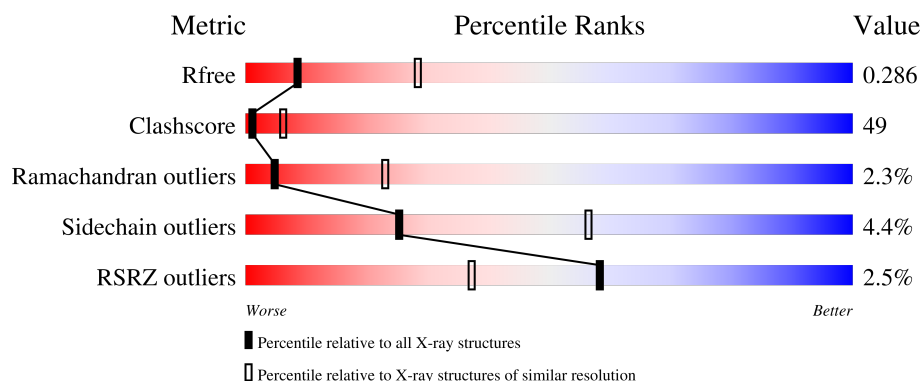
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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     | 968    |                  |
| 1   | B     | 968    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14787 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 Importin alpha re-exporter.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 925      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7435  | 4818 | 1208 | 1391 | 18 |         |         |       |
| 1   | B     | 914      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7351  | 4774 | 1189 | 1370 | 18 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 961     | ARG      | -      | expression tag | UNP P33307 |
| A     | 962     | SER      | -      | expression tag | UNP P33307 |
| A     | 963     | HIS      | -      | expression tag | UNP P33307 |
| A     | 964     | HIS      | -      | expression tag | UNP P33307 |
| A     | 965     | HIS      | -      | expression tag | UNP P33307 |
| A     | 966     | HIS      | -      | expression tag | UNP P33307 |
| A     | 967     | HIS      | -      | expression tag | UNP P33307 |
| A     | 968     | HIS      | -      | expression tag | UNP P33307 |
| B     | 961     | ARG      | -      | expression tag | UNP P33307 |
| B     | 962     | SER      | -      | expression tag | UNP P33307 |
| B     | 963     | HIS      | -      | expression tag | UNP P33307 |
| B     | 964     | HIS      | -      | expression tag | UNP P33307 |
| B     | 965     | HIS      | -      | expression tag | UNP P33307 |
| B     | 966     | HIS      | -      | expression tag | UNP P33307 |
| B     | 967     | HIS      | -      | expression tag | UNP P33307 |
| B     | 968     | HIS      | -      | expression tag | UNP P33307 |

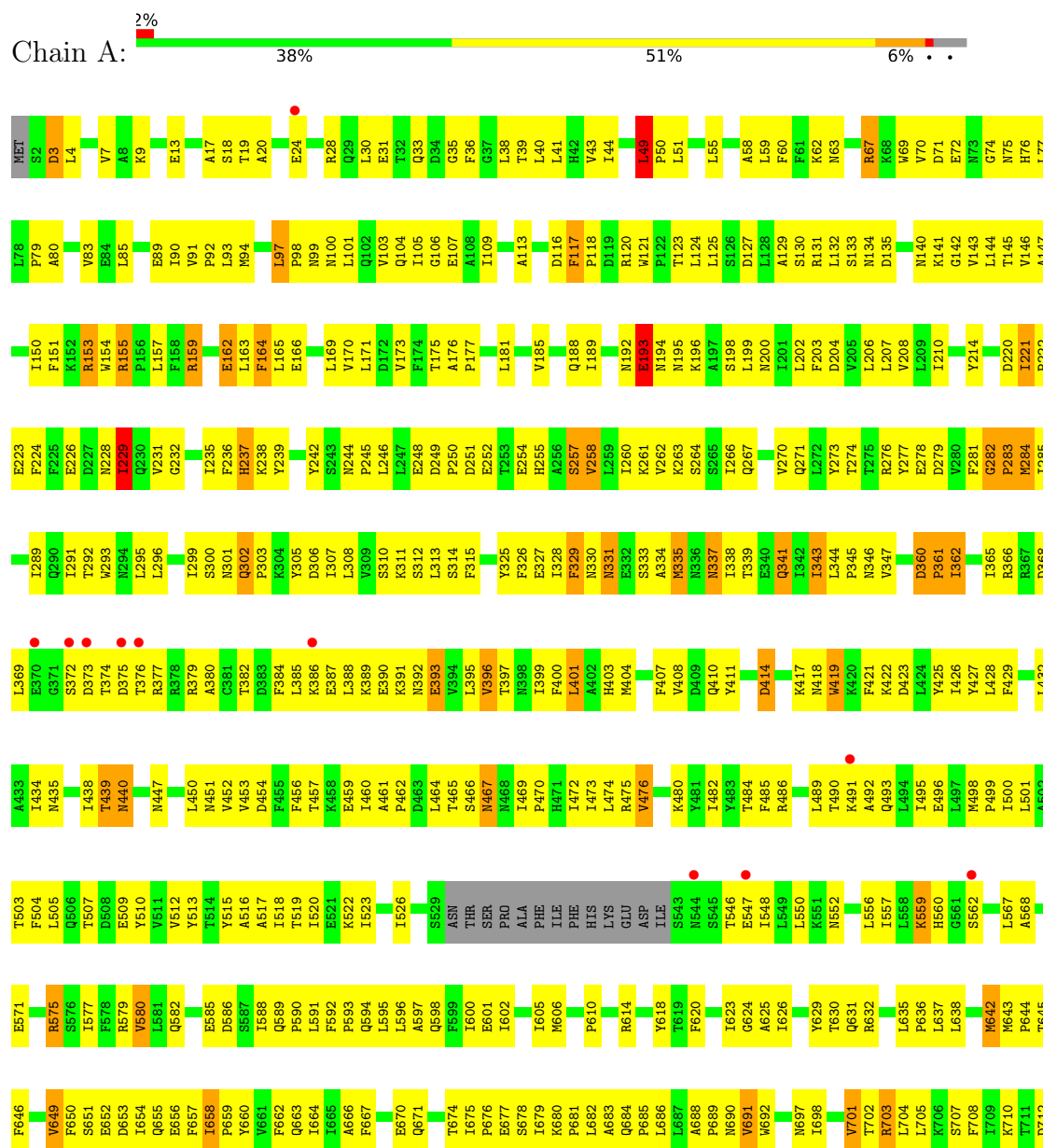
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

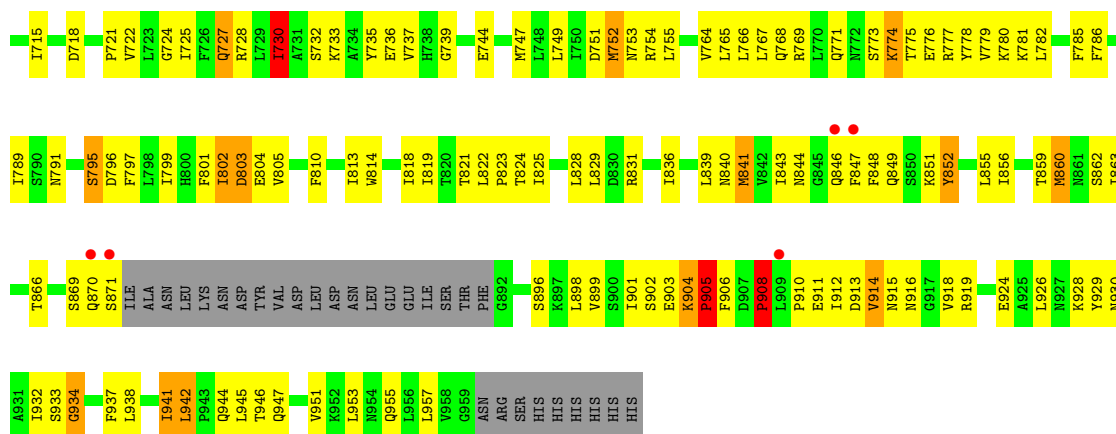
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

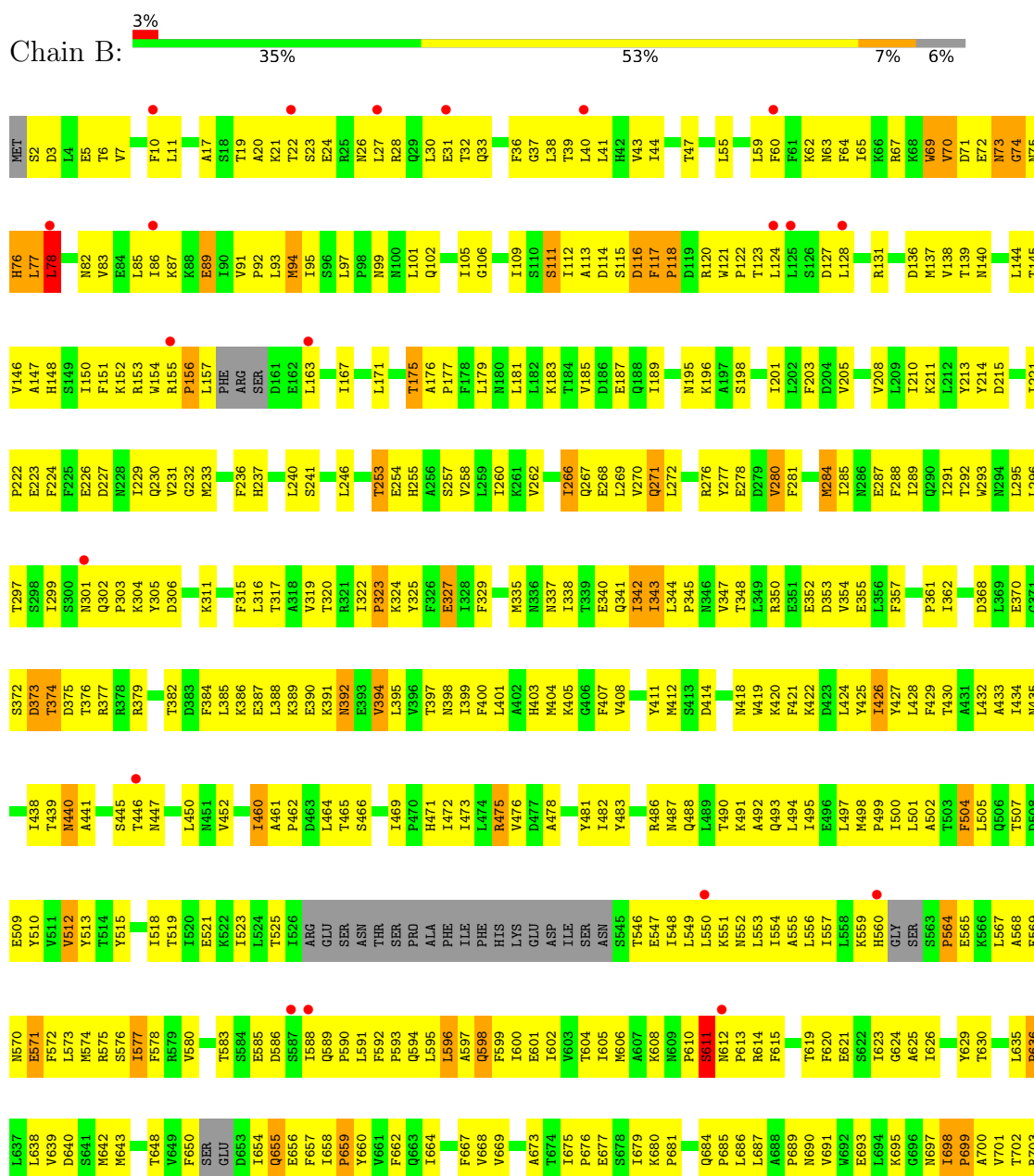
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

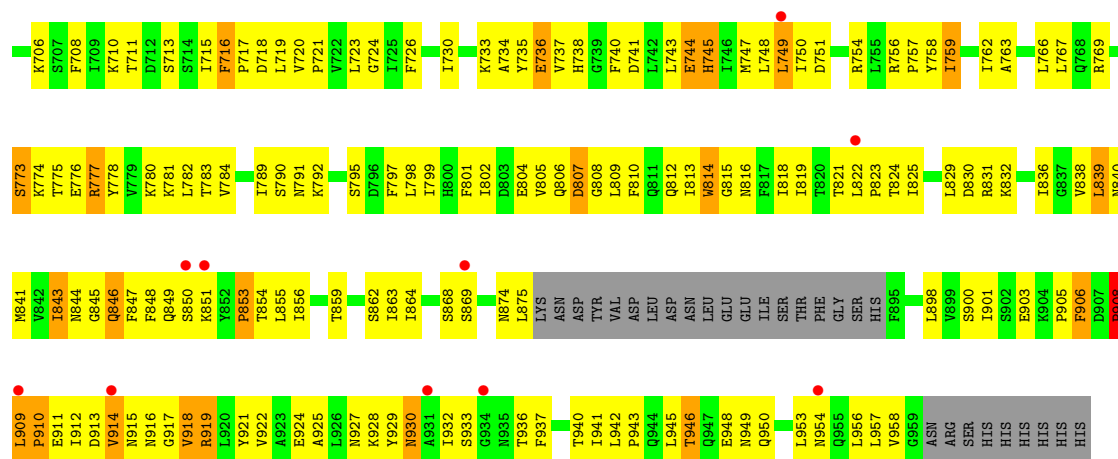
#### • Molecule 1: Importin alpha re-exporter





• Molecule 1: Importin alpha re-exporter





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 162.52Å 113.04Å 122.97Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 122.00 – 3.10<br>122.00 – 3.10                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (122.00-3.10)<br>99.6 (122.00-3.10)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.39 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.241 , 0.288<br>0.239 , 0.286                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2291 reflections (4.99%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 75.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.499                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 71.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 14787                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 77.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.65         | 3/7584 (0.0%)   | 1.14        | 46/10306 (0.4%)  |
| 1   | B     | 0.74         | 13/7495 (0.2%)  | 1.16        | 55/10185 (0.5%)  |
| All | All   | 0.70         | 16/15079 (0.1%) | 1.15        | 101/20491 (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   | B     | 0                   | 3                   |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 807 | ASP  | C-O   | -30.95 | 0.84        | 1.24     |
| 1   | B     | 807 | ASP  | CA-C  | 10.73  | 1.67        | 1.52     |
| 1   | B     | 807 | ASP  | C-N   | 10.64  | 1.49        | 1.33     |
| 1   | B     | 908 | PRO  | CA-C  | -10.28 | 1.41        | 1.52     |
| 1   | B     | 73  | ASN  | C-O   | -10.06 | 1.11        | 1.23     |
| 1   | B     | 73  | ASN  | CA-C  | 9.76   | 1.64        | 1.53     |
| 1   | B     | 808 | GLY  | N-CA  | 7.56   | 1.56        | 1.45     |
| 1   | B     | 73  | ASN  | N-CA  | -7.23  | 1.37        | 1.47     |
| 1   | B     | 611 | SER  | C-N   | 6.68   | 1.42        | 1.33     |
| 1   | B     | 909 | LEU  | C-N   | 6.45   | 1.41        | 1.34     |
| 1   | B     | 74  | GLY  | N-CA  | 6.42   | 1.54        | 1.45     |
| 1   | B     | 73  | ASN  | CA-CB | 6.41   | 1.63        | 1.52     |
| 1   | A     | 310 | SER  | C-N   | 5.28   | 1.41        | 1.34     |
| 1   | B     | 868 | SER  | CA-C  | -5.14  | 1.47        | 1.53     |
| 1   | A     | 658 | ILE  | CA-CB | -5.11  | 1.51        | 1.54     |
| 1   | A     | 155 | ARG  | N-CA  | -5.11  | 1.41        | 1.46     |



All (101) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | B     | 73  | ASN  | O-C-N   | -21.84 | 93.36       | 123.06   |
| 1   | B     | 807 | ASP  | CA-C-O  | 13.41  | 139.69      | 120.51   |
| 1   | A     | 908 | PRO  | CA-N-CD | -11.85 | 95.41       | 112.00   |
| 1   | B     | 807 | ASP  | N-CA-C  | 11.27  | 134.81      | 110.80   |
| 1   | B     | 918 | VAL  | N-CA-C  | -10.77 | 103.07      | 112.12   |
| 1   | B     | 342 | ILE  | N-CA-C  | 10.14  | 119.96      | 110.42   |
| 1   | B     | 73  | ASN  | CB-CA-C | -9.82  | 98.27       | 111.82   |
| 1   | B     | 78  | LEU  | N-CA-C  | -9.80  | 99.31       | 108.13   |
| 1   | B     | 807 | ASP  | CA-C-N  | -9.39  | 103.00      | 121.41   |
| 1   | B     | 807 | ASP  | C-N-CA  | -9.39  | 103.00      | 121.41   |
| 1   | B     | 909 | LEU  | CB-CA-C | 9.18   | 124.51      | 109.46   |
| 1   | B     | 343 | ILE  | N-CA-C  | 8.91   | 119.71      | 110.62   |
| 1   | A     | 329 | PHE  | N-CA-C  | -8.10  | 102.86      | 114.12   |
| 1   | B     | 240 | LEU  | N-CA-C  | -8.05  | 103.46      | 113.28   |
| 1   | A     | 426 | ILE  | N-CA-C  | -7.49  | 102.98      | 110.62   |
| 1   | B     | 440 | ASN  | N-CA-C  | -7.26  | 104.56      | 113.19   |
| 1   | B     | 909 | LEU  | N-CA-C  | -7.21  | 99.82       | 109.84   |
| 1   | B     | 736 | GLU  | N-CA-C  | -7.20  | 103.75      | 112.54   |
| 1   | B     | 698 | ILE  | CB-CA-C | -7.07  | 106.98      | 113.70   |
| 1   | A     | 229 | ILE  | N-CA-C  | 7.03   | 117.17      | 110.42   |
| 1   | A     | 335 | MET  | N-CA-C  | -7.01  | 102.85      | 111.40   |
| 1   | B     | 254 | GLU  | N-CA-C  | 7.01   | 118.57      | 111.07   |
| 1   | A     | 310 | SER  | O-C-N   | 6.99   | 131.89      | 122.59   |
| 1   | A     | 771 | GLN  | N-CA-C  | 6.98   | 119.78      | 111.33   |
| 1   | A     | 3   | ASP  | N-CA-C  | -6.97  | 103.37      | 110.97   |
| 1   | A     | 90  | ILE  | N-CA-C  | 6.78   | 118.35      | 110.62   |
| 1   | A     | 782 | LEU  | N-CA-C  | -6.74  | 103.62      | 110.97   |
| 1   | B     | 460 | ILE  | N-CA-C  | 6.70   | 116.82      | 110.53   |
| 1   | B     | 908 | PRO  | CA-N-CD | -6.68  | 102.64      | 112.00   |
| 1   | B     | 807 | ASP  | CB-CA-C | -6.63  | 97.22       | 110.42   |
| 1   | B     | 89  | GLU  | N-CA-C  | 6.59   | 119.47      | 111.82   |
| 1   | A     | 302 | GLN  | N-CA-C  | 6.54   | 119.11      | 109.50   |
| 1   | A     | 343 | ILE  | N-CA-C  | 6.53   | 116.56      | 110.42   |
| 1   | B     | 266 | ILE  | N-CA-C  | -6.49  | 103.20      | 112.35   |
| 1   | A     | 97  | LEU  | CA-C-N  | 6.31   | 126.22      | 119.85   |
| 1   | A     | 97  | LEU  | C-N-CA  | 6.31   | 126.22      | 119.85   |
| 1   | B     | 426 | ILE  | N-CA-C  | -6.29  | 104.37      | 110.72   |
| 1   | B     | 17  | ALA  | N-CA-C  | 6.20   | 118.83      | 111.33   |
| 1   | B     | 919 | ARG  | N-CA-C  | -6.14  | 104.59      | 111.28   |
| 1   | A     | 255 | HIS  | N-CA-C  | 6.09   | 118.66      | 108.73   |
| 1   | A     | 703 | ARG  | N-CA-C  | -6.07  | 104.22      | 111.69   |
| 1   | A     | 852 | TYR  | CA-C-N  | 6.03   | 125.24      | 118.97   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 852 | TYR  | C-N-CA  | 6.03  | 125.24      | 118.97   |
| 1   | B     | 614 | ARG  | O-C-N   | -6.02 | 115.74      | 122.12   |
| 1   | A     | 649 | VAL  | N-CA-C  | -5.86 | 104.80      | 110.72   |
| 1   | B     | 390 | GLU  | N-CA-C  | -5.83 | 104.92      | 111.28   |
| 1   | B     | 614 | ARG  | N-CA-C  | 5.81  | 117.61      | 111.28   |
| 1   | B     | 237 | HIS  | N-CA-C  | -5.80 | 105.03      | 111.36   |
| 1   | B     | 914 | VAL  | CB-CA-C | -5.79 | 101.80      | 111.29   |
| 1   | B     | 355 | GLU  | N-CA-C  | -5.78 | 104.89      | 111.07   |
| 1   | A     | 302 | GLN  | CA-C-N  | 5.77  | 125.90      | 119.32   |
| 1   | A     | 302 | GLN  | C-N-CA  | 5.77  | 125.90      | 119.32   |
| 1   | B     | 512 | VAL  | N-CA-C  | 5.75  | 115.93      | 110.53   |
| 1   | A     | 452 | VAL  | N-CA-C  | 5.65  | 117.06      | 110.62   |
| 1   | A     | 154 | TRP  | N-CA-C  | -5.54 | 107.17      | 114.04   |
| 1   | B     | 583 | THR  | N-CA-C  | -5.53 | 104.07      | 112.04   |
| 1   | A     | 258 | VAL  | N-CA-C  | -5.48 | 105.03      | 111.00   |
| 1   | B     | 846 | GLN  | CA-C-N  | 5.42  | 127.99      | 120.29   |
| 1   | B     | 846 | GLN  | C-N-CA  | 5.42  | 127.99      | 120.29   |
| 1   | B     | 777 | ARG  | N-CA-C  | -5.42 | 104.24      | 112.04   |
| 1   | B     | 179 | LEU  | N-CA-C  | 5.42  | 116.87      | 111.07   |
| 1   | A     | 910 | PRO  | N-CA-C  | 5.40  | 122.53      | 113.78   |
| 1   | B     | 111 | SER  | N-CA-C  | -5.38 | 105.06      | 111.03   |
| 1   | B     | 749 | LEU  | N-CA-C  | 5.37  | 118.84      | 112.72   |
| 1   | B     | 716 | PHE  | CA-C-N  | 5.36  | 125.00      | 119.05   |
| 1   | B     | 716 | PHE  | C-N-CA  | 5.36  | 125.00      | 119.05   |
| 1   | A     | 744 | GLU  | N-CA-C  | -5.36 | 104.68      | 111.11   |
| 1   | A     | 423 | ASP  | N-CA-C  | -5.33 | 105.37      | 111.07   |
| 1   | B     | 946 | THR  | N-CA-C  | -5.31 | 103.12      | 110.35   |
| 1   | B     | 839 | LEU  | N-CA-C  | -5.30 | 105.50      | 111.28   |
| 1   | B     | 255 | HIS  | N-CA-C  | 5.27  | 117.42      | 109.41   |
| 1   | A     | 779 | VAL  | N-CA-C  | 5.26  | 115.88      | 110.36   |
| 1   | B     | 908 | PRO  | CB-CA-C | -5.22 | 103.03      | 110.75   |
| 1   | A     | 360 | ASP  | CA-C-N  | 5.20  | 126.34      | 119.84   |
| 1   | A     | 360 | ASP  | C-N-CA  | 5.20  | 126.34      | 119.84   |
| 1   | A     | 911 | GLU  | N-CA-C  | 5.17  | 118.37      | 111.75   |
| 1   | B     | 759 | ILE  | N-CA-C  | 5.16  | 115.93      | 110.72   |
| 1   | A     | 341 | GLN  | N-CA-C  | 5.15  | 117.68      | 111.40   |
| 1   | A     | 440 | ASN  | N-CA-C  | -5.14 | 105.86      | 111.82   |
| 1   | A     | 414 | ASP  | CA-C-N  | 5.13  | 126.26      | 119.84   |
| 1   | A     | 414 | ASP  | C-N-CA  | 5.13  | 126.26      | 119.84   |
| 1   | A     | 204 | ASP  | N-CA-C  | -5.13 | 106.53      | 112.89   |
| 1   | B     | 504 | PHE  | N-CA-C  | -5.13 | 105.87      | 111.82   |
| 1   | A     | 419 | TRP  | N-CA-C  | -5.11 | 106.21      | 112.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 846 | GLN  | N-CA-C  | 5.09  | 116.83      | 111.28   |
| 1   | B     | 577 | ILE  | N-CA-C  | -5.08 | 105.75      | 110.53   |
| 1   | A     | 485 | PHE  | N-CA-C  | 5.08  | 119.12      | 113.02   |
| 1   | A     | 580 | VAL  | N-CA-C  | -5.08 | 105.46      | 111.00   |
| 1   | B     | 940 | THR  | N-CA-C  | 5.06  | 116.79      | 111.28   |
| 1   | A     | 117 | PHE  | N-CA-C  | 5.05  | 120.98      | 109.81   |
| 1   | B     | 280 | VAL  | N-CA-C  | -5.04 | 105.24      | 112.35   |
| 1   | B     | 77  | LEU  | CA-C-N  | 5.04  | 130.52      | 122.56   |
| 1   | B     | 77  | LEU  | C-N-CA  | 5.04  | 130.52      | 122.56   |
| 1   | A     | 476 | VAL  | N-CA-C  | -5.03 | 105.42      | 110.30   |
| 1   | A     | 801 | PHE  | N-CA-C  | 5.03  | 116.45      | 110.97   |
| 1   | B     | 253 | THR  | N-CA-C  | -5.03 | 107.28      | 113.41   |
| 1   | A     | 941 | ILE  | CB-CA-C | -5.01 | 105.41      | 111.87   |
| 1   | A     | 49  | LEU  | CA-C-N  | 5.01  | 125.16      | 119.90   |
| 1   | A     | 49  | LEU  | C-N-CA  | 5.01  | 125.16      | 119.90   |
| 1   | B     | 117 | PHE  | CA-C-N  | 5.00  | 126.09      | 119.84   |
| 1   | B     | 117 | PHE  | C-N-CA  | 5.00  | 126.09      | 119.84   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | B     | 73  | ASN  | Mainchain,Peptide |
| 1   | B     | 910 | PRO  | Mainchain         |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 7435  | 0        | 7576     | 644     | 0            |
| 1   | B     | 7351  | 0        | 7510     | 830     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 14787 | 0        | 15086    | 1474    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (1474) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:546:THR:CG2  | 1:B:588:ILE:HD11 | 1.38                     | 1.53              |
| 1:B:6:THR:HG22   | 1:B:10:PHE:CE1   | 1.51                     | 1.44              |
| 1:B:791:ASN:ND2  | 1:B:909:LEU:CD1  | 1.78                     | 1.43              |
| 1:B:69:TRP:CD1   | 1:B:70:VAL:CG2   | 2.04                     | 1.39              |
| 1:B:6:THR:CG2    | 1:B:10:PHE:HE1   | 1.37                     | 1.36              |
| 1:A:374:THR:HA   | 1:A:379:ARG:NH1  | 1.38                     | 1.32              |
| 1:B:28:ARG:O     | 1:B:31:GLU:HG2   | 1.24                     | 1.31              |
| 1:B:791:ASN:ND2  | 1:B:909:LEU:HD12 | 1.37                     | 1.26              |
| 1:B:116:ASP:CB   | 1:B:120:ARG:HB2  | 1.66                     | 1.24              |
| 1:B:850:SER:O    | 1:B:851:LYS:HG2  | 1.30                     | 1.24              |
| 1:B:87:LYS:HG2   | 1:B:121:TRP:CZ2  | 1.72                     | 1.23              |
| 1:B:63:ASN:O     | 1:B:67:ARG:HG2   | 1.39                     | 1.22              |
| 1:B:117:PHE:HB2  | 1:B:118:PRO:CD   | 1.70                     | 1.21              |
| 1:B:676:PRO:HG2  | 1:B:679:ILE:CG1  | 1.71                     | 1.20              |
| 1:B:117:PHE:CB   | 1:B:118:PRO:HD3  | 1.71                     | 1.20              |
| 1:B:93:LEU:O     | 1:B:97:LEU:HG    | 1.39                     | 1.19              |
| 1:B:87:LYS:HB3   | 1:B:121:TRP:CH2  | 1.78                     | 1.17              |
| 1:A:585:GLU:HB3  | 1:A:629:TYR:CE2  | 1.79                     | 1.16              |
| 1:B:2:SER:O      | 1:B:5:GLU:HG2    | 1.46                     | 1.15              |
| 1:B:69:TRP:CD1   | 1:B:70:VAL:HG23  | 1.70                     | 1.15              |
| 1:B:914:VAL:HG12 | 1:B:915:ASN:N    | 1.59                     | 1.15              |
| 1:A:585:GLU:CB   | 1:A:629:TYR:CE2  | 2.29                     | 1.14              |
| 1:B:97:LEU:CD1   | 1:B:105:ILE:CD1  | 2.25                     | 1.14              |
| 1:B:36:PHE:HE2   | 1:B:40:LEU:HD21  | 1.01                     | 1.13              |
| 1:A:799:ILE:HD12 | 1:A:847:PHE:CZ   | 1.83                     | 1.12              |
| 1:B:93:LEU:HG    | 1:B:97:LEU:HD11  | 1.17                     | 1.12              |
| 1:B:954:ASN:O    | 1:B:958:VAL:HG23 | 1.47                     | 1.12              |
| 1:B:155:ARG:NH1  | 1:B:214:TYR:HD2  | 1.45                     | 1.12              |
| 1:B:94:MET:HE1   | 1:B:109:ILE:HG21 | 1.19                     | 1.12              |
| 1:B:117:PHE:HB2  | 1:B:118:PRO:HD2  | 1.28                     | 1.12              |
| 1:B:117:PHE:CB   | 1:B:118:PRO:CD   | 2.25                     | 1.12              |
| 1:A:585:GLU:O    | 1:A:586:ASP:OD2  | 1.68                     | 1.11              |
| 1:B:97:LEU:CD1   | 1:B:105:ILE:HD12 | 1.81                     | 1.10              |
| 1:A:374:THR:CA   | 1:A:379:ARG:HH11 | 1.65                     | 1.10              |
| 1:B:69:TRP:NE1   | 1:B:70:VAL:CG2   | 2.12                     | 1.10              |
| 1:B:546:THR:O    | 1:B:550:LEU:HG   | 1.50                     | 1.09              |
| 1:B:69:TRP:CD1   | 1:B:70:VAL:HG22  | 1.78                     | 1.09              |
| 1:B:116:ASP:HB3  | 1:B:120:ARG:CB   | 1.81                     | 1.09              |
| 1:B:472:ILE:HG21 | 1:B:509:GLU:HG3  | 1.34                     | 1.09              |
| 1:B:848:PHE:CD2  | 1:B:856:ILE:HD13 | 1.85                     | 1.09              |
| 1:B:848:PHE:HD2  | 1:B:856:ILE:CD1  | 1.65                     | 1.08              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:643:MET:HE3  | 1:B:679:ILE:CG2  | 1.82                     | 1.08              |
| 1:B:832:LYS:NZ   | 1:B:908:PRO:HB3  | 1.69                     | 1.08              |
| 1:A:736:GLU:HG2  | 1:A:769:ARG:HH21 | 1.18                     | 1.08              |
| 1:B:546:THR:HG22 | 1:B:588:ILE:HD11 | 1.25                     | 1.08              |
| 1:B:87:LYS:CB    | 1:B:121:TRP:CH2  | 2.36                     | 1.07              |
| 1:B:676:PRO:HG2  | 1:B:679:ILE:HG12 | 1.08                     | 1.07              |
| 1:B:690:ASN:HA   | 1:B:693:GLU:OE2  | 1.55                     | 1.07              |
| 1:A:908:PRO:HD2  | 1:A:908:PRO:O    | 1.50                     | 1.07              |
| 1:B:912:ILE:HG22 | 1:B:912:ILE:O    | 1.53                     | 1.06              |
| 1:B:116:ASP:HB3  | 1:B:120:ARG:HB2  | 1.08                     | 1.06              |
| 1:B:469:ILE:HG21 | 1:B:475:ARG:NH1  | 1.70                     | 1.06              |
| 1:B:822:LEU:HD11 | 1:B:838:VAL:HG21 | 1.35                     | 1.05              |
| 1:A:597:ALA:O    | 1:A:601:GLU:HG3  | 1.56                     | 1.05              |
| 1:B:546:THR:CG2  | 1:B:588:ILE:CD1  | 2.33                     | 1.05              |
| 1:B:848:PHE:CD2  | 1:B:856:ILE:CD1  | 2.40                     | 1.05              |
| 1:B:914:VAL:CG1  | 1:B:915:ASN:N    | 2.19                     | 1.05              |
| 1:A:490:THR:HB   | 1:A:493:GLN:HB2  | 1.37                     | 1.05              |
| 1:B:155:ARG:NH1  | 1:B:214:TYR:CD2  | 2.26                     | 1.04              |
| 1:B:87:LYS:CG    | 1:B:121:TRP:CZ2  | 2.42                     | 1.03              |
| 1:B:117:PHE:HB3  | 1:B:118:PRO:HD3  | 1.35                     | 1.03              |
| 1:B:137:MET:HE1  | 1:B:185:VAL:HG22 | 1.39                     | 1.03              |
| 1:B:382:THR:HG22 | 1:B:386:LYS:HE3  | 1.40                     | 1.02              |
| 1:B:65:ILE:HD11  | 1:B:112:ILE:HG12 | 1.42                     | 1.02              |
| 1:B:36:PHE:CE2   | 1:B:40:LEU:HD21  | 1.93                     | 1.01              |
| 1:A:802:ILE:HD11 | 1:A:810:PHE:HA   | 1.02                     | 1.01              |
| 1:A:307:ILE:HG12 | 1:A:375:ASP:OD2  | 1.59                     | 1.01              |
| 1:A:799:ILE:CD1  | 1:A:847:PHE:CZ   | 2.44                     | 1.01              |
| 1:A:560:HIS:NE2  | 1:A:567:LEU:HA   | 1.76                     | 1.00              |
| 1:B:7:VAL:HG21   | 1:B:39:THR:HG21  | 1.40                     | 1.00              |
| 1:B:340:GLU:HA   | 1:B:344:LEU:HD12 | 1.41                     | 1.00              |
| 1:B:832:LYS:HZ3  | 1:B:908:PRO:HB3  | 1.20                     | 1.00              |
| 1:B:97:LEU:HD12  | 1:B:105:ILE:HD12 | 1.43                     | 1.00              |
| 1:B:546:THR:HG21 | 1:B:588:ILE:HD11 | 1.04                     | 0.99              |
| 1:A:802:ILE:HD11 | 1:A:810:PHE:CA   | 1.91                     | 0.99              |
| 1:B:630:THR:HG21 | 1:B:638:LEU:HD11 | 1.43                     | 0.99              |
| 1:B:546:THR:HG21 | 1:B:588:ILE:CD1  | 1.92                     | 0.98              |
| 1:A:76:HIS:HE1   | 1:A:116:ASP:OD2  | 1.46                     | 0.98              |
| 1:B:792:LYS:HE2  | 1:B:909:LEU:HD22 | 1.44                     | 0.98              |
| 1:B:69:TRP:HD1   | 1:B:70:VAL:HG23  | 1.22                     | 0.98              |
| 1:B:910:PRO:O    | 1:B:912:ILE:N    | 1.95                     | 0.98              |
| 1:A:802:ILE:CD1  | 1:A:810:PHE:HA   | 1.93                     | 0.97              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:382:THR:O    | 1:B:386:LYS:HG3  | 1.65                     | 0.97              |
| 1:A:585:GLU:CB   | 1:A:629:TYR:HE2  | 1.71                     | 0.97              |
| 1:A:237:HIS:CE1  | 1:A:291:ILE:HD11 | 2.00                     | 0.97              |
| 1:B:469:ILE:HG21 | 1:B:475:ARG:HH11 | 1.23                     | 0.97              |
| 1:A:697:ASN:O    | 1:A:701:VAL:HG23 | 1.63                     | 0.97              |
| 1:B:789:ILE:HD11 | 1:B:798:LEU:HD13 | 1.46                     | 0.97              |
| 1:B:504:PHE:O    | 1:B:507:THR:HG22 | 1.65                     | 0.97              |
| 1:B:6:THR:CG2    | 1:B:10:PHE:CE1   | 2.27                     | 0.96              |
| 1:A:498:MET:HE1  | 1:A:520:ILE:HG23 | 1.46                     | 0.96              |
| 1:B:412:MET:HA   | 1:B:412:MET:HE2  | 1.48                     | 0.96              |
| 1:B:370:GLU:OE2  | 1:B:438:ILE:HB   | 1.65                     | 0.95              |
| 1:B:791:ASN:HD21 | 1:B:909:LEU:HD12 | 1.23                     | 0.95              |
| 1:B:850:SER:O    | 1:B:851:LYS:CG   | 2.14                     | 0.95              |
| 1:B:555:ALA:O    | 1:B:559:LYS:HG3  | 1.68                     | 0.94              |
| 1:B:676:PRO:HG2  | 1:B:679:ILE:CD1  | 1.99                     | 0.93              |
| 1:A:267:GLN:HG2  | 1:A:312:SER:HA   | 1.51                     | 0.93              |
| 1:B:853:PRO:HD2  | 1:B:854:THR:H    | 1.32                     | 0.93              |
| 1:B:791:ASN:HD22 | 1:B:909:LEU:HD12 | 1.28                     | 0.92              |
| 1:B:155:ARG:HH12 | 1:B:214:TYR:HD2  | 1.12                     | 0.92              |
| 1:B:59:LEU:O     | 1:B:62:LYS:HG2   | 1.70                     | 0.92              |
| 1:A:585:GLU:HB2  | 1:A:629:TYR:CE2  | 2.02                     | 0.92              |
| 1:A:376:THR:HG22 | 1:A:377:ARG:N    | 1.85                     | 0.92              |
| 1:B:117:PHE:HD2  | 1:B:153:ARG:HH22 | 1.17                     | 0.92              |
| 1:B:70:VAL:HA    | 1:B:76:HIS:HA    | 1.52                     | 0.92              |
| 1:B:83:VAL:O     | 1:B:87:LYS:HG3   | 1.70                     | 0.91              |
| 1:B:69:TRP:NE1   | 1:B:70:VAL:HG22  | 1.81                     | 0.91              |
| 1:B:94:MET:CE    | 1:B:109:ILE:HG21 | 2.01                     | 0.91              |
| 1:A:334:ALA:O    | 1:A:338:ILE:HG13 | 1.70                     | 0.91              |
| 1:A:799:ILE:HG21 | 1:A:847:PHE:CZ   | 2.04                     | 0.91              |
| 1:B:23:SER:O     | 1:B:27:LEU:HG    | 1.70                     | 0.91              |
| 1:A:585:GLU:HB3  | 1:A:629:TYR:HE2  | 1.27                     | 0.91              |
| 1:B:229:ILE:HD13 | 1:B:280:VAL:HG13 | 1.51                     | 0.91              |
| 1:B:546:THR:HG22 | 1:B:588:ILE:CD1  | 1.97                     | 0.91              |
| 1:B:557:ILE:HD11 | 1:B:577:ILE:CD1  | 2.00                     | 0.91              |
| 1:B:469:ILE:CG2  | 1:B:475:ARG:NH1  | 2.33                     | 0.91              |
| 1:B:848:PHE:HD2  | 1:B:856:ILE:HD13 | 1.22                     | 0.91              |
| 1:B:914:VAL:CG1  | 1:B:915:ASN:H    | 1.81                     | 0.90              |
| 1:B:662:PHE:CE1  | 1:B:701:VAL:HG22 | 2.06                     | 0.90              |
| 1:B:65:ILE:HD11  | 1:B:112:ILE:CG1  | 2.01                     | 0.90              |
| 1:B:549:LEU:O    | 1:B:553:LEU:HG   | 1.72                     | 0.90              |
| 1:B:83:VAL:HG12  | 1:B:87:LYS:HE3   | 1.53                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:461:ALA:HB3  | 1:B:462:PRO:HD3  | 1.54                     | 0.90              |
| 1:A:937:PHE:CE1  | 1:A:941:ILE:HD11 | 2.06                     | 0.89              |
| 1:A:937:PHE:CZ   | 1:A:941:ILE:HD11 | 2.05                     | 0.89              |
| 1:A:72:GLU:HG2   | 1:A:735:TYR:CZ   | 2.07                     | 0.89              |
| 1:B:638:LEU:O    | 1:B:642:MET:HG2  | 1.71                     | 0.89              |
| 1:B:676:PRO:CG   | 1:B:679:ILE:CD1  | 2.50                     | 0.89              |
| 1:B:791:ASN:ND2  | 1:B:909:LEU:HD13 | 1.86                     | 0.88              |
| 1:A:736:GLU:HG2  | 1:A:769:ARG:NH2  | 1.89                     | 0.88              |
| 1:B:490:THR:HB   | 1:B:493:GLN:HG3  | 1.54                     | 0.88              |
| 1:A:588:ILE:HB   | 1:A:591:LEU:HD12 | 1.55                     | 0.88              |
| 1:A:162:GLU:HA   | 1:A:165:LEU:HD13 | 1.55                     | 0.88              |
| 1:B:124:LEU:O    | 1:B:128:LEU:HG   | 1.74                     | 0.88              |
| 1:B:93:LEU:HG    | 1:B:97:LEU:CD1   | 2.03                     | 0.87              |
| 1:B:848:PHE:CE2  | 1:B:937:PHE:HE1  | 1.92                     | 0.87              |
| 1:A:814:TRP:HE1  | 1:A:859:THR:HG21 | 1.37                     | 0.87              |
| 1:A:276:ARG:HB3  | 1:A:277:TYR:CE1  | 2.08                     | 0.87              |
| 1:A:374:THR:CA   | 1:A:379:ARG:NH1  | 2.32                     | 0.86              |
| 1:B:792:LYS:HE2  | 1:B:909:LEU:CD2  | 2.05                     | 0.86              |
| 1:A:376:THR:HG22 | 1:A:377:ARG:H    | 1.36                     | 0.86              |
| 1:A:325:TYR:O    | 1:A:328:ILE:HG12 | 1.74                     | 0.86              |
| 1:B:97:LEU:HD13  | 1:B:105:ILE:CD1  | 2.05                     | 0.86              |
| 1:B:676:PRO:HD2  | 1:B:679:ILE:HD11 | 1.57                     | 0.86              |
| 1:A:329:PHE:HD2  | 1:A:338:ILE:HD11 | 1.39                     | 0.85              |
| 1:B:588:ILE:HG22 | 1:B:588:ILE:O    | 1.75                     | 0.85              |
| 1:A:855:LEU:O    | 1:A:859:THR:HG23 | 1.76                     | 0.85              |
| 1:B:241:SER:HB2  | 1:B:291:ILE:HD11 | 1.57                     | 0.85              |
| 1:B:319:VAL:O    | 1:B:322:ILE:HG12 | 1.77                     | 0.84              |
| 1:A:841:MET:HE1  | 1:A:848:PHE:HB2  | 1.59                     | 0.84              |
| 1:B:348:THR:HA   | 1:B:424:LEU:HD21 | 1.59                     | 0.84              |
| 1:A:652:GLU:O    | 1:A:654:ILE:HG13 | 1.77                     | 0.84              |
| 1:A:62:LYS:HZ2   | 1:A:104:GLN:HE22 | 1.23                     | 0.84              |
| 1:B:36:PHE:HE2   | 1:B:40:LEU:CD2   | 1.86                     | 0.84              |
| 1:A:226:GLU:O    | 1:A:229:ILE:HG22 | 1.78                     | 0.83              |
| 1:B:65:ILE:CD1   | 1:B:112:ILE:CG1  | 2.55                     | 0.83              |
| 1:B:87:LYS:HG2   | 1:B:121:TRP:HZ2  | 1.36                     | 0.83              |
| 1:B:792:LYS:CE   | 1:B:909:LEU:HD22 | 2.08                     | 0.83              |
| 1:B:152:LYS:O    | 1:B:155:ARG:HG2  | 1.77                     | 0.83              |
| 1:B:401:LEU:O    | 1:B:405:LYS:HG3  | 1.76                     | 0.83              |
| 1:B:592:PHE:CD2  | 1:B:626:ILE:HG23 | 2.12                     | 0.83              |
| 1:A:870:GLN:HG3  | 1:A:871:SER:H    | 1.44                     | 0.83              |
| 1:B:791:ASN:HD21 | 1:B:909:LEU:CD1  | 1.73                     | 0.82              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:VAL:HG21   | 1:A:39:THR:HG21  | 1.60                     | 0.82              |
| 1:A:76:HIS:CE1   | 1:A:116:ASP:OD2  | 2.31                     | 0.82              |
| 1:B:295:LEU:O    | 1:B:299:ILE:HG13 | 1.79                     | 0.82              |
| 1:A:828:LEU:HB3  | 1:A:914:VAL:HG12 | 1.59                     | 0.82              |
| 1:B:317:THR:HG23 | 1:B:387:GLU:HG3  | 1.59                     | 0.82              |
| 1:A:150:ILE:O    | 1:A:153:ARG:HG2  | 1.79                     | 0.82              |
| 1:B:676:PRO:CG   | 1:B:679:ILE:HG12 | 2.03                     | 0.82              |
| 1:A:331:ASN:HD21 | 1:A:334:ALA:H    | 1.25                     | 0.82              |
| 1:A:591:LEU:O    | 1:A:594:GLN:HG2  | 1.80                     | 0.82              |
| 1:A:596:LEU:HD22 | 1:A:638:LEU:HD22 | 1.61                     | 0.82              |
| 1:B:93:LEU:CG    | 1:B:97:LEU:HD11  | 2.07                     | 0.82              |
| 1:A:175:THR:HG23 | 1:A:224:PHE:CD2  | 2.14                     | 0.82              |
| 1:B:774:LYS:O    | 1:B:774:LYS:HG3  | 1.80                     | 0.82              |
| 1:B:791:ASN:HD22 | 1:B:909:LEU:CD1  | 1.81                     | 0.82              |
| 1:B:433:ALA:C    | 1:B:446:THR:HG23 | 2.05                     | 0.81              |
| 1:B:912:ILE:O    | 1:B:912:ILE:CG2  | 2.28                     | 0.81              |
| 1:B:404:MET:O    | 1:B:408:VAL:HG23 | 1.80                     | 0.81              |
| 1:A:870:GLN:HG3  | 1:A:871:SER:N    | 1.95                     | 0.81              |
| 1:B:87:LYS:CA    | 1:B:121:TRP:HH2  | 1.93                     | 0.81              |
| 1:A:799:ILE:HG21 | 1:A:847:PHE:CE1  | 2.14                     | 0.81              |
| 1:B:65:ILE:O     | 1:B:69:TRP:HB3   | 1.80                     | 0.81              |
| 1:B:853:PRO:CD   | 1:B:854:THR:H    | 1.92                     | 0.81              |
| 1:A:331:ASN:HD21 | 1:A:334:ALA:CB   | 1.94                     | 0.81              |
| 1:B:643:MET:HE3  | 1:B:679:ILE:HG22 | 1.61                     | 0.81              |
| 1:B:568:ALA:HB3  | 1:B:611:SER:CB   | 2.09                     | 0.81              |
| 1:B:814:TRP:CZ2  | 1:B:841:MET:HG2  | 2.15                     | 0.81              |
| 1:A:814:TRP:HE1  | 1:A:859:THR:CG2  | 1.94                     | 0.81              |
| 1:B:439:THR:HG22 | 1:B:440:ASN:H    | 1.45                     | 0.81              |
| 1:A:547:GLU:HG2  | 1:A:591:LEU:CD1  | 2.11                     | 0.80              |
| 1:B:28:ARG:O     | 1:B:31:GLU:CG    | 2.20                     | 0.80              |
| 1:A:571:GLU:OE1  | 1:A:614:ARG:HD2  | 1.81                     | 0.80              |
| 1:B:176:ALA:HB3  | 1:B:177:PRO:HD3  | 1.63                     | 0.80              |
| 1:B:591:LEU:HD11 | 1:B:594:GLN:OE1  | 1.82                     | 0.80              |
| 1:B:557:ILE:HG22 | 1:B:567:LEU:HD11 | 1.64                     | 0.80              |
| 1:B:547:GLU:O    | 1:B:551:LYS:HG3  | 1.81                     | 0.80              |
| 1:B:929:TYR:CE1  | 1:B:932:ILE:HD12 | 2.16                     | 0.80              |
| 1:A:847:PHE:CD1  | 1:A:851:LYS:HD2  | 2.18                     | 0.79              |
| 1:A:786:PHE:CD1  | 1:A:818:ILE:HD11 | 2.17                     | 0.79              |
| 1:B:6:THR:HG22   | 1:B:10:PHE:HE1   | 0.64                     | 0.79              |
| 1:B:97:LEU:HD12  | 1:B:105:ILE:CD1  | 2.05                     | 0.79              |
| 1:A:192:ASN:HD22 | 1:A:202:LEU:HD11 | 1.47                     | 0.79              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:660:TYR:HD2  | 1:B:898:LEU:HD21 | 1.45                     | 0.79              |
| 1:B:710:LYS:HA   | 1:B:749:LEU:HD13 | 1.64                     | 0.79              |
| 1:A:799:ILE:CB   | 1:A:847:PHE:HZ   | 1.95                     | 0.79              |
| 1:A:856:ILE:O    | 1:A:860:MET:HB2  | 1.82                     | 0.79              |
| 1:B:65:ILE:CD1   | 1:B:112:ILE:HG12 | 2.12                     | 0.79              |
| 1:B:832:LYS:HE3  | 1:B:913:ASP:HB2  | 1.63                     | 0.79              |
| 1:B:10:PHE:HB3   | 1:B:27:LEU:HD21  | 1.62                     | 0.79              |
| 1:A:206:LEU:HG   | 1:A:210:ILE:HD11 | 1.65                     | 0.79              |
| 1:B:557:ILE:HG22 | 1:B:567:LEU:CD1  | 2.12                     | 0.79              |
| 1:B:655:GLN:HA   | 1:B:658:ILE:HD12 | 1.65                     | 0.79              |
| 1:B:233:MET:HB2  | 1:B:284:MET:CE   | 2.13                     | 0.78              |
| 1:B:791:ASN:ND2  | 1:B:909:LEU:HD11 | 1.93                     | 0.78              |
| 1:A:62:LYS:NZ    | 1:A:104:GLN:HE22 | 1.79                     | 0.78              |
| 1:B:155:ARG:HB2  | 1:B:156:PRO:HD3  | 1.64                     | 0.78              |
| 1:B:848:PHE:CD2  | 1:B:856:ILE:HD11 | 2.16                     | 0.78              |
| 1:A:422:LYS:HA   | 1:A:425:TYR:CE2  | 2.18                     | 0.78              |
| 1:A:507:THR:HG22 | 1:A:509:GLU:H    | 1.48                     | 0.78              |
| 1:B:411:TYR:CD2  | 1:B:412:MET:HE3  | 2.17                     | 0.78              |
| 1:B:229:ILE:HD13 | 1:B:280:VAL:CG1  | 2.14                     | 0.78              |
| 1:B:832:LYS:O    | 1:B:836:ILE:HG12 | 1.82                     | 0.78              |
| 1:A:331:ASN:ND2  | 1:A:334:ALA:H    | 1.80                     | 0.78              |
| 1:B:433:ALA:O    | 1:B:446:THR:HG23 | 1.84                     | 0.78              |
| 1:B:658:ILE:HB   | 1:B:659:PRO:HD3  | 1.66                     | 0.78              |
| 1:B:87:LYS:CA    | 1:B:121:TRP:CH2  | 2.67                     | 0.77              |
| 1:B:7:VAL:HG21   | 1:B:39:THR:CG2   | 2.15                     | 0.77              |
| 1:B:97:LEU:HD13  | 1:B:105:ILE:HD12 | 1.62                     | 0.77              |
| 1:B:874:ASN:O    | 1:B:875:LEU:HD23 | 1.83                     | 0.77              |
| 1:A:263:LYS:O    | 1:A:266:ILE:HG22 | 1.84                     | 0.77              |
| 1:B:546:THR:O    | 1:B:550:LEU:CG   | 2.33                     | 0.77              |
| 1:B:552:ASN:O    | 1:B:556:LEU:HG   | 1.84                     | 0.77              |
| 1:B:397:THR:O    | 1:B:401:LEU:HG   | 1.84                     | 0.76              |
| 1:A:267:GLN:HG2  | 1:A:312:SER:CA   | 2.15                     | 0.76              |
| 1:A:329:PHE:CD2  | 1:A:338:ILE:HD11 | 2.20                     | 0.76              |
| 1:B:501:LEU:HA   | 1:B:504:PHE:HD1  | 1.50                     | 0.76              |
| 1:B:116:ASP:HB3  | 1:B:120:ARG:CG   | 2.15                     | 0.76              |
| 1:A:375:ASP:O    | 1:A:376:THR:OG1  | 2.04                     | 0.76              |
| 1:A:296:LEU:HD21 | 1:A:312:SER:OG   | 1.85                     | 0.76              |
| 1:B:71:ASP:OD1   | 1:B:77:LEU:HG    | 1.86                     | 0.76              |
| 1:B:439:THR:HG22 | 1:B:440:ASN:N    | 2.00                     | 0.76              |
| 1:A:870:GLN:CG   | 1:A:871:SER:H    | 1.98                     | 0.76              |
| 1:B:557:ILE:HD11 | 1:B:577:ILE:HD12 | 1.66                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:382:THR:HG22 | 1:A:386:LYS:HE3  | 1.66                     | 0.75              |
| 1:B:69:TRP:NE1   | 1:B:70:VAL:HG21  | 1.98                     | 0.75              |
| 1:B:919:ARG:HG2  | 1:B:956:LEU:CD1  | 2.16                     | 0.75              |
| 1:A:376:THR:CG2  | 1:A:377:ARG:H    | 2.00                     | 0.75              |
| 1:B:386:LYS:HA   | 1:B:389:LYS:HE2  | 1.66                     | 0.75              |
| 1:A:799:ILE:CG2  | 1:A:847:PHE:HZ   | 2.00                     | 0.75              |
| 1:B:36:PHE:HD2   | 1:B:40:LEU:HG    | 1.51                     | 0.75              |
| 1:B:596:LEU:CD2  | 1:B:626:ILE:HG21 | 2.16                     | 0.75              |
| 1:A:490:THR:HG22 | 1:A:492:ALA:H    | 1.51                     | 0.75              |
| 1:A:285:ILE:O    | 1:A:289:ILE:HG13 | 1.86                     | 0.75              |
| 1:B:229:ILE:HG22 | 1:B:284:MET:HE1  | 1.69                     | 0.75              |
| 1:B:706:LYS:HE2  | 1:B:745:HIS:ND1  | 2.01                     | 0.75              |
| 1:B:372:SER:OG   | 1:B:379:ARG:NH2  | 2.20                     | 0.75              |
| 1:A:492:ALA:O    | 1:A:496:GLU:HG3  | 1.87                     | 0.75              |
| 1:B:70:VAL:HG13  | 1:B:76:HIS:CA    | 2.17                     | 0.75              |
| 1:A:585:GLU:HB2  | 1:A:629:TYR:CD2  | 2.21                     | 0.74              |
| 1:B:94:MET:HE1   | 1:B:109:ILE:CG2  | 2.10                     | 0.74              |
| 1:B:469:ILE:CG2  | 1:B:475:ARG:HH12 | 1.98                     | 0.74              |
| 1:A:117:PHE:HB3  | 1:A:118:PRO:HD3  | 1.69                     | 0.74              |
| 1:B:730:ILE:HD11 | 1:B:766:LEU:HD23 | 1.69                     | 0.74              |
| 1:B:690:ASN:O    | 1:B:693:GLU:HG3  | 1.88                     | 0.74              |
| 1:A:786:PHE:HD1  | 1:A:818:ILE:CD1  | 2.01                     | 0.74              |
| 1:A:847:PHE:HB2  | 1:A:851:LYS:HE3  | 1.68                     | 0.74              |
| 1:B:568:ALA:HB3  | 1:B:611:SER:OG   | 1.88                     | 0.74              |
| 1:A:780:LYS:HE2  | 1:A:824:THR:HG22 | 1.70                     | 0.74              |
| 1:A:94:MET:CE    | 1:A:146:VAL:HA   | 2.16                     | 0.74              |
| 1:B:65:ILE:CD1   | 1:B:112:ILE:HG13 | 2.17                     | 0.74              |
| 1:B:382:THR:CG2  | 1:B:386:LYS:HE3  | 2.16                     | 0.74              |
| 1:A:361:PRO:O    | 1:A:365:ILE:HG13 | 1.88                     | 0.73              |
| 1:A:786:PHE:HD1  | 1:A:818:ILE:HD11 | 1.53                     | 0.73              |
| 1:A:698:ILE:HD12 | 1:A:735:TYR:CE1  | 2.23                     | 0.73              |
| 1:A:941:ILE:HG22 | 1:A:945:LEU:HG   | 1.69                     | 0.73              |
| 1:B:591:LEU:CD1  | 1:B:594:GLN:OE1  | 2.36                     | 0.73              |
| 1:A:373:ASP:O    | 1:A:379:ARG:NH1  | 2.21                     | 0.73              |
| 1:B:296:LEU:HA   | 1:B:299:ILE:HD12 | 1.69                     | 0.73              |
| 1:A:194:ASN:HA   | 1:A:246:LEU:HD11 | 1.70                     | 0.73              |
| 1:A:331:ASN:HD22 | 1:A:331:ASN:C    | 1.96                     | 0.73              |
| 1:B:91:VAL:HG12  | 1:B:131:ARG:NH1  | 2.03                     | 0.73              |
| 1:B:116:ASP:OD2  | 1:B:116:ASP:N    | 2.22                     | 0.73              |
| 1:A:192:ASN:O    | 1:A:194:ASN:N    | 2.22                     | 0.73              |
| 1:B:22:THR:HG22  | 1:B:26:ASN:HD21  | 1.52                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:914:VAL:HG12 | 1:B:916:ASN:H    | 1.51                     | 0.73              |
| 1:A:329:PHE:O    | 1:A:335:MET:HE2  | 1.89                     | 0.73              |
| 1:A:257:SER:H    | 1:A:260:ILE:HD12 | 1.53                     | 0.73              |
| 1:A:860:MET:HG2  | 1:A:941:ILE:HD13 | 1.69                     | 0.73              |
| 1:B:157:LEU:CD2  | 1:B:163:LEU:HD13 | 2.19                     | 0.73              |
| 1:B:596:LEU:HD11 | 1:B:638:LEU:HD22 | 1.71                     | 0.73              |
| 1:B:70:VAL:HG12  | 1:B:75:ASN:O     | 1.88                     | 0.72              |
| 1:B:592:PHE:HD2  | 1:B:626:ILE:HG23 | 1.52                     | 0.72              |
| 1:A:799:ILE:HD12 | 1:A:847:PHE:CE2  | 2.23                     | 0.72              |
| 1:B:557:ILE:HD11 | 1:B:577:ILE:HD11 | 1.71                     | 0.72              |
| 1:B:93:LEU:CD1   | 1:B:97:LEU:HD21  | 2.20                     | 0.72              |
| 1:B:676:PRO:CG   | 1:B:679:ILE:HD13 | 2.17                     | 0.72              |
| 1:B:684:GLN:HE22 | 1:B:717:PRO:HD2  | 1.54                     | 0.72              |
| 1:B:210:ILE:CD1  | 1:B:262:VAL:HG13 | 2.19                     | 0.72              |
| 1:B:767:LEU:HD12 | 1:B:805:VAL:HG21 | 1.71                     | 0.72              |
| 1:A:389:LYS:HA   | 1:A:396:VAL:HG11 | 1.72                     | 0.72              |
| 1:B:466:SER:OG   | 1:B:469:ILE:HG22 | 1.90                     | 0.72              |
| 1:B:639:VAL:HG13 | 1:B:643:MET:HE2  | 1.72                     | 0.72              |
| 1:A:38:LEU:CD1   | 1:A:85:LEU:HD23  | 2.20                     | 0.72              |
| 1:B:116:ASP:HB2  | 1:B:120:ARG:HB2  | 1.72                     | 0.72              |
| 1:B:643:MET:HE3  | 1:B:679:ILE:HG21 | 1.68                     | 0.72              |
| 1:A:195:ASN:HB2  | 1:A:198:SER:HB2  | 1.71                     | 0.72              |
| 1:A:419:TRP:HB2  | 1:A:474:LEU:HD11 | 1.72                     | 0.72              |
| 1:B:819:ILE:HD11 | 1:B:859:THR:OG1  | 1.89                     | 0.72              |
| 1:A:7:VAL:HG21   | 1:A:39:THR:CG2   | 2.19                     | 0.71              |
| 1:A:94:MET:HB2   | 1:A:105:ILE:HG21 | 1.72                     | 0.71              |
| 1:A:116:ASP:OD1  | 1:A:120:ARG:NH2  | 2.23                     | 0.71              |
| 1:B:137:MET:HE1  | 1:B:185:VAL:CG2  | 2.19                     | 0.71              |
| 1:B:769:ARG:HG3  | 1:B:769:ARG:HH11 | 1.53                     | 0.71              |
| 1:A:698:ILE:HD12 | 1:A:735:TYR:CZ   | 2.24                     | 0.71              |
| 1:B:832:LYS:NZ   | 1:B:908:PRO:CB   | 2.49                     | 0.71              |
| 1:B:924:GLU:O    | 1:B:928:LYS:HG3  | 1.90                     | 0.71              |
| 1:A:376:THR:CG2  | 1:A:377:ARG:N    | 2.53                     | 0.71              |
| 1:A:513:TYR:CD1  | 1:A:556:LEU:HD13 | 2.24                     | 0.71              |
| 1:B:94:MET:HE3   | 1:B:146:VAL:HG22 | 1.72                     | 0.71              |
| 1:B:266:ILE:O    | 1:B:270:VAL:HG23 | 1.89                     | 0.71              |
| 1:A:335:MET:HB3  | 1:A:399:ILE:HD13 | 1.71                     | 0.71              |
| 1:A:796:ASP:OD1  | 1:A:847:PHE:CE2  | 2.43                     | 0.71              |
| 1:A:828:LEU:CD1  | 1:A:915:ASN:OD1  | 2.38                     | 0.71              |
| 1:A:904:LYS:N    | 1:A:905:PRO:HD3  | 2.05                     | 0.71              |
| 1:B:589:GLN:HA   | 1:B:592:PHE:CD1  | 2.25                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:301:ASN:HA   | 1:A:377:ARG:HH12 | 1.56                     | 0.71              |
| 1:A:486:ARG:NH1  | 1:A:522:LYS:HD2  | 2.05                     | 0.71              |
| 1:B:233:MET:HB2  | 1:B:284:MET:HE2  | 1.72                     | 0.71              |
| 1:B:589:GLN:HA   | 1:B:592:PHE:CE1  | 2.25                     | 0.71              |
| 1:B:598:GLN:O    | 1:B:602:ILE:HG13 | 1.90                     | 0.71              |
| 1:A:341:GLN:O    | 1:A:345:PRO:HG3  | 1.91                     | 0.71              |
| 1:B:703:ARG:HD2  | 1:B:903:GLU:OE2  | 1.91                     | 0.71              |
| 1:A:589:GLN:NE2  | 1:A:631:GLN:HE21 | 1.88                     | 0.71              |
| 1:A:692:TRP:HZ3  | 1:A:702:THR:HG22 | 1.56                     | 0.71              |
| 1:B:87:LYS:HA    | 1:B:121:TRP:CH2  | 2.25                     | 0.71              |
| 1:A:267:GLN:CG   | 1:A:312:SER:HA   | 2.20                     | 0.71              |
| 1:B:372:SER:O    | 1:B:374:THR:N    | 2.24                     | 0.71              |
| 1:A:104:GLN:HA   | 1:A:104:GLN:NE2  | 2.06                     | 0.71              |
| 1:B:361:PRO:HB2  | 1:B:510:TYR:HD2  | 1.55                     | 0.71              |
| 1:B:568:ALA:HB3  | 1:B:611:SER:HB2  | 1.71                     | 0.71              |
| 1:B:374:THR:HA   | 1:B:379:ARG:HH11 | 1.56                     | 0.70              |
| 1:A:185:VAL:O    | 1:A:189:ILE:HG13 | 1.91                     | 0.70              |
| 1:B:106:GLY:O    | 1:B:109:ILE:HG22 | 1.90                     | 0.70              |
| 1:B:848:PHE:CE2  | 1:B:856:ILE:HD13 | 2.25                     | 0.70              |
| 1:B:6:THR:O      | 1:B:10:PHE:HD1   | 1.74                     | 0.70              |
| 1:B:94:MET:HG2   | 1:B:146:VAL:CG2  | 2.21                     | 0.70              |
| 1:B:706:LYS:HE3  | 1:B:741:ASP:O    | 1.91                     | 0.70              |
| 1:B:848:PHE:CE2  | 1:B:937:PHE:CE1  | 2.78                     | 0.70              |
| 1:B:914:VAL:HG13 | 1:B:915:ASN:H    | 1.57                     | 0.70              |
| 1:A:461:ALA:HB3  | 1:A:462:PRO:HD3  | 1.72                     | 0.70              |
| 1:B:730:ILE:CD1  | 1:B:766:LEU:HD23 | 2.21                     | 0.70              |
| 1:A:747:MET:SD   | 1:A:785:PHE:HZ   | 2.14                     | 0.70              |
| 1:A:828:LEU:HD13 | 1:A:915:ASN:OD1  | 1.91                     | 0.70              |
| 1:B:36:PHE:CD2   | 1:B:40:LEU:HG    | 2.25                     | 0.70              |
| 1:B:87:LYS:HA    | 1:B:121:TRP:HH2  | 1.55                     | 0.70              |
| 1:B:401:LEU:HD21 | 1:B:450:LEU:HD21 | 1.73                     | 0.70              |
| 1:A:691:VAL:HG22 | 1:A:692:TRP:CD1  | 2.27                     | 0.70              |
| 1:A:819:ILE:HD11 | 1:A:859:THR:HG22 | 1.74                     | 0.70              |
| 1:B:94:MET:HG2   | 1:B:146:VAL:HG22 | 1.73                     | 0.70              |
| 1:B:776:GLU:O    | 1:B:780:LYS:HG3  | 1.92                     | 0.70              |
| 1:A:270:VAL:HG12 | 1:A:315:PHE:CD1  | 2.27                     | 0.70              |
| 1:B:6:THR:O      | 1:B:10:PHE:CD1   | 2.45                     | 0.69              |
| 1:A:600:ILE:HD11 | 1:A:642:MET:HB3  | 1.73                     | 0.69              |
| 1:B:281:PHE:O    | 1:B:285:ILE:HG13 | 1.92                     | 0.69              |
| 1:B:948:GLU:HG3  | 1:B:949:ASN:H    | 1.56                     | 0.69              |
| 1:A:464:LEU:HD11 | 1:A:482:ILE:HD11 | 1.74                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:40:LEU:O     | 1:B:44:ILE:HG13  | 1.93                     | 0.69              |
| 1:B:210:ILE:HG12 | 1:B:236:PHE:HE2  | 1.58                     | 0.69              |
| 1:B:374:THR:HG22 | 1:B:374:THR:O    | 1.91                     | 0.69              |
| 1:B:486:ARG:O    | 1:B:494:LEU:HD11 | 1.92                     | 0.69              |
| 1:A:400:PHE:HB3  | 1:A:404:MET:HE3  | 1.73                     | 0.69              |
| 1:A:181:LEU:O    | 1:A:185:VAL:HG23 | 1.93                     | 0.69              |
| 1:B:690:ASN:HA   | 1:B:693:GLU:CD   | 2.17                     | 0.69              |
| 1:B:70:VAL:HG13  | 1:B:76:HIS:HB3   | 1.75                     | 0.69              |
| 1:B:660:TYR:CD2  | 1:B:898:LEU:HD21 | 2.27                     | 0.69              |
| 1:B:789:ILE:HD11 | 1:B:798:LEU:CD1  | 2.22                     | 0.69              |
| 1:B:736:GLU:OE1  | 1:B:769:ARG:NH2  | 2.22                     | 0.68              |
| 1:A:847:PHE:HD1  | 1:A:851:LYS:HD2  | 1.59                     | 0.68              |
| 1:A:924:GLU:HG3  | 1:A:928:LYS:HE3  | 1.74                     | 0.68              |
| 1:A:175:THR:HG23 | 1:A:224:PHE:CE2  | 2.28                     | 0.68              |
| 1:A:244:ASN:O    | 1:A:248:GLU:HG2  | 1.92                     | 0.68              |
| 1:A:666:ALA:O    | 1:A:670:GLU:HG3  | 1.91                     | 0.68              |
| 1:A:592:PHE:HA   | 1:A:595:LEU:HD12 | 1.74                     | 0.68              |
| 1:B:348:THR:HA   | 1:B:424:LEU:CD2  | 2.24                     | 0.68              |
| 1:B:730:ILE:O    | 1:B:769:ARG:HD3  | 1.93                     | 0.68              |
| 1:A:667:PHE:CD1  | 1:A:901:ILE:HG23 | 2.27                     | 0.68              |
| 1:B:69:TRP:HE1   | 1:B:70:VAL:HG21  | 1.58                     | 0.68              |
| 1:B:509:GLU:HB2  | 1:B:512:VAL:HB   | 1.76                     | 0.68              |
| 1:B:848:PHE:HD2  | 1:B:856:ILE:HD11 | 1.52                     | 0.68              |
| 1:A:270:VAL:HG12 | 1:A:315:PHE:CE1  | 2.28                     | 0.68              |
| 1:A:775:THR:O    | 1:A:776:GLU:C    | 2.37                     | 0.67              |
| 1:B:30:LEU:HA    | 1:B:33:GLN:HG3   | 1.76                     | 0.67              |
| 1:A:326:PHE:CE2  | 1:A:391:LYS:HB3  | 2.30                     | 0.67              |
| 1:B:698:ILE:HB   | 1:B:699:PRO:HD3  | 1.75                     | 0.67              |
| 1:A:942:LEU:HD21 | 1:A:953:LEU:HD23 | 1.75                     | 0.67              |
| 1:B:229:ILE:CD1  | 1:B:280:VAL:HG13 | 2.23                     | 0.67              |
| 1:A:62:LYS:NZ    | 1:A:104:GLN:NE2  | 2.43                     | 0.67              |
| 1:A:257:SER:O    | 1:A:261:LYS:HG3  | 1.94                     | 0.67              |
| 1:B:697:ASN:O    | 1:B:701:VAL:HG23 | 1.94                     | 0.67              |
| 1:A:228:ASN:O    | 1:A:231:VAL:HG22 | 1.94                     | 0.67              |
| 1:A:331:ASN:HD21 | 1:A:334:ALA:HB3  | 1.59                     | 0.67              |
| 1:B:498:MET:HE1  | 1:B:523:ILE:HG22 | 1.77                     | 0.67              |
| 1:B:155:ARG:NH1  | 1:B:215:ASP:OD1  | 2.27                     | 0.67              |
| 1:B:546:THR:HG22 | 1:B:550:LEU:HD11 | 1.75                     | 0.67              |
| 1:B:585:GLU:HB2  | 1:B:629:TYR:CE2  | 2.30                     | 0.67              |
| 1:B:702:THR:O    | 1:B:706:LYS:HB2  | 1.95                     | 0.67              |
| 1:A:331:ASN:ND2  | 1:A:334:ALA:HB3  | 2.11                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:547:GLU:CD   | 1:A:591:LEU:HD11 | 2.20                     | 0.66              |
| 1:A:795:SER:HB3  | 1:A:841:MET:SD   | 2.35                     | 0.66              |
| 1:B:362:ILE:CD1  | 1:B:569:GLU:OE1  | 2.42                     | 0.66              |
| 1:A:829:LEU:HD11 | 1:A:908:PRO:HB3  | 1.76                     | 0.66              |
| 1:B:2:SER:C      | 1:B:5:GLU:HG2    | 2.21                     | 0.66              |
| 1:B:465:THR:HG22 | 1:B:465:THR:O    | 1.95                     | 0.66              |
| 1:B:513:TYR:CD1  | 1:B:556:LEU:HD13 | 2.29                     | 0.66              |
| 1:A:331:ASN:HD21 | 1:A:334:ALA:N    | 1.92                     | 0.66              |
| 1:A:546:THR:HG23 | 1:A:580:VAL:CG1  | 2.26                     | 0.66              |
| 1:A:133:SER:C    | 1:A:134:ASN:HD22 | 2.02                     | 0.66              |
| 1:B:97:LEU:CD1   | 1:B:105:ILE:HD13 | 2.21                     | 0.66              |
| 1:B:223:GLU:O    | 1:B:227:ASP:CG   | 2.38                     | 0.66              |
| 1:A:70:VAL:CG1   | 1:A:74:GLY:HA2   | 2.26                     | 0.66              |
| 1:A:589:GLN:HE22 | 1:A:631:GLN:HE21 | 1.43                     | 0.66              |
| 1:B:185:VAL:O    | 1:B:189:ILE:HG13 | 1.96                     | 0.66              |
| 1:B:557:ILE:CD1  | 1:B:577:ILE:CD1  | 2.72                     | 0.66              |
| 1:B:183:LYS:HE2  | 1:B:231:VAL:HG11 | 1.78                     | 0.66              |
| 1:B:76:HIS:CD2   | 1:B:83:VAL:HG21  | 2.31                     | 0.66              |
| 1:B:70:VAL:HG12  | 1:B:75:ASN:C     | 2.21                     | 0.66              |
| 1:B:70:VAL:HG13  | 1:B:76:HIS:CB    | 2.26                     | 0.65              |
| 1:B:167:ILE:O    | 1:B:171:LEU:HG   | 1.96                     | 0.65              |
| 1:B:272:LEU:HD11 | 1:B:276:ARG:HG3  | 1.78                     | 0.65              |
| 1:B:343:ILE:HD13 | 1:B:385:LEU:HD21 | 1.77                     | 0.65              |
| 1:B:175:THR:HG23 | 1:B:224:PHE:CE2  | 2.32                     | 0.65              |
| 1:A:221:ILE:HG13 | 1:A:277:TYR:CE2  | 2.31                     | 0.65              |
| 1:A:464:LEU:HD13 | 1:A:500:ILE:HD11 | 1.78                     | 0.65              |
| 1:A:585:GLU:CB   | 1:A:629:TYR:CD2  | 2.77                     | 0.65              |
| 1:B:564:PRO:HG2  | 1:B:565:GLU:H    | 1.61                     | 0.65              |
| 1:A:369:LEU:HD11 | 1:A:515:TYR:HE2  | 1.60                     | 0.65              |
| 1:B:673:ALA:O    | 1:B:711:THR:HG23 | 1.96                     | 0.65              |
| 1:B:825:ILE:O    | 1:B:831:ARG:HG3  | 1.96                     | 0.65              |
| 1:A:404:MET:HE2  | 1:A:428:LEU:HB3  | 1.79                     | 0.65              |
| 1:B:404:MET:HA   | 1:B:407:PHE:HD1  | 1.61                     | 0.65              |
| 1:A:262:VAL:O    | 1:A:266:ILE:HB   | 1.96                     | 0.65              |
| 1:A:456:PHE:HD1  | 1:A:460:ILE:HB   | 1.60                     | 0.65              |
| 1:B:281:PHE:HD2  | 1:B:285:ILE:HG12 | 1.61                     | 0.65              |
| 1:B:550:LEU:HD11 | 1:B:588:ILE:CD1  | 2.27                     | 0.65              |
| 1:A:343:ILE:CD1  | 1:A:385:LEU:HD13 | 2.27                     | 0.65              |
| 1:A:513:TYR:HD1  | 1:A:556:LEU:HD13 | 1.62                     | 0.65              |
| 1:B:22:THR:HG22  | 1:B:26:ASN:ND2   | 2.12                     | 0.65              |
| 1:B:150:ILE:O    | 1:B:153:ARG:CD   | 2.44                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:649:VAL:HA   | 1:A:654:ILE:HD12 | 1.78                     | 0.65              |
| 1:B:10:PHE:CB    | 1:B:27:LEU:HD21  | 2.27                     | 0.65              |
| 1:B:27:LEU:HB3   | 1:B:60:PHE:CZ    | 2.32                     | 0.65              |
| 1:A:799:ILE:CG2  | 1:A:847:PHE:CZ   | 2.75                     | 0.65              |
| 1:A:30:LEU:HD12  | 1:A:33:GLN:NE2   | 2.12                     | 0.64              |
| 1:B:20:ALA:O     | 1:B:24:GLU:HG3   | 1.98                     | 0.64              |
| 1:B:400:PHE:CE2  | 1:B:428:LEU:HD22 | 2.32                     | 0.64              |
| 1:B:735:TYR:HB3  | 1:B:738:HIS:HD2  | 1.62                     | 0.64              |
| 1:A:598:GLN:O    | 1:A:602:ILE:HG13 | 1.98                     | 0.64              |
| 1:A:799:ILE:HB   | 1:A:847:PHE:HZ   | 1.60                     | 0.64              |
| 1:A:908:PRO:O    | 1:A:908:PRO:CD   | 2.30                     | 0.64              |
| 1:A:663:GLN:NE2  | 1:A:896:SER:O    | 2.30                     | 0.64              |
| 1:B:510:TYR:HA   | 1:B:513:TYR:CE2  | 2.32                     | 0.64              |
| 1:B:546:THR:HG22 | 1:B:550:LEU:CD1  | 2.27                     | 0.64              |
| 1:B:933:SER:HB2  | 1:B:936:THR:HB   | 1.80                     | 0.64              |
| 1:B:157:LEU:HG   | 1:B:163:LEU:CD1  | 2.27                     | 0.64              |
| 1:B:690:ASN:C    | 1:B:693:GLU:HG3  | 2.23                     | 0.64              |
| 1:A:7:VAL:CG2    | 1:A:39:THR:HG21  | 2.28                     | 0.64              |
| 1:A:736:GLU:OE1  | 1:A:777:ARG:HD2  | 1.98                     | 0.64              |
| 1:B:74:GLY:O     | 1:B:75:ASN:OD1   | 2.15                     | 0.64              |
| 1:B:914:VAL:HG12 | 1:B:916:ASN:N    | 2.12                     | 0.64              |
| 1:B:210:ILE:HD11 | 1:B:262:VAL:HG13 | 1.80                     | 0.64              |
| 1:A:491:LYS:NZ   | 1:A:526:ILE:HG21 | 2.12                     | 0.64              |
| 1:A:498:MET:N    | 1:A:499:PRO:HD2  | 2.12                     | 0.64              |
| 1:B:836:ILE:HD12 | 1:B:921:TYR:CE2  | 2.33                     | 0.63              |
| 1:A:62:LYS:HZ2   | 1:A:104:GLN:NE2  | 1.92                     | 0.63              |
| 1:A:144:LEU:HB3  | 1:A:208:VAL:HG11 | 1.80                     | 0.63              |
| 1:B:720:VAL:HG22 | 1:B:758:TYR:HE2  | 1.63                     | 0.63              |
| 1:B:754:ARG:O    | 1:B:757:PRO:HD2  | 1.99                     | 0.63              |
| 1:A:602:ILE:O    | 1:A:606:MET:HG3  | 1.99                     | 0.63              |
| 1:B:95:ILE:HD12  | 1:B:131:ARG:HH11 | 1.63                     | 0.63              |
| 1:B:392:ASN:ND2  | 1:B:395:LEU:HB2  | 2.14                     | 0.63              |
| 1:B:596:LEU:HD23 | 1:B:626:ILE:HG21 | 1.78                     | 0.63              |
| 1:B:910:PRO:C    | 1:B:912:ILE:H    | 2.05                     | 0.63              |
| 1:B:948:GLU:HG3  | 1:B:949:ASN:N    | 2.12                     | 0.63              |
| 1:A:159:ARG:NH2  | 1:A:220:ASP:OD1  | 2.29                     | 0.63              |
| 1:B:93:LEU:HD11  | 1:B:97:LEU:HD21  | 1.79                     | 0.63              |
| 1:B:695:LYS:NZ   | 1:B:734:ALA:HB1  | 2.14                     | 0.63              |
| 1:A:155:ARG:NH2  | 1:A:214:TYR:HB3  | 2.13                     | 0.63              |
| 1:B:592:PHE:N    | 1:B:593:PRO:HD2  | 2.13                     | 0.63              |
| 1:A:94:MET:SD    | 1:A:105:ILE:HG22 | 2.39                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:932:ILE:HG13 | 1:A:933:SER:N    | 2.13                     | 0.62              |
| 1:A:44:ILE:HD13  | 1:A:58:ALA:HA    | 1.81                     | 0.62              |
| 1:A:72:GLU:OE2   | 1:A:728:ARG:NH2  | 2.31                     | 0.62              |
| 1:B:137:MET:HA   | 1:B:140:ASN:HD22 | 1.64                     | 0.62              |
| 1:B:690:ASN:O    | 1:B:693:GLU:CG   | 2.46                     | 0.62              |
| 1:B:843:ILE:CG1  | 1:B:844:ASN:ND2  | 2.62                     | 0.62              |
| 1:A:38:LEU:HD11  | 1:A:85:LEU:HD23  | 1.79                     | 0.62              |
| 1:A:646:PHE:HA   | 1:A:649:VAL:HG23 | 1.81                     | 0.62              |
| 1:A:151:PHE:CE2  | 1:A:170:VAL:HG11 | 2.35                     | 0.62              |
| 1:A:347:VAL:HG11 | 1:A:427:TYR:CD2  | 2.34                     | 0.62              |
| 1:B:7:VAL:O      | 1:B:11:LEU:HG    | 1.98                     | 0.62              |
| 1:B:233:MET:HB2  | 1:B:284:MET:HE1  | 1.81                     | 0.62              |
| 1:B:635:LEU:HA   | 1:B:638:LEU:HD12 | 1.81                     | 0.62              |
| 1:B:38:LEU:HD11  | 1:B:85:LEU:CD1   | 2.30                     | 0.62              |
| 1:A:727:GLN:HG3  | 1:A:765:LEU:HD11 | 1.81                     | 0.62              |
| 1:B:36:PHE:CE2   | 1:B:40:LEU:CD2   | 2.72                     | 0.62              |
| 1:B:789:ILE:HG13 | 1:B:790:SER:N    | 2.14                     | 0.62              |
| 1:B:832:LYS:HZ2  | 1:B:908:PRO:HB3  | 1.62                     | 0.62              |
| 1:B:595:LEU:HA   | 1:B:598:GLN:OE1  | 1.99                     | 0.62              |
| 1:B:213:TYR:CD2  | 1:B:269:LEU:HD21 | 2.35                     | 0.62              |
| 1:B:769:ARG:NH1  | 1:B:773:SER:O    | 2.32                     | 0.62              |
| 1:B:810:PHE:C    | 1:B:810:PHE:CD2  | 2.78                     | 0.62              |
| 1:B:850:SER:C    | 1:B:851:LYS:HG2  | 2.21                     | 0.62              |
| 1:B:914:VAL:HB   | 1:B:917:GLY:H    | 1.65                     | 0.61              |
| 1:A:189:ILE:HD13 | 1:A:203:PHE:CE1  | 2.34                     | 0.61              |
| 1:A:276:ARG:HB3  | 1:A:277:TYR:CD1  | 2.35                     | 0.61              |
| 1:A:117:PHE:CE1  | 1:A:124:LEU:HD23 | 2.35                     | 0.61              |
| 1:A:655:GLN:HE22 | 1:A:697:ASN:ND2  | 1.98                     | 0.61              |
| 1:A:795:SER:O    | 1:A:799:ILE:HG13 | 1.99                     | 0.61              |
| 1:A:904:LYS:N    | 1:A:905:PRO:CD   | 2.64                     | 0.61              |
| 1:A:143:VAL:O    | 1:A:146:VAL:HG12 | 2.01                     | 0.61              |
| 1:A:492:ALA:HA   | 1:A:495:ILE:HG12 | 1.81                     | 0.61              |
| 1:B:175:THR:HG23 | 1:B:224:PHE:CZ   | 2.34                     | 0.61              |
| 1:B:471:HIS:HD2  | 1:B:473:ILE:H    | 1.46                     | 0.61              |
| 1:B:676:PRO:CD   | 1:B:679:ILE:HD11 | 2.27                     | 0.61              |
| 1:B:735:TYR:CB   | 1:B:738:HIS:HD2  | 2.13                     | 0.61              |
| 1:A:117:PHE:CZ   | 1:A:125:LEU:HD11 | 2.35                     | 0.61              |
| 1:B:676:PRO:HG3  | 1:B:679:ILE:HD13 | 1.83                     | 0.61              |
| 1:A:392:ASN:HB3  | 1:A:395:LEU:HB3  | 1.82                     | 0.61              |
| 1:A:600:ILE:HG23 | 1:A:645:THR:HG21 | 1.83                     | 0.61              |
| 1:B:183:LYS:O    | 1:B:187:GLU:HG3  | 2.00                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:20:ALA:O     | 1:A:24:GLU:HG3   | 2.00                     | 0.61              |
| 1:A:28:ARG:NH1   | 1:A:67:ARG:CZ    | 2.64                     | 0.61              |
| 1:B:31:GLU:OE1   | 1:B:67:ARG:NH2   | 2.33                     | 0.61              |
| 1:B:268:GLU:HG2  | 1:B:311:LYS:HD2  | 1.82                     | 0.61              |
| 1:B:568:ALA:HB2  | 1:B:606:MET:HE3  | 1.82                     | 0.61              |
| 1:A:937:PHE:CZ   | 1:A:941:ILE:CD1  | 2.81                     | 0.61              |
| 1:A:264:SER:HA   | 1:A:308:LEU:HD12 | 1.82                     | 0.61              |
| 1:A:400:PHE:HB3  | 1:A:404:MET:CE   | 2.31                     | 0.61              |
| 1:A:635:LEU:N    | 1:A:636:PRO:CD   | 2.64                     | 0.61              |
| 1:B:394:VAL:HG13 | 1:B:398:ASN:ND2  | 2.16                     | 0.61              |
| 1:B:550:LEU:HD21 | 1:B:580:VAL:CG1  | 2.31                     | 0.61              |
| 1:A:331:ASN:ND2  | 1:A:331:ASN:C    | 2.57                     | 0.60              |
| 1:A:347:VAL:HG11 | 1:A:427:TYR:CE2  | 2.36                     | 0.60              |
| 1:B:394:VAL:HG13 | 1:B:398:ASN:HD21 | 1.66                     | 0.60              |
| 1:B:792:LYS:CE   | 1:B:909:LEU:CD2  | 2.73                     | 0.60              |
| 1:A:643:MET:N    | 1:A:644:PRO:HD2  | 2.17                     | 0.60              |
| 1:A:951:VAL:O    | 1:A:955:GLN:HG3  | 2.01                     | 0.60              |
| 1:B:706:LYS:NZ   | 1:B:741:ASP:HB3  | 2.16                     | 0.60              |
| 1:B:814:TRP:CE3  | 1:B:818:ILE:HD12 | 2.36                     | 0.60              |
| 1:A:655:GLN:HE22 | 1:A:697:ASN:HD21 | 1.47                     | 0.60              |
| 1:B:571:GLU:HG2  | 1:B:572:PHE:H    | 1.66                     | 0.60              |
| 1:B:635:LEU:HB2  | 1:B:636:PRO:HD3  | 1.83                     | 0.60              |
| 1:B:550:LEU:CD1  | 1:B:588:ILE:HD13 | 2.32                     | 0.60              |
| 1:A:942:LEU:CD2  | 1:A:953:LEU:HD23 | 2.32                     | 0.60              |
| 1:B:843:ILE:CG1  | 1:B:844:ASN:N    | 2.65                     | 0.60              |
| 1:A:89:GLU:O     | 1:A:92:PRO:HG2   | 2.02                     | 0.60              |
| 1:A:194:ASN:HA   | 1:A:246:LEU:CD1  | 2.31                     | 0.60              |
| 1:B:115:SER:OG   | 1:B:116:ASP:OD2  | 2.15                     | 0.60              |
| 1:A:221:ILE:HG13 | 1:A:277:TYR:CD2  | 2.36                     | 0.60              |
| 1:B:400:PHE:HE2  | 1:B:428:LEU:HD22 | 1.67                     | 0.60              |
| 1:A:712:ASP:O    | 1:A:715:ILE:HG22 | 2.01                     | 0.60              |
| 1:A:237:HIS:HE1  | 1:A:291:ILE:HD11 | 1.65                     | 0.60              |
| 1:B:341:GLN:O    | 1:B:345:PRO:HG2  | 2.01                     | 0.60              |
| 1:A:785:PHE:CZ   | 1:A:789:ILE:HD11 | 2.37                     | 0.60              |
| 1:B:304:LYS:HE3  | 1:B:305:TYR:CZ   | 2.36                     | 0.60              |
| 1:A:596:LEU:CD2  | 1:A:638:LEU:HD22 | 2.29                     | 0.59              |
| 1:A:859:THR:O    | 1:A:863:ILE:HG13 | 2.01                     | 0.59              |
| 1:A:903:GLU:C    | 1:A:905:PRO:CD   | 2.75                     | 0.59              |
| 1:B:804:GLU:HG3  | 1:B:804:GLU:O    | 2.01                     | 0.59              |
| 1:B:822:LEU:HB2  | 1:B:823:PRO:HD3  | 1.83                     | 0.59              |
| 1:B:304:LYS:HE3  | 1:B:305:TYR:CE1  | 2.37                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:843:ILE:HG13 | 1:B:844:ASN:N    | 2.17                     | 0.59              |
| 1:A:828:LEU:HB3  | 1:A:914:VAL:CG1  | 2.30                     | 0.59              |
| 1:B:38:LEU:HD11  | 1:B:85:LEU:HD13  | 1.85                     | 0.59              |
| 1:B:155:ARG:HB2  | 1:B:156:PRO:CD   | 2.32                     | 0.59              |
| 1:B:281:PHE:CD2  | 1:B:285:ILE:HG12 | 2.37                     | 0.59              |
| 1:B:592:PHE:H    | 1:B:593:PRO:HD2  | 1.66                     | 0.59              |
| 1:A:62:LYS:HD2   | 1:A:107:GLU:OE2  | 2.02                     | 0.59              |
| 1:A:99:ASN:O     | 1:A:103:VAL:HG23 | 2.02                     | 0.59              |
| 1:B:157:LEU:HD23 | 1:B:163:LEU:HD13 | 1.83                     | 0.59              |
| 1:B:395:LEU:O    | 1:B:399:ILE:HG23 | 2.03                     | 0.59              |
| 1:B:144:LEU:O    | 1:B:147:ALA:HB3  | 2.03                     | 0.59              |
| 1:A:425:TYR:HE1  | 1:A:459:GLU:OE1  | 1.84                     | 0.59              |
| 1:A:547:GLU:HG2  | 1:A:591:LEU:HD11 | 1.85                     | 0.59              |
| 1:A:557:ILE:O    | 1:A:560:HIS:CE1  | 2.55                     | 0.59              |
| 1:A:796:ASP:OD1  | 1:A:847:PHE:HE2  | 1.84                     | 0.59              |
| 1:B:39:THR:O     | 1:B:43:VAL:HG23  | 2.02                     | 0.59              |
| 1:B:267:GLN:OE1  | 1:B:267:GLN:HA   | 2.01                     | 0.59              |
| 1:B:596:LEU:HD11 | 1:B:638:LEU:CD2  | 2.32                     | 0.59              |
| 1:B:853:PRO:CD   | 1:B:854:THR:N    | 2.61                     | 0.59              |
| 1:A:94:MET:HE1   | 1:A:146:VAL:HA   | 1.84                     | 0.59              |
| 1:B:148:HIS:CE1  | 1:B:211:LYS:HB3  | 2.38                     | 0.59              |
| 1:B:414:ASP:O    | 1:B:418:ASN:ND2  | 2.36                     | 0.59              |
| 1:B:780:LYS:HE2  | 1:B:824:THR:HG22 | 1.83                     | 0.59              |
| 1:B:70:VAL:HG13  | 1:B:76:HIS:HA    | 1.84                     | 0.59              |
| 1:B:102:GLN:NE2  | 1:B:145:THR:HG21 | 2.16                     | 0.59              |
| 1:B:157:LEU:HG   | 1:B:163:LEU:HD11 | 1.84                     | 0.59              |
| 1:B:643:MET:CE   | 1:B:679:ILE:CG2  | 2.71                     | 0.59              |
| 1:A:451:ASN:C    | 1:A:451:ASN:HD22 | 2.11                     | 0.59              |
| 1:B:469:ILE:CD1  | 1:B:472:ILE:HA   | 2.33                     | 0.59              |
| 1:A:117:PHE:HE1  | 1:A:124:LEU:HD23 | 1.67                     | 0.58              |
| 1:A:239:TYR:HA   | 1:A:242:TYR:HB2  | 1.84                     | 0.58              |
| 1:A:510:TYR:HA   | 1:A:513:TYR:CE2  | 2.37                     | 0.58              |
| 1:A:799:ILE:HD13 | 1:A:847:PHE:CZ   | 2.38                     | 0.58              |
| 1:B:91:VAL:N     | 1:B:92:PRO:HD2   | 2.18                     | 0.58              |
| 1:B:472:ILE:CG2  | 1:B:509:GLU:HG3  | 2.22                     | 0.58              |
| 1:B:573:LEU:O    | 1:B:577:ILE:HG13 | 2.02                     | 0.58              |
| 1:B:845:GLY:C    | 1:B:847:PHE:H    | 2.10                     | 0.58              |
| 1:A:339:THR:HG22 | 1:A:344:LEU:CD1  | 2.33                     | 0.58              |
| 1:B:568:ALA:CB   | 1:B:611:SER:HB2  | 2.33                     | 0.58              |
| 1:A:24:GLU:O     | 1:A:28:ARG:HG2   | 2.03                     | 0.58              |
| 1:A:799:ILE:O    | 1:A:803:ASP:HB2  | 2.03                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:927:ASN:O    | 1:B:930:ASN:HB2  | 2.04                     | 0.58              |
| 1:B:937:PHE:CE1  | 1:B:941:ILE:HD11 | 2.39                     | 0.58              |
| 1:A:133:SER:H    | 1:A:140:ASN:HD21 | 1.52                     | 0.58              |
| 1:A:369:LEU:HD11 | 1:A:515:TYR:CE2  | 2.38                     | 0.58              |
| 1:B:30:LEU:O     | 1:B:33:GLN:HB2   | 2.03                     | 0.58              |
| 1:B:109:ILE:HD13 | 1:B:146:VAL:HG13 | 1.85                     | 0.58              |
| 1:B:335:MET:HB3  | 1:B:399:ILE:HD13 | 1.85                     | 0.58              |
| 1:B:791:ASN:CG   | 1:B:909:LEU:CD1  | 2.72                     | 0.58              |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:N    | 2.19                     | 0.58              |
| 1:A:504:PHE:O    | 1:A:513:TYR:HB3  | 2.04                     | 0.58              |
| 1:B:344:LEU:HB2  | 1:B:345:PRO:HD3  | 1.86                     | 0.58              |
| 1:B:599:PHE:HA   | 1:B:602:ILE:HD12 | 1.85                     | 0.58              |
| 1:B:841:MET:SD   | 1:B:847:PHE:CD1  | 2.97                     | 0.58              |
| 1:A:237:HIS:ND1  | 1:A:291:ILE:HD11 | 2.18                     | 0.58              |
| 1:B:476:VAL:HG13 | 1:B:515:TYR:CD2  | 2.39                     | 0.58              |
| 1:B:715:ILE:HG23 | 1:B:716:PHE:CD1  | 2.39                     | 0.58              |
| 1:A:710:LYS:HD3  | 1:A:749:LEU:HD13 | 1.85                     | 0.57              |
| 1:A:736:GLU:CG   | 1:A:769:ARG:NH2  | 2.66                     | 0.57              |
| 1:A:924:GLU:OE2  | 1:A:924:GLU:HA   | 2.04                     | 0.57              |
| 1:B:317:THR:CG2  | 1:B:387:GLU:HG3  | 2.33                     | 0.57              |
| 1:B:643:MET:CE   | 1:B:679:ILE:HG22 | 2.31                     | 0.57              |
| 1:A:36:PHE:CE2   | 1:A:40:LEU:HD22  | 2.38                     | 0.57              |
| 1:A:69:TRP:CH2   | 1:A:83:VAL:HG13  | 2.39                     | 0.57              |
| 1:A:252:GLU:OE1  | 1:A:252:GLU:HA   | 2.04                     | 0.57              |
| 1:A:414:ASP:OD2  | 1:A:417:LYS:HD2  | 2.03                     | 0.57              |
| 1:B:2:SER:O      | 1:B:5:GLU:CG     | 2.38                     | 0.57              |
| 1:B:28:ARG:C     | 1:B:31:GLU:HG2   | 2.19                     | 0.57              |
| 1:B:775:THR:HG22 | 1:B:777:ARG:H    | 1.70                     | 0.57              |
| 1:A:38:LEU:HD13  | 1:A:85:LEU:HD23  | 1.87                     | 0.57              |
| 1:A:192:ASN:ND2  | 1:A:202:LEU:HD11 | 2.17                     | 0.57              |
| 1:A:476:VAL:HG13 | 1:A:515:TYR:CD1  | 2.38                     | 0.57              |
| 1:A:799:ILE:HD13 | 1:A:847:PHE:CE1  | 2.38                     | 0.57              |
| 1:B:726:PHE:CE1  | 1:B:743:LEU:HB2  | 2.40                     | 0.57              |
| 1:B:849:GLN:C    | 1:B:851:LYS:H    | 2.12                     | 0.57              |
| 1:B:87:LYS:CB    | 1:B:121:TRP:CZ2  | 2.75                     | 0.57              |
| 1:B:94:MET:CE    | 1:B:146:VAL:HG22 | 2.34                     | 0.57              |
| 1:B:138:VAL:HG22 | 1:B:201:ILE:HD12 | 1.87                     | 0.57              |
| 1:B:708:PHE:HB3  | 1:B:716:PHE:HE1  | 1.69                     | 0.57              |
| 1:A:132:LEU:HD11 | 1:A:143:VAL:HG21 | 1.86                     | 0.57              |
| 1:A:491:LYS:HZ2  | 1:A:526:ILE:HG21 | 1.68                     | 0.57              |
| 1:A:767:LEU:HD12 | 1:A:805:VAL:HG21 | 1.86                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:836:ILE:O    | 1:A:840:ASN:HB2  | 2.05                     | 0.57              |
| 1:A:70:VAL:HG11  | 1:A:74:GLY:HA2   | 1.87                     | 0.57              |
| 1:B:117:PHE:HD2  | 1:B:153:ARG:NH2  | 1.95                     | 0.57              |
| 1:B:680:LYS:N    | 1:B:681:PRO:HD2  | 2.20                     | 0.57              |
| 1:A:585:GLU:HB2  | 1:A:629:TYR:HE2  | 1.50                     | 0.57              |
| 1:A:942:LEU:HD23 | 1:A:945:LEU:HD12 | 1.87                     | 0.57              |
| 1:A:143:VAL:O    | 1:A:146:VAL:CG1  | 2.53                     | 0.56              |
| 1:A:736:GLU:OE2  | 1:A:769:ARG:NH2  | 2.38                     | 0.56              |
| 1:A:632:ARG:HE   | 1:A:671:GLN:HE21 | 1.53                     | 0.56              |
| 1:A:295:LEU:O    | 1:A:299:ILE:HG13 | 2.05                     | 0.56              |
| 1:A:568:ALA:HB2  | 1:A:606:MET:HE3  | 1.86                     | 0.56              |
| 1:B:113:ALA:O    | 1:B:117:PHE:HA   | 2.04                     | 0.56              |
| 1:B:127:ASP:O    | 1:B:131:ARG:HG3  | 2.05                     | 0.56              |
| 1:B:230:GLN:OE1  | 1:B:284:MET:HE3  | 2.04                     | 0.56              |
| 1:B:297:THR:HG22 | 1:B:297:THR:O    | 2.05                     | 0.56              |
| 1:B:439:THR:CG2  | 1:B:440:ASN:H    | 2.16                     | 0.56              |
| 1:A:94:MET:HE3   | 1:A:146:VAL:HA   | 1.86                     | 0.56              |
| 1:A:382:THR:CG2  | 1:A:386:LYS:HE3  | 2.34                     | 0.56              |
| 1:B:719:LEU:HD12 | 1:B:758:TYR:CE1  | 2.41                     | 0.56              |
| 1:B:726:PHE:O    | 1:B:730:ILE:HG22 | 2.06                     | 0.56              |
| 1:B:822:LEU:HB2  | 1:B:823:PRO:CD   | 2.35                     | 0.56              |
| 1:A:680:LYS:N    | 1:A:681:PRO:HD2  | 2.21                     | 0.56              |
| 1:B:602:ILE:O    | 1:B:606:MET:HG3  | 2.05                     | 0.56              |
| 1:A:104:GLN:HA   | 1:A:104:GLN:HE21 | 1.70                     | 0.56              |
| 1:A:113:ALA:O    | 1:A:117:PHE:N    | 2.37                     | 0.56              |
| 1:A:951:VAL:HG12 | 1:A:955:GLN:HE21 | 1.70                     | 0.56              |
| 1:B:10:PHE:CE1   | 1:B:30:LEU:HD11  | 2.41                     | 0.56              |
| 1:B:591:LEU:O    | 1:B:591:LEU:HG   | 2.05                     | 0.56              |
| 1:B:769:ARG:HG3  | 1:B:769:ARG:NH1  | 2.21                     | 0.56              |
| 1:B:946:THR:HB   | 1:B:948:GLU:HG2  | 1.86                     | 0.56              |
| 1:A:69:TRP:CD1   | 1:A:70:VAL:HG23  | 2.40                     | 0.56              |
| 1:A:72:GLU:HG2   | 1:A:735:TYR:CE1  | 2.41                     | 0.56              |
| 1:A:109:ILE:HD13 | 1:A:146:VAL:HG23 | 1.88                     | 0.56              |
| 1:B:82:ASN:O     | 1:B:86:ILE:HG13  | 2.06                     | 0.56              |
| 1:B:419:TRP:NE1  | 1:B:471:HIS:HB3  | 2.19                     | 0.56              |
| 1:A:501:LEU:HA   | 1:A:504:PHE:CD1  | 2.41                     | 0.56              |
| 1:B:124:LEU:HD21 | 1:B:150:ILE:HD13 | 1.88                     | 0.56              |
| 1:B:720:VAL:N    | 1:B:721:PRO:HD2  | 2.21                     | 0.56              |
| 1:A:164:PHE:CD2  | 1:A:165:LEU:HD12 | 2.40                     | 0.56              |
| 1:B:10:PHE:CE2   | 1:B:26:ASN:HB3   | 2.40                     | 0.56              |
| 1:B:87:LYS:HB3   | 1:B:121:TRP:CZ3  | 2.36                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:114:ASP:O    | 1:B:117:PHE:CZ   | 2.58                     | 0.56              |
| 1:A:335:MET:HG3  | 1:A:399:ILE:CD1  | 2.37                     | 0.55              |
| 1:A:469:ILE:CG1  | 1:A:470:PRO:HD2  | 2.37                     | 0.55              |
| 1:B:28:ARG:HA    | 1:B:31:GLU:CD    | 2.30                     | 0.55              |
| 1:B:472:ILE:HD13 | 1:B:509:GLU:CD   | 2.31                     | 0.55              |
| 1:B:550:LEU:CD1  | 1:B:588:ILE:CD1  | 2.83                     | 0.55              |
| 1:B:684:GLN:HA   | 1:B:684:GLN:OE1  | 2.05                     | 0.55              |
| 1:A:72:GLU:CG    | 1:A:735:TYR:CZ   | 2.87                     | 0.55              |
| 1:A:389:LYS:CA   | 1:A:396:VAL:HG11 | 2.36                     | 0.55              |
| 1:B:354:VAL:HG21 | 1:B:420:LYS:NZ   | 2.21                     | 0.55              |
| 1:B:262:VAL:O    | 1:B:266:ILE:HG13 | 2.06                     | 0.55              |
| 1:B:667:PHE:HB2  | 1:B:901:ILE:HG21 | 1.86                     | 0.55              |
| 1:B:737:VAL:HG21 | 1:B:777:ARG:HH21 | 1.70                     | 0.55              |
| 1:A:547:GLU:CG   | 1:A:591:LEU:HD11 | 2.36                     | 0.55              |
| 1:B:513:TYR:OH   | 1:B:560:HIS:NE2  | 2.38                     | 0.55              |
| 1:B:718:ASP:O    | 1:B:721:PRO:HD2  | 2.06                     | 0.55              |
| 1:B:942:LEU:N    | 1:B:943:PRO:HD2  | 2.21                     | 0.55              |
| 1:A:475:ARG:HD2  | 1:A:504:PHE:HE2  | 1.71                     | 0.55              |
| 1:A:799:ILE:CD1  | 1:A:847:PHE:CE1  | 2.89                     | 0.55              |
| 1:B:322:ILE:HG13 | 1:B:325:TYR:HB2  | 1.87                     | 0.55              |
| 1:B:599:PHE:O    | 1:B:602:ILE:HB   | 2.07                     | 0.55              |
| 1:B:680:LYS:O    | 1:B:715:ILE:HD11 | 2.06                     | 0.55              |
| 1:A:469:ILE:HG12 | 1:A:470:PRO:HD2  | 1.88                     | 0.55              |
| 1:A:903:GLU:O    | 1:A:903:GLU:HG2  | 2.07                     | 0.55              |
| 1:B:550:LEU:HD12 | 1:B:588:ILE:HD13 | 1.89                     | 0.55              |
| 1:A:843:ILE:HG13 | 1:A:844:ASN:OD1  | 2.06                     | 0.55              |
| 1:A:335:MET:HG2  | 1:A:395:LEU:HG   | 1.89                     | 0.55              |
| 1:B:38:LEU:HD22  | 1:B:89:GLU:OE2   | 2.07                     | 0.55              |
| 1:B:65:ILE:HD13  | 1:B:112:ILE:HG13 | 1.88                     | 0.55              |
| 1:B:31:GLU:HA    | 1:B:36:PHE:CD1   | 2.42                     | 0.55              |
| 1:B:905:PRO:O    | 1:B:906:PHE:C    | 2.50                     | 0.55              |
| 1:A:335:MET:CB   | 1:A:399:ILE:HD13 | 2.38                     | 0.54              |
| 1:A:519:THR:O    | 1:A:523:ILE:HG13 | 2.07                     | 0.54              |
| 1:B:509:GLU:CB   | 1:B:512:VAL:HB   | 2.36                     | 0.54              |
| 1:B:376:THR:HG22 | 1:B:377:ARG:N    | 2.22                     | 0.54              |
| 1:B:610:PRO:HG2  | 1:B:656:GLU:OE1  | 2.07                     | 0.54              |
| 1:B:72:GLU:OE1   | 1:B:734:ALA:HB2  | 2.08                     | 0.54              |
| 1:B:137:MET:HA   | 1:B:140:ASN:ND2  | 2.23                     | 0.54              |
| 1:A:829:LEU:HD11 | 1:A:908:PRO:CB   | 2.37                     | 0.54              |
| 1:B:469:ILE:HD12 | 1:B:472:ILE:HA   | 1.90                     | 0.54              |
| 1:B:743:LEU:HD11 | 1:B:762:ILE:HG21 | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:392:ASN:O    | 1:A:395:LEU:N    | 2.41                     | 0.54              |
| 1:B:36:PHE:CD2   | 1:B:40:LEU:CG    | 2.91                     | 0.54              |
| 1:A:7:VAL:HG22   | 1:A:30:LEU:HD21  | 1.88                     | 0.54              |
| 1:B:774:LYS:O    | 1:B:774:LYS:CG   | 2.51                     | 0.54              |
| 1:A:134:ASN:HD22 | 1:A:134:ASN:N    | 2.01                     | 0.54              |
| 1:B:36:PHE:CE2   | 1:B:40:LEU:HD11  | 2.42                     | 0.54              |
| 1:B:404:MET:HE3  | 1:B:428:LEU:HB2  | 1.89                     | 0.54              |
| 1:B:815:GLY:HA2  | 1:B:819:ILE:HD12 | 1.90                     | 0.54              |
| 1:A:780:LYS:HE2  | 1:A:824:THR:CG2  | 2.36                     | 0.54              |
| 1:B:10:PHE:HB3   | 1:B:27:LEU:CD2   | 2.33                     | 0.54              |
| 1:B:291:ILE:HG23 | 1:B:292:THR:N    | 2.22                     | 0.54              |
| 1:B:814:TRP:CH2  | 1:B:841:MET:HG2  | 2.43                     | 0.54              |
| 1:A:94:MET:HE2   | 1:A:146:VAL:HB   | 1.88                     | 0.54              |
| 1:A:732:SER:O    | 1:A:733:LYS:C    | 2.51                     | 0.54              |
| 1:A:924:GLU:CG   | 1:A:928:LYS:HE3  | 2.37                     | 0.54              |
| 1:B:270:VAL:HG12 | 1:B:315:PHE:CD1  | 2.42                     | 0.54              |
| 1:B:676:PRO:O    | 1:B:679:ILE:HG12 | 2.08                     | 0.54              |
| 1:A:210:ILE:CD1  | 1:A:262:VAL:HG13 | 2.38                     | 0.54              |
| 1:A:899:VAL:HA   | 1:A:902:SER:HB3  | 1.89                     | 0.54              |
| 1:A:271:GLN:HG3  | 1:A:314:SER:OG   | 2.08                     | 0.53              |
| 1:B:70:VAL:CG1   | 1:B:76:HIS:HA    | 2.37                     | 0.53              |
| 1:B:422:LYS:O    | 1:B:426:ILE:HG13 | 2.08                     | 0.53              |
| 1:B:610:PRO:CG   | 1:B:656:GLU:OE1  | 2.56                     | 0.53              |
| 1:A:490:THR:HG22 | 1:A:492:ALA:N    | 2.21                     | 0.53              |
| 1:A:515:TYR:HA   | 1:A:518:ILE:HD12 | 1.90                     | 0.53              |
| 1:B:684:GLN:N    | 1:B:685:PRO:HD2  | 2.24                     | 0.53              |
| 1:B:733:LYS:HE3  | 1:B:775:THR:OG1  | 2.09                     | 0.53              |
| 1:B:31:GLU:HA    | 1:B:36:PHE:HD1   | 1.73                     | 0.53              |
| 1:B:157:LEU:CD2  | 1:B:163:LEU:CD1  | 2.86                     | 0.53              |
| 1:B:565:GLU:OE1  | 1:B:569:GLU:OE2  | 2.26                     | 0.53              |
| 1:B:605:ILE:HA   | 1:B:608:LYS:HE3  | 1.91                     | 0.53              |
| 1:B:221:ILE:HG13 | 1:B:277:TYR:CE2  | 2.44                     | 0.53              |
| 1:B:335:MET:HG3  | 1:B:399:ILE:HD11 | 1.90                     | 0.53              |
| 1:B:412:MET:HA   | 1:B:412:MET:CE   | 2.30                     | 0.53              |
| 1:B:446:THR:HG22 | 1:B:447:ASN:N    | 2.22                     | 0.53              |
| 1:B:914:VAL:HG12 | 1:B:915:ASN:CA   | 2.36                     | 0.53              |
| 1:A:397:THR:O    | 1:A:401:LEU:HD13 | 2.07                     | 0.53              |
| 1:A:646:PHE:HA   | 1:A:649:VAL:CG2  | 2.38                     | 0.53              |
| 1:B:150:ILE:O    | 1:B:153:ARG:HG2  | 2.08                     | 0.53              |
| 1:B:452:VAL:HG13 | 1:B:481:TYR:OH   | 2.08                     | 0.53              |
| 1:B:954:ASN:O    | 1:B:958:VAL:CG2  | 2.37                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:144:LEU:O    | 1:A:147:ALA:HB3  | 2.08                     | 0.53              |
| 1:A:335:MET:HG3  | 1:A:399:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:385:LEU:HD11 | 1:A:400:PHE:CE1  | 2.44                     | 0.53              |
| 1:B:357:PHE:CE1  | 1:B:473:ILE:HG12 | 2.43                     | 0.53              |
| 1:B:839:LEU:HD21 | 1:B:925:ALA:HB3  | 1.89                     | 0.53              |
| 1:B:472:ILE:HG21 | 1:B:509:GLU:CG   | 2.22                     | 0.53              |
| 1:A:372:SER:O    | 1:A:373:ASP:HB2  | 2.09                     | 0.53              |
| 1:B:83:VAL:CG1   | 1:B:87:LYS:HE3   | 2.32                     | 0.53              |
| 1:A:117:PHE:HZ   | 1:A:125:LEU:HD11 | 1.74                     | 0.53              |
| 1:A:498:MET:HE1  | 1:A:520:ILE:CG2  | 2.31                     | 0.53              |
| 1:A:498:MET:CE   | 1:A:520:ILE:HG23 | 2.31                     | 0.53              |
| 1:A:692:TRP:CZ3  | 1:A:702:THR:HG22 | 2.40                     | 0.53              |
| 1:B:476:VAL:HG13 | 1:B:515:TYR:CE2  | 2.43                     | 0.53              |
| 1:A:903:GLU:OE1  | 1:A:903:GLU:N    | 2.38                     | 0.53              |
| 1:A:930:ASN:OD1  | 1:A:938:LEU:HG   | 2.08                     | 0.53              |
| 1:B:483:TYR:O    | 1:B:486:ARG:HD3  | 2.09                     | 0.53              |
| 1:B:498:MET:HB3  | 1:B:499:PRO:CD   | 2.39                     | 0.53              |
| 1:B:848:PHE:CZ   | 1:B:937:PHE:CE1  | 2.97                     | 0.53              |
| 1:B:501:LEU:O    | 1:B:504:PHE:HB2  | 2.09                     | 0.52              |
| 1:A:559:LYS:O    | 1:A:559:LYS:HG3  | 2.08                     | 0.52              |
| 1:A:769:ARG:NH1  | 1:A:773:SER:O    | 2.42                     | 0.52              |
| 1:B:419:TRP:HZ2  | 1:B:473:ILE:HB   | 1.74                     | 0.52              |
| 1:A:736:GLU:OE1  | 1:A:777:ARG:CD   | 2.58                     | 0.52              |
| 1:A:132:LEU:N    | 1:A:132:LEU:HD12 | 2.25                     | 0.52              |
| 1:A:392:ASN:O    | 1:A:393:GLU:C    | 2.52                     | 0.52              |
| 1:A:799:ILE:CB   | 1:A:847:PHE:CZ   | 2.86                     | 0.52              |
| 1:B:284:MET:O    | 1:B:287:GLU:HG2  | 2.08                     | 0.52              |
| 1:B:195:ASN:HB3  | 1:B:198:SER:OG   | 2.09                     | 0.52              |
| 1:A:400:PHE:HB2  | 1:A:432:LEU:HD11 | 1.92                     | 0.52              |
| 1:B:285:ILE:O    | 1:B:289:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:94:MET:CE    | 1:A:146:VAL:HB   | 2.40                     | 0.52              |
| 1:A:513:TYR:O    | 1:A:516:ALA:HB3  | 2.09                     | 0.52              |
| 1:B:695:LYS:HZ1  | 1:B:734:ALA:HB1  | 1.74                     | 0.52              |
| 1:A:157:LEU:N    | 1:A:157:LEU:HD12 | 2.25                     | 0.52              |
| 1:A:400:PHE:CB   | 1:A:432:LEU:HD11 | 2.40                     | 0.52              |
| 1:B:144:LEU:CB   | 1:B:208:VAL:HG11 | 2.40                     | 0.52              |
| 1:B:272:LEU:CD1  | 1:B:276:ARG:HG3  | 2.39                     | 0.52              |
| 1:B:429:PHE:CE1  | 1:B:450:LEU:HD13 | 2.45                     | 0.52              |
| 1:B:469:ILE:HG13 | 1:B:469:ILE:O    | 2.09                     | 0.52              |
| 1:A:132:LEU:CD1  | 1:A:143:VAL:HG21 | 2.40                     | 0.52              |
| 1:B:93:LEU:O     | 1:B:97:LEU:CG    | 2.33                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:109:ILE:CD1  | 1:B:146:VAL:HG13 | 2.40                     | 0.52              |
| 1:A:71:ASP:HB3   | 1:A:77:LEU:HD21  | 1.92                     | 0.52              |
| 1:A:596:LEU:HD11 | 1:A:642:MET:HE3  | 1.92                     | 0.52              |
| 1:A:686:LEU:HG   | 1:A:686:LEU:O    | 2.10                     | 0.52              |
| 1:A:718:ASP:O    | 1:A:721:PRO:HD2  | 2.09                     | 0.51              |
| 1:B:486:ARG:HG2  | 1:B:487:ASN:N    | 2.24                     | 0.51              |
| 1:B:588:ILE:O    | 1:B:588:ILE:CG2  | 2.48                     | 0.51              |
| 1:B:836:ILE:O    | 1:B:840:ASN:HB2  | 2.10                     | 0.51              |
| 1:A:562:SER:O    | 1:A:605:ILE:HG21 | 2.10                     | 0.51              |
| 1:B:501:LEU:HA   | 1:B:504:PHE:CD1  | 2.38                     | 0.51              |
| 1:A:106:GLY:O    | 1:A:109:ILE:HG22 | 2.10                     | 0.51              |
| 1:A:557:ILE:HD11 | 1:A:577:ILE:HD11 | 1.91                     | 0.51              |
| 1:A:676:PRO:HG2  | 1:A:679:ILE:HD12 | 1.91                     | 0.51              |
| 1:A:764:VAL:O    | 1:A:768:GLN:HG2  | 2.10                     | 0.51              |
| 1:B:301:ASN:HA   | 1:B:377:ARG:HH12 | 1.75                     | 0.51              |
| 1:B:723:LEU:O    | 1:B:724:GLY:C    | 2.54                     | 0.51              |
| 1:A:722:VAL:C    | 1:A:724:GLY:N    | 2.66                     | 0.51              |
| 1:A:819:ILE:CD1  | 1:A:859:THR:HG22 | 2.40                     | 0.51              |
| 1:B:268:GLU:CG   | 1:B:311:LYS:HD2  | 2.40                     | 0.51              |
| 1:B:233:MET:HE1  | 1:B:269:LEU:CD2  | 2.40                     | 0.51              |
| 1:B:44:ILE:HG21  | 1:B:105:ILE:HD11 | 1.92                     | 0.51              |
| 1:B:392:ASN:HD21 | 1:B:395:LEU:HB2  | 1.73                     | 0.51              |
| 1:B:513:TYR:HH   | 1:B:560:HIS:CD2  | 2.29                     | 0.51              |
| 1:B:610:PRO:HB3  | 1:B:657:PHE:CE1  | 2.45                     | 0.51              |
| 1:A:451:ASN:C    | 1:A:451:ASN:ND2  | 2.69                     | 0.51              |
| 1:B:324:LYS:O    | 1:B:327:GLU:CD   | 2.53                     | 0.51              |
| 1:B:403:HIS:HB3  | 1:B:407:PHE:HE1  | 1.75                     | 0.51              |
| 1:B:812:GLN:O    | 1:B:816:ASN:HB2  | 2.10                     | 0.51              |
| 1:A:361:PRO:HB2  | 1:A:510:TYR:CD2  | 2.46                     | 0.51              |
| 1:B:362:ILE:HD13 | 1:B:569:GLU:HB3  | 1.92                     | 0.51              |
| 1:B:676:PRO:CD   | 1:B:679:ILE:CD1  | 2.88                     | 0.51              |
| 1:B:814:TRP:HE3  | 1:B:818:ILE:HD12 | 1.76                     | 0.51              |
| 1:A:472:ILE:HD13 | 1:A:509:GLU:CD   | 2.36                     | 0.51              |
| 1:A:730:ILE:HG23 | 1:A:730:ILE:O    | 2.10                     | 0.51              |
| 1:A:870:GLN:CG   | 1:A:871:SER:N    | 2.55                     | 0.51              |
| 1:B:97:LEU:HD11  | 1:B:105:ILE:CD1  | 2.30                     | 0.51              |
| 1:B:233:MET:HE1  | 1:B:269:LEU:HD23 | 1.92                     | 0.51              |
| 1:B:316:LEU:HB3  | 1:B:384:PHE:CE1  | 2.46                     | 0.51              |
| 1:B:950:GLN:O    | 1:B:954:ASN:ND2  | 2.44                     | 0.51              |
| 1:A:285:ILE:HG22 | 1:A:289:ILE:HD11 | 1.93                     | 0.50              |
| 1:A:775:THR:O    | 1:A:778:TYR:N    | 2.45                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:221:ILE:CG2  | 1:B:226:GLU:HB2  | 2.41                     | 0.50              |
| 1:B:461:ALA:CB   | 1:B:462:PRO:HD3  | 2.35                     | 0.50              |
| 1:B:625:ALA:O    | 1:B:629:TYR:HD1  | 1.94                     | 0.50              |
| 1:B:953:LEU:O    | 1:B:957:LEU:HG   | 2.10                     | 0.50              |
| 1:A:500:ILE:O    | 1:A:503:THR:HB   | 2.12                     | 0.50              |
| 1:A:786:PHE:CD1  | 1:A:818:ILE:CD1  | 2.83                     | 0.50              |
| 1:B:19:THR:HG22  | 1:B:19:THR:O     | 2.12                     | 0.50              |
| 1:B:233:MET:CB   | 1:B:284:MET:HE2  | 2.40                     | 0.50              |
| 1:B:91:VAL:N     | 1:B:92:PRO:CD    | 2.75                     | 0.50              |
| 1:B:557:ILE:CG2  | 1:B:567:LEU:HD11 | 2.40                     | 0.50              |
| 1:A:513:TYR:HA   | 1:A:516:ALA:HB3  | 1.92                     | 0.50              |
| 1:A:727:GLN:HG3  | 1:A:765:LEU:CD1  | 2.41                     | 0.50              |
| 1:B:337:ASN:O    | 1:B:338:ILE:C    | 2.54                     | 0.50              |
| 1:B:490:THR:HG22 | 1:B:492:ALA:H    | 1.76                     | 0.50              |
| 1:B:554:ILE:HD11 | 1:B:595:LEU:HD22 | 1.94                     | 0.50              |
| 1:B:557:ILE:CG2  | 1:B:567:LEU:CD1  | 2.87                     | 0.50              |
| 1:A:278:GLU:O    | 1:A:282:GLY:N    | 2.44                     | 0.50              |
| 1:B:7:VAL:CG2    | 1:B:39:THR:HG21  | 2.27                     | 0.50              |
| 1:A:40:LEU:O     | 1:A:44:ILE:HG13  | 2.11                     | 0.50              |
| 1:A:339:THR:HG22 | 1:A:344:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:751:ASP:CG   | 1:A:753:ASN:OD1  | 2.54                     | 0.50              |
| 1:B:374:THR:O    | 1:B:374:THR:CG2  | 2.60                     | 0.50              |
| 1:B:710:LYS:CA   | 1:B:749:LEU:HD13 | 2.36                     | 0.50              |
| 1:B:750:ILE:HG22 | 1:B:751:ASP:O    | 2.12                     | 0.50              |
| 1:A:125:LEU:HB3  | 1:A:173:VAL:HG11 | 1.94                     | 0.50              |
| 1:A:270:VAL:CG1  | 1:A:315:PHE:CE1  | 2.94                     | 0.50              |
| 1:A:662:PHE:CE1  | 1:A:701:VAL:HG22 | 2.47                     | 0.50              |
| 1:A:767:LEU:HD22 | 1:A:813:ILE:HD13 | 1.94                     | 0.50              |
| 1:B:93:LEU:HD12  | 1:B:97:LEU:HD21  | 1.91                     | 0.50              |
| 1:B:570:ASN:CG   | 1:B:573:LEU:HB2  | 2.37                     | 0.50              |
| 1:A:929:TYR:O    | 1:A:932:ILE:HG12 | 2.12                     | 0.50              |
| 1:B:70:VAL:CG1   | 1:B:76:HIS:CA    | 2.89                     | 0.50              |
| 1:B:472:ILE:HD13 | 1:B:509:GLU:CG   | 2.42                     | 0.50              |
| 1:B:839:LEU:HA   | 1:B:863:ILE:HD13 | 1.94                     | 0.50              |
| 1:A:326:PHE:CZ   | 1:A:391:LYS:CB   | 2.95                     | 0.50              |
| 1:A:425:TYR:CE1  | 1:A:459:GLU:OE1  | 2.64                     | 0.50              |
| 1:A:453:VAL:O    | 1:A:456:PHE:HB3  | 2.11                     | 0.50              |
| 1:A:841:MET:CE   | 1:A:848:PHE:HB2  | 2.34                     | 0.50              |
| 1:B:150:ILE:O    | 1:B:153:ARG:HD3  | 2.11                     | 0.50              |
| 1:A:9:LYS:HE2    | 1:A:13:GLU:OE2   | 2.12                     | 0.49              |
| 1:A:753:ASN:OD1  | 1:A:753:ASN:N    | 2.44                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:36:PHE:CE2   | 1:B:40:LEU:CG    | 2.95                     | 0.49              |
| 1:B:181:LEU:O    | 1:B:185:VAL:HG23 | 2.12                     | 0.49              |
| 1:B:546:THR:CG2  | 1:B:550:LEU:HD11 | 2.42                     | 0.49              |
| 1:A:117:PHE:CD1  | 1:A:117:PHE:C    | 2.83                     | 0.49              |
| 1:B:94:MET:HE3   | 1:B:146:VAL:HA   | 1.93                     | 0.49              |
| 1:B:550:LEU:HD21 | 1:B:580:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:476:VAL:HG13 | 1:A:515:TYR:HD1  | 1.77                     | 0.49              |
| 1:A:300:SER:C    | 1:A:302:GLN:H    | 2.19                     | 0.49              |
| 1:A:638:LEU:O    | 1:A:642:MET:HG2  | 2.12                     | 0.49              |
| 1:B:513:TYR:OH   | 1:B:560:HIS:CD2  | 2.65                     | 0.49              |
| 1:B:624:GLY:HA2  | 1:B:901:ILE:HD11 | 1.93                     | 0.49              |
| 1:B:851:LYS:O    | 1:B:851:LYS:HG3  | 2.10                     | 0.49              |
| 1:A:624:GLY:HA2  | 1:A:901:ILE:HD11 | 1.94                     | 0.49              |
| 1:B:464:LEU:HD11 | 1:B:482:ILE:HD11 | 1.95                     | 0.49              |
| 1:A:207:LEU:HA   | 1:A:210:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:254:GLU:HA   | 1:A:303:PRO:HB2  | 1.94                     | 0.49              |
| 1:A:373:ASP:C    | 1:A:379:ARG:HH12 | 2.20                     | 0.49              |
| 1:A:722:VAL:C    | 1:A:724:GLY:H    | 2.20                     | 0.49              |
| 1:B:151:PHE:C    | 1:B:153:ARG:N    | 2.70                     | 0.49              |
| 1:B:418:ASN:O    | 1:B:421:PHE:HD1  | 1.96                     | 0.49              |
| 1:A:389:LYS:NZ   | 1:A:432:LEU:O    | 2.42                     | 0.49              |
| 1:A:736:GLU:O    | 1:A:739:GLY:N    | 2.45                     | 0.49              |
| 1:A:814:TRP:HD1  | 1:A:855:LEU:HD22 | 1.78                     | 0.49              |
| 1:B:518:ILE:O    | 1:B:521:GLU:HB3  | 2.12                     | 0.49              |
| 1:B:588:ILE:C    | 1:B:590:PRO:HD2  | 2.38                     | 0.49              |
| 1:A:79:PRO:O     | 1:A:80:ALA:C     | 2.56                     | 0.49              |
| 1:A:231:VAL:O    | 1:A:235:ILE:HG13 | 2.13                     | 0.49              |
| 1:A:293:TRP:CD1  | 1:A:293:TRP:C    | 2.91                     | 0.49              |
| 1:B:937:PHE:CZ   | 1:B:941:ILE:CD1  | 2.95                     | 0.49              |
| 1:A:127:ASP:O    | 1:A:131:ARG:HG3  | 2.13                     | 0.49              |
| 1:A:392:ASN:HB3  | 1:A:395:LEU:CB   | 2.43                     | 0.49              |
| 1:B:439:THR:C    | 1:B:441:ALA:H    | 2.20                     | 0.49              |
| 1:B:648:THR:C    | 1:B:650:PHE:N    | 2.68                     | 0.49              |
| 1:B:686:LEU:HD11 | 1:B:701:VAL:HG13 | 1.95                     | 0.49              |
| 1:A:94:MET:HB2   | 1:A:105:ILE:CG2  | 2.40                     | 0.48              |
| 1:A:329:PHE:O    | 1:A:335:MET:CE   | 2.60                     | 0.48              |
| 1:A:589:GLN:HB2  | 1:A:590:PRO:HD3  | 1.95                     | 0.48              |
| 1:A:825:ILE:HG21 | 1:A:831:ARG:HA   | 1.94                     | 0.48              |
| 1:B:21:LYS:HG3   | 1:B:22:THR:N     | 2.26                     | 0.48              |
| 1:B:47:THR:O     | 1:B:47:THR:HG22  | 2.12                     | 0.48              |
| 1:B:55:LEU:O     | 1:B:59:LEU:HG    | 2.12                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:691:VAL:C    | 1:B:693:GLU:H    | 2.21                     | 0.48              |
| 1:A:384:PHE:CE2  | 1:A:388:LEU:HD11 | 2.47                     | 0.48              |
| 1:A:946:THR:O    | 1:A:947:GLN:C    | 2.56                     | 0.48              |
| 1:B:519:THR:O    | 1:B:523:ILE:HG13 | 2.12                     | 0.48              |
| 1:B:948:GLU:CG   | 1:B:949:ASN:H    | 2.26                     | 0.48              |
| 1:A:4:LEU:HD12   | 1:A:43:VAL:HG22  | 1.95                     | 0.48              |
| 1:A:368:ASP:OD1  | 1:A:480:LYS:NZ   | 2.28                     | 0.48              |
| 1:A:411:TYR:OH   | 1:A:470:PRO:HG2  | 2.13                     | 0.48              |
| 1:A:451:ASN:OD1  | 1:A:454:ASP:CG   | 2.56                     | 0.48              |
| 1:A:632:ARG:NE   | 1:A:671:GLN:HE21 | 2.11                     | 0.48              |
| 1:A:667:PHE:HB2  | 1:A:901:ILE:HG21 | 1.95                     | 0.48              |
| 1:A:841:MET:HE1  | 1:A:848:PHE:CB   | 2.38                     | 0.48              |
| 1:B:361:PRO:HB2  | 1:B:510:TYR:CD2  | 2.42                     | 0.48              |
| 1:B:789:ILE:CD1  | 1:B:798:LEU:HD13 | 2.33                     | 0.48              |
| 1:B:809:LEU:HD21 | 1:B:813:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:41:LEU:HD22  | 1:A:93:LEU:HD23  | 1.95                     | 0.48              |
| 1:A:125:LEU:CD2  | 1:A:170:VAL:HA   | 2.43                     | 0.48              |
| 1:A:237:HIS:ND1  | 1:A:291:ILE:CD1  | 2.76                     | 0.48              |
| 1:B:362:ILE:HD13 | 1:B:569:GLU:OE1  | 2.14                     | 0.48              |
| 1:B:677:GLU:HA   | 1:B:680:LYS:HG3  | 1.96                     | 0.48              |
| 1:A:276:ARG:HD3  | 1:A:277:TYR:OH   | 2.13                     | 0.48              |
| 1:A:698:ILE:CD1  | 1:A:735:TYR:CE1  | 2.95                     | 0.48              |
| 1:A:836:ILE:CD1  | 1:A:912:ILE:HD13 | 2.44                     | 0.48              |
| 1:B:175:THR:HG23 | 1:B:224:PHE:CD2  | 2.47                     | 0.48              |
| 1:B:271:GLN:HG3  | 1:B:272:LEU:N    | 2.24                     | 0.48              |
| 1:B:461:ALA:HB3  | 1:B:462:PRO:CD   | 2.36                     | 0.48              |
| 1:B:730:ILE:O    | 1:B:769:ARG:CD   | 2.60                     | 0.48              |
| 1:A:153:ARG:O    | 1:A:157:LEU:HD13 | 2.14                     | 0.48              |
| 1:A:814:TRP:O    | 1:A:819:ILE:HG13 | 2.14                     | 0.48              |
| 1:A:836:ILE:HD11 | 1:A:912:ILE:HD13 | 1.94                     | 0.48              |
| 1:B:27:LEU:HD13  | 1:B:60:PHE:CE1   | 2.49                     | 0.48              |
| 1:B:669:VAL:HG22 | 1:B:679:ILE:CD1  | 2.42                     | 0.48              |
| 1:B:706:LYS:HZ1  | 1:B:741:ASP:HB3  | 1.79                     | 0.48              |
| 1:A:70:VAL:HG13  | 1:A:74:GLY:HA2   | 1.95                     | 0.48              |
| 1:A:117:PHE:CB   | 1:A:118:PRO:HD3  | 2.38                     | 0.48              |
| 1:A:331:ASN:ND2  | 1:A:334:ALA:CB   | 2.67                     | 0.48              |
| 1:A:571:GLU:OE1  | 1:A:614:ARG:CD   | 2.60                     | 0.48              |
| 1:A:819:ILE:HG23 | 1:A:862:SER:OG   | 2.14                     | 0.48              |
| 1:A:839:LEU:HD11 | 1:A:926:LEU:HD11 | 1.96                     | 0.48              |
| 1:B:288:PHE:HA   | 1:B:291:ILE:HG22 | 1.96                     | 0.48              |
| 1:B:612:ASN:HB3  | 1:B:613:PRO:HD2  | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:447:ASN:HD22 | 1:A:450:LEU:CD1  | 2.27                     | 0.48              |
| 1:A:870:GLN:NE2  | 1:A:919:ARG:HD2  | 2.28                     | 0.48              |
| 1:B:30:LEU:HA    | 1:B:33:GLN:CG    | 2.44                     | 0.48              |
| 1:B:210:ILE:HG12 | 1:B:236:PHE:CE2  | 2.44                     | 0.48              |
| 1:B:843:ILE:HG13 | 1:B:844:ASN:ND2  | 2.28                     | 0.48              |
| 1:B:918:VAL:O    | 1:B:922:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:30:LEU:CD1   | 1:A:33:GLN:NE2   | 2.77                     | 0.48              |
| 1:A:195:ASN:O    | 1:A:196:LYS:C    | 2.57                     | 0.48              |
| 1:A:382:THR:O    | 1:A:386:LYS:HG3  | 2.13                     | 0.48              |
| 1:B:689:PRO:O    | 1:B:693:GLU:HG3  | 2.14                     | 0.48              |
| 1:A:171:LEU:HD21 | 1:A:222:PRO:CB   | 2.44                     | 0.47              |
| 1:A:224:PHE:O    | 1:A:228:ASN:HB2  | 2.13                     | 0.47              |
| 1:A:274:THR:HG1  | 1:A:315:PHE:HE1  | 1.61                     | 0.47              |
| 1:A:366:ARG:O    | 1:A:369:LEU:O    | 2.31                     | 0.47              |
| 1:A:655:GLN:NE2  | 1:A:697:ASN:HD21 | 2.12                     | 0.47              |
| 1:B:740:PHE:CE2  | 1:B:782:LEU:HA   | 2.49                     | 0.47              |
| 1:B:799:ILE:HA   | 1:B:810:PHE:CD1  | 2.48                     | 0.47              |
| 1:A:94:MET:CE    | 1:A:146:VAL:CA   | 2.91                     | 0.47              |
| 1:A:343:ILE:HD13 | 1:A:385:LEU:HD13 | 1.94                     | 0.47              |
| 1:A:347:VAL:CG1  | 1:A:427:TYR:CD2  | 2.96                     | 0.47              |
| 1:A:547:GLU:CG   | 1:A:591:LEU:CD1  | 2.88                     | 0.47              |
| 1:B:2:SER:O      | 1:B:5:GLU:N      | 2.47                     | 0.47              |
| 1:B:491:LYS:O    | 1:B:495:ILE:HG13 | 2.14                     | 0.47              |
| 1:B:679:ILE:C    | 1:B:681:PRO:HD2  | 2.38                     | 0.47              |
| 1:A:326:PHE:CZ   | 1:A:391:LYS:HB3  | 2.50                     | 0.47              |
| 1:A:368:ASP:HB3  | 1:A:515:TYR:OH   | 2.13                     | 0.47              |
| 1:A:385:LEU:HD11 | 1:A:400:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:752:MET:C    | 1:A:754:ARG:H    | 2.22                     | 0.47              |
| 1:B:22:THR:O     | 1:B:26:ASN:ND2   | 2.47                     | 0.47              |
| 1:B:63:ASN:O     | 1:B:67:ARG:CG    | 2.34                     | 0.47              |
| 1:B:343:ILE:HD13 | 1:B:385:LEU:CD2  | 2.45                     | 0.47              |
| 1:B:586:ASP:OD1  | 1:B:586:ASP:O    | 2.31                     | 0.47              |
| 1:B:675:ILE:HB   | 1:B:680:LYS:HE2  | 1.96                     | 0.47              |
| 1:A:235:ILE:O    | 1:A:238:LYS:HB3  | 2.13                     | 0.47              |
| 1:A:453:VAL:HG13 | 1:A:493:GLN:HE22 | 1.79                     | 0.47              |
| 1:B:374:THR:HA   | 1:B:379:ARG:NH1  | 2.27                     | 0.47              |
| 1:B:635:LEU:O    | 1:B:638:LEU:N    | 2.42                     | 0.47              |
| 1:A:91:VAL:N     | 1:A:92:PRO:HD2   | 2.30                     | 0.47              |
| 1:B:37:GLY:O     | 1:B:41:LEU:HG    | 2.13                     | 0.47              |
| 1:B:394:VAL:CG1  | 1:B:398:ASN:ND2  | 2.78                     | 0.47              |
| 1:B:588:ILE:CG2  | 1:B:591:LEU:HB3  | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:737:VAL:HG21 | 1:B:777:ARG:NH2  | 2.29                     | 0.47              |
| 1:B:767:LEU:HD13 | 1:B:809:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:134:ASN:N    | 1:A:134:ASN:ND2  | 2.63                     | 0.47              |
| 1:A:375:ASP:C    | 1:A:376:THR:HG1  | 2.14                     | 0.47              |
| 1:B:24:GLU:O     | 1:B:28:ARG:HG3   | 2.13                     | 0.47              |
| 1:B:502:ALA:O    | 1:B:505:LEU:HB2  | 2.15                     | 0.47              |
| 1:B:589:GLN:N    | 1:B:590:PRO:HD2  | 2.29                     | 0.47              |
| 1:B:855:LEU:O    | 1:B:859:THR:OG1  | 2.31                     | 0.47              |
| 1:A:501:LEU:HA   | 1:A:504:PHE:HD1  | 1.79                     | 0.47              |
| 1:A:941:ILE:O    | 1:A:942:LEU:C    | 2.56                     | 0.47              |
| 1:B:97:LEU:HD11  | 1:B:105:ILE:HD13 | 1.94                     | 0.47              |
| 1:B:347:VAL:HG11 | 1:B:427:TYR:CD2  | 2.50                     | 0.47              |
| 1:B:354:VAL:HG21 | 1:B:420:LYS:HZ3  | 1.79                     | 0.47              |
| 1:B:505:LEU:HA   | 1:B:513:TYR:HB2  | 1.96                     | 0.47              |
| 1:B:946:THR:O    | 1:B:950:GLN:HG3  | 2.15                     | 0.47              |
| 1:A:142:GLY:O    | 1:A:143:VAL:C    | 2.58                     | 0.47              |
| 1:B:736:GLU:OE1  | 1:B:778:TYR:HB2  | 2.15                     | 0.47              |
| 1:B:821:THR:O    | 1:B:824:THR:HB   | 2.15                     | 0.47              |
| 1:A:472:ILE:O    | 1:A:473:ILE:C    | 2.56                     | 0.47              |
| 1:A:692:TRP:CZ2  | 1:A:725:ILE:HD13 | 2.49                     | 0.47              |
| 1:B:317:THR:HG23 | 1:B:387:GLU:CG   | 2.39                     | 0.47              |
| 1:B:589:GLN:HA   | 1:B:592:PHE:HE1  | 1.78                     | 0.47              |
| 1:B:908:PRO:O    | 1:B:909:LEU:C    | 2.56                     | 0.47              |
| 1:A:50:PRO:O     | 1:A:51:LEU:C     | 2.56                     | 0.47              |
| 1:A:292:THR:HG23 | 1:A:312:SER:HB2  | 1.96                     | 0.47              |
| 1:A:301:ASN:OD1  | 1:A:301:ASN:C    | 2.58                     | 0.47              |
| 1:B:6:THR:HG23   | 1:B:10:PHE:CE1   | 2.42                     | 0.47              |
| 1:B:370:GLU:CD   | 1:B:438:ILE:HB   | 2.38                     | 0.47              |
| 1:A:692:TRP:CE2  | 1:A:725:ILE:HD13 | 2.50                     | 0.46              |
| 1:B:137:MET:HB3  | 1:B:205:VAL:HG21 | 1.97                     | 0.46              |
| 1:B:428:LEU:O    | 1:B:432:LEU:HG   | 2.15                     | 0.46              |
| 1:B:521:GLU:OE2  | 1:B:525:THR:OG1  | 2.31                     | 0.46              |
| 1:A:4:LEU:CD1    | 1:A:43:VAL:HG22  | 2.45                     | 0.46              |
| 1:A:188:GLN:O    | 1:A:192:ASN:ND2  | 2.48                     | 0.46              |
| 1:A:390:GLU:O    | 1:A:390:GLU:HG2  | 2.15                     | 0.46              |
| 1:A:505:LEU:O    | 1:A:556:LEU:HD21 | 2.14                     | 0.46              |
| 1:A:550:LEU:HD21 | 1:A:580:VAL:CG1  | 2.46                     | 0.46              |
| 1:B:518:ILE:HG13 | 1:B:519:THR:N    | 2.31                     | 0.46              |
| 1:B:591:LEU:HD12 | 1:B:594:GLN:CD   | 2.40                     | 0.46              |
| 1:A:70:VAL:HG13  | 1:A:74:GLY:CA    | 2.45                     | 0.46              |
| 1:B:38:LEU:HD11  | 1:B:85:LEU:HD12  | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:221:ILE:HG22 | 1:B:226:GLU:HB2  | 1.95                     | 0.46              |
| 1:B:466:SER:HG   | 1:B:469:ILE:HG22 | 1.78                     | 0.46              |
| 1:B:726:PHE:CZ   | 1:B:743:LEU:HD22 | 2.50                     | 0.46              |
| 1:A:414:ASP:OD2  | 1:A:417:LYS:CD   | 2.63                     | 0.46              |
| 1:A:660:TYR:CD2  | 1:A:898:LEU:HD21 | 2.51                     | 0.46              |
| 1:A:660:TYR:HD2  | 1:A:898:LEU:HD21 | 1.80                     | 0.46              |
| 1:B:567:LEU:HD21 | 1:B:602:ILE:HG23 | 1.97                     | 0.46              |
| 1:A:374:THR:HA   | 1:A:379:ARG:HH11 | 0.69                     | 0.46              |
| 1:A:473:ILE:O    | 1:A:476:VAL:HB   | 2.14                     | 0.46              |
| 1:A:710:LYS:CD   | 1:A:749:LEU:HD13 | 2.46                     | 0.46              |
| 1:B:253:THR:HG23 | 1:B:302:GLN:HB3  | 1.98                     | 0.46              |
| 1:B:829:LEU:CD1  | 1:B:908:PRO:HG3  | 2.46                     | 0.46              |
| 1:A:849:GLN:HA   | 1:A:856:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:117:PHE:CD2  | 1:B:153:ARG:NH2  | 2.75                     | 0.46              |
| 1:B:137:MET:HE2  | 1:B:205:VAL:HG11 | 1.97                     | 0.46              |
| 1:B:155:ARG:NH1  | 1:B:214:TYR:CE2  | 2.79                     | 0.46              |
| 1:B:706:LYS:HG2  | 1:B:745:HIS:CG   | 2.51                     | 0.46              |
| 1:A:346:ASN:OD1  | 1:A:377:ARG:NH1  | 2.48                     | 0.46              |
| 1:A:585:GLU:O    | 1:A:586:ASP:CG   | 2.54                     | 0.46              |
| 1:B:2:SER:HB2    | 1:B:5:GLU:OE2    | 2.16                     | 0.46              |
| 1:B:372:SER:HG   | 1:B:379:ARG:HH22 | 1.56                     | 0.46              |
| 1:B:385:LEU:O    | 1:B:389:LYS:HG2  | 2.15                     | 0.46              |
| 1:B:433:ALA:CA   | 1:B:446:THR:HG23 | 2.44                     | 0.46              |
| 1:B:568:ALA:CB   | 1:B:606:MET:HE3  | 2.46                     | 0.46              |
| 1:B:831:ARG:HH12 | 1:B:869:SER:HB3  | 1.81                     | 0.46              |
| 1:A:916:ASN:OD1  | 1:A:916:ASN:C    | 2.59                     | 0.46              |
| 1:B:601:GLU:O    | 1:B:604:THR:HB   | 2.15                     | 0.46              |
| 1:A:144:LEU:HB3  | 1:A:208:VAL:CG1  | 2.46                     | 0.46              |
| 1:A:222:PRO:O    | 1:A:223:GLU:C    | 2.58                     | 0.46              |
| 1:A:841:MET:CE   | 1:A:848:PHE:CB   | 2.94                     | 0.46              |
| 1:B:69:TRP:CE2   | 1:B:70:VAL:HG22  | 2.50                     | 0.46              |
| 1:B:706:LYS:HE3  | 1:B:741:ASP:C    | 2.41                     | 0.46              |
| 1:A:403:HIS:HB3  | 1:A:407:PHE:CE1  | 2.51                     | 0.46              |
| 1:A:404:MET:HA   | 1:A:407:PHE:HD1  | 1.81                     | 0.46              |
| 1:B:635:LEU:N    | 1:B:636:PRO:CD   | 2.79                     | 0.46              |
| 1:B:723:LEU:HD11 | 1:B:758:TYR:HB3  | 1.96                     | 0.46              |
| 1:B:797:PHE:C    | 1:B:797:PHE:CD2  | 2.94                     | 0.46              |
| 1:A:236:PHE:HA   | 1:A:266:ILE:HD11 | 1.97                     | 0.45              |
| 1:A:279:ASP:C    | 1:A:281:PHE:N    | 2.74                     | 0.45              |
| 1:A:307:ILE:O    | 1:A:311:LYS:HG2  | 2.16                     | 0.45              |
| 1:B:232:GLY:O    | 1:B:236:PHE:HD1  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:439:THR:C    | 1:B:441:ALA:N    | 2.73                     | 0.45              |
| 1:B:596:LEU:O    | 1:B:597:ALA:C    | 2.58                     | 0.45              |
| 1:B:620:PHE:HD2  | 1:B:664:ILE:HD12 | 1.81                     | 0.45              |
| 1:B:822:LEU:HA   | 1:B:825:ILE:HD12 | 1.99                     | 0.45              |
| 1:B:822:LEU:N    | 1:B:823:PRO:HD2  | 2.31                     | 0.45              |
| 1:A:557:ILE:HD11 | 1:A:577:ILE:CD1  | 2.45                     | 0.45              |
| 1:B:414:ASP:HB3  | 1:B:418:ASN:ND2  | 2.31                     | 0.45              |
| 1:B:919:ARG:CG   | 1:B:956:LEU:CD1  | 2.92                     | 0.45              |
| 1:A:489:LEU:HD22 | 1:A:493:GLN:NE2  | 2.31                     | 0.45              |
| 1:A:630:THR:HG21 | 1:A:638:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:646:PHE:O    | 1:A:649:VAL:HB   | 2.16                     | 0.45              |
| 1:A:823:PRO:HB3  | 1:A:866:THR:OG1  | 2.16                     | 0.45              |
| 1:B:3:ASP:O      | 1:B:7:VAL:HG23   | 2.17                     | 0.45              |
| 1:B:62:LYS:HG3   | 1:B:63:ASN:N     | 2.30                     | 0.45              |
| 1:B:373:ASP:O    | 1:B:375:ASP:N    | 2.50                     | 0.45              |
| 1:B:684:GLN:NE2  | 1:B:717:PRO:HD2  | 2.26                     | 0.45              |
| 1:A:683:ALA:O    | 1:A:686:LEU:HB3  | 2.17                     | 0.45              |
| 1:A:799:ILE:HD11 | 1:A:841:MET:HE1  | 1.99                     | 0.45              |
| 1:A:839:LEU:HD11 | 1:A:926:LEU:CD1  | 2.46                     | 0.45              |
| 1:B:10:PHE:CZ    | 1:B:30:LEU:HD11  | 2.51                     | 0.45              |
| 1:B:392:ASN:ND2  | 1:B:395:LEU:CB   | 2.79                     | 0.45              |
| 1:A:434:ILE:HD11 | 1:A:484:THR:HG21 | 1.98                     | 0.45              |
| 1:A:547:GLU:HG2  | 1:A:591:LEU:HD13 | 1.96                     | 0.45              |
| 1:B:6:THR:HG22   | 1:B:10:PHE:CD1   | 2.31                     | 0.45              |
| 1:B:123:THR:HG22 | 1:B:127:ASP:OD2  | 2.16                     | 0.45              |
| 1:B:350:ARG:HG2  | 1:B:353:ASP:OD2  | 2.16                     | 0.45              |
| 1:B:384:PHE:CE2  | 1:B:388:LEU:HD11 | 2.51                     | 0.45              |
| 1:B:385:LEU:HD21 | 1:B:400:PHE:CZ   | 2.52                     | 0.45              |
| 1:B:620:PHE:CG   | 1:B:660:TYR:HB3  | 2.51                     | 0.45              |
| 1:B:769:ARG:HH11 | 1:B:769:ARG:CG   | 2.25                     | 0.45              |
| 1:A:70:VAL:HA    | 1:A:75:ASN:O     | 2.16                     | 0.45              |
| 1:A:199:LEU:O    | 1:A:200:ASN:C    | 2.60                     | 0.45              |
| 1:A:301:ASN:HA   | 1:A:377:ARG:NH1  | 2.28                     | 0.45              |
| 1:A:666:ALA:O    | 1:A:670:GLU:CG   | 2.61                     | 0.45              |
| 1:A:674:THR:HG22 | 1:A:675:ILE:N    | 2.32                     | 0.45              |
| 1:A:901:ILE:HG22 | 1:A:901:ILE:O    | 2.16                     | 0.45              |
| 1:B:30:LEU:HD22  | 1:B:33:GLN:OE1   | 2.17                     | 0.45              |
| 1:B:564:PRO:CG   | 1:B:565:GLU:H    | 2.27                     | 0.45              |
| 1:A:491:LYS:HZ1  | 1:A:526:ILE:CG2  | 2.30                     | 0.45              |
| 1:A:847:PHE:CB   | 1:A:851:LYS:HE3  | 2.44                     | 0.45              |
| 1:A:231:VAL:HG23 | 1:A:232:GLY:N    | 2.31                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:333:SER:O    | 1:A:337:ASN:N    | 2.43                     | 0.45              |
| 1:B:144:LEU:HB2  | 1:B:208:VAL:HG11 | 1.98                     | 0.45              |
| 1:B:291:ILE:CG2  | 1:B:292:THR:N    | 2.80                     | 0.45              |
| 1:B:548:ILE:HG22 | 1:B:552:ASN:ND2  | 2.32                     | 0.45              |
| 1:B:564:PRO:HG2  | 1:B:565:GLU:N    | 2.28                     | 0.45              |
| 1:B:763:ALA:HB2  | 1:B:801:PHE:CE1  | 2.52                     | 0.45              |
| 1:B:767:LEU:HD13 | 1:B:809:LEU:CD2  | 2.47                     | 0.45              |
| 1:A:72:GLU:HG2   | 1:A:735:TYR:CE2  | 2.51                     | 0.45              |
| 1:A:475:ARG:HD2  | 1:A:504:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:643:MET:HE2  | 1:A:678:SER:O    | 2.17                     | 0.45              |
| 1:A:656:GLU:C    | 1:A:657:PHE:HD1  | 2.24                     | 0.45              |
| 1:A:786:PHE:CE1  | 1:A:818:ILE:HD11 | 2.52                     | 0.45              |
| 1:B:791:ASN:HA   | 1:B:840:ASN:HD22 | 1.82                     | 0.45              |
| 1:A:162:GLU:O    | 1:A:165:LEU:N    | 2.49                     | 0.45              |
| 1:A:235:ILE:HG23 | 1:A:239:TYR:HE1  | 1.82                     | 0.45              |
| 1:A:913:ASP:HB2  | 1:A:916:ASN:O    | 2.16                     | 0.45              |
| 1:B:654:ILE:O    | 1:B:658:ILE:HG13 | 2.17                     | 0.45              |
| 1:B:675:ILE:HG23 | 1:B:679:ILE:HD11 | 1.99                     | 0.45              |
| 1:B:802:ILE:CG2  | 1:B:813:ILE:HD12 | 2.47                     | 0.45              |
| 1:A:192:ASN:C    | 1:A:194:ASN:N    | 2.75                     | 0.44              |
| 1:A:404:MET:O    | 1:A:408:VAL:HG23 | 2.17                     | 0.44              |
| 1:B:150:ILE:O    | 1:B:153:ARG:CG   | 2.65                     | 0.44              |
| 1:B:372:SER:HG   | 1:B:379:ARG:NH2  | 2.12                     | 0.44              |
| 1:B:550:LEU:HD21 | 1:B:580:VAL:HG12 | 1.99                     | 0.44              |
| 1:B:945:LEU:HB2  | 1:B:950:GLN:HG2  | 1.99                     | 0.44              |
| 1:A:44:ILE:CD1   | 1:A:58:ALA:HA    | 2.46                     | 0.44              |
| 1:A:237:HIS:HD1  | 1:A:291:ILE:CD1  | 2.30                     | 0.44              |
| 1:A:684:GLN:N    | 1:A:685:PRO:HD2  | 2.32                     | 0.44              |
| 1:B:36:PHE:CZ    | 1:B:60:PHE:CE2   | 3.05                     | 0.44              |
| 1:B:70:VAL:HG21  | 1:B:115:SER:HB3  | 1.99                     | 0.44              |
| 1:B:232:GLY:O    | 1:B:236:PHE:CD1  | 2.70                     | 0.44              |
| 1:B:482:ILE:HD13 | 1:B:497:LEU:HD13 | 1.99                     | 0.44              |
| 1:B:747:MET:HE2  | 1:B:747:MET:HB3  | 1.87                     | 0.44              |
| 1:B:813:ILE:O    | 1:B:814:TRP:C    | 2.60                     | 0.44              |
| 1:A:273:TYR:HD2  | 1:A:281:PHE:CD1  | 2.36                     | 0.44              |
| 1:A:707:SER:O    | 1:A:708:PHE:C    | 2.60                     | 0.44              |
| 1:B:136:ASP:CG   | 1:B:139:THR:OG1  | 2.60                     | 0.44              |
| 1:B:320:THR:O    | 1:B:391:LYS:HE3  | 2.17                     | 0.44              |
| 1:B:404:MET:HE1  | 1:B:429:PHE:HB2  | 1.98                     | 0.44              |
| 1:B:574:MET:HE2  | 1:B:615:PHE:CZ   | 2.53                     | 0.44              |
| 1:B:610:PRO:HB3  | 1:B:657:PHE:HE1  | 1.83                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:843:ILE:HD11 | 1:B:844:ASN:HD21 | 1.81                     | 0.44              |
| 1:A:135:ASP:OD1  | 1:A:135:ASP:O    | 2.36                     | 0.44              |
| 1:A:635:LEU:O    | 1:A:638:LEU:HB2  | 2.16                     | 0.44              |
| 1:A:797:PHE:CD2  | 1:A:797:PHE:C    | 2.95                     | 0.44              |
| 1:A:903:GLU:C    | 1:A:905:PRO:HD3  | 2.40                     | 0.44              |
| 1:A:918:VAL:HG13 | 1:A:919:ARG:N    | 2.33                     | 0.44              |
| 1:B:293:TRP:CD2  | 1:B:342:ILE:HD11 | 2.53                     | 0.44              |
| 1:B:703:ARG:HH22 | 1:B:901:ILE:HG22 | 1.83                     | 0.44              |
| 1:A:49:LEU:HD12  | 1:A:49:LEU:HA    | 1.82                     | 0.44              |
| 1:A:592:PHE:O    | 1:A:593:PRO:C    | 2.59                     | 0.44              |
| 1:A:625:ALA:O    | 1:A:629:TYR:HD1  | 1.99                     | 0.44              |
| 1:A:691:VAL:CG2  | 1:A:692:TRP:CD1  | 2.98                     | 0.44              |
| 1:B:27:LEU:HB3   | 1:B:60:PHE:CE1   | 2.52                     | 0.44              |
| 1:B:783:THR:HG21 | 1:B:822:LEU:HD23 | 2.00                     | 0.44              |
| 1:A:284:MET:H    | 1:A:284:MET:HG2  | 1.42                     | 0.44              |
| 1:A:682:LEU:O    | 1:A:685:PRO:HG2  | 2.17                     | 0.44              |
| 1:A:930:ASN:HD21 | 1:A:937:PHE:HB3  | 1.83                     | 0.44              |
| 1:B:87:LYS:CD    | 1:B:121:TRP:CZ2  | 3.00                     | 0.44              |
| 1:B:564:PRO:HB3  | 1:B:605:ILE:HG22 | 2.00                     | 0.44              |
| 1:B:784:VAL:HG21 | 1:B:830:ASP:HB3  | 1.99                     | 0.44              |
| 1:A:334:ALA:O    | 1:A:338:ILE:CG1  | 2.53                     | 0.44              |
| 1:A:930:ASN:ND2  | 1:A:937:PHE:HB3  | 2.33                     | 0.44              |
| 1:B:94:MET:CE    | 1:B:109:ILE:HD13 | 2.48                     | 0.44              |
| 1:B:97:LEU:HD13  | 1:B:105:ILE:HD11 | 1.91                     | 0.44              |
| 1:B:151:PHE:C    | 1:B:153:ARG:H    | 2.24                     | 0.44              |
| 1:B:352:GLU:OE1  | 1:B:352:GLU:HA   | 2.18                     | 0.44              |
| 1:B:635:LEU:HA   | 1:B:638:LEU:CD1  | 2.46                     | 0.44              |
| 1:B:643:MET:CE   | 1:B:679:ILE:HG21 | 2.43                     | 0.44              |
| 1:B:654:ILE:O    | 1:B:654:ILE:HG22 | 2.18                     | 0.44              |
| 1:B:687:LEU:HD21 | 1:B:716:PHE:CE2  | 2.53                     | 0.44              |
| 1:A:237:HIS:CE1  | 1:A:291:ILE:CD1  | 2.88                     | 0.44              |
| 1:A:362:ILE:O    | 1:A:366:ARG:HG3  | 2.18                     | 0.44              |
| 1:B:708:PHE:O    | 1:B:711:THR:O    | 2.35                     | 0.44              |
| 1:B:919:ARG:HG2  | 1:B:956:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:210:ILE:HD11 | 1:A:262:VAL:HG13 | 1.99                     | 0.44              |
| 1:A:326:PHE:CZ   | 1:A:391:LYS:HB2  | 2.53                     | 0.44              |
| 1:A:373:ASP:C    | 1:A:379:ARG:NH1  | 2.75                     | 0.44              |
| 1:B:404:MET:HE2  | 1:B:425:TYR:HB2  | 1.99                     | 0.44              |
| 1:B:596:LEU:O    | 1:B:600:ILE:HG12 | 2.17                     | 0.44              |
| 1:A:63:ASN:ND2   | 1:A:67:ARG:HH21  | 2.16                     | 0.43              |
| 1:A:94:MET:CE    | 1:A:146:VAL:CB   | 2.96                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:295:LEU:O    | 1:A:295:LEU:HD12 | 2.18                     | 0.43              |
| 1:A:821:THR:O    | 1:A:822:LEU:C    | 2.60                     | 0.43              |
| 1:B:253:THR:O    | 1:B:303:PRO:HG2  | 2.17                     | 0.43              |
| 1:B:507:THR:HG23 | 1:B:509:GLU:H    | 1.83                     | 0.43              |
| 1:B:719:LEU:HB2  | 1:B:758:TYR:CZ   | 2.53                     | 0.43              |
| 1:A:59:LEU:HD12  | 1:A:59:LEU:HA    | 1.78                     | 0.43              |
| 1:A:475:ARG:HH11 | 1:A:504:PHE:HE2  | 1.65                     | 0.43              |
| 1:A:821:THR:C    | 1:A:823:PRO:HD2  | 2.43                     | 0.43              |
| 1:B:38:LEU:HD21  | 1:B:85:LEU:HB3   | 1.98                     | 0.43              |
| 1:B:433:ALA:HB1  | 1:B:446:THR:CG2  | 2.48                     | 0.43              |
| 1:B:557:ILE:CD1  | 1:B:577:ILE:HD11 | 2.42                     | 0.43              |
| 1:A:704:LEU:O    | 1:A:705:LEU:C    | 2.61                     | 0.43              |
| 1:A:901:ILE:O    | 1:A:902:SER:C    | 2.60                     | 0.43              |
| 1:A:930:ASN:O    | 1:A:934:GLY:N    | 2.52                     | 0.43              |
| 1:B:843:ILE:CG1  | 1:B:844:ASN:H    | 2.30                     | 0.43              |
| 1:A:151:PHE:HE2  | 1:A:170:VAL:HG21 | 1.83                     | 0.43              |
| 1:A:335:MET:C    | 1:A:399:ILE:HD13 | 2.43                     | 0.43              |
| 1:A:391:LYS:O    | 1:A:392:ASN:ND2  | 2.47                     | 0.43              |
| 1:A:571:GLU:H    | 1:A:571:GLU:HG2  | 1.49                     | 0.43              |
| 1:A:814:TRP:NE1  | 1:A:859:THR:HG21 | 2.19                     | 0.43              |
| 1:A:841:MET:HE2  | 1:A:841:MET:HB3  | 1.71                     | 0.43              |
| 1:B:111:SER:O    | 1:B:112:ILE:C    | 2.61                     | 0.43              |
| 1:B:329:PHE:CD2  | 1:B:338:ILE:HD11 | 2.52                     | 0.43              |
| 1:B:557:ILE:HG22 | 1:B:567:LEU:HD12 | 1.94                     | 0.43              |
| 1:B:570:ASN:ND2  | 1:B:573:LEU:HD22 | 2.33                     | 0.43              |
| 1:B:914:VAL:CG1  | 1:B:916:ASN:H    | 2.23                     | 0.43              |
| 1:A:143:VAL:HG13 | 1:A:144:LEU:N    | 2.34                     | 0.43              |
| 1:A:360:ASP:N    | 1:A:361:PRO:HD3  | 2.33                     | 0.43              |
| 1:A:645:THR:O    | 1:A:649:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:689:PRO:O    | 1:A:690:ASN:C    | 2.61                     | 0.43              |
| 1:A:821:THR:HG22 | 1:A:825:ILE:CD1  | 2.49                     | 0.43              |
| 1:A:852:TYR:HB3  | 1:A:855:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:70:VAL:CG1   | 1:B:75:ASN:C     | 2.91                     | 0.43              |
| 1:B:460:ILE:HG23 | 1:B:478:ALA:HA   | 1.99                     | 0.43              |
| 1:A:635:LEU:HD12 | 1:A:635:LEU:HA   | 1.89                     | 0.43              |
| 1:A:652:GLU:O    | 1:A:654:ILE:N    | 2.52                     | 0.43              |
| 1:A:657:PHE:CD1  | 1:A:657:PHE:N    | 2.87                     | 0.43              |
| 1:A:752:MET:C    | 1:A:754:ARG:N    | 2.75                     | 0.43              |
| 1:B:230:GLN:OE1  | 1:B:230:GLN:HA   | 2.18                     | 0.43              |
| 1:B:322:ILE:HA   | 1:B:323:PRO:HD3  | 1.88                     | 0.43              |
| 1:B:759:ILE:HG22 | 1:B:804:GLU:OE2  | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:798:LEU:O    | 1:B:801:PHE:HB3  | 2.19                     | 0.43              |
| 1:B:864:ILE:HD13 | 1:B:953:LEU:HB2  | 2.01                     | 0.43              |
| 1:B:948:GLU:CG   | 1:B:949:ASN:N    | 2.80                     | 0.43              |
| 1:A:129:ALA:O    | 1:A:132:LEU:HD13 | 2.19                     | 0.43              |
| 1:A:162:GLU:O    | 1:A:163:LEU:C    | 2.61                     | 0.43              |
| 1:A:575:ARG:HB2  | 1:A:618:TYR:CD1  | 2.54                     | 0.43              |
| 1:A:822:LEU:HB3  | 1:A:823:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:97:LEU:CD1   | 1:A:105:ILE:HD12 | 2.49                     | 0.43              |
| 1:B:203:PHE:HB3  | 1:B:258:VAL:CG1  | 2.49                     | 0.43              |
| 1:B:434:ILE:HD13 | 1:B:438:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:720:VAL:CG2  | 1:B:758:TYR:HE2  | 2.30                     | 0.43              |
| 1:A:192:ASN:O    | 1:A:193:GLU:C    | 2.62                     | 0.43              |
| 1:B:387:GLU:O    | 1:B:391:LYS:HG2  | 2.19                     | 0.43              |
| 1:B:781:LYS:HD2  | 1:B:781:LYS:HA   | 1.80                     | 0.43              |
| 1:B:930:ASN:HD22 | 1:B:930:ASN:HA   | 1.55                     | 0.43              |
| 1:A:40:LEU:HD21  | 1:A:60:PHE:HD2   | 1.84                     | 0.43              |
| 1:A:63:ASN:ND2   | 1:A:67:ARG:HE    | 2.17                     | 0.43              |
| 1:A:732:SER:O    | 1:A:735:TYR:N    | 2.48                     | 0.43              |
| 1:B:361:PRO:CG   | 1:B:510:TYR:CD2  | 3.02                     | 0.43              |
| 1:A:313:LEU:HB2  | 1:A:380:ALA:HB1  | 2.01                     | 0.42              |
| 1:A:387:GLU:OE1  | 1:A:387:GLU:HA   | 2.19                     | 0.42              |
| 1:A:465:THR:O    | 1:A:466:SER:C    | 2.61                     | 0.42              |
| 1:A:703:ARG:HH22 | 1:A:901:ILE:HG22 | 1.84                     | 0.42              |
| 1:B:32:THR:O     | 1:B:32:THR:HG22  | 2.19                     | 0.42              |
| 1:B:65:ILE:HD11  | 1:B:112:ILE:HG13 | 1.85                     | 0.42              |
| 1:B:221:ILE:HA   | 1:B:222:PRO:HD3  | 1.85                     | 0.42              |
| 1:B:446:THR:CG2  | 1:B:447:ASN:N    | 2.82                     | 0.42              |
| 1:B:621:GLU:O    | 1:B:900:SER:HB3  | 2.19                     | 0.42              |
| 1:B:814:TRP:HA   | 1:B:818:ILE:HD12 | 2.01                     | 0.42              |
| 1:B:843:ILE:HG12 | 1:B:844:ASN:HD22 | 1.84                     | 0.42              |
| 1:A:331:ASN:ND2  | 1:A:331:ASN:O    | 2.45                     | 0.42              |
| 1:A:347:VAL:CG1  | 1:A:427:TYR:CE2  | 3.01                     | 0.42              |
| 1:A:932:ILE:CG1  | 1:A:933:SER:N    | 2.82                     | 0.42              |
| 1:A:941:ILE:O    | 1:A:944:GLN:N    | 2.40                     | 0.42              |
| 1:B:223:GLU:O    | 1:B:227:ASP:OD2  | 2.37                     | 0.42              |
| 1:B:488:GLN:OE1  | 1:B:488:GLN:HA   | 2.19                     | 0.42              |
| 1:B:498:MET:HB3  | 1:B:499:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:249:ASP:O    | 1:A:251:ASP:N    | 2.51                     | 0.42              |
| 1:B:31:GLU:C     | 1:B:33:GLN:H     | 2.27                     | 0.42              |
| 1:B:625:ALA:N    | 1:B:900:SER:HB2  | 2.35                     | 0.42              |
| 1:A:117:PHE:O    | 1:A:121:TRP:HB3  | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:ASN:HD22 | 1:A:202:LEU:CD1  | 2.23                     | 0.42              |
| 1:A:366:ARG:NH2  | 1:A:571:GLU:OE2  | 2.52                     | 0.42              |
| 1:A:410:GLN:OE1  | 1:A:421:PHE:CZ   | 2.73                     | 0.42              |
| 1:A:428:LEU:O    | 1:A:429:PHE:C    | 2.60                     | 0.42              |
| 1:A:625:ALA:O    | 1:A:626:ILE:C    | 2.62                     | 0.42              |
| 1:A:664:ILE:O    | 1:A:667:PHE:HB3  | 2.19                     | 0.42              |
| 1:A:736:GLU:O    | 1:A:737:VAL:C    | 2.60                     | 0.42              |
| 1:A:953:LEU:O    | 1:A:957:LEU:HG   | 2.19                     | 0.42              |
| 1:B:121:TRP:CE3  | 1:B:124:LEU:HB2  | 2.54                     | 0.42              |
| 1:B:323:PRO:O    | 1:B:324:LYS:C    | 2.63                     | 0.42              |
| 1:B:476:VAL:CG1  | 1:B:515:TYR:CE2  | 3.01                     | 0.42              |
| 1:B:657:PHE:CD1  | 1:B:657:PHE:N    | 2.87                     | 0.42              |
| 1:B:695:LYS:HZ3  | 1:B:734:ALA:HB1  | 1.82                     | 0.42              |
| 1:A:70:VAL:HG12  | 1:A:71:ASP:O     | 2.20                     | 0.42              |
| 1:A:94:MET:HE3   | 1:A:146:VAL:CA   | 2.50                     | 0.42              |
| 1:A:327:GLU:HA   | 1:A:330:ASN:HB2  | 2.01                     | 0.42              |
| 1:A:781:LYS:HD3  | 1:A:781:LYS:HA   | 1.90                     | 0.42              |
| 1:B:783:THR:CG2  | 1:B:822:LEU:HD23 | 2.48                     | 0.42              |
| 1:A:795:SER:HB3  | 1:A:841:MET:HG2  | 2.02                     | 0.42              |
| 1:B:619:THR:O    | 1:B:623:ILE:HG13 | 2.20                     | 0.42              |
| 1:B:621:GLU:O    | 1:B:900:SER:CB   | 2.67                     | 0.42              |
| 1:B:689:PRO:O    | 1:B:693:GLU:CG   | 2.67                     | 0.42              |
| 1:B:706:LYS:NZ   | 1:B:906:PHE:CZ   | 2.88                     | 0.42              |
| 1:B:151:PHE:HD2  | 1:B:154:TRP:CH2  | 2.37                     | 0.42              |
| 1:B:500:ILE:HG22 | 1:B:504:PHE:CE1  | 2.55                     | 0.42              |
| 1:B:805:VAL:HG12 | 1:B:806:GLN:HG3  | 2.01                     | 0.42              |
| 1:B:937:PHE:CZ   | 1:B:941:ILE:HD11 | 2.53                     | 0.42              |
| 1:A:98:PRO:HB2   | 1:A:100:ASN:OD1  | 2.19                     | 0.42              |
| 1:A:567:LEU:HD21 | 1:A:602:ILE:HG23 | 2.00                     | 0.42              |
| 1:A:828:LEU:C    | 1:A:914:VAL:CG1  | 2.93                     | 0.42              |
| 1:B:10:PHE:CB    | 1:B:27:LEU:CD2   | 2.96                     | 0.42              |
| 1:B:295:LEU:O    | 1:B:299:ILE:CG1  | 2.59                     | 0.42              |
| 1:B:316:LEU:HB3  | 1:B:384:PHE:HE1  | 1.83                     | 0.42              |
| 1:B:373:ASP:C    | 1:B:375:ASP:H    | 2.27                     | 0.42              |
| 1:B:435:ASN:OD1  | 1:B:445:SER:OG   | 2.36                     | 0.42              |
| 1:B:575:ARG:O    | 1:B:578:PHE:HB3  | 2.20                     | 0.42              |
| 1:A:106:GLY:C    | 1:A:109:ILE:HG22 | 2.45                     | 0.42              |
| 1:A:397:THR:HA   | 1:A:432:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:620:PHE:CD2  | 1:A:660:TYR:HB3  | 2.55                     | 0.42              |
| 1:A:799:ILE:HG21 | 1:A:847:PHE:HE1  | 1.76                     | 0.42              |
| 1:B:77:LEU:O     | 1:B:78:LEU:HD23  | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:157:LEU:CG   | 1:B:163:LEU:CD1  | 2.94                     | 0.42              |
| 1:B:203:PHE:HB3  | 1:B:258:VAL:HG12 | 2.02                     | 0.42              |
| 1:B:382:THR:HG22 | 1:B:386:LYS:CE   | 2.30                     | 0.42              |
| 1:B:630:THR:HG21 | 1:B:638:LEU:CD1  | 2.32                     | 0.42              |
| 1:B:635:LEU:N    | 1:B:636:PRO:HD2  | 2.35                     | 0.42              |
| 1:A:439:THR:OG1  | 1:A:440:ASN:N    | 2.52                     | 0.42              |
| 1:A:659:PRO:O    | 1:A:663:GLN:HG3  | 2.19                     | 0.42              |
| 1:B:769:ARG:HG3  | 1:B:769:ARG:O    | 2.19                     | 0.42              |
| 1:A:263:LYS:C    | 1:A:266:ILE:HG22 | 2.45                     | 0.41              |
| 1:B:94:MET:HG2   | 1:B:146:VAL:HG23 | 2.00                     | 0.41              |
| 1:B:475:ARG:HE   | 1:B:504:PHE:HE2  | 1.68                     | 0.41              |
| 1:A:145:THR:O    | 1:A:146:VAL:C    | 2.63                     | 0.41              |
| 1:A:166:GLU:O    | 1:A:169:LEU:HB3  | 2.20                     | 0.41              |
| 1:A:505:LEU:HD23 | 1:A:505:LEU:HA   | 1.92                     | 0.41              |
| 1:B:306:ASP:HA   | 1:B:377:ARG:HE   | 1.85                     | 0.41              |
| 1:B:648:THR:C    | 1:B:650:PHE:H    | 2.27                     | 0.41              |
| 1:A:28:ARG:HH11  | 1:A:67:ARG:NH1   | 2.19                     | 0.41              |
| 1:A:31:GLU:OE2   | 1:A:67:ARG:NH1   | 2.53                     | 0.41              |
| 1:A:124:LEU:HD21 | 1:A:150:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:151:PHE:CE2  | 1:A:170:VAL:CG1  | 3.02                     | 0.41              |
| 1:A:419:TRP:C    | 1:A:421:PHE:N    | 2.76                     | 0.41              |
| 1:A:461:ALA:O    | 1:A:462:PRO:C    | 2.63                     | 0.41              |
| 1:A:657:PHE:HD1  | 1:A:657:PHE:N    | 2.18                     | 0.41              |
| 1:B:841:MET:HE2  | 1:B:841:MET:HB2  | 1.91                     | 0.41              |
| 1:B:919:ARG:CG   | 1:B:956:LEU:HD13 | 2.49                     | 0.41              |
| 1:A:62:LYS:HZ3   | 1:A:104:GLN:NE2  | 2.17                     | 0.41              |
| 1:A:210:ILE:HD13 | 1:A:262:VAL:HG13 | 2.00                     | 0.41              |
| 1:A:344:LEU:N    | 1:A:345:PRO:HD2  | 2.35                     | 0.41              |
| 1:A:579:ARG:HA   | 1:A:582:GLN:HB2  | 2.03                     | 0.41              |
| 1:A:606:MET:HE2  | 1:A:606:MET:HB3  | 1.94                     | 0.41              |
| 1:B:31:GLU:C     | 1:B:33:GLN:N     | 2.77                     | 0.41              |
| 1:B:55:LEU:HD23  | 1:B:101:LEU:HD23 | 2.01                     | 0.41              |
| 1:B:229:ILE:H    | 1:B:229:ILE:HG13 | 1.70                     | 0.41              |
| 1:B:664:ILE:O    | 1:B:668:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:791:ASN:HD21 | 1:B:909:LEU:HD13 | 1.63                     | 0.41              |
| 1:A:55:LEU:HA    | 1:A:101:LEU:CD2  | 2.50                     | 0.41              |
| 1:A:176:ALA:O    | 1:A:177:PRO:C    | 2.64                     | 0.41              |
| 1:A:331:ASN:HD21 | 1:A:334:ALA:CA   | 2.31                     | 0.41              |
| 1:A:447:ASN:HD22 | 1:A:450:LEU:HD11 | 1.86                     | 0.41              |
| 1:B:557:ILE:CG2  | 1:B:567:LEU:HD12 | 2.50                     | 0.41              |
| 1:A:244:ASN:HA   | 1:A:245:PRO:HD3  | 1.92                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:411:TYR:CE1  | 1:A:419:TRP:HA   | 2.55                     | 0.41              |
| 1:A:475:ARG:NH1  | 1:A:504:PHE:CE2  | 2.89                     | 0.41              |
| 1:A:799:ILE:HB   | 1:A:847:PHE:CZ   | 2.47                     | 0.41              |
| 1:B:257:SER:OG   | 1:B:260:ILE:HG13 | 2.21                     | 0.41              |
| 1:B:744:GLU:O    | 1:B:748:LEU:HG   | 2.21                     | 0.41              |
| 1:B:789:ILE:HG13 | 1:B:790:SER:H    | 1.84                     | 0.41              |
| 1:A:124:LEU:HD21 | 1:A:150:ILE:HD12 | 2.01                     | 0.41              |
| 1:A:151:PHE:HE2  | 1:A:170:VAL:CG2  | 2.34                     | 0.41              |
| 1:A:281:PHE:CD2  | 1:A:285:ILE:HG12 | 2.56                     | 0.41              |
| 1:A:596:LEU:HD11 | 1:A:642:MET:CE   | 2.51                     | 0.41              |
| 1:A:596:LEU:CD1  | 1:A:623:ILE:HG23 | 2.50                     | 0.41              |
| 1:A:804:GLU:O    | 1:A:805:VAL:C    | 2.64                     | 0.41              |
| 1:B:699:PRO:O    | 1:B:700:ALA:C    | 2.63                     | 0.41              |
| 1:A:93:LEU:O     | 1:A:97:LEU:HG    | 2.21                     | 0.41              |
| 1:A:97:LEU:HD12  | 1:A:105:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:162:GLU:O    | 1:A:165:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:335:MET:C    | 1:A:399:ILE:CD1  | 2.94                     | 0.41              |
| 1:A:548:ILE:HG22 | 1:A:552:ASN:HD21 | 1.84                     | 0.41              |
| 1:A:631:GLN:O    | 1:A:632:ARG:C    | 2.64                     | 0.41              |
| 1:B:64:PHE:HE2   | 1:B:78:LEU:HD11  | 1.86                     | 0.41              |
| 1:B:196:LYS:HB2  | 1:B:246:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:585:GLU:CB   | 1:B:629:TYR:CE2  | 3.03                     | 0.41              |
| 1:B:832:LYS:HZ2  | 1:B:908:PRO:CB   | 2.25                     | 0.41              |
| 1:A:117:PHE:CE1  | 1:A:125:LEU:HD11 | 2.56                     | 0.41              |
| 1:A:140:ASN:O    | 1:A:141:LYS:C    | 2.64                     | 0.41              |
| 1:A:147:ALA:HB1  | 1:A:151:PHE:HE1  | 1.86                     | 0.41              |
| 1:A:592:PHE:N    | 1:A:593:PRO:HD2  | 2.36                     | 0.41              |
| 1:A:767:LEU:HD22 | 1:A:813:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:938:LEU:HD13 | 1:A:957:LEU:HD11 | 2.02                     | 0.41              |
| 1:B:730:ILE:HD12 | 1:B:766:LEU:HD23 | 1.99                     | 0.41              |
| 1:B:769:ARG:NH1  | 1:B:769:ARG:CG   | 2.80                     | 0.41              |
| 1:B:789:ILE:O    | 1:B:790:SER:C    | 2.60                     | 0.41              |
| 1:B:941:ILE:O    | 1:B:942:LEU:C    | 2.63                     | 0.41              |
| 1:B:2:SER:CA     | 1:B:5:GLU:HG2    | 2.51                     | 0.41              |
| 1:B:475:ARG:NE   | 1:B:504:PHE:HE2  | 2.19                     | 0.41              |
| 1:B:713:SER:CB   | 1:B:754:ARG:HH22 | 2.33                     | 0.41              |
| 1:B:733:LYS:HE3  | 1:B:775:THR:CG2  | 2.51                     | 0.41              |
| 1:A:192:ASN:C    | 1:A:194:ASN:H    | 2.29                     | 0.40              |
| 1:A:903:GLU:C    | 1:A:905:PRO:HD2  | 2.45                     | 0.40              |
| 1:B:114:ASP:O    | 1:B:117:PHE:CE1  | 2.74                     | 0.40              |
| 1:B:233:MET:CB   | 1:B:284:MET:CE   | 2.92                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:311:LYS:HA   | 1:B:311:LYS:HD3  | 1.91                     | 0.40              |
| 1:B:472:ILE:HD13 | 1:B:509:GLU:OE2  | 2.21                     | 0.40              |
| 1:B:710:LYS:CB   | 1:B:749:LEU:HD13 | 2.51                     | 0.40              |
| 1:B:743:LEU:HD21 | 1:B:766:LEU:HD11 | 2.02                     | 0.40              |
| 1:A:36:PHE:CZ    | 1:A:40:LEU:HD22  | 2.56                     | 0.40              |
| 1:A:140:ASN:HA   | 1:A:143:VAL:HG12 | 2.02                     | 0.40              |
| 1:A:257:SER:OG   | 1:A:258:VAL:N    | 2.53                     | 0.40              |
| 1:A:636:PRO:O    | 1:A:637:LEU:C    | 2.65                     | 0.40              |
| 1:B:335:MET:HG3  | 1:B:399:ILE:CD1  | 2.50                     | 0.40              |
| 1:B:433:ALA:O    | 1:B:446:THR:CG2  | 2.62                     | 0.40              |
| 1:B:571:GLU:CG   | 1:B:572:PHE:N    | 2.84                     | 0.40              |
| 1:B:843:ILE:HG12 | 1:B:844:ASN:H    | 1.86                     | 0.40              |
| 1:A:404:MET:O    | 1:A:407:PHE:N    | 2.55                     | 0.40              |
| 1:A:644:PRO:HG2  | 1:A:645:THR:H    | 1.86                     | 0.40              |
| 1:B:106:GLY:HA2  | 1:B:109:ILE:HG22 | 2.02                     | 0.40              |
| 1:B:124:LEU:HD21 | 1:B:150:ILE:CD1  | 2.51                     | 0.40              |
| 1:B:429:PHE:O    | 1:B:430:THR:C    | 2.65                     | 0.40              |
| 1:B:576:SER:O    | 1:B:580:VAL:HG23 | 2.21                     | 0.40              |
| 1:B:706:LYS:HZ3  | 1:B:906:PHE:HE2  | 1.68                     | 0.40              |
| 1:B:942:LEU:N    | 1:B:943:PRO:CD   | 2.85                     | 0.40              |
| 1:A:125:LEU:N    | 1:A:125:LEU:CD1  | 2.82                     | 0.40              |
| 1:A:516:ALA:O    | 1:A:517:ALA:C    | 2.65                     | 0.40              |
| 1:A:650:PHE:O    | 1:A:651:SER:C    | 2.64                     | 0.40              |
| 1:A:688:ALA:O    | 1:A:691:VAL:HG13 | 2.21                     | 0.40              |
| 1:B:28:ARG:O     | 1:B:31:GLU:N     | 2.54                     | 0.40              |
| 1:B:106:GLY:O    | 1:B:109:ILE:CG2  | 2.63                     | 0.40              |
| 1:B:368:ASP:OD2  | 1:B:515:TYR:OH   | 2.39                     | 0.40              |
| 1:B:565:GLU:OE1  | 1:B:565:GLU:C    | 2.65                     | 0.40              |
| 1:B:565:GLU:O    | 1:B:569:GLU:HG3  | 2.22                     | 0.40              |
| 1:B:589:GLN:HA   | 1:B:592:PHE:HD1  | 1.78                     | 0.40              |
| 1:B:792:LYS:NZ   | 1:B:909:LEU:HD22 | 2.34                     | 0.40              |
| 1:A:63:ASN:O     | 1:A:67:ARG:HG3   | 2.21                     | 0.40              |
| 1:A:305:TYR:O    | 1:A:306:ASP:C    | 2.64                     | 0.40              |
| 1:A:447:ASN:HB3  | 1:A:450:LEU:HD12 | 2.04                     | 0.40              |
| 1:A:504:PHE:HB3  | 1:A:512:VAL:HG12 | 2.04                     | 0.40              |
| 1:A:825:ILE:HG21 | 1:A:831:ARG:CA   | 2.50                     | 0.40              |
| 1:B:69:TRP:CH2   | 1:B:112:ILE:HG23 | 2.57                     | 0.40              |
| 1:B:469:ILE:HD12 | 1:B:471:HIS:O    | 2.21                     | 0.40              |
| 1:B:471:HIS:CD2  | 1:B:473:ILE:H    | 2.32                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 919/968 (95%)   | 814 (89%)  | 83 (9%)  | 22 (2%)  | 4           | 22 |
| 1   | B     | 902/968 (93%)   | 800 (89%)  | 82 (9%)  | 20 (2%)  | 5           | 24 |
| All | All   | 1821/1936 (94%) | 1614 (89%) | 165 (9%) | 42 (2%)  | 5           | 23 |

All (42) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 193 | GLU  |
| 1   | A     | 653 | ASP  |
| 1   | A     | 905 | PRO  |
| 1   | A     | 908 | PRO  |
| 1   | B     | 99  | ASN  |
| 1   | B     | 118 | PRO  |
| 1   | B     | 374 | THR  |
| 1   | B     | 564 | PRO  |
| 1   | B     | 611 | SER  |
| 1   | B     | 807 | ASP  |
| 1   | B     | 853 | PRO  |
| 1   | B     | 911 | GLU  |
| 1   | A     | 282 | GLY  |
| 1   | A     | 438 | ILE  |
| 1   | A     | 934 | GLY  |
| 1   | B     | 373 | ASP  |
| 1   | A     | 17  | ALA  |
| 1   | A     | 130 | SER  |
| 1   | A     | 159 | ARG  |
| 1   | A     | 467 | ASN  |
| 1   | A     | 559 | LYS  |
| 1   | A     | 677 | GLU  |
| 1   | A     | 904 | LYS  |
| 1   | B     | 392 | ASN  |
| 1   | B     | 655 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 814 | TRP  |
| 1   | B     | 906 | PHE  |
| 1   | A     | 393 | GLU  |
| 1   | A     | 153 | ARG  |
| 1   | B     | 278 | GLU  |
| 1   | B     | 640 | ASP  |
| 1   | A     | 35  | GLY  |
| 1   | A     | 730 | ILE  |
| 1   | A     | 774 | LYS  |
| 1   | B     | 699 | PRO  |
| 1   | A     | 250 | PRO  |
| 1   | B     | 156 | PRO  |
| 1   | B     | 323 | PRO  |
| 1   | A     | 283 | PRO  |
| 1   | A     | 610 | PRO  |
| 1   | B     | 122 | PRO  |
| 1   | B     | 394 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 849/890 (95%)   | 800 (94%)  | 49 (6%)  | 18          | 48 |
| 1   | B     | 839/890 (94%)   | 813 (97%)  | 26 (3%)  | 35          | 64 |
| All | All   | 1688/1780 (95%) | 1613 (96%) | 75 (4%)  | 25          | 56 |

All (75) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ASP  |
| 1   | A     | 18  | SER  |
| 1   | A     | 19  | THR  |
| 1   | A     | 49  | LEU  |
| 1   | A     | 67  | ARG  |
| 1   | A     | 123 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 162 | GLU  |
| 1   | A     | 164 | PHE  |
| 1   | A     | 193 | GLU  |
| 1   | A     | 221 | ILE  |
| 1   | A     | 229 | ILE  |
| 1   | A     | 237 | HIS  |
| 1   | A     | 257 | SER  |
| 1   | A     | 283 | PRO  |
| 1   | A     | 284 | MET  |
| 1   | A     | 331 | ASN  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 361 | PRO  |
| 1   | A     | 362 | ILE  |
| 1   | A     | 396 | VAL  |
| 1   | A     | 401 | LEU  |
| 1   | A     | 418 | ASN  |
| 1   | A     | 435 | ASN  |
| 1   | A     | 439 | THR  |
| 1   | A     | 457 | THR  |
| 1   | A     | 467 | ASN  |
| 1   | A     | 575 | ARG  |
| 1   | A     | 642 | MET  |
| 1   | A     | 658 | ILE  |
| 1   | A     | 691 | VAL  |
| 1   | A     | 701 | VAL  |
| 1   | A     | 727 | GLN  |
| 1   | A     | 730 | ILE  |
| 1   | A     | 752 | MET  |
| 1   | A     | 755 | LEU  |
| 1   | A     | 766 | LEU  |
| 1   | A     | 774 | LYS  |
| 1   | A     | 791 | ASN  |
| 1   | A     | 795 | SER  |
| 1   | A     | 802 | ILE  |
| 1   | A     | 803 | ASP  |
| 1   | A     | 841 | MET  |
| 1   | A     | 860 | MET  |
| 1   | A     | 869 | SER  |
| 1   | A     | 905 | PRO  |
| 1   | A     | 906 | PHE  |
| 1   | A     | 908 | PRO  |
| 1   | A     | 914 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 942 | LEU  |
| 1   | B     | 69  | TRP  |
| 1   | B     | 70  | VAL  |
| 1   | B     | 76  | HIS  |
| 1   | B     | 78  | LEU  |
| 1   | B     | 94  | MET  |
| 1   | B     | 116 | ASP  |
| 1   | B     | 175 | THR  |
| 1   | B     | 271 | GLN  |
| 1   | B     | 284 | MET  |
| 1   | B     | 327 | GLU  |
| 1   | B     | 475 | ARG  |
| 1   | B     | 571 | GLU  |
| 1   | B     | 596 | LEU  |
| 1   | B     | 598 | GLN  |
| 1   | B     | 636 | PRO  |
| 1   | B     | 659 | PRO  |
| 1   | B     | 744 | GLU  |
| 1   | B     | 745 | HIS  |
| 1   | B     | 756 | ARG  |
| 1   | B     | 773 | SER  |
| 1   | B     | 795 | SER  |
| 1   | B     | 843 | ILE  |
| 1   | B     | 846 | GLN  |
| 1   | B     | 862 | SER  |
| 1   | B     | 908 | PRO  |
| 1   | B     | 930 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | GLN  |
| 1   | A     | 63  | ASN  |
| 1   | A     | 76  | HIS  |
| 1   | A     | 82  | ASN  |
| 1   | A     | 102 | GLN  |
| 1   | A     | 104 | GLN  |
| 1   | A     | 134 | ASN  |
| 1   | A     | 140 | ASN  |
| 1   | A     | 192 | ASN  |
| 1   | A     | 195 | ASN  |
| 1   | A     | 331 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 337 | ASN  |
| 1   | A     | 398 | ASN  |
| 1   | A     | 435 | ASN  |
| 1   | A     | 447 | ASN  |
| 1   | A     | 487 | ASN  |
| 1   | A     | 493 | GLN  |
| 1   | A     | 552 | ASN  |
| 1   | A     | 589 | GLN  |
| 1   | A     | 609 | ASN  |
| 1   | A     | 612 | ASN  |
| 1   | A     | 655 | GLN  |
| 1   | A     | 671 | GLN  |
| 1   | A     | 791 | ASN  |
| 1   | A     | 927 | ASN  |
| 1   | A     | 949 | ASN  |
| 1   | A     | 955 | GLN  |
| 1   | B     | 26  | ASN  |
| 1   | B     | 148 | HIS  |
| 1   | B     | 180 | ASN  |
| 1   | B     | 188 | GLN  |
| 1   | B     | 228 | ASN  |
| 1   | B     | 237 | HIS  |
| 1   | B     | 398 | ASN  |
| 1   | B     | 418 | ASN  |
| 1   | B     | 437 | ASN  |
| 1   | B     | 451 | ASN  |
| 1   | B     | 471 | HIS  |
| 1   | B     | 487 | ASN  |
| 1   | B     | 493 | GLN  |
| 1   | B     | 552 | ASN  |
| 1   | B     | 570 | ASN  |
| 1   | B     | 633 | GLN  |
| 1   | B     | 634 | ASN  |
| 1   | B     | 738 | HIS  |
| 1   | B     | 745 | HIS  |
| 1   | B     | 768 | GLN  |
| 1   | B     | 791 | ASN  |
| 1   | B     | 844 | ASN  |
| 1   | B     | 930 | ASN  |
| 1   | B     | 949 | ASN  |
| 1   | B     | 954 | ASN  |
| 1   | B     | 955 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------|-------|-----------------------|-------|
| 1   | A     | 925/968 (95%)   | -0.20  | 16 (1%) | 69 48 | 22, 55, 114, 154      | 0     |
| 1   | B     | 914/968 (94%)   | 0.28   | 30 (3%) | 49 29 | 37, 89, 150, 172      | 0     |
| All | All   | 1839/1936 (94%) | 0.04   | 46 (2%) | 58 37 | 22, 70, 141, 172      | 0     |

All (46) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 847 | PHE  | 4.5  |
| 1   | A     | 375 | ASP  | 4.1  |
| 1   | A     | 376 | THR  | 3.6  |
| 1   | A     | 909 | LEU  | 3.4  |
| 1   | B     | 869 | SER  | 3.3  |
| 1   | A     | 547 | GLU  | 3.2  |
| 1   | B     | 125 | LEU  | 3.2  |
| 1   | A     | 372 | SER  | 3.2  |
| 1   | B     | 909 | LEU  | 3.0  |
| 1   | B     | 27  | LEU  | 2.9  |
| 1   | A     | 373 | ASP  | 2.8  |
| 1   | B     | 587 | SER  | 2.8  |
| 1   | B     | 851 | LYS  | 2.8  |
| 1   | A     | 562 | SER  | 2.8  |
| 1   | B     | 40  | LEU  | 2.7  |
| 1   | B     | 954 | ASN  | 2.7  |
| 1   | B     | 155 | ARG  | 2.6  |
| 1   | B     | 128 | LEU  | 2.6  |
| 1   | B     | 301 | ASN  | 2.6  |
| 1   | B     | 446 | THR  | 2.6  |
| 1   | A     | 870 | GLN  | 2.5  |
| 1   | B     | 124 | LEU  | 2.5  |
| 1   | B     | 60  | PHE  | 2.4  |
| 1   | B     | 850 | SER  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 544 | ASN  | 2.3  |
| 1   | B     | 10  | PHE  | 2.3  |
| 1   | B     | 560 | HIS  | 2.3  |
| 1   | B     | 31  | GLU  | 2.3  |
| 1   | A     | 370 | GLU  | 2.2  |
| 1   | B     | 749 | LEU  | 2.2  |
| 1   | B     | 86  | ILE  | 2.2  |
| 1   | B     | 78  | LEU  | 2.2  |
| 1   | B     | 934 | GLY  | 2.2  |
| 1   | A     | 24  | GLU  | 2.2  |
| 1   | B     | 612 | ASN  | 2.1  |
| 1   | B     | 22  | THR  | 2.1  |
| 1   | A     | 491 | LYS  | 2.1  |
| 1   | A     | 846 | GLN  | 2.1  |
| 1   | B     | 550 | LEU  | 2.1  |
| 1   | B     | 822 | LEU  | 2.1  |
| 1   | A     | 871 | SER  | 2.1  |
| 1   | B     | 931 | ALA  | 2.0  |
| 1   | B     | 163 | LEU  | 2.0  |
| 1   | B     | 588 | ILE  | 2.0  |
| 1   | A     | 386 | LYS  | 2.0  |
| 1   | B     | 914 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MG   | A     | 969 | 1/1   | 1.00 | 0.06 | 1,1,1,1                     | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.